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Structures of Technetium and Rhenium Complexes

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Structures of Technetium and Rhenium Complexes

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1. Introduction

Investigations in the technetium-99m chemistry [1] are stimulated by the search for new radiopharmaceuticals for nuclear medical applications. To understand the coordination mode of technetium with various complexing agents, macroscopic studies of technetium coordination chemistry are often performed in the milligram level using the low energy β-emitting radionuclide ^{99}Tc, which has a much longer half life ($t_{1/2}$ = 2.12 x 10^5 years) than ^{99m}Tc (6 hours).

Investigations of rhenium coordination chemistry are done in conjunction with Tc studies because Re possesses chemical properties similar to those of Tc. For some chemical tasks, Re provides a non-radioactive alternative to work with Tc radioisotopes. In addition, ^{186}Re and ^{188}Re are of great interest to nuclear medicine as they possess nuclear properties favorable for use in therapeutic radiopharmaceuticals.

Our investigations of Tc and Re coordination chemistry are toward this goal. A large series of technetium and rhenium complexes resulting from this studies have been characterized by X-ray crystal structure determinations.

This survey covers the structural investigations performed by P.Leibnitz and G.Reck (BAM) from 1992 till 12/2000. It summarizes results obtained in the Rossendorf technetium group and is not intended to compete with the well-written reviews published so far [2,3].

Data of all crystal structures described here are deposited at the Cambridge Crystallographic Data Centre (CCDC). Furthermore, all relevant crystal data as well as some service computer programs are stored on a CD provided together with this atlas[1]. This shall enable the interested reader to extract additional information concerning molecular configurations and conformations, bond lengths and angles, torsion angles, intra- and intermolecular interactions as well as molecular packings.

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[1]Data from this CD-ROM are available on request. Address correspondence to

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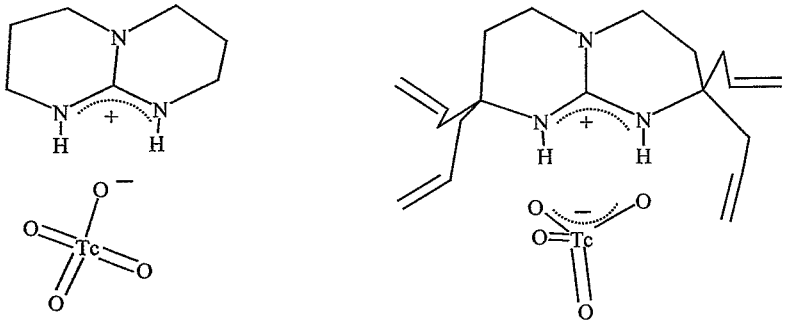
2. Chemistry of Tc and Re complexes

This chapter gives an overview on the compounds studied. Complexes are arranged in sections with respect to the oxidation state of the metal centre.

2.1. Oxoanions of Tc(VII) and Re(VII)

Salts of the tetrahedral oxoanions $[MO_4]^-$ are among the most important compounds of technetium and rhenium and appear in several crystallographic studies (see in [1]). We are interested in efficient binding of pertechnetate at physiological pH values in view of radiotracer design. Since there has been no effective chemistry for pertechnetate so far, we looked for supramolecular hosts able to bind pertechnetate and perrhenate anions with high selectivity and stability by multi-point fixation [4]. Preliminary structural studies refer on binding of Re and Tc oxoanions with bicyclic guanidinium compounds, thought as essential constituents in supramolecular hosts (**Tc1-Tc3; Re1,Re2**). Figure 1 shows binding of pertechnetate by bicyclic guanidinium compounds, where the guanidinium part is able to interact with one (**Tc1**) or with two (**Tc2**) pertechnetate oxygen atoms.



Tc1 **Tc2**

Fig. 1. Different interaction modes of bicyclic guanidinium compounds with the pertechnetate ion

2.2. Technetium and Rhenium on the oxidation state V

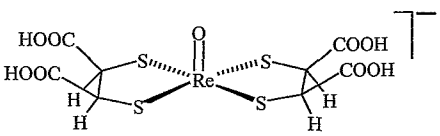
2.2.1. Bi- and tetradentate N,S ligands

The dominant feature of Tc(V) and Re(V) chemistry is the occurrence of the metal-oxo core which is preferably stabilized by a set of four S, N donor atoms [5]. The complexes described here are arranged according to their ligand denticity, following the order

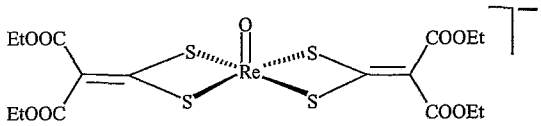
bidentate, tetradentate and mixed tridentate/monodentate. Additionally, complexes with neutral dithioether ligands and thiacrown ethers are shown.

An important aspect in complexes of dimercaptosuccinic acid and its derivatives is the occurrrence of isomers [6] due to different orientation of the carboxylic groups *syn* or *anti* to the metal oxo bond. **Re4** shows one of such isomers. In **Re5** the oxo group is changed by a substituted nitrogen [7].

Bis[1,1-di(carbethoxy)ethylene-dithiolato]oxorhenate(V) (**Re6**) is an example where the mercapto groups in the ligand are positioned *geminal* [8].



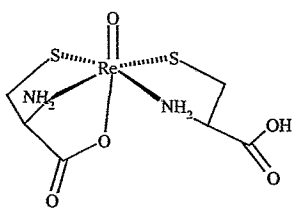
Re4



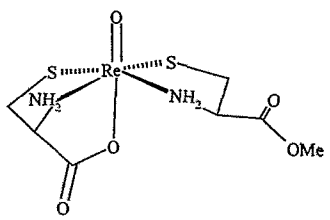
Re6

Fig. 2. Re dithiolato complexes with DMSA (*syn* isomer) (Re4) and a *geminal* dithiolato ligand (Re6)

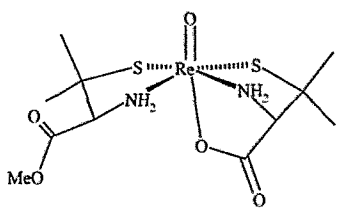
Complex formation of the oxorhenium(V) core with the aminothiols cysteamine, cysteine and penicillamine was studied in order to get basic information on what may happen in the labelling of peptides [9]. Different coordination mode has to be considered with these ligands since - beside highly stable bonding of the thiolate group - the amino group may act in neutral or deprotonated form, and a carboxylic group can additionally coordinate. (**Re7-Tc11**)



Re8



Re9



Re11

Fig. 3. Oxorhenium(V) complexes with S, N, O donor ligands

In the tetradentate ligand series studies were made with the aim to develop novel types of stable chelates for coupling the metal to biologically active molecules. N,S chelates (**Tc13**,

Re12-Re16) and MAG-like (MAG = mercaptoacetyl glycine) species (**Re17-Re19**) dominate. Figure 4 shows the Re complex of a novel N,N,N,S ligand (**Re16**) [10a,b], the Tc complex of mercaptoacetyldiglycine (MAG_2) with S,N,N,O coordination (**Tc18**) [11c] and a S,S,N,N coordinated Re complex bearing a receptor-binding moiety (Re**12**).

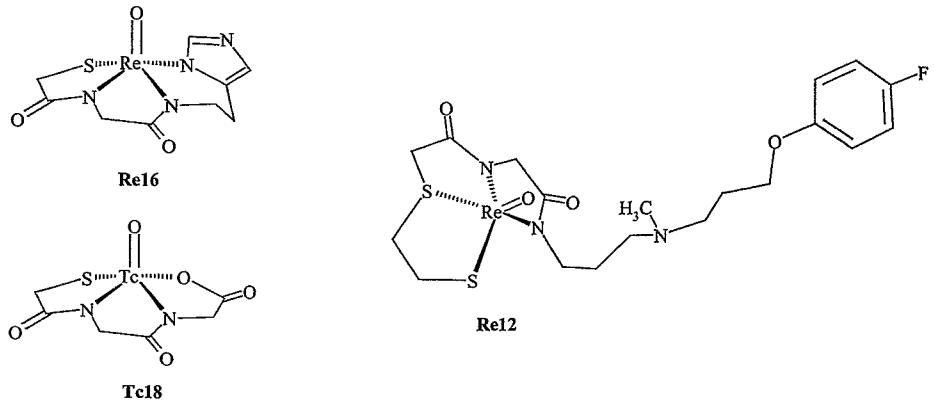
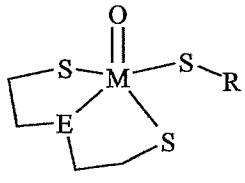


Fig. 4. Examples for Tc/Re complexes with tetradentate N,S chelators

2.2.2. "3+1" mixed-ligand complexes

Many studies refer to mixed-ligand complexes, where the equatorial coordination sphere is formed by a combination of a tridentate with a monodentate ligand [12]. This class of complexes claims special attention because it enables coupling of biological relevant groups to a relatively small-sized chelate [13] and has therefore been widely used in the search for new radiotracers. Since all the complexes are neutral species, they found application preferably in the design of neuroreceptor-affine Tc and Re complexes [14].

Most of the complexes in this section contain the thia dithiolate HS-CH_2CH_2-S-CH_2CH_2-SH (SSS), but aza and oxa ligands (SNS and SOS) are also involved. "3+1" complexes on basis of N-functionalized SNS aza ligands have also been described by Chiotellis et al. [15], among them are species where the aza group bears a diethylaminoethyl group (E = N-CH_2CH_2-NEt_2).



M = Tc, Re
E = O, $N(CH_3)$, S
R = alkyl, aryl, carboxylic, ester and amine groups, steroids, receptor-binding moieties

Fig. 5. General structure of "3+1" mixed-ligand complexes **Tc20-Re42**

The "3+1" mixed-ligand Tc and Re complexes can be prepared in a one-pot procedure by common action of the monodentate and the tridentate ligand with appropriate M(V) precursor molecules (Figure 6). An alternative route involves two steps. Firstly, the reaction of the tridentate ligand with tetrachlorooxo-metalates delivers relatively stable complexes, [MO(SES)Cl], that can be isolated and stored. In a subsequent reaction the chlorine atom is substituted by the monodentate ligand.

Side reactions give rise to the formation of dimeric complexes, where one S-E-S ligand acts as dithiolate forming a bridge between two [MO(S-E-S)] centres (**Re22**) [12,16].

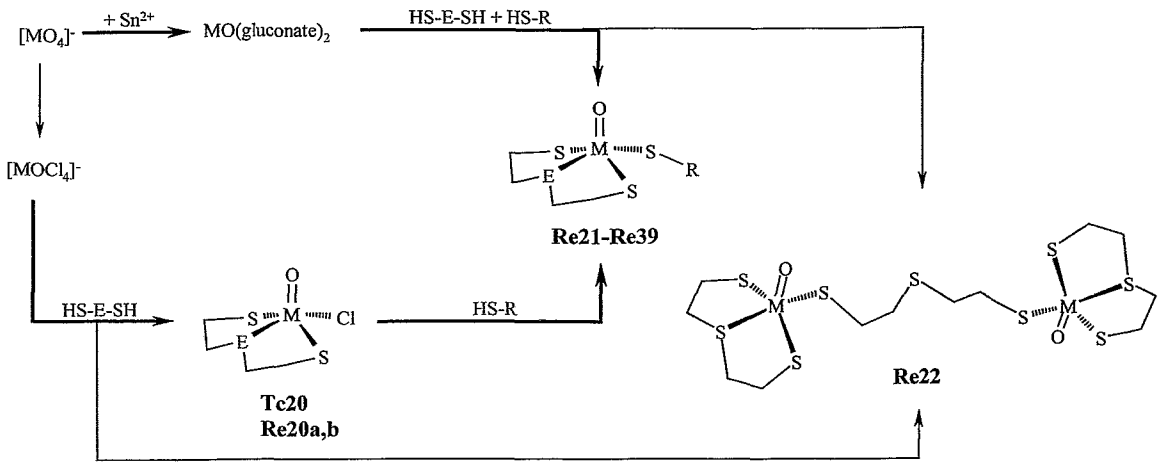


Fig. 6. Reaction routes to "3+1" mixed-ligand complexes

Our structural studies involve both simple chlorine-containing complexes **Re20a,b** and **Tc20** [17] used as precursor for more complicated complexes, but also so-called functionalized chelates bearing organic groups [18] or biologically active moieties [13] (**Re21-Tc40**). Complexes **Re24** and **Re34** exemplify binding of rhenium to a carbohydrate or a steroid moiety.

The "3+1" approach found broad application in the search for steroid-like [19] and neuroreceptor-affine [20] Tc and Re complexes. Coupling of "3+1" chelates with organic receptor-binding units resulted in complexes having high affinity to the 5-HT_{2A} receptor with K_i values in the subnanomolar range.

Re42 is a representative of "3+1" complexes based on tridendate Schiff base ligands with O,N,S donor set. Figure 7 compiles some typical representatives of precursors and functionalized "3+1" complexes.

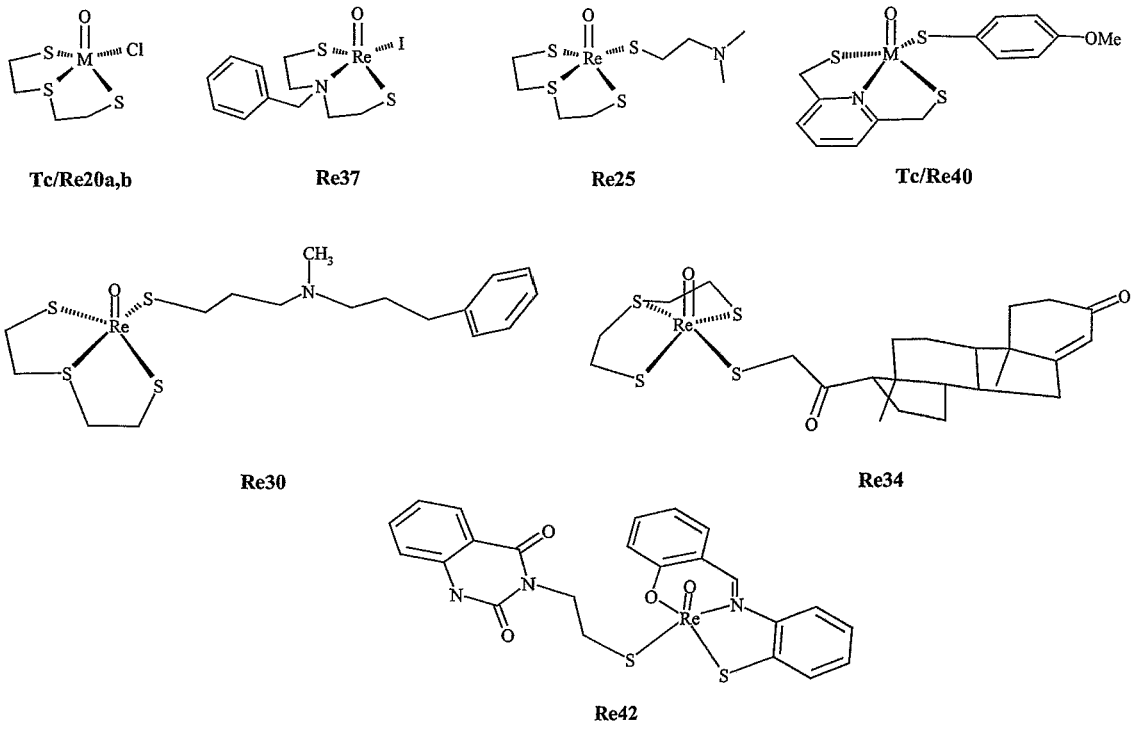


Fig. 7. Typical representatives of precursors and functionalized "3+1" complexes

Efforts to extend the concept [21] aim at less lipophilic and more stable chelates. Thus, when the tribasic SNO ligand mercaptoacetyl glycine reacts with $[MOCl_4]^-$ the chlorine containing compound $[MO(SNO)Cl]^-$ results (**Tc41, Re41**). That delivers, on attack of a monothiolate ligand, the anionic species $[MO(SNO)(SR)]^-$. Being more hydrophilic these chelates extend the potencies of the "3+1" approach [21].

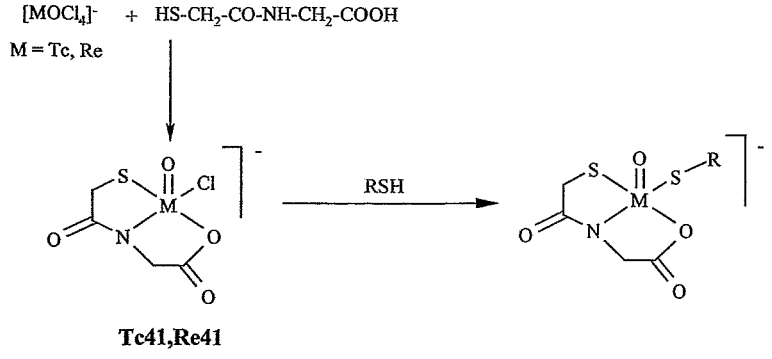


Fig. 8. Negatively charged "3+1" complexes with S, N, O/S coordination

Further contributions to molecular structures of novel "3+1" mixed-ligand rhenium complexes were given by Zubieta et al. [22] and Chiotellis et al. [23]. From the latter authors, mixed-ligand complexes derived from the tridentate S,N,N ligand have been described.

2.2.2.1 Square-pyramidal *vs.* trigonal-bipyramidal geometry in "3+1" complexes

Five-coordinated oxo(V) species of technetium and rhenium show, as a rule, distorted square-pyramidal configuration with tendency to trigonal-bipyramidal geometry. To describe the degree of distortion the parameter τ is used. This value is 0 for ideal square-pyramidal and 1 for trigonal-bipyramidal arrangement [37]. In Table 1 τ-values for a series of "3+1" mixed-ligand Re complexes [ReO(SES)(SR)] with E = S, O, NR are summarized.

Table 1. τ-values of some "3+1" mixed-ligand complexes

Complex	E	τ-value	ref.
Re 36	O	0.09	[18b]
Re 35	O	0.17	[18a]
Re 24	S	0.25	[18d]
Re 26	S	0.33	[18d]
Re 29	S	0.37	[18d]
Re 21	S	0.38	[18d]
Re 30	S	0.40	[18d]
Re 20a	S	0.41	[18d]
---	NH	0.61	[30]
---	N-$(CH_2)_2NEt_2$	0.63	[40]
Re 38	NMe	0.67	[18d]
Re 37	NBz	0.73	[17c]

Distorted square-pyramidal arrangement is found for E = O, S. Low τ-values are observed for E = O indicating small distortion of square-pyramidal geometry, while in complexes

with E = S τ-values between 0.25 and 0.4 reveal a considerably deviation towards trigonal-bipyramidal coordination.

When SN(R)S chelators are used, *syn* and *anti* isomerism is observed [38]. Unlike the *anti* isomer that tends to a square-pyramidal arrangement, trigonal-bipyramidal geometry is frequently observed for the *syn* oriented compounds. Within the NR series, one may expect that stronger distortion is a function of the alkyl chain lenght at the chelating moiety. However, comparison between NR complexes that differ in size of R (see Table 1) does not confirm this trend. So, only small differences in τ-values have been observed between compounds with R = methyl and R = diethylaminoethyl. The non-sensitivity of the τ-value concerning R is impressively shown for the complex with R = H, that has a τ-value of 0.61.

2.2.3. Dithioether ligands, thiacrown ethers

Studies have also been devoted to thioether ligands and their Tc/Re chemistry. Although the domaine of thioether ligands are complexes at lower oxidation states, some representatives of Re=O and Tc=O complexes have been obtained with bidentate thioether ligands (**Re43-Re51, Tc48,Tc50**) in the presence of anionic co-ligands [24]. The latter allows the compensation of the positive charge of the $[MO]^{3+}$ core. The requirement of charge compensation is obviously responsible for possessing the *trans* position of the M=O group by an additional donor group. In the absence of such groups, formation of binuclear M-O-M species is favoured.

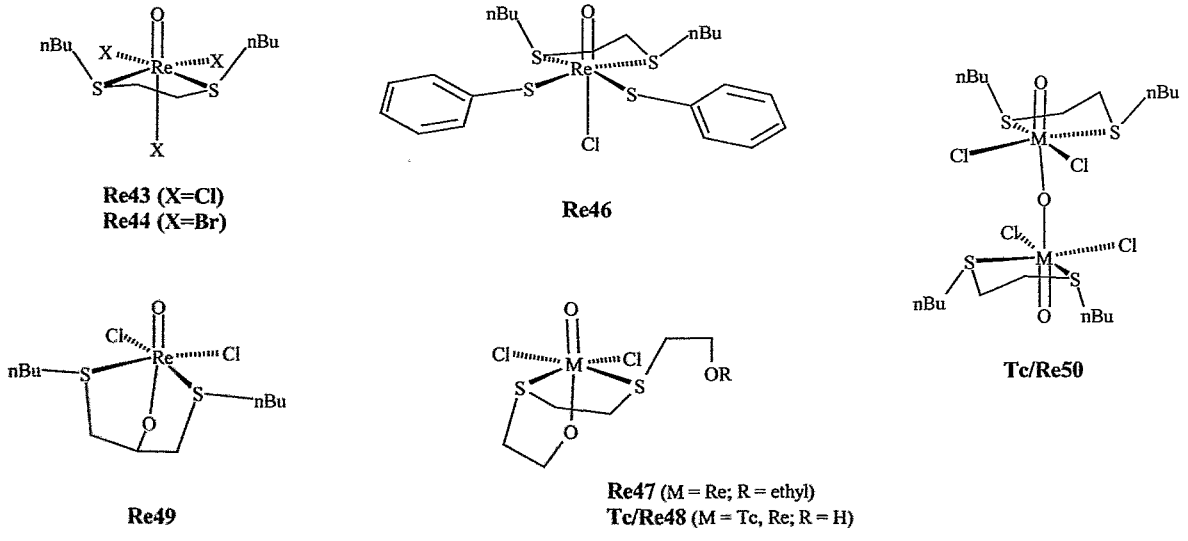
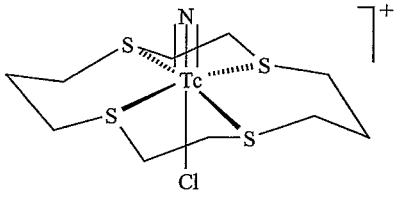
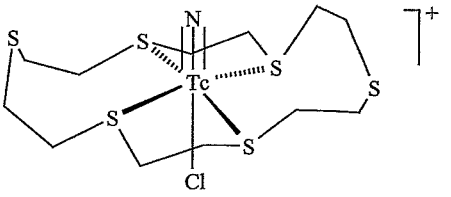


Fig. 9. Tc/Re(V) complexes with dithioether ligands

Thiacrown ethers form cationic nitridotechnetium(V) complexes. Charge compensation is achieved by a *trans*-positioned chlorine ligand (**Tc52-Tc54**) [25].



Tc52



Tc54

Fig. 10. Cationic TcN complexes with thiacrown ethers

A phosphine containing complex having some importance as precursor for oxorhenium(V) complexes $[ReOCl_3(PMe_2Ph)_2]$ (**Re55**) has been investigated [26].

2.3. Rhenium on the oxidation state IV

The only studied compound of Re(IV) is $[ReCl_4(PMe_2Ph)_2]$ (**Re56**) used as a precursor molecule [27].

2.4. Technetium and Rhenium on the oxidation state III

As for M(V), the M(III) chemistry was exploited with the aim to create simply structured, small-sized and stable chelates able to conjugate the metal centre to biologically active molecules.

There are two strategies. The first one comprises mixed-ligand complexes derived from "3+1" chelates by reduction of the metal centre leading to "3+1+1" and "3+2" ligand arrangements (**Tc57-Tc61**) [28,29]. The other makes use of the tripodal NS_3 ligand nitrilotris(ethanethiol) combined with phosphines or functionalized isonitriles as co-ligands (**Tc62-Tc66,Re67**) [30]. X-ray structural studies of such compounds have also been performed by E. Hahn et al. [30,31].

Furthermore, the combination of acyclic tetrathioether ligands with two dithiolates resulted in cationic "4+2" species (**Tc68**) [32].

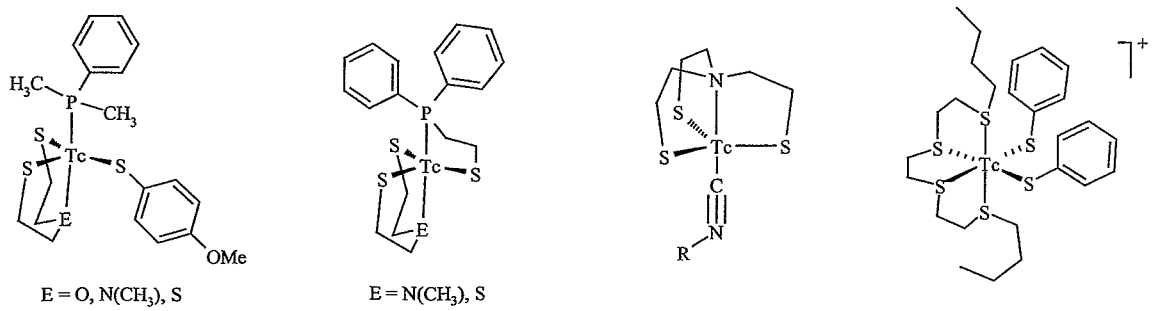
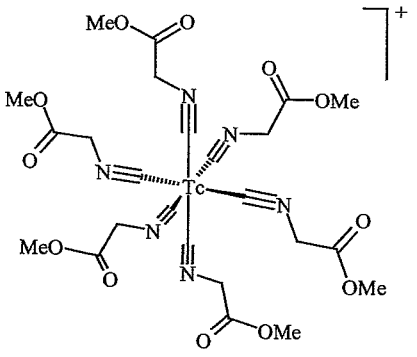


Fig 11. Tc(III) complexes with "3+1+1", "3+2", "4+1" and "4+2" donor-atom arrangement

The crystal structure of a mixed ligand Tc complex with DPPE and oxalic acid was performed earlier (**Tc69**) [33].

2.5. Technetium and Rhenium on the oxidation state I

A cationic hexakisisonitrile Tc(I) complex (**Tc70**) having pertechnetate as counter ion was formed, when Tc(V) disproportionates after attack of an isonitrile ligand [34] (Figure 12).

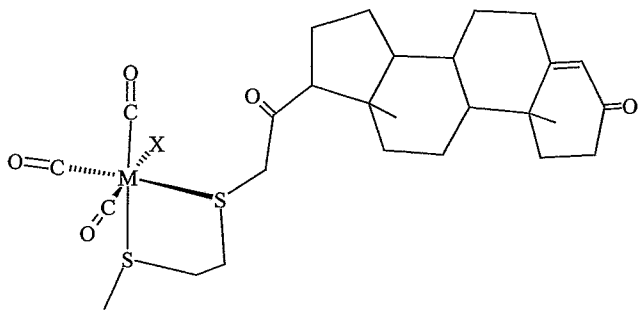


Tc70

Fig. 12. Cationic hexakisisonitrile Tc(I) complex

Studies on M(I) complexes focus on complexes derived from the $[M(CO)_3]^{3+}$ core. Since Alberto et al. succeeded in one-step synthesis of metal carbonyl precursors $[M(H_2O)_3(CO)_3]^+$ [35], the $[M(CO)_3]^+$ unit found increasing interest in Tc radiotracer design. Cooperating with R. Alberto (University of Zürich), we combined the $[M(CO)_3]^+$ moiety with multidentate thioether ligands bearing biomolecules [35a].

Two structural studies has been performed showing the binding of the $[M(CO)_3]^{3+}$ core to steroids (**Tc71, Re71**) [36] (Figure 13).



Tc71 (X=Cl)
Re71 (X=Br)

Fig. 13. Steroid-bearing Tc(I) and Re(I) carbonyl complexes

3. Crystallographic aspects

This chapter contains a concise report on crystal and molecular structure determinations, accuracy and significancy of structural parameters, and on the identificaton of crystalline forms of Tc and Re complexes by powder diffraction patterns.

Several structures reported here show order-disorder phenomena. These problems are treated in Chapter 3.5.1.. Generally, molecular structures presented here are in the ordered form. In some cases the disordered positions are shown in strange colors.

3.1. X-ray structure analyses

3.1.1. Structure determination from single-crystal data

Molecular and crystal structures of almost all Re and Tc complexes were determined by single-crystal structure analysis. For two compounds no suitable crystals were available. Their structures were solved from powder diffraction data (see Chapter 3.1.2.).

Crystal data and reflection intensities of about two thirds of all complexes were collected on an Enraf-Nonius CAD-4 diffractometer using monochromatized MoK_α radiation. Data of the remaining compounds were measured on a Siemens SMART diffractometer equipped with a CCD area detector. Intensities were corrected for Lorentz- and polarization effects. In most cases empirical absorption corrections were applied.

Structures were solved by the heavy-atom technique or by direct methods using MULTAN-82 [41] or SHELXS-90 [42]. Atomic coordinates and anisotropic displacement parameters were refined by full-matrix least-squares calculations using MOLEN [43], SHELXL-93 [44] or SHELXL-97 [45]. In most cases positions of hydrogen atoms were calculated according to ideal geometries and included into the structure refinement riding on the attached atoms.

Some crystals were disordered or/and of poor quality. In these cases more or less weighted restraints were used in the structure refinement.

Computing publication materials were produced by SHELXL-97. Drawings of the complexes were made by the programs PowderCell [46] and CELLGRAF [47]

3.1.2. X-ray structure determination from powder diffraction data

No single crystals were available for the structure analyses of the complexes **Re7** and **Re20b**. Therefore, these structures were determined from powder diffraction data using a conventional X-ray source. The powder diffraction patterns were measured on a SIEMENS D5000 diffractometer using following parameters:

geometry:	Bragg-Brentano
radiation:	CuK_α (λ = 1.5406/1.5444 Å)
divergence slit:	2Θ compensating
detection:	linear PSD (used length 20 mm)
sample carrier:	diameter 15 mm, depth 2 mm.

After the determination of lattice parameters approximate integral reflection intensities were extracted from the powder pattern by the IPAP method (Intensity Partion by Approximated Patterson function) [48]. This method is implemented in the program PowderCell [46]. The determination of intensities is combined with a special Rietveld refinement of lattice constants and profile parameters as well as with a selection of possible space groups. After these procedures the structure of **Re7** was solved by direct methods using SHELXS-90. In the case of **Re20b** the structure of a further crystalline form (**Re20a**) could be determined by single crystal structure analysis. Thus, the resulting molecular geometry could be used for the structure analysis of **Re30b** using the program POSIT [49]. Introducing restraints for bond lengths and angles structural parameters and reflection intensities were refined by a cyclic procedure consisting of least-squares calculations by SHELXL-97 and intensity partition using the actual molecular model. The correctness of the determined crystal structures of **Re7** and **Re20b** were proved by a comparison of the experimental powder patterns (see Figures 14a and 14a).

As shown in Figure 14b the powder sample of **Re20b** also contains crystals of the other polymorphic form **Re20a**. A quantitative phase analysis using the Rietveld method indicated a composition 90.6 % of **Re20b** and 9.4% of **Re20a.**

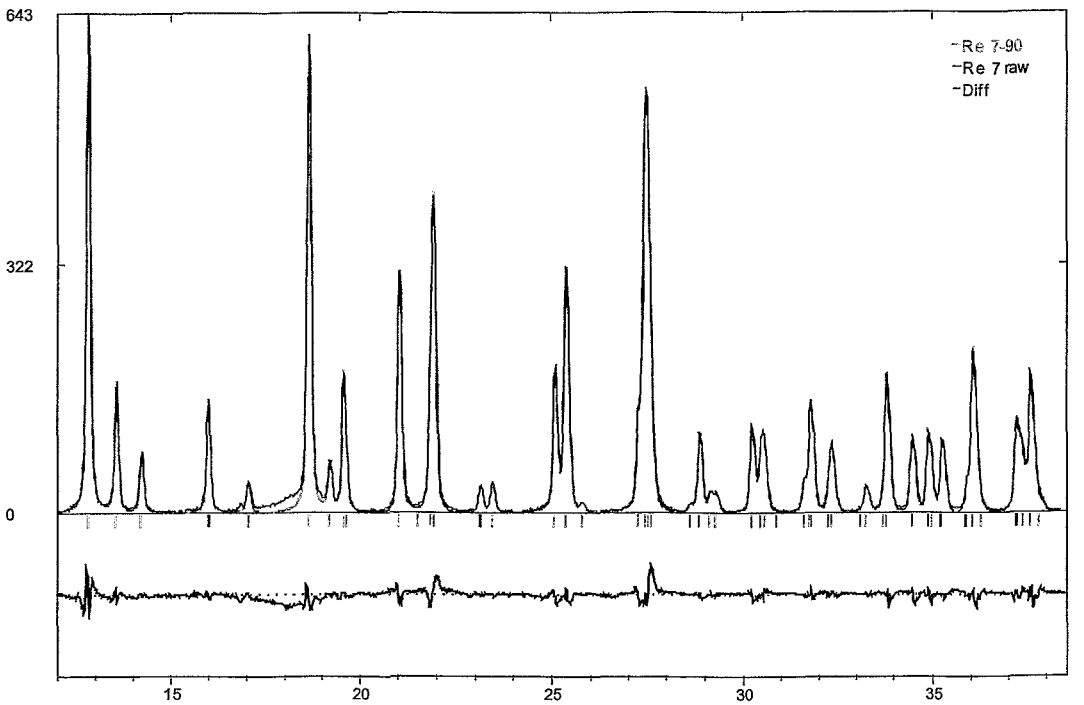


Fig. 14a. Comparison of calculated (red line) and experimental (blue) powder diffraction pattern of **Re7**

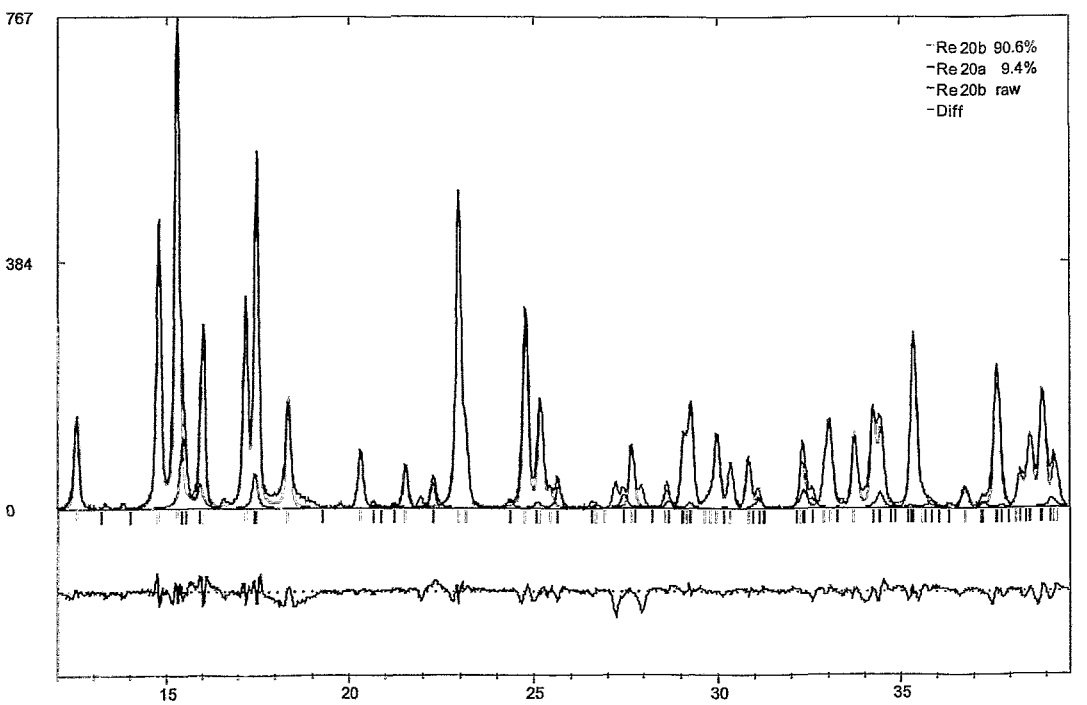


Fig. 14b. Comparison of calculated (red line) and experimental (blue) powder diffraction pattern of **Re20b.** The calculated pattern of **Re20a** occuring together with **Re20b** is marked by green lines.

3.2. Accuracy and stability of crystal structures

The accuracy of the structural parameters as bond lengths and angles depends mainly on the quality of the available single crystals. The quality is influenced by size, perfection and stability of the crystals. Special problems arise if crystals are twinned or if they consist of two or more pieces twisted to each other.

A raw criterion for the accuracy of the structure determinations is the conventional R-value which is defined by

$$R = \Sigma(|F_o|-|F_c|) / \Sigma|F_o|$$

with

F_o = observed stucture factors

F_c = calculated structure factors

R values for each structure determination are given in Chapter 5.

A better criterion for the accuracy of the structure determination are the standard deviations of bond lengts and angles resulting from the least-squares refinements. These are stored together with corresponding structural parameters on the provided CD (see footnote on p. 3).

Generally, the crystals of all investigated Tc and Re complexes were stable under normal ambient conditions. The structure determination of **Re9** and **Re5** were repeated after five and seven years, respectively. No changes of the molecular and crystal structeres were observed.

3.3. Identification of Tc and Re complexes by powder diffraction patterns

Using structural parameters obtained by single crystal structure analyses theoretical powder diffraction patterns were calculated by PowderCell for all Re and Tc complexes. These theoretical patterns can be used for the identification of the corresponding Re and Tc complexes in crystalline powder samples. This can be done by a comparison of theoretical and experimental patterns.

The theoretical diagrams were calculated using following conditions:

Diffraction geometry:	Bragg-Brentano
X-ray:	Cu-Kα
Wavelength	1.5406 / 1.5444 Å
Profile function	Pseudo Voigt 1 (na = 0.5, nb = 0)

FWHM	const., 0.16°
Divergence slit	const.
2theta range	0 – 30°

Using an automatic peak search procedure 2theta values, d values, and integral intensities were calculated for the 30 strongest reflections. These values and the corresponding diagrams are given for each compound in Chapter 6.

3.4. Storage and deposition of structure data

All crystallographic and structural data have been deposited at the Cambridge Crystallographic Data Centre (CCDC). Any request to the CCDC for data should quote the corresponding reference numbers given for each compound in Chapter 5.

All relevant informations on crystal structures and their solutions are stored on a CD provided together with this atlas. Data from this CD are available on request (see footnote on p.5). The CD contains the following files:

*.cif: crystallographic information file sent to the CCDC. Besides crystallographic data and details of structure analyses these files contain all bond lengths and angles including their estimated standard deviations.

*.res: out put file of SHEXL-97 with atomic coordinates and displacement parameters, input file for PowderCell and CELLGRAF

*.cel atomic coordinates, input file for PowderCell,

*.bas atomic coordinates; input file for CELLGRAF

The files *.res, *.cel, and *.bas contain atomic coordinates of the asymmetric unit. There are several binuclear complexes consisting of two symmetry-equivalent parts or the molecule has a symmetry element coinciding with the same element of the space group. In these cases the number of atoms in the drawings of chapter 5 is larger than the number of atoms in the asymmetric unit.

The reader has the possibilty to make drawings of molecular and crystal structures using PowderCell an /or CELLGRAF. PowderCell is a WINDOWS program (self-extracting executable). CELLGRAF is a DOS program consisting of following files: CG.EXE, ATOMS.INI, CELG.INI, SYMM1, and SYMM2. CELLGRAF.doc contains a description of the program.

3.5. Special crystallographic problems

3.5.1. Order-disorder phenomena

Several structures of the Re and Tc complexes show order-disorder phenomena. These can be divided into three groups:

1. *Rotational disorder:* There are at least two arrangements of substituents which are statistically realized in the crystal structure. This was observed in the following complexes: **Re2, Re15a, Re15b, Re25, Re26, Re41.**

2. *Flip-flop disorder:* Some rings change their conformation by a flip-flop mechanism giving rise to a statistical distribution if different conformations occur in the crystal structures. This kind of disorder was found in **Tc61, Tc66.**

3. *Symmetry disorder*: In this case one or more symmetry elements of the space group are fulfilled only statistically. This kind of order-disorder exists probably in **Re22.** In Chapter 5 space group $P2_1$ is given for this structure. From systematic absences of h0l reflections with h+l=2n+1 follows the existence of the space group $P2_1/n$. The resulting centre of symmetry causes steric hindrances between the central sulfur atoms S(5) and S(5').

3.5.2. Intermolecular interactions of selected compounds

In Chapter 5 only molecular structures of Re and Tc complexes are depicted. In some cases the reader may be interested to study intermolecular interactions using drawings of molecular packings. These drawings (stereo plots or mono pictures) can be produced using PowderCell or CELLGRAF and the corresponding structure files (*res, *cel, *.bas).

In the crystal the complexes are connected with each other by *van der Waals contacts*, *hydrogen bonds* or/and *π-π electron interaction*. Here we present one typical example for each kind of interaction.

- *van der Waals contacts*

Figure 15 shows a stereo plot of the very interesting arrangement of **Re71** bearing a steroid moiety. The molecules are hold together only by van der Waals interactions. The compound crystallizes in the unusual space group $P4_22_12$. There are wide channels (14 x 17 Å) extending in the z-direction of the crystal structure.

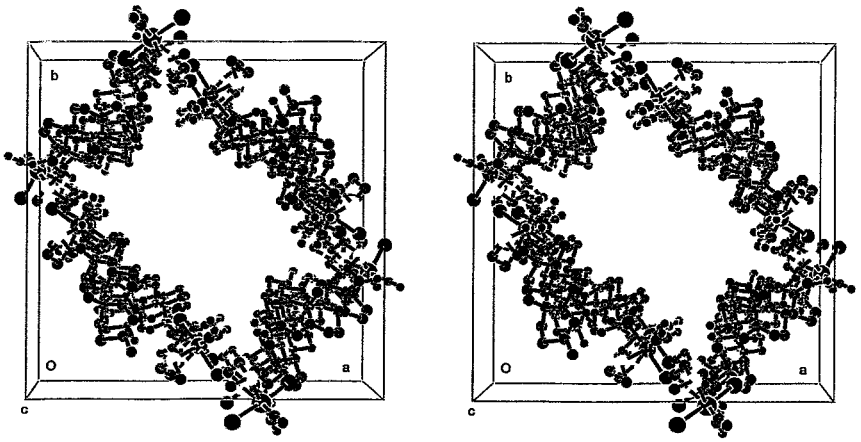


Fig. 15. Stereo plot of the molecular packing of **Re71**

- *hydrogen bonds*

The dominant interactions in the crystal structure of **Re24** are hydrogen bonds which form a complicate two-dimensional network. This is illustrated in Figure 16.

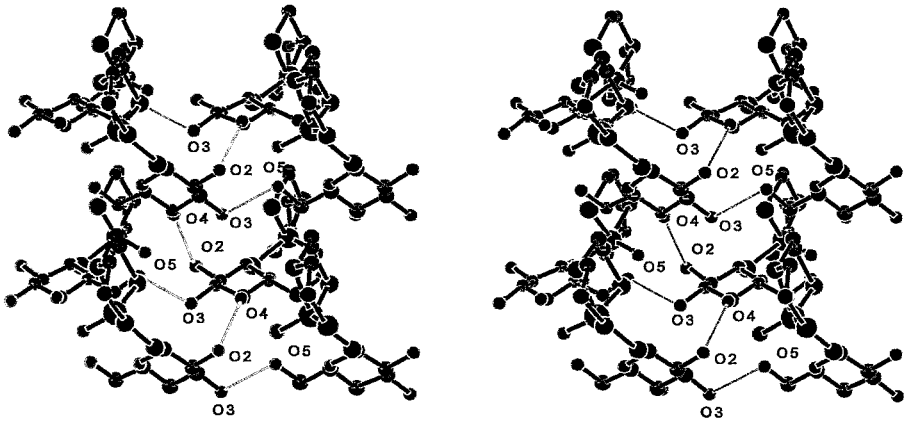


Fig. 16. Stereo plot of the two-dimensional hydrogen-bond network of **Re24**

- *π-π-Electron interactions*

π-π-Electron interactions of benzene rings occur in the crystal structure of **Re28**. The distances between the benzene planes are shorter than 3.4 Å. These interactions connect the molecules forming infinite stacks in x-direction.

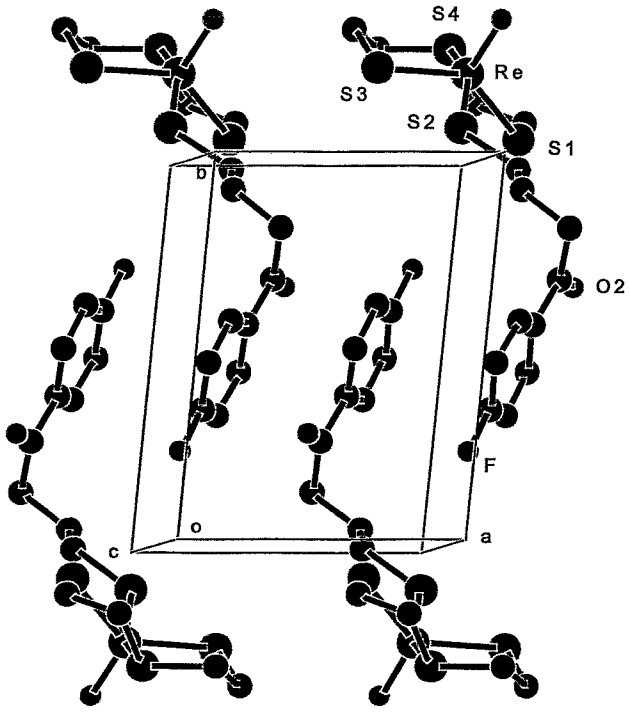


Fig. 17. Molecular stacks formed by π-π electron interactions in **Re28**

4. References

[1] K.Schwochau:
Technetium. Chemistry and Radiopharmaceutical Application
Wiley-VCH, 2000, p. 127 ff.

[2a] G.Bandoli, U.Mazzi, E.Roncari, E.Deutsch:
Crystal Structures of Technetium Compounds
Coord. Chem. Rev. 44 (1982) 57

[2b] M.Melnik, J.Van Lier:
Analyses of structural data of technetium compounds
Coord. Chem. Rev. 77 (1987) 275

[3] F.Tisato, F.Refosco, G.Bandoli:
Structural survey of technetium complexes
Coord. Chem. Rev. 135/136 (1994) 325-397

[4] H.Stephan, H.Spies, B.Johannsen, L.Klein, F.Vögtle:
Lipophilic urea-functionalized dendrimers as efficient carriers for oxoanions
Chem. Commun. 1999, 1875 - 1876

[5a] H.Stephan, R.Berger, H.Spies, B.Johannsen, F.P.Schmidtchen:
Efficient phase tranfer of pertechnetate with bicyclic guanidinium compounds
J.Radioanal.Nucl.Chem. 242 (1999) 399 - 403

[5b] B.Johannsen, H.Spies:
Chemistry of technetium(V) as relevant for nuclear medicine
Topics Curr.Chem. 176 (1996) 77-121

[6a] Spies, H., D.Scheller:
Chemical and ^{1}H NMR spectroscopic investigations of stereoisomeric Tc(V) DMSA complexes
Inorg.Chim.Acta 116 (1986) 1-4

[6b] Bandoli, G., M.Nicolini, U.Mazzi, H.Spies, R.Münze:
Synthesis and X-ray crystal structure of tetraethylammonium bis(1.2-di(carbmethoxy)ethane-1.2-dithiolato)oxotechnetate(V)
Transition Met.Chem. 9 (1984) 127-129

[6c] S. Seifert, H.Spies, P. Leibnitz, G. Reck
Rhenium (V) complexes with meso-DMSA PART (III): X-ray crystal structure of $Rh_4As[ReO(DMSA)_2] \times 2$ acetone and identification of the possible isomers
FZR-32 (1993) 91-95

[7] S.Seifert, P.Leibnitz, H.Spies:
Nitridorhenium(V)-Komplexe mit Dimercaptobernsteinsäuredimethylester. Präparation, Charakterisierung und Kristallstruktur von $[Re\{NC(CH_3)_2PPhMe_2\}(DMSMe_2)_2]$
Z. Anorg. Allg. Chem. 625 (1999) 1037 - 1040

[8] S. Seifert, unpublished results

[9a] S.Kirsch, B.Noll, H.Spies, P.Leibnitz, D.Scheller, T.Krueger, B.Johannsen:
Preparation and structural studies of neutral oxorhenium(V) complexes with D-penicillamine methyl ester
J.Chem.Soc., Dalton Trans. 1998, 455-460

[9b] S.Kirsch, R.Jankowsky, P.Leibnitz, H.Spies, B.Johannsen:
Crystal and solution structure of oxorhenium(V) complexes with cysteine and cysteine methyl ester
J.Biol.Inorg.Chem., 4 (1999) 48 - 55

[10a] C.S. Hilger, F. Blume, B. Noll, P. Leibnitz, H.Spies:
Tc (V) and Re (V) complexes of N-('MAG_1)-histamine
Technetium, Rhenium and Other Metals in Chemistry and Nuclear Medicine SGE Editoriali-Italy (1999) 221-224

[10b] C.S. Hilger, F. Blume, P. Leibnitz, B. Johannsen
Tc (V) and Re (V) complexes of N-(mercaptoacetyl-glycyl))-histamine
Annual Report FZR 200 (1997) 92 - 94

[10c] B.Noll, C.S. Hilger, P. Leibnitz, H.Spies, L.Dinkelborg, B.Johannsen:
A novel amide thioether dithiolate ligand derived from cysteine
Annual Report FZR 165 (1996) 59 - 61

[11a] B. Noll, St. Noll, P. Leibnitz, H. Spies, B. Johannsen
Technetium and rhenium complexes of mercaptoacetyl glycine ligands. 6. Preparation and X-ray structure of $Ph_4As[ReO(MAG_1)Cl]$
Annual Report FZR 122 (1995) 105 - 107

[11b] B. Noll, St. Noll, P. Leibnitz, H. Spies, P.E. Schulze, W. Semmler and B. Johannsen
Technetium and rhenium complexes of mercaptoacetyl glycine ligands. II. Formation and molecular structure of Re (V) complexes with mercaptoacetyl glycine and mercaptoacetyl glycine ethylester
Inorg.Chim.Acta 255 (1997) 399-403

[11c] B. Johannsen, B.Noll, P.Leibnitz, G.Reck, St.Noll, H.Spies:
Technetium and rhenium complexes of mercapto containing peptides.
1. Tc(V) and Re(V) complexes with mercaptoacetyl diglycine (MAG_2) and X-ray structure of $AsPh_4[TcO(MAG_2)] \times C_2H_5OH$
Inorg.Chim.Acta, 210 (2) (1993) 209 - 214

[12] Pietzsch, H.-J., H.Spies, S.Hoffmann:
Lipophilic Technetium Complexes. VI. Neutral Tc(V) complexes with tridentate dithiole/monothiole ligand coordination
Inorg.Chim.Acta 165 (1989) 163-166

[13a] H.Spies, Th.Fietz, M.Glaser, H.-J.Pietzsch, B.Johannsen:
The "n+1" concept in the strategy of novel technetium and rhenium tracers
4th Int.Symp. on Technetium in chemistry and nuclear medicine, 12.-14.Sept. Bressanone, 243-246.

[13b] Spies, H. and B.Johannsen:
Functionalization of Technetium complexes to make them active in vivo
Analyst 120 (1995) 775-777

[14] B.Johannsen and H.Spies:
Advances in technetium chemistry towards ^{99m}Tc receptor imaging agents
Transition Met.Chem. 22 (1997) 318-320.

[15a] Spyriounis, D.M., Pelecanou, M., Stassinopoulou, C.I., Raptopoulou, C.P., Terzis, A., Chiotellis, E.
Synthesis and Characterization of Oxotechnetium(V) Complexes with Aza-Substituted 2,6-Dimethyl-4-azaheptane-2,6-dithiol Ligands and Benzyl Mercaptan as Coligand
Inorg. Chem. 34(1995)1077-1082

[15b] Pirmettis, I.C.; Papadopoulos, M.S.; Mastrostamatis, S.G.; Raptopoulou, C.P.; Terzis, A.; Chiotellis, E.
Synthesis and characterization of oxotechnetium(V) mixed-ligand complexes containing a tridentate N-substituted bis(2-mercaptoethyl)amine and a monodentate thiol
Inorg.Chem. 35 (1996), S. 1685-1691

[15c] B.Nock, H.-J.Pietzsch, F.Tisato, T.Maina, P.Leibnitz, H.Spies, E.Chiotellis:
Oxorhenium mixed-ligand "3+1" and "3+2" complexes with the 2,6-dithiomethylpyridine ligand. Crystal structure of [2,6-dimethylthiopyridinato][p-methoxybenzenethiolato]oxo-rhenium.
Inorg.Chim.Acta 304(1) (2000) 26 - 32

[16] H.-J.Pietzsch, unpublished results

[17a] Fietz, T, H.Spies, H-J.Pietzsch and P.Leibnitz:
Synthesis and Molecular Structure of Chloro(3-thiapentane-1,5-dithiolato)oxorhenium(V)
Inorg.Chim.Acta 231 (1995) 233-236

[17b] T.Fietz, P.Leibnitz:
Reactions of hydroxy group bcontaining "3+1" mixed-ligand rhenium(V) complexes. Part 3: Unexpected reaction of "3+1" mixed-ligand complexes with thionyl and acyl halides and methyl iodide. Structural considerations for a new modification of chlorooxo(3-thiapentane-1,5-dithiolato)rhenium(V)
Annual Report FZR 200 (1999) 119 - 123

[17c] T. Fietz, P.Leibnitz, H. Spies, B.Johannsen:
Synthesis and Reactions of New Oxorhenium(V) Complexes with Re–Halogen Bonds. X–Ray Crystal Structure of (3–(Benzyl)azapentane-1,5-dithiolato)iodo-oxorhenium(V).
Polyhedron 18 (1999) 1793 - 1797

[17d] B.Noll, P.Leibnitz, H.Spies:
Synthesis and molecular structure of chloro(3-thiapentane-1,5-dithiolato)oxotechnetium(V)
Annual Report FZR 270 (1999) 151 - 152

[18a] H.Spies, Fietz, T, H-J.Pietzsch, B.Johannsen, P.Leibnitz, G.Reck, D.Scheller, K.Klostermann:
Neutral Oxorhenium(V) Complexes with Tridentate Dithiol Ligands and Monodentate Alkyl/Aryl Thiols as Co-ligands
J.Chem.Soc. Dalton Trans. 1995, 2277-2280

[18b] Fietz, T., H.Spies, P.Leibnitz, D.Scheller:
Mixed-ligand oxorhenium(V) complexes with rhenium-selenium bonds. Molecular structure of (3-oxapentane-1,5-dithiolato)(benzeneselenolato)oxorhenium(V)
J.Coord.Chem. 38 (1996) 227-235.

[18c] B.Noll. P.Leibnitz, St.Noll, R.M.Mahfouz, H.Spies:
Structure and reactivity of a "3+1" mixed-ligand rhenium complex containing thiobenzoate as a monodentate ligand [ReO(SSS)(C(O)Ph)]
Annual Report FZR 165 (1996) 93 - 95

[18d] T. Fietz, Oxorhenium(V)-Komplexe mit "3+1"-Gemischtligand-Koordination
Thesis, Dresden 1996

[19a] F.Wüst, P.Leibnitz, H.Spies:
Technetium and rhenium-labelled steroids: 4. Synthesis of "3+1" mixed-ligand oxorhenium(V) complexes with 17α-mercaptoalkynyl derivatives of 3,17β-estradiol
Annual Report FZR 200 (1997) 43 - 45

[19b] F.Wüst, M.B.Skaddan, P.Leibnitz, H.Spies, J.A.Katzenellenbogen, B.Johannsen:
Synthesis of novel progestin-rhenium conjugates as potential ligands for the progesterone receptor
Bioorg.Med. Chem. 7 (1999) 1827 - 1835

[20a] Johannsen,B., M.Scheunemann, H.Spies, P.Brust, J.Wober, R.Syhre, H.-J.Pietzsch:
Technetium(V) and rhenium(V) complexes for 5-HT_{2A} serotonin receptor binding: Structure-affinity considerations
Nucl.Med.Biol. 23 (1996) 429-438.

[20b] H. Spies, B. Noll, St. Noll, M. Findeisen, P.Leibnitz, P. E.Schulze and B.Johannsen:
Synthesis and Molecular Structure of a Rhenium Complex derived from 8α-amino-6-methylergoline
Chem.Ber., 130 (1997) 839-841

[20c] A.Hoepping, P.Brust, R.Berger, P.Leibnitz, H.Spies, S.Machill, D.Scheller, B.Johannsen:
Novel rhenium complexes derived from α-tropanol as potential ligands for the dopamine transporter
Bioorg.Med.Chem., 6 (1998) 1663 – 1672

[20d] H. Spies, P. Leibnitz, St. Noll, B. Noll:
Technetium-and rhenium complexes derived from spiperone II. X-ray crystal structure of [(3-thiapentane-1,5-dithiolato)(p-fluorophenyl-1-oxobutanethiolato-4)] oxorhenium (V)
Annual Report FZR 32 (1993) 40-42

[21] H.Spies, H.-J.Pietzsch, B.Johannsen:
The "n+1" mixed-ligand approach in the design of specific technetium radio-pharmaceuticals: Potentials and problems
5th Int. Symp. on Technetium in chemistry and nuclear medicine, 6.-9.Sept. 1998, Bressanone,101 - 108.

[22] K.V.Mareska, G.H.Bonavia, J.W.Babich, J.Zubieta:
Synthesis and characterization of oxorhenium "3+1" mixed thiolate complexes. Crystal and molecular structures of $[ReO\{\eta^3\text{-}(SCH_2CH_2)_2S\}(C_6H_4X\text{-}4\text{-}CH_2S)]$ (X = F, Cl, Br, OMe) and of the pendent thiolate compounds $[ReO\{\eta^3\text{-}(SCH_2CH_2)_2S\}(\eta^1\text{-}SCH_2CH_2SCH_2CH_2SH)]$ and $[ReO\{\eta^3\text{-}(SCH_2CH_2)_2S\}\{\eta^1\text{-}SCH_2CH(OH)CH(OH)CH_2SH\}]$.
Inorg.Chim.Acta 284 (2) (1999) 252-257

[23] Papadopoulos, M. S.; Pelecanou, M.; Pirmettis, I. C.; Spyriounis, D. M.; Raptopoulou, C. P.; Terzis, A.; Stassinopoulou, C. I.; Chiotellis, E.
A new donor atom system [(SNN)(S)] for the synthesis of neutral oxotechnetium(V) mixed-ligand complexes.
Inorg. Chem. 35 (1996) 15, S. 4478-4483

[24a] Pietzsch, H.-J., H.Spies, P.Leibnitz, G.Reck, J.Beger, R.Jacobi:
Technetium Complexes with Thioether Ligands. 2. Synthesis and Structural Characterization of Neutral Oxotechnetium(V) Complexes with Dithioethers. X-Ray Structure Analysis of μ-Oxo-bis(5,8dithiadodecane)-dichlorooxotechnetium(V) and (8-hdroxy-3,6-dthiaoctane-1-olato)dichlorooxotechnetium(V)
Polyhedron, 12 (1993) 187 - 193

[24b] H.-J.Pietzsch, M.Reisgys, H.Spies, P.Leibnitz, B.Johannsen:
Technetium and rhenium complexes with thioether ligands. 5. Synthesis and structural characterization of neutral oxorhenium(V) complexes with tridentate dithioethers
Chem. Ber. 130 (1997) 357 - 361

[24c] M.Reisgys, H.Spies, B.Johannsen, P.Leibnitz, H.-J.Pietzsch:
Technetium and rhenium complexes with thioether ligands. VI. Synthesis and structural characterization of mixed-ligand oxorhenium(V) complexes containing bidentate dithioethers and monothiolato ligands.
Chem.Ber. 130 (1997) 1343 - 1347.

[24d] M.Reisgys, H.-J.Pietzsch, H.Spies, P.Leibnitz:
Technetium and rhenium complexes with thioether ligands. 7. Mononuclear trichlorooxorhenium(V) complexes with bidentate and tetradentate thioethers.
Annual Report FZR 122 (1995) 116 - 119.

[24e] M.Reisgys, H.-J.Pietzsch, H.Spies, P.Leibnitz:
Technetium and rhenium complexes with thioether ligands. 8. X-ray structure of mononuclear oxorhenium(V) complexes with bidentate thioethers and dithiaalcohol ligands.
Annual Report FZR 165 (1996) 79 - 81.

[24f] H.-J. Pietzsch, H. Spies, P. Leibnitz, G. Reck
Technetium and Rhenium complexes with Thioether LigandsIV. Synthesis and structural characterization of Binuclear Oxorhenium(V) complexes with bidentate thioether Coordination
Polyhedron 13-14 (1995) 1849-1853

[25] Pietzsch, H.-J., H.Spies, P.Leibnitz, G.Reck:
Technetium Complexes with Thioether Ligands. 3. Synthesis and Structural Characterization of Cationic Nitridotechnetium(V) Complexes with Thiacrown Ethers.
Polyhedron, 12 (1993) 2995 – 3002

[26] H.-J. Pietzsch, unpublished results

[27] H.-J. Pietzsch, unpublished results

[28] H.-J.Pietzsch, H.Spies, S.Hoffmann;
Lipophilic Technetium Complexes.IX. The reduction of (3-oxapentane-1,5-dithiolato)(p-carbmethoxybenzenethiolato)oxotechnetium(V) by tertiary phosphines
Inorg. Chim. Acta 168 (1990) 7-9

[29a] H.-J.Pietzsch, S.Seifert, A.Drews, P.Leibnitz, H.Spies:
Synthesis and characterization of novel mixed-ligand technetium(III) complexes containing tridentate/monodentate thiol ligands and monodentate phosphines
Annual Report FZR 283 (1999) 74 - 75

[29b] H.-J.Pietzsch, F.Tisato, F.Refosco, P.Leibnitz, A.Drews, S.Seifert, H.Spies:
Synthesis and characterization of novel trigonal-bipyramidal technetium(III) mixed-ligand complexes with SES/S/P coordination (E = O, $N(CH_3)$, S)
Inorg. Chem. 40, 2001, 59 - 64

[30a] Spies, H., M.Glaser, H.-J.Pietzsch, F.E.Hahn, O.Kintzel, T.Lügger:
Trigonal-bipyramidale Technetium- und Rhenium-Komplexe mit vierzähnigen tripodalen NS_3-Liganden
Angew.Chem., 106 (1994) 1416-1419

[30b] Spies, H., M.Glaser, H.-J.Pietzsch, F.E.Hahn, O.Kintzel, T.Lügger:
Synthesis and reactions of trigonal bipyramidal rhenium and technetium complexes with a tripodal NS_3 ligand
Inorg.Chim.Acta 240 (1995) 465-478

[31] M. Glaser, H.Spies, T.Lügger, F.E.Hahn:
Formation of a rhenium(III) carbonyl complex by electrophilic attack on rhenium isocyanides. Synthesis and molecular structure of $\{Re[N(CH_2CH_2S)_3][CNC(CH_3)_3]\}$ and $\{Re[N(CH_2CH_2S)_3](CO)]\}$
J.Organomet.Chem. 503 (1995) C32-C35

[32] H.-J. Pietzsch, H.Spies, P.Leibnitz, G.Reck, J.Beger, R.Jacobi:
Technetium Complexes with Thioether Ligands. 1. Cationic Technetium(III) Complexes Containing Tetradentate Thioether/Monothiole Ligands; X-Ray Structure Analysis of Bis(benzenethiolato)(5,8,11,14-tetrathiaoctadecane)technetium(III)hexafluorophosphate
Polyhedron, 11 (1992) 1623 - 1628

[33] S. Seifert, R. Muenze, P. Leibnitz, G. Reck and J. Stach:
Preparation , characterization and crystal structure of a mixed ligand complex of technetium with DPPE and oxalic acid: Oxalato-bis[1.2-bis- (diphenylphosphino)-ethane] technetium (III)
Inorg.Chim.Acta 193 (1992) 167-172

[34] B. Noll, P. Leibnitz, H. Spies
Synthesis and molecular structure of $[Tc(CN\text{-}CH_2\text{-}COOH_3)_6]TcO_4$
Annual Report FZR 270 (1999) 153

[35] R.Alberto,R.Schibli, A.Egli, A.P.Schubiger T. A. Kaden:
A Novel Organometallic Aqua Complex of Technetium for the Labeling of Biomolecules: Synthesis of $[^{99m}Tc(OH_2)_3(CO)_3]^+$ from $[^{99m}TcO_4]^-$ in Aqueous Solution and Its Reaction with a Bifunctional Ligand,
J.Am.Chem.Soc 1998 120(31) 7987-7988

[35a] Pietzsch H.-J., Gupta A., Reisgys M., Drews A., Seifert S., Syhre R., Spies H., Alberto R., Abram U., Schubiger P. A., Johannsen B.
Chemical and biological characterization of technetium(I) and rhenium(I) tricarbonyl complexes with dithioether ligands serving as linkers for coupling the $Tc(CO)_3$ and $Re(CO)_3$ moieties to biologically active molecules
Bioconjugate Chem. 2000, 11, 414-424

[36] F.Wüst, unpublished results

[37] A.W.Addison, T.N.Rao, J.Reedijk, J.van Rijn, G.C.Verschoor:
Synthesis, structure, and spectroscopic properties of copper(II) compounds containing nitrogen-sulphur donor ligands; the crystal and molecular structure of aqua[1,7-bis(N-methylbenzimidazol-2'-yl)-2,6-dithiaheptane]copper(II) perchlorate
JCS, Dalton Trans. 1984, 1349

[38] Papadopoulos, M. S.; Pirmettis, I. C.; Pelecanou, M.; Raptopoulou, C. P.; Terzis, A.; Stassinopoulou, C. I.; Chiotellis, E.:
Syn-anti isomerism in a mixed-ligand oxorhenium complex, ReO[SN(R)S][S]
Inorg Chem 35 (1996) 25, S. 7377-7383

[39] M.Glaser, H.Spies, R.Berger, F. E. Hahn,T. Lügger, B.Johannsen:
Unexpected formation of the new oxorhenium(V) complex $ReO(NH(CH_2CH_2S)_2)(SC_6H_5)$ obtained by N-C cleavage of the tripodal ligand $N(CH_2CH_2SH)_2$
Inorg.Chim.Acta 257 (1997) 143 - 147.

[40] M.Papadopoulos, I.Pirmettis, C.Raptopoulou, E.Chiotellis, M.Friebe, R.Berger, H.Spies, B.Johannsen:
Synthesis, structure, lipophilicity and protonation behaviour of mixed-ligand rhenium chelates functionalized by amine groups
Appl.Radiat.Isot. 49 (1998)961 – 965

[41] P. Main, S.,J. Fiske, S. E. Hull, L. Lessinger, G. Germain, J. P. Declercq, M. M. Woolfson: MULTAN-82. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data. University of York, England, 1982

[42] G. M. Sheldrick: SHELXS-90 Acta Cryst., Sect. A (1990) 46, 467

[43] B.A. Frenz & Associates, INC.,College Station, Texas 77840 and ENRAF-NONIUS, Delft, Holland MOLEN-SDP Structure Determination Package

[44] G. M. Sheldrick: SHELXL-93. University of Göttingen: Göttingen, Germany, 1993

[45] G. M. Sheldrick: SHELXL-97. University of Göttingen: Göttingen, Germany, 1997

[46] W. Kraus, G. Nolze: PowderCell, a Program for the Representation and Manipulation of Crystal Structures and Calculation of the Resulting X-ray Powder Patterns J. App. Cryst. (1996) 29, 301-303

[47] G. Reck, G. Walther, R.-G. Kretschmer: CELLGRAF, Bundesanstalt für Materialforschung und –prüfung, Berlin, Germany, 1996

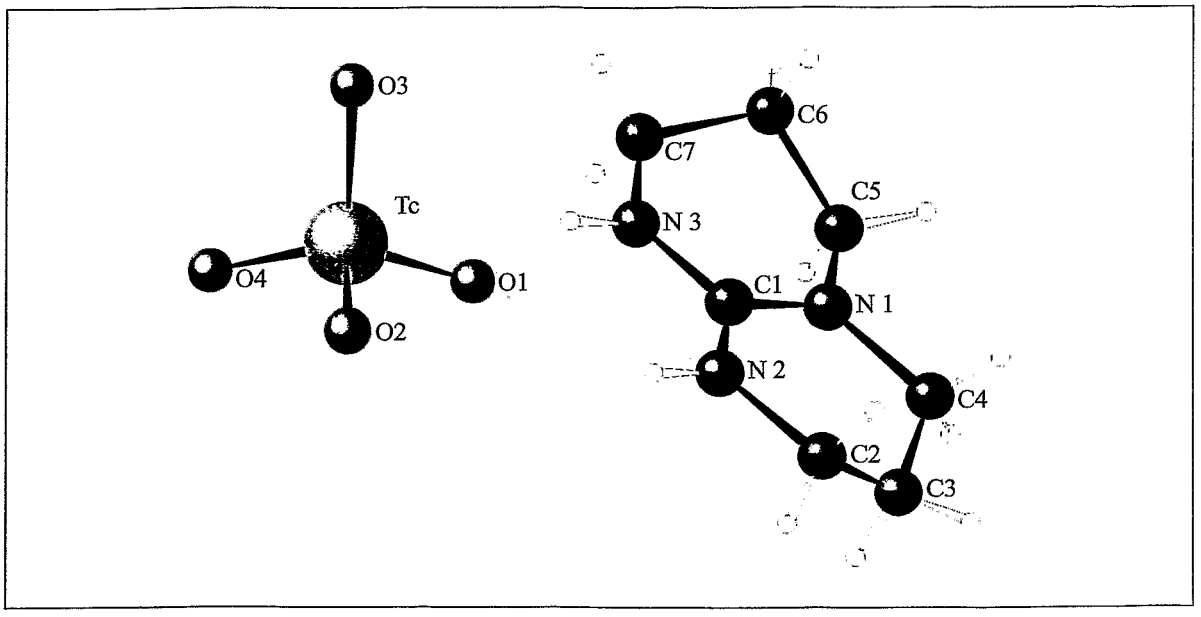
[48] G. Reck: Röntgenstrukturanalyse aus Pulverdiffraktionsdaten Workshop, Frankfurt am Main 27.-30.09.1999. Tagungsband der Johann Wolfgang Goethe-Universität, Frankfurt am Main, Germany

[49] G. Reck, R.-G. Kretschmer, L. Kutschabsky, W. Pritzkow: POSIT – a Method for Structure Determination of Small Partially Known Molecules from Powder Diffraction Data, Acta Cryst. A44 (1988) 417-421

5. Tables of Structures

5.1. Oxoanions of Tc(VII) and Re(VII)

Tc 1



[3,4,6,7,8,9-Hexahydro-2H-pyrimidino(1,2-a)pyridinium]pertechnetate

$C_7H_{14}N_3O_4Tc$

7.7065Å	15.9182Å	8.7084Å	
90.0000°	98.5560°	90.0000°	V=1056.0Å^3
$P2_1/c$; 14	Z=4; F(000)=608	ρ=1.900g/cm^3	R=11.3%
monoclinic			

H. Stephan (1999)
not published
CCDC 159493

Tc 1

Selected Bonds (Å) and Angles (°)

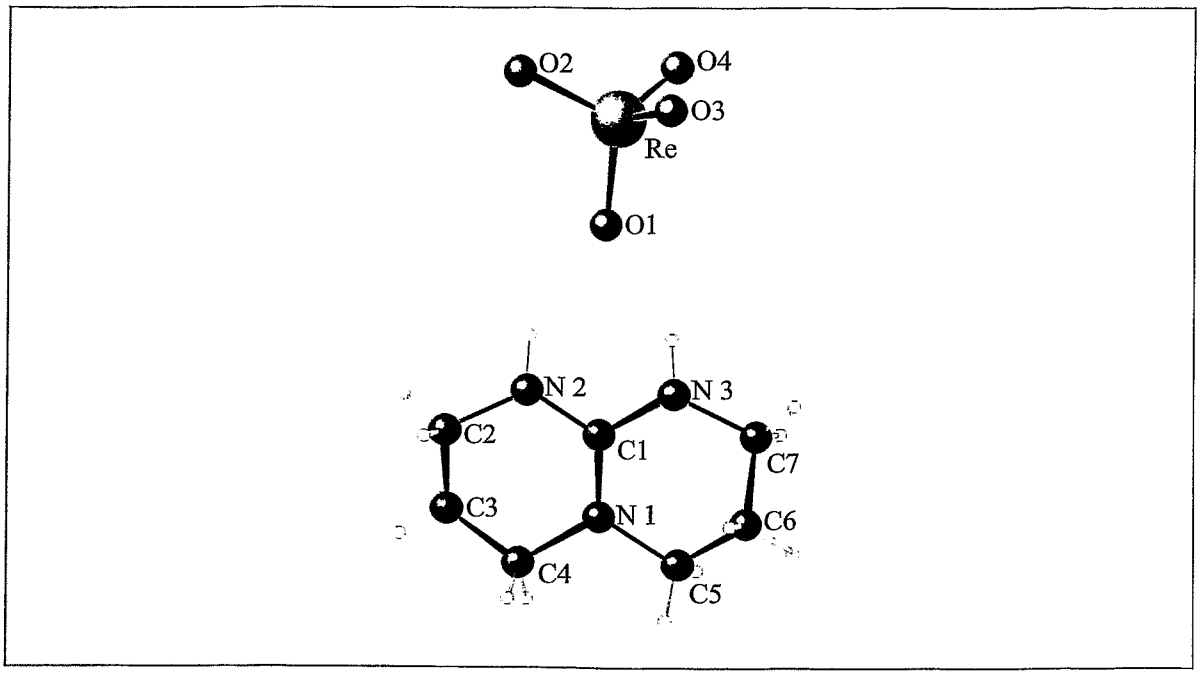
Bonds

Tc-O(3)	1.684
Tc-O(4)	1.688
Tc-O(2)	1.695
Tc-O(1)	1.702
N(1)-C(1)	1.305
N(1)-C(5)	1.454
N(1)-C(4)	1.461
N(2)-C(1)	1.325
N(2)-C(2)	1.455
N(3)-C(1)	1.325
N(3)-C(7)	1.457
C(2)-C(3)	1.427
C(3)-C(4)	1.442
C(5)-C(6)	1.496
C(6)-C(7)	1.478

Angles

O(3)-Tc-O(4)	108.80
O(3)-Tc-O(2)	108.40
O(4)-Tc-O(2)	109.10
O(3)-Tc-O(1)	111.20
O(4)-Tc-O(1)	109.70
O(2)-Tc-O(1)	109.60
C(1)-N(1)-C(5)	121.30
C(1)-N(1)-C(4)	122.20
C(5)-N(1)-C(4)	116.60
C(1)-N(2)-C(2)	123.00
C(1)-N(3)-C(7)	123.30
N(1)-C(1)-N(3)	120.80
N(1)-C(1)-N(2)	120.60
N(3)-C(1)-N(2)	118.60
C(3)-C(2)-N(2)	110.70

Re 1



[3,4,6,7,8,9-Hexahydro-2H-pyrimidino(1,2-a)pyridinium]perrhenate

$C_7H_{14}N_3O_4Re$

7.7835Å	16.1240Å	8.7342Å	
90.0000°	98.5960°	90.0000°	V=1083.8Å^3
$P2_1/c$; 14	Z=4; F(000)=736	ρ=2.393g/cm^3	R=3.0%
monoclinic			

H. Stephan (1999)
not published
CCDC 161728

Re 1

Selected Bonds (Å) and Angles (^{0})

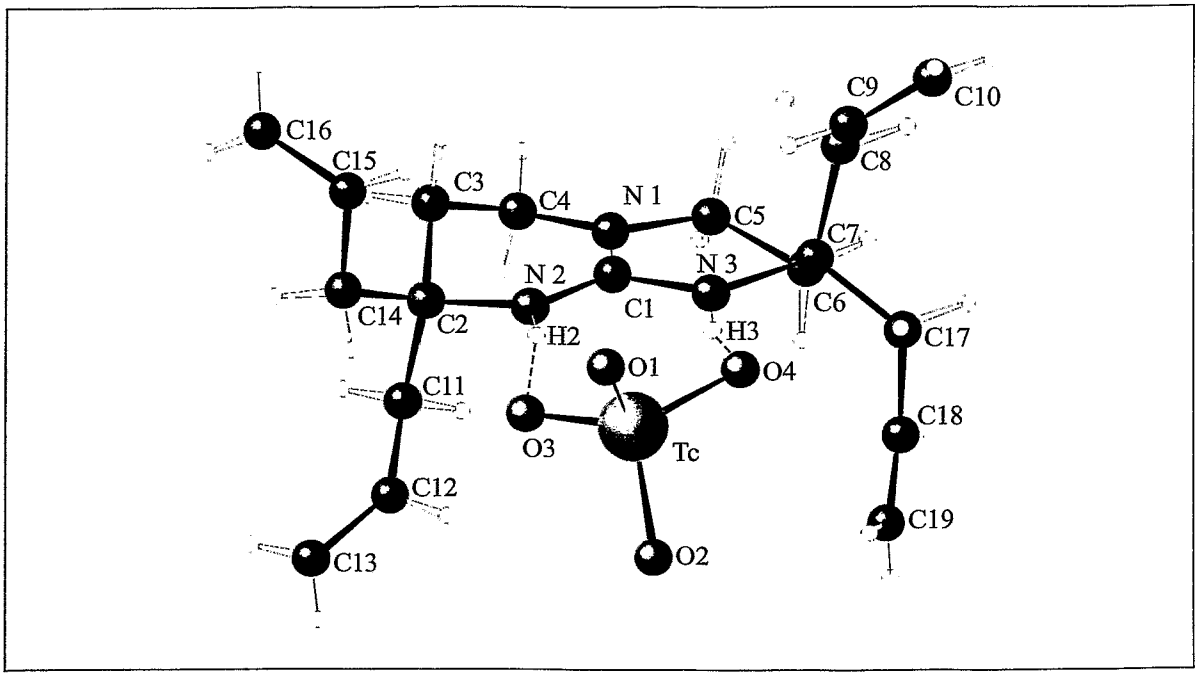
Bonds

Re(1)-O(3)	1.696
Re(1)-O(4)	1.697
Re(1)-O(2)	1.702
Re(1)-O(1)	1.715
N(1)-C(1)	1.325
N(1)-C(4)	1.457
N(1)-C(5)	1.470
N(2)-C(1)	1.336
N(2)-C(2)	1.420
N(3)-C(1)	1.335
N(3)-C(7)	1.465
C(2)-C(3)	1.420
C(3)-C(4)	1.450
C(5)-C(6)	1.480
C(6)-C(7)	1.490

Angles

O(3)-Re(1)-O(4)	108.30
O(3)-Re(1)-O(2)	108.80
O(4)-Re(1)-O(2)	108.90
O(3)-Re(1)-O(1)	111.60
O(4)-Re(1)-O(1)	109.60
O(2)-Re(1)-O(1)	109.40
C(1)-N(1)-C(4)	122.60
C(1)-N(1)-C(5)	120.70
C(4)-N(1)-C(5)	116.70
C(1)-N(2)-C(2)	121.90
C(1)-N(3)-C(7)	123.60
N(1)-C(1)-N(3)	120.50
N(1)-C(1)-N(2)	120.60
N(3)-C(1)-N(2)	118.80
C(3)-C(2)-N(2)	113.10

Tc 2



[2,2,8,8-Tetraallyl-3,4,6,7,8,9-hexahydro-2H-pyrimidino(1,2-a)pyrimidinium] pertechnetate

$C_{19}H_{30}N_3O_4Tc$

14.8363Å	11.0422Å	14.6124Å	
90.0000°	114.4950°	90.0000°	V=2178.4Å^3
C2/c; 15	Z=4; F(000)=960	ρ=1.410g/cm^3	R=3.9%
monoclinic			

H. Stephan (1999)
not published
CCDC 159494

Tc 2

Selected Bonds (Å) and Angles (°)

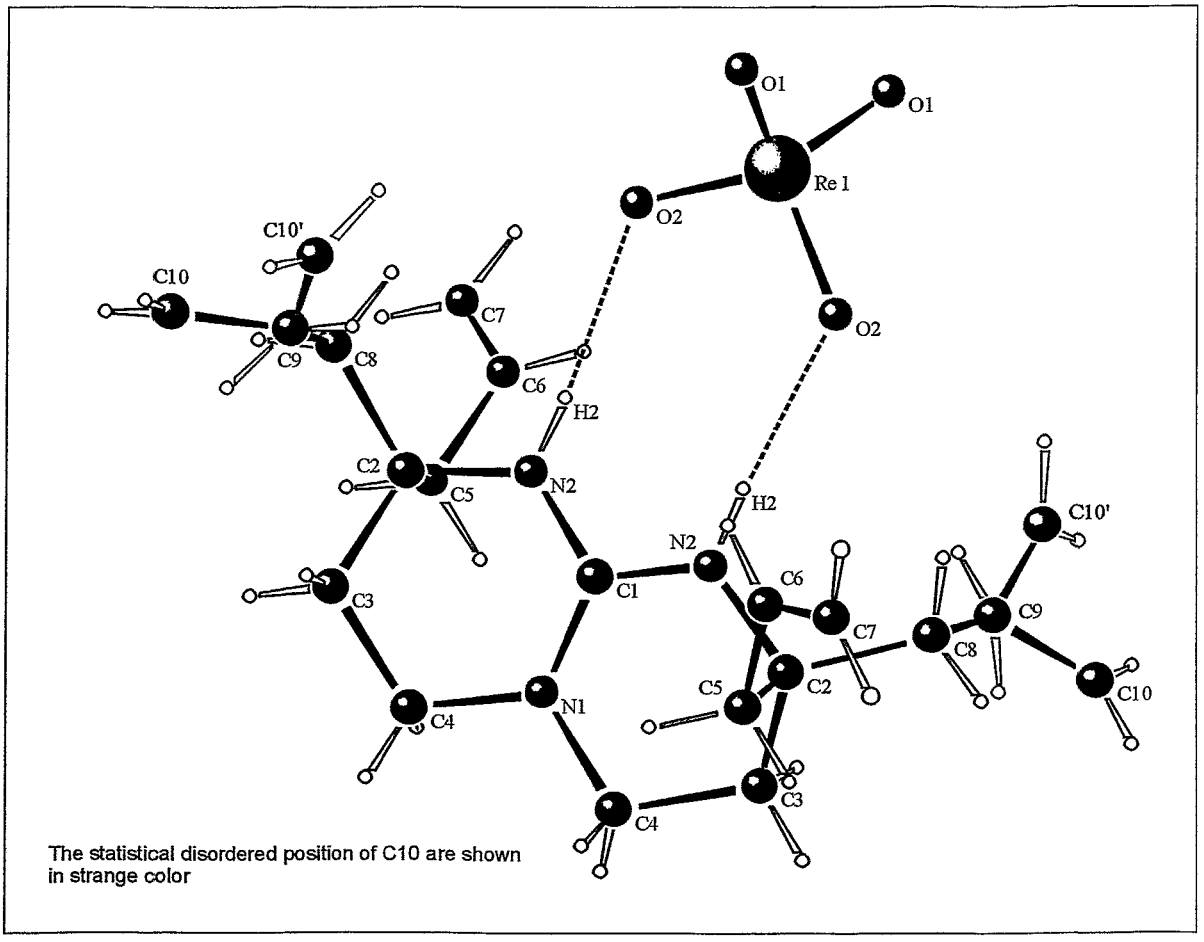
Bonds

Tc(1)-O(1)	1.643
Tc(1)-O(3)	1.668
Tc(1)-O(2)	1.705
Tc(1)-O(4)	1.733
N(1)-C(1)	1.354
N(1)-C(4)	1.430
N(1)-C(5)	1.510
N(2)-C(1)	1.240
N(2)-C(2)	1.450
N(3)-C(1)	1.420
N(3)-C(7)	1.490
C(2)-C(14)	1.540
C(2)-C(11)	1.570
C(2)-C(3)	1.590
C(3)-C(4)	1.500
C(5)-C(6)	1.490
C(6)-C(7)	1.470
C(7)-C(8)	1.510
C(7)-C(17)	1.530
C(8)-C(9)	1.510
C(9)-C(10)	1.310
C(11)-C(12)	1.400
C(12)-C(13)	1.290

Angles

O(1)-Tc(1)-O(3)	108.70
O(1)-Tc(1)-O(2)	106.50
O(3)-Tc(1)-O(2)	110.40
O(1)-Tc(1)-O(4)	112.30
O(3)-Tc(1)-O(4)	106.40
O(2)-Tc(1)-O(4)	112.50
C(1)-N(1)-C(4)	123.30
C(1)-N(1)-C(5)	120.00
C(4)-N(1)-C(5)	116.20
C(1)-N(2)-C(2)	124.70
C(1)-N(3)-C(7)	124.90
N(2)-C(1)-N(1)	122.40
N(2)-C(1)-N(3)	119.30
N(1)-C(1)-N(3)	117.90
N(2)-C(2)-C(14)	109.50
N(2)-C(2)-C(11)	109.00
C(14)-C(2)-C(11)	108.20
N(2)-C(2)-C(3)	104.80
C(14)-C(2)-C(3)	113.40
C(11)-C(2)-C(3)	111.70
C(4)-C(3)-C(2)	110.50
N(1)-C(4)-C(3)	106.70
C(6)-C(5)-N(1)	115.60

Re 2



[2,2,8,8-Tetraallyl-3,4,6,7,8,9-hexahydro-2H-pyrimidino(1,2-a)pyrimidinium] pertechnetate

$C_{19}H_{30}N_3O_4Re$

14.8585Å	11.0679Å	14.6128Å	
90.0000°	114.5660°	90.0000°	V=2185.6Å^3
C2/c; 15	Z=4; F(000)=1088	ρ=1.673g/cm^3	R=3.95%
monoclinic			

H. Stephan (2000)
not published
CCDC 159496

Re 2

Selected Bonds (Å) and Angles (°)

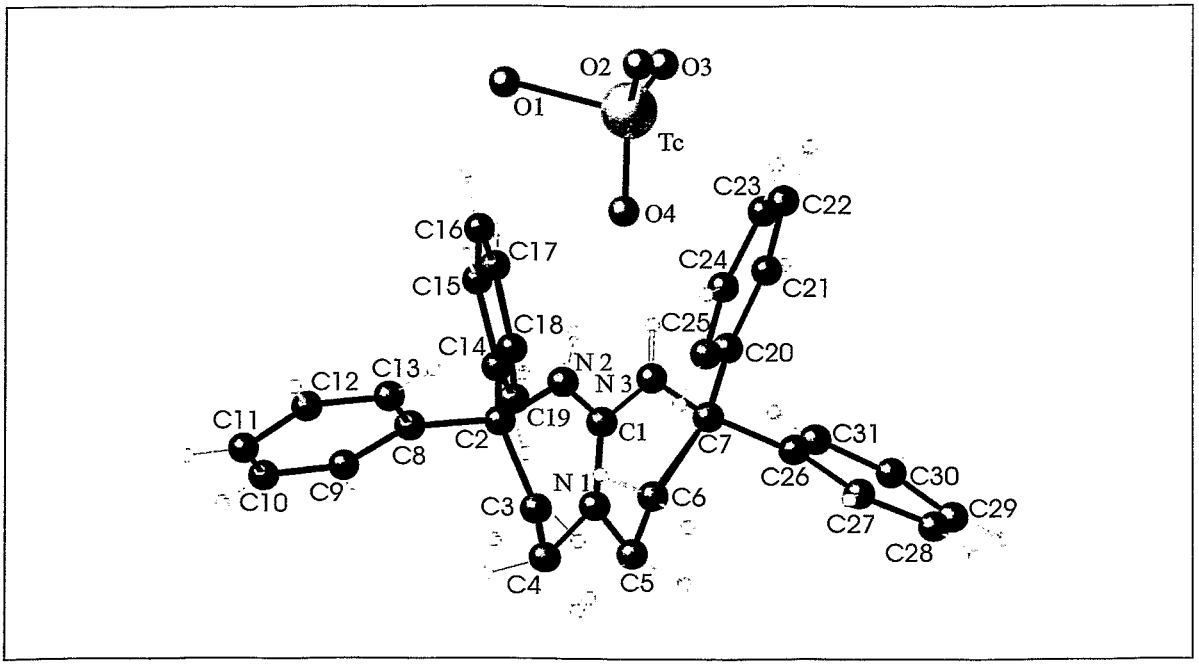
Bonds

Re(1)-O(1)1	1.679
Re(1)-O(1)	1.679
Re(1)-O(2)1	1.719
Re(1)-O(2)	1.719
N(1)-C(1)	1.334
N(1)-C(4)1	1.472
N(1)-C(4)	1.472
N(2)-C(1)	1.334
N(2)-C(2)	1.470
C(1)-N(2)1	1.334
C(2)-C(3)	1.532
C(2)-C(5)	1.535
C(2)-C(8)	1.536
C(3)-C(4)	1.504
C(5)-C(6)	1.480
C(6)-C(7)	1.321
C(8)-C(9')	1.451
C(8)-C(9)	1.451
C(9)-C(10)	1.290
C(9')-C(10')	1.280

Angles

O(1)1-Re(1)-O(1)	107.40
O(1)1-Re(1)-O(2)1	111.10
O(1)-Re(1)-O(2)1	110.20
O(1)1-Re(1)-O(2)	110.20
O(1)-Re(1)-O(2)	111.10
O(2)1-Re(1)-O(2)	106.90
C(1)-N(1)-C(4)1	121.90
C(1)-N(1)-C(4)	121.90
C(4)1-N(1)-C(4)	116.20
C(1)-N(2)-C(2)	124.20
N(1)-C(1)-N(2)1	120.60
N(1)-C(1)-N(2)	120.60
N(2)1-C(1)-N(2)	118.80
N(2)-C(2)-C(3)	105.90
N(2)-C(2)-C(5)	111.60
C(3)-C(2)-C(5)	110.00
N(2)-C(2)-C(8)	108.40
C(3)-C(2)-C(8)	111.30
C(5)-C(2)-C(8)	109.50
C(4)-C(3)-C(2)	110.90

Tc 3



[2,2,8,8-Tetraphenyl-3,4,6,7,8,9-hexahydro-2H-pyrimidino(1,2-a)pyrimidinium] pertechnetate (toluene adduct)

$C_{31}H_{30}N_3O_4Tc \times (C_7H_8)_n$
(The toluene molecule has been omitted for clarity.)

9.8982Å	18.8347Å	23.3568Å	
109.1020°	94.0900°	90.5780°	V=4101.6Å^3
P-1; 2	Z=4; F(000)=1616	ρ=1.258g/cm^3	R=5.0%
triclinic			

H. Stephan (2000)
not published
CCDC 159495

Tc 3

Selected Bonds (Å) and Angles (°)

Bonds

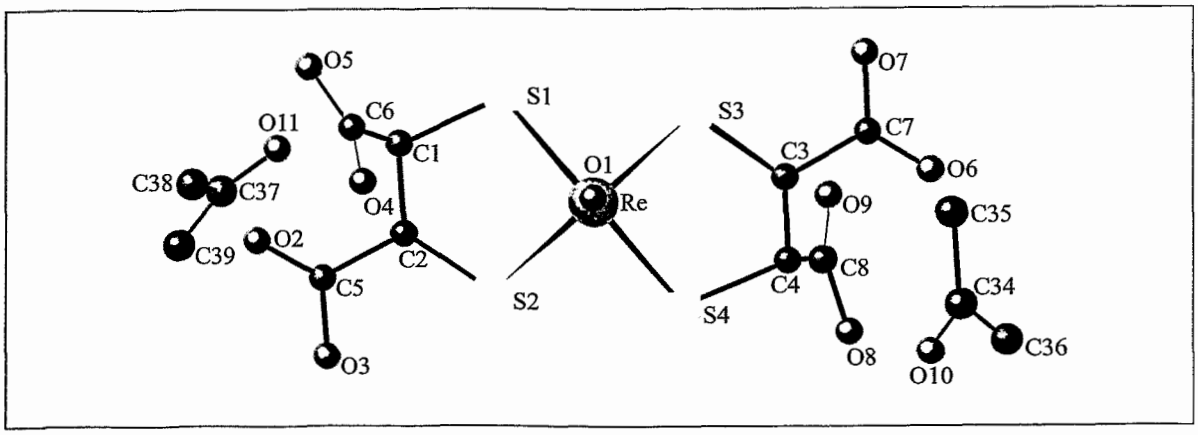
Tc(1)-O(2)	1.566
Tc(1)-O(1)	1.651
Tc(1)-O(3)	1.685
Tc(1)-O(4)	1.728
N(1)-C(1)	1.327
N(1)-C(4)	1.452
N(1)-C(5)	1.457
N(2)-C(1)	1.336
N(2)-C(2)	1.469
N(2)-H(2B)	0.860
N(3)-C(1)	1.347
N(3)-C(7)	1.474
N(3)-H(3B)	0.860
C(2)-C(14)	1.520
C(2)-C(8)	1.530
C(2)-C(3)	1.542
C(3)-C(4)	1.506
C(3)-H(3C)	0.970
C(3)-H(3D)	0.970
C(4)-H(4B)	0.970
Tc(2)-O(3')	1.467
Tc(2)-O(4')	1.631
Tc(2)-O(2')	1.656
Tc(2)-O(1')	2.030

Angles

O(2)-Tc(1)-O(1)	109.40
O(2)-Tc(1)-O(3)	112.60
O(1)-Tc(1)-O(3)	111.10
O(2)-Tc(1)-O(4)	109.80
O(1)-Tc(1)-O(4)	104.90
O(3)-Tc(1)-O(4)	108.70
C(1)-N(1)-C(4)	121.30
C(1)-N(1)-C(5)	121.30
C(4)-N(1)-C(5)	117.40
C(1)-N(2)-C(2)	123.90
C(1)-N(2)-H(2B)	118.10
C(2)-N(2)-H(2B)	118.10
C(1)-N(3)-C(7)	123.70
C(1)-N(3)-H(3B)	118.10
C(7)-N(3)-H(3B)	118.10
N(1)-C(1)-N(2)	121.60
N(1)-C(1)-N(3)	120.60
N(2)-C(1)-N(3)	117.80
O(3')-Tc(2)-O(4')	122.10
O(3')-Tc(2)-O(2')	118.20
O(4')-Tc(2)-O(2')	113.20
O(3')-Tc(2)-O(1')	90.10
O(4')-Tc(2)-O(1')	102.00
O(2')-Tc(2)-O(1')	104.20

5.2. Technetium and Rhenium on the oxidation state V

5.2.1. Bi- and tetradendate N,S ligands



Tetraphenylarsonium bis[1,2-di(carboxy)ethane-1,2-dithiolato]oxorhenate(V)

$C_{39}H_{24}AsO_9ReS_4 \times (CH_3COCH_3)_2$
(The tetraphenylarsonium counterion has been omitted for clarity.)

12.79152Å	13.95322Å	14.84152Å	
116.3891°	101.6331°	104.2781°	V=2146.5Å^3
P-1; 2	Z=2; F(000)=920	ρ=1.456g/cm^3	R=2.7%
triclinic			

S. Seifert, H.Spies, P. Leibnitz, G. Reck
"Rhenium (V) complexes with meso-DMSA Part III: X-ray crystal structure of $Rh_4As[ReO(DMSA)_2] \times 2$ acetone and identification of the possible isomers"
FZR-32 (1993) 91-95
CCDC 156798

Re 4

Selected Bonds (Å) and Angles (°)

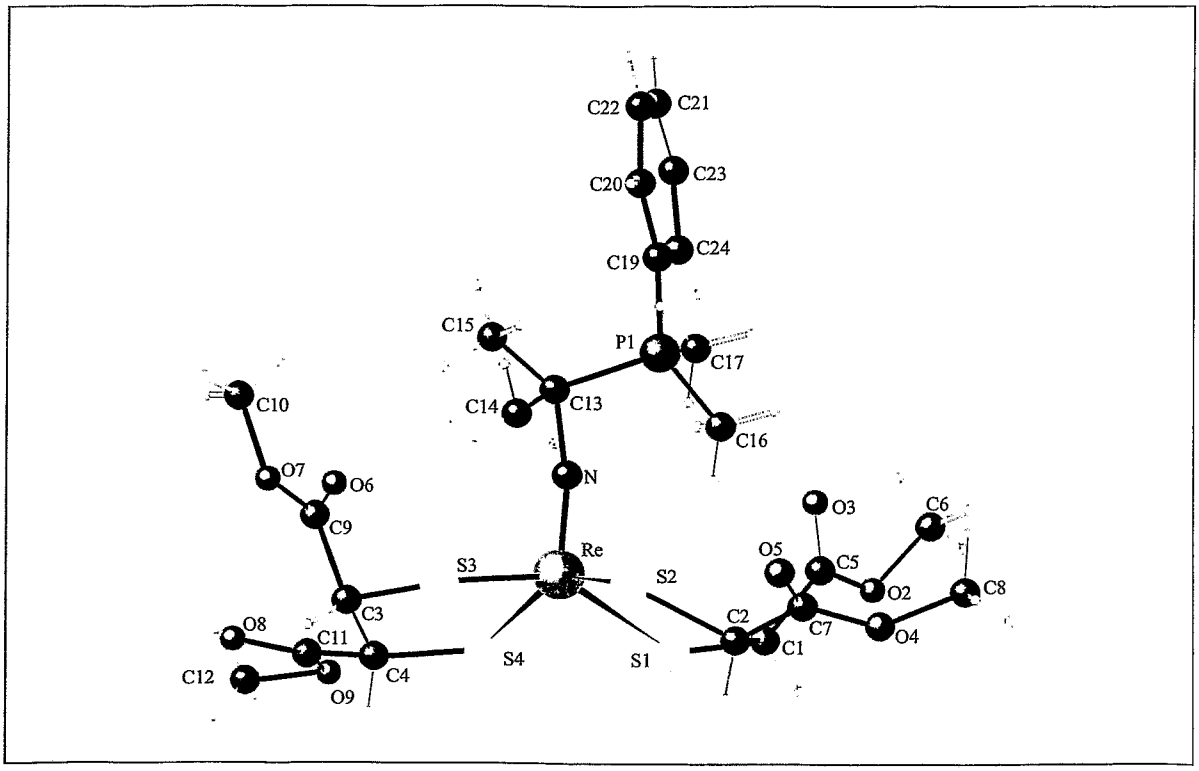
Bonds

Re-O(1)	1.676
Re-S(2)	2.292
Re-S(3)	2.313
Re-S(1)	2.315
Re-S(4)	2.319
S(1)-C(1)	1.844
S(2)-C(2)	1.847
S(3)-C(3)	1.844
S(4)-C(4)	1.831
O(2)-C(5)	1.229
O(3)-C(5)	1.288
O(4)-C(6)	1.323
O(5)-C(6)	1.213
O(6)-C(7)	1.222
O(7)-C(7)	1.276
O(8)-C(8)	1.317
O(9)-C(8)	1.198
C(1)-C(6)	1.473
C(1)-C(2)	1.511
C(2)-C(5)	1.503
C(3)-C(7)	1.500
C(3)-C(4)	1.515
C(4)-C(8)	1.510

Angles

O(1)-Re-S(2)	109.11
O(1)-Re-S(3)	109.95
S(2)-Re-S(3)	140.93
O(1)-Re-S(1)	108.24
S(2)-Re-S(1)	86.34
S(3)-Re-S(1)	82.38
O(1)-Re-S(4)	108.20
S(2)-Re-S(4)	82.00
S(3)-Re-S(4)	85.28
S(1)-Re-S(4)	143.56
C(1)-S(1)-Re	107.20
C(2)-S(2)-Re	108.14
C(3)-S(3)-Re	108.09
C(4)-S(4)-Re	105.35
C(15)-As-C(9)	111.00
C(15)-As-C(21)	108.30
C(9)-As-C(21)	109.60
C(15)-As-C(27)	110.70
C(9)-As-C(27)	107.00
C(21)-As-C(27)	110.20
C(10)-C(9)-C(14)	121.40
C(10)-C(9)-As	118.40
C(14)-C(9)-As	120.20

Re 5



[Bis(dimercaptobernsteinsäuredimethylester)-dimethylphenylphosphine isopropylimido]rhenium(V)

$C_{23}H_{33}NO_8PReS_4$

12.3347Å	12.4127Å	12.4148Å	
60.1430°	67.9830°	80.6360°	$V=1527.2Å^3$
P-1; 2	Z=2; F(000)=1527	$\rho=1.733g/cm^3$	R=5.4%
triclinic			

S. Seifert, P. Leibnitz und H. Spies
"Nitridorhenium (V)-Komplexe mit Dimercaptobernsteinsäuredimethylester. Präparation, Charakterisierung und Kristallstruktur von $\{Re[NC(CH_3)_2PPhMe_2](DMSMe_2)_2\}$"
Z.anorg.allg.Chem. 625 (1999) 1037-1040
CSD No. 410513

Re 5

Selected Bonds (Å) and Angles (°)

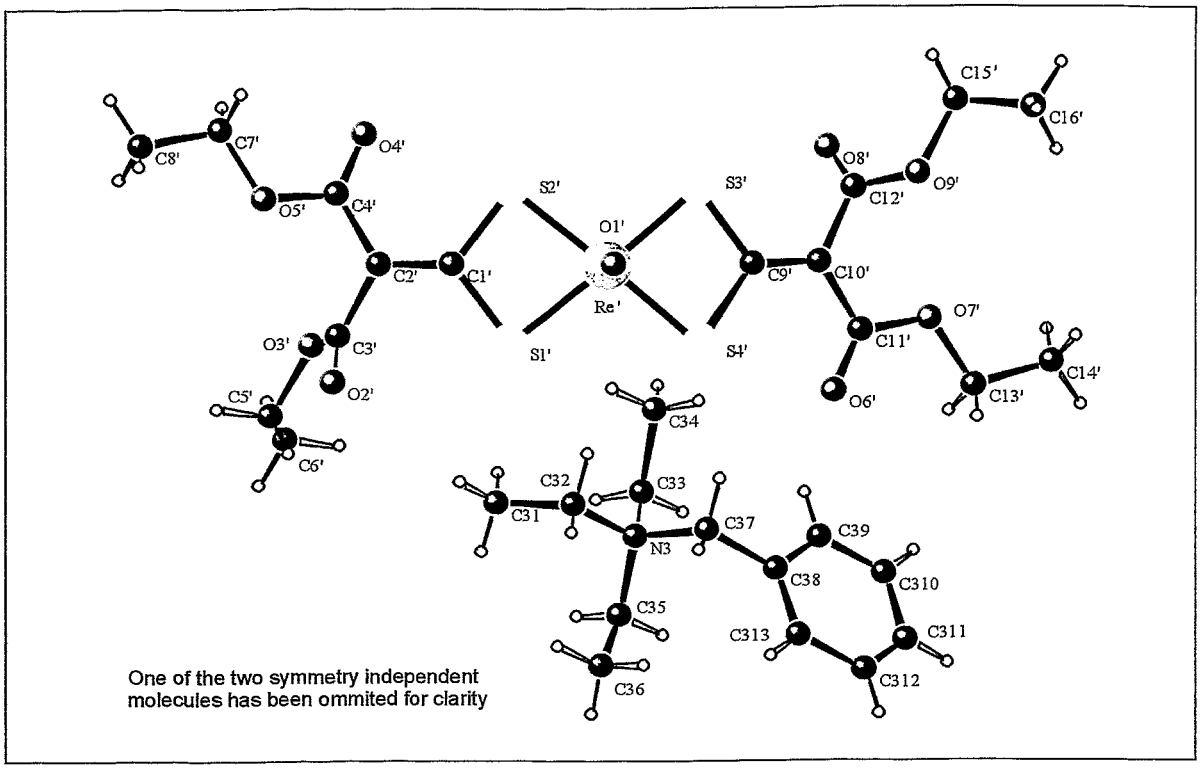
Bonds

Re(1)-N(1)	1.697
Re(1)-S(4)	2.292
Re(1)-S(3)	2.316
Re(1)-S(2)	2.318
Re(1)-S(1)	2.329
S(1)-C(1)	1.830
S(2)-C(2)	1.850
S(3)-C(3)	1.830
S(4)-C(4)	1.830
P(1)-C(17)	1.740
P(1)-C(13)	1.760
P(1)-C(16)	1.760
P(1)-C(19)	1.760
N(1)-C(13)	1.620
O(2)-C(5)	1.350
O(2)-C(6)	1.500
O(3)-C(5)	1.180
O(4)-C(7)	1.280
O(4)-C(8)	1.410
O(5)-C(7)	1.210
O(6)-C(9)	1.360
O(6)-C(10)	1.440
O(7)-C(9)	1.180

Angles

N(1)-Re(1)-S(4)	106.30
N(1)-Re(1)-S(3)	107.70
S(4)-Re(1)-S(3)	85.30
N(1)-Re(1)-S(2)	110.70
S(4)-Re(1)-S(2)	143.00
S(3)-Re(1)-S(2)	82.00
N(1)-Re(1)-S(1)	109.30
S(4)-Re(1)-S(1)	84.30
S(3)-Re(1)-S(1)	143.00
S(2)-Re(1)-S(1)	85.30
C(1)-S(1)-Re(1)	107.90
C(2)-S(2)-Re(1)	108.90
C(3)-S(3)-Re(1)	107.50
C(4)-S(4)-Re(1)	108.10
C(17)-P(1)-C(13)	107.90
C(17)-P(1)-C(16)	112.50
C(13)-P(1)-C(16)	106.30
C(17)-P(1)-C(19)	114.30
C(13)-P(1)-C(19)	105.00
C(16)-P(1)-C(19)	110.40
C(13)-N(1)-Re(1)	167.50
C(5)-O(2)-C(6)	118.00
C(7)-O(4)-C(8)	133.00

Re 6



Triethylbenzylammonium bis(1,1-dicarbethoxyethene-2,2-dithiolato)oxorhenate(V)

$C_{58}H_{84}N_2O_{18}Re_2S_8$

27.7466Å	12.9948Å	22.0970Å	
90.0000°	112.2740°	90.0000°	V=7343.7Å^3
P2(1)/c; 14	Z=4; F(000)=3472	ρ=1.561g/cm^3	R=5.0%
monoclinic			

S.Seifert (1997)
not published
CCDC 156807

Re 6

Selected Bonds (Å) and Angles (°)

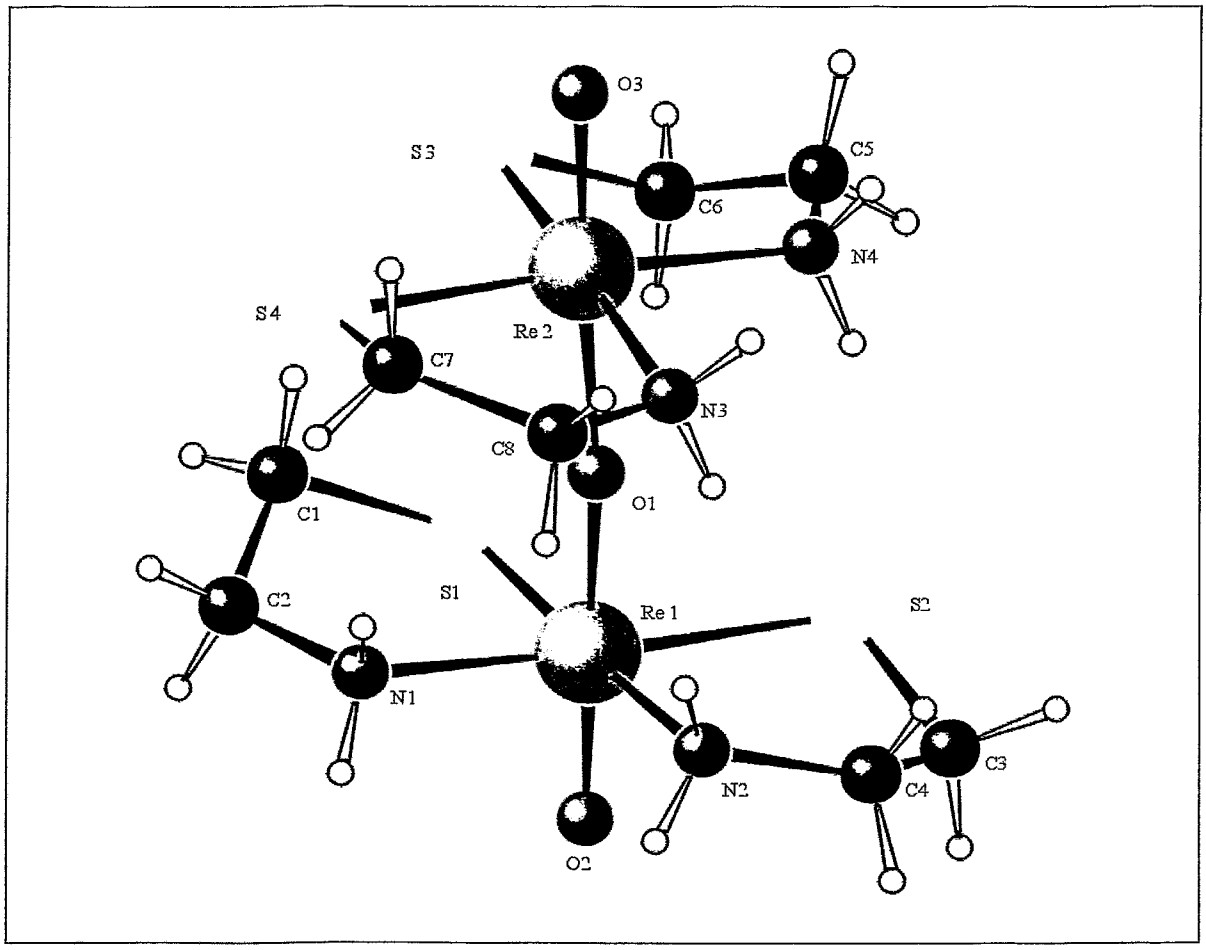
Bonds

Re-O(1)	1.672
Re-S(3)	2.329
Re-S(2)	2.331
Re-S(4)	2.335
Re-S(1)	2.335
S(1)-C(1)	1.753
S(2)-C(1)	1.762
S(3)-C(9)	1.768
S(4)-C(9)	1.760
O(2)-C(3)	1.150
O(3)-C(3)	1.242
O(3)-C(5)	1.460
O(4)-C(4)	1.195
O(5)-C(4)	1.316
O(5)-C(7)	1.550
O(6)-C(11)	1.189
O(7)-C(11)	1.306
O(7)-C(13)	1.453
O(8)-C(12)	1.178
O(9)-C(12)	1.326
O(9)-C(15)	1.471
C(1)-C(2)	1.343
C(2)-C(4)	1.444
C(2)-C(3)	1.490
C(5)-C(6)	1.420
C(7)-C(8)	1.419
C(9)-C(10)	1.345
C(10)-C(11)	1.485
C(10)-C(12)	1.491
C(13)-C(14)	1.370
C(15)-C(16)	1.340

Angles

O(1)-Re-S(3)	111.10
O(1)-Re-S(2)	109.60
S(3)-Re-S(2)	92.07
O(1)-Re-S(4)	111.10
S(3)-Re-S(4)	73.57
S(2)-Re-S(4)	139.24
O(1)-Re-S(1)	112.10
S(3)-Re-S(1)	136.77
S(2)-Re-S(1)	73.40
S(4)-Re-S(1)	91.11
C(1)-S(1)-Re	90.80
C(1)-S(2)-Re	90.70
C(9)-S(3)-Re	90.70
C(9)-S(4)-Re	90.70
C(3)-O(3)-C(5)	114.90
C(4)-O(5)-C(7)	111.80
C(11)-O(7)-C(13)	118.10
C(12)-O(9)-C(15)	116.10
C(2)-C(1)-S(1)	126.50
C(2)-C(1)-S(2)	128.40
S(1)-C(1)-S(2)	105.00
C(1)-C(2)-C(4)	122.60
C(1)-C(2)-C(3)	118.70
C(4)-C(2)-C(3)	118.70
O(2)-C(3)-O(3)	122.20
O(2)-C(3)-C(2)	125.30
O(3)-C(3)-C(2)	112.30
O(4)-C(4)-O(5)	121.30
O(4)-C(4)-C(2)	124.60
O(5)-C(4)-C(2)	114.00
C(6)-C(5)-O(3)	108.40
C(8)-C(7)-O(5)	104.20
C(10)-C(9)-S(4)	128.00
C(10)-C(9)-S(3)	127.30
S(4)-C(9)-S(3)	104.70
C(9)-C(10)-C(11)	120.10
C(9)-C(10)-C(12)	119.90

Re 7



μ-Oxo[bis (2-aminoethylthiolato)oxorhenium (V)]

$C_8H_{24}N_4O_3Re_2S_4$

9.2322Å	9.2322Å	20.7902	
90.0000°	90.0000°	90.0000°	$V=1779.3Å^3$
$P4_12_12$; 92	Z=4; F(000)=1352	$\rho=2.706 g/cm^3$	R=11.89%
tetragonal			

S. Kirsch (1996)
not published

Re 7

Selected Bonds (Å) and Angles (°)

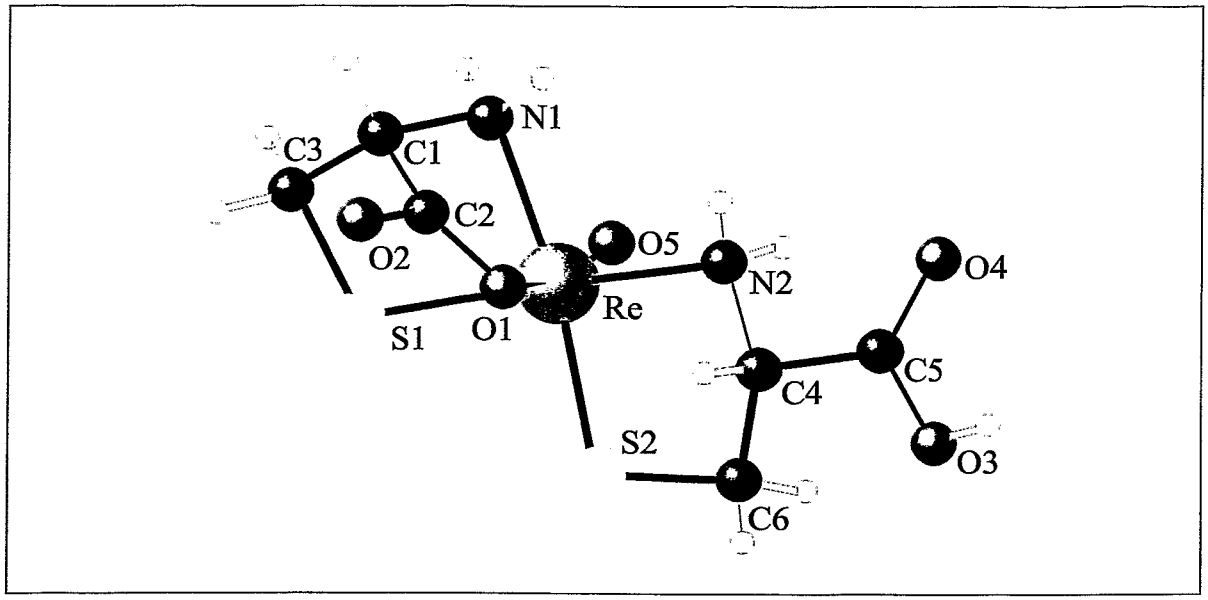
Bonds

Re(1)-O(2)	1.716
Re(1)-O(1)	1.911
Re(1)-N(1)	2.099
Re(1)-N(2)	2.159
Re(1)-S(1)	2.232
Re(1)-S(2)	2.305
S(1)-C(1)	1.870
S(2)-C(3)	1.830
Re(2)-O(2)	1.716
Re(2)-O(1)	1.911
Re(2)-N(3)	2.159
Re(2)-N(4)	2.099
Re(2)-S(3)	2.231
Re(2)-S(4)	2.305
S(3)-C(6)	1.870
S(4)-C(7)	1.830

Angles

O(2)-Re(1)-S(1)	105.30
N(1)-Re(1)-N(2)	98.80
S(1)-Re(1)-S(2)	95.20
N(2)-Re(1)-S(2)	81.40
N(1)-Re(1)-S(1)	84.30
O(3)-Re(1)-O(1)	151.90
O(1)-Re(1)-S(1)	96.20
O(3)-Re(2)-S(3)	105.30
N(4)-Re(2)-N(3)	98.80
S(3)-Re(2)-S(4)	95.20
N(3)-Re(2)-S(4)	81.40
N(4)-Re(2)-S(3)	84.30
O(3)-Re(2)-O(1)	151.90
O(3)-Re(2)-S(3)	96.20

Re 8



[(D-cysteinato-N,S,O)(D-cysteinato-N,S)]oxorhenium(V)
(One of the two symmetry-indepndent molecules has been omitted.)
$C_6H_{11}N_2O_5ReS_2$

6.0660Å	20.1550Å	9.7450Å	
90.0000°	93.0900°	90.0000°	V=1189.7Å^3
$P2_1$; 4	Z=2; F(000)=828	ρ=2.459g/cm^3	R=9.1%
Monoclinic			

Kirsch (1997)
not published
CCDC 159487

Re 8

Selected Bonds (Å) and Angles (°)

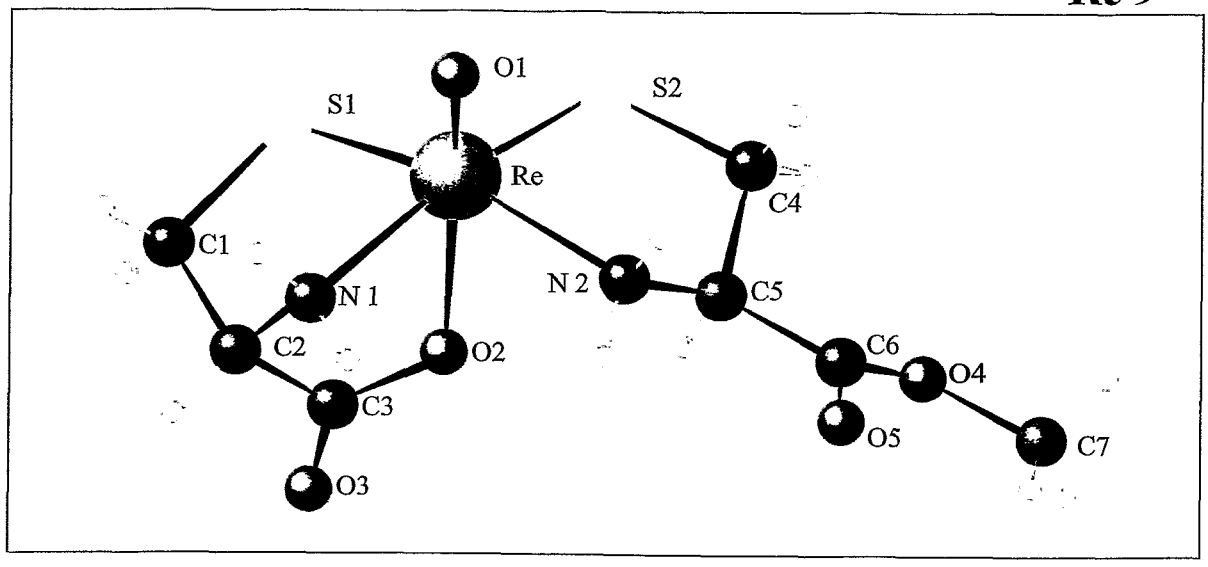
Bonds

Re(1)-O(5)	1.660
Re(1)-O(1)	2.150
Re(1)-N(2)	2.180
Re(1)-N(1)	2.200
Re(1)-S(2)	2.284
Re(1)-S(1)	2.286
S(1)-C(3)	1.840
S(2)-C(6)	1.810
O(1)-C(2)	1.280
O(2)-C(2)	1.200
O(3)-C(5)	1.230
O(4)-C(5)	1.270
N(1)-C(1)	1.540
N(2)-C(4)	1.530
C(1)-C(3)	1.480
C(1)-C(2)	1.560
C(4)-C(5)	1.490
C(4)-C(6)	1.500

Angles

O(5)-Re(1)-O(1)	161.00
O(5)-Re(1)-N(2)	93.00
O(1)-Re(1)-N(2)	78.00
O(5)-Re(1)-N(1)	91.00
O(1)-Re(1)-N(1)	72.00
N(2)-Re(1)-N(1)	94.60
O(5)-Re(1)-S(2)	106.00
O(1)-Re(1)-S(2)	90.00
N(2)-Re(1)-S(2)	83.50
N(1)-Re(1)-S(2)	162.20
O(5)-Re(1)-S(1)	107.00
O(1)-Re(1)-S(1)	82.50
N(2)-Re(1)-S(1)	160.00
N(1)-Re(1)-S(1)	83.00
S(2)-Re(1)-S(1)	92.70
C(3)-S(1)-Re(1)	99.00
C(6)-S(2)-Re(1)	105.00
C(2)-O(1)-Re(1)	123.00
C(1)-N(1)-Re(1)	103.00
C(4)-N(2)-Re(1)	110.00

Re 9



[(D-cysteinato-N,S,O)(O-methyl-D-cysteinato-N,S)]oxorhenium(V)

$C_7H_{13}N_2O_5ReS_2$

8.4138Å	9.3850Å	15.6200Å	
90.0000°	90.0000°	90.0000°	$V=1233.5Å^3$
$P2_12_12_1$; 19 orthorhombic	Z=4; F(000)=864	$\rho=2.453 g/cm^3$	R=2.2%

S. Kirsch, R. Jankowsky, P. Leibnitz, H. Spies, B. Johannsen
"Crystal and solution structure of oxorhenium (V) complexes with cysteine and cysteine methyl ester"
J.Biol.Inorg.Chem. 4 (1999) 48-55
CSD No. 410514

Re 9

Selected Bonds (Å) and Angles (°)

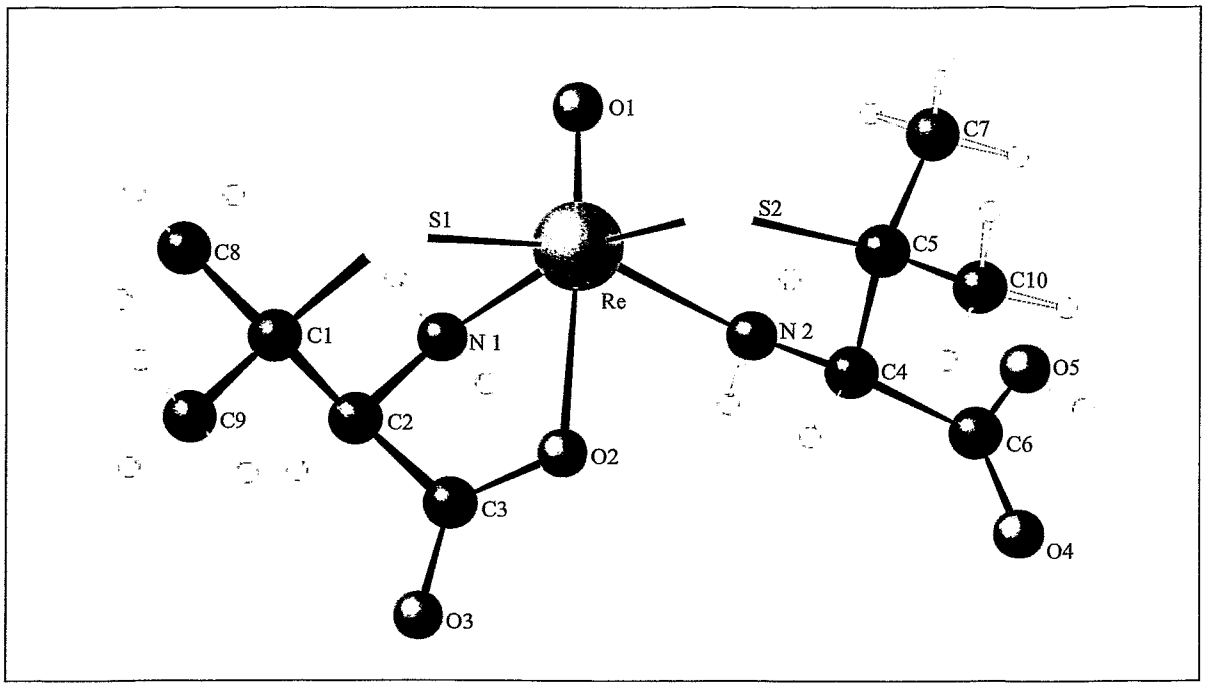
Bonds

Re-O(1)	1.670
Re-N(2)	2.158
Re-O(2)	2.159
Re-N(1)	2.202
Re-S(2)	2.290
Re-S(1)	2.305
S(1)-C(1)	1.830
S(2)-C(4)	1.820
O(2)-C(3)	1.289
O(3)-C(3)	1.240
O(4)-C(6)	1.332
O(4)-C(7)	1.438
O(5)-C(6)	1.192
N(1)-C(2)	1.470
N(1)-H(1A)	0.900
N(1)-H(1B)	0.900
N(2)-C(5)	1.475
N(2)-H(2A)	0.900
N(2)-H(2B)	0.900
C(1)-C(2)	1.510
C(1)-H(1C)	0.970
C(1)-H(1D)	0.970
C(2)-C(3)	1.506
C(2)-H(2)	0.980

Angles

O(1)-Re-N(2)	94.60
O(1)-Re-O(2)	157.30
N(2)-Re-O(2)	75.60
O(1)-Re-N(1)	90.80
N(2)-Re-N(1)	96.90
O(2)-Re-N(1)	70.50
O(1)-Re-S(2)	105.30
N(2)-Re-S(2)	82.23
O(2)-Re-S(2)	93.81
N(1)-Re-S(2)	163.80
O(1)-Re-S(1)	106.80
N(2)-Re-S(1)	158.59
O(2)-Re-S(1)	84.03
N(1)-Re-S(1)	82.22
S(2)-Re-S(1)	92.67
C(1)-S(1)-Re	100.80
C(4)-S(2)-Re	102.40
C(3)-O(2)-Re	116.20
C(2)-N(1)-Re	105.00
Re-N(1)-H(1A)	110.75
Re-N(1)-H(1B)	110.75
C(5)-N(2)-Re	113.20
Re-N(2)-H(2A)	108.94
Re-N(2)-H(2B)	108.94

Re 10



[(D-penicillaminato-N,S,O)(D-penicillaminato-N,S)]oxorhenium(V)

$C_{10}H_{19}N_2O_5ReS_2$

5.9304Å	11.7094Å	21.7504Å	
90.0000°	90.0000°	90.0000°	V=1510.1Å
$P2_12_12_1$; 19	Z=4; F(000)=960	ρ=2.189g/cm^3	R=3.0%
orthorhombic			

S. Kirsch, B. Noll, H. Spies, P. Leibnitz, D. Scheller, T. Krueger, B. Johannsen
"Preparation and structural studies of neutral oxorhenium (V) complexes with D-penicillamine methyl ester"
J.Chem.Soc.Dalton Trans. (1998) 455-460
CCDC 407094

Selected Bonds (Å) and Angles (°)

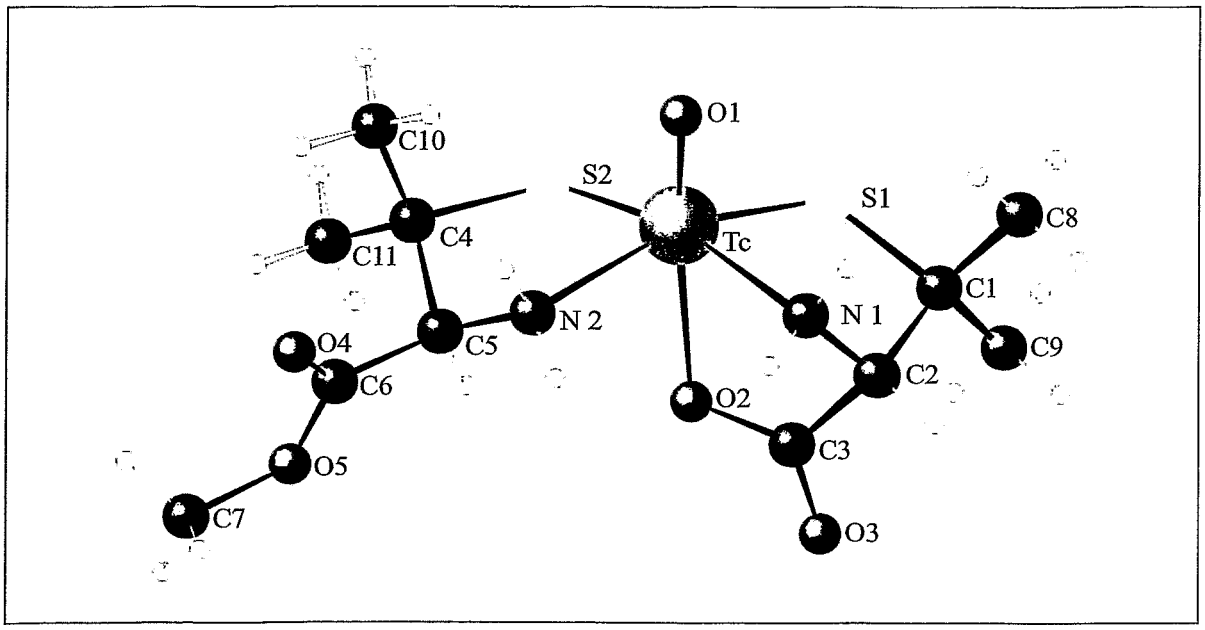
Bonds

Re-O(1)	1.684
Re-O(2)	2.181
Re-N(2)	2.187
Re-N(1)	2.213
Re-S(2)	2.285
Re-S(1)	2.297
S(1)-C(1)	1.845
S(2)-C(5)	1.853
O(2)-C(3)	1.272
O(3)-C(3)	1.238
O(4)-C(6)	1.203
O(5)-C(6)	1.293
O(5)-H(5)	0.820
N(1)-C(2)	1.486
N(1)-H(1A)	0.900
N(1)-H(1B)	0.900
N(2)-C(4)	1.480
N(2)-H(2A)	0.900
N(2)-H(2B)	0.900
C(1)-C(9)	1.518
C(1)-C(8)	1.530
C(1)-C(2)	1.536
C(2)-C(3)	1.518
C(2)-H(2)	0.980

Angles

O(1)-Re-O(2)	157.50
O(1)-Re-N(2)	98.20
O(2)-Re-N(2)	73.50
O(1)-Re-N(1)	90.30
O(2)-Re-N(1)	69.90
N(2)-Re-N(1)	93.80
O(1)-Re-S(2)	106.70
O(2)-Re-S(2)	93.27
N(2)-Re-S(2)	83.11
N(1)-Re-S(2)	163.04
O(1)-Re-S(1)	105.70
O(2)-Re-S(1)	83.25
N(2)-Re-S(1)	155.95
N(1)-Re-S(1)	83.88
S(2)-Re-S(1)	92.16
C(1)-S(1)-Re	101.20
C(5)-S(2)-Re	101.30
C(3)-O(2)-Re	116.00
C(2)-N(1)-Re	103.90
Re-N(1)-H(1A)	111.00
Re-N(1)-H(1B)	111.00
C(4)-N(2)-Re	111.40
Re-N(2)-H(2A)	109.30
Re-N(2)-H(2B)	109.30

Tc 11



[(D-penicillaminato-N,S,O)(O-methyl-D-penicillaminato-N,S)oxotechnetium(V)

$C_{11}H_{21}N_2O_5S_2Tc$

6.1249Å	13.8679Å	19.7389Å	
90.0000°	90.0000°	90.0000°	V=1676.6Å^3
$P2_12_12_1$; 19	Z=4; F(000)=864	ρ=1.677g/cm^3	R=2.0%
orthorhombic			

S. Kirsch (1997)
not published
CCDC159504

Tc 11

Selected Bonds (Å) and Angles (°)

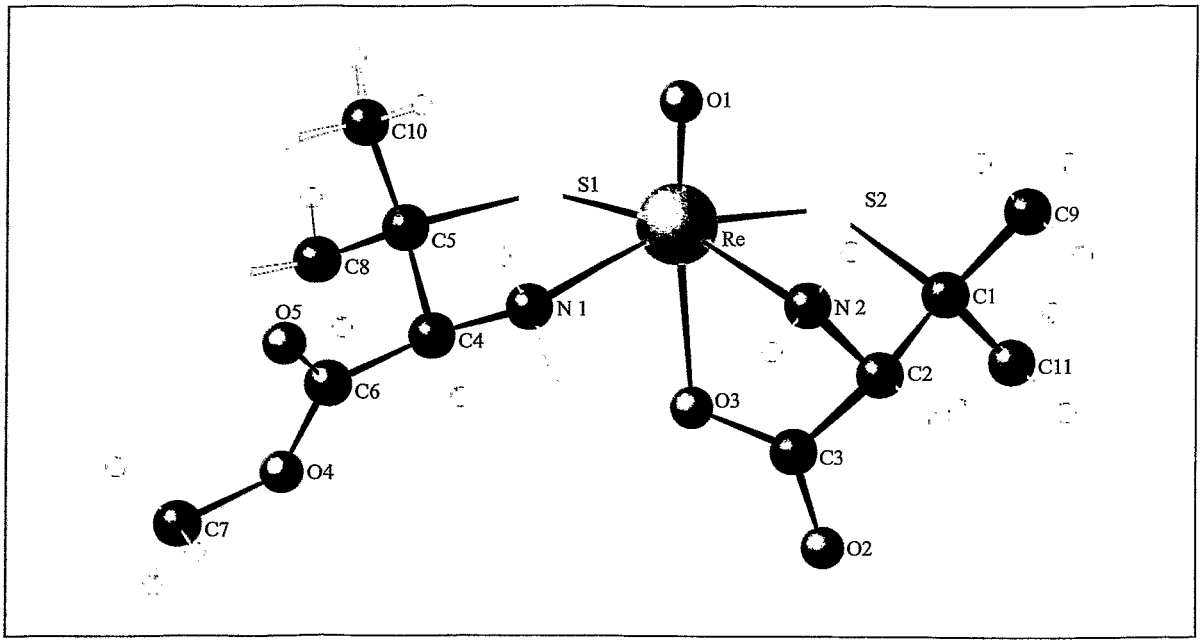
Bonds

Tc(1)-O(1)	1.659
Tc(1)-N(2)	2.171
Tc(1)-N(1)	2.212
Tc(1)-O(2)	2.213
Tc(1)-S(2)	2.284
Tc(1)-S(1)	2.300
S(1)-C(1)	1.854
S(2)-C(4)	1.864
O(2)-C(3)	1.281
O(3)-C(3)	1.229
O(4)-C(6)	1.194
O(5)-C(6)	1.323
O(5)-C(7)	1.457
N(1)-C(2)	1.475
N(2)-C(5)	1.469
C(1)-C(9)	1.536
C(1)-C(8)	1.546
C(1)-C(2)	1.554
C(2)-C(3)	1.524
C(4)-C(11)	1.512
C(4)-C(10)	1.528
C(4)-C(5)	1.546
C(5)-C(6)	1.519

Angles

O(1)-Tc(1)-N(2)	97.72
O(1)-Tc(1)-N(1)	90.56
N(2)-Tc(1)-N(1)	93.21
O(1)-Tc(1)-O(2)	157.72
N(2)-Tc(1)-O(2)	73.84
N(1)-Tc(1)-O(2)	69.79
O(1)-Tc(1)-S(2)	106.97
N(2)-Tc(1)-S(2)	83.35
N(1)-Tc(1)-S(2)	162.42
O(2)-Tc(1)-S(2)	92.73
O(1)-Tc(1)-S(1)	105.99
N(2)-Tc(1)-S(1)	156.24
N(1)-Tc(1)-S(1)	85.19
O(2)-Tc(1)-S(1)	83.42
S(2)-Tc(1)-S(1)	91.04
C(1)-S(1)-Tc(1)	100.18
C(4)-S(2)-Tc(1)	101.13
C(3)-O(2)-Tc(1)	115.20
C(6)-O(5)-C(7)	116.20
C(2)-N(1)-Tc(1)	103.30
C(5)-N(2)-Tc(1)	112.90
C(9)-C(1)-C(8)	110.10
C(9)-C(1)-C(2)	110.80

Re 11



[(D-penicillaminato-N,S,O)(O-methyl-D-penicillaminato-N,S)]oxorhenium(V)

$C_{11}H_{21}N_2O_5ReS_2$

6.0852Å	13.8804Å	19.7023Å	
90.0000°	90.0000°	90.0000°	V=1664.1Å^3
$P2_12_12_1$; 19	Z=4; F(000)=992	ρ=2.042g/cm^3	R=3.1%
orthorhombic			

S. Kirsch, B. Noll, H. Spies, P. Leibnitz, D. Scheller, T. Krueger, B. Johannsen
"Preparation and structural studies of neutral oxorhenium (V) complexes with D-penicillamine methyl ester"
J.Chem.Soc.Dalton Trans. (1998) 455-460
CCDC 407093

Re 11

Selected Bonds (Å) and Angles (°)

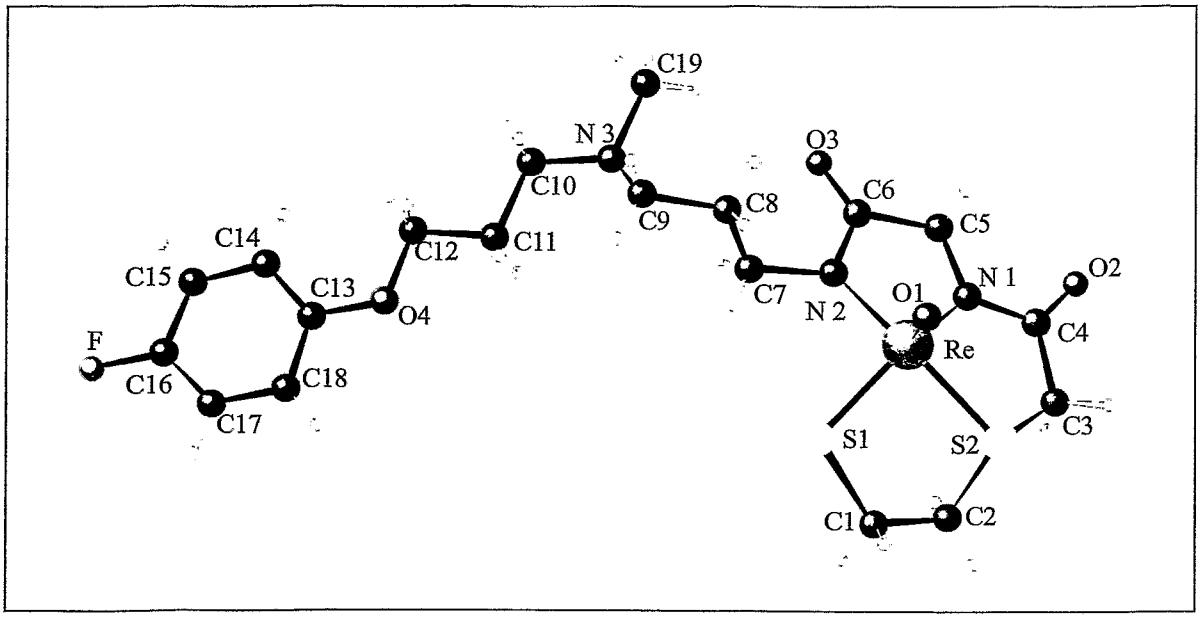
Bonds

Re-O(1)	1.663
Re-N(1)	2.162
Re-O(3)	2.179
Re-N(2)	2.194
Re-S(1)	2.280
Re-S(2)	2.300
S(1)-C(5)	1.859
S(2)-C(1)	1.851
O(2)-C(3)	1.220
O(3)-C(3)	1.282
O(4)-C(6)	1.311
O(4)-C(7)	1.412
O(5)-C(6)	1.197
N(1)-C(4)	1.486
N(1)-H(1A)	0.900
N(1)-H(1B)	0.900
N(2)-C(2)	1.476
N(2)-H(2A)	0.900
N(2)-H(2B)	0.900
C(1)-C(11)	1.500
C(1)-C(9)	1.545
C(1)-C(2)	1.554
C(2)-C(3)	1.526
C(2)-H(2)	0.980

Angles

O(1)-Re-N(1)	97.90
O(1)-Re-O(3)	157.90
N(1)-Re-O(3)	74.30
O(1)-Re-N(2)	90.20
N(1)-Re-N(2)	93.20
O(3)-Re-N(2)	70.10
O(1)-Re-S(1)	106.00
N(1)-Re-S(1)	83.10
O(3)-Re-S(1)	93.73
N(2)-Re-S(1)	163.80
O(1)-Re-S(2)	104.60
N(1)-Re-S(2)	157.30
O(3)-Re-S(2)	83.77
N(2)-Re-S(2)	84.60
S(1)-Re-S(2)	92.80
C(5)-S(1)-Re	101.30
C(1)-S(2)-Re	101.00
C(3)-O(3)-Re	116.10
C(4)-N(1)-Re	113.20
Re-N(1)-H(1A)	108.93
Re-N(1)-H(1B)	108.90
C(2)-N(2)-Re	103.80
Re-N(2)-H(2A)	111.01
Re-N(2)-H(2B)	111.00

Re 12



[N-(3-{N-[3-(4-fluorophenoxy)-propyl]-N-methylamino}-propylamino)-6,9-diaza-3-thia-5,8-dioxononanethiolato]oxorhenium(V)

$C_{19}H_{27}FN_3O_4ReS_2$

14.2314Å	11.4396Å	29.4245Å	
90.0000°	102.2170°	90.0000°	V=4681.9Å^3
$P2_1/n$; 14	Z=8; F(000)=2480	ρ=1.790g/cm^3	R=4.8%
monoclinic			

M. Scheunemann (1997)
not published
CCDC 159490

Re 12

Selected Bonds (Å) and Angles (°)

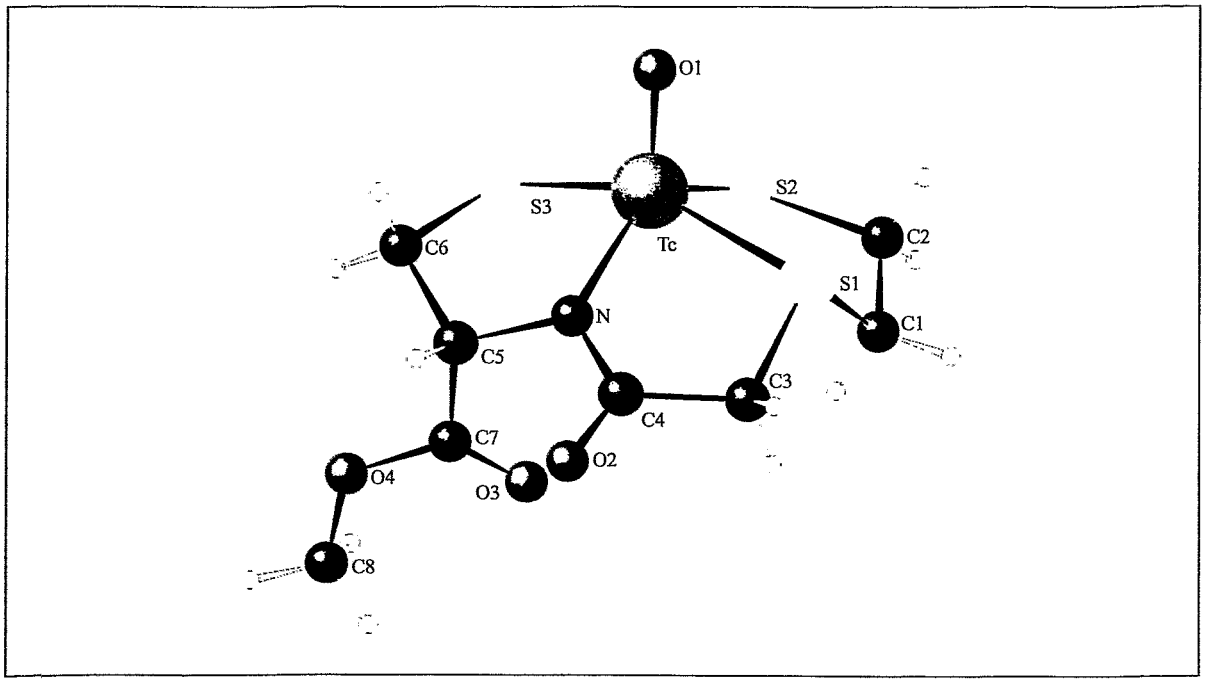
Bonds

Re(1)-O(1)	1.673
Re(1)-N(1)	2.010
Re(1)-N(2)	2.020
Re(1)-S(1)	2.280
Re(1)-S(2)	2.355
S(1)-C(1)	1.840
S(2)-C(3)	1.810
S(2)-C(2)	1.830
F(1)-C(16)	1.420
O(2)-C(4)	1.170
O(3)-C(6)	1.220
O(4)-C(13)	1.390
O(4)-C(12)	1.440
N(1)-C(4)	1.360
N(1)-C(5)	1.480
N(2)-C(6)	1.340
N(2)-C(7)	1.480
N(3)-C(10)	1.450
N(3)-C(9)	1.460
N(3)-C(19)	1.460
C(1)-C(2)	1.560
C(3)-C(4)	1.510
C(5)-C(6)	1.530
C(7)-C(8)	1.460
C(8)-C(9)	1.490
C(10)-C(11)	1.520
C(11)-C(12)	1.460
C(13)-C(14)	1.350
C(13)-C(18)	1.360
C(14)-C(15)	1.360
C(15)-C(16)	1.340
C(16)-C(17)	1.340
C(17)-C(18)	1.380

Angles

O(1)-Re(1)-N(1)	116.50
O(1)-Re(1)-N(2)	105.70
N(1)-Re(1)-N(2)	80.70
O(1)-Re(1)-S(1)	115.00
N(1)-Re(1)-S(1)	128.50
N(2)-Re(1)-S(1)	88.40
O(1)-Re(1)-S(2)	103.30
N(1)-Re(1)-S(2)	80.20
N(2)-Re(1)-S(2)	150.20
S(1)-Re(1)-S(2)	85.70
C(1)-S(1)-Re(1)	106.00
C(3)-S(2)-C(2)	104.90
C(3)-S(2)-Re(1)	102.00
C(2)-S(2)-Re(1)	106.80
C(4)-N(1)-Re(1)	128.40
C(5)-N(1)-Re(1)	113.80
C(6)-N(2)-Re(1)	117.00
C(7)-N(2)-Re(1)	128.90

Tc 13



(2-Carbmethoxy-3-aza-4-oxo-6-thiaoctane-1,8-dithiolato-S,N,S,S)oxotechnetium(V)

$C_8H_{12}NO_4S_3Tc$

6.6325Å	10.7503Å	18.2549Å	
90.0000°	90.0000°	90.0000°	V=1301.6Å^3
$P2_12_12_1$; 19	Z=4; F(000)=760	ρ=1.941g/cm^3	R=2.1%
orthorhombic			

B. Noll, (1998)
not published
CCDC 14093

Tc 13

Selected Bonds (Å) and Angles (°)

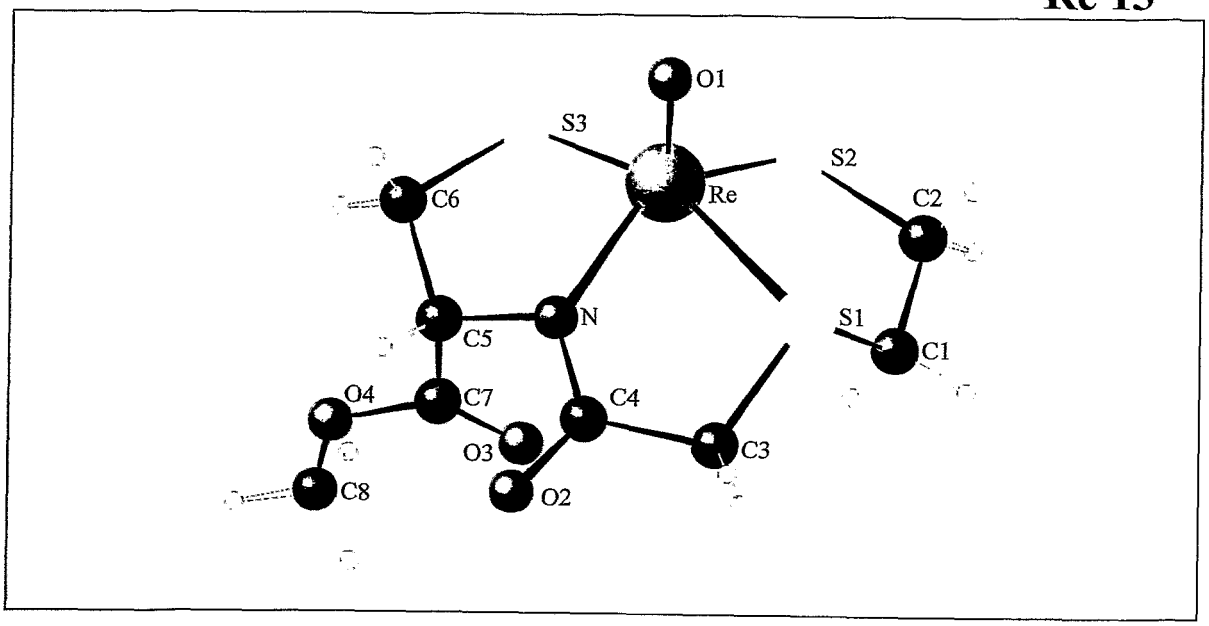
Bonds

Tc(1)-O(1)	1.668
Tc(1)-N(1)	1.995
Tc(1)-S(2)	2.275
Tc(1)-S(3)	2.292
Tc(1)-S(1)	2.376
S(1)-C(3)	1.797
S(1)-C(1)	1.815
S(2)-C(2)	1.824
S(3)-C(6)	1.821
O(2)-C(4)	1.217
O(3)-C(7)	1.196
O(4)-C(7)	1.320
O(4)-C(8)	1.452
N(1)-C(4)	1.379
N(1)-C(5)	1.475
C(1)-C(2)	1.527
C(3)-C(4)	1.519
C(5)-C(6)	1.523
C(5)-C(7)	1.528

Angles

O(1)-Tc(1)-N(1)	118.19
O(1)-Tc(1)-S(2)	115.37
N(1)-Tc(1)-S(2)	126.29
O(1)-Tc(1)-S(3)	107.99
N(1)-Tc(1)-S(3)	82.81
S(2)-Tc(1)-S(3)	84.70
O(1)-Tc(1)-S(1)	100.52
N(1)-Tc(1)-S(1)	81.65
S(2)-Tc(1)-S(1)	85.35
S(3)-Tc(1)-S(1)	151.38
C(3)-S(1)-C(1)	105.00
C(3)-S(1)-Tc(1)	102.21
C(1)-S(1)-Tc(1)	103.84
C(2)-S(2)-Tc(1)	106.16
C(6)-S(3)-Tc(1)	97.51
C(7)-O(4)-C(8)	116.30
C(4)-N(1)-C(5)	112.20
C(4)-N(1)-Tc(1)	125.20
C(5)-N(1)-Tc(1)	122.40

Re 13



(2-Carbmethoxy-3-aza-4-oxo-6-thiaoctane-1,8-dithiolato-S,N,S,S)oxorhenium(V)

$C_8H_{12}NO_4ReS_3$

6.5750Å	10.7590Å	18.2250Å	
90.0000°	90.0000°	90.0000°	V=1289.2Å^3
$P2_12_12_1$; 19	Z=4; F(000)=856	ρ=2.332g/cm^3	R=2.1%
orthorhombic			

B. Noll, S.C. Hilger, P. Leibnitz, H. Spies, L. Dinkelborg, B. Johannsen
"A novel amide thioether dithiolate ligand derived from cysteine"
FZR-165 (1996) 59-61
CSD 406750

Re 13

Selected Bonds (Å) and Angles (°)

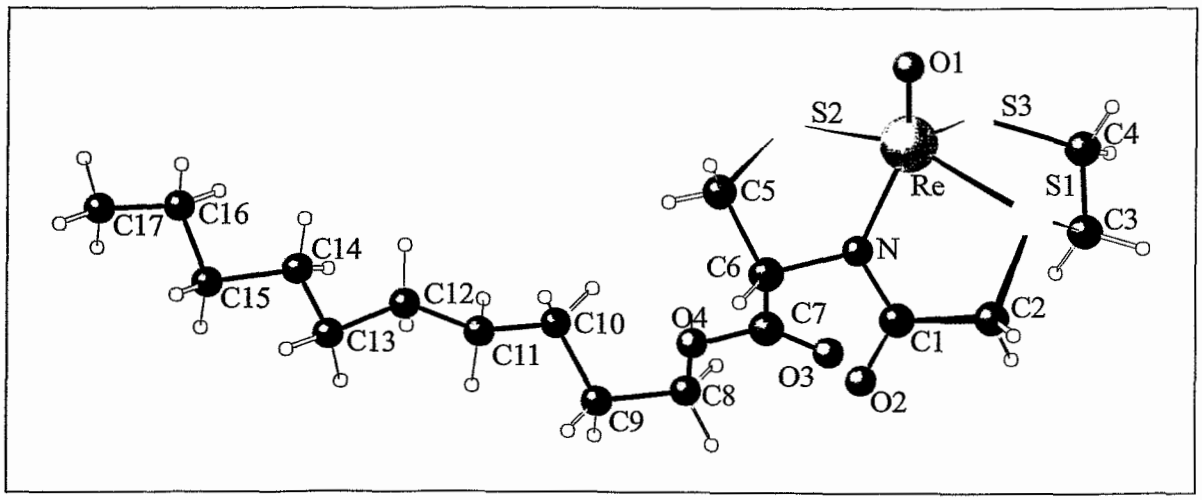
Bonds

Re-O(1)	1.676
Re-N	1.991
Re-S(2)	2.266
Re-S(3)	2.290
Re-S(1)	2.359
S(1)-C(3)	1.785
S(1)-C(1)	1.811
S(2)-C(2)	1.823
S(3)-C(6)	1.813
O(2)-C(4)	1.201
O(3)-C(7)	1.196
O(4)-C(7)	1.325
O(4)-C(8)	1.439
N-C(4)	1.377
N-C(5)	1.471
C(1)-C(2)	1.497
C(1)-H(1A)	0.970
C(1)-H(1B)	0.970
C(2)-H(2A)	0.970
C(2)-H(2B)	0.970
C(3)-C(4)	1.524
C(3)-H(3A)	0.970
C(3)-H(3B)	0.970

Angles

O(1)-Re-N	117.80
O(1)-Re-S(2)	115.00
N-Re-S(2)	127.03
O(1)-Re-S(3)	107.00
N-Re-S(3)	82.69
S(2)-Re-S(3)	85.72
O(1)-Re-S(1)	100.70
N-Re-S(1)	81.64
S(2)-Re-S(1)	85.48
S(3)-Re-S(1)	152.09
C(3)-S(1)-C(1)	105.60
C(3)-S(1)-Re	102.70
C(1)-S(1)-Re	103.80
C(2)-S(2)-Re	106.00
C(6)-S(3)-Re	98.10
C(7)-O(4)-C(8)	117.10
C(4)-N-C(5)	112.10
C(4)-N-Re	125.40
C(5)-N-Re	122.40
C(2)-C(1)-S(1)	107.00
C(2)-C(1)-H(1A)	110.30
S(1)-C(1)-H(1A)	110.30
C(2)-C(1)-H(1B)	110.30

Re 14



(2-Carbdecoxy-3-aza-4-oxo-6-thiaoctane-1,8-dithiolato-S,N,S,S)oxorhenium(V)

$C_{17}H_{30}NO_4ReS_3$

31.4500Å	10.7390Å	6.7790Å	
90.0000°	90.0000°	90.0000°	V=2289.5Å^3
$P2_12_12_1$; 19	Z=4; F(000)=1760	ρ=1.726g/cm^3	R=8.9%
orthorhombic			

B. Noll, (1998)
not published
CCDC 149092

Re 14

Selected Bonds (Å) and Angles (°)

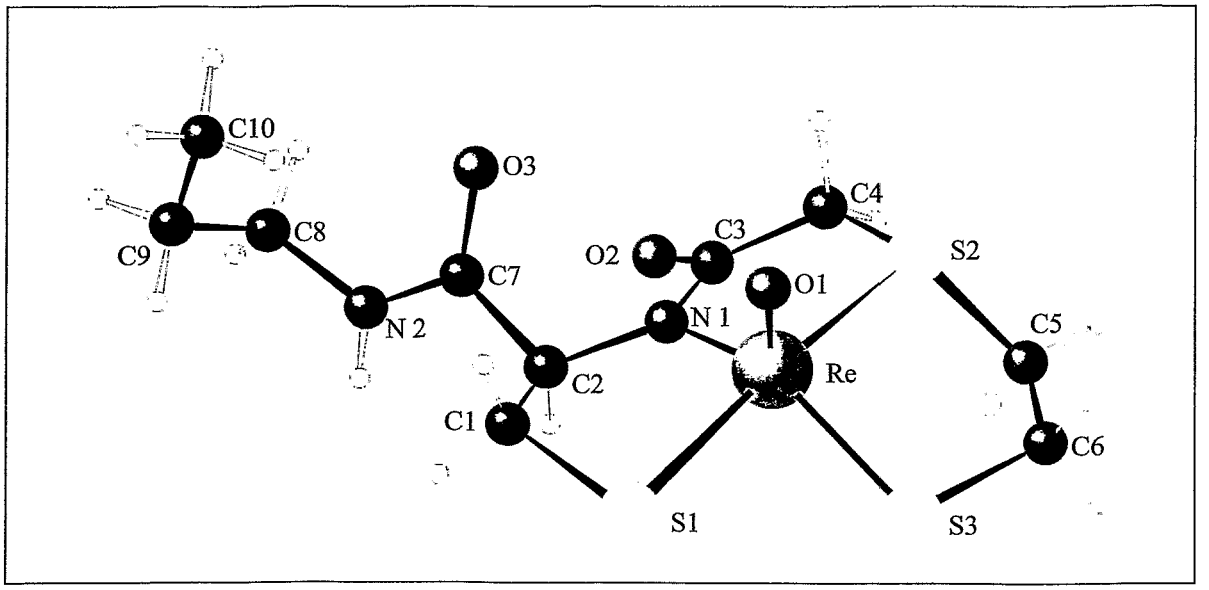
Bonds

Re-O(1)	1.676
Re-N	1.981
Re-S(3)	2.270
Re-S(2)	2.291
Re-S(1)	2.361
S(1)-C(3)	1.810
S(1)-C(2)	1.820
S(2)-C(5)	1.850
S(3)-C(4)	1.870
O(2)-C(1)	1.180
O(3)-C(7)	1.220
O(4)-C(7)	1.280
O(4)-C(8)	1.420
N-C(1)	1.380
N-C(6)	1.530
C(1)-C(2)	1.520
C(2)-H(2A)	0.970
C(2)-H(2B)	0.970
C(3)-C(4)	1.520
C(3)-H(3A)	0.970
C(3)-H(3B)	0.970
C(4)-H(4A)	0.970
C(4)-H(4B)	0.970

Angles

O(1)-Re-N	117.60
O(1)-Re-S(3)	116.60
N-Re-S(3)	125.60
O(1)-Re-S(2)	104.40
N-Re-S(2)	83.30
S(3)-Re-S(2)	86.60
O(1)-Re-S(1)	100.80
N-Re-S(1)	81.10
S(3)-Re-S(1)	86.10
S(2)-Re-S(1)	154.40
C(3)-S(1)-C(2)	104.70
C(3)-S(1)-Re	104.70
C(2)-S(1)-Re	102.70
C(5)-S(2)-Re	97.30
C(4)-S(3)-Re	104.60
C(7)-O(4)-C(8)	115.70
C(1)-N-C(6)	109.20
C(1)-N-Re	127.60
C(6)-N-Re	122.80
O(2)-C(1)-N	126.10
O(2)-C(1)-C(2)	117.30
N-C(1)-C(2)	116.40
C(1)-C(2)-S(1)	111.10

Re 15a



[2-(N-propyl)carbamoyl-3-aza-4-oxo-6-thiaoctane-1,8-dithiolato-S,N,S,S)oxorhenium(V)

$C_{10}H_{17}N_2O_3ReS_3$

9.4550Å	15.3589Å	22.1470Å	
90.0000°	90.0000°	90.0000°	V=3216.1Å^3
$P2_12_12_1$; 19	Z=8; F(000)=1904	ρ=2.047g/cm^3	R=6.6%
orthorhombic			

B. Noll, (1999)
not published
CCDC 161726

Re 15a

Selected Bonds (Å) and Angles (°)

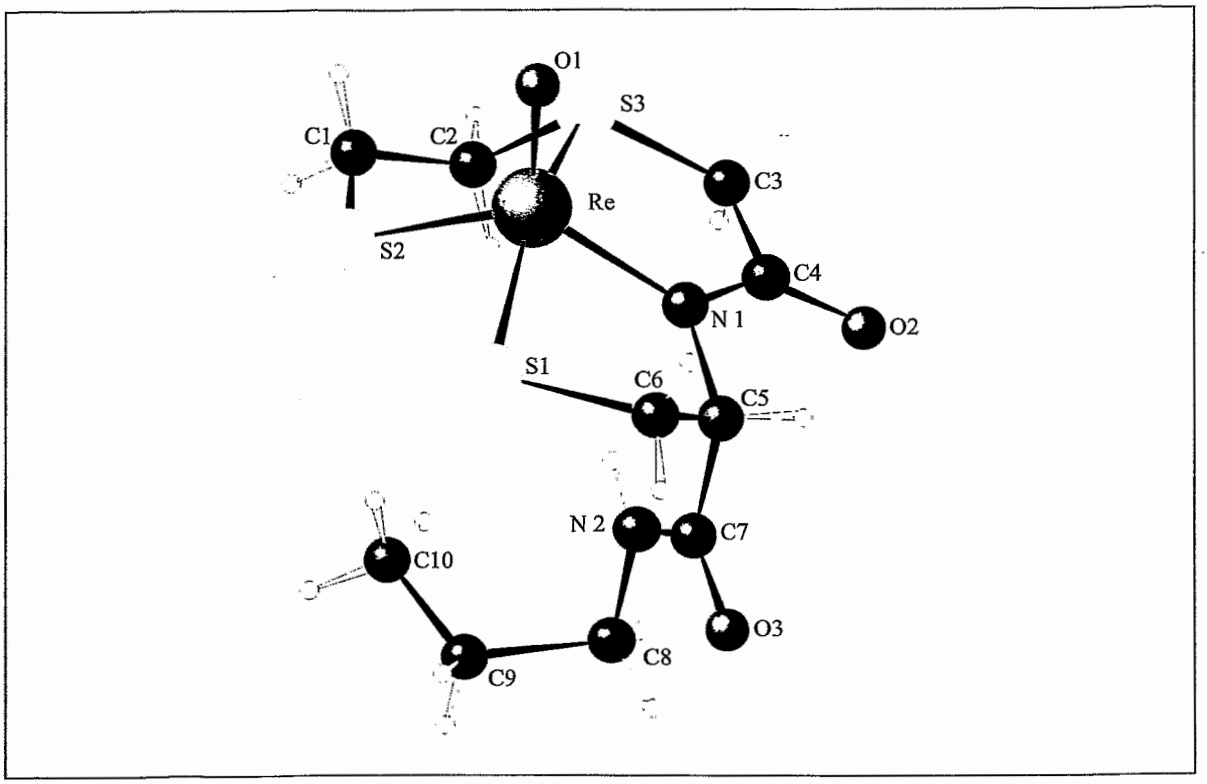
Bonds

Re(1)-O(1)	1.687
Re(1)-N(1)	1.990
Re(1)-S(3)	2.264
Re(1)-S(1)	2.279
Re(1)-S(2)	2.371
S(1)-C(1)	1.800
S(2)-C(4)	1.760
S(2)-C(5)	1.840
S(3)-C(6)	1.810
O(2)-C(3)	1.230
O(3)-C(7)	1.290
N(1)-C(3)	1.410
N(1)-C(2)	1.470
N(2)-C(7)	1.300
N(2)-C(8)	1.470
C(1)-C(2)	1.480
C(2)-C(7)	1.470
C(3)-C(4)	1.500
C(5)-C(6)	1.450
C(8)-C(9)	1.510
C(9)-C(101)	1.540
C(9)-C(10)	1.550
Re(2)-O(1')	1.691
Re(2)-N(1')	2.000
Re(2)-S(1')	2.290
Re(2)-S(3')	2.293
Re(2)-S(2')	2.362
S(1')-C(1')	1.790
S(2')-C(5')	1.790
S(2')-C(4')	1.860
S(3')-C(6')	1.800
O(2')-C(3')	1.230

Angles

O(1)-Re(1)-N(1)	119.70
O(1)-Re(1)-S(3)	114.00
N(1)-Re(1)-S(3)	126.10
O(1)-Re(1)-S(1)	106.90
N(1)-Re(1)-S(1)	81.30
S(3)-Re(1)-S(1)	87.50
O(1)-Re(1)-S(2)	98.00
N(1)-Re(1)-S(2)	83.30
S(3)-Re(1)-S(2)	85.70
S(1)-Re(1)-S(2)	154.90
C(1)-S(1)-Re(1)	96.20
C(4)-S(2)-Re(1)	100.80
C(5)-S(2)-Re(1)	104.80
C(6)-S(3)-Re(1)	104.20
C(3)-N(1)-Re(1)	122.30
C(2)-N(1)-Re(1)	123.20
O(1')-Re(2)-N(1')	115.50
O(1')-Re(2)-S(1')	107.50
N(1')-Re(2)-S(1')	81.90
O(1')-Re(2)-S(3')	113.40
N(1')-Re(2)-S(3')	131.00
S(1')-Re(2)-S(3')	85.80
O(1')-Re(2)-S(2')	101.90
N(1')-Re(2)-S(2')	82.90
S(1')-Re(2)-S(2')	150.40
S(3')-Re(2)-S(2')	85.30
C(1')-S(1')-Re(2)	96.10
C(5')-S(2')-Re(2)	103.30
C(4')-S(2')-Re(2)	101.80
C(6')-S(3')-Re(2)	106.20
C(3')-N(1')-Re(2)	123.90
C(2')-N(1')-Re(2)	123.00

Re 15b



[2-(N-propyl)carbamoyl-3-aza-4-oxo-6-thiaoctane-1,8-dithiolato-S,N,S,S]oxorhenium(V)

$C_{10}H_{17}N_2O_3ReS_3$

6.8230Å	13.7920Å	16.3790Å	
90.0000°	90.0000°	90.0000°	V=1541.3Å^3
$P2_12_12_1$; 19	Z=4; F(000)=952	ρ=2.136g/cm^3	R=2.2%
orthorhombic			

B. Noll, (1997)
not published
CCDC 156812

Re 15b

Selected Bonds (Å) and Angles (°)

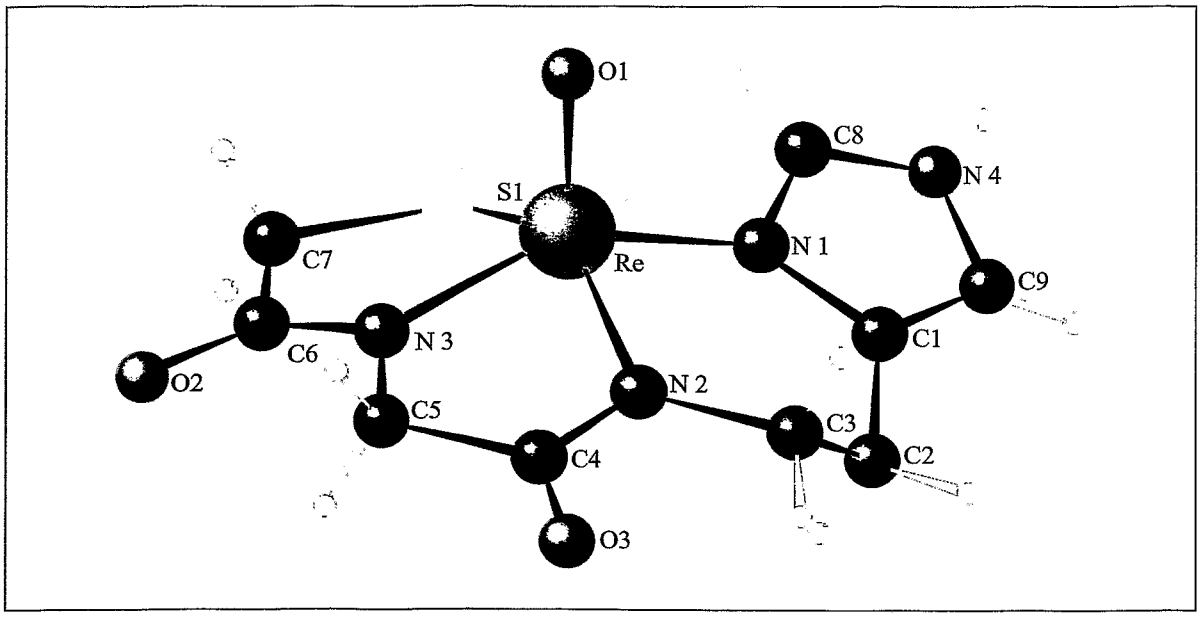
Bonds

Re(1)-O(1)	1.687
Re(1)-N(1)	2.014
Re(1)-S(2)	2.267
Re(1)-S(1)	2.301
Re(1)-S(3)	2.371
S(1)-C(6)	1.832
S(2)-C(1)	1.844
S(3)-C(3)	1.804
S(3)-C(2)	1.825
O(2)-C(4)	1.209
O(3)-C(7)	1.225
N(1)-C(4)	1.379
N(1)-C(5)	1.499
N(2)-C(7)	1.319
N(2)-C(8)	1.440
N(2)-C(8')	1.470
C(1)-C(2)	1.481
C(3)-C(4)	1.504
C(5)-C(6)	1.506
C(5)-C(7)	1.538
C(8)-C(9)	1.370

Angles

O(1)-Re(1)-N(1)	121.10
O(1)-Re(1)-S(2)	114.80
N(1)-Re(1)-S(2)	124.00
O(1)-Re(1)-S(1)	104.90
N(1)-Re(1)-S(1)	82.40
S(2)-Re(1)-S(1)	87.92
O(1)-Re(1)-S(3)	98.90
N(1)-Re(1)-S(3)	81.90
S(2)-Re(1)-S(3)	85.68
S(1)-Re(1)-S(3)	155.82
C(6)-S(1)-Re(1)	96.30
C(1)-S(2)-Re(1)	105.50
C(3)-S(3)-C(2)	107.00
C(3)-S(3)-Re(1)	101.60
C(2)-S(3)-Re(1)	103.80
C(4)-N(1)-C(5)	113.40
C(4)-N(1)-Re(1)	124.90
C(5)-N(1)-Re(1)	121.60
C(7)-N(2)-C(8)	122.70
C(7)-N(2)-C(8')	125.80
C(2)-C(1)-S(2)	111.40

Re 16



[1-(1H-imidazol-5-yl)-3,6-diaza-4,7-dioxooctane-8-thiolato-N,N,N,S]oxorhenium(V)

$C_9H_{11}N_4O_3ReS$

7.7553Å	9.0445Å	9.7643Å	
74.6950°	69.7100°	70.0650°	V=595.6Å^3
P-1; 2	Z=2; F(000)=460	ρ=2.462g/cm^3	R=3.1%
triclinic			

C.S. Hilger, B. Noll, F. Blume, P. Leibnitz, B. Johannsen
"Tc (V) and Re (V) complexes of N-(MAG_1)-histamine"
Technetium, Rhenium and Other Metals in Chemistry and Nuclear Medicine
SGE Editoriali-Italy (1999) 221-224
CCDC 156811

Re 16

Selected Bonds (Å) and Angles (°)

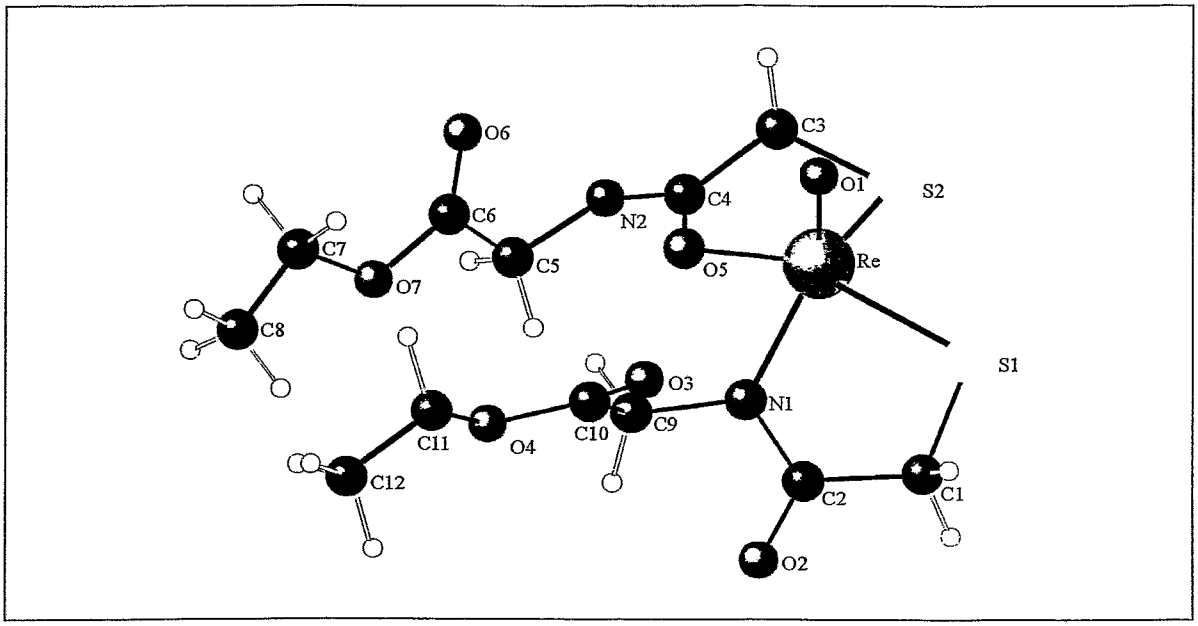
Bonds

Re(1)-O(1)	1.672
Re(1)-N(3)	1.990
Re(1)-N(2)	2.008
Re(1)-N(1)	2.090
Re(1)-S(1)	2.288
S(1)-C(7)	1.827
O(2)-C(6)	1.237
O(3)-C(4)	1.229
N(1)-C(8)	1.345
N(1)-C(1)	1.390
N(2)-C(4)	1.359
N(2)-C(3)	1.491
N(3)-C(6)	1.333
N(3)-C(5)	1.464
N(4)-C(8)	1.308
N(4)-C(9)	1.383
C(1)-C(9)	1.339
C(1)-C(2)	1.499
C(2)-C(3)	1.508
C(4)-C(5)	1.514
C(6)-C(7)	1.515

Angles

O(1)-Re(1)-N(3)	107.90
O(1)-Re(1)-N(2)	111.80
N(3)-Re(1)-N(2)	78.90
O(1)-Re(1)-N(1)	106.50
N(3)-Re(1)-N(1)	145.60
N(2)-Re(1)-N(1)	87.20
O(1)-Re(1)-S(1)	109.90
N(3)-Re(1)-S(1)	82.40
N(2)-Re(1)-S(1)	137.80
N(1)-Re(1)-S(1)	87.40
C(7)-S(1)-Re(1)	99.90
C(8)-N(1)-C(1)	106.40
C(8)-N(1)-Re(1)	123.00
C(1)-N(1)-Re(1)	129.90
C(4)-N(2)-C(3)	116.30
C(4)-N(2)-Re(1)	116.70
C(3)-N(2)-Re(1)	126.20
C(6)-N(3)-C(5)	118.30
C(6)-N(3)-Re(1)	125.50
C(5)-N(3)-Re(1)	116.30
C(8)-N(4)-C(9)	108.30

Re 17



[(O-ethyl-mercaptoacetylglycinato-S,O)(O-ethyl-2-mercaptoacetylglycinato-S.N)]oxorhenium(V)

$C_{12}H_{19}N_2O_7ReS_2$

12.2910Å	8.4760Å	18.3750Å	
90.0000°	109.0430°	90.0000°	V=1809.6Å^3
$P2_1$; 1014	Z=4; F(000)=1072	ρ=2.032g/cm^3	R=4.5%
monoclinc			

B. Noll, St. Noll, P. Leibnitz, H. Spies, P.E. Schulze, W. Semmler and B. Johannsen
"Technetium and rhenium complexes of mercaptoacetyl glycine ligands. II. Formation and molecular structure of Re (V) complexes with mercaptoacetyl glycine and mercaptoacetyl glycine ethylester"
Inorg.Chim.Acta 255 (1997) 399-403
CSD No. 404912

Re 17

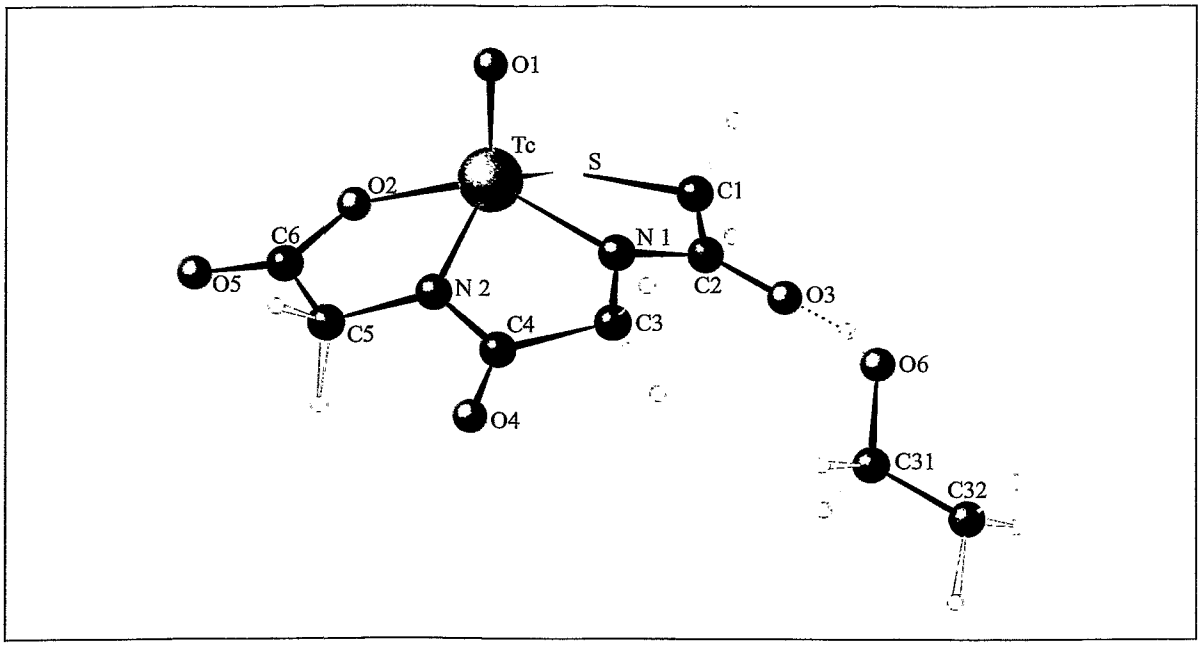
Selected Bonds (Å) and Angles (°)

Bonds

Re(1)-O(1)	1.673
Re(1)-N(1)	2.018
Re(1)-O(5)	2.051
Re(1)-S(1)	2.246
Re(1)-S(2)	2.273
S(1)-C(1)	1.803
S(2)-C(3)	1.795
N(1)-C(2)	1.355
N(1)-C(9)	1.464
N(2)-C(4)	1.285
N(2)-C(5)	1.446
N(2)-H(2)	0.860
O(2)-C(2)	1.234
O(3)-C(10)	1.177
O(4)-C(10)	1.302
O(4)-C(11)	1.460
O(5)-C(4)	1.272
O(6)-C(6)	1.187
O(7)-C(6)	1.292
O(7)-C(7)	1.464
C(1)-C(2)	1.459

Angles

O(1)-Re(1)-N(1)	110.60
O(1)-Re(1)-O(5)	111.30
N(1)-Re(1)-O(5)	83.00
O(1)-Re(1)-S(1)	107.10
N(1)-Re(1)-S(1)	83.10
O(5)-Re(1)-S(1)	141.60
O(1)-Re(1)-S(2)	108.70
N(1)-Re(1)-S(2)	140.70
O(5)-Re(1)-S(2)	81.30
S(1)-Re(1)-S(2)	87.24
C(1)-S(1)-Re(1)	101.10
C(3)-S(2)-Re(1)	99.90
C(2)-N(1)-C(9)	113.00
C(2)-N(1)-Re(1)	122.00
C(9)-N(1)-Re(1)	123.90
C(4)-N(2)-C(5)	122.30
C(4)-N(2)-H(2)	118.80
C(5)-N(2)-H(2)	118.80
C(10)-O(4)-C(11)	117.00
C(4)-O(5)-Re(1)	122.00
C(6)-O(7)-C(7)	119.60



Tetraphenylarsonium (2-mercaptoacetyl-diglycinato-S,N,N,O)oxotechnetate(V) (ethanol adduct)
$C_{30}H_{25}N_2O_5SAsTc \times C_2H_5OH$
(The tetraphenylarsonium counterion has been omitted for clarity.)

12.4785Å	14.9225Å	17.1839Å	
90.0340°	103.1340°	90.0230°	V=3115.9Å^3
$P2_1/n$; 1014	Z=4; F(000)=1380	ρ=1.587g/cm^3	R=3.3%
monoclinic			

B. Johannsen, B. Noll, P. Leibnitz, G. Reck, St. Noll, H. Spies
"Technetium and rhenium complexes of mercapto containing peptides. I. Tc (V) and Re (V) complexes with mercaptoacetyl diglycine (MAG_2) and X-ray structure of $AsPh_4(TcO(MAG_2)) \times C_2H_5OH$"
Inorg.Chim.Acta 210 (1993) 209-214
CSD No. 57135

Tc 18

Selected Bonds (Å) and Angles (°)

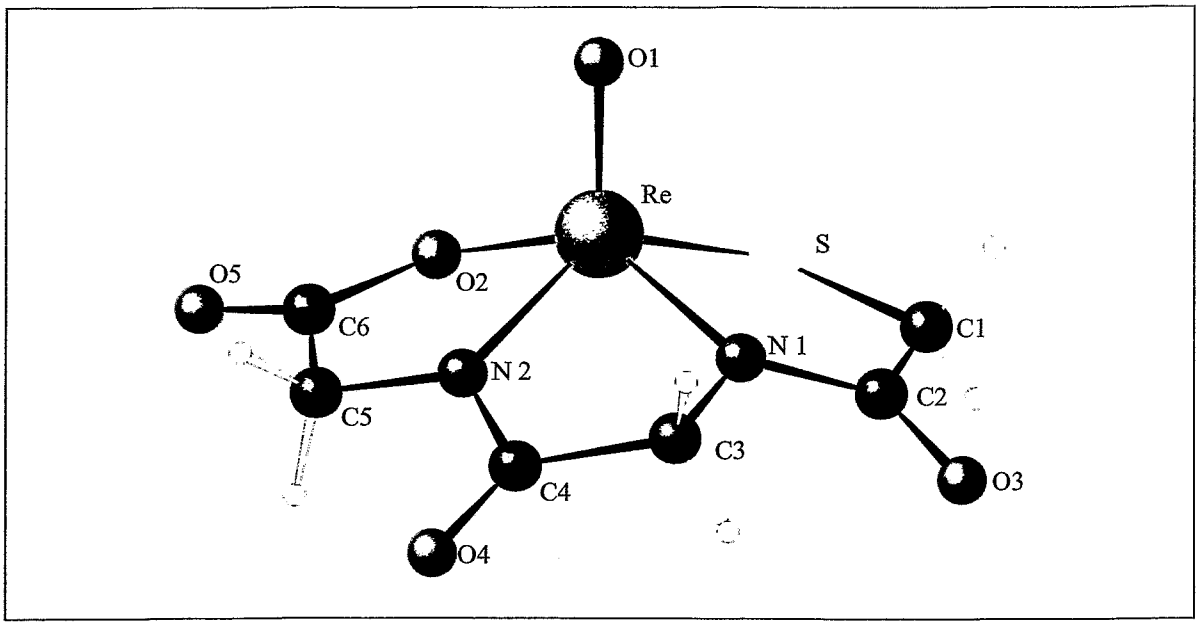
Bonds

Tc-O(1)	1.645
Tc-N(1)	1.966
Tc-N(2)	1.968
Tc-O(2)	2.016
Tc-S	2.272
As-C(13)	1.905
As-C(25)	1.912
As-C(19)	1.914
As-C(7)	1.922
S-C(1)	1.815
O(2)-C(6)	1.323
O(3)-C(2)	1.233
O(4)-C(4)	1.224
O(5)-C(6)	1.211
O(6)-C(31)	1.378
N(1)-C(2)	1.362
N(1)-C(3)	1.451
N(2)-C(4)	1.345
N(2)-C(5)	1.449
C(1)-C(2)	1.500
C(3)-C(4)	1.522
C(5)-C(6)	1.504
C(7)-C(12)	1.369
C(7)-C(8)	1.373

Angles

O(1)-Tc-N(1)	109.60
O(1)-Tc-N(2)	115.80
N(1)-Tc-N(2)	78.90
O(1)-Tc-O(2)	110.30
N(1)-Tc-O(2)	139.60
N(2)-Tc-O(2)	78.70
O(1)-Tc-S	110.30
N(1)-Tc-S	83.56
N(2)-Tc-S	133.79
O(2)-Tc-S	88.35
C(13)-As-C(25)	112.20
C(13)-As-C(19)	109.70
C(25)-As-C(19)	107.10
C(13)-As-C(7)	107.10
C(25)-As-C(7)	111.60
C(19)-As-C(7)	109.00
C(1)-S-Tc	98.40
C(6)-O(2)-Tc	118.10
C(2)-N(1)-C(3)	118.80
C(2)-N(1)-Tc	124.40
C(3)-N(1)-Tc	116.30
C(4)-N(2)-C(5)	121.50
C(4)-N(2)-Tc	120.00
C(5)-N(2)-Tc	118.00

Re 18a



Tetraphenylarsonium (mercaptoacetyldiglycine-S,N,N,O)oxorhenate(V)

$C_{30}H_{26}AsN_2O_5ReS$
(The tetraphenylarsonium counterion has been omitted for clarity.)

23.8429Å	8.8272Å	14.0605Å	
90.0000°	90.0000°	90.0000°	V=2959.2Å
$Pna2_1$; 33	Z=4; F(000)=1536	ρ=1.786g/cm^3	R=3.0%
orthorhombic			

B. Johannnsen, B. Noll, P. Leibnitz, G. Reck, St. Noll, and H. Spies
"Occurrence and nature of different Tc (V) and Re (V) complexes with mercapto/amide ligands"
Radiochim.Acta 63 (1993) 133-137
CCDC 156311

Re 18a

Selected Bonds (Å) and Angles (°)

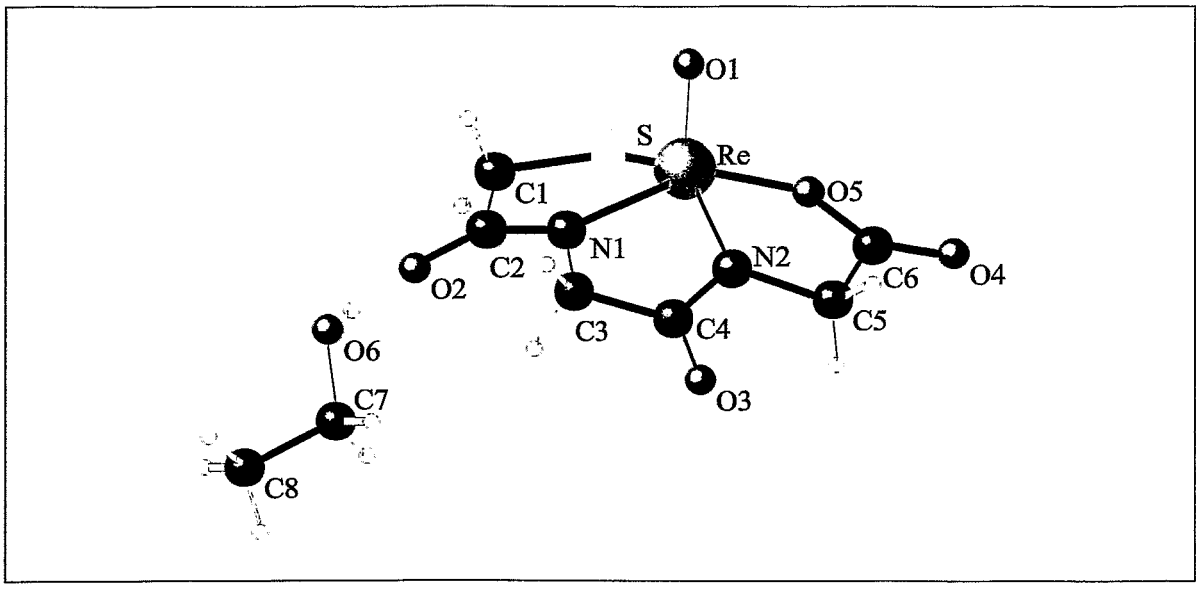
Bonds

Re-O(1)	1.667
Re-N(2)	1.961
Re-N(1)	1.976
Re-O(2)	2.023
Re-S	2.260
As-C(7)	1.897
As-C(19)	1.910
As-C(13)	1.911
As-C(25)	1.920
S-C(1)	1.780
O(2)-C(6)	1.320
O(3)-C(2)	1.220
O(4)-C(4)	1.215
O(5)-C(6)	1.190
N(1)-C(2)	1.340
N(1)-C(3)	1.450
N(2)-C(4)	1.380
N(2)-C(5)	1.440
C(1)-C(2)	1.520
C(1)-H(1A)	0.970
C(1)-H(1B)	0.970
C(3)-C(4)	1.460
C(3)-H(3A)	0.970
C(3)-H(3B)	0.970
C(5)-C(6)	1.530
C(5)-H(5A)	0.970
C(5)-H(5B)	0.970
C(7)-C(8)	1.379
C(7)-C(12)	1.393
C(8)-C(9)	1.380
C(8)-H(8)	0.930
C(9)-C(10)	1.390

Angles

O(1)-Re-N(2)	115.90
O(1)-Re-N(1)	109.60
N(2)-Re-N(1)	78.10
O(1)-Re-O(2)	109.20
N(2)-Re-O(2)	78.20
N(1)-Re-O(2)	140.40
O(1)-Re-S	110.20
N(2)-Re-S	133.80
N(1)-Re-S	84.00
O(2)-Re-S	90.10
C(7)-As-C(19)	106.10
C(7)-As-C(13)	112.30
C(19)-As-C(13)	110.60
C(7)-As-C(25)	110.50
C(19)-As-C(25)	109.60
C(13)-As-C(25)	107.80
C(1)-S-Re	99.90
C(6)-O(2)-Re	118.10
C(2)-N(1)-C(3)	118.70
C(2)-N(1)-Re	124.40
C(3)-N(1)-Re	115.50
C(4)-N(2)-C(5)	120.90
C(4)-N(2)-Re	119.80
C(5)-N(2)-Re	118.80
C(8)-C(7)-As	120.30
C(12)-C(7)-As	119.80
C(18)-C(13)-As	119.00
C(14)-C(13)-As	119.30
C(24)-C(19)-As	120.90
C(20)-C(19)-As	120.30
C(26)-C(25)-As	119.50
C(30)-C(25)-As	117.60

Re 18b



Tetraphenylarsonium (2-mercaptoacetyl diglycinato-S,N,N,O)oxorhenate(V) (ethanol adduct)
$C_{32}H_{32}AsN_2O_6ReS$
(The tetraphenylarsonium counterion has been omitted for clarity.)

12.4779Å	14.8913Å	17.1259Å	
90.0000°	103.1150°	90.0000°	V=3099.2Å^3
$Pna2_1/n$; 1014	Z=4; F(000)=1640	ρ=1.787g/cm^3	R=5.5%
monoclinic			

B. Noll (1995)
not published
CCDC 156806

Re 18b

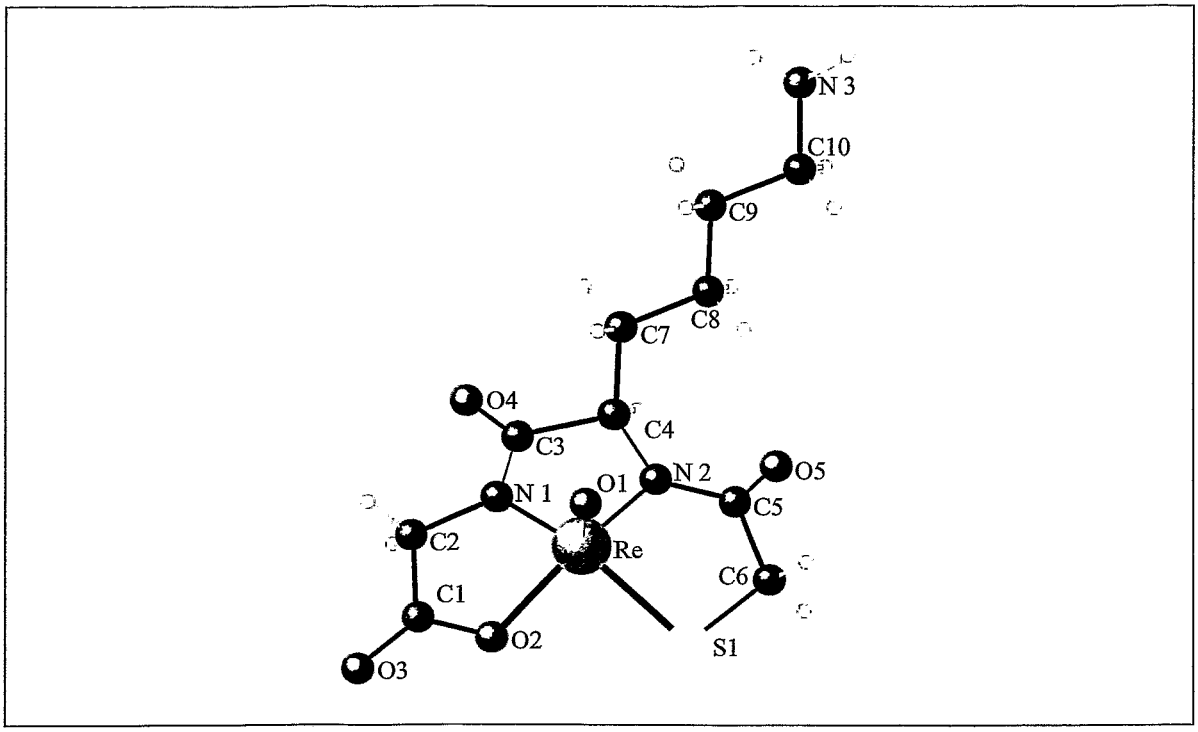
Selected Bonds (Å) and Angles (°)

Bonds

Re-O(1)	1.678
Re-N(2)	1.961
Re-N(1)	1.968
Re-O(5)	2.011
Re-S	2.266
S-C(1)	1.816
O(2)-C(2)	1.229
O(3)-C(4)	1.221
O(4)-C(6)	1.212
O(5)-C(6)	1.328
N(1)-C(2)	1.364
N(1)-C(3)	1.463
N(2)-C(4)	1.356
N(2)-C(5)	1.453
C(1)-C(2)	1.489
C(3)-C(4)	1.505
C(5)-C(6)	1.483
O(6)-C(7)	1.378
C(7)-C(8)	1.450
As-C(27)	1.896
As-C(9)	1.899
As-C(21)	1.904
As-C(15)	1.917
C(9)-C(14)	1.381

Angles

O(1)-Re-N(2)	115.30
O(1)-Re-N(1)	109.50
N(2)-Re-N(1)	78.90
O(1)-Re-O(5)	110.10
N(2)-Re-O(5)	78.20
N(1)-Re-O(5)	139.80
O(1)-Re-S	110.20
N(2)-Re-S	134.40
N(1)-Re-S	83.40
O(5)-Re-S	89.61
C(1)-S-Re	98.90
C(6)-O(5)-Re	118.30
C(2)-N(1)-C(3)	119.10
C(2)-N(1)-Re	124.40
C(3)-N(1)-Re	115.90
C(4)-N(2)-C(5)	121.40
C(4)-N(2)-Re	119.80
C(5)-N(2)-Re	118.50
C(2)-C(1)-S	112.10
O(2)-C(2)-N(1)	123.40
O(2)-C(2)-C(1)	121.70
N(1)-C(2)-C(1)	114.90
N(1)-C(3)-C(4)	108.90
O(3)-C(4)-N(2)	123.90



Tetraphenylarsonium (2-mercaptoacetyl lysylglycinato-S.N.N.O)oxorhenate(V)

$C_{10}H_{15}N_3O_5ReS$
(The tetraphenylarsonium counterion has been omitted for clarity.)

8.5721Å	9.1358Å	10.4571Å	
82.0190°	66.1690°	73.2800°	V=717.2Å^3
P-1; 2	Z=2; F(000)=454	ρ=2.202g/cm^3	R=5.5%
triclinic			

B. Noll, (1998)
not published
CCDC 161727

Re 19

Selected Bonds (Å) and Angles (°)

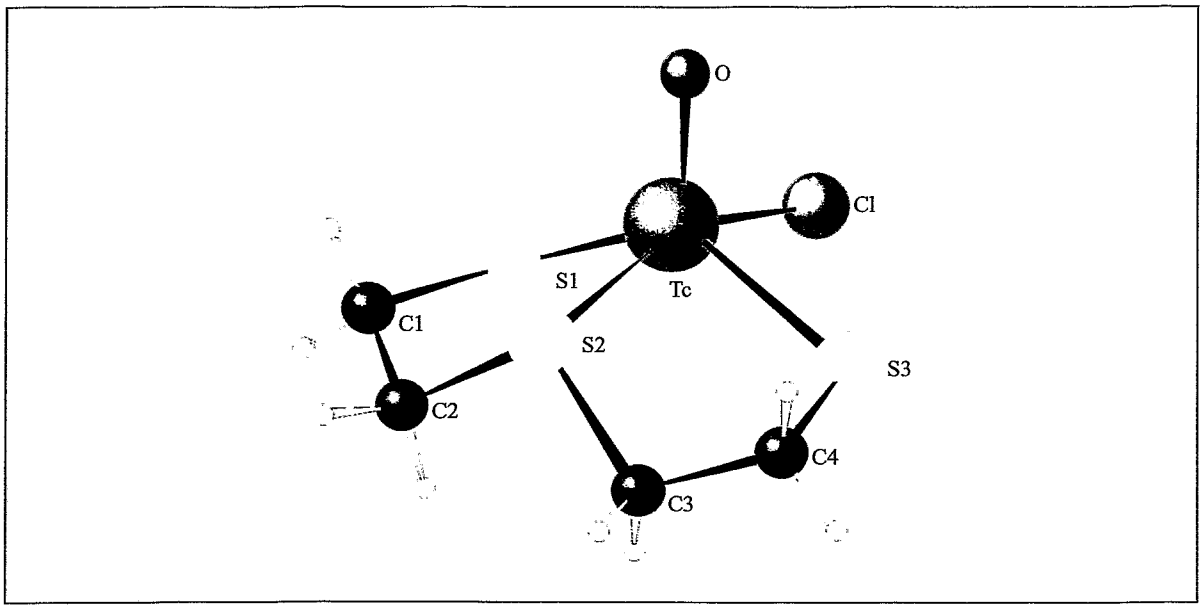
Bonds

Re-O(1)	1.705
Re-N(2)	1.980
Re-N(1)	1.988
Re-O(2)	2.032
Re-S(1)	2.284
S(1)-C(6)	1.800
O(2)-C(1)	1.290
O(3)-C(1)	1.250
O(4)-C(3)	1.240
O(5)-C(5)	1.230
N(1)-C(3)	1.340
N(1)-C(2)	1.471
N(2)-C(5)	1.390
N(2)-C(4)	1.480
N(3)-C(10)	1.510
C(1)-C(2)	1.500
C(3)-C(4)	1.570
C(4)-C(7)	1.560
C(5)-C(6)	1.540
C(7)-C(8)	1.500
C(8)-C(9)	1.520
C(9)-C(10)	1.500

Angles

O(1)-Re-N(2)	109.10
O(1)-Re-N(1)	115.40
N(2)-Re-N(1)	78.40
O(1)-Re-O(2)	110.00
N(2)-Re-O(2)	140.10
N(1)-Re-O(2)	77.80
O(1)-Re-S(1)	110.60
N(2)-Re-S(1)	85.10
N(1)-Re-S(1)	134.00
O(2)-Re-S(1)	88.90
C(6)-S(1)-Re	97.80
C(1)-O(2)-Re	117.60
C(3)-N(1)-C(2)	120.10
C(3)-N(1)-Re	121.50
C(2)-N(1)-Re	118.10
C(5)-N(2)-C(4)	117.00
C(5)-N(2)-Re	123.70
C(4)-N(2)-Re	117.60
O(3)-C(1)-O(2)	120.10
O(3)-C(1)-C(2)	122.20
O(2)-C(1)-C(2)	117.60
N(1)-C(2)-C(1)	106.20

5.2.2. "3+1" mixed-ligand complexes



Chloro(3-thiapentane-1,5-dithiolato)oxotechnetium(V)

$C_4H_8ClOS_3Tc$

13.4257Å	6.2867Å	11.1543Å	
90.0000°	90.0000°	90.0000°	V=941.5Å^3
$Pca2_1$; 29	Z=4; F(0009=592	ρ=2.129g/cm^3	R=4.8%
orthorhombic			

B. Noll, (1998)
not published
CCDC 161725

Selected Bonds (Å) and Angles (°)

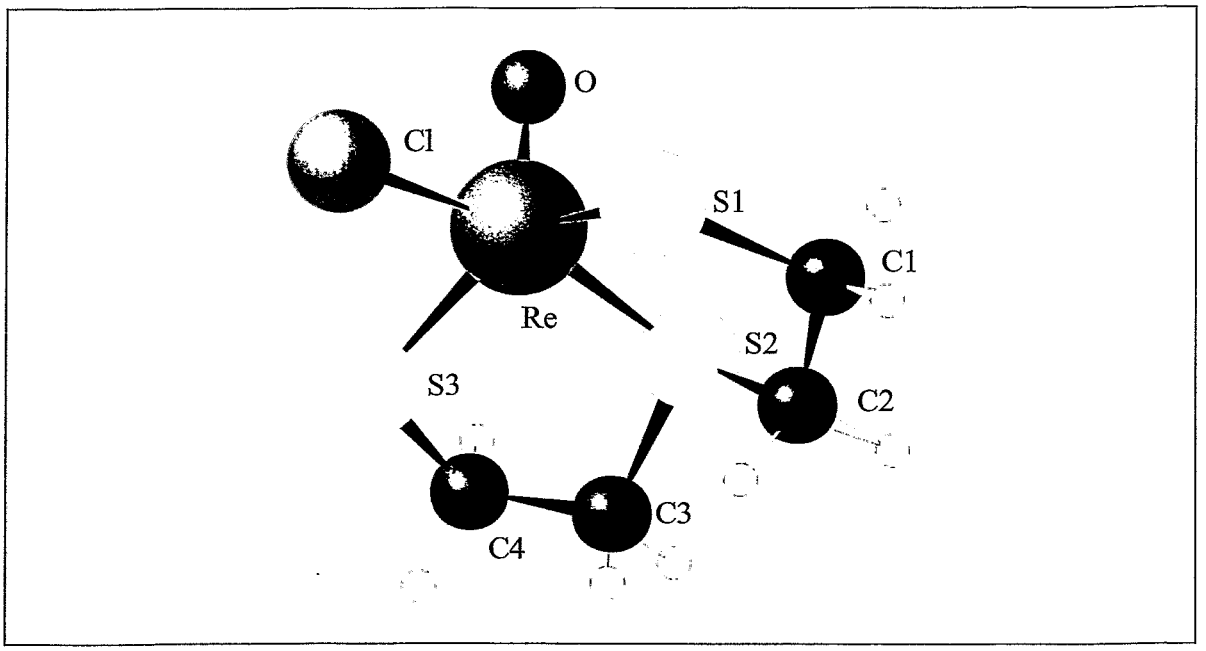
Bonds

Tc(1)-O(1)	1.654
Tc(1)-S(1)	2.278
Tc(1)-S(3)	2.279
Tc(1)-S(2)	2.349
Tc(1)-Cl(1)	2.360
S(1)-C(1)	1.814
S(2)-C(3)	1.816
S(2)-C(2)	1.818
S(3)-C(4)	1.846
C(1)-C(2)	1.496
C(3)-C(4)	1.483

Angles

O(1)-Tc(1)-S(1)	116.20
O(1)-Tc(1)-S(3)	115.40
S(1)-Tc(1)-S(3)	128.33
O(1)-Tc(1)-S(2)	101.60
S(1)-Tc(1)-S(2)	84.75
S(3)-Tc(1)-S(2)	84.94
O(1)-Tc(1)-Cl(1)	104.50
S(1)-Tc(1)-Cl(1)	84.13
S(3)-Tc(1)-Cl(1)	83.54
S(2)-Tc(1)-Cl(1)	153.83
C(1)-S(1)-Tc(1)	106.10
C(3)-S(2)-Tc(1)	105.10
C(2)-S(2)-Tc(1)	107.60
C(4)-S(3)-Tc(1)	106.20

Re 20a



Chloro(3-thiapentane-1,5-dithiolato)oxorhenium(V)

$C_4H_8ClOS_3Re$

13.4244Å	6.3146Å	11.1339Å	
90.0000°	90.0000°	90.0000°	V=943.8Å^3
$Pca2_1$; 29	Z=4; F(000)=720	ρ=2.744g/cm^3	R=4.0%
orthorhombic			

T.Fietz, H.Spies, H.-J. Pietzsch, and P.Leibnitz
"Synthesis and molecular structure of chloro(3-thiapentane-1.5-dithiolato) oxorhenium (V)"
Inorg.Chim.Acta 231 (1995) 233-236
CSD No. 401490

Re 20a

Selected Bonds (Å) and Angles (°)

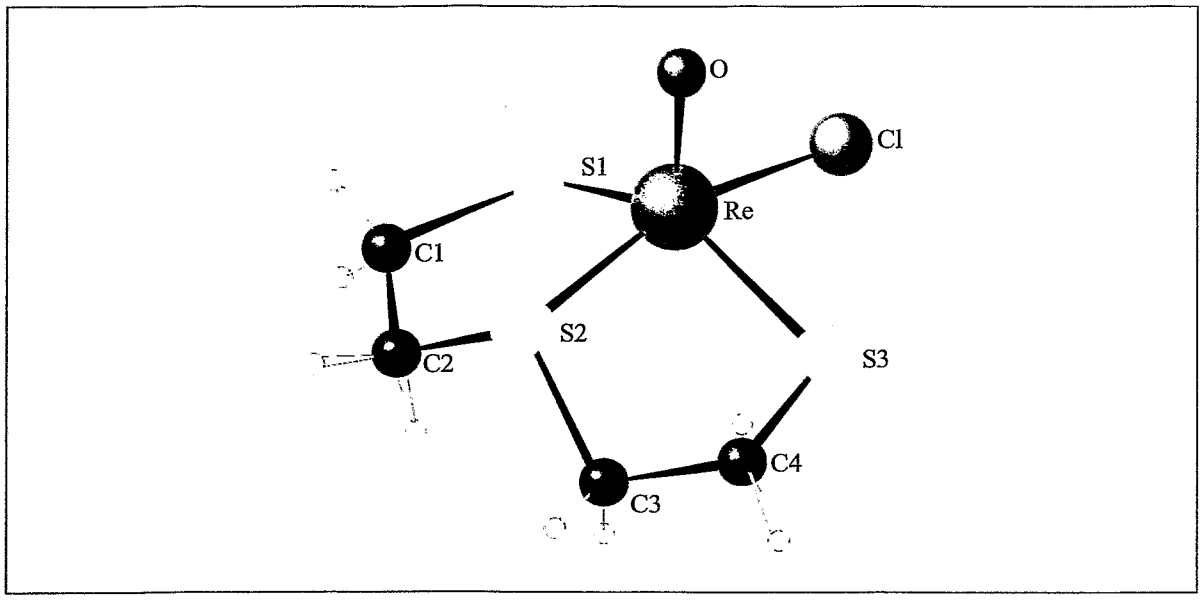
Bonds

Re-O	1.705
Re-S(3)	2.260
Re-S(1)	2.272
Re-S(2)	2.295
Re-Cl	2.372
S(1)-C(1)	1.842
S(2)-C(3)	1.813
S(2)-C(2)	1.848
S(3)-C(4)	1.838
C(1)-C(2)	1.500
C(3)-C(4)	1.470

Angles

O-Re-S(3)	115.20
O-Re-S(1)	114.10
S(3)-Re-S(1)	130.70
O-Re-S(2)	101.80
S(3)-Re-S(2)	86.36
S(1)-Re-S(2)	86.30
O-Re-Cl	102.00
S(3)-Re-Cl	84.31
S(1)-Re-Cl	83.34
S(2)-Re-Cl	156.20
C(1)-S(1)-Re	105.40
C(3)-S(2)-C(2)	102.90
C(3)-S(2)-Re	106.90
C(2)-S(2)-Re	105.00
C(4)-S(3)-Re	105.40

Re 20b



Chloro(3-thiapentane-1,5-dithiolato)oxorhenium(V)

$C_4H_8ClOS_3Re$

14.1385Å	6.6190Å	10.1460Å	
90.0000°	90.0000°	90.0000°	$V=949.3Å^3$
$Pna2_1$; 33	Z=4; F(000)=720	$\rho=2.728 g/cm^3$	R=11.94%
orthorhombic			

T.Fietz (1997)
not published

Re 20b

Selected Bonds (Å) and Angles (°)

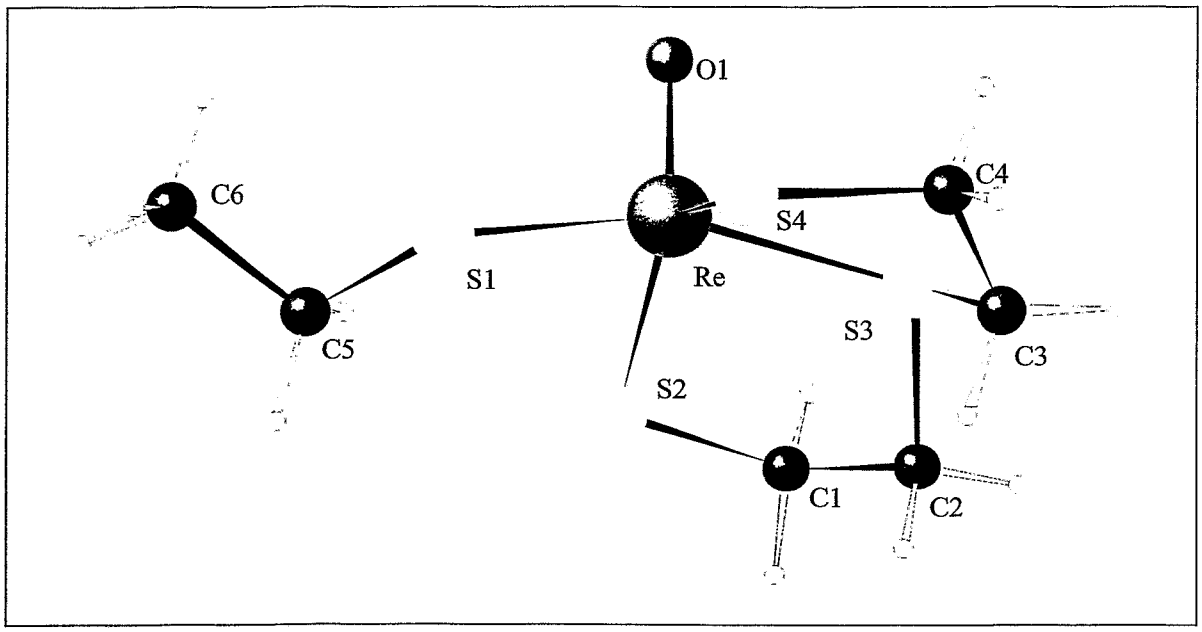
Bonds

Re-O	1.757
Re-S(1)	2.210
Re-S(2)	2.231
Re-S(3)	2.285
Re-Cl	2.398
S(1)-C(1)	1.827
S(2)-C(2)	1.802
S(2)-C(3)	1.820
S(3)-C(4)	1.811
C(1)-C(2)	1.468
C(3)-C(4)	1.493

Angles

O-Re-S(1)	114.20
O-Re-S(2)	101.30
S(1)-Re-S(2)	88.80
O-Re-S(3)	110.00
S(1)-Re-S(3)	135.50
S(2)-Re-S(3)	87.50
O-Re-Cl	99.20
S(1)-Re-Cl	85.30
S(2)-Re-Cl	159.20
S(3)-Re-Cl	82.80
C(1)-S(1)-Re	106.60
C(2)-S(2)-C(3)	110.00
C(2)-S(2)-Re	106.60
C(3)-S(2)-Re	106.00
C(4)-S(3)-Re	105.10
C(2)-C(1)-S(1)	112.90
C(1)-C(2)-S(2)	113.90
C(4)-C(3)-S(2)	110.90
C(3)-C(4)-S(3)	110.10

Re 21



(3-Thiapentane-1,5-dithiolato)(ethanethiolato)oxorhenium(V)

$C_6H_{13}ORES_4$

18.5495Å	18.5504Å	7.2432Å	
90.0000°	90.0000°	90.0000°	V=2492.1Å^3
P42/n; 86	Z=8; F(000)=1568	ρ=2.560g/cm^3	R=7.2%
tetragonal			

T. Fietz (1993)
not published
CCDC 156310

Re 21

Selected Bonds (Å) and Angles (°)

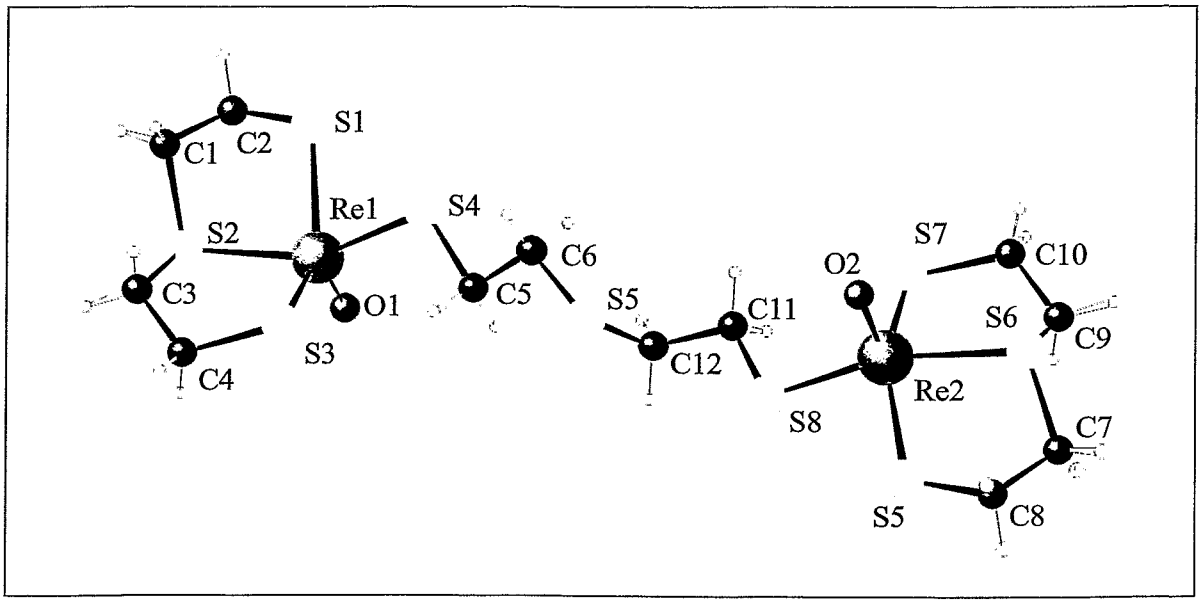
Bonds

Re-O(1)	1.670
Re-S(1)	2.288
Re-S(2)	2.294
Re-S(4)	2.301
Re-S(3)	2.368
S(1)-C(5)	1.780
S(2)-C(1)	1.810
S(3)-C(2)	1.790
S(3)-C(3)	1.800
S(4)-C(4)	1.800
C(1)-C(2)	1.560
C(1)-H(1B)	0.970
C(1)-H(1C)	0.970
C(2)-H(2A)	0.970
C(2)-H(2B)	0.970
C(3)-C(4)	1.480
C(3)-H(3A)	0.970
C(3)-H(3B)	0.970
C(4)-H(4A)	0.970
C(4)-H(4B)	0.970
C(5)-C(6)	1.410
C(5)-H(5A)	0.970
C(5)-H(5B)	0.970

Angles

O(1)-Re-S(1)	104.80
O(1)-Re-S(2)	115.20
S(1)-Re-S(2)	88.60
O(1)-Re-S(4)	113.70
S(1)-Re-S(4)	82.20
S(2)-Re-S(4)	131.00
O(1)-Re-S(3)	101.20
S(1)-Re-S(3)	153.70
S(2)-Re-S(3)	83.80
S(4)-Re-S(3)	83.90
C(5)-S(1)-Re	112.60
C(1)-S(2)-Re	106.00
C(2)-S(3)-C(3)	104.10
C(2)-S(3)-Re	108.50
C(3)-S(3)-Re	106.90
C(4)-S(4)-Re	104.30
C(2)-C(1)-S(2)	110.90
C(2)-C(1)-H(1B)	109.50
S(2)-C(1)-H(1B)	109.50
C(2)-C(1)-H(1C)	109.50
S(2)-C(1)-H(1C)	109.50
H(1B)-C(1)-H(1C)	108.10
C(1)-C(2)-S(3)	105.40

Re 22



μ-(3-thiapentane-1,5-dithiolato)-bis[(3-thiapentane-1,5-dithiolato)-oxorhenium(V)]

$C_{14}H_{14}NO_2ReS_3$

7.3530Å	15.1990Å	10.4660Å	
90.0000°	94.4800°	90.0000°	V=1166.1Å^3
$P2_1$; 4	Z=4; F(000)=812	ρ=2.453g/cm^3	R=2.7%
monoclinic			

H.-J. Pietzsch (1997)
not published
CCDC 159502

Re 22

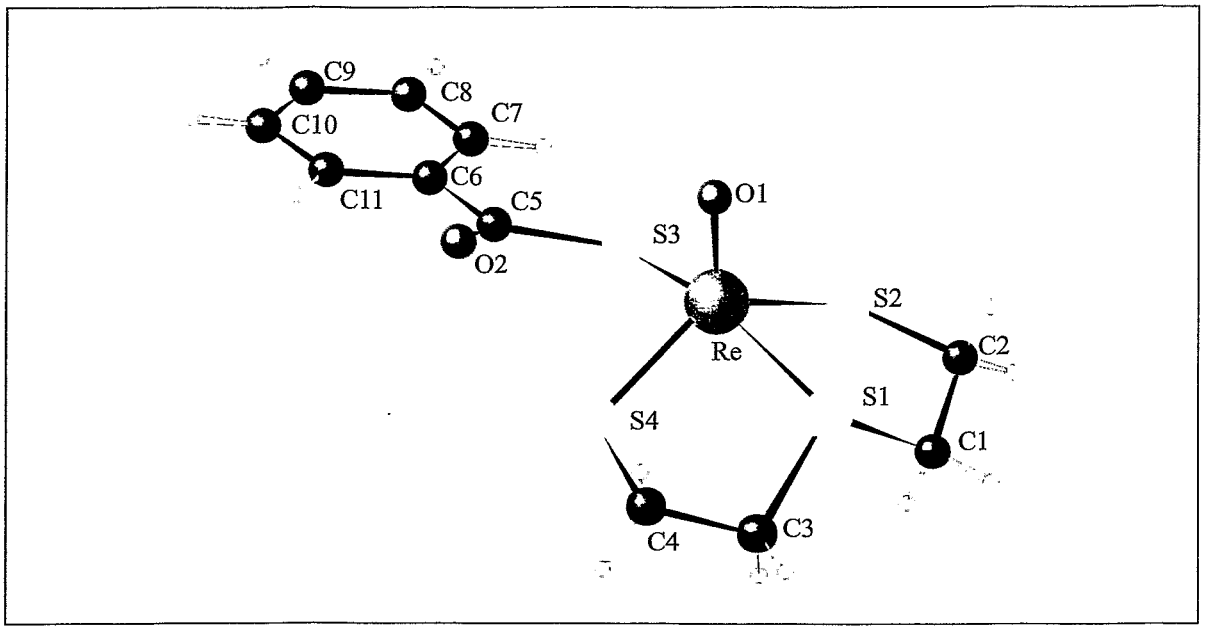
Selected Bonds (Å) and Angles (°)

Bonds

Re-O(1)	1.770
Re-S(1)	2.157
Re-S(3)	2.270
Re-S(4)	2.300
Re-S(2)	2.380
S(1)-C(2)	1.580
S(2)-C(1)	1.810
S(2)-C(3)	1.840
S(4)-C(5)	1.900
S(3)-C(4)	1.780
S(5)-C(6)	1.680
S(5)-C(6')	1.690
C(1)-C(2)	1.420
C(3)-C(4)	1.430
C(5)-C(6)	1.440
Re'-O(1')	1.680
Re'-S(3')	2.239
Re'-S(4')	2.330
Re'-S(2')	2.360
Re'-S(1')	2.369
S(1')-C(2')	1.490
S(2')-C(3')	1.840
S(2')-C(1')	1.860
S(4')-C(5')	1.900
S(3')-C(4')	1.810
C(1')-C(2')	1.400
C(3')-C(4')	1.410
C(5')-C(6')	1.450

Angles

O(1)-Re-S(1)	119.10
O(1)-Re-S(3)	108.50
S(1)-Re-S(3)	131.50
O(1)-Re-S(4)	106.30
S(1)-Re-S(4)	85.90
S(3)-Re-S(4)	89.50
O(1)-Re-S(2)	97.60
S(1)-Re-S(2)	82.00
S(3)-Re-S(2)	83.30
S(4)-Re-S(2)	156.10
C(2)-S(1)-Re	111.40
C(1)-S(2)-C(3)	109.50
C(1)-S(2)-Re	105.40
C(3)-S(2)-Re	103.40
C(5)-S(4)-Re	112.50
C(4)-S(3)-Re	108.30
O(1')-Re'-S(3')	115.50
O(1')-Re'-S(4')	109.80
S(3')-Re'-S(4')	89.10
O(1')-Re'-S(2')	101.90
S(3')-Re'-S(2')	84.40
S(4')-Re'-S(2')	147.20
O(1')-Re'-S(1')	113.80
S(3')-Re'-S(1')	130.50
S(4')-Re'-S(1')	78.40
S(2')-Re'-S(1')	81.70
C(2')-S(1')-Re'	105.90
C(3')-S(2')-Re'	104.70
C(1')-S(2')-Re'	104.20
C(5')-S(4')-Re'	114.00
C(4')-S(3')-Re'	107.10



[S-benzoylthiolato(3-thiapentane-1,5-dithiolato)]oxorhenium(V)

$C_{11}H_{13}O_2ReS_4$

8.6120Å	14.5350Å	12.2140Å	
90.0000°	90.0000°	90.0000°	V=1528.9Å
$P2_12_12_1$; 19	Z=4; F(000)=936	ρ=2.136g/cm^3	R=2.4%
orthorhombic			

B. Noll, P. Leibnitz, St. Noll, R.M. Mahfouz, H. Spies
"Structure and reactivity of a "3+1" mixed-ligand rhenium complex containing thiobenzoate as a monodentate ligand [ReO(SSS)(SC(O)Ph)]"
FZR-165 (1996) 93-95
CCDC 156808

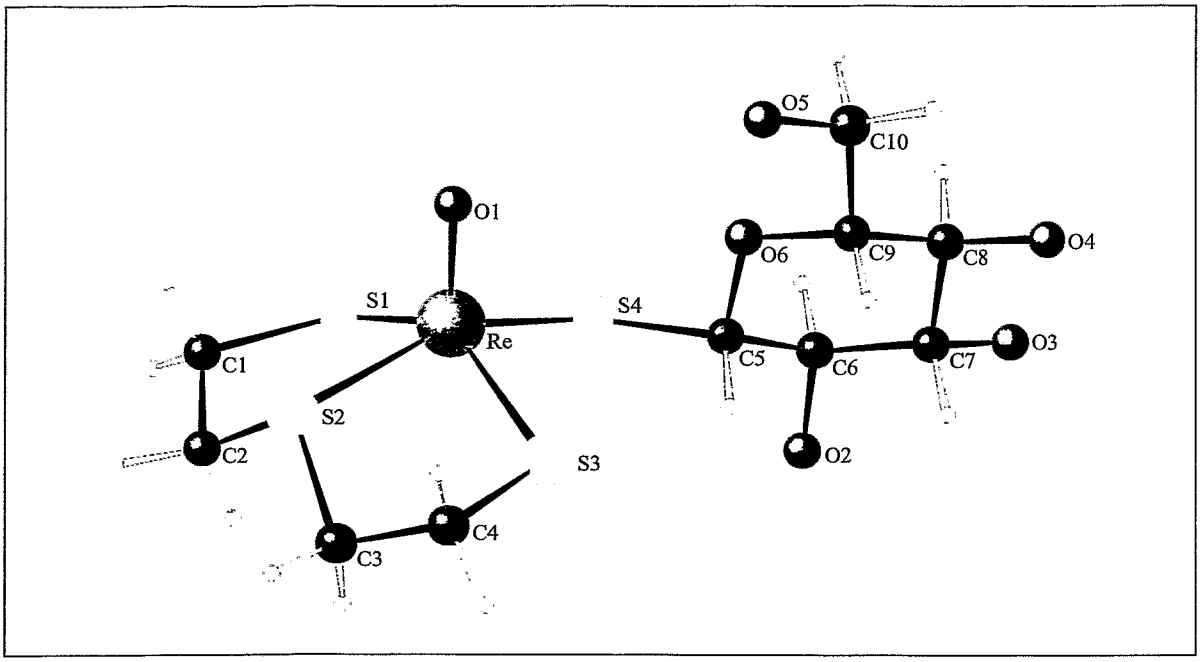
Selected Bonds (Å) and Angles (°)

Bonds

Re-O(1)	1.682
Re-S(4)	2.276
Re-S(2)	2.293
Re-S(1)	2.348
Re-S(3)	2.351
S(1)-C(3)	1.808
S(1)-C(1)	1.814
S(2)-C(2)	1.818
S(3)-C(5)	1.790
S(4)-C(4)	1.817
O(2)-C(5)	1.192
C(1)-C(2)	1.489
C(1)-H(1A)	0.970
C(1)-H(1B)	0.970
C(2)-H(2A)	0.970
C(2)-H(2B)	0.970
C(3)-C(4)	1.476
C(3)-H(3A)	0.970
C(3)-H(3B)	0.970
C(4)-H(4A)	0.970
C(4)-H(4B)	0.970
C(5)-C(6)	1.499

Angles

O(1)-Re-S(4)	115.90
O(1)-Re-S(2)	114.90
S(4)-Re-S(2)	129.17
O(1)-Re-S(1)	102.00
S(4)-Re-S(1)	83.65
S(2)-Re-S(1)	84.36
O(1)-Re-S(3)	103.80
S(4)-Re-S(3)	89.59
S(2)-Re-S(3)	80.36
S(1)-Re-S(3)	153.75
C(3)-S(1)-C(1)	103.70
C(3)-S(1)-Re	108.30
C(1)-S(1)-Re	106.80
C(2)-S(2)-Re	105.40
C(5)-S(3)-Re	108.20
C(4)-S(4)-Re	106.80
C(2)-C(1)-S(1)	106.90
C(2)-C(1)-H(1A)	110.30
S(1)-C(1)-H(1A)	110.30
C(2)-C(1)-H(1B)	110.30
S(1)-C(1)-H(1B)	110.30
H(1A)-C(1)-H(1B)	108.60



[(3-Thiapentane-1,5-dithiolato)(D-glucose-1-thiolato)]oxorhenium(V)

$C_{10}H_{18}O_6ReS_4$

8.2294Å	8.4879Å	23.2168Å	
90.0000°	90.0000°	90.0000°	V=1628.7Å^3
$P2_12_12_1$; 19	Z=4; F(000)=1028	ρ=2.180g/cm^3	R=2.0%
orthorhombic			

H. Spies, B. Johannsen
"Functionalization of Tc complexes to make them active *in vivo*"
Analyst 120 (1995) 775-777
CCDC 156801

Re 24

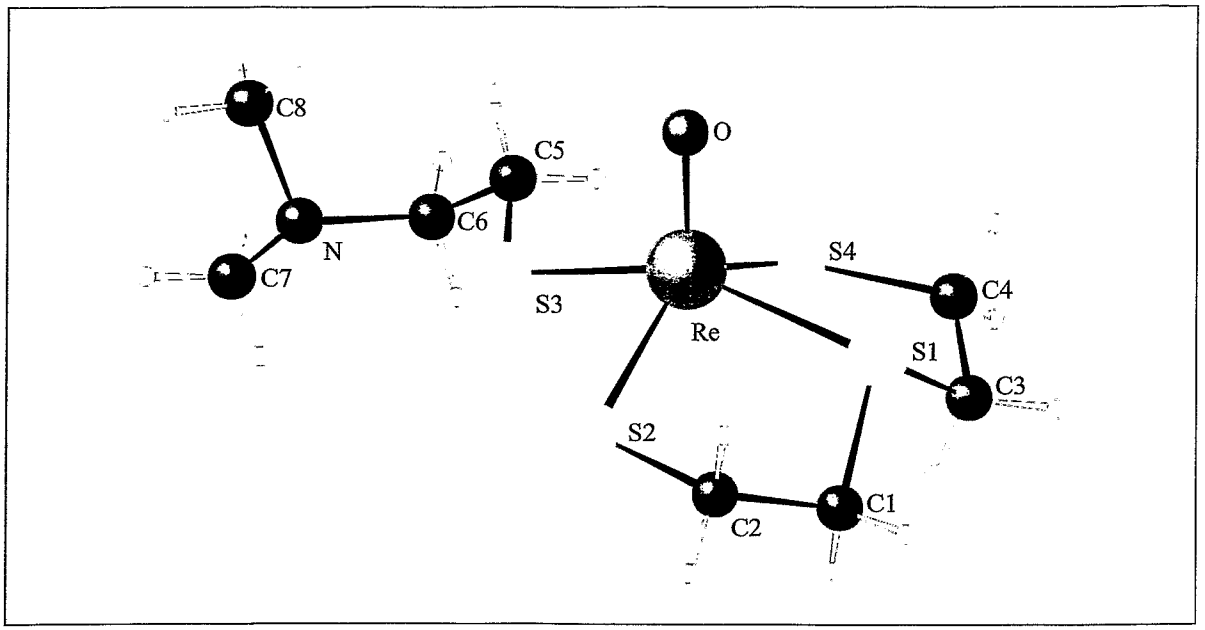
Selected Bonds (Å) and Angles (°)

Bonds

Re-O(1)	1.685
Re-S(3)	2.298
Re-S(1)	2.309
Re-S(4)	2.327
Re-S(2)	2.352
S(1)-C(1)	1.825
S(2)-C(3)	1.799
S(2)-C(2)	1.815
S(3)-C(4)	1.838
S(4)-C(5)	1.820
O(2)-C(6)	1.443
O(2)-H(2)	0.820
O(3)-C(7)	1.413
O(3)-H(3)	0.820
O(4)-C(8)	1.417
O(4)-H(4)	0.820
O(5)-C(10)	1.407
O(5)-H(5)	0.820
O(6)-C(5)	1.420
O(6)-C(9)	1.433
C(1)-C(2)	1.500
C(1)-H(1A)	0.970
C(1)-H(1B)	0.970
C(2)-H(2A)	0.970

Angles

O(1)-Re-S(3)	113.50
O(1)-Re-S(1)	112.30
S(3)-Re-S(1)	134.11
O(1)-Re-S(4)	107.40
S(3)-Re-S(4)	87.93
S(1)-Re-S(4)	81.29
O(1)-Re-S(2)	103.30
S(3)-Re-S(2)	83.19
S(1)-Re-S(2)	83.83
S(4)-Re-S(2)	149.05
C(1)-S(1)-Re	105.20
C(3)-S(2)-C(2)	104.70
C(3)-S(2)-Re	109.40
C(2)-S(2)-Re	107.90
C(4)-S(3)-Re	106.80
C(5)-S(4)-Re	109.70
C(6)-O(2)-H(2)	109.50
C(7)-O(3)-H(3)	109.50
C(8)-O(4)-H(4)	109.50
C(10)-O(5)-H(5)	109.50
C(5)-O(6)-C(9)	113.40
C(2)-C(1)-S(1)	111.70
C(2)-C(1)-H(1A)	109.30
S(1)-C(1)-H(1A)	109.30



[(N.N-dimethylamino)ethylthiolato](3-thiapentane-1,5-dithiolato)oxorhenium(V)

$C_8H_{18}NOReS_4$

10.6598Å	13.3647Å	10.5825Å	
90.0004°	111.3816°	90.0004°	V=1403.9Å^3
$P2_1/c$; 14	Z=4; F(000)=880	ρ=2.170g/cm^3	R=4.4%
monoclinic			

T. Fietz (1996)
not published
CCDC 156804

Re 25

Selected Bonds (Å) and Angles (°)

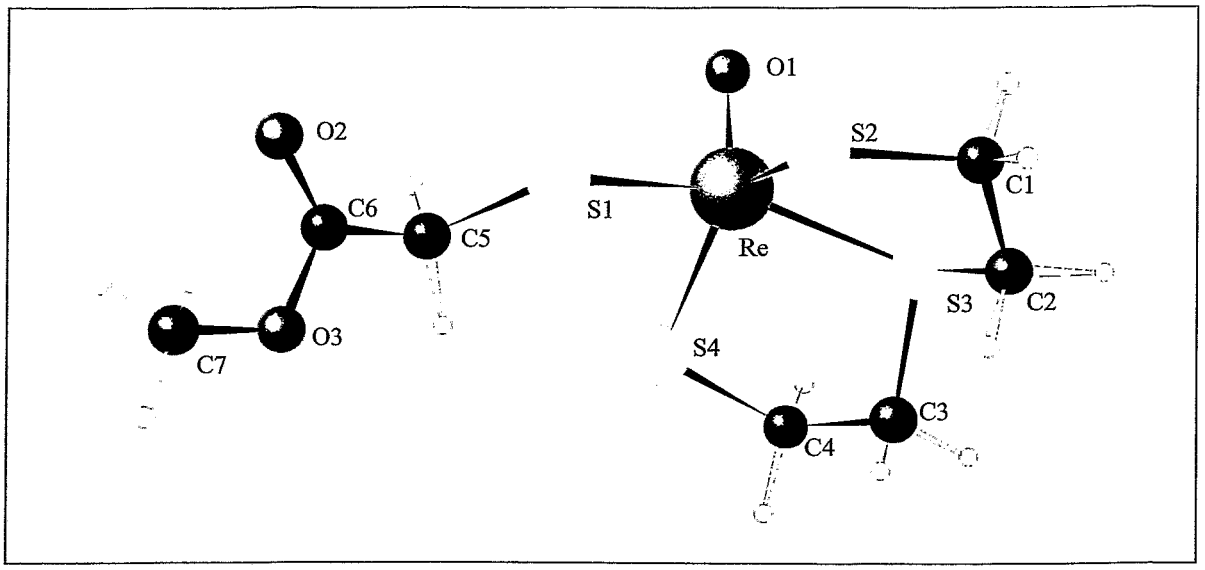
Bonds

Re-O	1.683
Re-S(4)	2.290
Re-S(2)	2.291
Re-S(3)	2.315
Re-S(1)	2.369
S(1)-C(3)	1.803
S(1)-C(1)	1.804
S(2)-C(2)	1.851
S(3)-C(5)	1.813
S(4)-C(4)	1.806
N-C(8)	1.422
N-C(7)	1.430
N-C(6)	1.469
C(1)-C(2)	1.496
C(1)-H(1A)	0.970
C(1)-H(1B)	0.970
C(2)-H(2A)	0.970
C(2)-H(2B)	0.970
C(3)-C(4)	1.485
C(3)-H(3A)	0.970
C(3)-H(3B)	0.970
C(4)-H(4A)	0.970
C(4)-H(4B)	0.970
C(5)-C(6)	1.468

Angles

O-Re-S(4)	115.40
O-Re-S(2)	114.40
S(4)-Re-S(2)	130.07
O-Re-S(3)	105.90
S(4)-Re-S(3)	88.50
S(2)-Re-S(3)	81.58
O-Re-S(1)	100.60
S(4)-Re-S(1)	83.62
S(2)-Re-S(1)	84.05
S(3)-Re-S(1)	153.21
C(3)-S(1)-C(1)	103.50
C(3)-S(1)-Re	106.70
C(1)-S(1)-Re	107.80
C(2)-S(2)-Re	104.90
C(5)-S(3)-Re	112.30
C(4)-S(4)-Re	107.20
C(8)-N-C(7)	108.80
C(8)-N-C(6)	112.50
C(7)-N-C(6)	109.30
C(2)-C(1)-S(1)	107.10
C(2)-C(1)-H(1A)	110.30
S(1)-C(1)-H(1A)	110.30
C(2)-C(1)-H(1B)	110.30
S(1)-C(1)-H(1B)	110.30

Re 26



(2-Carbmethoxymethylthiolato)(3-thiapentane-1,5-dithiolato)oxorhenium(V)

$C_7H_{13}O_3ReS_4$

18.7610Å	18.7570Å	7.4186Å	
90.0000°	90.0000°	90.0000°	V=2610.4Å^3
P42/n; 86	Z=8; F(000)=1744	ρ=2.339g/cm^3	R=2.1%
orthorhombic			

T. Fietz (1995)
not published
CCDC 159501

Re 26

Selected Bonds (Å) and Angles (°)

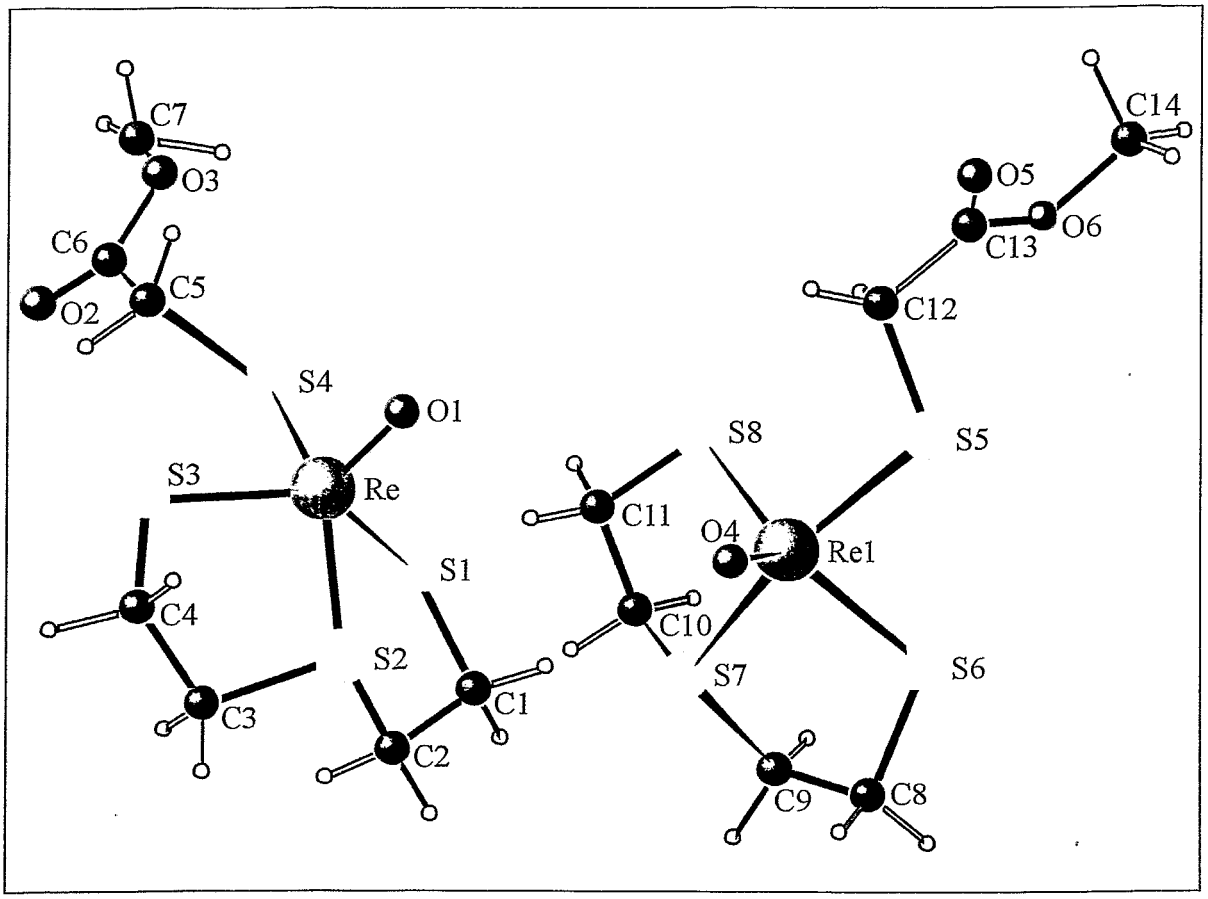
Bonds

Re(1)-O(1)	1.675
Re(1)-S(1)	2.294
Re(1)-S(3)	2.294
Re(1)-S(4)	2.301
Re(1)-S(2)	2.369
S(1)-C(1)	1.837
S(2)-C(2)	1.806
S(2)-C(3)	1.808
S(3)-C(4)	1.827
S(4)-C(5)	1.818
C(1)-C(2)	1.491
C(3)-C(4)	1.503
C(6)-O(2)	1.187
C(6)-O(3)	1.312
C(6)-C(5)	1.480
O(3)-C(7)	1.449

Angles

O(1)-Re(1)-S(1)	114.90
O(1)-Re(1)-S(3)	113.40
S(1)-Re(1)-S(3)	131.56
O(1)-Re(1)-S(4)	105.31
S(1)-Re(1)-S(4)	88.84
S(3)-Re(1)-S(4)	81.28
O(1)-Re(1)-S(2)	101.35
S(1)-Re(1)-S(2)	83.92
S(3)-Re(1)-S(2)	84.18
S(4)-Re(1)-S(2)	152.97
C(1)-S(1)-Re(1)	106.70
C(2)-S(2)-C(3)	104.30
C(2)-S(2)-Re(1)	106.40
C(3)-S(2)-Re(1)	107.30
C(4)-S(3)-Re(1)	104.70
C(5)-S(4)-Re(1)	113.10

Re26a



(Carbmethoxymethylthiolato)(3-thiapentane-1,5-dithiolato)oxorhenium(V)

$C_7H_{13}O_3ReS_4$

7.634Å	18.898Å	17.867Å	
90.0000°	91.52°	90.0000°	V=2577.0Å^3
$P2_1/n$; 1014	Z=8; F(000)=1744	ρ=2.37g/cm^3	R=5.7%
monoclinic			

T. Fietz (1995)
not published
CCDC 159500

Re 26a

Selected Bonds (Å) and Angles (°)

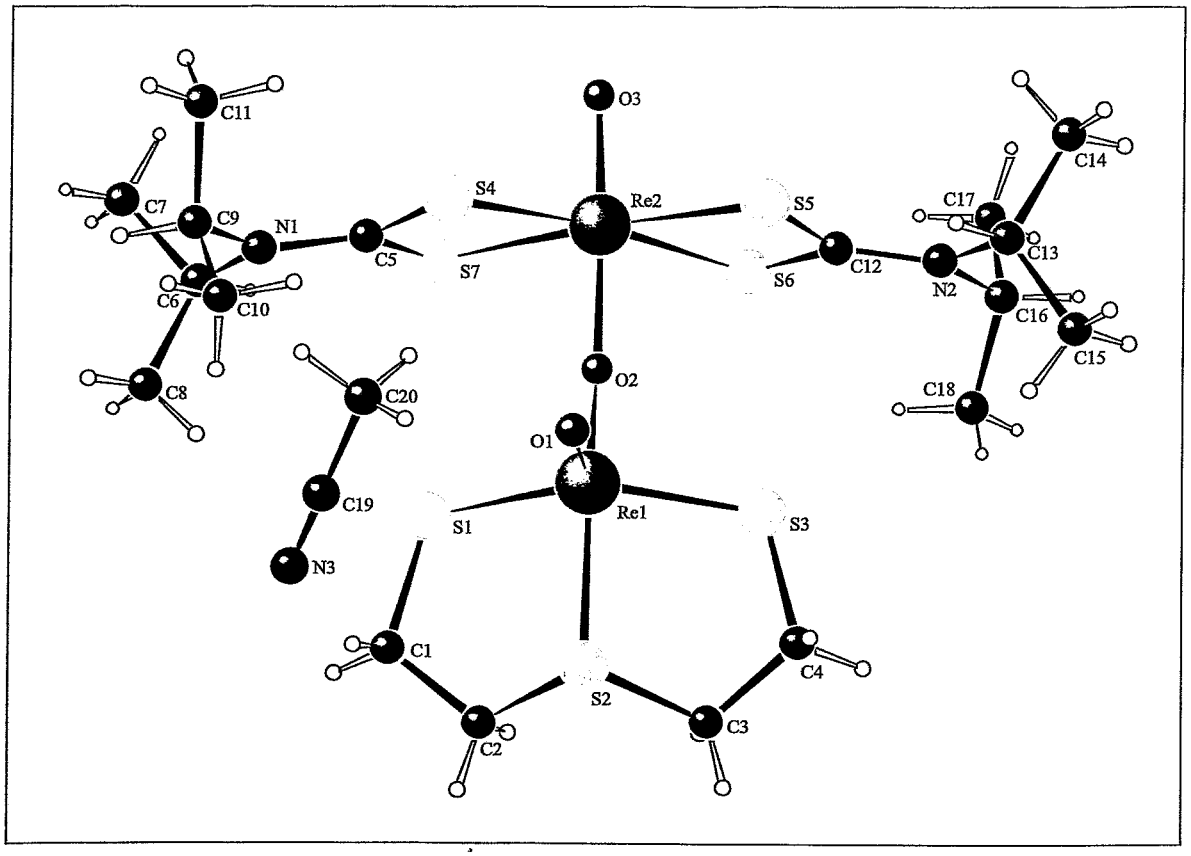
Bonds

Re-O(1)	1.656
Re-S(1)	2.260
Re-S(3)	2.284
Re-S(4)	2.288
Re-S(2)	2.340
Re(1)-O(4)	1.664
Re(1)-S(6)	2.258
Re(1)-S(8)	2.274
Re(1)-S(5)	2.298
Re(1)-S(7)	2.345
S(1)-C(1)	1.804
S(2)-C(2)	1.760
S(2)-C(3)	1.804
S(3)-C(4)	1.833
S(4)-C(5)	1.830
S(5)-C(12)	1.810
S(6)-C(8)	1.795
S(7)-C(9)	1.773
S(7)-C(10)	1.800
S(8)-C(11)	1.820
O(2)-C(6)	1.190
O(3)-C(6)	1.280
O(3)-C(7)	1.450
O(5)-C(13)	1.160
O(6)-C(13)	1.320
O(6)-C(14)	1.430
C(1)-C(2)	1.490
C(1)-H(1A)	0.970
C(1)-H(1B)	0.970
C(2)-H(2A)	0.970

Angles

O(1)-Re-S(1)	112.50
O(1)-Re-S(3)	115.40
S(1)-Re-S(3)	131.99
O(1)-Re-S(4)	106.60
S(1)-Re-S(4)	80.12
S(3)-Re-S(4)	89.38
O(1)-Re-S(2)	100.30
S(1)-Re-S(2)	85.12
S(3)-Re-S(2)	83.59
S(4)-Re-S(2)	152.71
O(4)-Re(1)-S(6)	114.10
O(4)-Re(1)-S(8)	114.90
S(6)-Re(1)-S(8)	130.82
O(4)-Re(1)-S(5)	106.70
S(6)-Re(1)-S(5)	79.91
S(8)-Re(1)-S(5)	89.58
O(4)-Re(1)-S(7)	100.50
S(6)-Re(1)-S(7)	85.01
S(8)-Re(1)-S(7)	82.95
S(5)-Re(1)-S(7)	152.41
C(1)-S(1)-Re	104.30
C(2)-S(2)-Re	105.60
C(3)-S(2)-Re	106.20
C(4)-S(3)-Re	107.70
C(5)-S(4)-Re	112.90
C(12)-S(5)-Re(1)	110.30
C(8)-S(6)-Re(1)	104.60
C(9)-S(7)-Re(1)	105.80
C(10)-S(7)-Re(1)	106.10
C(11)-S(8)-Re(1)	108.30

Re 26b



μ-Oxo-bis{[(N-diethyldithiocarbamato)oxorhenium(V)][(3-thiapentane-1,5-dithiolato)oxorhenium(V)]}
(acetonitrile adduct)

$C_{20}H_{39}N_3O_3Re_2S_7$

10.0242Å	13.7551Å	14.1497Å	
66.1200°	74.2350°	72.7680°	V=1678.0Å^3
P-1; 2	Z=2; F(000)=932	ρ=1.913g/cm^3	R=8.3%
triclinic			

H.-J. Pietzsch (2000)
not published
CCDC 159497

Re 26b

Selected Bonds (Å) and Angles (°)

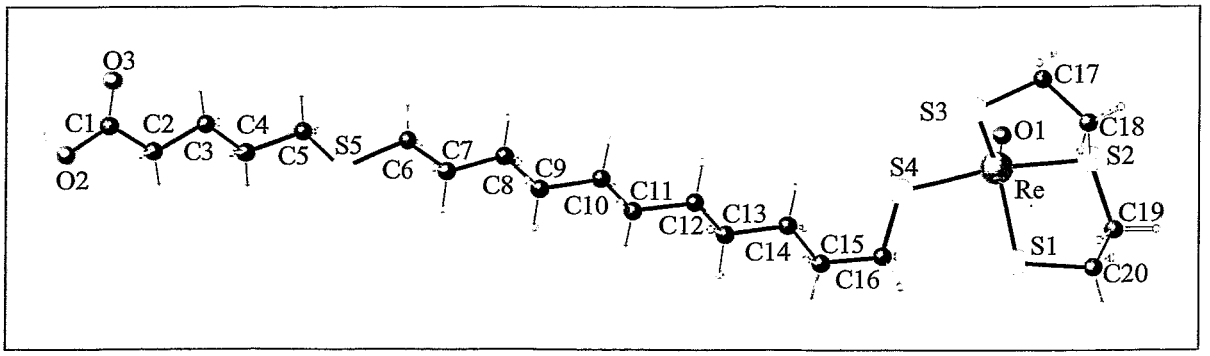
Bonds

Re(1)-O(1)	1.667
Re(1)-O(2)	1.941
Re(1)-S(3)	2.301
Re(1)-S(1)	2.312
Re(1)-S(2)	2.344
Re(2)-O(3)	1.695
Re(2)-O(2)	1.889
Re(2)-S(6)	2.444
Re(2)-S(4)	2.445
Re(2)-S(7)	2.450
Re(2)-S(5)	2.451
S(1)-C(1)	1.815
S(2)-C(3)	1.810
S(2)-C(2)	1.810
S(3)-C(4)	1.850
S(4)-C(5)	1.709
S(5)-C(12)	1.720
S(6)-C(12)	1.730
S(7)-C(5)	1.727
N(1)-C(5)	1.330
N(1)-C(9)	1.470
N(1)-C(6)	1.470
N(2)-C(12)	1.320
N(2)-C(13)	1.480
N(2)-C(16)	1.500
C(1)-C(2)	1.500
C(3)-C(4)	1.510
C(6)-C(7)	1.490
C(6)-C(8)	1.500
C(9)-C(10)	1.550
C(9)-C(11)	1.560
C(13)-C(15)	1.500
C(13)-C(14)	1.530
C(16)-C(18)	1.520

Angles

O(1)-Re(1)-O(2)	107.90
O(1)-Re(1)-S(3)	114.00
O(2)-Re(1)-S(3)	82.70
O(1)-Re(1)-S(1)	114.60
O(2)-Re(1)-S(1)	83.30
S(3)-Re(1)-S(1)	131.30
O(1)-Re(1)-S(2)	101.40
O(2)-Re(1)-S(2)	150.70
S(3)-Re(1)-S(2)	85.25
S(1)-Re(1)-S(2)	84.74
O(3)-Re(2)-O(2)	178.20
O(3)-Re(2)-S(6)	94.40
O(2)-Re(2)-S(6)	87.00
O(3)-Re(2)-S(4)	91.50
O(2)-Re(2)-S(4)	87.00
S(6)-Re(2)-S(4)	174.02
O(3)-Re(2)-S(7)	92.50
O(2)-Re(2)-S(7)	88.00
S(6)-Re(2)-S(7)	108.88
S(4)-Re(2)-S(7)	71.23
O(3)-Re(2)-S(5)	91.60
O(2)-Re(2)-S(5)	87.80
S(6)-Re(2)-S(5)	71.28
S(4)-Re(2)-S(5)	108.15
S(7)-Re(2)-S(5)	175.85
C(1)-S(1)-Re(1)	105.20
C(3)-S(2)-Re(1)	107.60
C(2)-S(2)-Re(1)	107.20
C(4)-S(3)-Re(1)	104.30
C(5)-S(4)-Re(2)	88.50
C(12)-S(5)-Re(2)	88.60
C(12)-S(6)-Re(2)	88.60
C(5)-S(7)-Re(2)	88.00
Re(2)-O(2)-Re(1)	154.50

Re 27



(15-Carboxy-12-thiahexadecanethiolato)(3-thiapentane-1,5-dithiolato)oxorhenium(V)

$C_{20}H_{39}O_3ReS_5$

9.0585Å	13.1617Å	45.3602Å	
90.0000°	90.0000°	90.0000°	V=5408.1Å^3
Pbca; 61	Z=8; F(000)=2704	ρ=1.656g/cm^3	R=3.7%
orthorhombic			

C. Jung (2000)
not published
CCDC 156312

Re 27

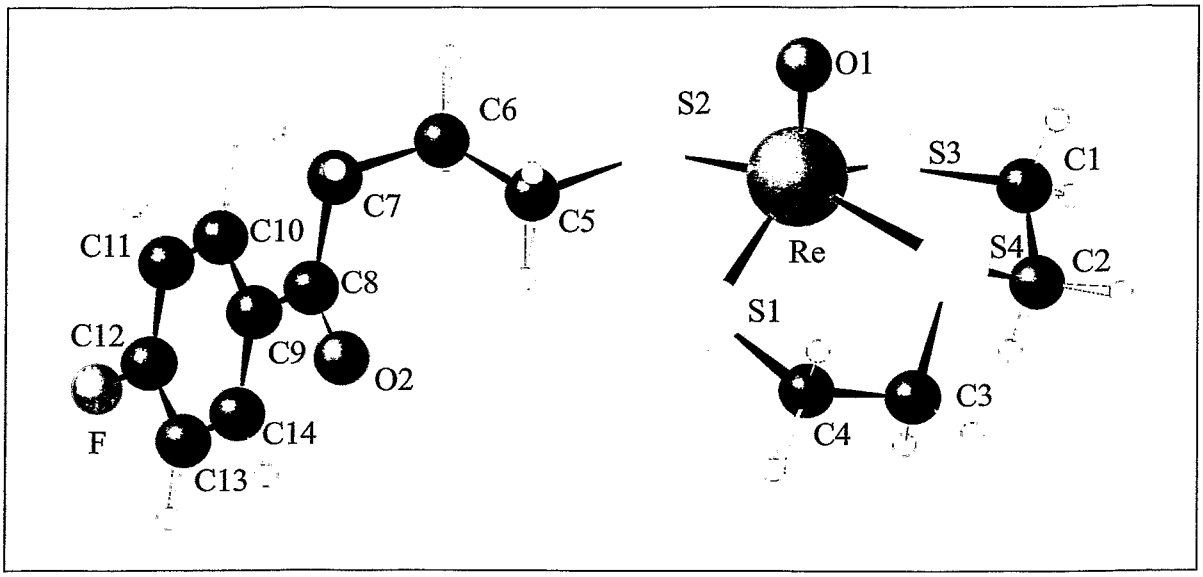
Selected Bonds (Å) and Angles (°)

Bonds

Re(1)-O(1)	1.684
Re(1)-S(3)	2.293
Re(1)-S(4)	2.301
Re(1)-S(1)	2.303
Re(1)-S(2)	2.377
S(1)-C(20)	1.821
S(2)-C(18)	1.790
S(2)-C(19)	1.810
S(3)-C(17)	1.840
S(4)-C(16)	1.831
S(5)-C(5)	1.779
S(5)-C(6)	1.791
C(20)-C(19)	1.530
C(18)-C(17)	1.460
C(16)-C(15)	1.510
C(15)-C(14)	1.500
C(14)-C(13)	1.520
C(13)-C(12)	1.500
C(12)-C(11)	1.510
C(11)-C(10)	1.500
C(10)-C(9)	1.530
C(9)-C(8)	1.500
C(8)-C(7)	1.480
C(7)-C(6)	1.520
C(5)-C(4)	1.500

Angles

O(1)-Re(1)-S(3)	115.70
O(1)-Re(1)-S(4)	106.60
S(3)-Re(1)-S(4)	81.05
O(1)-Re(1)-S(1)	114.20
S(3)-Re(1)-S(1)	129.88
S(4)-Re(1)-S(1)	88.76
O(1)-Re(1)-S(2)	100.30
S(3)-Re(1)-S(2)	83.41
S(4)-Re(1)-S(2)	152.78
S(1)-Re(1)-S(2)	84.22
C(20)-S(1)-Re(1)	106.50
C(18)-S(2)-C(19)	103.00
C(18)-S(2)-Re(1)	107.80
C(19)-S(2)-Re(1)	106.40
C(17)-S(3)-Re(1)	105.90
C(16)-S(4)-Re(1)	113.00
C(5)-S(5)-C(6)	105.30
C(19)-C(20)-S(1)	110.30
C(20)-C(19)-S(2)	107.40
C(17)-C(18)-S(2)	108.60
C(18)-C(17)-S(3)	111.40
C(15)-C(16)-S(4)	110.10
C(14)-C(15)-C(16)	115.40
C(15)-C(14)-C(13)	113.90
C(12)-C(13)-C(14)	116.10



(4-Fluorophenyl-1-oxobutan-4-thiolato)(3-thiapentane-1,5-dithiolato)oxorhenium(V)

$C_{14}H_{18}FO_2ReS_4$

7.2533Å	9.8473Å	12.5172Å	
87.4720°	79.8020°	84.6030°	V=875.7Å
P-1; 2	Z=2; F(000)=660	ρ=2.092g/cm^3	R=3.4%
triclinic			

H. Spies, P. Leibnitz, St. Noll, B. Noll
"Technetium-and rhenium complexes derived from spiperone II. X-ray crystal structure of (4-fluorophenyl-1-oxobutane-4-thiolato)(3-thiapentane-1.5-dithiolato)(oxorhenium(V)"
FZR-32 (1993) 40-42
CCDC 156799

Selected Bonds (Å) and Angles (°)

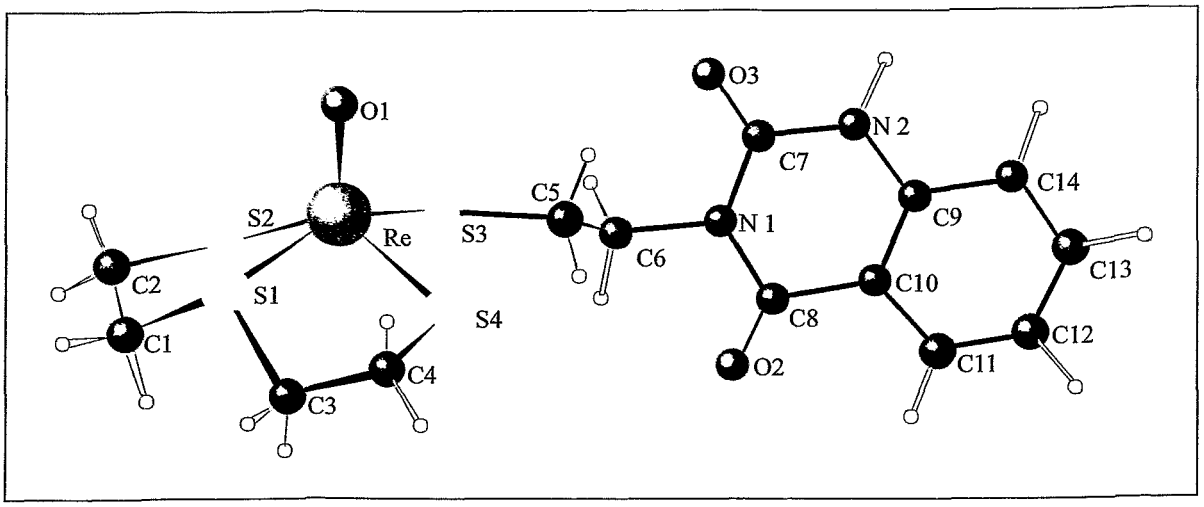
Bonds

Re-O(1)	1.683
Re-S(1)	2.287
Re-S(3)	2.296
Re-S(2)	2.303
Re-S(4)	2.372
S(1)-C(4)	1.826
S(2)-C(5)	1.831
S(3)-C(1)	1.824
S(4)-C(2)	1.813
S(4)-C(3)	1.822
F-C(12)	1.355
O(2)-C(8)	1.216
C(1)-C(2)	1.512
C(3)-C(4)	1.501
C(5)-C(6)	1.513
C(6)-C(7)	1.534
C(7)-C(8)	1.498
C(8)-C(9)	1.487
C(9)-C(10)	1.390
C(9)-C(14)	1.394
C(10)-C(11)	1.376
C(11)-C(12)	1.370
C(12)-C(13)	1.373
C(13)-C(14)	1.381

Angles

O(1)-Re-S(1)	114.80
O(1)-Re-S(3)	114.90
S(1)-Re-S(3)	130.15
O(1)-Re-S(2)	105.50
S(1)-Re-S(2)	88.09
S(3)-Re-S(2)	82.21
O(1)-Re-S(4)	100.30
S(1)-Re-S(4)	84.06
S(3)-Re-S(4)	84.08
S(2)-Re-S(4)	154.04
C(4)-S(1)-Re	107.40
C(5)-S(2)-Re	111.40
C(1)-S(3)-Re	105.70
C(2)-S(4)-C(3)	104.20
C(2)-S(4)-Re	107.30
C(3)-S(4)-Re	106.90
C(2)-C(1)-S(3)	110.30
C(1)-C(2)-S(4)	107.70
C(4)-C(3)-S(4)	107.70
C(3)-C(4)-S(1)	111.40
C(6)-C(5)-S(2)	109.80
C(5)-C(6)-C(7)	112.10
C(8)-C(7)-C(6)	112.10
O(2)-C(8)-C(9)	119.20

Re 29



[2-(Chinazoline)ethylthiolato](3-thiapentane-1,5-dithiolato)oxorhenium(V)

$C_{13}H_{17}N_2O_3ReS_4$
(DMF adduct, the DMF molecule has been omitted for clarity.)

10.2290Å	7.0990Å	31.5730Å	
90.0000°	91.1710°	90.0000°	$V=2287.4Å^3$
$P2_1/n_1$; 14	Z=4; F(000)=1272	$\rho=1.884 g/cm^3$	R=6.6%
monoclinc			

H.-J. Pietzsch (1995)
not published
CCDC 156803

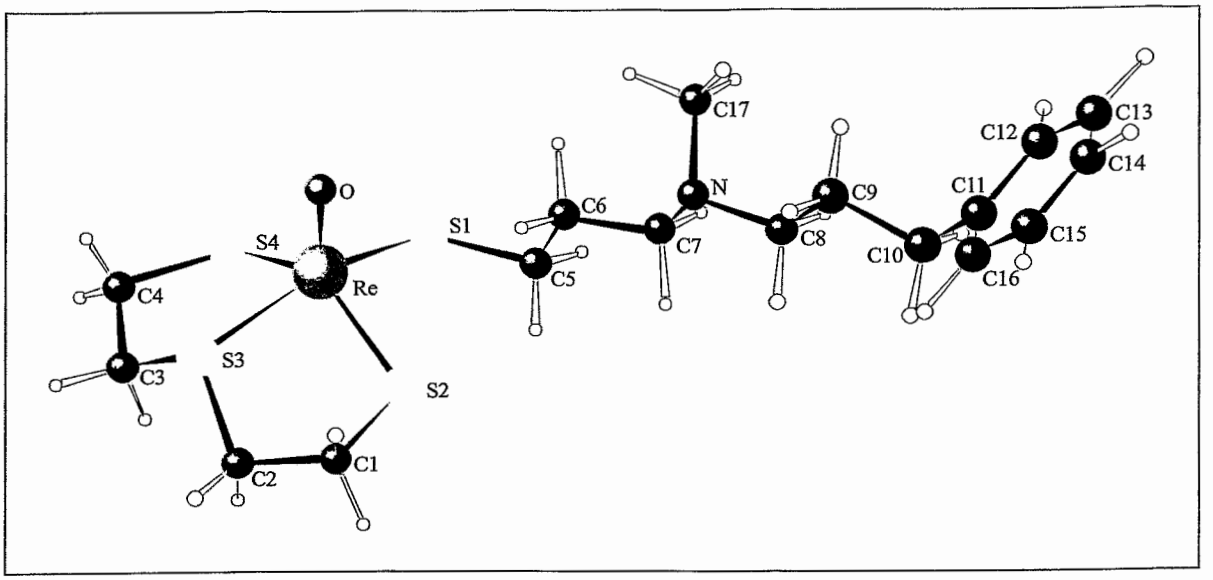
Selected Bonds (Å) and Angles (°)

Bonds

Re-O(1)	1.662
Re-S(4)	2.265
Re-S(2)	2.310
Re-S(3)	2.343
Re-S(1)	2.383
S(1)-C(3)	1.740
S(1)-C(1)	1.830
S(2)-C(2)	1.850
S(3)-C(5)	1.830
S(4)-C(4)	1.819
O(2)-C(8)	1.210
O(3)-C(7)	1.180
N(1)-C(8)	1.360
N(1)-C(7)	1.390
N(1)-C(6)	1.490
N(2)-C(7)	1.360
N(2)-C(9)	1.390
N(2)-H(2)	0.860
C(1)-C(2)	1.470
C(1)-H(1A)	0.970
C(1)-H(1B)	0.970
C(2)-H(2A)	0.970
C(2)-H(2B)	0.970
C(3)-C(4)	1.480
C(3)-H(3A)	0.970
C(3)-H(3B)	0.970
C(4)-H(4A)	0.970
C(4)-H(4B)	0.970
C(5)-C(6)	1.550
C(5)-H(5A)	0.970
C(5)-H(5B)	0.970
C(6)-H(6A)	0.970
C(6)-H(6B)	0.970
C(8)-C(10)	1.430
C(9)-C(10)	1.360

Angles

O(1)-Re-S(4)	113.00
O(1)-Re-S(2)	114.90
S(4)-Re-S(2)	131.90
O(1)-Re-S(3)	107.90
S(4)-Re-S(3)	88.30
S(2)-Re-S(3)	81.20
O(1)-Re-S(1)	98.70
S(4)-Re-S(1)	85.40
S(2)-Re-S(1)	83.70
S(3)-Re-S(1)	153.00
C(3)-S(1)-C(1)	105.60
C(3)-S(1)-Re	104.20
C(1)-S(1)-Re	107.40
C(2)-S(2)-Re	105.00
C(5)-S(3)-Re	112.80
C(4)-S(4)-Re	105.50
C(8)-N(1)-C(7)	122.40
C(8)-N(1)-C(6)	120.80
C(7)-N(1)-C(6)	116.80
C(7)-N(2)-C(9)	124.20
C(7)-N(2)-H(2)	117.90
C(9)-N(2)-H(2)	117.90
C(2)-C(1)-S(1)	108.00
C(2)-C(1)-H(1A)	110.10
S(1)-C(1)-H(1A)	110.10
C(2)-C(1)-H(1B)	110.10
S(1)-C(1)-H(1B)	110.10
H(1A)-C(1)-H(1B)	108.40
C(1)-C(2)-S(2)	110.80
C(1)-C(2)-H(2A)	109.50
S(2)-C(2)-H(2A)	109.50
C(1)-C(2)-H(2B)	109.50
S(2)-C(2)-H(2B)	109.50
H(2A)-C(2)-H(2B)	108.10
C(4)-C(3)-S(1)	110.50



{3-[N-(3-phenylpropyl)-N-methylamino]propane-thiolato}(3-thiapentane-1,5-dithiolato)oxorhenium(V)

$C_{17}H_{28}NOReS_4$

8.7148Å	9.2865Å	14.9298Å	
88.3089°	81.1704°	65.3270°	V=1084.2Å^3
P-1; 2	Z=2; F(000)=568;	ρ=1.767g/cm^3	R=4.2%
triclinic			

T. Fietz; H.-J. Pietzsch (1995)
not published
CSD 404673

Re 30

Selected Bonds (Å) and Angles (°)

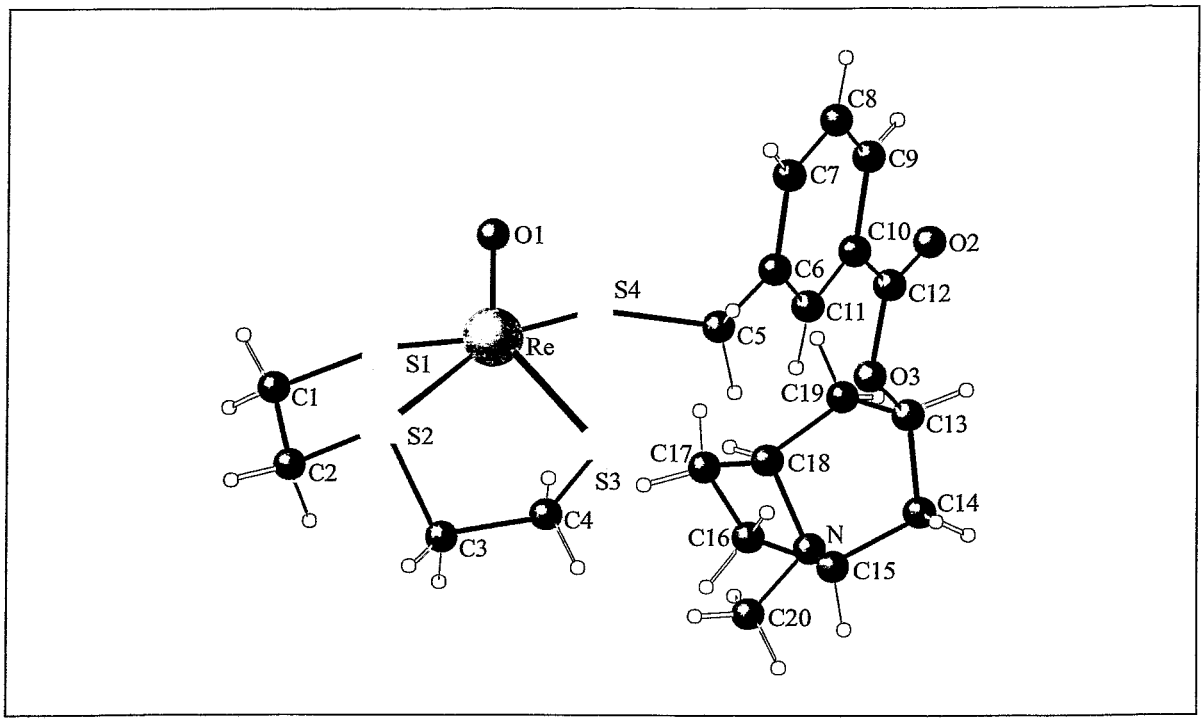
Bonds

Re-O	1.672
Re-S(2)	2.285
Re-S(4)	2.291
Re-S(1)	2.316
Re-S(3)	2.376
S(1)-C(5)	1.810
S(2)-C(1)	1.825
S(3)-C(3)	1.797
S(3)-C(2)	1.816
S(4)-C(4)	1.827
N-C(17)	1.443
N-C(7)	1.450
N-C(8)	1.458
C(1)-C(2)	1.508
C(1)-H(1A)	0.970
C(1)-H(1B)	0.970
C(2)-H(2A)	0.970
C(2)-H(2B)	0.970
C(3)-C(4)	1.479
C(3)-H(3A)	0.970
C(3)-H(3B)	0.970
C(4)-H(4A)	0.970
C(4)-H(4B)	0.970

Angles

O-Re-S(2)	114.70
O-Re-S(4)	115.20
S(2)-Re-S(4)	129.99
O-Re-S(1)	105.30
S(2)-Re-S(1)	88.64
S(4)-Re-S(1)	81.50
O-Re-S(3)	100.50
S(2)-Re-S(3)	84.04
S(4)-Re-S(3)	84.17
S(1)-Re-S(3)	153.93
C(5)-S(1)-Re	111.30
C(1)-S(2)-Re	106.50
C(3)-S(3)-C(2)	103.60
C(3)-S(3)-Re	106.50
C(2)-S(3)-Re	108.00
C(4)-S(4)-Re	106.20
C(17)-N-C(7)	110.40
C(17)-N-C(8)	110.10
C(7)-N-C(8)	106.90
C(2)-C(1)-S(2)	112.40
C(2)-C(1)-H(1A)	109.10
S(2)-C(1)-H(1A)	109.10
C(2)-C(1)-H(1B)	109.10

Re 31



(3-Thiapentane-1,5-dithiolato)(3-thiolatomethyl benzoic acid trop-3α-yl ester)oxorhenium(V)

$C_{20}H_{28}NO_3ReS_4$

11.3740Å	17.9450Å	12.0680Å	
90.0000°	106.9200°	90.0000°	V=2356.5Å^3
P12_1/c1; 14	Z=4; F(000)=1272	ρ=1.817g/cm^3	R=2.6%
monoclinic			

A. Hoepping, P. Brust, R. Berger, P. Leibnitz, H. Spies, S. Machill, D. Scheller, B. Johannsen
"Novel rhenium complexes derived from α-tropanol as potential ligands for the dopamine transporter"
Bioorg.Med.Chem. 6 (1998) 1663-1672
CSD No. 407092

Re 31

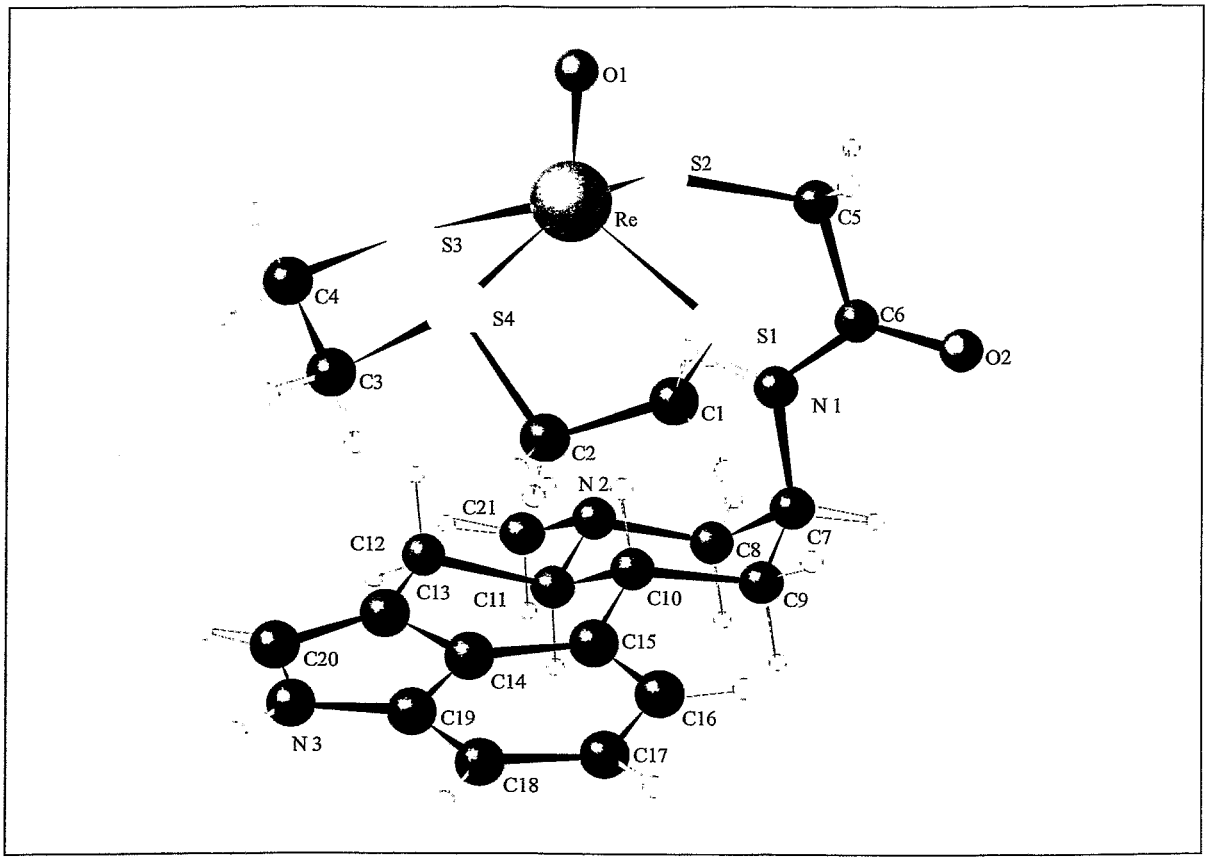
Selected Bonds (Å) and Angles (°)

Bonds

Re-O(1)	1.692
Re-S(3)	2.281
Re-S(1)	2.291
Re-S(4)	2.309
Re-S(2)	2.382
S(1)-C(1)	1.862
S(2)-C(2)	1.822
S(2)-C(3)	1.827
S(3)-C(4)	1.839
S(4)-C(5)	1.850
O(2)-C(12)	1.215
O(3)-C(12)	1.353
O(3)-C(13)	1.466
N(1)-C(20)	1.460
N(1)-C(15)	1.476
N(1)-C(18)	1.492
C(1)-C(2)	1.530
C(3)-C(4)	1.510
C(5)-C(6)	1.490
C(6)-C(7)	1.410

Angles

O(1)-Re-S(3)	115.20
O(1)-Re-S(1)	116.00
S(3)-Re-S(1)	128.75
O(1)-Re-S(4)	104.70
S(3)-Re-S(4)	87.87
S(1)-Re-S(4)	81.73
O(1)-Re-S(2)	101.20
S(3)-Re-S(2)	84.35
S(1)-Re-S(2)	83.74
S(4)-Re-S(2)	153.77
C(1)-S(1)-Re	106.70
C(2)-S(2)-C(3)	103.30
C(2)-S(2)-Re	108.00
C(3)-S(2)-Re	107.00
C(4)-S(3)-Re	107.30
C(5)-S(4)-Re	112.60
C(12)-O(3)-C(13)	116.10
C(20)-N(1)-C(15)	115.10
C(20)-N(1)-C(18)	112.70
C(15)-N(1)-C(18)	99.70



[N-(6-methyl-8α-ergolinyl) carbamoylmethylthiolato](3-thiapentane-1,5-dithiolato)oxorhenium(V)

$C_{21}H_{28}N_3O_2ReS_4$

9.2651Å	11.7824Å	11.2332Å	
90.0000°	94.2510°	90.0000°	V=1223.1Å^3
$P2_1$; 4	Z=2; F(000)=658	ρ=1.813g/cm^3	R=2.5%
monoclinic			

H. Spies, B. Noll, St. Noll, M. Findeisen, P. Leibnitz, P.E. Schulze, B. Johannsen
"Sythesis and molecular structure of a rhenium complex derived from 8α-amino-6-methyl-ergoline"
Chem.Ber. 130 (1997) 357-361
CSD No. 405989

Re 32

Selected Bonds (Å) and Angles (°)

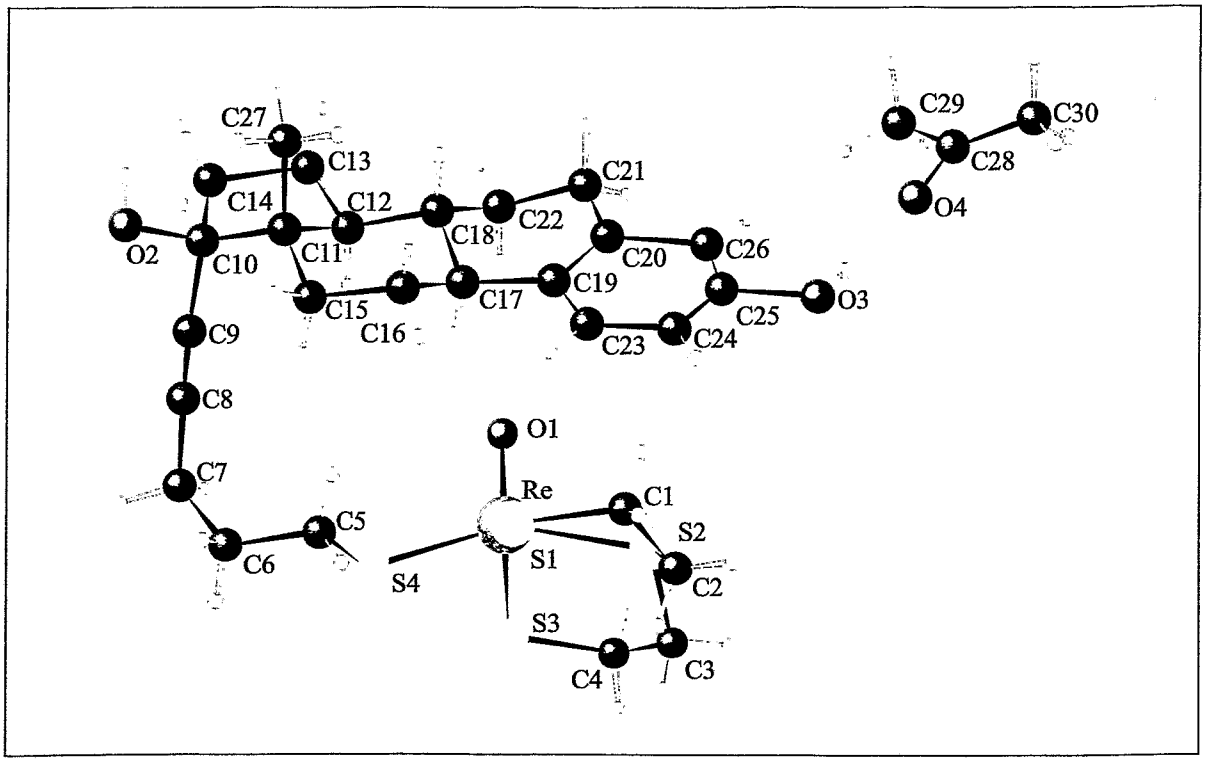
Bonds

Re-O(1)	1.659
Re-S(1)	2.282
Re-S(3)	2.299
Re-S(2)	2.315
Re-S(4)	2.364
S(1)-C(1)	1.829
S(2)-C(5)	1.815
S(3)-C(4)	1.819
S(4)-C(2)	1.801
S(4)-C(3)	1.829
O(2)-C(6)	1.243
N(1)-C(6)	1.322
N(1)-C(7)	1.447
N(2)-C(8)	1.451
N(2)-C(11)	1.461
N(2)-C(21)	1.480
N(3)-C(19)	1.379
N(3)-C(20)	1.377
C(1)-C(2)	1.490
C(3)-C(4)	1.500
C(5)-C(6)	1.505
C(7)-C(8)	1.507
C(7)-C(9)	1.518
C(9)-C(10)	1.509

Angles

O(1)-Re-S(1)	114.50
O(1)-Re-S(3)	115.60
S(1)-Re-S(3)	129.74
O(1)-Re-S(2)	105.50
S(1)-Re-S(2)	89.61
S(3)-Re-S(2)	80.82
O(1)-Re-S(4)	99.70
S(1)-Re-S(4)	84.48
S(3)-Re-S(4)	83.88
S(2)-Re-S(4)	154.36
C(1)-S(1)-Re	105.90
C(5)-S(2)-Re	114.50
C(4)-S(3)-Re	106.50
C(2)-S(4)-C(3)	103.00
C(2)-S(4)-Re	107.00
C(3)-S(4)-Re	107.00
C(6)-N(1)-C(7)	124.60
C(8)-N(2)-C(11)	111.90
C(8)-N(2)-C(21)	109.50
C(11)-N(2)-C(21)	111.30
C(19)-N(3)-C(20)	108.70
C(2)-C(1)-S(1)	111.40
C(1)-C(2)-S(4)	108.00
C(4)-C(3)-S(4)	107.20

Re 33



(3-Thiapentane-1,5-dithiolato)[17α-(5-thiolato-1-pentyn-1-yl)-estra-1,3,5(10)-triene-3,17α-diol]oxorhenium(V)
(acetone adduct)

$C_{27}H_{37}O_3ReS_4$

14.2049Å	12.0944Å	37.1033Å	
90.0000°	95.2350°	90.0000°	V=6347.7Å^3
$P2_1$; 4	Z=8; F(000)=3064	ρ=1.595g/cm^3	R=4.8%
monoclinic			

F. Wüst (1997)
not published
CCDC 156810

Re 33

Selected Bonds (Å) and Angles (°)

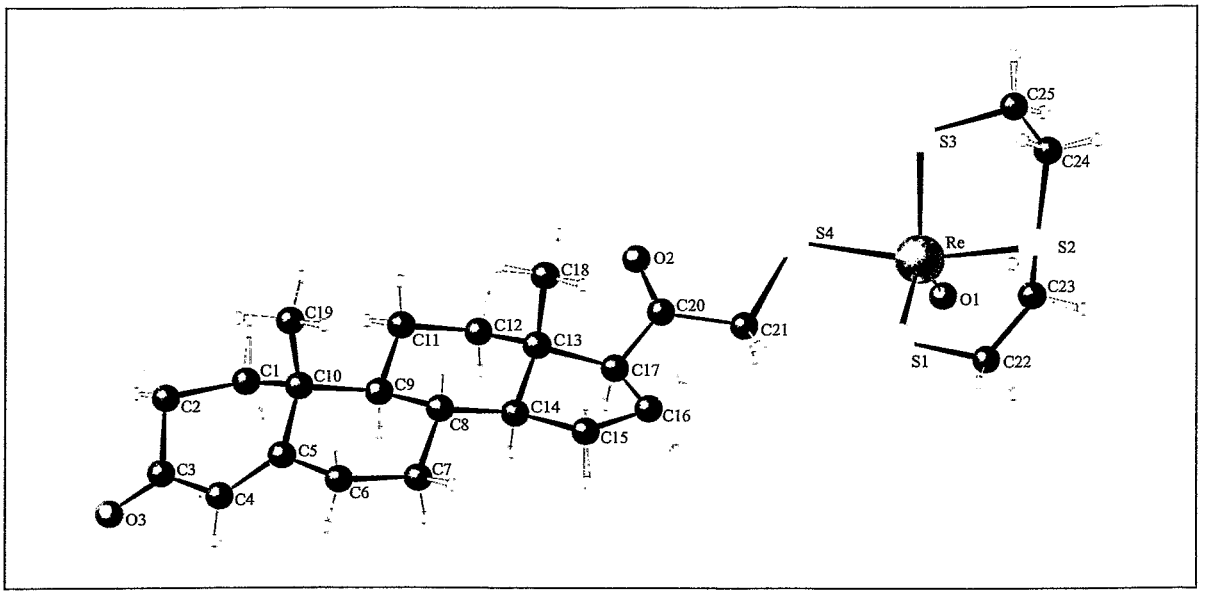
Bonds

Re(1)-O(101)	1.691
Re(1)-S(13)	2.296
Re(1)-S(11)	2.302
Re(1)-S(14)	2.308
Re(1)-S(12)	2.379
S(11)-C(104)	1.790
S(12)-C(101)	1.800
S(12)-C(103)	1.840
S(13)-C(102)	1.870
S(14)-C(105)	1.806
O(102)-C(110)	1.450
O(103)-C(125)	1.400
C(101)-C(102)	1.490
C(103)-C(104)	1.420
C(105)-C(106)	1.500
C(106)-C(107)	1.540
C(107)-C(108)	1.470
C(108)-C(109)	1.160
C(109)-C(110)	1.520
C(110)-C(111)	1.470
C(110)-C(114)	1.550
C(111)-C(127)	1.550
C(111)-C(115)	1.560
C(111)-C(112)	1.570

Angles

O(101)-Re(1)-S(13)	116.10
O(101)-Re(1)-S(11)	114.40
S(13)-Re(1)-S(11)	129.40
O(101)-Re(1)-S(14)	105.60
S(13)-Re(1)-S(14)	81.30
S(11)-Re(1)-S(14)	88.40
O(101)-Re(1)-S(12)	100.70
S(13)-Re(1)-S(12)	83.70
S(11)-Re(1)-S(12)	84.20
S(14)-Re(1)-S(12)	153.40
C(104)-S(11)-Re(1)	103.60
C(101)-S(12)-C(103)	105.60
C(101)-S(12)-Re(1)	107.80
C(103)-S(12)-Re(1)	104.30
C(102)-S(13)-Re(1)	107.10
C(105)-S(14)-Re(1)	113.40
C(102)-C(101)-S(12)	109.70
C(101)-C(102)-S(13)	110.20
C(104)-C(103)-S(12)	106.60
C(103)-C(104)-S(11)	111.80
C(106)-C(105)-S(14)	109.90
C(105)-C(106)-C(107)	114.20
C(108)-C(107)-C(106)	111.20
C(109)-C(108)-C(107)	173.00

Re 34



(4-Pregnene-20-dionyl-21-thiolato)(3-thiapentane-1,5-dithiolato)oxorhenium(V)

$C_{25}H_{37}O_3ReS_4$

10.9440Å	8.2060Å	30.3428Å	
90.0000°	97.2390°	90.0000°	V=2703.3Å
$P2_1$; 4	Z=4; F(000)=1400	ρ=1.720g/cm^3	R=5.0%
monoclinc			

F. Wüst, M.B. Skaddan, P. Leibnitz, H. Spies, J.A. Katzenellenbogen and B. Johannsen
"Synthesis of novel progestin-rhenium conjugates as potential ligands for the progesterone receptor"
Bioorg.Med.Chem. 7 (1999) 1827-1835
CCDC 114993

Re 34

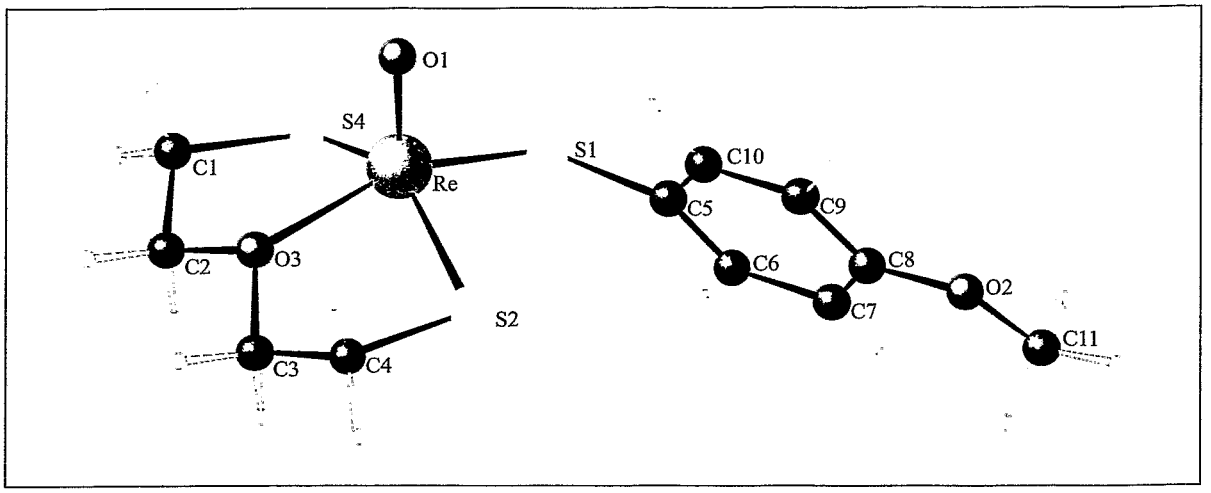
Selected Bonds (Å) and Angles (°)

Bonds

Re-O(1)	1.664
Re-S(1)	2.300
Re-S(4)	2.305
Re-S(3)	2.307
Re-S(2)	2.379
S(1)-C(22)	1.800
S(2)-C(24)	1.830
S(2)-C(23)	1.850
S(3)-C(25)	1.820
S(4)-C(21)	1.850
O(20)-C(20)	1.190
O(3)-C(3)	1.220
C(1)-C(10)	1.510
C(1)-C(2)	1.530
C(2)-C(3)	1.480
C(3)-C(4)	1.470
C(4)-C(5)	1.330
C(5)-C(6)	1.490
C(5)-C(10)	1.510
C(6)-C(7)	1.500
C(7)-C(8)	1.510
C(8)-C(14)	1.530
C(8)-C(9)	1.570
C(9)-C(10)	1.550
C(9)-C(11)	1.560
C(10)-C(19)	1.550
Re'-O(1')	1.693
Re'-S(1')	2.293
Re'-S(3')	2.295
Re'-S(4')	2.309
Re'-S(2')	2.375

Angles

O(1)-Re-S(1)	115.10
O(1)-Re-S(4)	105.00
S(1)-Re-S(4)	88.60
O(1)-Re-S(3)	115.10
S(1)-Re-S(3)	129.70
S(4)-Re-S(3)	81.20
O(1)-Re-S(2)	101.40
S(1)-Re-S(2)	83.30
S(4)-Re-S(2)	153.40
S(3)-Re-S(2)	84.50
C(22)-S(1)-Re	107.20
C(24)-S(2)-C(23)	103.60
C(24)-S(2)-Re	106.60
C(23)-S(2)-Re	107.20
C(25)-S(3)-Re	106.00
C(21)-S(4)-Re	110.90
O(1')-Re'-S(1')	114.90
O(1')-Re'-S(3')	115.40
S(1')-Re'-S(3')	129.50
O(1')-Re'-S(4')	106.80
S(1')-Re'-S(4')	81.80
S(3')-Re'-S(4')	87.50
O(1')-Re'-S(2')	99.70
S(1')-Re'-S(2')	84.20
S(3')-Re'-S(2')	84.10
S(4')-Re'-S(2')	153.30
C(22')-S(1')-Re'	106.50
C(23')-S(2')-Re'	106.00
C(24')-S(2')-Re'	107.60
C(25')-S(3')-Re'	105.80
C(21')-S(4')-Re'	113.00



(3-Oxapentane-1,5-dithiolato)(4-methoxybenzenethiolato)oxorhenium(V)

$C_{11}H_{15}O_3ReS_3$

7.5144Å	14.7674Å	13.9622Å	
90.0000°	103.7020°	90.0000°	V=1476.1Å^3
$P2_1/c$; 14	Z=4; F(000)=912	ρ=2.150g/cm^3	R=2.5%
monoclinc			

H. Spies, T. Fietz, H.-J. Pietzsch, B. Johannsen, P. Leibnitz, G. Reck, D. Scheller and K. Klostermann
"Neutral oxorhenium (V) complexes with tridentate dithiol ligands and monodentate alkyl/aryl thiols as co-ligands"
J.Chem.Soc.Dalton Trans. (1995) 2277-2280
CSD No. 401649

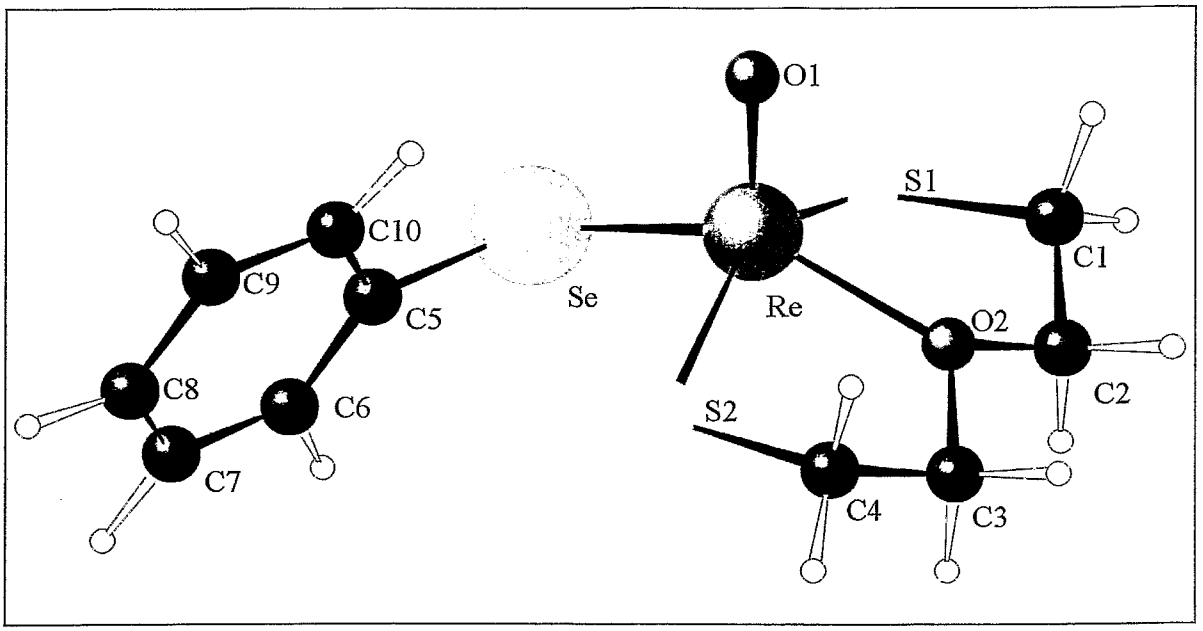
Selected Bonds (Å) and Angles (°)

Bonds

Re-O(1)	1.660
Re-O(3)	2.102
Re-S(1)	2.267
Re-S(2)	2.277
Re-S(4)	2.292
S(1)-C(5)	1.782
S(2)-C(4)	1.826
S(4)-C(1)	1.811
O(2)-C(8)	1.375
O(2)-C(11)	1.402
O(3)-C(2)	1.456
O(3)-C(3)	1.471
C(1)-C(2)	1.493
C(1)-H(1A)	0.970
C(1)-H(1B)	0.970
C(2)-H(2A)	0.970
C(2)-H(2B)	0.970
C(3)-C(4)	1.468
C(3)-H(3A)	0.970
C(3)-H(3B)	0.970
C(4)-H(4A)	0.970
C(4)-H(4B)	0.970
C(5)-C(10)	1.370

Angles

O(1)-Re-O(3)	107.10
O(1)-Re-S(1)	105.70
O(3)-Re-S(1)	146.84
O(1)-Re-S(2)	111.40
O(3)-Re-S(2)	81.23
S(1)-Re-S(2)	91.01
O(1)-Re-S(4)	111.60
O(3)-Re-S(4)	80.16
S(1)-Re-S(4)	83.80
S(2)-Re-S(4)	136.50
C(5)-S(1)-Re	114.30
C(4)-S(2)-Re	99.00
C(1)-S(4)-Re	99.20
C(8)-O(2)-C(11)	118.40
C(2)-O(3)-C(3)	109.70
C(2)-O(3)-Re	121.70
C(3)-O(3)-Re	121.10
C(2)-C(1)-S(4)	107.90
C(2)-C(1)-H(1A)	110.10
S(4)-C(1)-H(1A)	110.10
C(2)-C(1)-H(1B)	110.10
S(4)-C(1)-H(1B)	110.10
H(1A)-C(1)-H(1B)	108.40



(Benzeneselenolato)(3-oxapentane-1,5-dithiolato)oxorhenium(V)

$C_{10}H_{13}O_2ReS_2Se$

18.1224Å	12.6683Å	12.0088Å	
90.0000°	90.0000°	90.0000°	$V=2756.9Å^3$
Pbca; 61	Z=8; F(000)=1840	$\rho=2.383 g/cm^3$	R=6.4%
orthorhombic			

T.Fietz, H. Spies, P. Leibnitz and D. Scheller
"Mixed-ligand oxorhenium (V) complexes with rhenium-selenium Bonds. Molecular structure of (Benzeneselenolato)(3-oxapentane-1,5-dithiolato)-oxorhenium(V)"
J.Coord.Chem. 38 (1996) 227-235
CCDC 156800

Re 36

Selected Bonds (Å) and Angles (°)

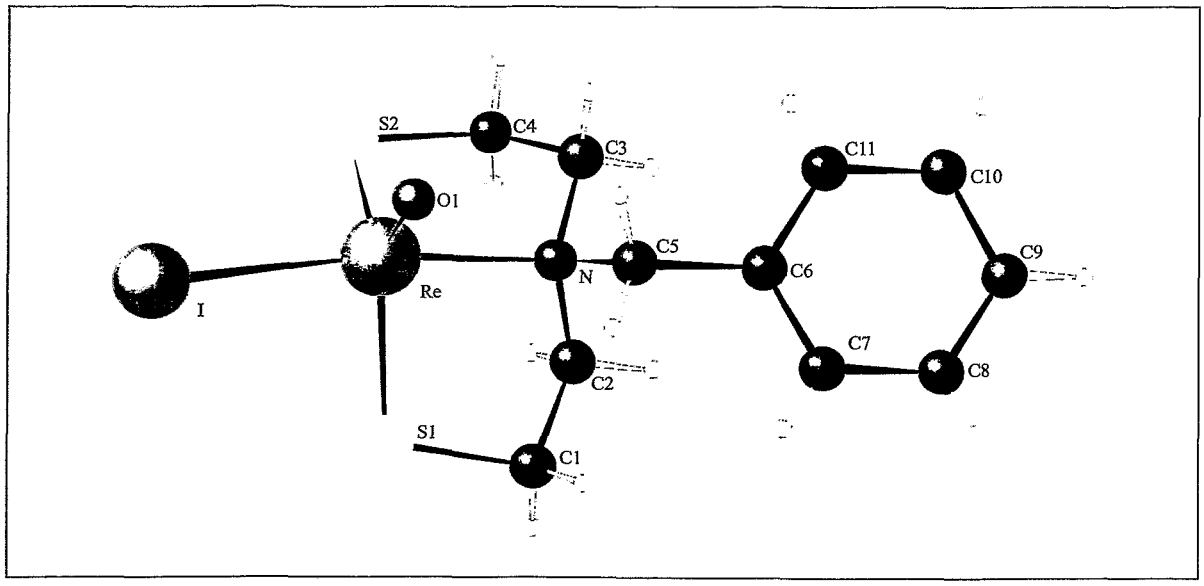
Bonds

Re-O(1)	1.662
Re-O(2)	2.123
Re-S(2)	2.270
Re-S(1)	2.285
Re-Se	2.411
Se-C(5)	1.860
S(1)-C(1)	1.820
S(2)-C(4)	1.850
O(2)-C(2)	1.420
O(2)-C(3)	1.450
C(1)-C(2)	1.510
C(3)-C(4)	1.510
C(5)-C(6)	1.340
C(5)-C(10)	1.410
C(6)-C(7)	1.410
C(7)-C(8)	1.350
C(8)-C(9)	1.360
C(9)-C(10)	1.420

Angles

O(1)-Re-O(2)	110.40
O(1)-Re-S(2)	110.70
O(2)-Re-S(2)	81.00
O(1)-Re-S(1)	109.30
O(2)-Re-S(1)	79.80
S(2)-Re-S(1)	139.50
O(1)-Re-Se	105.20
O(2)-Re-Se	144.20
S(2)-Re-Se	90.30
S(1)-Re-Se	84.92
C(5)-Se-Re	109.40
C(1)-S(1)-Re	99.20
C(4)-S(2)-Re	98.40
C(2)-O(2)-C(3)	112.00
C(2)-O(2)-Re	122.20
C(3)-O(2)-Re	122.10
C(2)-C(1)-S(1)	108.00
O(2)-C(2)-C(1)	110.00

Re 37



(3-Benzyl-azapentane-1,5-dithiolato)iodooxorhenium(V)

$C_{11}H_{15}INOReS_2$

7.6495Å	9.5225Å	10.7170Å	
90.2481°	109.6941°	91.8771°	V=734.5Å^3
P1; 2	Z=2; F(000)=512	ρ=2.507g/cm^3	R=4.0%
triclinic			

T. Fietz, P. Leibnitz, H. Spies, B. Johannsen
"Sythesis and reactions of new oxorhenium (V) complexes with Re-halogen Bonds. X-ray crystal structure of [3-benzyl-azapentane-1,5-dithiolato)iodo-oxorhenium(V)"
Polyhedron 18 (1999) 1793-1797
CSD No. 408902

Re 37

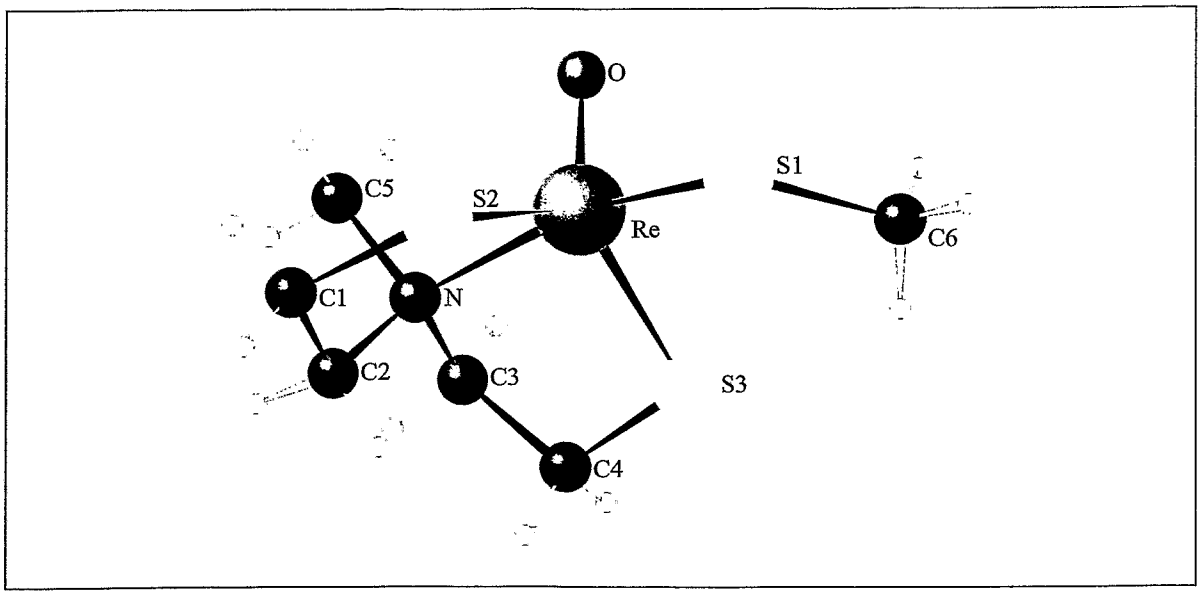
Selected Bonds (Å) and Angles (°)

Bonds

Re(1)-O(1)	1.672
Re(1)-N(1)	2.170
Re(1)-S(1)	2.264
Re(1)-S(2)	2.269
Re(1)-I(1)	2.694
S(1)-C(1)	1.825
S(2)-C(4)	1.845
N(1)-C(2)	1.505
N(1)-C(3)	1.517
N(1)-C(5)	1.523
C(1)-C(2)	1.517
C(3)-C(4)	1.490
C(5)-C(6)	1.519
C(6)-C(7)	1.374
C(6)-C(11)	1.382
C(7)-C(8)	1.380
C(8)-C(9)	1.360
C(9)-C(10)	1.380
C(10)-C(11)	1.380

Angles

O(1)-Re(1)-N(1)	96.20
O(1)-Re(1)-S(1)	119.80
N(1)-Re(1)-S(1)	84.50
O(1)-Re(1)-S(2)	119.40
N(1)-Re(1)-S(2)	84.80
S(1)-Re(1)-S(2)	120.58
O(1)-Re(1)-I(1)	99.60
N(1)-Re(1)-I(1)	164.20
S(1)-Re(1)-I(1)	86.55
S(2)-Re(1)-I(1)	88.62
C(1)-S(1)-Re(1)	102.80
C(4)-S(2)-Re(1)	102.90
C(2)-N(1)-C(3)	108.50
C(2)-N(1)-C(5)	110.80
C(3)-N(1)-C(5)	109.80
C(2)-N(1)-Re(1)	110.50
C(3)-N(1)-Re(1)	110.70
C(5)-N(1)-Re(1)	106.60
C(2)-C(1)-S(1)	109.30



[(3-(N-methyl)-azapentane-1.5-dithiolato](methylthiolato)oxorhenium(V)

$C_6H_{14}NOReS_3$

13.1835Å	6.8305Å	13.2244Å	
90.0000°	109.4800°	90.0000°	V=1122.7Å^3
$P2_1/c$; 14	Z=4; F(000)=752	ρ=2.358g/cm^3	R=2.6%
monoclinic			

T. Fietz (1995)
not published
CCDC 156805

Re 38

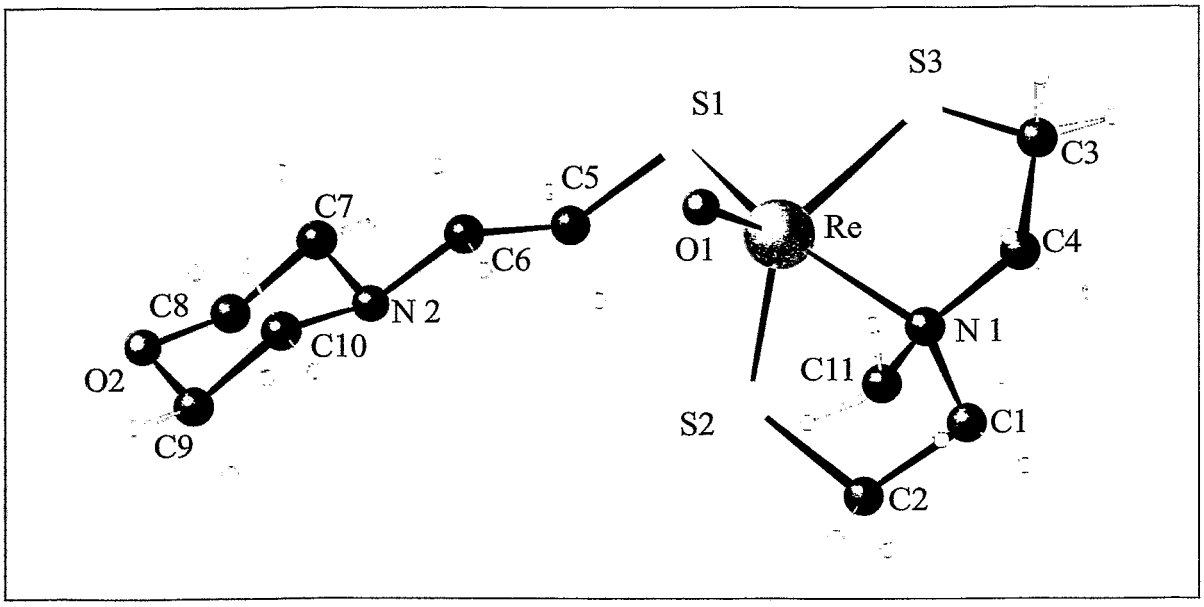
Selected Bonds (Å) and Angles (°)

Bonds

Re-O	1.683
Re-N	2.209
Re-S(3)	2.273
Re-S(2)	2.275
Re-S(1)	2.293
S(1)-C(6)	1.823
S(2)-C(1)	1.825
S(3)-C(4)	1.839
N-C(5)	1.480
N-C(2)	1.485
N-C(3)	1.497
C(1)-C(2)	1.500
C(1)-H(1A)	0.970
C(1)-H(1B)	0.970
C(2)-H(2A)	0.970
C(2)-H(2B)	0.970
C(3)-C(4)	1.469
C(3)-H(3A)	0.970
C(3)-H(3B)	0.970
C(4)-H(4A)	0.970
C(4)-H(4B)	0.970
C(5)-H(5A)	0.960
C(5)-H(5B)	0.960
C(5)-H(5C)	0.960

Angles

O-Re-N	95.10
O-Re-S(3)	119.20
N-Re-S(3)	82.90
O-Re-S(2)	119.50
N-Re-S(2)	83.00
S(3)-Re-S(2)	120.46
O-Re-S(1)	104.30
N-Re-S(1)	160.50
S(3)-Re-S(1)	89.54
S(2)-Re-S(1)	85.40
C(6)-S(1)-Re	111.30
C(1)-S(2)-Re	103.10
C(4)-S(3)-Re	103.30
C(5)-N-C(2)	109.80
C(5)-N-C(3)	105.60
C(2)-N-C(3)	111.00
C(5)-N-Re	109.70
C(2)-N-Re	109.90
C(3)-N-Re	110.70
C(2)-C(1)-S(2)	108.90
C(2)-C(1)-H(1A)	109.90
S(2)-C(1)-H(1A)	109.90
C(2)-C(1)-H(1B)	109.90
S(2)-C(1)-H(1B)	109.90



[3-(N-Methyl)-azapentane-1,5-dithiolato](2-N-morpholinoethyl-thiolato)oxorhenium(V)

$C_{11}H_{23}N_2O_2ReS_3$

11.7673Å	11.4723Å	13.2999Å	
90.0000°	111.1100°	90.0000°	V=1675.0Å^3
$P2_1/n$; 1014	Z=4; F(000)=484	ρ=1.974g/cm^3	R=5.3%
monoclinic			

M. Friebe (1998)
not published
CCDC 186/2005

Selected Bonds (Å) and Angles (°)

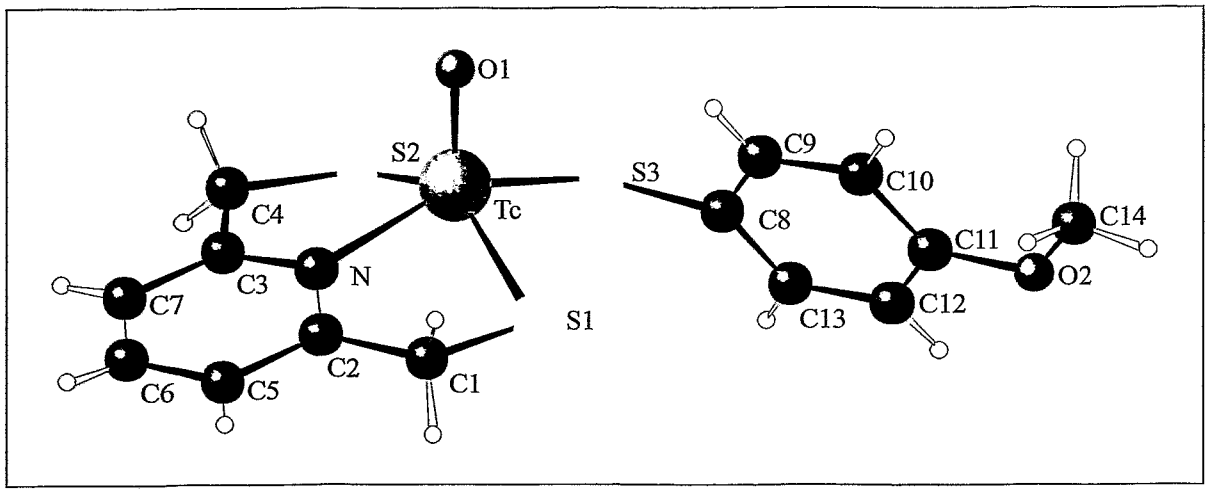
Bonds

Re-O(1)	1.663
Re-N(1)	2.153
Re-S(2)	2.270
Re-S(3)	2.278
Re-S(1)	2.293
S(1)-C(5)	1.805
S(2)-C(2)	1.834
S(3)-C(3)	1.810
S(3)-C(31)	1.830
O(2)-C(8)	1.420
O(2)-C(9)	1.431
N(1)-C(4)	1.454
N(1)-C(1)	1.474
N(1)-C(11)	1.540
N(2)-C(7)	1.431
N(2)-C(6)	1.469
N(2)-C(10)	1.475
C(1)-C(2)	1.500
C(1)-H(1A)	0.970
C(1)-H(1B)	0.970
C(2)-H(2A)	0.970
C(2)-H(2B)	0.970

Angles

O(1)-Re-N(1)	99.30
O(1)-Re-S(2)	117.70
N(1)-Re-S(2)	82.40
O(1)-Re-S(3)	115.90
N(1)-Re-S(3)	82.10
S(2)-Re-S(3)	125.82
O(1)-Re-S(1)	106.20
N(1)-Re-S(1)	154.00
S(2)-Re-S(1)	89.65
S(3)-Re-S(1)	82.65
C(5)-S(1)-Re	113.10
C(2)-S(2)-Re	103.30
C(3)-S(3)-C(31)	21.80
C(3)-S(3)-Re	102.70
C(31)-S(3)-Re	101.50
C(8)-O(2)-C(9)	109.90
C(4)-N(1)-C(1)	113.70
C(4)-N(1)-C(11)	102.70
C(1)-N(1)-C(11)	105.60
C(4)-N(1)-Re	113.00
C(1)-N(1)-Re	113.00
C(11)-N(1)-Re	107.80

Tc 40



(2,6-Dithiomethylpyridinato)(4-methoxy-benzenethiolato)oxotechnetium(V)

$C_{14}H_{14}NO_2S_3Tc$

5.8065Å	8.8033Å	16.0137Å	
90.0000°	98.8990°	90.0000°	$V=808.7Å^3$
$P2_1$; 4	Z=2; F(000)=424	$\rho=1.735 g/cm^3$	R=4.5%
monoclinic			

H.-J. Pietzsch (1999)
not published
CCDC 159492

Tc 40

Selected Bonds (Å) and Angles (°)

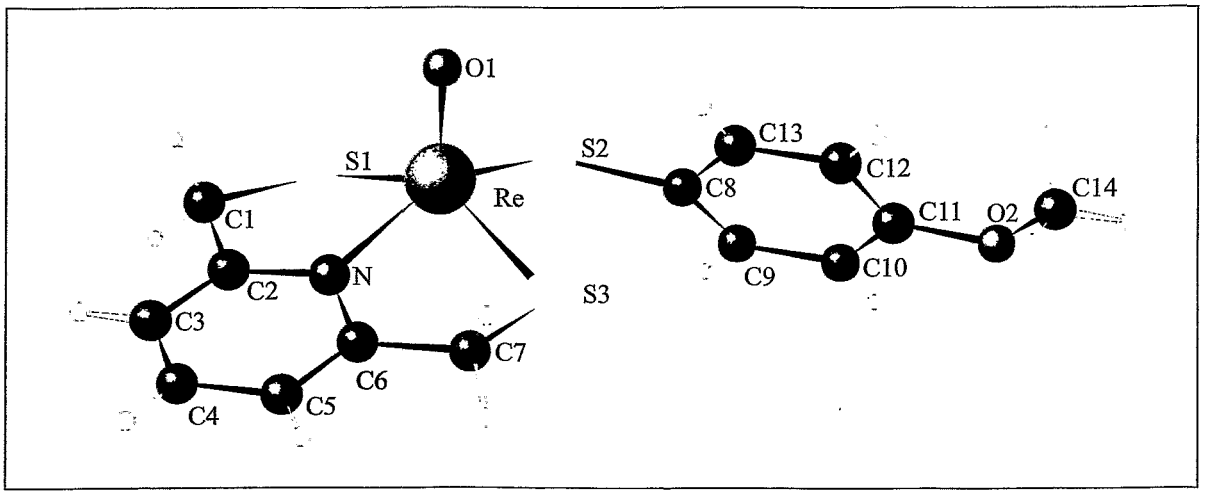
Bonds

Tc(1)-O(1)	1.662
Tc(1)-N(1)	2.128
Tc(1)-S(1)	2.287
Tc(1)-S(2)	2.288
Tc(1)-S(3)	2.298
S(2)-C(4)	1.806
S(1)-C(1)	1.821
S(3)-C(8)	1.776
O(2)-C(11)	1.356
O(2)-C(14)	1.414
N(1)-C(3)	1.345
N(1)-C(2)	1.357
C(1)-C(2)	1.493
C(2)-C(5)	1.408
C(3)-C(7)	1.387
C(3)-C(4)	1.478
C(5)-C(6)	1.355
C(6)-C(7)	1.382
C(8)-C(9)	1.378
C(8)-C(13)	1.401
C(9)-C(10)	1.377
C(10)-C(11)	1.397
C(11)-C(12)	1.393
C(12)-C(13)	1.373

Angles

O(1)-Tc(1)-N(1)	107.50
O(1)-Tc(1)-S(1)	114.24
N(1)-Tc(1)-S(1)	80.80
O(1)-Tc(1)-S(2)	111.64
N(1)-Tc(1)-S(2)	80.45
S(1)-Tc(1)-S(2)	133.76
O(1)-Tc(1)-S(3)	106.44
N(1)-Tc(1)-S(3)	145.87
S(1)-Tc(1)-S(3)	88.68
S(2)-Tc(1)-S(3)	83.88
C(4)-S(2)-Tc(1)	100.10
C(1)-S(1)-Tc(1)	100.00
C(8)-S(3)-Tc(1)	112.50
C(11)-O(2)-C(14)	118.60
C(3)-N(1)-C(2)	120.50
C(3)-N(1)-Tc(1)	120.00
C(2)-N(1)-Tc(1)	119.30
C(2)-C(1)-S(1)	111.20
N(1)-C(2)-C(5)	120.30
N(1)-C(2)-C(1)	118.20
C(5)-C(2)-C(1)	121.60
N(1)-C(3)-C(7)	120.60
N(1)-C(3)-C(4)	117.70
C(7)-C(3)-C(4)	121.70

Re 40



(2,6-Dithiomethylpyridinato)(4-methoxy-benzenethiolato)oxorhenium(V)

$C_{14}H_{14}NO_2ReS_3$

7.2600Å	7.9210Å	28.2000Å	
90.0000°	90.0000°	90.0000°	V=1621.7Å^3
$P2_12_12_1$; 19	Z=4; F(000)=976	ρ=2.091g/cm^3	R=3.6%
orthorhombic			

Nock B., Pietzsch H.-J., Tisato F., Maina T., Leibnitz P., Spies H., Chiotellis E
"Oxorhenium mixed-ligand complexes with the 2,6-dimercaptomethylpyridine ligand. Crystal structure of (2,6-dimercaptomethylpyridinato)(4-methoxy-benzenethiolato)oxorhenium(V)"
Inorg. Chim. Acta 304 (2000) 26-32
CCDC-136219

Re 40

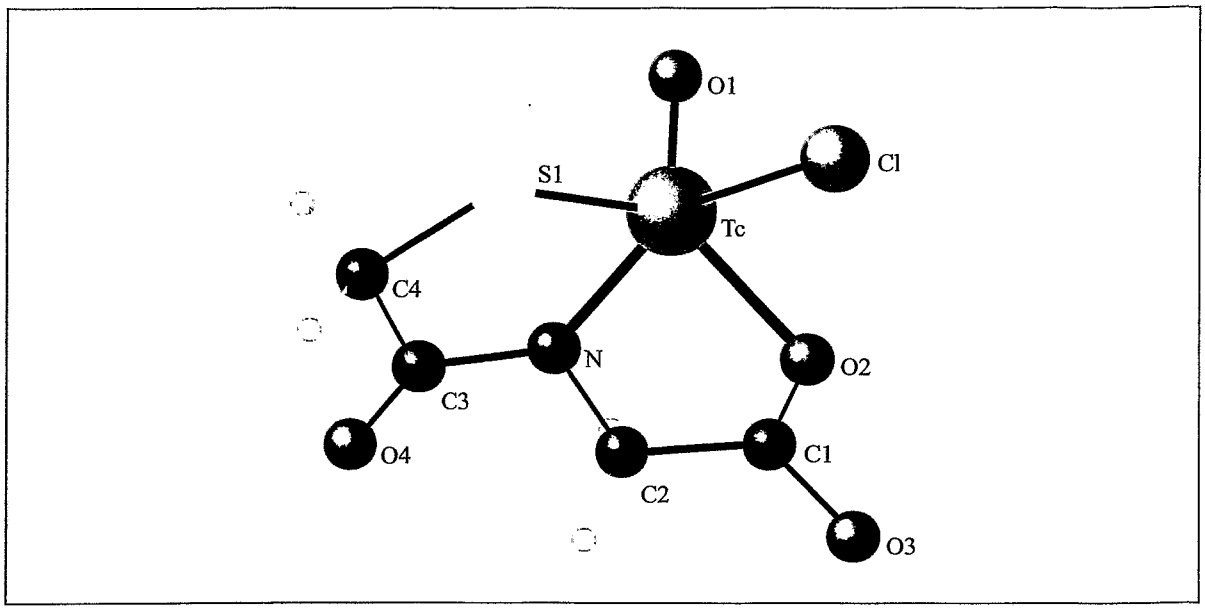
Selected Bonds (Å) and Angles (°)

Bonds

Re-O(1)	1.692
Re-N	2.106
Re-S(3)	2.279
Re-S(1)	2.286
Re-S(2)	2.290
S(1)-C(1)	1.793
S(2)-C(8)	1.790
S(3)-C(7)	1.809
O(2)-C(11)	1.361
O(2)-C(14)	1.420
N-C(2)	1.331
N-C(6)	1.388
C(1)-C(2)	1.510
C(1)-H(1A)	0.970
C(1)-H(1B)	0.970
C(2)-C(3)	1.370
C(3)-C(4)	1.400
C(3)-H(3)	0.930
C(4)-C(5)	1.350
C(4)-H(4)	0.930
C(5)-C(6)	1.390
C(5)-H(5)	0.930
C(6)-C(7)	1.470

Angles

O(1)-Re-N	106.30
O(1)-Re-S(3)	111.60
N-Re-S(3)	81.70
O(1)-Re-S(1)	111.00
N-Re-S(1)	80.10
S(3)-Re-S(1)	136.87
O(1)-Re-S(2)	107.30
N-Re-S(2)	146.10
S(3)-Re-S(2)	89.63
S(1)-Re-S(2)	84.37
C(1)-S(1)-Re	99.90
C(8)-S(2)-Re	113.80
C(7)-S(3)-Re	100.30
C(11)-O(2)-C(14)	118.90
C(2)-N-C(6)	118.00
C(2)-N-Re	122.10
C(6)-N-Re	119.70
C(2)-C(1)-S(1)	112.50
C(2)-C(1)-H(1A)	109.10
S(1)-C(1)-H(1A)	109.10
C(2)-C(1)-H(1B)	109.10
S(1)-C(1)-H(1B)	109.10
H(1A)-C(1)-H(1B)	107.80



Tetraphenylarsonium chloro(2-mercaptoacetylglycinato-S,N,O)oxotechnetate(V)

$C_{28}H_{24}ASClNO_4STc$
(The tetraphenylarsonium counterion has been omitted for clarity.)

10.1279Å	11.3003Å	13.3644Å	
91.2452°	112.1146°	102.5908°	V=1373.8Å^3
P1; 2	Z=2; F(000)=680	ρ=1.641g/cm^3	R=3.6%
triclinic			

B. Noll, (1996)
not published
CCDC 156809

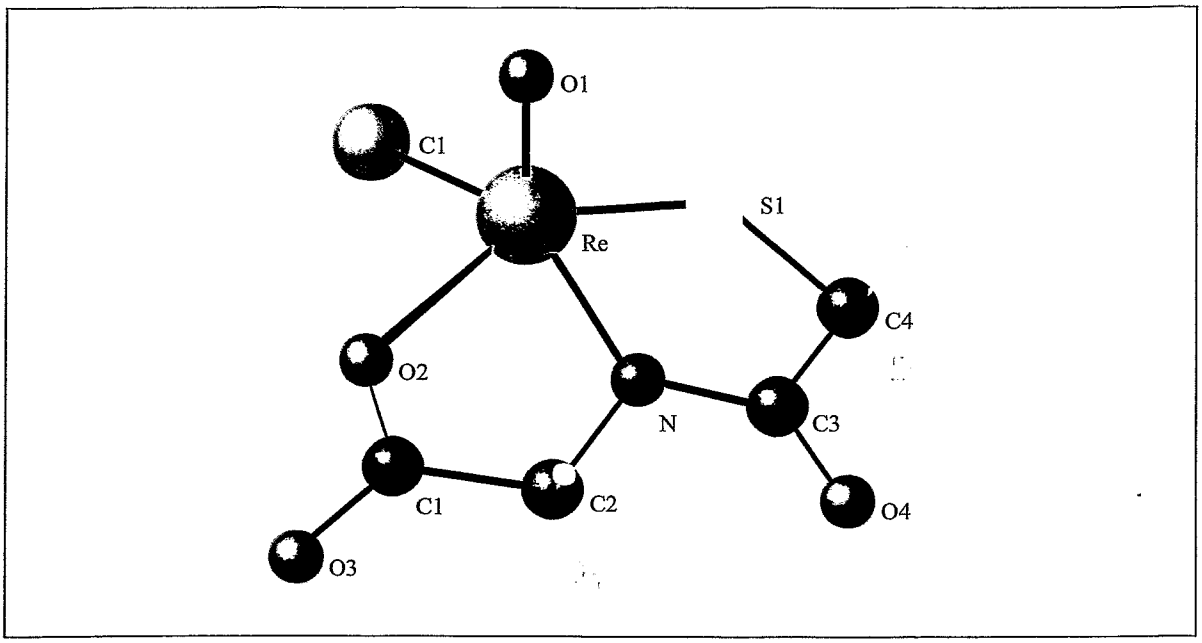
Selected Bonds (Å) and Angles (°)

Bonds

Tc-O(1)	1.645
Tc-N	1.938
Tc-O(2)	2.018
Tc-S(1)	2.231
Tc-Cl	2.348
As-C(5)	1.906
As-C(11)	1.911
As-C(17)	1.912
As-C(23)	1.917
S(1)-C(4)	1.797
O(2)-C(1)	1.155
O(3)-C(1)	1.314
O(4)-C(3)	1.214
N-C(3)	1.352
N-C(2)	1.469
C(1)-C(2)	1.490
C(2)-H(2A)	0.970
C(2)-H(2B)	0.970
C(3)-C(4)	1.528
C(4)-H(4A)	0.970
C(4)-H(4B)	0.970

Angles

O(1)-Tc-N	109.70
O(1)-Tc-O(2)	115.40
N-Tc-O(2)	76.10
O(1)-Tc-S(1)	110.30
N-Tc-S(1)	83.30
O(2)-Tc-S(1)	133.84
O(1)-Tc-Cl	106.70
N-Tc-Cl	143.30
O(2)-Tc-Cl	84.30
S(1)-Tc-Cl	88.59
C(5)-As-C(11)	108.30
C(5)-As-C(17)	108.60
C(11)-As-C(17)	110.20
C(5)-As-C(23)	112.40
C(11)-As-C(23)	108.30
C(17)-As-C(23)	109.10
C(4)-S(1)-Tc	99.90
C(1)-O(2)-Tc	118.70
C(3)-N-C(2)	115.80
C(3)-N-Tc	126.60
C(2)-N-Tc	117.50



Tetraphenylarsonium chloro(2-mercaptoacetylglycinato-S,N,O)oxorhenate(V)

$C_{28}H_{24}AsClNO_4ReS$
(The tetraphenylarsonium counterion has been omitted for clarity.)

10.1926Å	11.2823Å	13.3064Å	
91.0440°	112.1050°	102.7340°	V=1374.1Å^3
P1bar; 2	Z=2; F(000)=744	ρ=1.854g/cm^3	R=6.2%
triclinic			

B. Noll, St. Noll, P. Leibnitz, H. Spies, P.E. Schulze, W. Semmler and B. Johannsen
"Technetium and rhenium complexes of mercaptoacetyl glycine ligands. II. Formation and molecular structure of Re (V) complexes with mercaptoacetyl glycine and mercaptoacetyl glycine ethylester"
Inorg.Chim.Acta 255 (1997) 399-403
CSD No. 404911

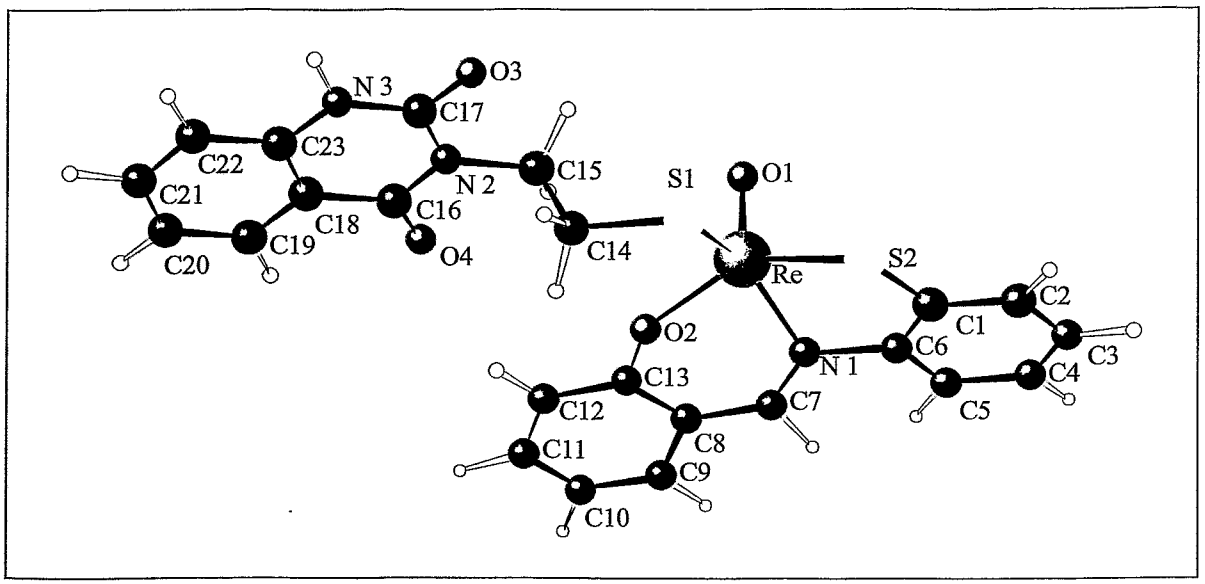
Selected Bonds (Å) and Angles (°)

Bonds

Re-O(1)	1.649
Re-N(1)	1.966
Re-O(2)	2.005
Re-S(1)	2.240
Re-Cl(1)	2.343
As-C(11)	1.899
As-C(17)	1.899
As-C(5)	1.906
As-C(23)	1.907
S(1)-C(4)	1.807
O(2)-C(1)	1.250
O(3)-C(1)	1.250
O(4)-C(3)	1.212
N(1)-C(3)	1.340
N(1)-C(2)	1.450
C(1)-C(2)	1.500
C(2)-H(2A)	0.970
C(2)-H(2B)	0.970
C(3)-C(4)	1.480
C(4)-H(4A)	0.970
C(4)-H(4B)	0.970

Angles

O(1)-Re-N(1)	109.10
O(1)-Re-O(2)	114.50
N(1)-Re-O(2)	78.00
O(1)-Re-S(1)	110.90
N(1)-Re-S(1)	82.90
O(2)-Re-S(1)	134.30
O(1)-Re-Cl(1)	106.80
N(1)-Re-Cl(1)	143.70
O(2)-Re-Cl(1)	82.70
S(1)-Re-Cl(1)	89.24
C(11)-As-C(17)	109.50
C(11)-As-C(5)	109.00
C(17)-As-C(5)	108.90
C(11)-As-C(23)	108.60
C(17)-As-C(23)	109.00
C(5)-As-C(23)	111.80
C(4)-S(1)-Re	99.50
C(1)-O(2)-Re	117.20
C(3)-N(1)-C(2)	117.10
C(3)-N(1)-Re	125.60
C(2)-N(1)-Re	117.00



[2-(Chinazoline)ethylthiolato][N-(2-mercaptophenyl) salicylideneiminato]oxorhenium(V)

$C_{23}H_{18}N_3O_4S_2Re$

9.2819Å	9.6082Å	13.9763Å	
107.1535°	103.9161°	100.0506°	V=1114.8Å^3
P-1; 2	Z=2; F(000)=632	ρ=1.938g/cm^3	R=4.5%
triclinic			

H.-J. Pietzsch (1994)
not published
CCDC 156802

Re 42

Selected Bonds (Å) and Angles (°)

Bonds

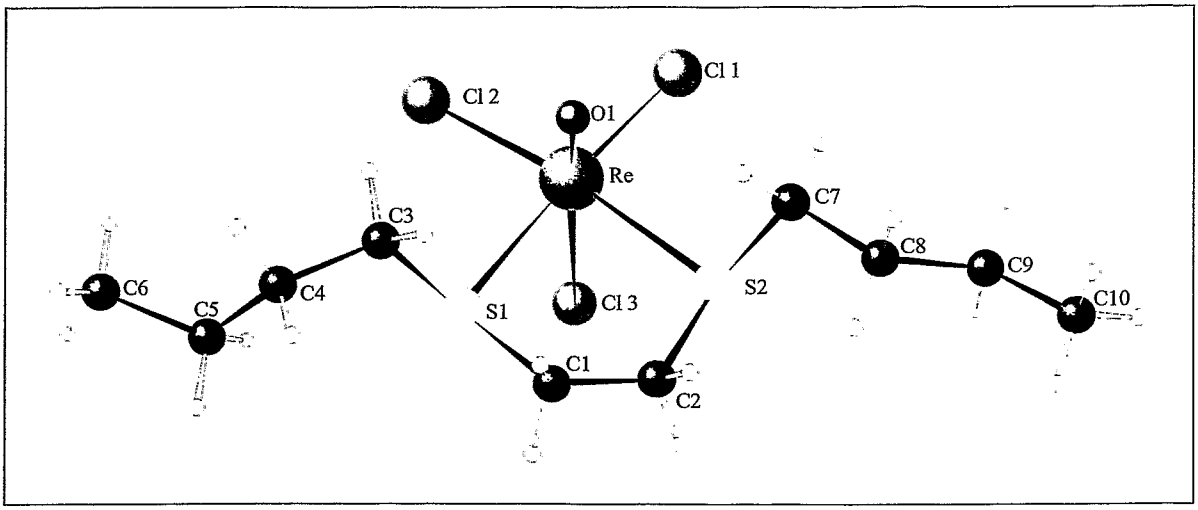
Re-O(1)	1.678
Re-O(2)	1.970
Re-N(1)	2.114
Re-S(1)	2.269
Re-S(2)	2.270
S(1)-C(14)	1.818
S(2)-C(1)	1.757
O(2)-C(13)	1.334
O(3)-C(17)	1.231
O(4)-C(16)	1.202
N(1)-C(7)	1.281
N(1)-C(6)	1.444
N(2)-C(17)	1.388
N(2)-C(16)	1.395
N(2)-C(15)	1.474
N(3)-C(17)	1.349
N(3)-C(23)	1.395
N(3)-H(3)	0.860
C(1)-C(6)	1.375
C(1)-C(2)	1.417
C(2)-C(3)	1.376
C(2)-H(2)	0.930
C(3)-C(4)	1.365

Angles

O(1)-Re-O(2)	114.10
O(1)-Re-N(1)	106.70
O(2)-Re-N(1)	85.50
O(1)-Re-S(1)	106.00
O(2)-Re-S(1)	84.50
N(1)-Re-S(1)	147.00
O(1)-Re-S(2)	108.50
O(2)-Re-S(2)	137.30
N(1)-Re-S(2)	81.68
S(1)-Re-S(2)	84.62
C(14)-S(1)-Re	111.10
C(1)-S(2)-Re	100.10
C(13)-O(2)-Re	129.20
C(7)-N(1)-C(6)	118.30
C(7)-N(1)-Re	125.80
C(6)-N(1)-Re	115.90
C(17)-N(2)-C(16)	124.40
C(17)-N(2)-C(15)	115.80
C(16)-N(2)-C(15)	119.80
C(17)-N(3)-C(23)	123.90
C(17)-N(3)-H(3)	118.10
C(23)-N(3)-H(3)	118.10
C(6)-C(1)-C(2)	120.10

5.2.3. Dithioether ligands thiacrown ethers dimethylphenyl phosphine

Re 43



(5,8-Dithiadodecane-S,S)trichlorooxorhenium(V)

$C_{10}H_{22}Cl_3OReS_2$

15.6679Å	13.0467Å	8.6871Å	
90.0000°	90.0000°	90.0000°	V=1775.8Å^3
$Pca2_1$	Z=4; F(000)=992	ρ=1.926g/cm^3	R=5.0%
orthorhombic			

H.-J. Pietzsch, M. Reisgys (1999)
not published
CCDC 159490

Re 43

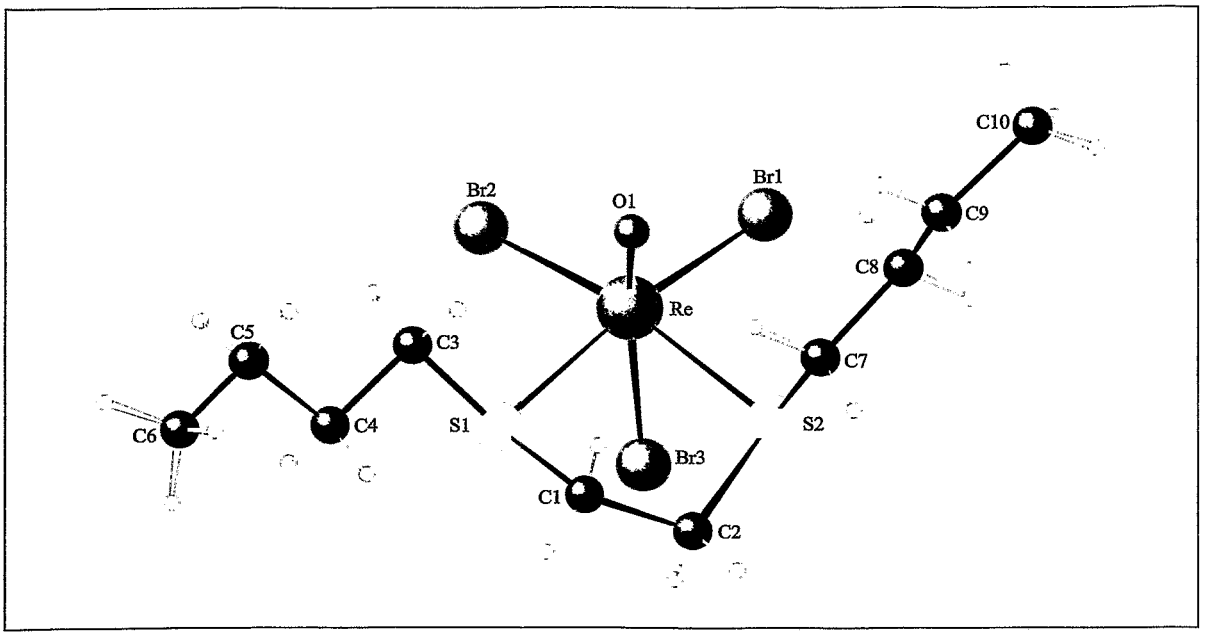
Selected Bonds (Å) and Angles (°)

Bonds

Re(1)-O(1)	1.668
Re(1)-Cl(1)	2.345
Re(1)-Cl(2)	2.368
Re(1)-S(2)	2.420
Re(1)-Cl(3)	2.420
Re(1)-S(1)	2.424
S(1)-C(1)	1.800
S(1)-C(3)	1.820
S(2)-C(2)	1.790
S(2)-C(7)	1.830
C(1)-C(2)	1.330
C(3)-C(4)	1.486
C(4)-C(5)	1.505
C(5)-C(6)	1.517
C(7)-C(8)	1.515
C(8)-C(9)	1.511
C(9)-C(10)	1.522

Angles

O(1)-Re(1)-Cl(1)	100.80
O(1)-Re(1)-Cl(2)	100.80
Cl(1)-Re(1)-Cl(2)	89.40
O(1)-Re(1)-S(2)	89.20
Cl(1)-Re(1)-S(2)	91.80
Cl(2)-Re(1)-S(2)	169.50
O(1)-Re(1)-Cl(3)	164.70
Cl(1)-Re(1)-Cl(3)	89.60
Cl(2)-Re(1)-Cl(3)	90.40
S(2)-Re(1)-Cl(3)	79.20
O(1)-Re(1)-S(1)	90.10
Cl(1)-Re(1)-S(1)	169.00
Cl(2)-Re(1)-S(1)	90.50
S(2)-Re(1)-S(1)	86.40
Cl(3)-Re(1)-S(1)	79.30
C(1)-S(1)-Re(1)	101.20
C(3)-S(1)-Re(1)	103.40
C(2)-S(2)-Re(1)	102.80
C(7)-S(2)-Re(1)	104.80



(5,8-Dithiadodecane-S,S)tribromooxorhenium(V)

$C_{10}H_{22}Br_3OReS_2$

24.1679Å	12.2574Å	14.042Å	
90.0000°	119.5050°	90.0000°	V=3619.4Å^3
C121/n1	Z=8; F(000)=2416	ρ=2.380g/cm^3	R=3.5%
monoclinic			

M. Reisgys, H.Spies, B. Johannsen, P. Leibnitz, H.-J. Pietzsch
"Technetium and rhenium complexes with thioether ligands. VI. Synthesis and structural characterization of mixed-ligand oxorhenium (V) complexes containing bidentate dithioethers and monothiolato ligands"
Chem.Ber. 130 (1997) 1343-1347
CSD No. 406680

Re 44

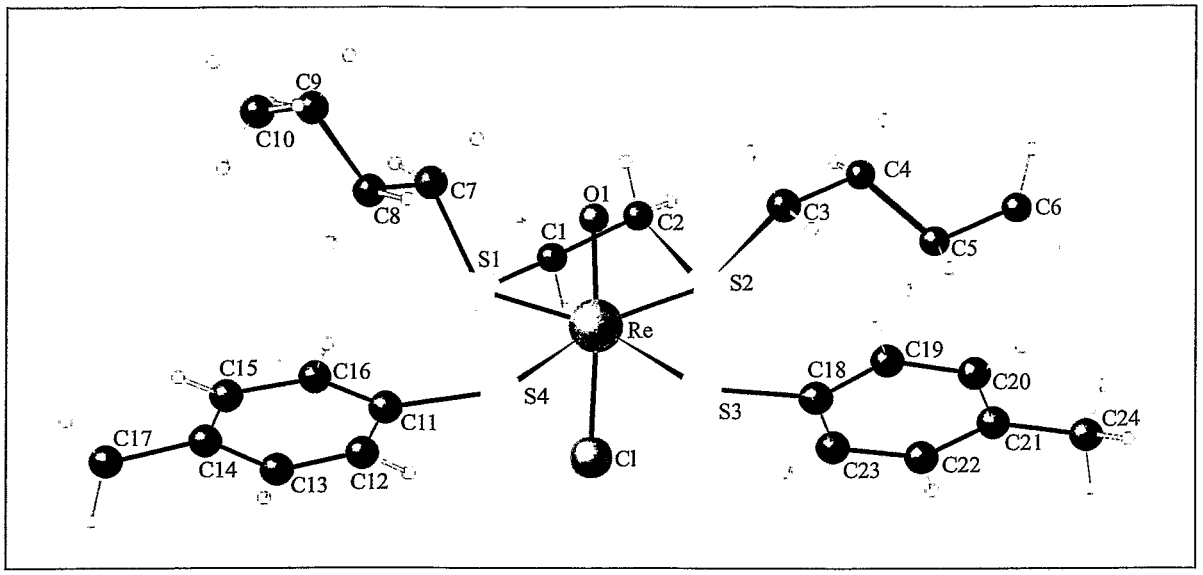
Selected Bonds (Å) and Angles (°)

Bonds

Re-O(1)	1.664
Re-S(1)	2.424
Re-S(2)	2.452
Re-Br(1)	2.487
Re-Br(2)	2.490
Re-Br(3)	2.598
S(1)-C(3')	1.830
S(1)-C(3)	1.780
S(1)-C(1)	1.828
S(2)-C(7)	1.816
S(2)-C(2)	1.826
C(1)-C(2)	1.505
C(1)-H(1A)	0.970
C(1)-H(1B)	0.970
C(2)-H(2A)	0.970
C(2)-H(2B)	0.970
C(3)-C(4)	1.535
C(3)-H(3A)	0.970
C(3)-H(3B)	0.970
C(4)-C(5)	1.490
C(4)-H(4A)	0.970
C(4)-H(4B)	0.970
C(5)-C(6)	1.512
C(5)-H(5A)	0.970

Angles

O(1)-Re-S(1)	90.10
O(1)-Re-S(2)	89.10
S(1)-Re-S(2)	86.05
O(1)-Re-Br(1)	100.90
S(1)-Re-Br(1)	168.83
S(2)-Re-Br(1)	92.32
O(1)-Re-Br(2)	102.80
S(1)-Re-Br(2)	90.17
S(2)-Re-Br(2)	167.56
Br(1)-Re-Br(2)	89.10
O(1)-Re-Br(3)	163.80
S(1)-Re-Br(3)	80.91
S(2)-Re-Br(3)	76.89
Br(1)-Re-Br(3)	87.95
Br(2)-Re-Br(3)	90.82
C(3')-S(1)-C(1)	93.00
C(3)-S(1)-C(1)	105.40
C(3')-S(1)-Re	103.60
C(3)-S(1)-Re	109.50
C(1)-S(1)-Re	102.00
C(7)-S(2)-C(2)	99.90
C(7)-S(2)-Re	107.40
C(2)-S(2)-Re	101.70
C(2)-C(1)-S(1)	110.20



Bis(4-methylbenzenethiolato)chloro(5,8-dithiadodecane-S,S)oxorhenium(V)

$C_{24}H_{36}ClOReS_4$

7.8662Å	11.0333Å	16.1373Å	
88.3801°	78.0201°	85.3901°	V=1365.9Å^3
P-1;2	Z=2; F(000)=688	ρ=1.679g/cm^3	R=5.8%
triclinic			

M. Reisgys, H.Spies, B. Johannsen, P. Leibnitz, H.-J. Pietzsch
"Technetium and rhenium complexes with thioether ligands. VI. Synthesis and structural characterization of mixed-ligand oxorhenium (V) complexes containing bidentate dithioethers and monothiolato ligands"
Chem.Ber. 130 (1997) 1343-1347
CSD No. 406681

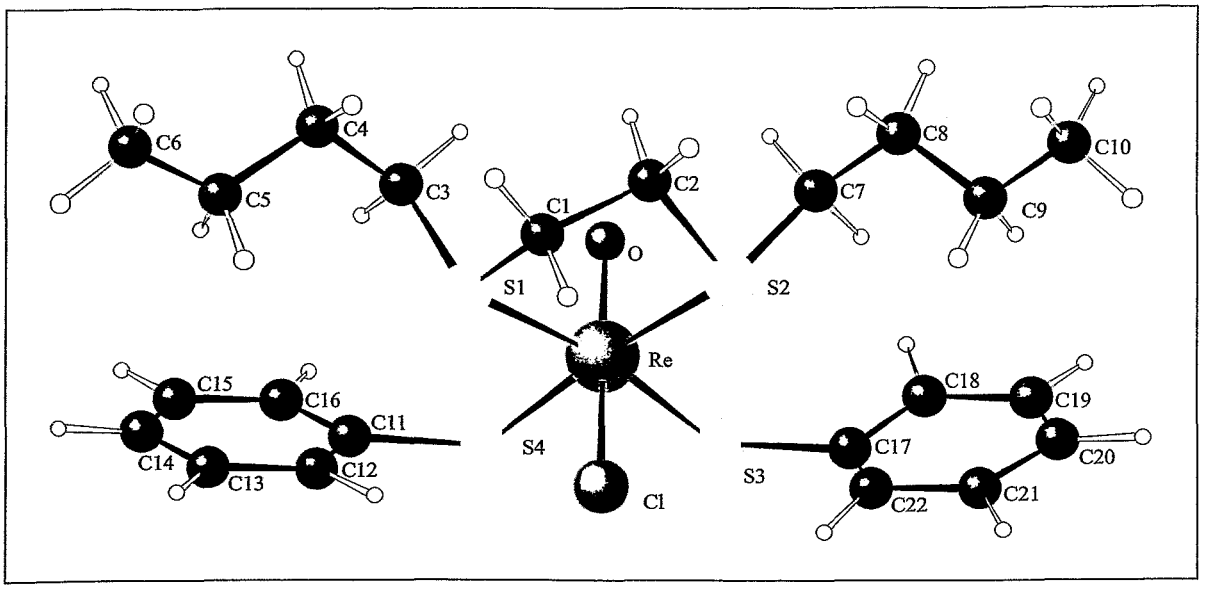
Selected Bonds (Å) and Angles (°)

Bonds

Re-O(1)	1.680
Re-S(3)	2.291
Re-S(4)	2.318
Re-Cl	2.453
Re-S(2)	2.483
Re-S(1)	2.534
S(1)-C(1)	1.820
S(1)-C(7)	1.830
S(2)-C(2)	1.780
S(2)-C(3)	1.820
S(3)-C(18)	1.800
S(4)-C(11)	1.790
C(1)-C(2)	1.470
C(1)-H(1A)	0.970
C(1)-H(1B)	0.970
C(2)-H(2A)	0.970
C(2)-H(2B)	0.970
C(3)-C(4)	1.510
C(3)-H(3A)	0.970
C(3)-H(3B)	0.970
C(7)-C(8)	1.510
C(7)-H(7A)	0.970
C(7)-H(7B)	0.970
C(11)-C(16)	1.380
C(11)-C(12)	1.420
C(18)-C(23)	1.370

Angles

O(1)-Re-S(3)	104.60
O(1)-Re-S(4)	102.70
S(3)-Re-S(4)	78.73
O(1)-Re-Cl	158.40
S(3)-Re-Cl	93.50
S(4)-Re-Cl	92.10
O(1)-Re-S(2)	87.60
S(3)-Re-S(2)	96.97
S(4)-Re-S(2)	169.53
Cl-Re-S(2)	78.51
O(1)-Re-S(1)	86.50
S(3)-Re-S(1)	168.83
S(4)-Re-S(1)	98.51
Cl-Re-S(1)	75.71
S(2)-Re-S(1)	83.88
C(1)-S(1)-C(7)	99.50
C(1)-S(1)-Re	101.30
C(7)-S(1)-Re	108.50
C(2)-S(2)-C(3)	100.40
C(2)-S(2)-Re	100.10
C(3)-S(2)-Re	108.00
C(18)-S(3)-Re	114.50
C(11)-S(4)-Re	115.50
C(2)-C(1)-S(1)	115.20
C(2)-C(1)-H(1A)	108.50
S(1)-C(1)-H(1A)	108.50



[Bis(benzenethiolato)chloro(5,8-dithiadodecane-S,S)]oxorhenium(V)

$C_{22}H_{32}ClOReS_4$

8.4380Å	12.3990Å	13.4540Å	
70.8800°	76.1800°	82.7400°	V=1289.7Å^3
$P2_1$; 4	Z=2; F(000)=656	ρ=1.706g/cm^3	R=4.5%
triclinic			

H.-J. Pietzsch (1996)
not published
CCDC 159489

Re 46

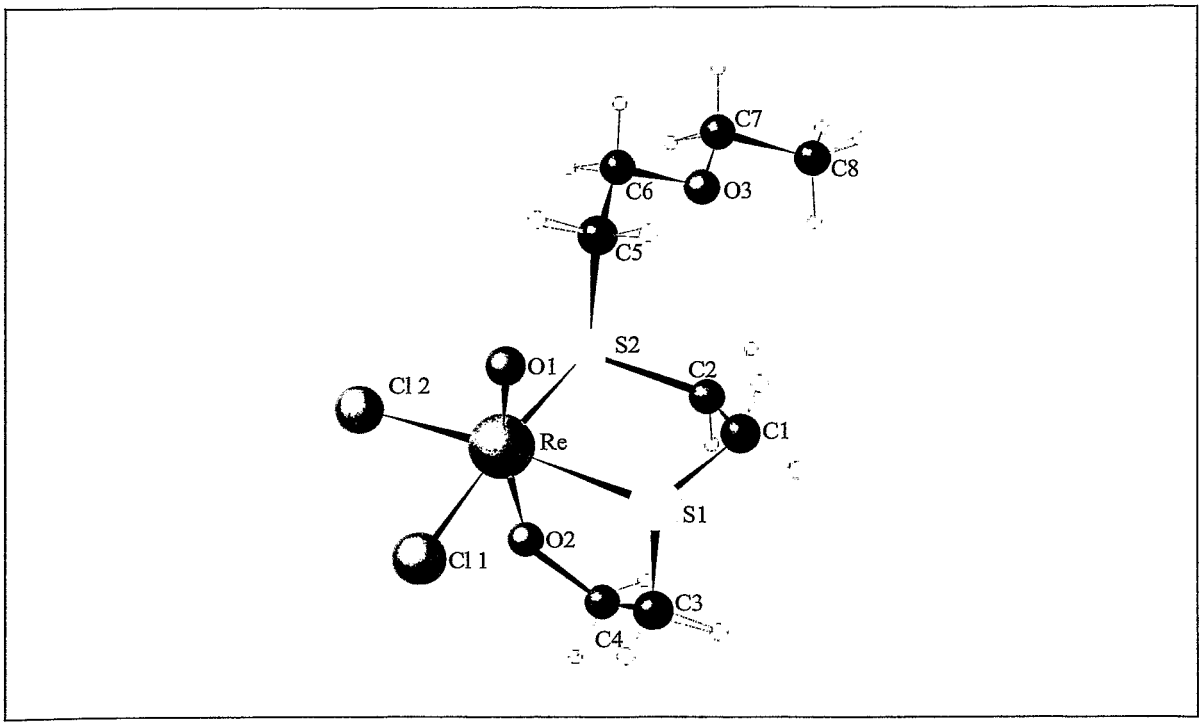
Selected Bonds (Å) and Angles (°)

Bonds

Re-O	1.660
Re-S(4)	2.302
Re-S(3)	2.308
Re-Cl	2.450
Re-S(1)	2.510
Re-S(2)	2.516
S(1)-C(3)	1.610
S(1)-C(1)	1.750
S(2)-C(7)	1.800
S(2)-C(2)	1.820
S(3)-C(17)	1.450
S(4)-C(23)	1.750
S(4)-C(11)	1.850
C(3)-C(4)	1.670
C(4)-C(5)	1.520
C(5)-C(6)	1.590
C(8)-C(9)	1.470
C(8)-C(7)	1.510
C(8)-C(24)#1	1.900
C(9)-C(10)	1.480
C(9)-C(24)#1	1.600
C(10)-C(24)#1	1.100
C(11)-C(16)	1.250
C(11)-C(12)	1.380
C(12)-C(13)	1.420

Angles

O-Re-S(4)	105.20
O-Re-S(3)	102.50
S(4)-Re-S(3)	79.50
O-Re-Cl	157.60
S(4)-Re-Cl	93.10
S(3)-Re-Cl	93.20
O-Re-S(1)	89.70
S(4)-Re-S(1)	97.10
S(3)-Re-S(1)	167.80
Cl-Re-S(1)	75.20
O-Re-S(2)	83.80
S(4)-Re-S(2)	171.00
S(3)-Re-S(2)	98.10
Cl-Re-S(2)	78.30
S(1)-Re-S(2)	83.40
C(3)-S(1)-C(1)	111.00
C(3)-S(1)-Re	102.00
C(1)-S(1)-Re	102.30
C(7)-S(2)-C(2)	77.00
C(7)-S(2)-Re	109.00
C(2)-S(2)-Re	107.40
C(17)-S(3)-Re	110.10
C(23)-S(4)-C(11)	102.00
C(23)-S(4)-Re	131.90
C(11)-S(4)-Re	117.00



[3,6-Dithia-9-oxaundecane-1-olato-(O,S,S)]dichlorooxorhenium(V)

$C_8H_{17}Cl_2O_2ReS_2$

7.2154Å	16.8456Å	12.1192Å	
90.0000°	99.3730°	90.0000°	V=1453.3Å^3
$P2_1/n$; 14	Z=4; F(000)=920	ρ=2.205g/cm^3	R=5.0%
monoclinic			

H.-J. Pietzsch, M. Reisgys, H. Spies, P. Leibnitz and B. Johannsen
"Technetium and rhenium complexes with thioether ligands. V. Synthesis and structural characterization of neutral oxorhenium (V) complexes with tridentate dithioethers"
Chem.Ber. 130 (1997) 357-361
CSD No. 405743

Re 47

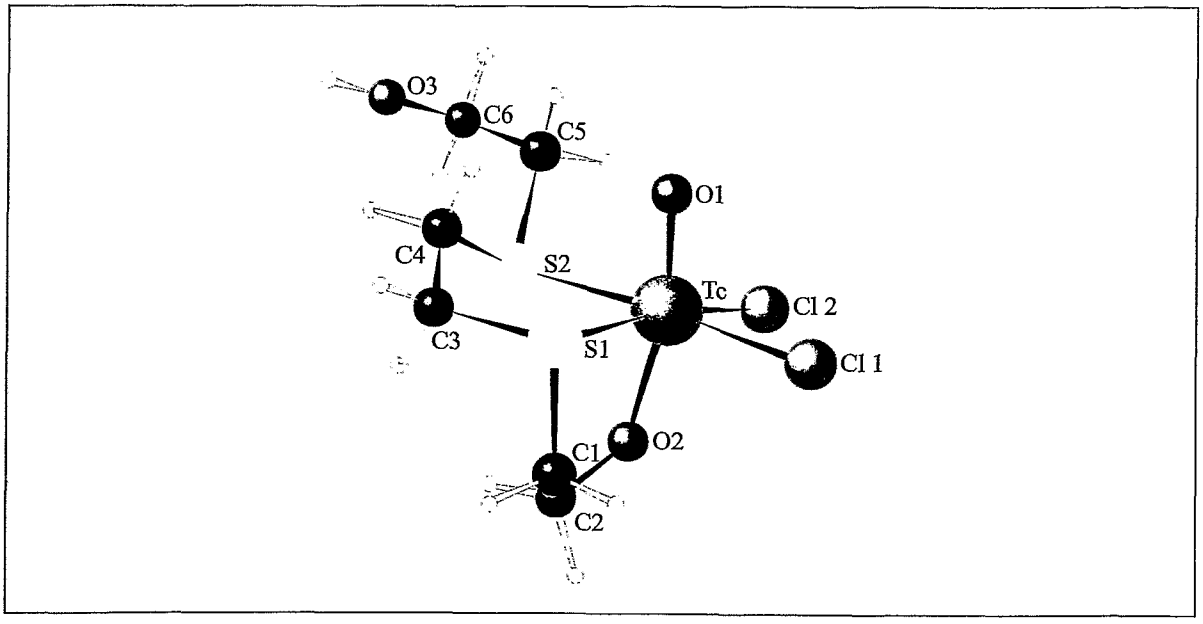
Selected Bonds (Å) and Angles (°)

Bonds

Re-O(1)	1.675
Re-O(2)	1.914
Re-Cl(2)	2.363
Re-Cl(1)	2.406
Re-S(2)	2.422
Re-S(1)	2.429
S(1)-C(3)	1.787
S(1)-C(1)	1.814
S(2)-C(5)	1.795
S(2)-C(2)	1.808
O(2)-C(4)	1.411
O(3)-C(6)	1.389
O(3)-C(7)	1.419
C(1)-C(2)	1.443
C(1)-H(1A)	0.970
C(1)-H(1B)	0.970
C(2)-H(2A)	0.970
C(2)-H(2B)	0.970
C(3)-C(4)	1.494
C(3)-H(3A)	0.970
C(3)-H(3B)	0.970
C(4)-H(4A)	0.970

Angles

O(1)-Re-O(2)	166.70
O(1)-Re-Cl(2)	103.20
O(2)-Re-Cl(2)	89.40
O(1)-Re-Cl(1)	94.30
O(2)-Re-Cl(1)	89.60
Cl(2)-Re-Cl(1)	91.29
O(1)-Re-S(2)	92.60
O(2)-Re-S(2)	83.00
Cl(2)-Re-S(2)	90.03
Cl(1)-Re-S(2)	172.52
O(1)-Re-S(1)	88.50
O(2)-Re-S(1)	78.70
Cl(2)-Re-S(1)	167.99
Cl(1)-Re-S(1)	90.70
S(2)-Re-S(1)	86.52
C(3)-S(1)-C(1)	104.40
C(3)-S(1)-Re	97.60
C(1)-S(1)-Re	103.30
C(5)-S(2)-C(2)	105.50
C(5)-S(2)-Re	107.70
C(2)-S(2)-Re	103.10
C(4)-O(2)-Re	131.40



Dichloro[8-hydroxy-3,6-dithiaoctane-2-olato(O,S,S)]oxotechnetium(V)

$C_6H_{12}Cl_2O_3S_2Tc$

8.0863Å	11.1899Å	27.4264Å	
90.0130°	90.0520°	90.1170°	V=2481.6Å^3
Pbca; 61	Z=8; F(000)=1472	ρ=1.966g/cm^3	R=6.9%
orthorhombic			

H.-J. Pietzsch, H. Spies, P. Leibnitz, G. Reck, J. Beger, R. Jacobi
"Technetium complexes with thioether ligands. II. Synthesis and structural characterization of neutral oxotechnetium (V) complexes with dithioethers. X-ray structure analysis of oxo-bis(5,8-dithiadodecane)dichlorooxotechnetium(V) and (8-hydroxy-3,6-dithiaoctane-1-olato)dichlorotechnetium(V)"
Polyhedron 12 (1993) 187-193
CSD No. 55698

Tc 48

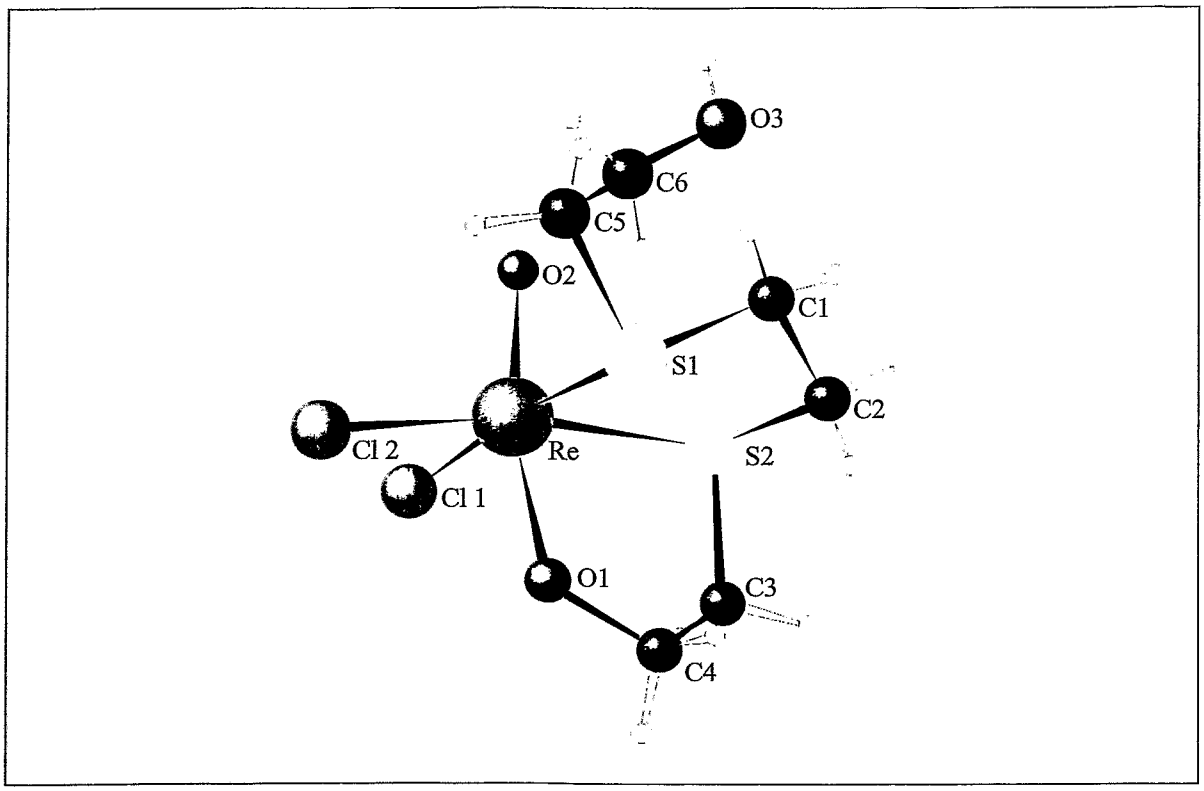
Selected Bonds (Å) and Angles (°)

Bonds

Tc-O(1)	1.677
Tc-O(2)	1.892
Tc-Cl(2)	2.410
Tc-S(2)	2.437
Tc-S(1)	2.447
Tc-Cl(1)	2.464
S(1)-C(1)	1.790
S(1)-C(3)	1.870
S(2)-C(5)	1.818
S(2)-C(4)	1.810
O(2)-C(2)	1.407
C(1)-C(2)	1.590
C(3)-C(4)	1.440
C(5)-C(6')	1.500
C(5)-C(6)	1.500
C(6)-O(3)	1.329
C(6')-O(3')	1.331

Angles

O(1)-Tc-O(2)	164.20
O(1)-Tc-Cl(2)	104.40
O(2)-Tc-Cl(2)	90.40
O(1)-Tc-S(2)	88.10
O(2)-Tc-S(2)	85.10
Cl(2)-Tc-S(2)	93.71
O(1)-Tc-S(1)	86.10
O(2)-Tc-S(1)	79.00
Cl(2)-Tc-S(1)	169.31
S(2)-Tc-S(1)	84.46
O(1)-Tc-Cl(1)	93.10
O(2)-Tc-Cl(1)	92.10
Cl(2)-Tc-Cl(1)	91.90
S(2)-Tc-Cl(1)	173.76
S(1)-Tc-Cl(1)	89.52
C(1)-S(1)-Tc	98.80
C(3)-S(1)-Tc	102.60
C(5)-S(2)-Tc	106.60
C(4)-S(2)-Tc	99.10
C(2)-O(2)-Tc	131.10



Dichloro[8-hydroxy-3,6-dithiaoctane-2-olato(O,S,S)]oxorhenium(V)

$C_6H_{13}Cl_2O_3ReS_2$

8.0864Å	11.2187Å	27.1627Å	
90.0000°	90.0000°	90.0000°	V=2464.2Å^3
Pbca; 61	Z=8; F(000)=1712	ρ=2.450g/cm^3	R=6.9%
orthorhombic			

H.-J. Pietzsch, M. Reisgys, H. Spies, P. Leibnitz, B. Johannsen
"Technetium and rhenium complexes with thioether ligands. V. Synthesis and structural characterzation of neutral oxorhenium (V) complexes with tridentate dithioethers"
Chem.Ber. 130 (1997) 357-361
CSD No. 405742

Re 48

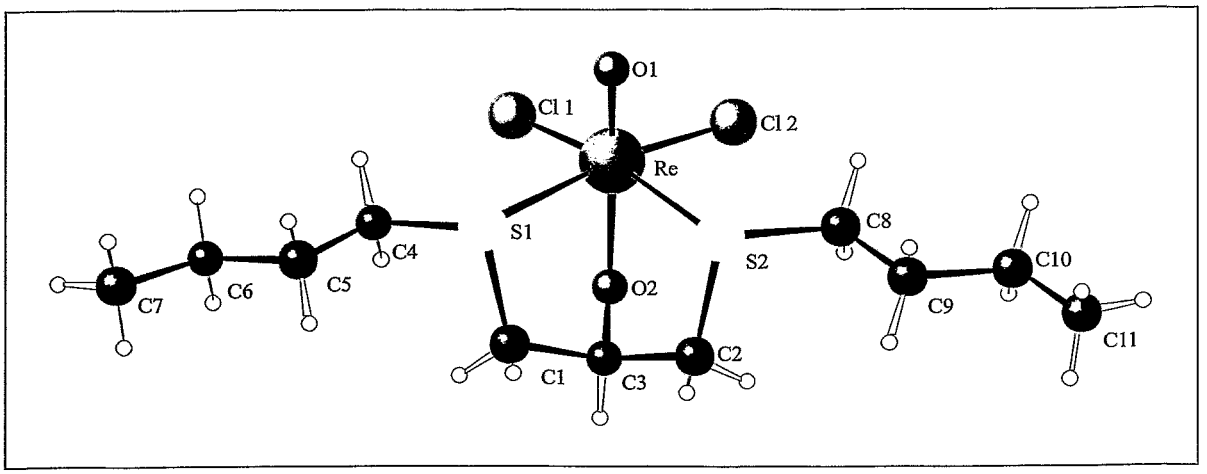
Selected Bonds (Å) and Angles (°)

Bonds

Re(1)-O(2)	1.710
Re(1)-O(1)	1.907
Re(1)-Cl(2)	2.394
Re(1)-S(1)	2.420
Re(1)-S(2)	2.442
Re(1)-Cl(1)	2.440
S(1)-C(5)	1.780
S(1)-C(1)	1.790
S(2)-C(3)	1.740
S(2)-C(2)	1.880
O(1)-C(4)	1.410
C(1)-C(2)	1.470
C(1)-H(1A)	0.970
C(1)-H(1B)	0.970
C(2)-H(2A)	0.970
C(2)-H(2B)	0.970
C(3)-C(4)	1.590
C(3)-H(3A)	0.970
C(3)-H(3B)	0.970
C(4)-H(4A)	0.970
C(4)-H(4B)	0.970
C(5)-C(6)	1.600
C(5)-H(5A)	0.970
C(5)-H(5B)	0.970

Angles

O(2)-Re(1)-O(1)	165.40
O(2)-Re(1)-Cl(2)	104.60
O(1)-Re(1)-Cl(2)	89.30
O(2)-Re(1)-S(1)	88.40
O(1)-Re(1)-S(1)	85.90
Cl(2)-Re(1)-S(1)	94.10
O(2)-Re(1)-S(2)	86.80
O(1)-Re(1)-S(2)	79.30
Cl(2)-Re(1)-S(2)	168.60
S(1)-Re(1)-S(2)	84.90
O(2)-Re(1)-Cl(1)	93.80
O(1)-Re(1)-Cl(1)	90.70
Cl(2)-Re(1)-Cl(1)	90.60
S(1)-Re(1)-Cl(1)	174.20
S(2)-Re(1)-Cl(1)	89.80
C(5)-S(1)-C(1)	102.60
C(5)-S(1)-Re(1)	106.50
C(1)-S(1)-Re(1)	99.70
C(3)-S(2)-C(2)	100.90
C(3)-S(2)-Re(1)	98.30
C(2)-S(2)-Re(1)	102.50
C(4)-O(1)-Re(1)	131.00
C(2)-C(1)-S(1)	111.00
C(2)-C(1)-H(1A)	109.00



Dichloro[5,9-dithiatridecane-7-olato-(O,S,S)]oxorhenium (V)

$C_{11}H_{23}Cl_2O_2ReS_2$

7.9045Å	9.5736	23.2455Å	
90.0000°	90.0000°	90.0000°	V=1759.1Å^3
$P2_12_12_1$	Z=4; F(000)=984	ρ=1.920g/cm^3	R=5.6%
orthorhombic			

H.-J. Pietzsch, M. Reisgys, H. Spies, P. Leibnitz, B. Johannsen
"Technetium and rhenium complexes with thioether ligands. V. Synthesis and structural characterzation of neutral oxorhenium (V) complexes with tridentate dithioethers"
Chem.Ber. 130 (1997) 357-361
CSD No.405741

Re 49

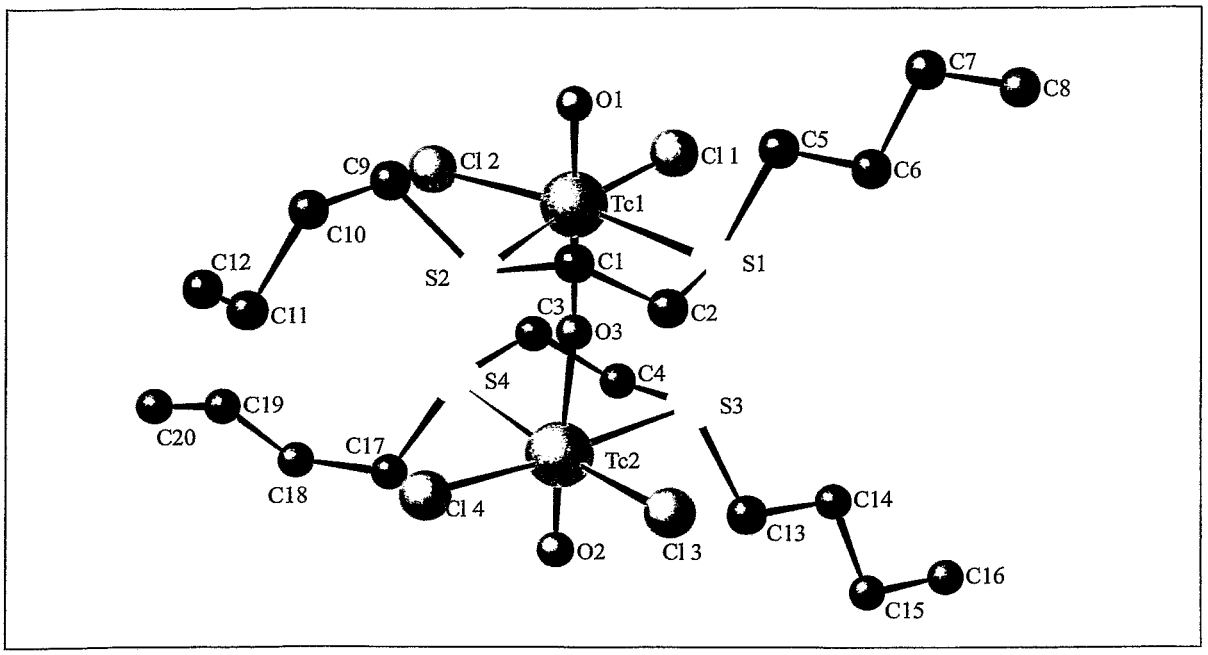
Selected Bonds (Å) and Angles (°)

Bonds

Re-O(1)	1.692
Re-O(2)	1.953
Re-Cl(2)	2.363
Re-Cl(1)	2.370
Re-S(2)	2.462
Re-S(1)	2.482
O(2)-C	1.384
C(1)-C	1.530
C(1)-S(1)	1.804
C-C(2)	1.540
C(2)-S(2)	1.785
S(1)-C(11)	1.829
C(11)-C(12)	1.520
C(12)-C(13)	1.530
C(13)-C(14)	1.480
S(2)-C(21)	1.804
C(21)-C(22)	1.530
C(22)-C(23)	1.480
C(23)-C(24)	1.530

Angles

O(1)-Re-O(2)	157.80
O(1)-Re-Cl(2)	103.40
O(2)-Re-Cl(2)	92.70
O(1)-Re-Cl(1)	103.00
O(2)-Re-Cl(1)	93.30
Cl(2)-Re-Cl(1)	85.80
O(1)-Re-S(2)	86.40
O(2)-Re-S(2)	77.30
Cl(2)-Re-S(2)	93.34
Cl(1)-Re-S(2)	170.49
O(1)-Re-S(1)	86.30
O(2)-Re-S(1)	77.70
Cl(2)-Re-S(1)	170.26
Cl(1)-Re-S(1)	93.04
S(2)-Re-S(1)	86.21
C-O(2)-Re	119.10
C(1)-S(1)-Re	98.10
C(11)-S(1)-Re	108.70
C(2)-S(2)-Re	98.80
C(21)-S(2)-Re	110.30



μ-Oxo-bis[(5.8-dithiadodecane)dichlorooxotechnetium(V)]

$C_{20}H_{44}Cl_4O_3S_4Tc_2$

16.4747Å	17.0446Å	23.7569Å	
89.9630°	89.7550°	90.0040°	V=6670.3Å^3
Pbca; 61	Z=8; F(000)=3248	ρ=1.562g/cm^3	R=7.8%
orthorhombic			

H.-J. Pietzsch, H. Spies, P. Leibnitz, G. Reck, J. Beger, R. Jacobi
"Technetium complexes with thioether ligands. II. Synthesis and structural characterization of neutral oxotechnetium (V) complexes with dithioethers. X-ray structure analysis of oxo-bis(5,8 dithiadodecane)dichlorooxotechnetium(V) and (8-hydroxy-3,6-dithiaoctane-1-olato)dichlorotechnetium(V)"
Polyhedron 12 (1993) 187-193
CSD No. 55698

Selected Bonds (Å) and Angles (°)

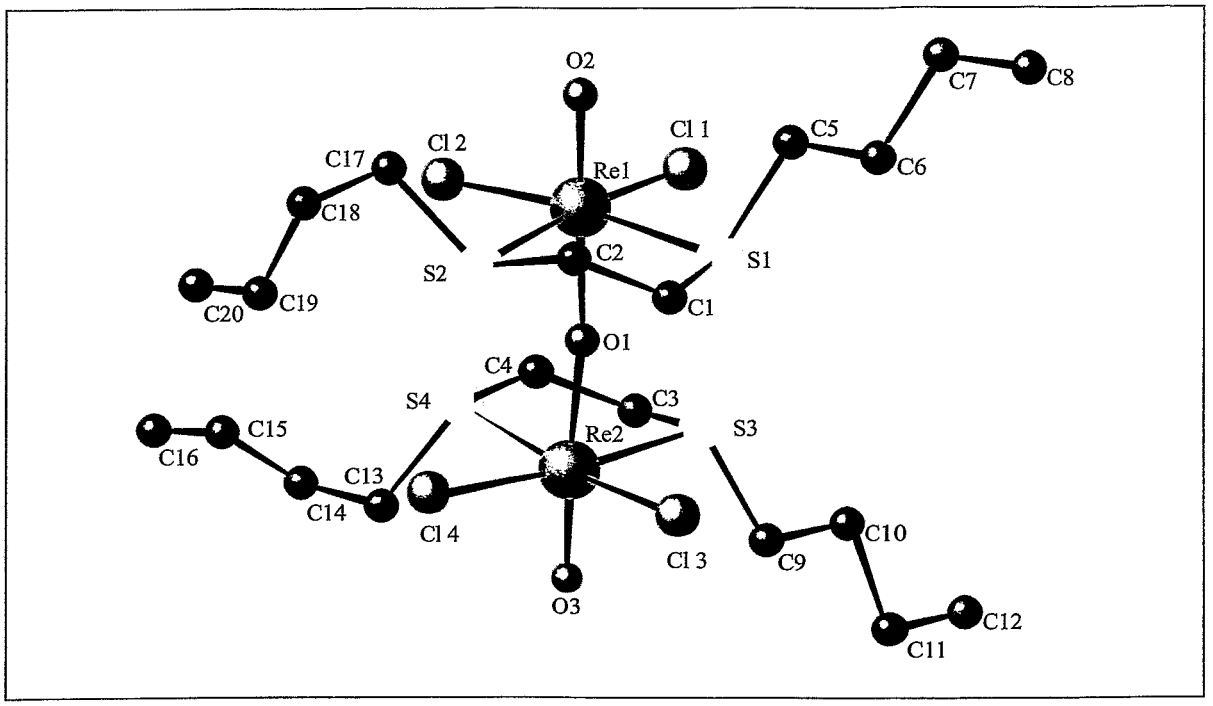
Bonds

Tc(1)-O(1)	1.676
Tc(1)-O(3)	1.896
Tc(1)-Cl(1)	2.398
Tc(1)-Cl(2)	2.402
Tc(1)-S(2)	2.431
Tc(1)-S(1)	2.448
Tc(2)-O(2)	1.672
Tc(2)-O(3)	1.895
Tc(2)-Cl(4)	2.391
Tc(2)-Cl(3)	2.393
Tc(2)-S(3)	2.433
Tc(2)-S(4)	2.438
S(1)-C(2)	1.797
S(1)-C(5)	1.838
S(2)-C(9)	1.805
S(2)-C(1)	1.841
S(3)-C(13)	1.824
S(3)-C(4)	1.880
S(4)-C(3)	1.740
S(4)-C(17)	1.767
C(1)-C(2)	1.440
C(3)-C(4)	1.360
C(5)-C(6)	1.470
C(6)-C(7)	1.490
C(7)-C(8)	1.470
C(9)-C(10)	1.370
C(10)-C(11)	1.520
C(11)-C(12)	1.390
C(13)-C(14)	1.430
C(14)-C(15)	1.490
C(15)-C(16)	1.450
C(17)-C(18)	1.310
C(18)-C(19)	1.400
C(19)-C(20)	1.460

Angles

O(1)-Tc(1)-O(3)	167.00
O(1)-Tc(1)-Cl(1)	97.50
O(3)-Tc(1)-Cl(1)	92.20
O(1)-Tc(1)-Cl(2)	97.30
O(3)-Tc(1)-Cl(2)	91.20
Cl(1)-Tc(1)-Cl(2)	90.85
O(1)-Tc(1)-S(2)	87.00
O(3)-Tc(1)-S(2)	82.60
Cl(1)-Tc(1)-S(2)	173.38
Cl(2)-Tc(1)-S(2)	93.39
O(1)-Tc(1)-S(1)	88.80
O(3)-Tc(1)-S(1)	82.50
Cl(1)-Tc(1)-S(1)	90.17
Cl(2)-Tc(1)-S(1)	173.68
S(2)-Tc(1)-S(1)	85.07
O(2)-Tc(2)-O(3)	166.00
O(2)-Tc(2)-Cl(4)	97.20
O(3)-Tc(2)-Cl(4)	93.00
O(2)-Tc(2)-Cl(3)	98.00
O(3)-Tc(2)-Cl(3)	91.40
Cl(4)-Tc(2)-Cl(3)	90.60
O(2)-Tc(2)-S(3)	87.50
O(3)-Tc(2)-S(3)	81.90
Cl(4)-Tc(2)-S(3)	174.35
Cl(3)-Tc(2)-S(3)	91.81
O(2)-Tc(2)-S(4)	88.30
O(3)-Tc(2)-S(4)	82.20
Cl(4)-Tc(2)-S(4)	90.03
Cl(3)-Tc(2)-S(4)	173.57
S(3)-Tc(2)-S(4)	87.03
C(2)-S(1)-Tc(1)	102.70
C(5)-S(1)-Tc(1)	104.30
C(9)-S(2)-Tc(1)	107.60
C(1)-S(2)-Tc(1)	97.20
C(13)-S(3)-Tc(2)	105.00

Re 50



μ-Oxo-bis[(5.8-dithiadodecane)dichlorooxorhenium(V)]

$C_{20}H_{44}Cl_4O_3Re_2S_4$

16.5912Å	17.1981Å	23.6051Å	
90.0000°	90.0000°	90.0000°	V=6735.3Å^3
Pbca; 61	Z=8; F(000)=3760	ρ=1.923g/cm^3	R=6.4%
orthorhombic			

H.-J. Pietzsch, H.Spies, P.Leibnitz, and G. Reck
"Technetium-and rhenium complexes with thioether ligands. IV. Synthesis and structural characterization of binuclear oxorhenium (V) complexes with bidentate thioether coordination"
Polyhedron 14 (1995) 1849-1853
CSD No. 401343

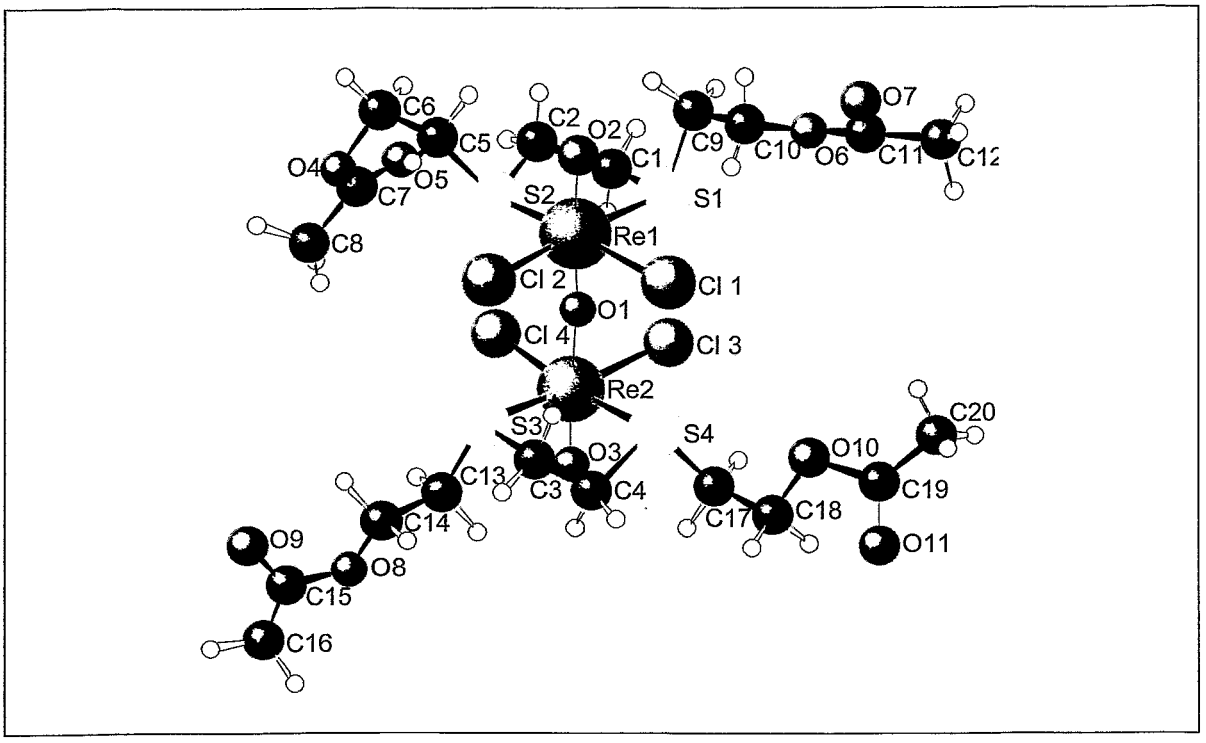
Selected Bonds (Å) and Angles (°)

Bonds

Re(1)-O(1)	1.683
Re(1)-O(3)	1.900
Re(1)-Cl(2)	2.399
Re(1)-Cl(1)	2.407
Re(1)-S(2)	2.411
Re(1)-S(1)	2.441
Re(2)-O(2)	1.689
Re(2)-O(3)	1.932
Re(2)-Cl(4)	2.394
Re(2)-Cl(3)	2.401
Re(2)-S(3)	2.423
Re(2)-S(4)	2.423
S(1)-C(2)	1.800
S(1)-C(5)	1.810
S(2)-C(9)	1.800
S(2)-C(1)	1.840
S(3)-C(4)	1.810
S(3)-C(13)	1.810
S(4)-C(3)	1.770
S(4)-C(17)	1.800
C(1)-C(2)	1.420
C(3)-C(4)	1.380
C(5)-C(6)	1.490
C(6)-C(7)	1.520
C(7)-C(8)	1.480
C(9)-C(10)	1.450
C(10)-C(11)	1.550
C(11)-C(12)	1.450
C(13)-C(14)	1.480
C(14)-C(15)	1.550

Angles

O(1)-Re(1)-O(3)	169.30
O(1)-Re(1)-Cl(2)	96.20
O(3)-Re(1)-Cl(2)	90.80
O(1)-Re(1)-Cl(1)	97.00
O(3)-Re(1)-Cl(1)	91.10
Cl(2)-Re(1)-Cl(1)	89.60
O(1)-Re(1)-S(2)	88.20
O(3)-Re(1)-S(2)	83.30
Cl(2)-Re(1)-S(2)	93.50
Cl(1)-Re(1)-S(2)	173.70
O(1)-Re(1)-S(1)	89.90
O(3)-Re(1)-S(1)	83.00
Cl(2)-Re(1)-S(1)	173.71
Cl(1)-Re(1)-S(1)	91.20
S(2)-Re(1)-S(1)	85.20
O(2)-Re(2)-O(3)	168.20
O(2)-Re(2)-Cl(4)	97.10
O(3)-Re(2)-Cl(4)	92.60
O(2)-Re(2)-Cl(3)	96.40
O(3)-Re(2)-Cl(3)	90.50
Cl(4)-Re(2)-Cl(3)	89.40
O(2)-Re(2)-S(3)	87.70
O(3)-Re(2)-S(3)	82.30
Cl(4)-Re(2)-S(3)	174.30
Cl(3)-Re(2)-S(3)	93.10
O(2)-Re(2)-S(4)	90.40
O(3)-Re(2)-S(4)	82.70
Cl(4)-Re(2)-S(4)	90.30
Cl(3)-Re(2)-S(4)	173.10
S(3)-Re(2)-S(4)	86.60



μ-Oxo-bis[(1.8-diacetoxy-3.6-dithiaoctane)]dichlorooxorhenium(V)

$C_{20}H_{36}Cl_4O_{11}Re_2S_4$

17.1354Å	8.5272Å	23.3449Å	
90.0000°	90.0000°	90.0000°	V=3411.2Å^3
$Pna2_1$; 33	Z=4; F(000)=2104	ρ=2.132g/cm^3	R=7.3%
orthorhombic			

H.-J. Pietzsch, M. Reisgys, H. Spies, P. Leibnitz and B. Johannsen
"Technetium and rhenium complexes with thioether ligands. V. Synthesis and structural characterization of neutral oxorhenium (V) complexes with tridentate dithioethers"
Chem.Ber. 130 (1997) 357-361
CSD No. 405744

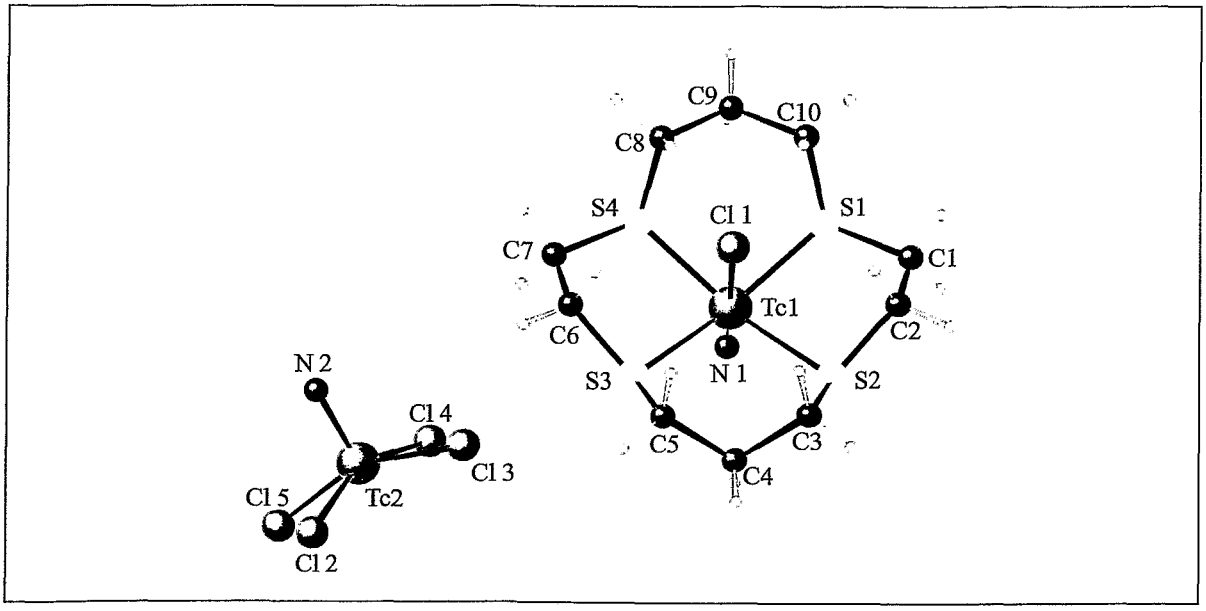
Selected Bonds (Å) and Angles (°)

Bonds

Re(1)-O(2)	1.730
Re(1)-O(1)	1.900
Re(1)-Cl(2)	2.361
Re(1)-S(2)	2.367
Re(1)-Cl(1)	2.480
Re(1)-S(1)	2.496
Re(2)-O(3)	1.680
Re(2)-O(1)	1.940
Re(2)-Cl(4)	2.374
Re(2)-S(3)	2.416
Re(2)-Cl(3)	2.439
Re(2)-S(4)	2.451
S(1)-C(1)	1.750
S(1)-C(9)	1.840
S(2)-C(2)	1.810
S(2)-C(5)	1.810
S(3)-C(13)	1.810
S(3)-C(3)	1.910
S(4)-C(17)	1.810
S(4)-C(4)	1.820
O(4)-C(7)	1.390
O(4)-C(6)	1.400
O(5)-C(7)	1.260
O(6)-C(11)	1.340
O(6)-C(10)	1.500
O(7)-C(11)	1.180
O(8)-C(14)	1.390
O(8)-C(15)	1.400
C(16)-C(15)	1.490
O(10)-C(18)	1.400
O(10)-C(19)	1.430
O(11)-C(19)	1.300
C(1)-C(2)	1.580
C(3)-C(4)	1.400
C(5)-C(6)	1.530
C(7)-C(8)	1.620

Angles

O(2)-Re(1)-O(1)	167.30
O(2)-Re(1)-Cl(2)	96.20
O(1)-Re(1)-Cl(2)	95.00
O(2)-Re(1)-S(2)	91.30
O(1)-Re(1)-S(2)	82.20
Cl(2)-Re(1)-S(2)	93.60
O(2)-Re(1)-Cl(1)	95.70
O(1)-Re(1)-Cl(1)	90.30
Cl(2)-Re(1)-Cl(1)	88.80
S(2)-Re(1)-Cl(1)	172.30
O(2)-Re(1)-S(1)	87.80
O(1)-Re(1)-S(1)	81.00
Cl(2)-Re(1)-S(1)	176.00
S(2)-Re(1)-S(1)	86.00
Cl(1)-Re(1)-S(1)	91.00
O(3)-Re(2)-O(1)	166.60
O(3)-Re(2)-Cl(4)	98.50
O(1)-Re(2)-Cl(4)	92.50
O(3)-Re(2)-S(3)	89.90
O(1)-Re(2)-S(3)	82.00
Cl(4)-Re(2)-S(3)	93.40
O(3)-Re(2)-Cl(3)	97.30
O(1)-Re(2)-Cl(3)	90.30
Cl(4)-Re(2)-Cl(3)	89.00
S(3)-Re(2)-Cl(3)	172.00
O(3)-Re(2)-S(4)	89.70
O(1)-Re(2)-S(4)	79.20
Cl(4)-Re(2)-S(4)	171.70
S(3)-Re(2)-S(4)	85.80
Cl(3)-Re(2)-S(4)	90.70
C(1)-S(1)-Re(1)	101.80
C(9)-S(1)-Re(1)	107.20
C(2)-S(2)-Re(1)	102.60
C(5)-S(2)-Re(1)	105.50
C(13)-S(3)-Re(2)	104.70
C(3)-S(3)-Re(2)	100.00



Chloro[1,4,8,11-tetrathiacyclotetradecane-(S,S,S,S)]nitridotechnetium(V) tetrachloronitridotechnetate(VI)

$C_{10}H_{20}Cl_5N_2S_4Tc_2$

13.2152	7.7255Å	21.6062Å	
90.0000°	105.8220°	90.0000°	V=2122.3Å^3
$P2_1/n$; 1014	Z=4; F(000)=1316	ρ=2.100g/cm^3	R=2.7%
monoclinic			

H.-J. Pietzsch, H. Spies, P. Leibnitz, G. Reck
"Technetium complexes with thioether ligands. III. Synthesis and structural characterization of cationic nitridotechnetium (V) complexes with thiacrown ethers"
Polyhedron 12 (1993) 2995-3002
CSD No. 56459

Tc 52

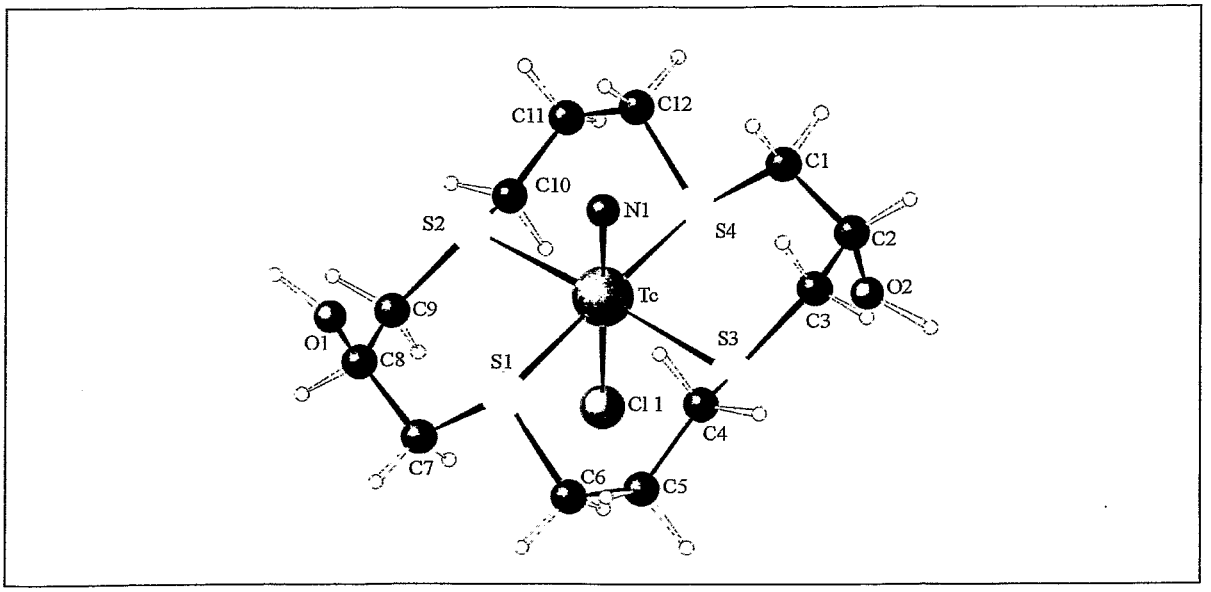
Selected Bonds (Å) and Angles (°)

Bonds

Tc(1)-N(1)	1.615
Tc(1)-S(4)	2.408
Tc(1)-S(3)	2.405
Tc(1)-S(2)	2.411
Tc(1)-S(1)	2.414
Tc(1)-Cl(1)	2.718
Tc(2)-N(2)	1.582
Tc(2)-Cl(2)	2.325
Tc(2)-Cl(3)	2.329
Tc(2)-Cl(5)	2.337
Tc(2)-Cl(4)	2.345
S(1)-C(1)	1.840
S(1)-C(10)	1.835
S(2)-C(3)	1.817
S(2)-C(2)	1.836
S(3)-C(5)	1.825
S(3)-C(6)	1.848
S(4)-C(8)	1.831
S(4)-C(7)	1.840
C(1)-C(2)	1.529
C(3)-C(4)	1.541
C(4)-C(5)	1.551
C(6)-C(7)	1.520
C(8)-C(9)	1.549
C(9)-C(10)	1.546

Angles

N(1)-Tc(1)-S(4)	95.20
N(1)-Tc(1)-S(3)	95.30
S(4)-Tc(1)-S(3)	85.29
N(1)-Tc(1)-S(2)	95.00
S(4)-Tc(1)-S(2)	169.10
S(3)-Tc(1)-S(2)	90.62
N(1)-Tc(1)-S(1)	97.70
S(4)-Tc(1)-S(1)	96.97
S(3)-Tc(1)-S(1)	167.50
S(2)-Tc(1)-S(1)	84.92
N(1)-Tc(1)-Cl(1)	176.40
S(4)-Tc(1)-Cl(1)	81.83
S(3)-Tc(1)-Cl(1)	86.84
S(2)-Tc(1)-Cl(1)	87.87
S(1)-Tc(1)-Cl(1)	81.34
N(2)-Tc(2)-Cl(2)	101.30
N(2)-Tc(2)-Cl(3)	102.50
Cl(2)-Tc(2)-Cl(3)	88.90
N(2)-Tc(2)-Cl(5)	100.90
Cl(2)-Tc(2)-Cl(5)	87.20
Cl(3)-Tc(2)-Cl(5)	156.58
N(2)-Tc(2)-Cl(4)	101.00
Cl(2)-Tc(2)-Cl(4)	157.62
Cl(3)-Tc(2)-Cl(4)	87.25
Cl(5)-Tc(2)-Cl(4)	87.59
C(1)-S(1)-C(10)	102.40
C(1)-S(1)-Tc(1)	100.70
C(10)-S(1)-Tc(1)	110.40
C(3)-S(2)-Tc(1)	108.30
C(2)-S(2)-Tc(1)	104.30
C(5)-S(3)-Tc(1)	107.10
C(6)-S(3)-Tc(1)	104.20
C(8)-S(4)-Tc(1)	110.60
C(7)-S(4)-Tc(1)	100.90



Chloro[1,5,9,13-tetrathiacyclohexadecane-3,11-diol-(S,S,S,S)]nitrido-technetium(V) chloride
(The counterion has been omitted.)
$C_{12}H_{24}Cl_2NO_2S_4Tc$

7.8891Å	10.8025Å	11.1362Å	
90.0000°	90.3520°	90.0000°	V=949.1Å^3
Pc; 7	Z=2; F(000)=520	ρ=1.790g/cm^3	R=4.6%
monoclinic			

H.-J. Pietzsch, H. Spies, P. Leibnitz, G. Reck
„Technetium complexes with thioether ligands. III. Synthesis and structural characterization of cationic nitridotechnetium (V) complexes with thiacrown ethers."
Polyhedron 12 (1993) 2995-3002
CSD No. 56459

Tc 53

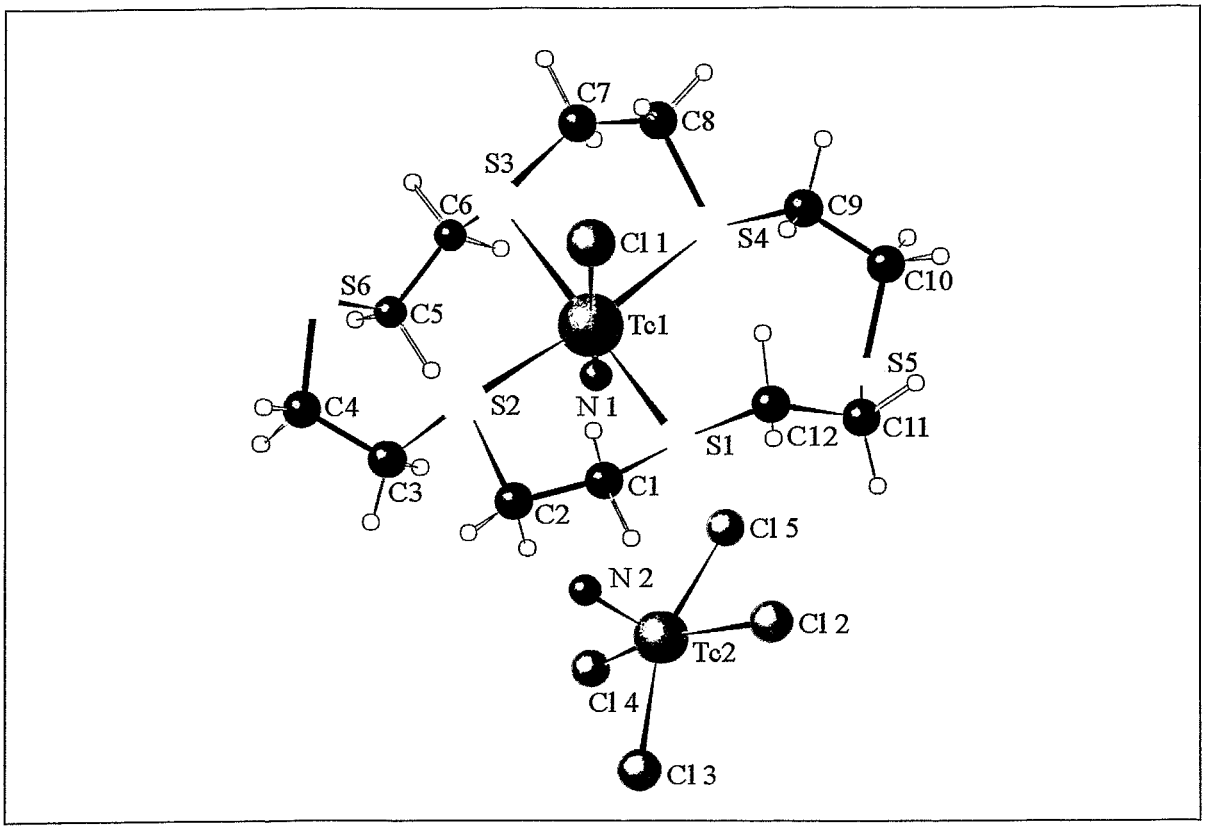
Selected Bonds (Å) and Angles (°)

Bonds

Tc-N(1)	1.974
Tc-S(3)	2.430
Tc-S(1)	2.432
Tc-S(4)	2.447
Tc-S(2)	2.451
Tc-Cl(1)	2.461
S(1)-C(6)	1.810
S(1)-C(7)	1.830
S(2)-C(10)	1.760
S(2)-C(9)	1.840
S(3)-C(3)	1.840
S(3)-C(4)	1.840
S(4)-C(1)	1.780
S(4)-C(12)	1.810
O(1)-C(8)	1.370
O(2)-C(2)	1.440
C(1)-C(2)	1.490
C(2)-C(3)	1.540
C(4)-C(5)	1.590
C(5)-C(6)	1.550
C(7)-C(8)	1.550
C(8)-C(9)	1.510
C(10)-C(11)	1.460
C(11)-C(12)	1.480

Angles

N(1)-Tc-S(3)	93.50
N(1)-Tc-S(1)	91.60
S(3)-Tc-S(1)	89.50
N(1)-Tc-S(4)	93.10
S(3)-Tc-S(4)	90.60
S(1)-Tc-S(4)	175.30
N(1)-Tc-S(2)	91.80
S(3)-Tc-S(2)	174.70
S(1)-Tc-S(2)	90.60
S(4)-Tc-S(2)	88.80
N(1)-Tc-Cl(1)	178.70
S(3)-Tc-Cl(1)	85.60
S(1)-Tc-Cl(1)	87.50
S(4)-Tc-Cl(1)	87.90
S(2)-Tc-Cl(1)	89.10
C(6)-S(1)-C(7)	97.50
C(6)-S(1)-Tc	105.60
C(7)-S(1)-Tc	108.70
C(10)-S(2)-Tc	105.10
C(9)-S(2)-Tc	111.60
C(3)-S(3)-Tc	104.90
C(4)-S(3)-Tc	104.20
C(1)-S(4)-Tc	105.50
C(12)-S(4)-Tc	104.20



Chloro[1,4,7,10,13,16-hexathiacyclooctadecane-($S^{4,7,13,16}$)]nitridotechnetium(V) tetrachloronitridotechnetate(VI)
$C_{12}H_{24}Cl_5N_2S_6Tc_2$

12.9426Å	16.7583Å	11.5776Å	
90.0000°	95.4540°	90.0000°	V=2499.6Å^3
$P2_1/c$; 14	Z=4; F(000)=1508	ρ=2.020g/cm^3	R=3.5%
monoclinic			

H.-J. Pietzsch, H. Spies, P. Leibnitz, G. Reck,
"Technetium complexes with thioether ligands. III. Synthesis and structural characterization of cationic nitridotechnetium(V) complexes with thiacrown ethers."
Polyhedron 12 (1993) 2995-3002
CSD No. 56459

Tc 54

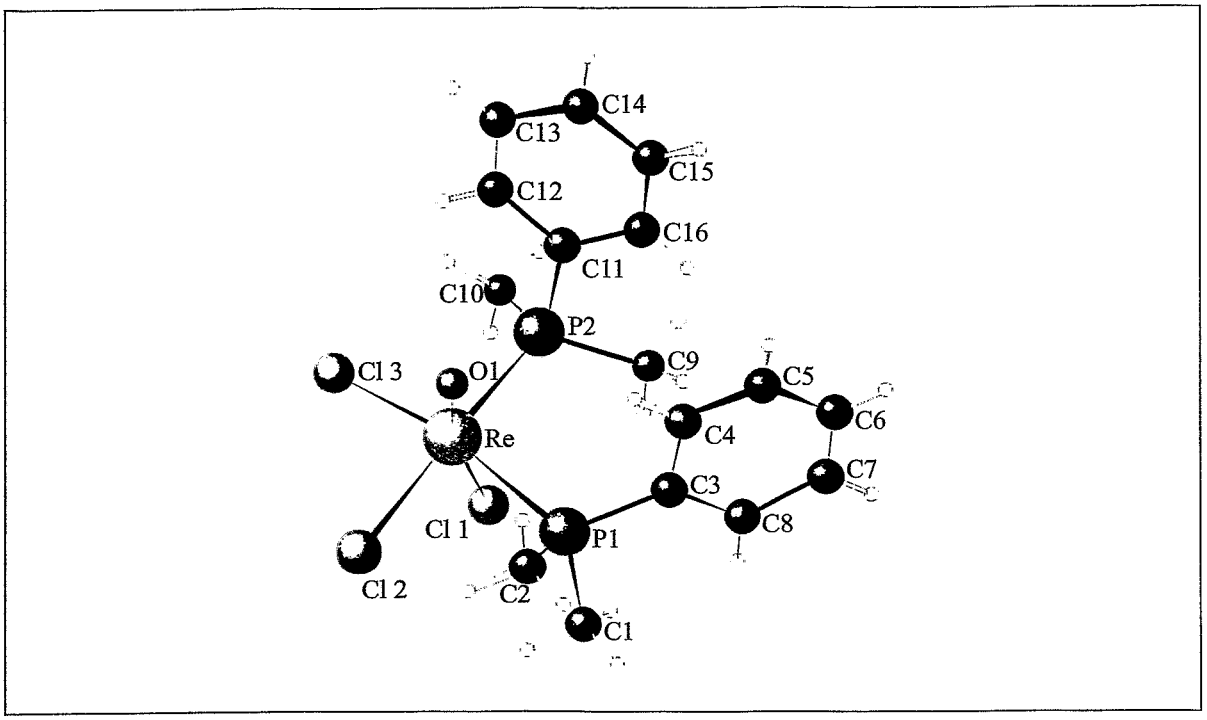
Selected Bonds (Å) and Angles (°)

Bonds

Tc(1)-N(1)	1.704
Tc(1)-S(4)	2.461
Tc(1)-S(3)	2.463
Tc(1)-S(1)	2.468
Tc(1)-S(2)	2.499
Tc(1)-Cl(1)	2.565
Tc(2)-N(2)	1.610
Tc(2)-Cl(3)	2.332
Tc(2)-Cl(5)	2.338
Tc(2)-Cl(4)	2.345
Tc(2)-Cl(2)	2.351
S(1)-C(1)	1.814
S(1)-C(12)	1.817
S(2)-C(3)	1.826
S(2)-C(2)	1.834
S(3)-C(6)	1.823
S(3)-C(7)	1.835
S(4)-C(9)	1.818
S(4)-C(8)	1.818
S(5)-C(11)	1.807
S(5)-C(10)	1.808
S(6)-C(4)	1.794
S(6)-C(5)	1.800
C(1)-C(2)	1.497
C(3)-C(4)	1.525
C(5)-C(6)	1.510
C(7)-C(8)	1.489
C(9)-C(10)	1.522
C(11)-C(12)	1.523

Angles

N(1)-Tc(1)-S(4)	90.60
N(1)-Tc(1)-S(3)	95.00
S(4)-Tc(1)-S(3)	82.36
N(1)-Tc(1)-S(1)	93.30
S(4)-Tc(1)-S(1)	100.04
S(3)-Tc(1)-S(1)	171.35
N(1)-Tc(1)-S(2)	100.90
S(4)-Tc(1)-S(2)	168.02
S(3)-Tc(1)-S(2)	93.21
S(1)-Tc(1)-S(2)	82.78
N(1)-Tc(1)-Cl(1)	177.30
S(4)-Tc(1)-Cl(1)	86.84
S(3)-Tc(1)-Cl(1)	83.95
S(1)-Tc(1)-Cl(1)	87.87
S(2)-Tc(1)-Cl(1)	81.61
N(2)-Tc(2)-Cl(3)	99.80
N(2)-Tc(2)-Cl(5)	99.90
Cl(3)-Tc(2)-Cl(5)	160.11
N(2)-Tc(2)-Cl(4)	98.20
Cl(3)-Tc(2)-Cl(4)	90.54
Cl(5)-Tc(2)-Cl(4)	89.41
N(2)-Tc(2)-Cl(2)	100.50
Cl(3)-Tc(2)-Cl(2)	87.87
Cl(5)-Tc(2)-Cl(2)	85.82
Cl(4)-Tc(2)-Cl(2)	161.22
C(1)-S(1)-Tc(1)	102.80
C(12)-S(1)-Tc(1)	115.90
C(3)-S(2)-Tc(1)	116.60
C(2)-S(2)-Tc(1)	102.80
C(6)-S(3)-Tc(1)	108.70
C(7)-S(3)-Tc(1)	105.20
C(9)-S(4)-Tc(1)	118.50
C(8)-S(4)-Tc(1)	101.90



[Bis(dimethylphenylphosphine)trichloro]oxorhenium (V)

$C_{16}H_{22}Cl_3OP_2Re$

12.5637Å	10.3345Å	16.9343Å	
90.0000°	110.7750°	90.0000°	V=2055.8Å^3
$P2_1$; 4	Z=4; F(000)=1128	ρ=1.890g/cm^3	R=8.1%
monoclinic			

H.-J. Pietzsch (1999)
not published
CCDC 161729

Re 55

Selected Bonds (Å) and Angles (°)

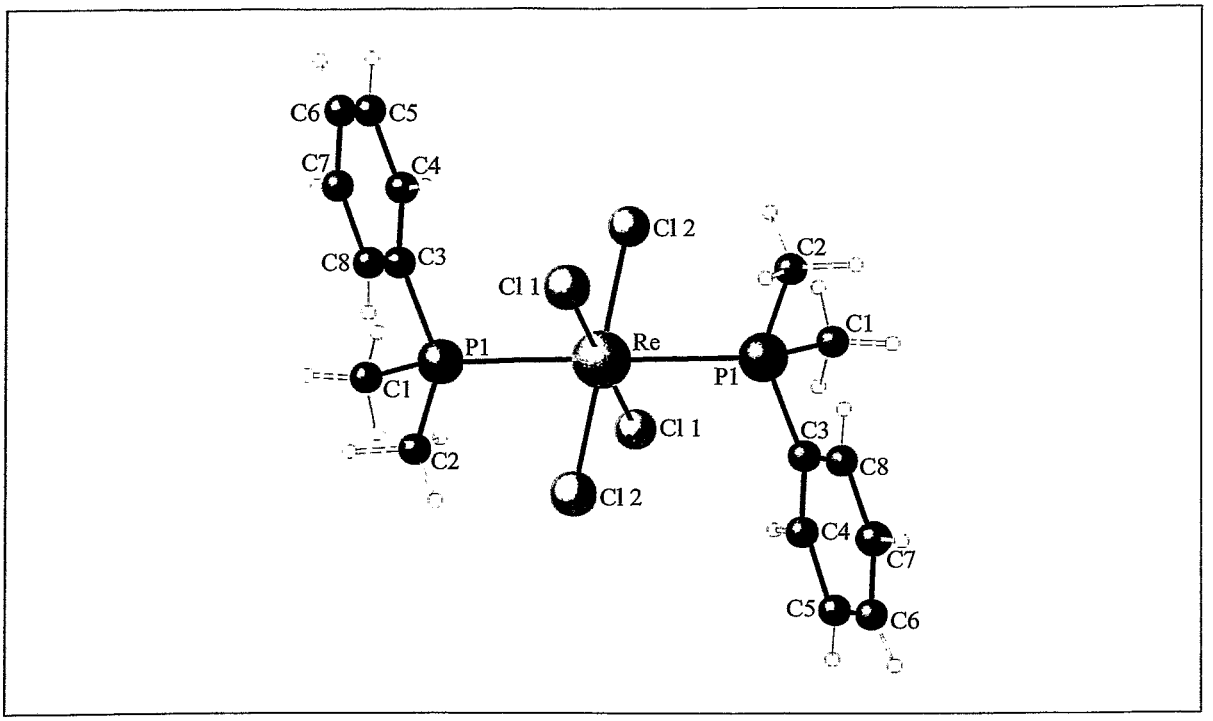
Bonds

Re(1)-O(1)	1.740
Re(1)-Cl(2)	2.385
Re(1)-Cl(3)	2.405
Re(1)-Cl(1)	2.427
Re(1)-P(2)	2.453
Re(1)-P(1)	2.481
P(1)-C(3)	1.800
P(1)-C(2)	1.800
P(1)-C(1)	1.810
P(2)-C(11)	1.790
P(2)-C(10)	1.790
P(2)-C(9)	1.810
C(3)-C(8)	1.400
C(3)-C(4)	1.410
C(4)-C(5)	1.370
C(5)-C(6)	1.400
C(6)-C(7)	1.390
C(7)-C(8)	1.410
C(11)-C(12)	1.370
C(11)-C(16)	1.400
C(12)-C(13)	1.380
C(13)-C(14)	1.370
C(14)-C(15)	1.380
C(15)-C(16)	1.410
Re(2)-O(1')	1.690
Re(2)-Cl(2')	2.373
Re(2)-Cl(3')	2.374
Re(2)-Cl(1')	2.443
Re(2)-P(1')	2.465
Re(2)-P(2')	2.489
P(1')-C(2')	1.780
P(1')-C(1')	1.810
P(1')-C(3')	1.830
P(2')-C(10')	1.770
P(2')-C(9')	1.790
P(2')-C(11')	1.800

Angles

O(1)-Re(1)-Cl(2)	102.60
O(1)-Re(1)-Cl(3)	100.60
Cl(2)-Re(1)-Cl(3)	86.70
O(1)-Re(1)-Cl(1)	166.60
Cl(2)-Re(1)-Cl(1)	87.00
Cl(3)-Re(1)-Cl(1)	89.10
O(1)-Re(1)-P(2)	92.30
Cl(2)-Re(1)-P(2)	164.90
Cl(3)-Re(1)-P(2)	88.00
Cl(1)-Re(1)-P(2)	78.80
O(1)-Re(1)-P(1)	87.20
Cl(2)-Re(1)-P(1)	83.50
Cl(3)-Re(1)-P(1)	168.60
Cl(1)-Re(1)-P(1)	84.60
P(2)-Re(1)-P(1)	100.00
C(3)-P(1)-Re(1)	118.50
C(2)-P(1)-Re(1)	107.80
C(1)-P(1)-Re(1)	114.80
C(11)-P(2)-Re(1)	111.00
C(10)-P(2)-Re(1)	114.00
C(9)-P(2)-Re(1)	117.20
O(1')-Re(2)-Cl(2')	96.50
O(1')-Re(2)-Cl(3')	104.50
Cl(2')-Re(2)-Cl(3')	88.30
O(1')-Re(2)-Cl(1')	166.70
Cl(2')-Re(2)-Cl(1')	89.70
Cl(3')-Re(2)-Cl(1')	87.40
O(1')-Re(2)-P(1')	90.10
Cl(2')-Re(2)-P(1')	89.10
Cl(3')-Re(2)-P(1')	165.40
Cl(1')-Re(2)-P(1')	78.20
O(1')-Re(2)-P(2')	88.10
Cl(2')-Re(2)-P(2')	171.50
Cl(3')-Re(2)-P(2')	83.60
Cl(1')-Re(2)-P(2')	87.20
P(1')-Re(2)-P(2')	98.10

5.3. Rhenium on the oxidation state IV



Bis(dimethylphenylphosphine)tetrachlororhenium(IV)

$C_{16}H_{22}Cl_4P_2Re$

9.7178Å	13.7333Å	8.3408Å	
90.0000°	106.8080°	90.0000°	V=1065.6Å^3
$P2_1/c$; 14	Z=2; F(000)=582	ρ=1.883g/cm^3	R=3.0%
monoclinic			

H.-J. Pietzsch (1999)
not published
CCDC 161730

Selected Bonds (Å) and Angles (°)

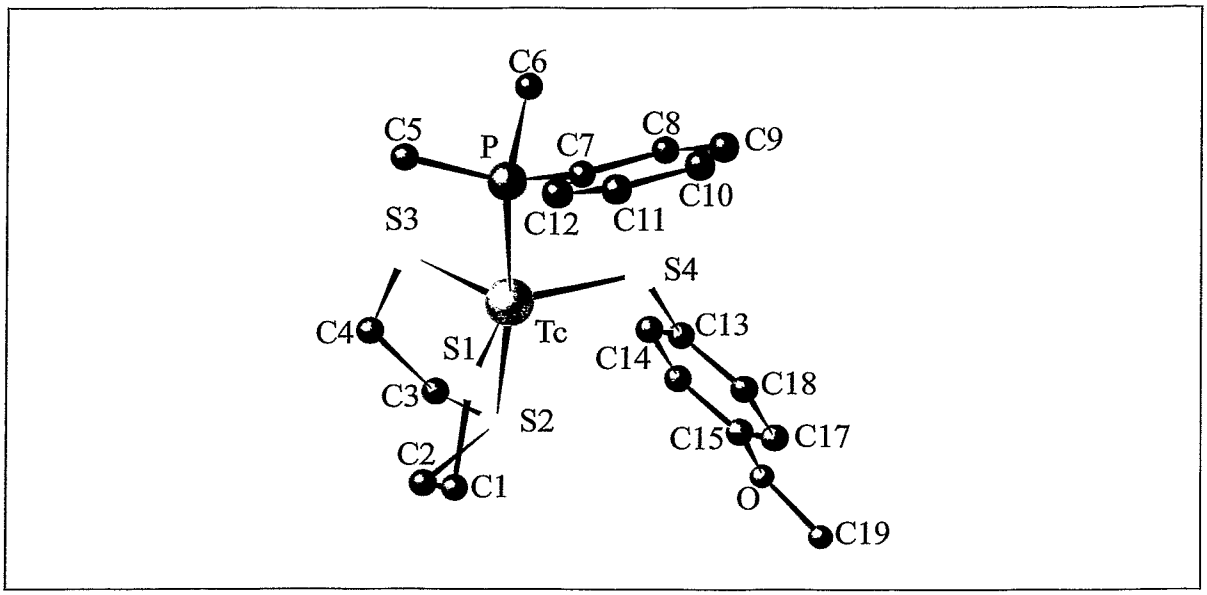
Bonds

Re(1)-Cl(1)1	2.321
Re(1)-Cl(1)	2.321
Re(1)-Cl(2)	2.338
Re(1)-Cl(2)1	2.338
Re(1)-P(1)1	2.510
Re(1)-P(1)	2.510
P(1)-C(2)	1.806
P(1)-C(3)	1.817
P(1)-C(1)	1.829
C(3)-C(8)	1.376
C(3)-C(4)	1.380
C(4)-C(5)	1.379
C(5)-C(6)	1.349
C(6)-C(7)	1.371
C(7)-C(8)	1.389

Angles

Cl(1)1-Re(1)-Cl(1)	180.00
Cl(1)1-Re(1)-Cl(2)	90.16
Cl(1)-Re(1)-Cl(2)	89.84
Cl(1)1-Re(1)-Cl(2)1	89.84
Cl(1)-Re(1)-Cl(2)1	90.16
Cl(2)-Re(1)-Cl(2)1	180.00
Cl(1)1-Re(1)-P(1)1	89.65
Cl(1)-Re(1)-P(1)1	90.35
Cl(2)-Re(1)-P(1)1	85.65
Cl(2)1-Re(1)-P(1)1	94.35
Cl(1)1-Re(1)-P(1)	90.35
Cl(1)-Re(1)-P(1)	89.65
Cl(2)-Re(1)-P(1)	94.35
Cl(2)1-Re(1)-P(1)	85.65
P(1)1-Re(1)-P(1)	180.00
C(2)-P(1)-Re(1)	112.70
C(3)-P(1)-Re(1)	115.40
C(1)-P(1)-Re(1)	112.20

5.4. Technetium and Rhenium on the oxidation state III



[(Dimethylphenylphosphine)(4-methoxybenzenethiolato)(thiapentane-1,5-dithiolato)]technetium(III)

$C_{19}H_{26}OPS_4Tc$

8.3869Å	11.1578Å	12.3806Å	
95.4960°	99.3760°	92.2350°	V=1136.1Å^3
P-1; 2	Z=2; F(000)=540	ρ=1.542g/cm^3	R=3.8%
triclinic			

H.-J. Pietzsch, F. Tisato, F. Refosco, P. Leibnitz, A. Drews, S. Seifert, H. Spies "Synthesis and characterization of novel trigonal-bipyramidal technetium(III) mixed-ligand complexes with SES/S/P coordination (E = O, N(CH_3), S)" Inorg. Chem. 40 (2001) 59-64
CCDC-146934

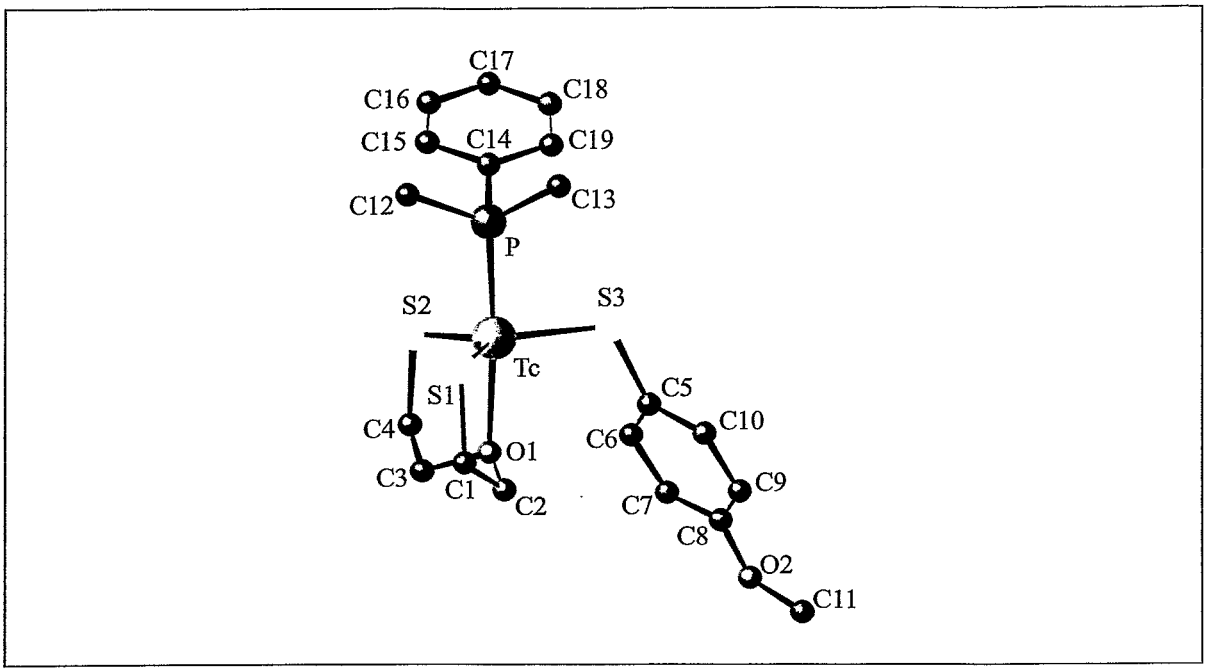
Selected Bonds (Å) and Angles (°)

Bonds

Tc(1)-S(1)	2.220
Tc(1)-S(3)	2.236
Tc(1)-S(4)	2.254
Tc(1)-P(1)	2.359
Tc(1)-S(2)	2.399
S(1)-C(1)	1.842
S(2)-C(2)	1.823
S(2)-C(3)	1.827
S(3)-C(4)	1.850
S(4)-C(13)	1.792
P(1)-C(6)	1.817
P(1)-C(7)	1.827
P(1)-C(5)	1.827
O(1)-C(16)	1.366
O(1)-C(19)	1.422
C(1)-C(2)	1.497
C(3)-C(4)	1.504
C(7)-C(12)	1.383
C(7)-C(8)	1.387
C(8)-C(9)	1.393
C(9)-C(10)	1.361
C(10)-C(11)	1.357
C(11)-C(12)	1.388
C(13)-C(18)	1.376

Angles

S(1)-Tc(1)-S(3)	116.23
S(1)-Tc(1)-S(4)	119.52
S(3)-Tc(1)-S(4)	124.26
S(1)-Tc(1)-P(1)	89.74
S(3)-Tc(1)-P(1)	91.87
S(4)-Tc(1)-P(1)	88.67
S(1)-Tc(1)-S(2)	87.09
S(3)-Tc(1)-S(2)	86.25
S(4)-Tc(1)-S(2)	96.08
P(1)-Tc(1)-S(2)	175.15
C(1)-S(1)-Tc(1)	109.00
C(2)-S(2)-C(3)	101.40
C(2)-S(2)-Tc(1)	103.92
C(3)-S(2)-Tc(1)	100.44
C(4)-S(3)-Tc(1)	107.02
C(13)-S(4)-Tc(1)	113.85
C(6)-P(1)-C(7)	103.00
C(6)-P(1)-C(5)	101.90
C(7)-P(1)-C(5)	102.80
C(6)-P(1)-Tc(1)	114.02
C(7)-P(1)-Tc(1)	118.02
C(5)-P(1)-Tc(1)	115.02
C(16)-O(1)-C(19)	117.70
C(2)-C(1)-S(1)	113.90



[(Dimethylphenylphosphine)(4-methoxybenzenethiolato)(oxapentane-1,5-dithiolato)]technetium(III)

$C_{19}H_{26}O_2S_3PTc$

7.6294Å	12.2524Å	12.8379Å	
73.0120°	81.8690°	79.7550°	V=1124.3Å^3
P-1; 2	Z=2; F(000)=524	ρ=1.511g/cm^3	R=3.0%
triclinic			

H.-J. Pietzsch, F. Tisato, F. Refosco, P. Leibnitz, A. Drews, S. Seifert, H. Spies "Synthesis and characterization of novel trigonal-bipyramidal technetium(III) mixed-ligand complexes with SES/S/P coordination (E = O, N(CH_3), S)" Inorg. Chem. 40 (2001) 59-64
CCDC-146936

Tc 58

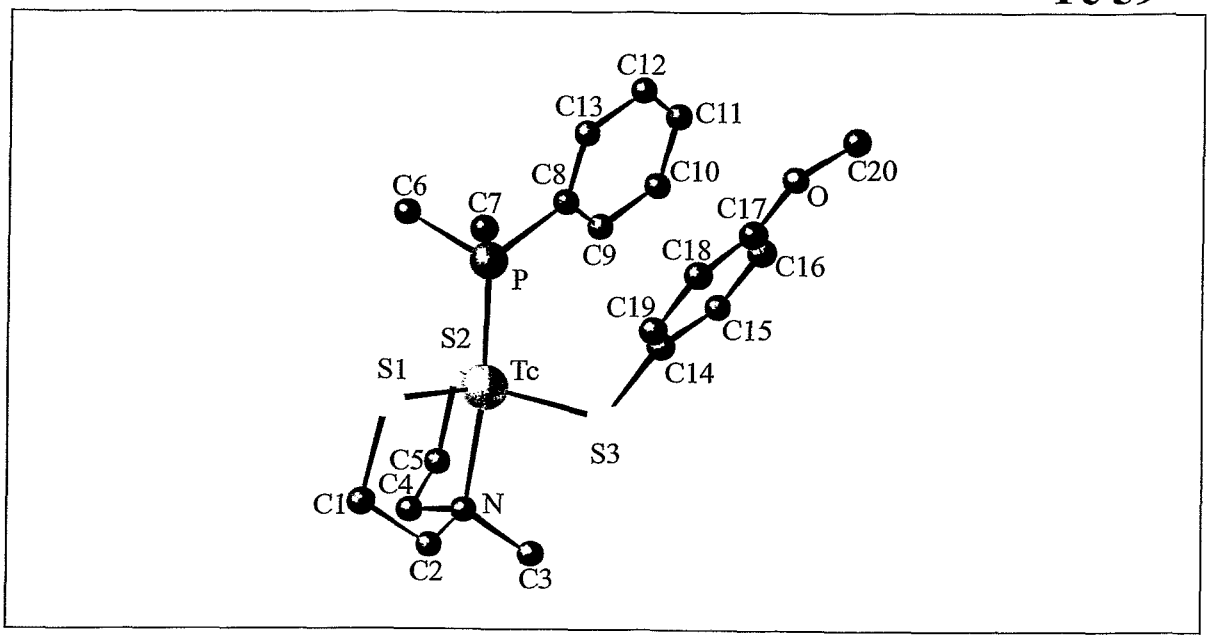
Selected Bonds (Å) and Angles (°)

Bonds

Tc(1)-S(2)	2.221
Tc(1)-S(1)	2.226
Tc(1)-O(1)	2.236
Tc(1)-S(3)	2.239
Tc(1)-P(1)	2.282
S(1)-C(1)	1.838
S(2)-C(4)	1.836
S(3)-C(5)	1.785
P(1)-C(13)	1.830
P(1)-C(12)	1.831
P(1)-C(14)	1.831
O(1)-C(2)	1.445
O(1)-C(3)	1.449
O(2)-C(8)	1.382
O(2)-C(11)	1.416
C(1)-C(2)	1.503
C(3)-C(4)	1.495
C(5)-C(6)	1.382
C(5)-C(10)	1.383
C(6)-C(7)	1.376
C(7)-C(8)	1.383
C(8)-C(9)	1.367

Angles

S(2)-Tc(1)-S(1)	119.97
S(2)-Tc(1)-O(1)	83.36
S(1)-Tc(1)-O(1)	83.58
S(2)-Tc(1)-S(3)	120.55
S(1)-Tc(1)-S(3)	119.03
O(1)-Tc(1)-S(3)	96.48
S(2)-Tc(1)-P(1)	94.59
S(1)-Tc(1)-P(1)	92.82
O(1)-Tc(1)-P(1)	174.21
S(3)-Tc(1)-P(1)	89.23
C(1)-S(1)-Tc(1)	103.69
C(4)-S(2)-Tc(1)	101.80
C(5)-S(3)-Tc(1)	112.52
C(13)-P(1)-C(12)	101.70
C(13)-P(1)-C(14)	102.80
C(12)-P(1)-C(14)	103.03
C(13)-P(1)-Tc(1)	116.30
C(12)-P(1)-Tc(1)	114.44
C(14)-P(1)-Tc(1)	116.54
C(2)-O(1)-C(3)	113.30
C(2)-O(1)-Tc(1)	110.00
C(3)-O(1)-Tc(1)	111.40



(Dimethylphenylphosphine)(4-methoxybenzenethiolato)[(3-N-methyl)azapentane-1,5-dithiolato]technetium(III)

$C_{20}H_{29}NOPS_3Tc$

13.3054Å	9.4678Å	18.7909Å	
90.0000°	100.7080°	90.0000°	V=2325.9Å^3
$P2_1/c$; 14	Z=4; F(000)=1080	ρ=1.498g/cm^3	R=2.4%
monoclinic			

H.-J. Pietzsch, F. Tisato, F. Refosco, P. Leibnitz, A. Drews, S. Seifert, H. Spies "Synthesis and characterization of novel trigonal-bipyramidal technetium(III) mixed-ligand complexes with SES/S/P coordination (E = O, $N(CH_3)$, S)" Inorg. Chem. 40 (2001) 59-64
CCDC-146935

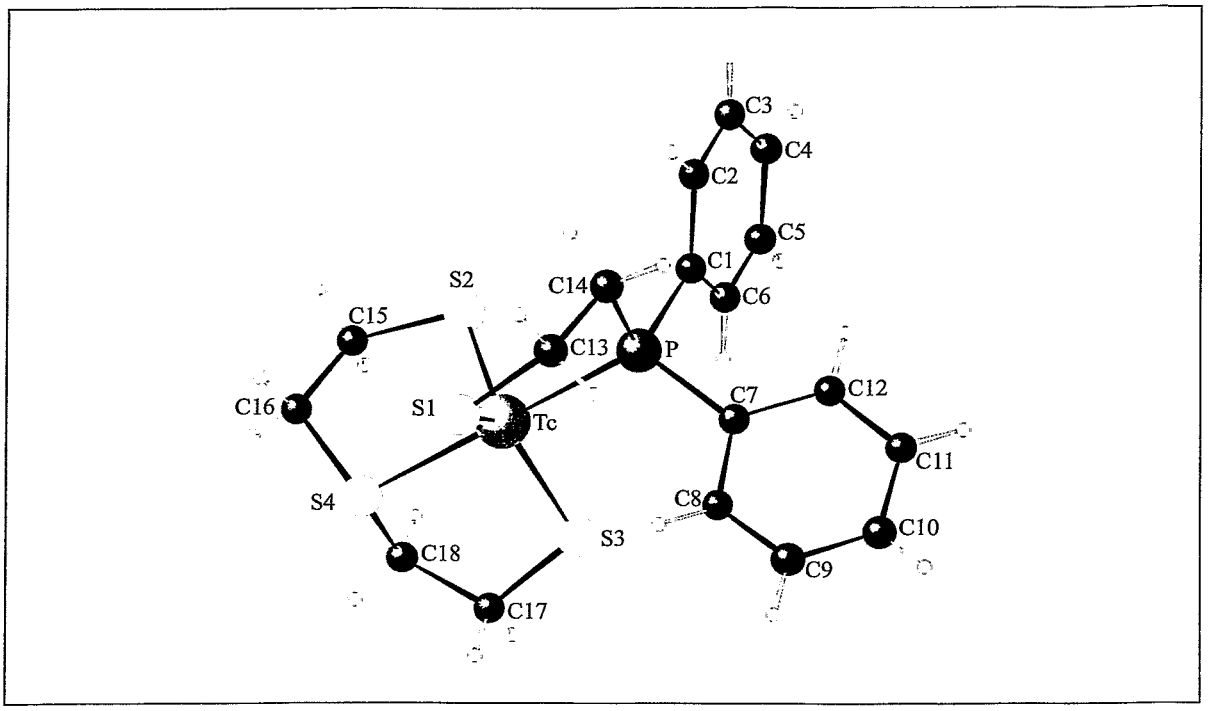
Selected Bonds (Å) and Angles (°)

Bonds

Tc(1)-S(1)	2.220
Tc(1)-S(2)	2.233
Tc(1)-S(3)	2.255
Tc(1)-N(1)	2.273
Tc(1)-P(1)	2.319
P(1)-C(7)	1.826
P(1)-C(6)	1.828
P(1)-C(8)	1.835
S(1)-C(1)	1.836
S(2)-C(5)	1.840
S(3)-C(14)	1.783
N(1)-C(3)	1.482
N(1)-C(2)	1.486
N(1)-C(4)	1.492
O(1)-C(17)	1.376
O(1)-C(20)	1.411
C(1)-C(2)	1.500
C(4)-C(5)	1.505
C(8)-C(9)	1.382
C(8)-C(13)	1.385
C(9)-C(10)	1.381
C(10)-C(11)	1.373

Angles

S(1)-Tc(1)-S(2)	116.77
S(1)-Tc(1)-S(3)	120.02
S(2)-Tc(1)-S(3)	121.87
S(1)-Tc(1)-N(1)	84.42
S(2)-Tc(1)-N(1)	84.70
S(3)-Tc(1)-N(1)	89.23
S(1)-Tc(1)-P(1)	90.00
S(2)-Tc(1)-P(1)	92.45
S(3)-Tc(1)-P(1)	98.82
N(1)-Tc(1)-P(1)	171.77
C(7)-P(1)-C(6)	99.57
C(7)-P(1)-C(8)	100.21
C(6)-P(1)-C(8)	103.63
C(7)-P(1)-Tc(1)	112.68
C(6)-P(1)-Tc(1)	117.49
C(8)-P(1)-Tc(1)	120.10
C(1)-S(1)-Tc(1)	104.23
C(5)-S(2)-Tc(1)	102.92
C(14)-S(3)-Tc(1)	117.69
C(3)-N(1)-Tc(1)	117.30
C(2)-N(1)-Tc(1)	107.50
C(4)-N(1)-Tc(1)	106.13



[2-(Diphenylphosphine)ethylthiolato](3-thiapentane-1,5-dithiolato)technetium(III)

$C_{18}H_{22}PS_4Tc$

7.1050Å	17.0160Å	19.1630Å	
64.0810°	88.7380°	87.8830°	V=2082.3Å^3
P-1; 2	Z=4; F(000)=1008	ρ=1.581g/cm^3	R=5.6%
triclinic			

H.-J. Pietzsch (2000)
not published
CCDC 156313

Tc 60

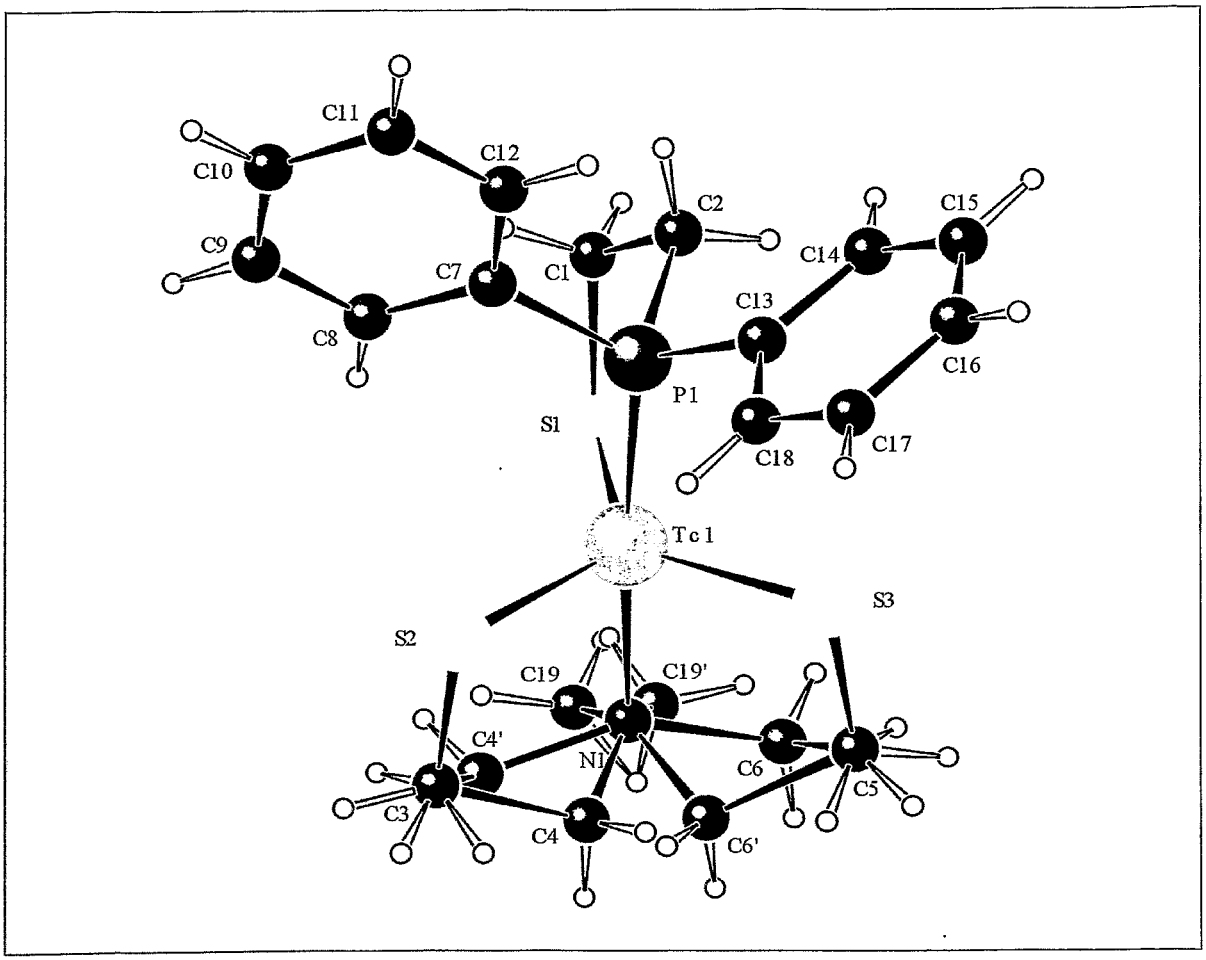
Selected Bonds (Å) and Angles (°)

Bonds

Tc-S(2)	2.216
Tc-S(3)	2.239
Tc-S(1)	2.251
Tc-P(1)	2.320
Tc-S(4)	2.402
S(1)-C(13)	1.830
S(2)-C(15)	1.847
S(3)-C(17)	1.840
S(4)-C(16)	1.801
S(4)-C(18)	1.821
P(1)-C(1)	1.812
P(1)-C(7)	1.822
P(1)-C(14)	1.848
C(1)-C(2)	1.390
C(1)-C(6)	1.390
C(2)-C(3)	1.400
C(3)-C(4)	1.380
C(4)-C(5)	1.360
C(5)-C(6)	1.390
C(7)-C(8)	1.400
C(7)-C(12)	1.410
C(8)-C(9)	1.380
C(9)-C(10)	1.360
C(10)-C(11)	1.390
C(11)-C(12)	1.390
C(13)-C(14)	1.510
C(15)-C(16)	1.520
C(17)-C(18)	1.510
Tc'-S(3')	2.213
Tc'-S(2')	2.234
Tc'-S(1')	2.252
Tc'-P(1')	2.319
Tc'-S(4')	2.401
S(1')-C(14')	1.843
S(3')-C(17')	1.839

Angles

S(2)-Tc-S(3)	114.90
S(2)-Tc-S(1)	118.50
S(3)-Tc-S(1)	126.40
S(2)-Tc-P(1)	93.80
S(3)-Tc-P(1)	94.40
S(1)-Tc-P(1)	85.20
S(2)-Tc-S(4)	87.90
S(3)-Tc-S(4)	87.00
S(1)-Tc-S(4)	91.90
P(1)-Tc-S(4)	177.04
C(13)-S(1)-Tc	108.70
C(15)-S(2)-Tc	108.40
C(17)-S(3)-Tc	106.80
C(16)-S(4)-C(18)	102.10
C(16)-S(4)-Tc	103.30
C(18)-S(4)-Tc	99.80
C(1)-P(1)-Tc	119.40
C(7)-P(1)-Tc	118.40
C(14)-P(1)-Tc	105.50
S(3')-Tc'-S(2')	115.20
S(3')-Tc'-S(1')	119.30
S(2')-Tc'-S(1')	125.40
S(3')-Tc'-P(1')	92.80
S(2')-Tc'-P(1')	94.90
S(1')-Tc'-P(1')	85.20
S(3')-Tc'-S(4')	87.90
S(2')-Tc'-S(4')	87.00
S(1')-Tc'-S(4')	92.30
P(1')-Tc'-S(4')	177.41
C(14')-S(1')-Tc'	109.70
C(17')-S(3')-Tc'	108.80
C(15')-S(2')-Tc'	107.10
C(18')-S(4')-C(16')	103.40
C(18')-S(4')-Tc'	103.20
C(16')-S(4')-Tc'	99.70



[2-(Diphenylphosphine)ethylthiolato][3-(N-methyl)azapentane-1.5-dithiolato]technetium(III)

$C_{19}H_{25}NPS_3Tc$

14.8299Å	8.0082Å	17.7414Å	
90.0000°	97.0470°	90.0000°	V=2091.1Å^3
$P2_1/n$; 14	Z=4; F(000)=1008	ρ=1.565g/cm^3	R=3.72%
monoclinic			

H.-J. Pietzsch (2000)
not published
CCDC 159498

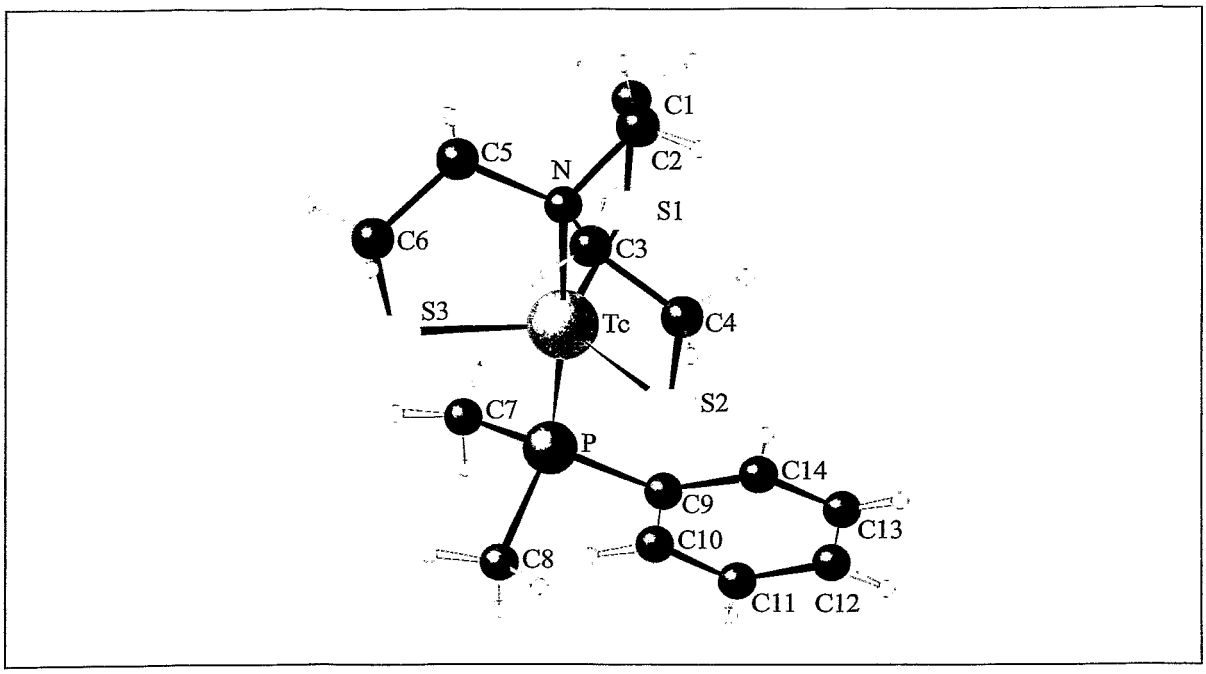
Selected Bonds (Å) and Angles (°)

Bonds

Tc(1)-S(3)	2.220
Tc(1)-S(1)	2.240
Tc(1)-S(2)	2.243
Tc(1)-N(1)	2.248
Tc(1)-P(1)	2.298
P(1)-C(13)	1.826
P(1)-C(7)	1.847
P(1)-C(2)	1.850
S(1)-C(1)	1.839
S(2)-C(3')	1.846
S(2)-C(3)	1.846
S(3)-C(5')	1.833
S(3)-C(5)	1.833
N(1)-C(4)	1.405
N(1)-C(19)	1.418
N(1)-C(6')	1.441
N(1)-C(19')	1.456
N(1)-C(6)	1.627
N(1)-C(4')	1.640
C(1)-C(2)	1.516
C(3)-C(4)	1.673
C(5)-C(6)	1.421
C(3')-C(4')	1.452
C(5')-C(6')	1.709
C(7)-C(8)	1.378
C(7)-C(12)	1.392
C(8)-C(9)	1.387

Angles

S(3)-Tc(1)-S(1)	121.27
S(3)-Tc(1)-S(2)	116.57
S(1)-Tc(1)-S(2)	121.73
S(3)-Tc(1)-N(1)	85.30
S(1)-Tc(1)-N(1)	92.64
S(2)-Tc(1)-N(1)	85.30
S(3)-Tc(1)-P(1)	92.29
S(1)-Tc(1)-P(1)	85.28
S(2)-Tc(1)-P(1)	99.27
N(1)-Tc(1)-P(1)	175.42
C(13)-P(1)-C(7)	100.85
C(13)-P(1)-C(2)	105.07
C(7)-P(1)-C(2)	100.67
C(13)-P(1)-Tc(1)	119.38
C(7)-P(1)-Tc(1)	122.36
C(2)-P(1)-Tc(1)	105.92
C(1)-S(1)-Tc(1)	109.69
C(3')-S(2)-Tc(1)	102.56
C(3)-S(2)-Tc(1)	102.56
C(5')-S(3)-Tc(1)	103.20
C(5)-S(3)-Tc(1)	103.20
C(4)-N(1)-Tc(1)	106.80
C(19)-N(1)-Tc(1)	115.60
C(6')-N(1)-Tc(1)	110.60
C(19')-N(1)-Tc(1)	118.00
C(6)-N(1)-Tc(1)	103.50
C(4')-N(1)-Tc(1)	106.50



(Dimethylphenylphosphine)[nitrilotris(ethanethiolato)]technetium(III)

$C_{14}H_{23}NPS_3Tc$

13.3502Å	9.4833Å	15.3085Å	
90.0000°	112.7420°	90.0000°	V=1787.4Å^3
$P2_1/c$; 14	Z=4; F(000)=880	ρ=1.600g/cm^3	R=2.2%
monoclinic			

H.-J. Pietzsch (1998)
not published
CCDC 159498

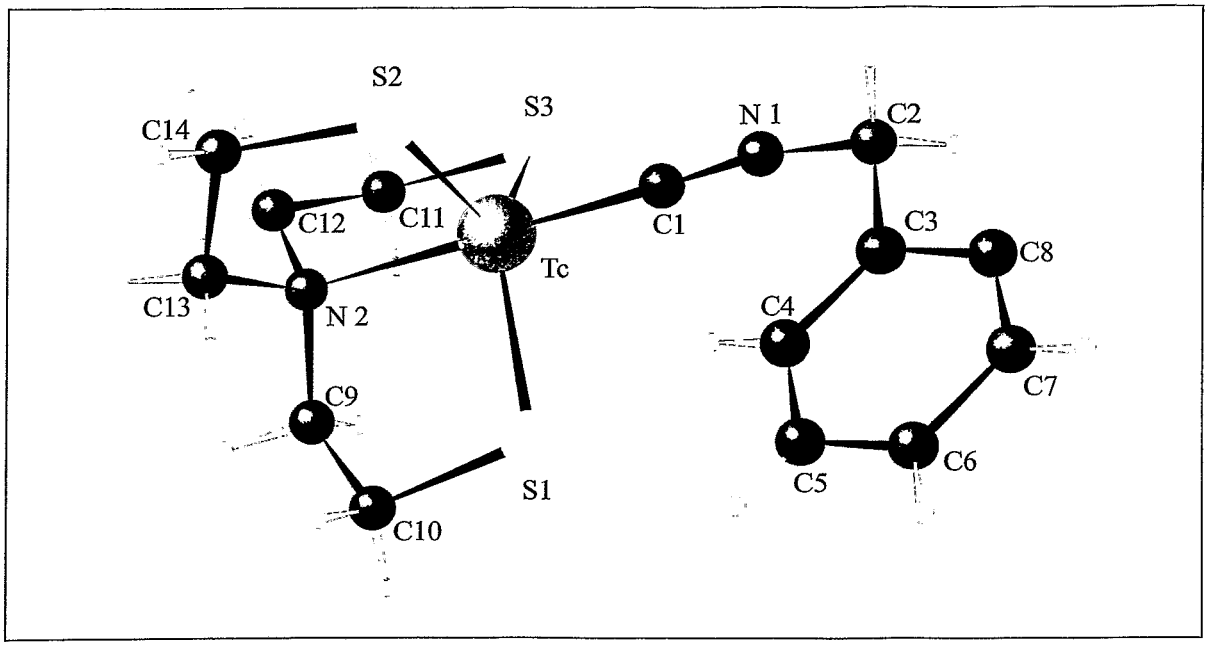
Selected Bonds (Å) and Angles (°)

Bonds

Tc(1)-N(1)	2.205
Tc(1)-S(2)	2.223
Tc(1)-S(1)	2.226
Tc(1)-S(3)	2.230
Tc(1)-P(1)	2.317
S(1)-C(1)	1.833
S(2)-C(4)	1.841
S(3)-C(6)	1.830
P(1)-C(7)	1.826
P(1)-C(8)	1.828
P(1)-C(9)	1.837
N(1)-C(2)	1.485
N(1)-C(3)	1.490
N(1)-C(5)	1.495
C(1)-C(2)	1.503
C(3)-C(4)	1.511
C(5)-C(6)	1.503
C(9)-C(14)	1.385
C(9)-C(10)	1.395
C(10)-C(11)	1.383
C(11)-C(12)	1.375
C(12)-C(13)	1.371

Angles

N(1)-Tc(1)-S(2)	85.72
N(1)-Tc(1)-S(1)	85.97
S(2)-Tc(1)-S(1)	118.39
N(1)-Tc(1)-S(3)	85.59
S(2)-Tc(1)-S(3)	119.46
S(1)-Tc(1)-S(3)	120.53
N(1)-Tc(1)-P(1)	176.10
S(2)-Tc(1)-P(1)	96.78
S(1)-Tc(1)-P(1)	95.44
S(3)-Tc(1)-P(1)	90.57
C(1)-S(1)-Tc(1)	102.51
C(4)-S(2)-Tc(1)	102.78
C(6)-S(3)-Tc(1)	102.62
C(7)-P(1)-C(8)	101.27
C(7)-P(1)-C(9)	102.78
C(8)-P(1)-C(9)	100.57
C(7)-P(1)-Tc(1)	113.65
C(8)-P(1)-Tc(1)	114.53
C(9)-P(1)-Tc(1)	121.35
C(2)-N(1)-Tc(1)	109.80
C(3)-N(1)-Tc(1)	110.13
C(5)-N(1)-Tc(1)	109.65



(Benzylisocyanido)[nitrilotris(ethanethiolato)]technetium(III)

$C_{14}H_{19}N_2S_3Tc$

8.2607Å	11.1868Å	17.6187Å	
90.0000°	93.8360°	90.0000°	V=1624.5Å^3
$P2_1/c$; 14	Z=4; F(000)=832	ρ=1.674g/cm^3	R=9.8%
monoclinic			

H.-J. Pietzsch (1999)
not published
CCDC 152319

Tc 63

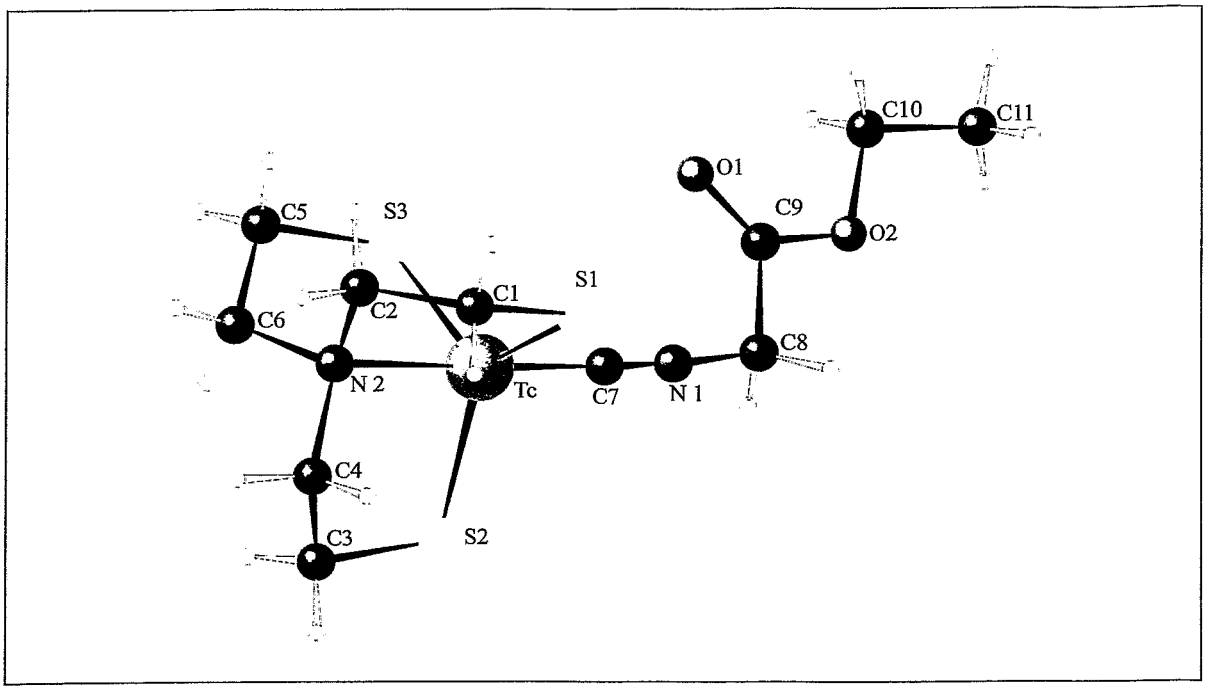
Selected Bonds (Å) and Angles (°)

Bonds

Tc(1)-C(1)	1.932
Tc(1)-N(2)	2.216
Tc(1)-S(3)	2.227
Tc(1)-S(2)	2.232
Tc(1)-S(1)	2.242
S(1)-C(10)	1.852
S(2)-C(12)	1.832
S(3)-C(14)	1.840
N(1)-C(1)	1.167
N(1)-C(2)	1.418
N(2)-C(13)	1.478
N(2)-C(11)	1.483
N(2)-C(9)	1.484
C(2)-C(3)	1.536
C(3)-C(4)	1.376
C(3)-C(8)	1.397
C(4)-C(5)	1.370
C(5)-C(6)	1.400
C(6)-C(7)	1.380
C(7)-C(8)	1.380
C(9)-C(10)	1.517
C(11)-C(12)	1.512
C(13)-C(14)	1.510

Angles

C(1)-Tc(1)-N(2)	178.00
C(1)-Tc(1)-S(3)	95.60
N(2)-Tc(1)-S(3)	86.10
C(1)-Tc(1)-S(2)	92.60
N(2)-Tc(1)-S(2)	85.60
S(3)-Tc(1)-S(2)	119.32
C(1)-Tc(1)-S(1)	93.80
N(2)-Tc(1)-S(1)	86.20
S(3)-Tc(1)-S(1)	120.04
S(2)-Tc(1)-S(1)	119.18
C(10)-S(1)-Tc(1)	101.70
C(12)-S(2)-Tc(1)	102.30
C(14)-S(3)-Tc(1)	102.00
C(1)-N(1)-C(2)	163.20
C(13)-N(2)-C(11)	110.00
C(13)-N(2)-C(9)	108.90
C(11)-N(2)-C(9)	109.50
C(13)-N(2)-Tc(1)	109.90
C(11)-N(2)-Tc(1)	109.80
C(9)-N(2)-Tc(1)	108.80
N(1)-C(1)-Tc(1)	178.80
N(1)-C(2)-C(3)	112.60
C(4)-C(3)-C(8)	118.80



(Isonitriloacetic acid ethylester)[nitrilotris(ethanethiolato)]technetium(III)

$C_{11}H_{19}N_2O_2S_3Tc$

9.9088Å	22.2839Å	7.5060Å	
90.0000°	107.6780°	90.0000°	V=1579.1Å^3
$P2_1/c$; 14	Z=4; F(000)=824	ρ=1.705g/cm^3	R=4.1%
monoclinic			

H.-J. Pietzsch (1999)
not published
CCDC 152321

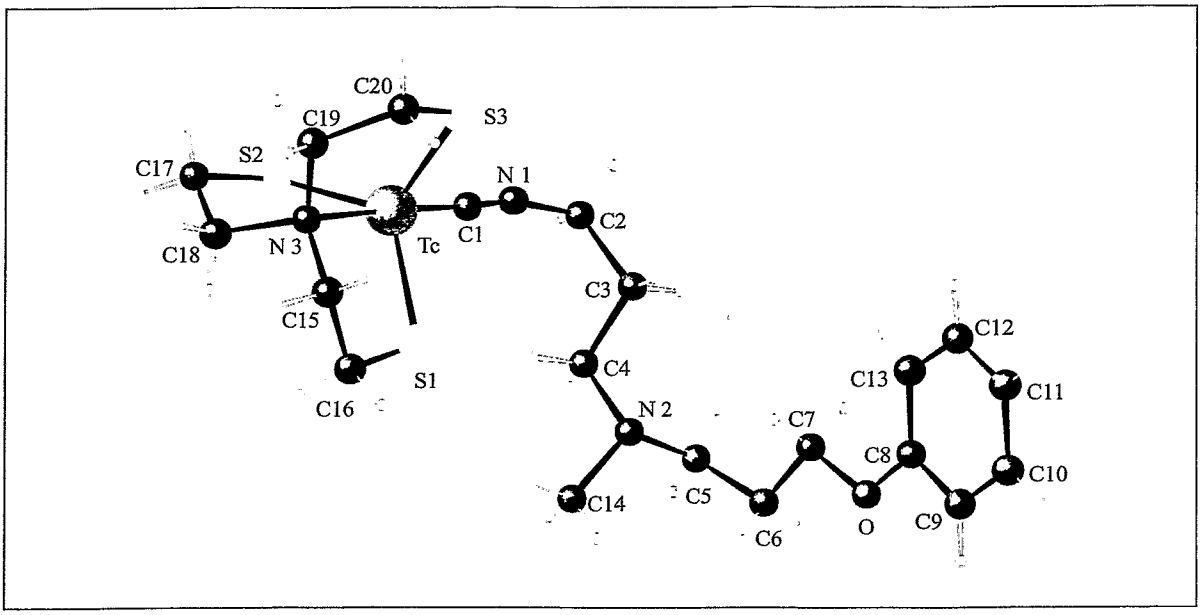
Selected Bonds (Å) and Angles (°)

Bonds

Tc(1)-C(7)	1.945
Tc(1)-N(2)	2.199
Tc(1)-S(3)	2.224
Tc(1)-S(2)	2.229
Tc(1)-S(1)	2.236
S(1)-C(1)	1.843
S(2)-C(3)	1.840
S(3)-C(5)	1.837
O(1)-C(9)	1.183
O(2)-C(9)	1.331
O(2)-C(10)	1.455
N(1)-C(7)	1.168
N(1)-C(8)	1.416
N(2)-C(4)	1.486
N(2)-C(2)	1.487
N(2)-C(6)	1.494
C(1)-C(2)	1.507
C(3)-C(4)	1.495
C(5)-C(6)	1.506
C(8)-C(9)	1.515
C(10)-C(11)	1.482

Angles

C(7)-Tc(1)-N(2)	178.09
C(7)-Tc(1)-S(3)	92.18
N(2)-Tc(1)-S(3)	85.91
C(7)-Tc(1)-S(2)	95.47
N(2)-Tc(1)-S(2)	85.50
S(3)-Tc(1)-S(2)	118.91
C(7)-Tc(1)-S(1)	95.32
N(2)-Tc(1)-S(1)	85.62
S(3)-Tc(1)-S(1)	120.22
S(2)-Tc(1)-S(1)	119.18
C(1)-S(1)-Tc(1)	102.31
C(3)-S(2)-Tc(1)	102.56
C(5)-S(3)-Tc(1)	102.41
C(9)-O(2)-C(10)	116.30
C(7)-N(1)-C(8)	177.20
C(4)-N(2)-C(2)	110.20
C(4)-N(2)-C(6)	108.90
C(2)-N(2)-C(6)	108.80
C(4)-N(2)-Tc(1)	110.00
C(2)-N(2)-Tc(1)	109.40
C(6)-N(2)-Tc(1)	109.60



{3-[N-(3-phenoxypropyl)-N-methylamino]-propaneisocyanido}[nitrilotris(ethanethiolato)]technetium(III)

$C_{20}H_{32}N_3OS_3Tc$

14.8550Å	8.0001Å	20.0173Å	
90.0000°	97.4580°	90.0000°	V=2358.8Å^3
$P2_1/c$; 14	Z=4; F(000)=1088	ρ=1.477g/cm^3	R=4.3%
monoclinic			

H.-J. Pietzsch (1999)
not published
CCDC 152322

Tc 65

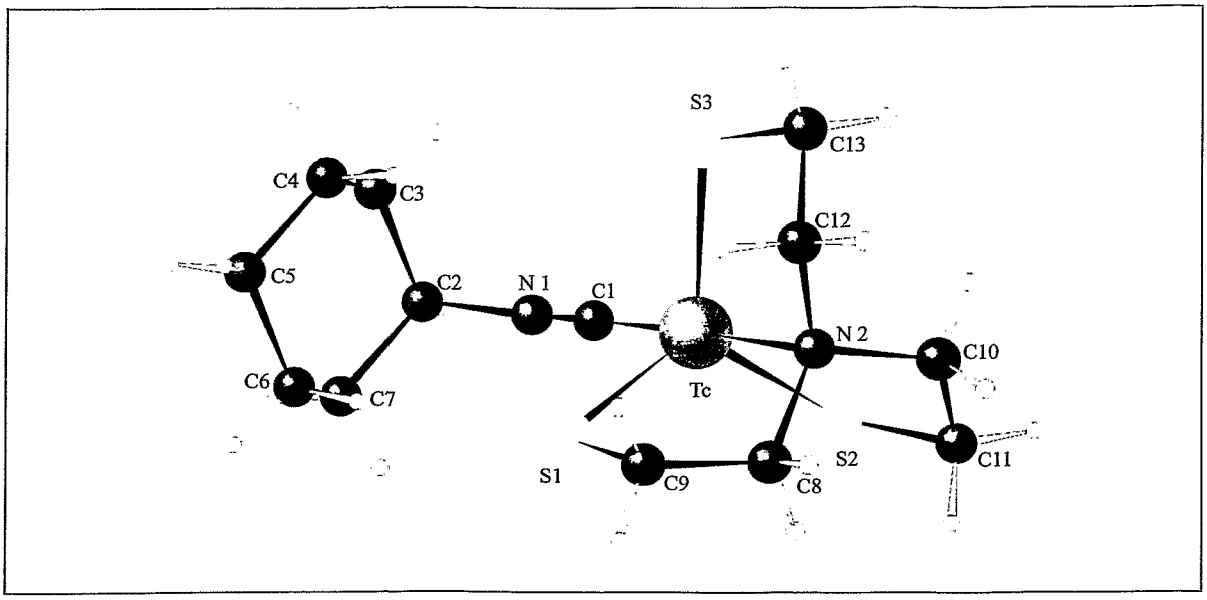
Selected Bonds (Å) and Angles (°)

Bonds

Tc(1)-C(1)	1.961
Tc(1)-N(3)	2.195
Tc(1)-S(1)	2.229
Tc(1)-S(3)	2.232
Tc(1)-S(2)	2.235
S(2)-C(18)	1.826
S(3)-C(20)	1.831
S(1)-C(16)	1.832
O(1)-C(8)	1.372
O(1)-C(7)	1.423
N(1)-C(1)	1.161
N(1)-C(2)	1.429
N(2)-C(5)	1.457
N(2)-C(4)	1.460
N(2)-C(14)	1.465
N(3)-C(15)	1.454
N(3)-C(19)	1.463
N(3)-C(17)	1.516
C(2)-C(3)	1.524
C(3)-C(4)	1.510
C(5)-C(6)	1.530
C(6)-C(7)	1.497
C(8)-C(13)	1.376
C(8)-C(9)	1.389
C(9)-C(10)	1.360

Angles

C(1)-Tc(1)-N(3)	178.30
C(1)-Tc(1)-S(1)	93.10
N(3)-Tc(1)-S(1)	86.13
C(1)-Tc(1)-S(3)	93.70
N(3)-Tc(1)-S(3)	85.41
S(1)-Tc(1)-S(3)	120.12
C(1)-Tc(1)-S(2)	95.69
N(3)-Tc(1)-S(2)	85.99
S(1)-Tc(1)-S(2)	119.41
S(3)-Tc(1)-S(2)	118.91
C(18)-S(2)-Tc(1)	102.20
C(20)-S(3)-Tc(1)	102.80
C(16)-S(1)-Tc(1)	101.80
C(8)-O(1)-C(7)	117.70
C(1)-N(1)-C(2)	163.90
C(5)-N(2)-C(4)	112.20
C(5)-N(2)-C(14)	110.80
C(4)-N(2)-C(14)	109.40
C(15)-N(3)-C(19)	110.80
C(15)-N(3)-C(17)	110.20
C(19)-N(3)-C(17)	105.00
C(15)-N(3)-Tc(1)	111.10
C(19)-N(3)-Tc(1)	110.60
C(17)-N(3)-Tc(1)	109.00
N(1)-C(1)-Tc(1)	177.40



(Cyclohexylisocyanido)[nitrilotris(ethanethiolato)]technetium(III)

$C_{13}H_{23}N_2S_3Tc$

11.0095Å	12.7034Å	24.5799Å	
90.0000°	90.0000°	90.0000°	V=3437.2Å^3
Pbca; 61	Z=8; F(000)=1648	ρ=1.552g/cm^3	R=4.3%
orthorhombic			

H.-J. Pietzsch (1999)
not published
CCDC156314

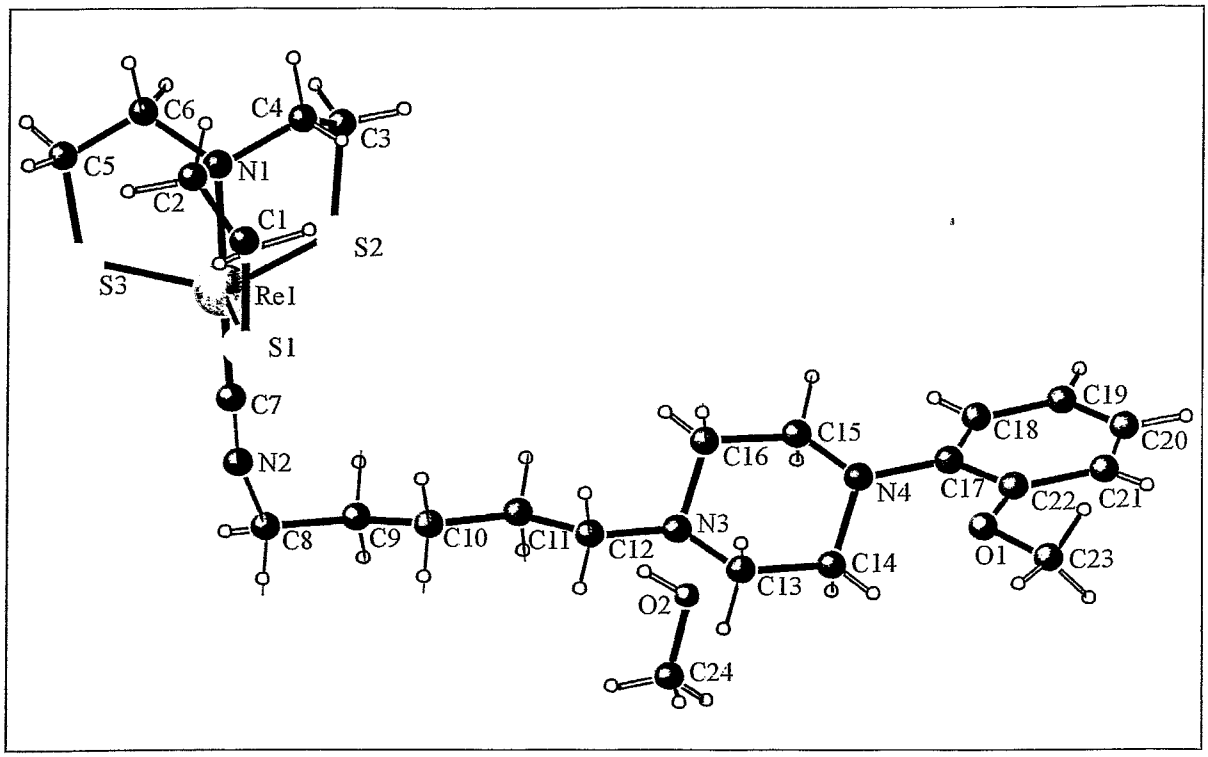
Selected Bonds (Angströms) and Angles (Degrees)

Bonds

Tc(1)-C(1)	1.942
Tc(1)-N(2)	2.184
Tc(1)-S(3)	2.214
Tc(1)-S(1)	2.215
Tc(1)-S(2)	2.242
S(1)-C(9)	1.798
S(2)-C(11)	1.823
S(3)-C(13)	1.814
N(1)-C(1)	1.174
N(1)-C(2)	1.481
N(2)-C(10)	1.400
N(2)-C(12)	1.530
N(2)-C(8)	1.589
C(2)-C(3)	1.458
C(2)-C(7)	1.499
C(3)-C(4)	1.444
C(4)-C(5)	1.470
C(5)-C(6)	1.481
C(6)-C(7)	1.432
C(8)-C(9)	1.410
C(10)-C(11)	1.570
C(12)-C(13)	1.549

Angles

C(1)-Tc(1)-N(2)	178.70
C(1)-Tc(1)-S(3)	95.20
N(2)-Tc(1)-S(3)	86.05
C(1)-Tc(1)-S(1)	92.80
N(2)-Tc(1)-S(1)	86.35
S(3)-Tc(1)-S(1)	117.74
C(1)-Tc(1)-S(2)	93.90
N(2)-Tc(1)-S(2)	85.61
S(3)-Tc(1)-S(2)	120.19
S(1)-Tc(1)-S(2)	120.62
C(9)-S(1)-Tc(1)	102.50
C(11)-S(2)-Tc(1)	101.90
C(13)-S(3)-Tc(1)	102.30
C(1)-N(1)-C(2)	158.40
C(10)-N(2)-C(12)	109.90
C(10)-N(2)-C(8)	111.20
C(12)-N(2)-C(8)	106.60
C(10)-N(2)-Tc(1)	112.50
C(12)-N(2)-Tc(1)	110.10
C(8)-N(2)-Tc(1)	106.20
N(1)-C(1)-Tc(1)	179.50



{5-[1-(2-Methoxyphenyl)-piperazine]-pentaneisocyanido}[nitrilotris(ethanethiolato)]technetium(III) (methanol adduct)

$C_{23}H_{37}N_4ORES_3 \times CH_3OH$

10.5518Å	11.8358Å	12.3413Å	
102.2870°	93.2850°	104.4790°	V=1448.17Å^3
P-1; 2	Z=2; F(000)=704	ρ=1.605g/cm^3	R=6.69%
triclinic			

H.-J. Pietzsch (2000)
not published
CCDC 159499

Re 67

Selected Bonds (Å) and Angles (°)

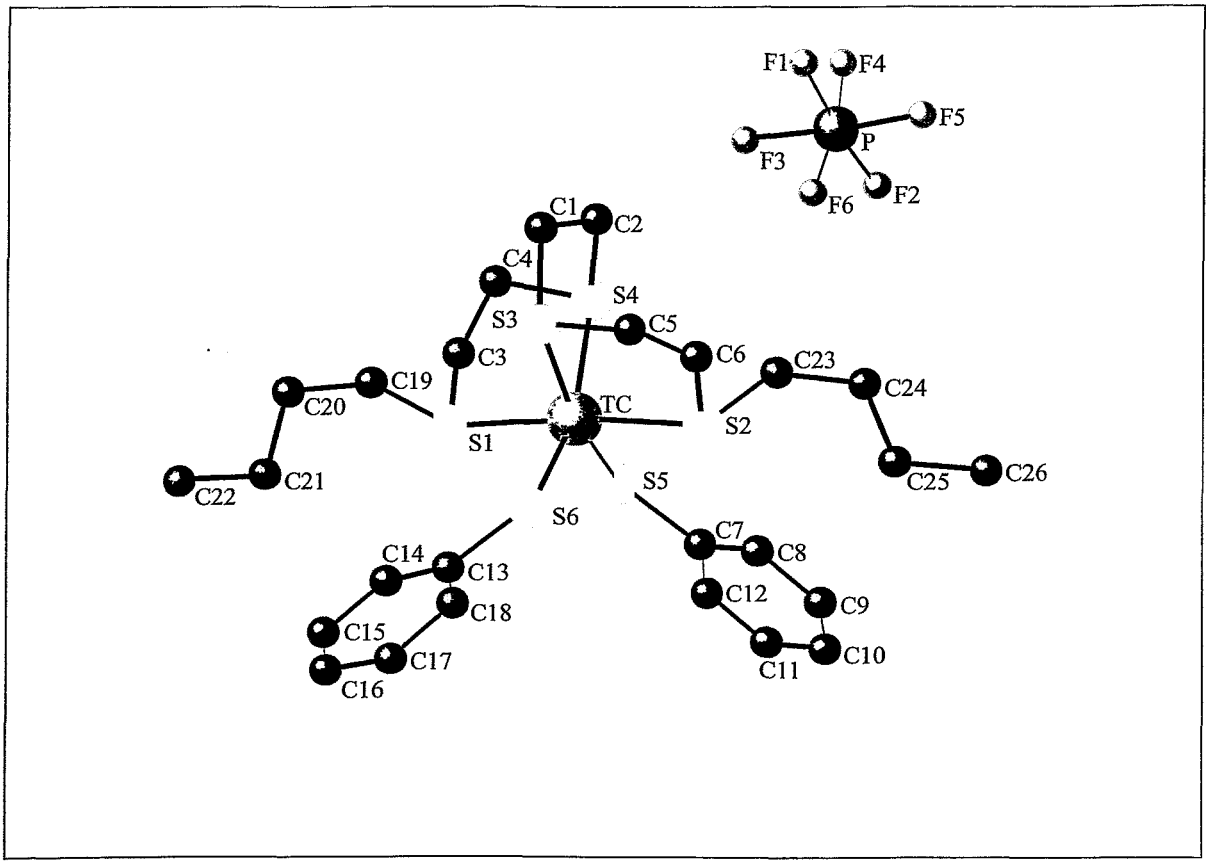
Bonds

Re(1)-C(7)	1.960
Re(1)-N(1)	2.206
Re(1)-S(1)	2.235
Re(1)-S(2)	2.237
Re(1)-S(3)	2.239
S(2)-C(3)	1.839
S(1)-C(1)	1.852
S(3)-C(5)	1.828
O(1)-C(22)	1.361
O(1)-C(23)	1.432
N(1)-C(4)	1.455
N(1)-C(6)	1.510
N(1)-C(2)	1.515
N(2)-C(7)	1.156
N(2)-C(8)	1.414
N(3)-C(13)	1.463
N(3)-C(12)	1.473
N(3)-C(16)	1.476
N(4)-C(17)	1.414
N(4)-C(15)	1.448
N(4)-C(14)	1.487
C(1)-C(2)	1.490
C(3)-C(4)	1.490

Angles

C(7)-Re(1)-N(1)	177.10
C(7)-Re(1)-S(1)	94.10
N(1)-Re(1)-S(1)	85.50
C(7)-Re(1)-S(2)	92.40
N(1)-Re(1)-S(2)	85.40
S(1)-Re(1)-S(2)	121.04
C(7)-Re(1)-S(3)	97.50
N(1)-Re(1)-S(3)	85.20
S(1)-Re(1)-S(3)	118.80
S(2)-Re(1)-S(3)	118.21
C(3)-S(2)-Re(1)	102.20
C(1)-S(1)-Re(1)	102.60
C(5)-S(3)-Re(1)	102.70
C(22)-O(1)-C(23)	118.20
C(4)-N(1)-C(6)	109.70
C(4)-N(1)-C(2)	110.70
C(6)-N(1)-C(2)	106.00
C(4)-N(1)-Re(1)	110.80
C(6)-N(1)-Re(1)	109.70
C(2)-N(1)-Re(1)	109.80
C(7)-N(2)-C(8)	165.10
C(13)-N(3)-C(12)	109.60
N(2)-C(7)-Re(1)	179.30

Tc 68



Bis-(benzenethiolato)(5,8,11,14-tetrathiaoctadecane)technetium(III) hexafluorophosphate

$C_{20}H_{40}F_6PS_6Tc$

8.9136Å	13.6853Å	15.2606Å	
115.4530°	93.1540°	91.5840°	$V=1675.7Å^3$
P-1; 2	Z=4; F(000)=808	$\rho=1.562g/cm^3$	R=8.4%
triclinic			

H.-J. Pietzsch, H. Spies, P. Leibnitz, G. Reck, J. Beger, R. Jacobi
"Technetium complexes with thioether ligands. I. Cationic technetium (III) complexes containing tetradentate thioether/monothiole ligands. X-ray structure analysis of technetium(III) hexafluorophosphate"
Polyhedron 11 (1992) 1623-1628
CSD No. 55810

Tc 68

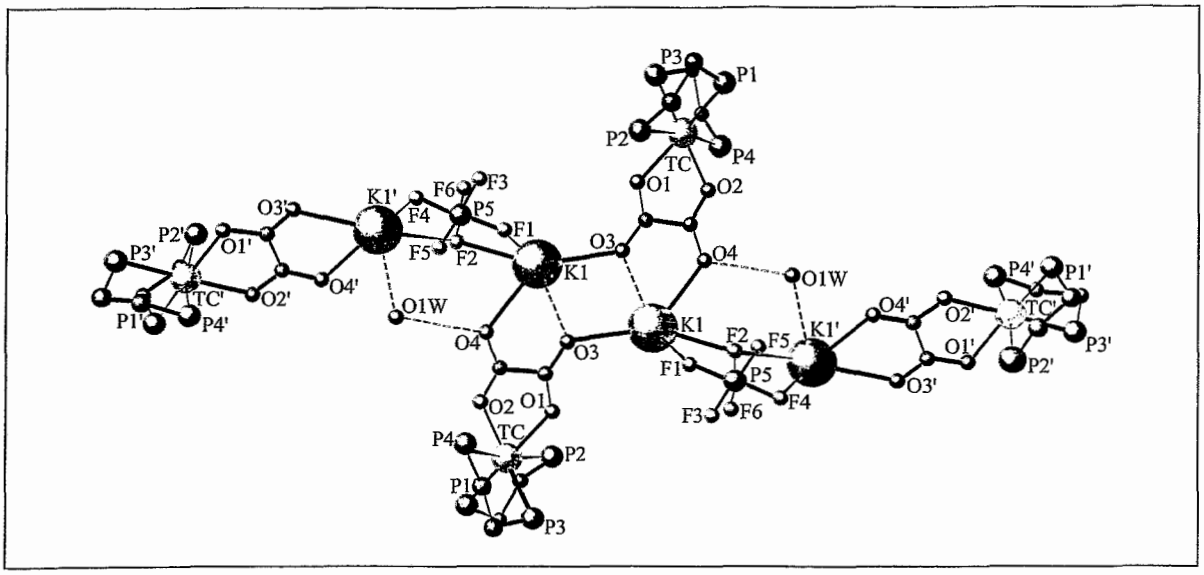
Selected Bonds (Angströms) and Angles (Degrees)

Bonds

Tc-S(6)	2.267
Tc-S(5)	2.289
Tc-S(1)	2.418
Tc-S(2)	2.425
Tc-S(4)	2.425
Tc-S(3)	2.463
S(1)-C(19)	1.798
S(1)-C(3)	1.810
S(2)-C(6)	1.820
S(2)-C(23)	1.828
S(2)-C(6')	1.860
S(3)-C(5)	1.640
S(3)-C(1)	1.811
S(3)-C(5')	2.040
S(4)-C(2)	1.814
S(4)-C(4)	1.825
S(5)-C(7)	1.774
S(6)-C(13)	1.782
C(1)-C(2)	1.510
C(3)-C(4)	1.488
C(5)-C(6)	1.620
C(5')-C(6')	1.120
C(7)-C(12)	1.376
C(7)-C(8)	1.387
C(8)-C(9)	1.368
C(9)-C(10)	1.370
C(10)-C(11)	1.370

Angles

S(6)-Tc-S(5)	109.49
S(6)-Tc-S(1)	92.21
S(5)-Tc-S(1)	83.14
S(6)-Tc-S(2)	87.09
S(5)-Tc-S(2)	92.37
S(1)-Tc-S(2)	174.95
S(6)-Tc-S(4)	161.40
S(5)-Tc-S(4)	88.08
S(1)-Tc-S(4)	83.67
S(2)-Tc-S(4)	98.54
S(6)-Tc-S(3)	82.00
S(5)-Tc-S(3)	167.68
S(1)-Tc-S(3)	101.26
S(2)-Tc-S(3)	83.60
S(4)-Tc-S(3)	81.04
C(19)-S(1)-Tc	110.70
C(3)-S(1)-Tc	104.30
C(6)-S(2)-Tc	106.20
C(23)-S(2)-Tc	109.90
C(6')-S(2)-Tc	104.40
C(5)-S(3)-Tc	106.00
C(1)-S(3)-Tc	109.20
C(5')-S(3)-Tc	101.50
C(2)-S(4)-Tc	108.70
C(4)-S(4)-Tc	105.80
C(7)-S(5)-Tc	114.70
C(13)-S(6)-Tc	115.80



Bis[1,2-bis(diphenylphosphino)ethane][oxalato-(O,O)]technetium(III)

$C_{54}H_{48}O_4P_4Tc \times KPF_6 \times ½\ H_2O$

16.9911Å	18.3018Å	19.1141Å	
91.0640°	113.0770°	91.2540°	V=5465.0Å^3
P-1; 2	Z=4; F(000)=2440	ρ=1.448g/cm^3	R=12.5%
triclinic			

S. Seifert, R. Muenze, P. Leibnitz, G. Reck and J. Stach
"Preparation , characterization and crystal structure of a mixed ligand complex of technetium with DPPE and oxalic acid: Oxalato-bis[1.2-bis-(diphenylphosphino)ethane]technetium(III)"
Inorg.Chim.Acta 193 (1992) 167-172

Selected Bonds (Å) and Angles (°)

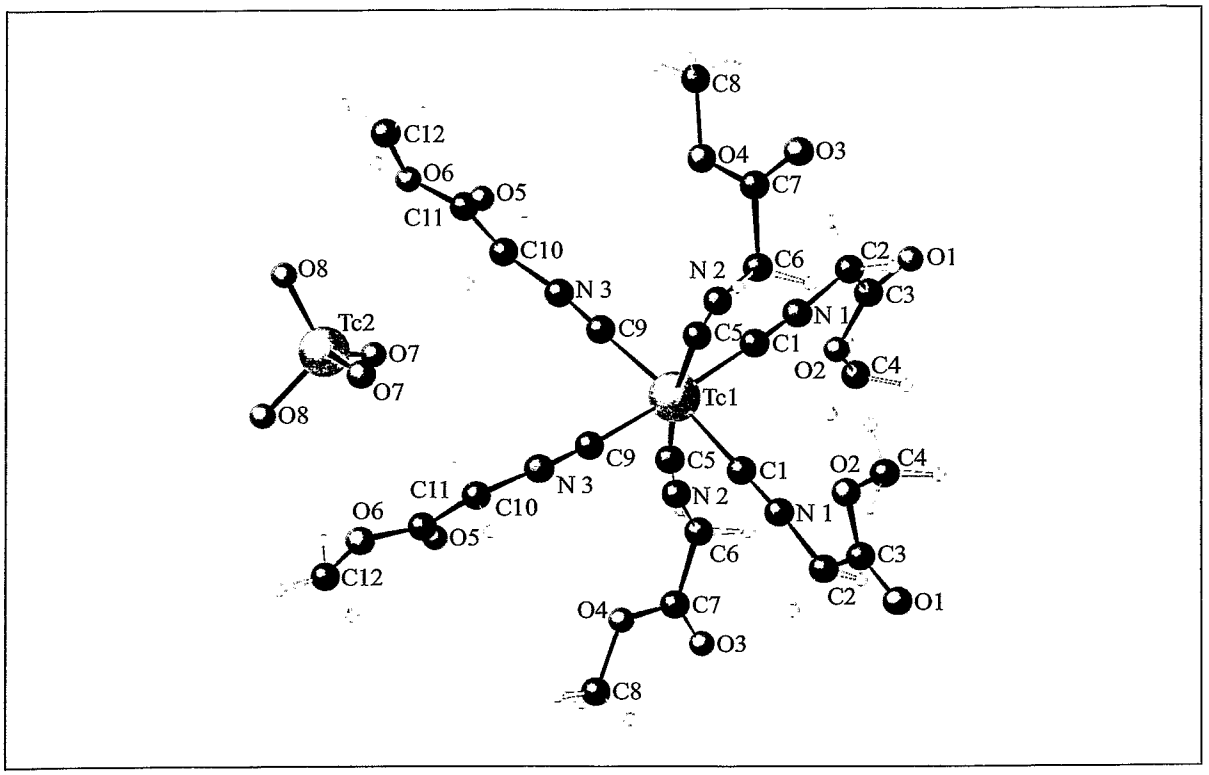
Bonds

Tc(1)-P(1)	2.408
Tc(1)-P(2)	2.440
Tc(1)-P(3)	2.404
Tc(1)-P(4)	2.422
Tc(1)-O(1)	2.141
Tc(1)-O(2)	2.118
P(1)-C(1)	1.841
P(2)-C(2)	1.848
P(3)-C(3)	1.838
P(4)-C(4)	1.815
C(1)-C(2)	1.564
C(3)-C(4)	1.535
O(1)-C(5)	1.303
O(2)-C(6)	1.274
O(3)-C(5)	1.224
O(4)-C(6)	1.208
C(5)-C(6)	1.533

Angles

P(1)-Tc(1)-P(2)	80.72
P(1)-Tc(1)-P(3)	88.82
P(1)-Tc(1)-P(4)	104.71
P(1)-Tc(1)-O(1)	165.03
P(1)-Tc(1)-O(2)	98.89
P(2)-Tc(1)-O(1)	85.24
P(2)-Tc(1)-O(2)	88.85
P(2)-Tc(1)-P(4)	172.24
P(2)-Tc(1)-P(3)	105.27
P(3)-Tc(1)-O(1)	99.91
P(3)-Tc(1)-O(2)	164.91
P(3)-Tc(1)-P(4)	80.63
P(4)-Tc(1)-O(1)	88.80
P(4)-Tc(1)-O(2)	84.86
O(1)-Tc(1)-O(2)	75.56
O(1)-C(5)-O(3)	126.75
O(2)-C(6)-O(4)	124.73

5.5. Technetium and Rhenium on the oxidation state I



Hexakis(carbmethoxymethylisocyanido)technetium(I) pertechnetate

$C_{24}H_{30}N_6O_{12}Tc \times [TcO_4]$

10.8130Å	20.3047Å	15.8330Å	
90.0000°	107.7620°	90.0000°	V=3310.5Å^3
C2/c; 15	Z=4; F(000)=1720	ρ=1.715g/cm^3	R=3.7%
monoclinic			

B. Noll, P. Leibnitz, H. Spies
"Synthesis and molecular structure of $[Tc(CN\text{-}CH_2\text{-}COOH_3)_6]TcO_4$"
FZR-270 (1999) 153
CCDC 159491

Tc 70

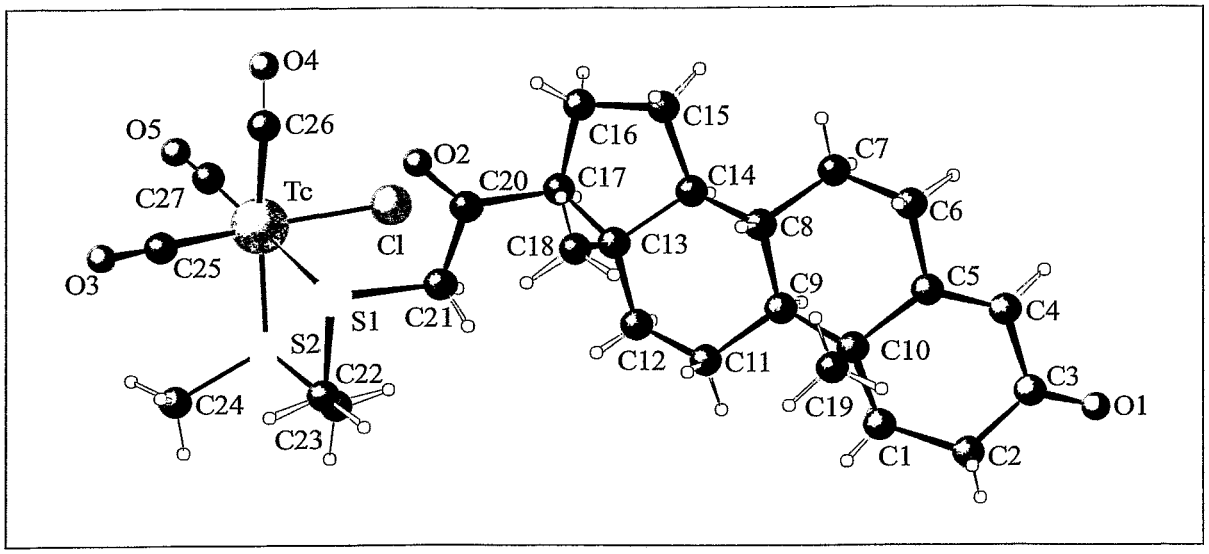
Selected Bonds (Å) and Angles (°)

Bonds

Tc(2)-O(8)	1.689
Tc(2)-O(7)	1.694
Tc(1)-C(1)	2.032
Tc(1)-C(5)	2.034
Tc(1)-C(9)	2.045
O(1)-C(3)	1.189
O(2)-C(3)	1.316
O(2)-C(4)	1.469
O(3)-C(7)	1.194
O(4)-C(7)	1.310
O(4)-C(8)	1.476
O(5)-C(11)	1.192
O(6)-C(11)	1.287
O(6)-C(12)	1.672
N(1)-C(1)	1.153
N(1)-C(2)	1.420
N(2)-C(5)	1.155
N(2)-C(6)	1.430
N(3)-C(9)	1.158
N(3)-C(10)	1.414

Angles

O(8)-Tc(2)-O(8')	109.40
O(8)-Tc(2)-O(7')	108.40
O(8)-Tc(2)-O(7)	109.30
O(7')-Tc(2)-O(7)	112.10
C(1')-Tc(1)-C(1)	93.90
C(1')-Tc(1)-C(5)	86.35
C(1)-Tc(1)-C(5)	86.96
C(5')-Tc(1)-C(5)	170.20
C(1)-Tc(1)-C(9')	176.21
C(1)-Tc(1)-C(9)	89.62
C(5)-Tc(1)-C(9)	92.53
C(3)-O(2)-C(4)	116.50
C(7)-O(4)-C(8)	116.80
C(11)-O(6)-C(12)	93.30
C(1)-N(1)-C(2)	175.60
C(5)-N(2)-C(6)	167.70
C(9)-N(3)-C(10)	176.30
N(1)-C(1)-Tc(1)	177.30
N(2)-C(5)-Tc(1)	172.90
N(3)-C(9)-Tc(1)	177.00



Chloro[21-(1,4-dithiapent-1-yl)progesterone]tricarbonyltechnetium(I)

$C_{27}H_{36}ClO_5S_2Tc$

31.2148Å	7.1275Å	15.0472Å	
90.0000°	113.7850°	90.0000°	V=3106.4Å^3
C2; 5	Z=4; F(000)=1384	ρ=1.433g/cm^3	R=7.3%
monoclinic			

F. Wüst (1999)
not published
CCDC 161724

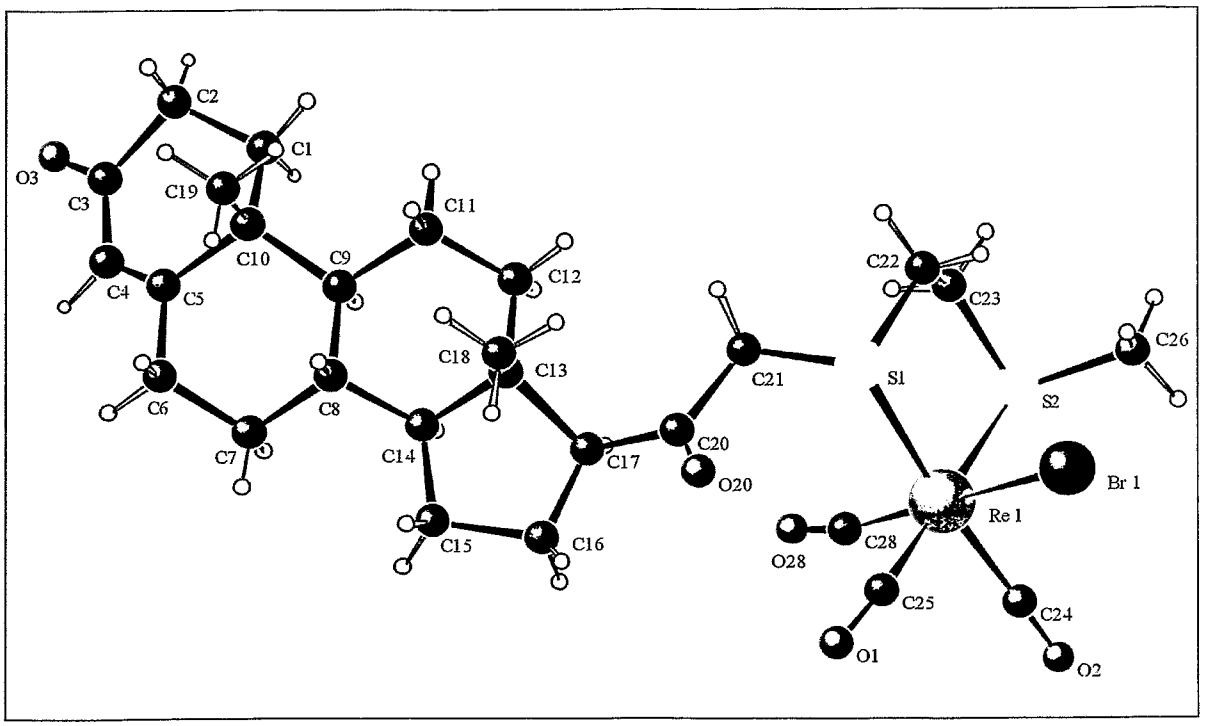
Selected Bonds (Å) and Angles (°)

Bonds

Tc(1)-C(25)	1.891
Tc(1)-C(27)	1.924
Tc(1)-C(26)	1.939
Tc(1)-S(2)	2.479
Tc(1)-Cl(1)	2.491
Tc(1)-S(1)	2.516
S(1)-C(22)	1.808
S(1)-C(21)	1.827
S(2)-C(24)	1.797
S(2)-C(23)	1.832
O(27)-C(27)	1.133
O(25)-C(25)	1.105
O(26)-C(26)	1.127
O(20)-C(20)	1.193
O(3)-C(3)	1.200
C(1)-C(10)	1.539
C(1)-C(2)	1.564
C(2)-C(3)	1.460
C(3)-C(4)	1.470
C(4)-C(5)	1.360
C(5)-C(6)	1.520
C(5)-C(10)	1.533
C(6)-C(7)	1.568
C(7)-C(8)	1.514

Angles

C(25)-Tc(1)-C(27)	91.50
C(25)-Tc(1)-C(26)	89.40
C(27)-Tc(1)-C(26)	91.30
C(25)-Tc(1)-S(2)	94.80
C(27)-Tc(1)-S(2)	89.80
C(26)-Tc(1)-S(2)	175.70
C(25)-Tc(1)-Cl(1)	176.70
C(27)-Tc(1)-Cl(1)	90.40
C(26)-Tc(1)-Cl(1)	93.30
S(2)-Tc(1)-Cl(1)	82.60
C(25)-Tc(1)-S(1)	89.20
C(27)-Tc(1)-S(1)	174.80
C(26)-Tc(1)-S(1)	93.80
S(2)-Tc(1)-S(1)	85.00
Cl(1)-Tc(1)-S(1)	88.61
C(22)-S(1)-C(21)	99.60
C(22)-S(1)-Tc(1)	102.10
C(21)-S(1)-Tc(1)	112.30
C(24)-S(2)-C(23)	100.20
C(24)-S(2)-Tc(1)	109.10
C(23)-S(2)-Tc(1)	102.60
O(25)-C(25)-Tc(1)	177.90
O(26)-C(26)-Tc(1)	176.10
O(27)-C(27)-Tc(1)	178.80



Bromo[21-(1,4-dithiapent-1-yl)progesterone]tricarbonylrhenium(I)

$C_{27}H_{36}BrO_5ReS_2$

27.8229Å	27.8229Å	11.3404Å	
90.0000°	90.0000°	90.0000°	V=8778.8Å^3
P4(2)2(1)2; 94	Z=8; F(000)=3040	ρ=1.166g/cm^3	R=6.88%
tetragonal			

F.Wüst (1998)
not published
CCDC 156813

Re 71

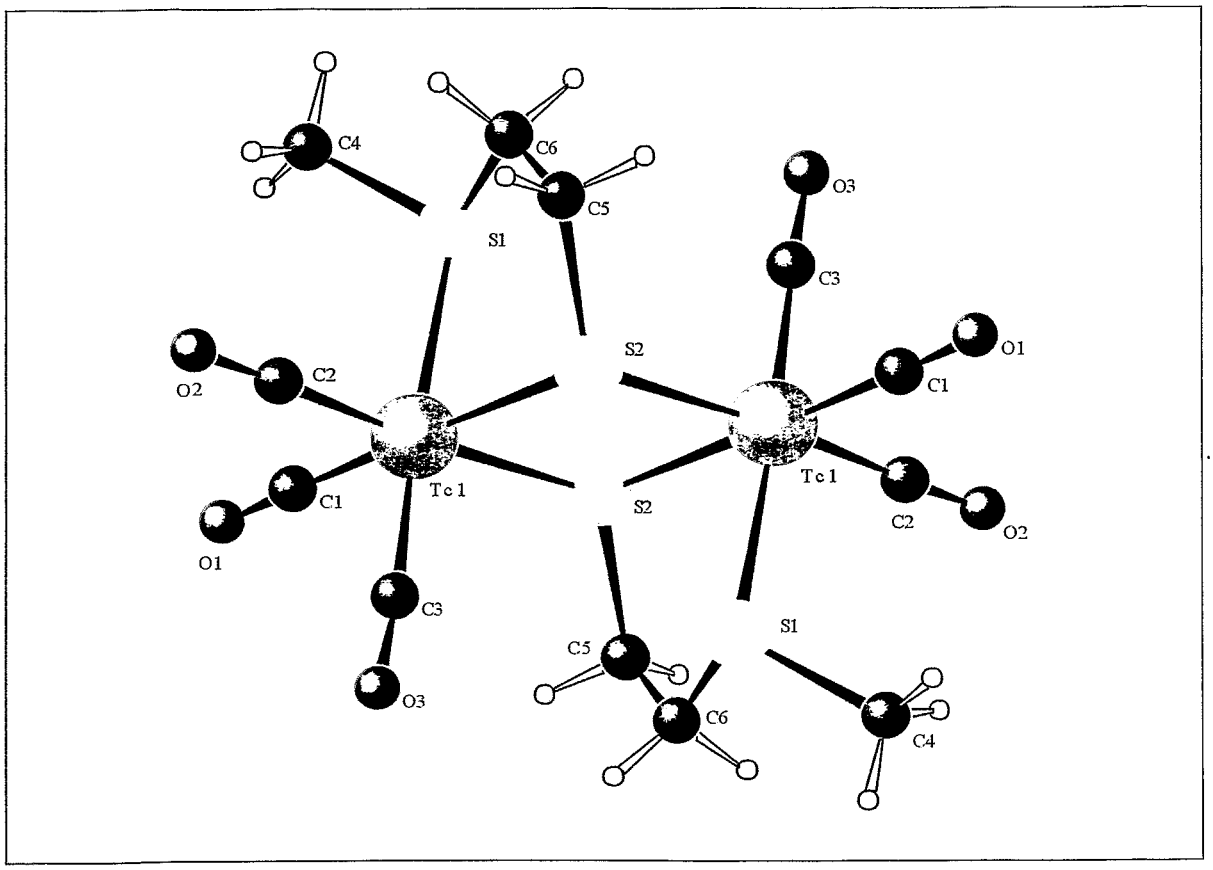
Selected Bonds (Å) and Angles (°)

Bonds

Re(1)-C(25)	1.830
Re(1)-C(24)	1.950
Re(1)-C(28)	1.960
Re(1)-C(27)	1.962
Re(1)-S(2)	2.478
Re(1)-S(1)	2.479
Re(1)-Br(2)	2.558
Re(1)-Br(1)	2.596
Br(1)-C(27)	0.656
Br(2)-O(28)	0.532
Br(2)-C(28)	0.649
C(27)-O(27)	1.117
C(28)-O(28)	1.118
S(1)-C(21)	1.818
S(1)-C(22)	1.823
S(2)-C(23)	1.789
S(2)-C(26)	1.835
O(3)-C(3)	1.230
O(2)-C(24)	1.100
O(1)-C(25)	1.250
O(20)-C(20)	1.180
C(1)-C(2)	1.530
C(1)-C(10)	1.580
C(2)-C(3)	1.580
C(3)-C(4)	1.360
C(4)-C(5)	1.310
C(5)-C(6)	1.530
C(5)-C(10)	1.530
C(6)-C(7)	1.520
C(7)-C(8)	1.500
C(8)-C(9)	1.480

Angles

C(25)-Re(1)-C(24)	85.20
C(25)-Re(1)-C(28)	84.60
C(24)-Re(1)-C(28)	89.90
C(25)-Re(1)-C(27)	88.40
C(24)-Re(1)-C(27)	89.70
C(28)-Re(1)-C(27)	173.00
C(25)-Re(1)-S(2)	175.40
C(24)-Re(1)-S(2)	93.50
C(28)-Re(1)-S(2)	91.00
C(27)-Re(1)-S(2)	96.00
C(25)-Re(1)-S(1)	97.50
C(24)-Re(1)-S(1)	173.70
C(28)-Re(1)-S(1)	96.00
C(27)-Re(1)-S(1)	84.60
S(2)-Re(1)-S(1)	84.25
C(25)-Re(1)-Br(2)	91.00
C(24)-Re(1)-Br(2)	91.00
C(28)-Re(1)-Br(2)	6.40
C(27)-Re(1)-Br(2)	179.00
S(2)-Re(1)-Br(2)	84.67
S(1)-Re(1)-Br(2)	94.64
C(25)-Re(1)-Br(1)	92.60
C(24)-Re(1)-Br(1)	91.20
C(28)-Re(1)-Br(1)	176.80
C(27)-Re(1)-Br(1)	4.30
S(2)-Re(1)-Br(1)	91.86
S(1)-Re(1)-Br(1)	82.99
Br(2)-Re(1)-Br(1)	175.98
C(27)-Br(1)-Re(1)	13.00
O(28)-Br(2)-Re(1)	160.00
C(28)-Br(2)-Re(1)	19.70



Di-μ-{[3-thiabutanethiolato(1-)]bis-(tricarbonyl)}technetium(I)

$C_6H_7O_3S_2Tc$

19.212Å	8.200Å	12.613Å	
90.0000°	103.59°	90.0000°	V=1931.3Å^3
C2/c; 15	Z=8; F(000)=1136	ρ=1.989g/cm^3	R=2.55%
monoclinic			

M. Reisgys (1997)
not published
CCDC 159505

Tc 72

Selected Bonds (Å) and Angles (°)

Bonds

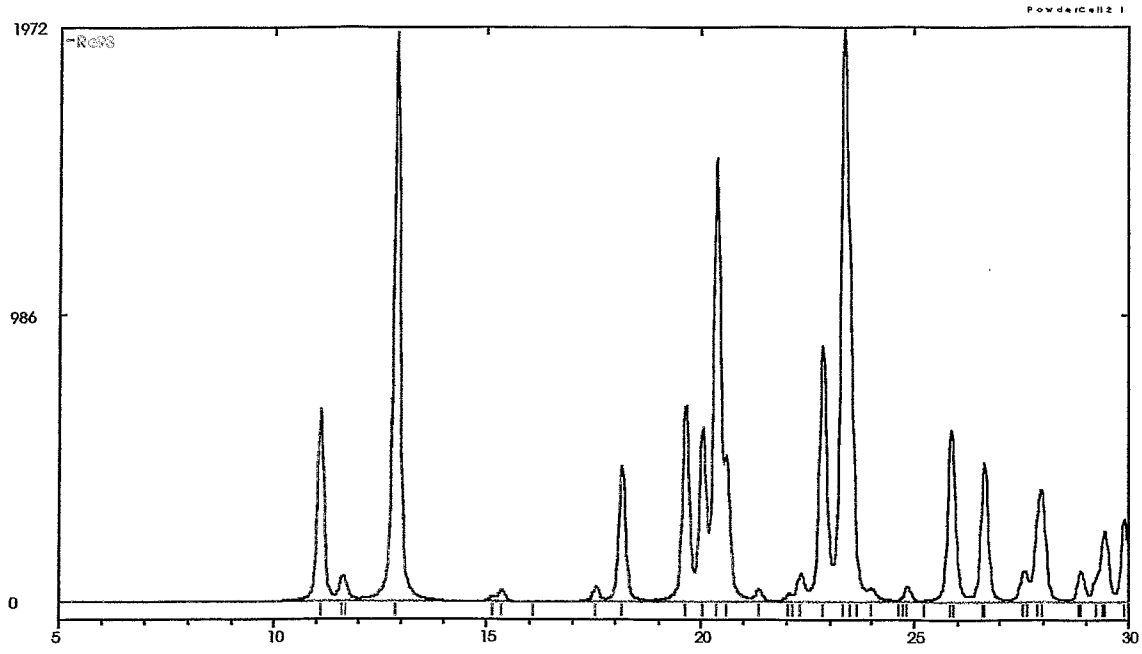
Tc(1)-C(2)	1.905
Tc(1)-C(3)	1.918
Tc(1)-C(1)	1.923
Tc(1)-S(1)	2.487
Tc(1)-S(2)	2.530
S(1)-C(4)	1.792
S(1)-C(6)	1.799
S(2)-C(5)	1.825
O(1)-C(1)	1.134
O(2)-C(2)	1.143
O(3)-C(3)	1.134

Angles

C(2)-Tc(1)-C(3)	87.10
C(2)-Tc(1)-C(1)	90.80
C(3)-Tc(1)-C(1)	88.30
C(2)-Tc(1)-S(1)	92.92
C(3)-Tc(1)-S(1)	175.33
C(1)-Tc(1)-S(1)	96.34
C(2)-Tc(1)-S(2)	94.00
C(3)-Tc(1)-S(2)	94.62
C(1)-Tc(1)-S(2)	174.48
S(1)-Tc(1)-S(2)	80.72
C(2)-Tc(1)-S(2)	174.99
C(3)-Tc(1)-S(2)	97.09
C(1)-Tc(1)-S(2)	92.14
S(1)-Tc(1)-S(2)	82.71
S(2)-Tc(1)-S(2)	82.86
C(4)-S(1)-Tc(1)	111.90
C(6)-S(1)-Tc(1)	104.10
C(5)-S(2)-Tc(1)	102.30
C(5)-S(2)-Tc(1)	111.70
Tc(1)-S(2)-Tc(1)	97.14
O(1)-C(1)-Tc(1)	178.00
O(2)-C(2)-Tc(1)	177.70
O(3)-C(3)-Tc(1)	176.60

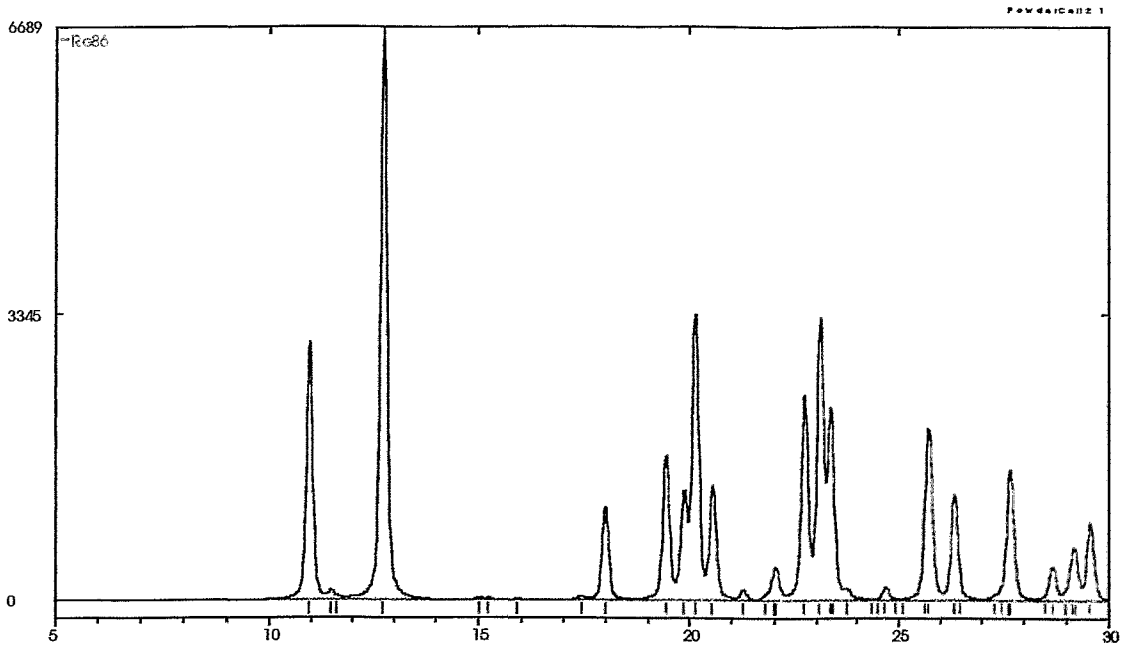
6. Supplement - Tables of calculated powder diffraction data

Tc 1



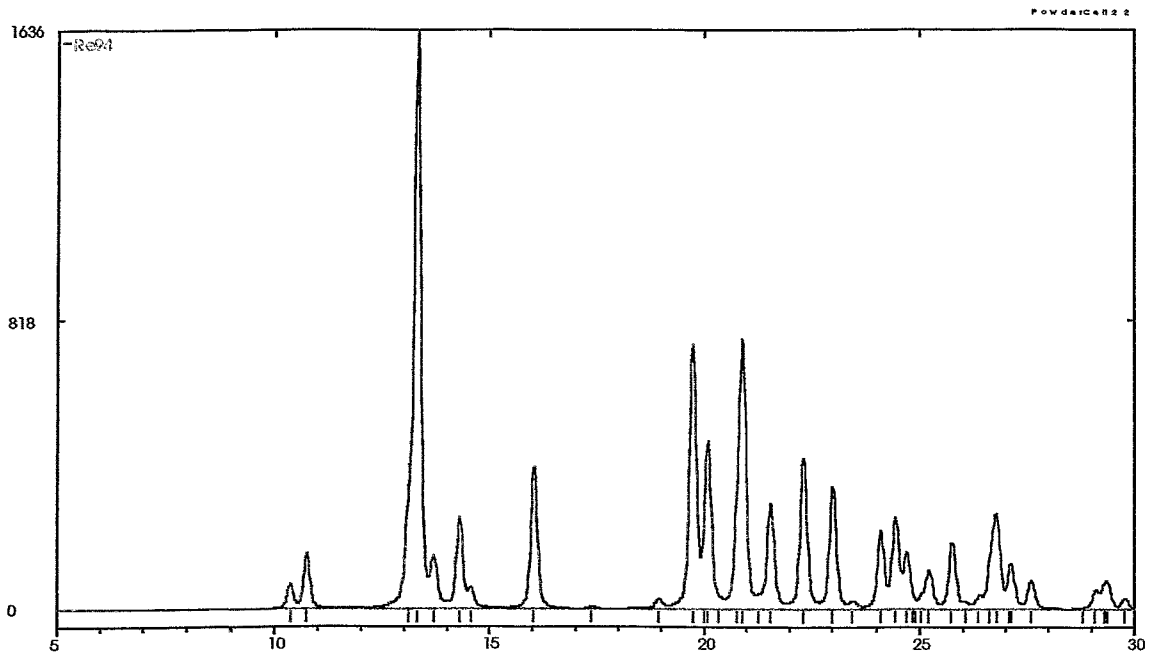
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	11.114	7.9545	34	16	23.369	3.8035	100
2	11.648	7.5912	5	17	23.991	3.7063	2
3	12.879	6.8683	99	18	24.845	3.5809	3
4	15.169	5.8362	1	19	25.847	3.4442	30
5	15.367	5.7614	2	20	26.634	3.3442	24
6	17.556	5.0475	3	21	27.574	3.2323	5
7	18.162	4.8804	24	22	27.943	3.1905	20
8	19.646	4.5151	34	23	28.888	3.0882	5
9	20.058	4.4233	30	24	29.238	3.0520	4
10	20.391	4.3519	77	25	29.444	3.0311	12
11	20.660	4.2957	25				
12	21.371	4.1544	2				
13	22.080	4.0226	1				
14	22.349	3.9748	5				
15	22.846	3.8894	45				

Re 1



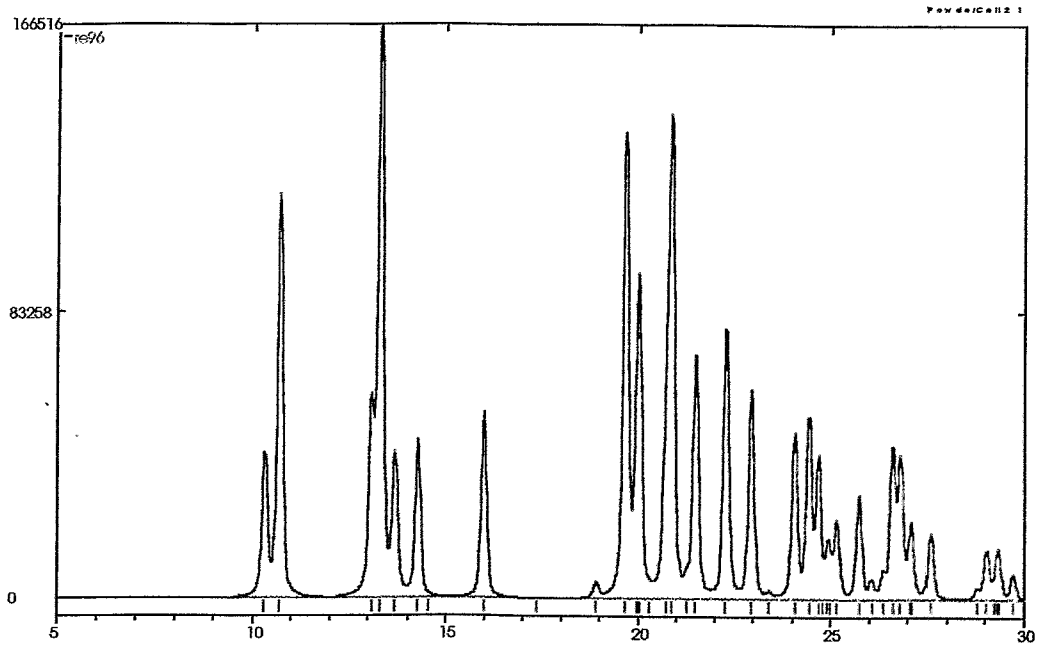
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	10.972	8.0571	45	16	23.752	3.7430	2
2	11.491	7.6947	2	17	24.689	3.6031	2
3	12.748	6.9387	100	18	25.709	3.4624	30
4	17.434	5.0827	1	19	26.333	3.3817	19
5	18.000	4.9242	16	20	27.668	3.2215	23
6	19.450	4.5601	25	21	28.672	3.1110	6
7	19.887	4.4609	19	22	29.176	3.0583	9
8	20.147	4.4040	50	23	29.564	3.0191	14
9	20.569	4.3146	20				
10	21.299	4.1682	2				
11	21.820	4.0699	1				
12	22.052	4.0276	6				
13	22.731	3.9088	36				
14	23.111	3.8455	49				
15	23.367	3.8039	34				

Tc 2



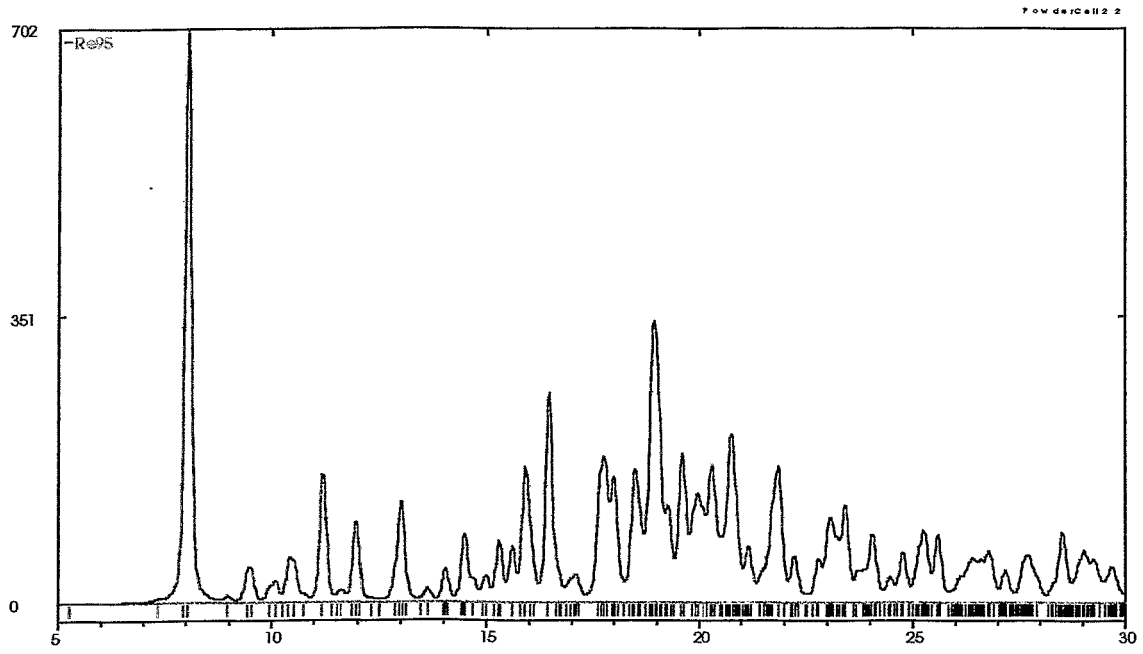
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	10.347	8.5430	4	16	23.003	3.8632	21
2	10.733	8.2359	10	17	23.473	3.7870	1
3	13.100	6.7528	21	18	24.117	3.6872	14
4	13.316	6.6440	100	19	24.452	3.6375	16
5	13.703	6.4570	9	20	24.713	3.5996	10
6	14.308	6.1852	16	21	25.234	3.5264	7
7	14.571	6.0743	4	22	25.771	3.4542	11
8	16.050	5.5177	25	23	26.414	3.3716	2
9	17.388	5.0961	1	24	26.796	3.3244	17
10	18.943	4.6810	2	25	27.140	3.2830	8
11	19.729	4.4962	46	26	27.611	3.2280	5
12	20.079	4.4187	29	27	29.107	3.0655	3
13	20.905	4.2458	47	28	29.347	3.0409	5
14	21.566	4.1173	18	29	29.782	2.9975	2
15	22.322	3.9794	26				

Re 2



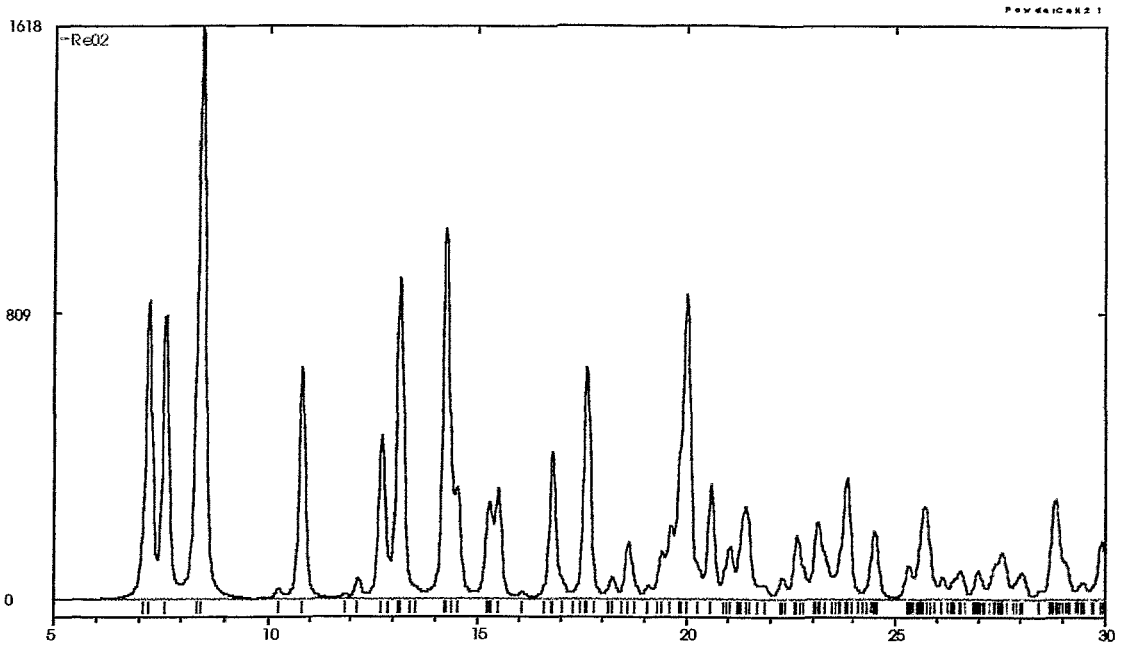
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	10.326	8.5602	26	17	24.064	3.6953	29
2	10.710	8.2537	71	18	24.428	3.6410	32
3	13.103	6.7512	36	19	24.684	3.6038	25
4	13.310	6.6470	100	20	24.941	3.5673	11
5	13.688	6.4640	26	21	25.162	3.5365	14
6	14.278	6.1983	28	22	25.739	3.4584	18
7	16.004	5.5336	32	23	26.066	3.4158	4
8	18.932	4.6838	3	24	26.358	3.3786	5
9	19.680	4.5074	81	25	26.604	3.3479	27
10	20.013	4.4332	57	26	26.812	3.3224	25
11	20.720	4.2834	47	27	27.075	3.2908	13
12	20.869	4.2532	84	28	27.573	3.2324	11
13	21.513	4.1272	43	30	29.029	3.0735	8
14	22.312	3.9813	47	31	29.331	3.0425	9
15	22.954	3.8713	37	32	29.720	3.0036	5

Tc 3



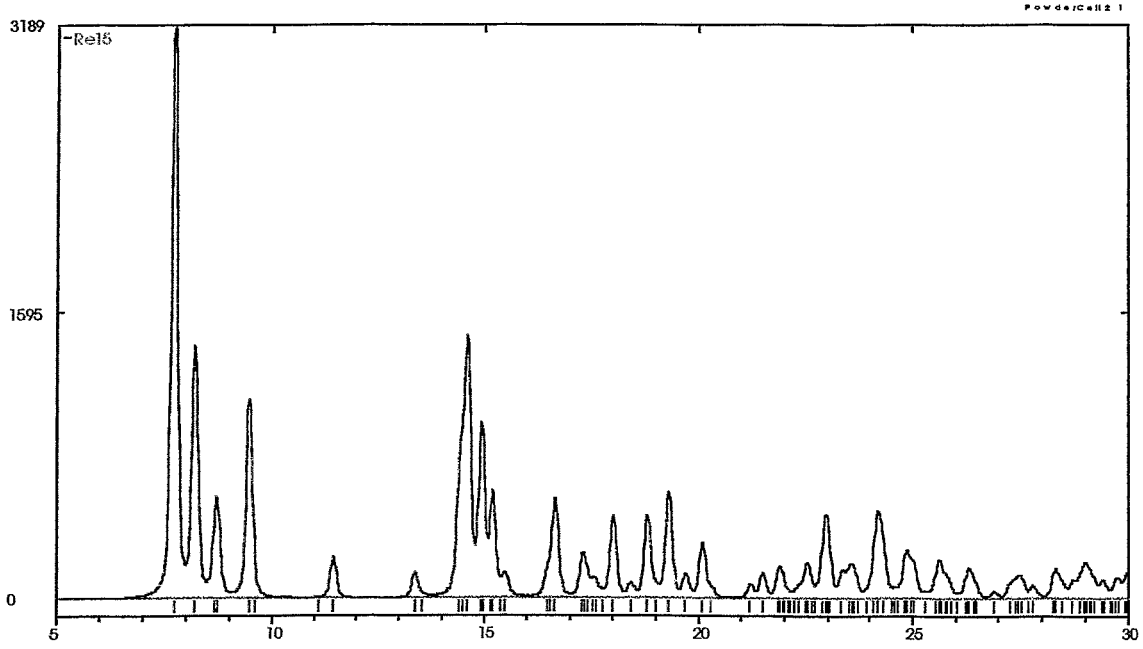
-N-	2 theta	---d---	I_{rel}	-N-	2 theta	---d---	I_{rel}
1	8.035	10.9944	100	24	19.246	4.6080	17
6	11.212	7.8854	22	25	19.590	4.5280	26
7	11.972	7.3864	14	26	19.951	4.4468	19
8	13.025	6.7913	18	27	20.291	4.3730	24
11	14.510	6.0996	12	28	20.763	4.2747	29
13	15.314	5.7811	11	29	21.160	4.1953	10
14	15.613	5.6710	10	30	21.852	4.0640	24
15	15.923	5.5613	24	33	23.069	3.8523	15
16	16.041	5.5208	14	34	23.429	3.7939	17
17	16.460	5.3812	37	35	24.067	3.6948	12
19	17.668	5.0158	21	38	25.262	3.5227	13
20	17.771	4.9870	25	39	25.596	3.4775	12
21	17.998	4.9247	22	41	26.793	3.3247	9
22	18.502	4.7915	23	44	28.532	3.1259	12
23	18.926	4.6853	49	45	29.034	3.0730	9

Re 4



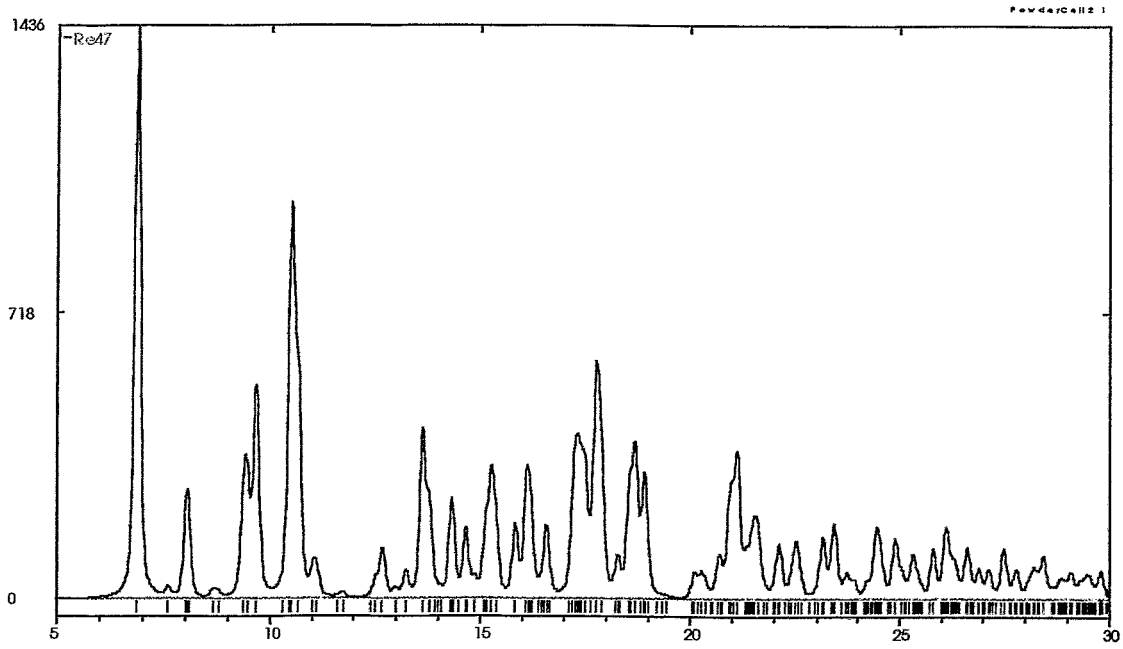
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	7.244	12.1929	52	22	19.865	4.4658	27
2	7.644	11.5563	50	23	20.016	4.4324	53
3	8.479	10.4197	100	24	20.600	4.3080	20
5	10.822	8.1686	41	25	21.042	4.2185	9
8	12.739	6.9432	29	26	21.426	4.1438	16
9	13.160	6.7223	56	29	22.647	3.9231	11
10	14.267	6.2029	65	30	23.140	3.8406	14
11	14.540	6.0871	20	31	23.840	3.7295	21
12	15.285	5.7921	17	32	24.510	3.6290	12
13	15.489	5.7162	19	33	25.320	3.5147	6
15	16.802	5.2723	26	34	25.692	3.4646	16
16	17.637	5.0245	41	38	27.382	3.2545	6
18	18.624	4.7605	10	39	27.559	3.2340	8
20	19.440	4.5625	8	41	28.825	3.0948	18
21	19.620	4.5210	13	42	29.069	3.0694	7

Re 5



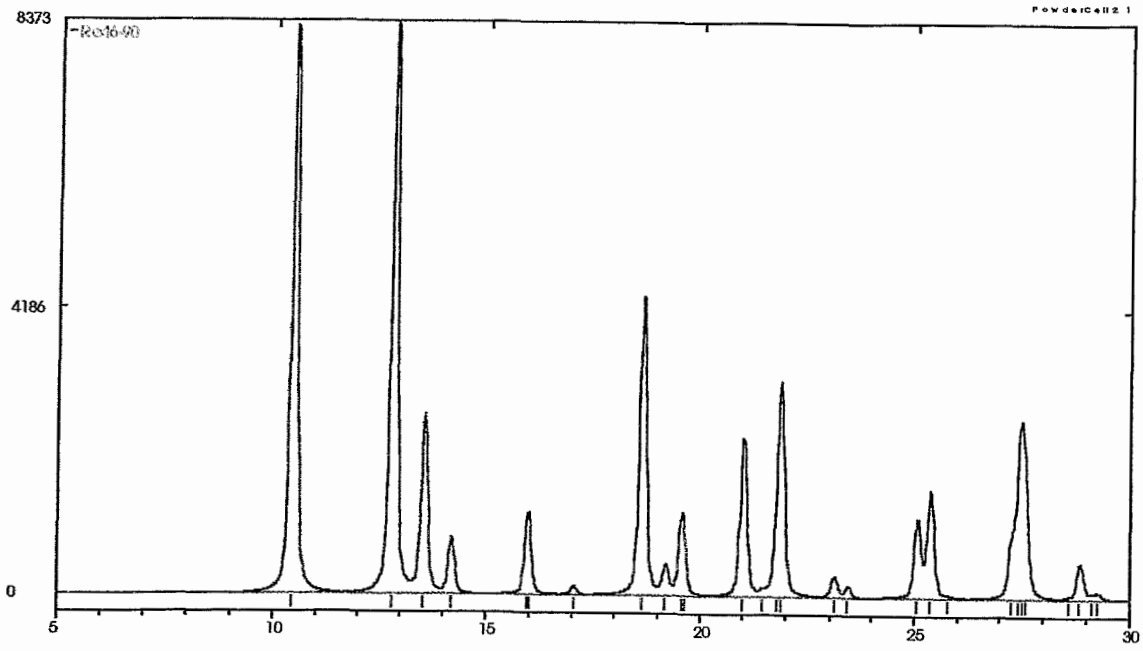
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	7.731	11.4263	100	19	19.303	4.5946	19
2	8.214	10.7557	44	21	20.096	4.4149	10
3	8.726	10.1254	18	23	21.528	4.1245	5
4	9.483	9.3190	35	24	21.920	4.0516	6
5	11.462	7.7140	7	25	22.557	3.9385	6
7	14.448	6.1258	28	26	22.971	3.8685	15
8	14.595	6.0643	46	27	23.360	3.8050	5
9	14.935	5.9272	31	28	23.567	3.7721	6
10	15.204	5.8227	19	29	24.213	3.6729	15
11	15.500	5.7122	5	30	24.878	3.5761	8
12	16.486	5.3727	6	31	25.014	3.5570	6
13	16.657	5.3178	17	32	25.616	3.4747	7
14	17.306	5.1199	8	33	26.315	3.3840	5
16	18.018	4.9191	14	37	28.308	3.1501	5
18	18.816	4.7123	15	38	29.005	3.0760	6

Re 6



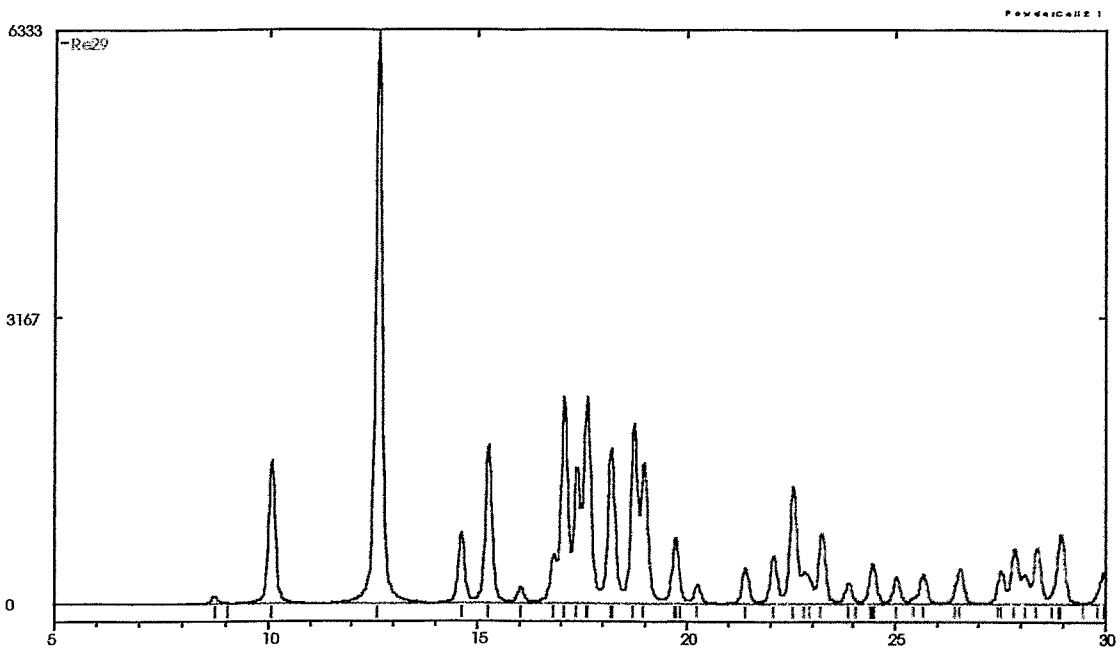
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	6.879	12.8388	100	25	17.317	5.1169	29
3	8.068	10.9493	19	26	17.451	5.0777	26
5	9.436	9.3655	25	27	17.788	4.9822	42
6	9.672	9.1370	37	29	18.585	4.7703	22
7	10.524	8.3991	69	30	18.694	4.7428	27
8	10.680	8.2769	44	31	18.924	4.6857	22
15	13.624	6.4943	30	35	21.000	4.2269	21
16	13.780	6.4211	19	36	21.128	4.2016	26
17	14.321	6.1797	18	37	21.580	4.1147	15
18	14.658	6.0384	13	39	22.530	3.9433	10
20	15.160	5.8396	17	40	23.170	3.8358	11
21	15.273	5.7966	23	41	23.434	3.7932	13
22	15.839	5.5907	13	45	24.459	3.6364	13
23	16.130	5.4906	23	46	24.891	3.5743	11
24	16.587	5.3404	13	50	26.101	3.4113	13

Re 7



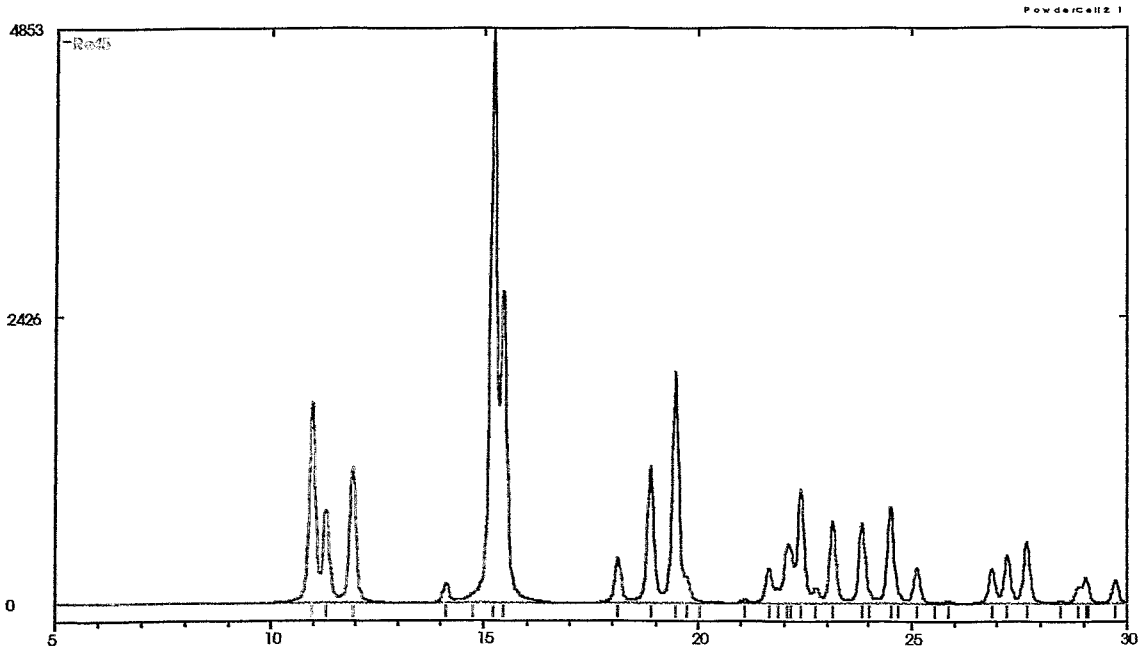
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	10.478	8.4360	99	16	27.291	3.2651	12
2	12.814	6.9027	100	17	27.502	3.2406	31
3	13.546	6.5313	31	18	28.861	3.0910	6
4	14.198	6.2330	10	19	29.225	3.0534	1
5	15.968	5.5460	14				
6	17.039	5.1997	2				
7	18.656	4.7524	52				
8	19.196	4.6200	6				
9	19.574	4.5315	15				
10	21.033	4.2203	28				
11	21.895	4.0562	38				
12	23.123	3.8435	4				
13	23.429	3.7939	2				
14	25.062	3.5503	14				
15	25.367	3.5082	19				

Re 8



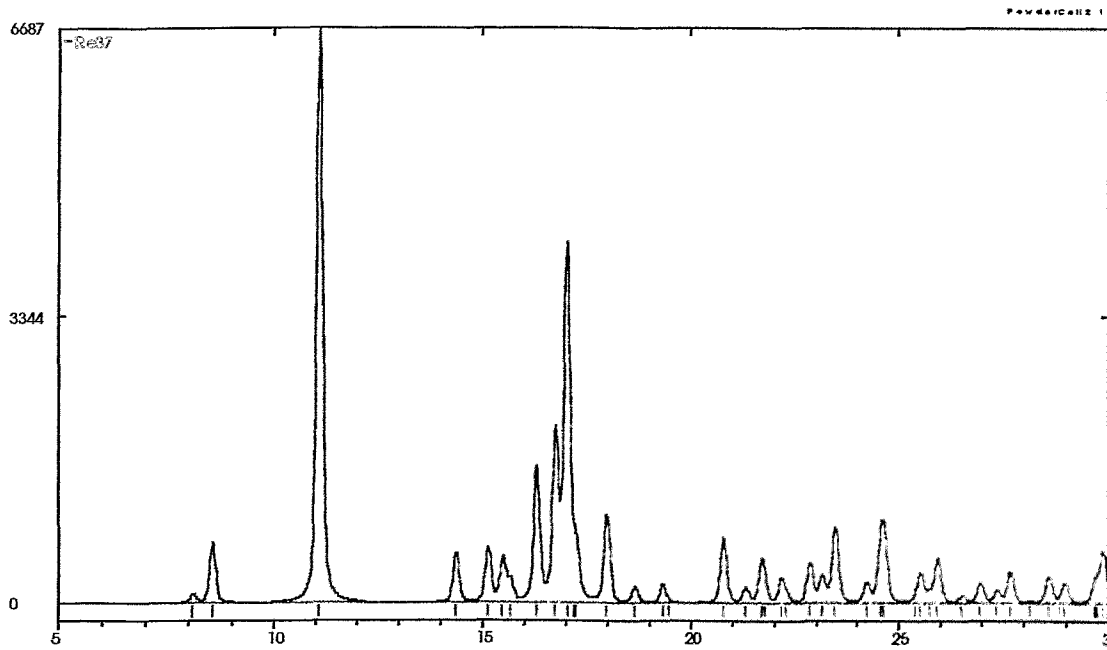
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	8.770	10.0745	1	16	21.432	4.1428	6
2	10.089	8.7602	25	17	22.098	4.0193	8
3	12.651	6.9916	100	18	22.567	3.9369	20
4	14.629	6.0505	12	19	22.844	3.8898	6
5	15.269	5.7982	28	20	23.250	3.8227	12
6	16.024	5.5267	3	21	23.888	3.7221	4
7	16.820	5.2668	9	22	24.462	3.6360	7
8	17.080	5.1873	36	23	25.027	3.5552	5
9	17.383	5.0976	24	24	25.666	3.4681	5
10	17.629	5.0270	36	25	26.548	3.3548	6
11	18.214	4.8668	27	26	27.532	3.2371	6
12	18.769	4.7240	31	27	27.861	3.1997	10
13	18.985	4.6708	25	28	28.103	3.1727	5
14	19.734	4.4952	11	29	28.397	3.1405	10
15	20.273	4.3768	3	30	28.953	3.0814	12

Re 9



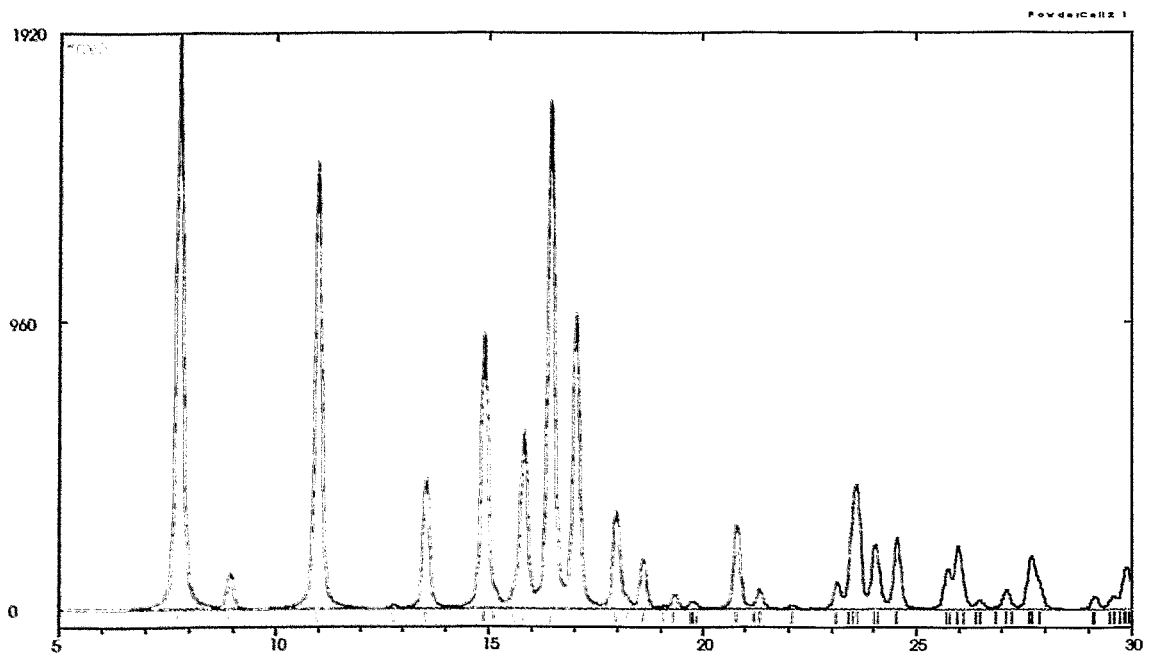
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	10.993	8.0419	35	16	23.146	3.8396	14
2	11.319	7.8113	16	17	23.846	3.7286	14
3	11.937	7.4082	24	18	24.514	3.6284	17
4	14.134	6.2610	3	19	25.120	3.5422	6
5	15.229	5.8133	100	20	25.838	3.4454	1
6	15.467	5.7244	54	21	26.883	3.3138	6
7	18.137	4.8871	8	22	27.226	3.2728	8
8	18.894	4.6932	24	23	27.676	3.2206	11
9	19.481	4.5530	40	24	28.470	3.1326	1
10	19.740	4.4938	5	25	28.891	3.0879	3
11	21.106	4.2060	1	26	29.054	3.0710	5
12	21.672	4.0973	6	27	29.739	3.0018	4
13	22.122	4.0150	10				
14	22.412	3.9637	20				
15	22.745	3.9064	3				

Re 10



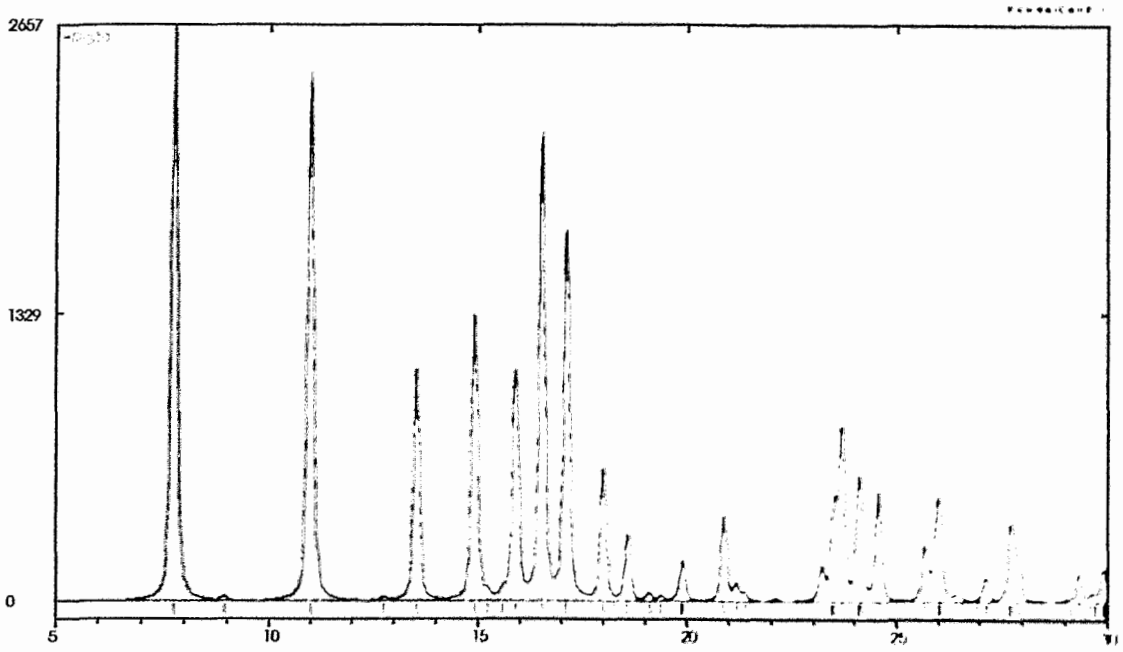
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	8.127	10.8710	2	16	21.723	4.0878	8
2	8.573	10.3053	11	17	22.186	4.0036	4
3	11.107	7.9594	100	18	22.858	3.8873	7
4	14.378	6.1555	9	19	23.140	3.8406	5
5	15.129	5.8514	10	20	23.463	3.7886	13
6	15.492	5.7153	8	21	24.218	3.6720	4
7	15.720	5.6328	4	22	24.609	3.6146	15
8	16.304	5.4323	24	23	25.518	3.4878	5
9	16.765	5.2839	31	24	25.923	3.4343	8
10	17.023	5.2044	63	26	26.960	3.3044	4
11	17.992	4.9263	15	27	27.352	3.2580	2
12	18.645	4.7551	3	28	27.671	3.2211	5
13	19.340	4.5858	3	29	28.586	3.1201	5
14	20.791	4.2689	11	30	28.963	3.0804	4
15	21.336	4.1611	3	31	29.869	2.9890	9

Tc 11



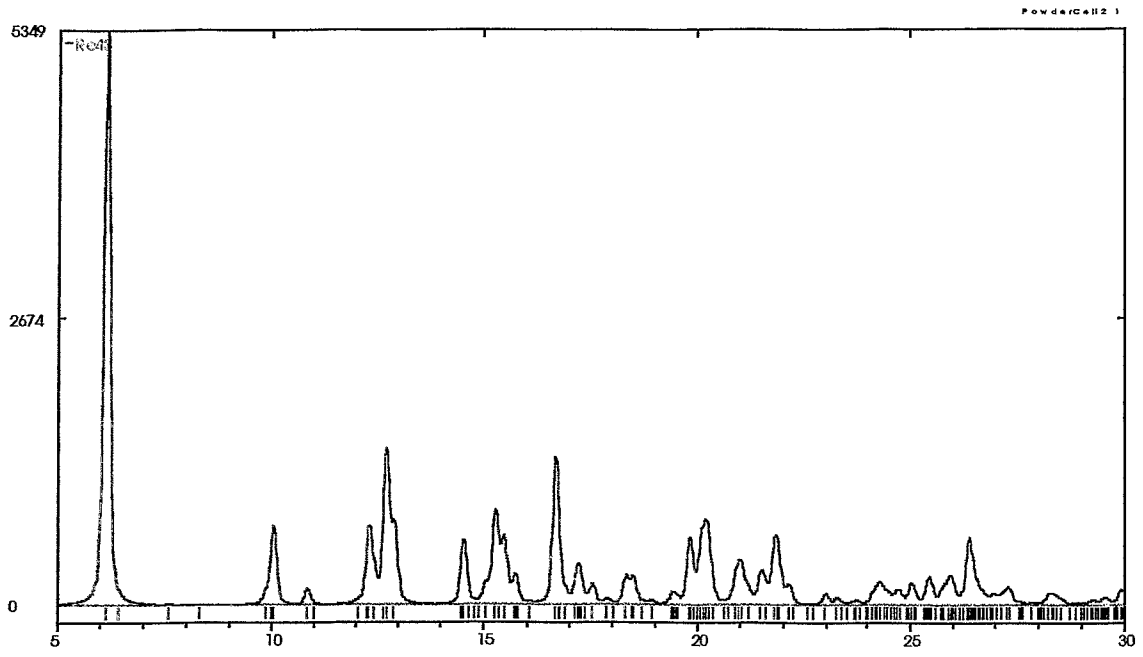
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	7.783	11.3494	100	16	22.116	4.0160	1
2	8.957	9.8647	6	17	23.159	3.8375	5
3	11.006	8.0323	78	18	23.594	3.7677	22
4	12.761	6.9316	1	19	24.041	3.6987	11
5	13.531	6.5388	23	20	24.546	3.6238	12
6	14.906	5.9386	48	21	25.727	3.4600	7
7	15.814	5.5993	31	22	25.973	3.4278	11
8	16.452	5.3836	88	23	26.492	3.3618	2
9	17.035	5.2008	51	24	27.108	3.2868	3
10	17.972	4.9318	17	25	27.691	3.2189	9
11	18.599	4.7670	9	26	29.156	3.0604	2
12	19.331	4.5879	3	27	29.600	3.0155	2
13	19.755	4.4903	1	28	29.884	2.9875	7
14	20.826	4.2618	15				
15	21.348	4.1589	3				

Re 11



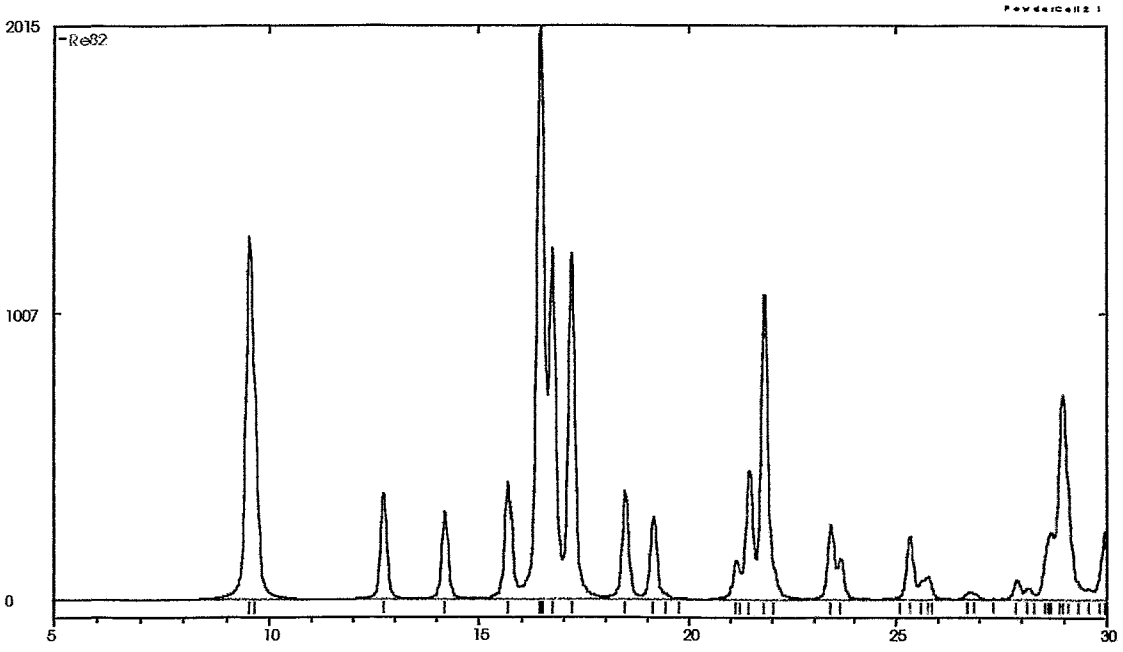
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	7.787	11.3437	100	19	21.400	4.1488	2
3	11.007	8.0319	92	21	23.218	3.8279	6
5	13.515	6.5465	41	22	23.523	3.7790	18
6	14.908	5.9378	50	23	23.676	3.7548	31
7	15.240	5.8091	3	24	24.107	3.6888	22
8	15.620	5.6686	3	25	24.574	3.6197	19
9	15.894	5.5714	41	26	25.654	3.4697	10
10	16.516	5.3629	82	27	25.987	3.4260	19
11	17.111	5.1778	65	28	26.410	3.3721	1
12	17.993	4.9261	23	30	27.132	3.2839	4
13	18.588	4.7695	12	31	27.731	3.2143	14
14	19.101	4.6426	2	32	27.900	3.1953	8
16	19.906	4.4567	7	34	29.328	3.0428	5
17	20.893	4.2484	15	35	29.643	3.0112	2
18	21.195	4.1884	3	36	29.916	2.9843	6

Re 12



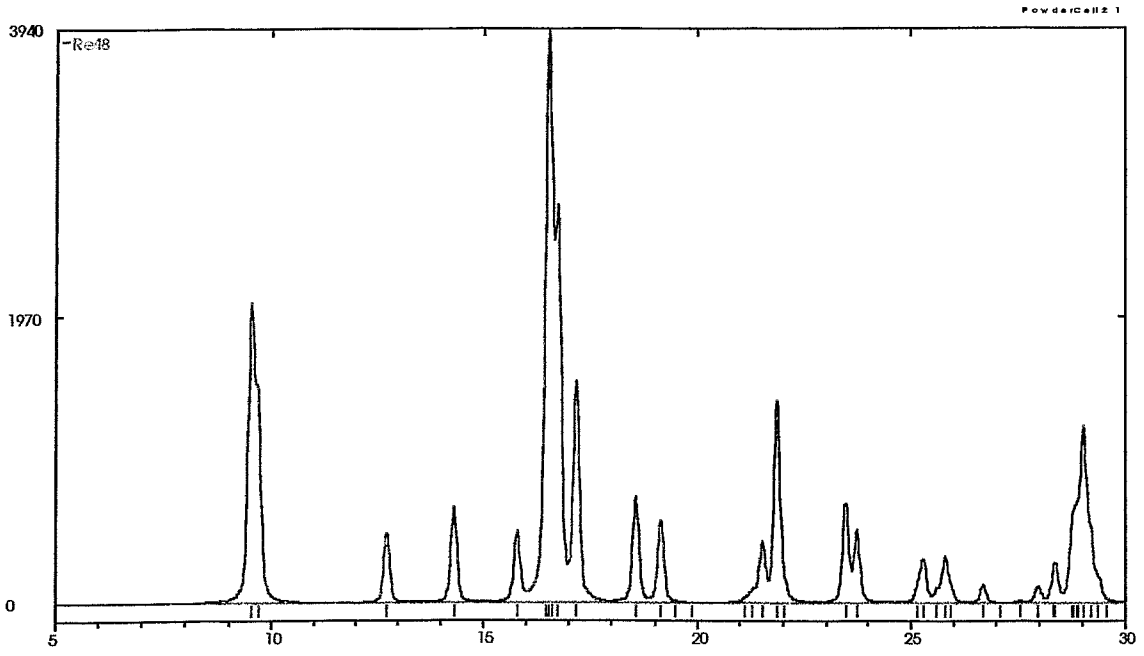
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	6.153	14.3527	100	17	18.496	4.7931	5
2	10.065	8.7812	14	19	19.457	4.5586	2
3	10.867	8.1350	3	20	19.835	4.4726	12
4	12.328	7.1742	14	21	20.196	4.3933	15
5	12.727	6.9497	27	22	21.007	4.2255	8
6	12.940	6.8360	14	23	21.530	4.1241	6
7	14.545	6.0852	11	24	21.852	4.0641	12
8	15.088	5.8672	4	25	22.160	4.0082	4
9	15.287	5.7912	17	29	24.288	3.6616	4
10	15.460	5.7269	12	30	24.713	3.5996	3
11	15.729	5.6295	5	31	25.041	3.5533	4
12	16.688	5.3081	26	32	25.451	3.4969	5
13	17.216	5.1464	7	33	25.933	3.4330	5
14	17.542	5.0517	4	34	26.394	3.3741	12
16	18.351	4.8308	5	36	27.296	3.2646	3

Tc 13



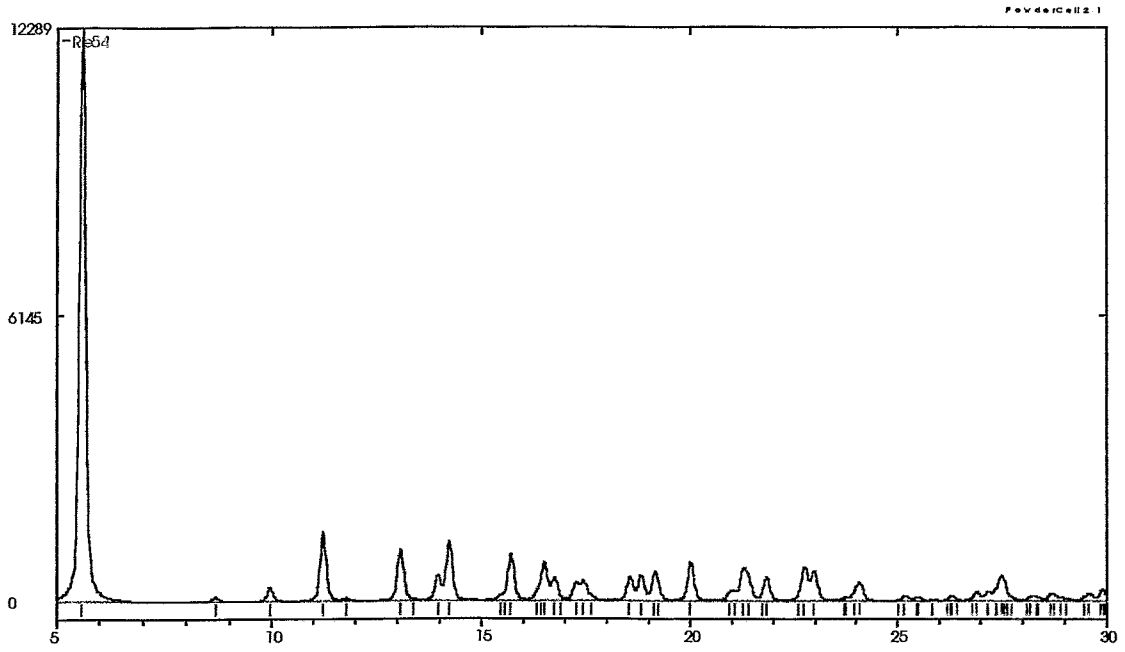
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	9.554	9.2496	63	16	23.654	3.7583	7
2	9.700	9.1109	38	17	25.329	3.5135	11
3	12.724	6.9517	19	18	25.620	3.4742	3
4	14.210	6.2276	15	19	25.750	3.4570	4
5	15.699	5.6401	21	20	26.745	3.3305	1
6	16.456	5.3825	100	21	26.869	3.3155	1
7	16.738	5.2925	61	22	27.890	3.1964	3
8	17.195	5.1528	61	23	28.155	3.1670	2
9	18.481	4.7970	19	24	28.703	3.1077	12
10	19.162	4.6280	14	25	28.973	3.0793	36
11	19.460	4.5578	1	26	29.564	3.0191	2
12	21.158	4.1957	7				
13	21.469	4.1356	23				
14	21.828	4.0684	53				
15	23.428	3.7941	13				

Re 13



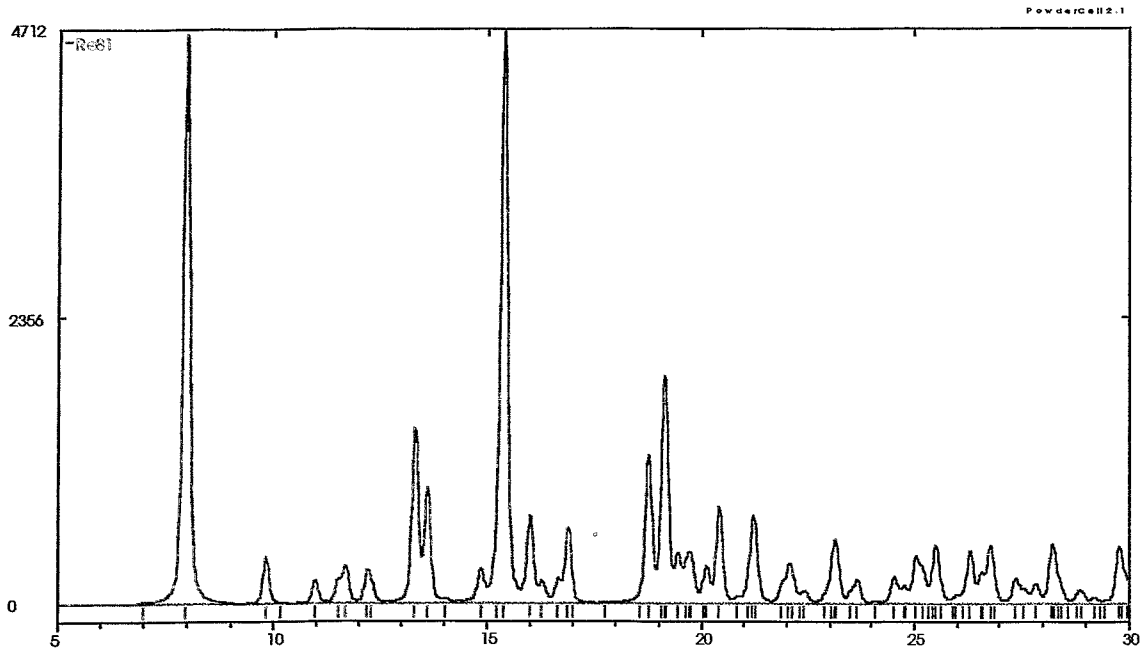
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	9.549	9.2544	53	16	25.285	3.5194	8
2	9.656	9.1519	38	17	25.600	3.4769	3
3	12.721	6.9534	12	18	25.793	3.4513	8
4	14.314	6.1828	17	19	26.688	3.3376	3
5	15.786	5.6092	13	21	27.970	3.1874	3
6	16.532	5.3579	100	22	28.358	3.1446	7
7	16.737	5.2926	69	23	28.840	3.0932	17
8	17.169	5.1605	39	24	29.031	3.0733	31
9	18.557	4.7776	19	25	29.400	3.0356	5
10	19.145	4.6321	14				
11	21.320	4.1642	3				
12	21.547	4.1208	11				
13	21.881	4.0588	35				
14	23.471	3.7872	17				
15	23.738	3.7453	13				

Re 14



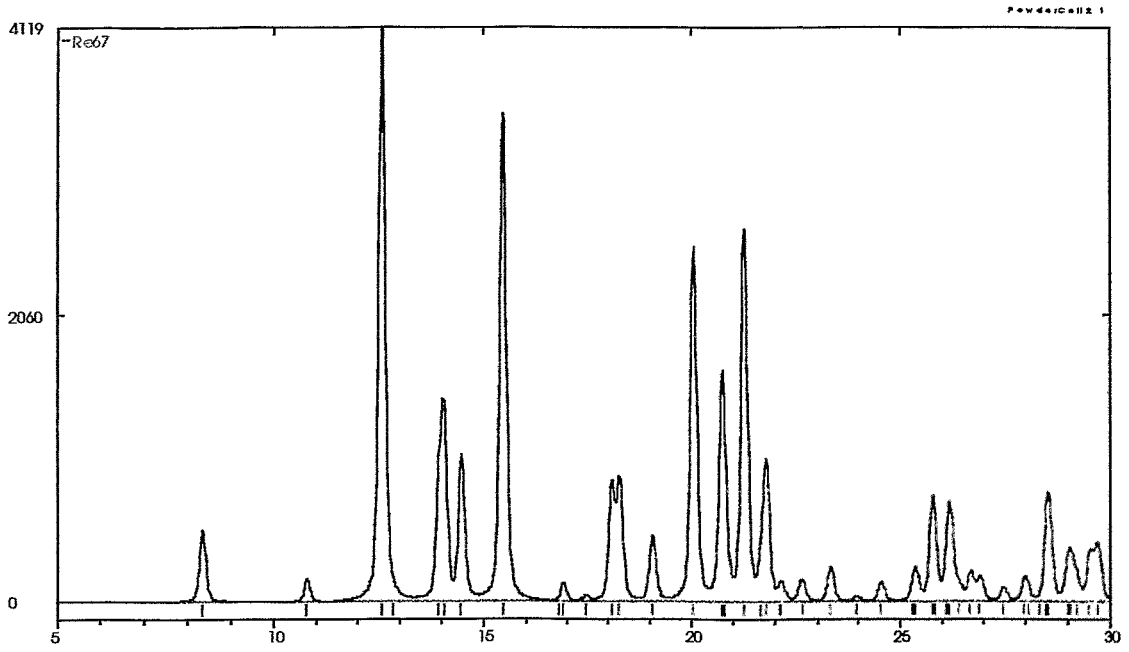
-N-	2 theta	---d---	I_{rel}	-N-	2 theta	---d---	I_{rel}
1	5.620	15.7115	100	18	20.028	4.4299	7
3	9.969	8.8659	2	19	21.020	4.2230	2
4	11.249	7.8598	12	20	21.332	4.1618	6
6	13.060	6.7734	9	21	21.855	4.0635	4
7	13.969	6.3347	5	22	22.779	3.9007	6
8	14.234	6.2174	10	23	22.982	3.8666	5
9	15.462	5.7262	1	25	24.080	3.6928	3
10	15.707	5.6374	8	26	25.188	3.5329	1
11	16.502	5.3675	7	29	26.293	3.3868	1
12	16.753	5.2876	4	30	26.897	3.3121	2
13	17.286	5.1260	3	31	27.200	3.2759	2
14	17.443	5.0801	4	32	27.495	3.2414	5
15	18.575	4.7728	4	34	28.700	3.1080	1
16	18.837	4.7073	5	36	29.580	3.0175	1
17	19.168	4.6267	5	37	29.918	2.9842	2

Re 15a



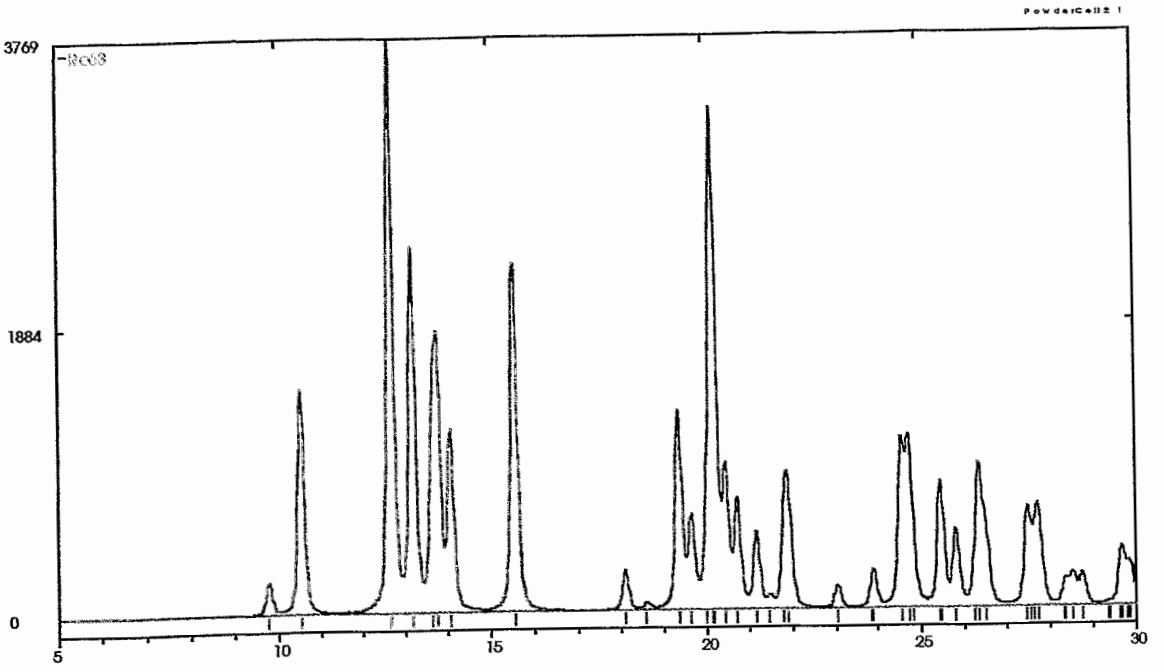
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	7.988	11.0592	99	20	20.115	4.4108	7
2	9.854	8.9690	8	21	20.431	4.3434	17
4	11.554	7.6527	4	22	21.251	4.1776	15
5	11.679	7.5710	7	24	22.087	4.0213	7
6	12.226	7.2333	6	26	23.131	3.8422	11
7	13.315	6.6443	31	28	24.544	3.6240	5
8	13.591	6.5098	20	30	25.063	3.5502	8
10	14.877	5.9502	6	31	25.155	3.5373	7
11	15.386	5.7543	100	32	25.497	3.4907	10
12	16.012	5.5307	15	34	26.316	3.3839	9
15	16.882	5.2476	13	35	26.609	3.3473	6
16	18.763	4.7254	26	36	26.789	3.3252	10
17	19.148	4.6313	40	37	27.391	3.2535	5
18	19.480	4.5532	9	40	28.232	3.1584	10
19	19.708	4.5010	9	43	29.790	2.9968	10

Re 15b



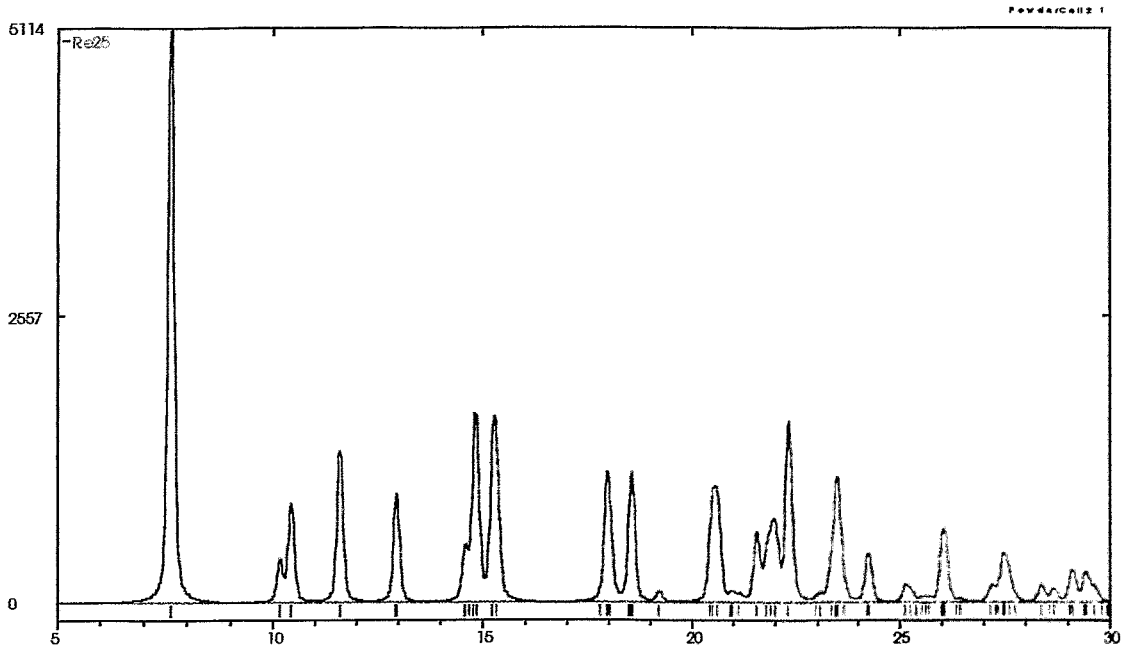
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	8.382	10.5399	13	16	22.176	4.0053	4
2	10.806	8.1807	4	17	22.644	3.9237	4
3	12.563	7.0405	100	18	23.323	3.8109	6
4	14.026	6.3091	35	20	24.542	3.6243	3
5	14.486	6.1098	26	21	25.366	3.5084	6
6	15.472	5.7226	85	22	25.773	3.4540	19
7	16.909	5.2393	3	23	26.166	3.4030	18
8	17.469	5.0725	1	24	26.682	3.3383	5
9	18.105	4.8957	21	25	26.900	3.3117	4
10	18.270	4.8520	21	26	27.475	3.2437	3
11	19.086	4.6462	12	27	27.992	3.1850	5
12	20.061	4.4227	62	28	28.546	3.1244	19
13	20.757	4.2758	40	29	29.060	3.0703	9
14	21.282	4.1715	65	30	29.561	3.0194	9
15	21.813	4.0712	25	31	29.689	3.0067	10

Re 16



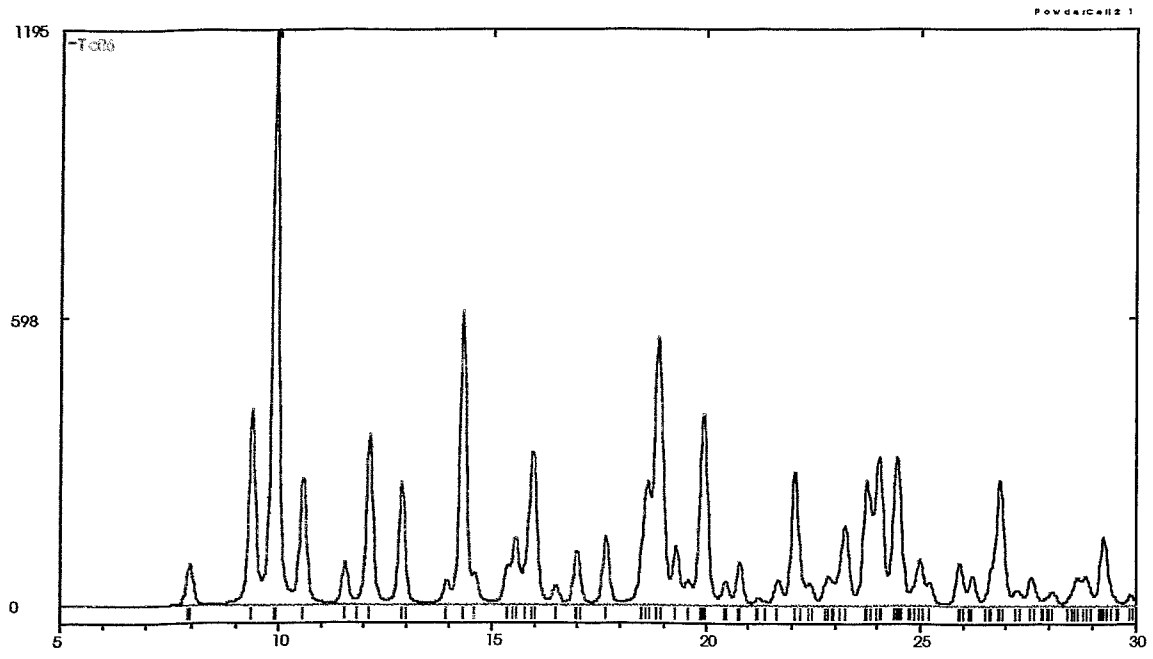
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	9.787	9.0298	6	17	21.889	4.0572	24
2	10.558	8.3720	39	18	23.046	3.8561	4
3	12.660	6.9866	100	19	23.904	3.7196	7
4	13.169	6.7175	64	20	24.578	3.6192	30
5	13.666	6.4743	43	21	24.722	3.5983	30
6	13.729	6.4449	49	22	25.448	3.4973	22
7	14.076	6.2870	32	23	25.809	3.4492	14
8	15.566	5.6883	61	24	26.354	3.3790	25
9	18.119	4.8921	7	25	26.496	3.3613	16
11	19.367	4.5794	35	26	27.516	3.2389	18
12	19.653	4.5136	17	27	27.712	3.2165	18
13	20.177	4.3974	88	28	28.377	3.1426	5
14	20.480	4.3331	26	29	28.543	3.1248	6
15	20.732	4.2809	20	30	28.758	3.1019	6
16	21.196	4.1883	14	31	29.696	3.0060	10

Re 17



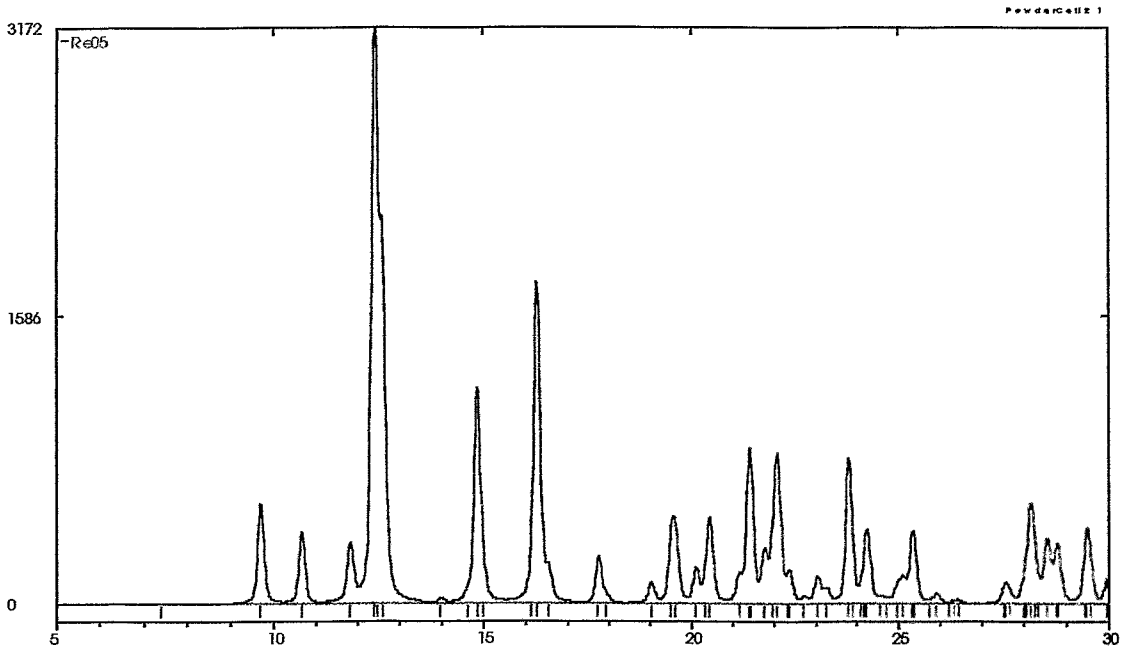
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	7.643	11.5581	100	16	21.975	4.0416	15
2	10.204	8.6622	8	17	22.336	3.9771	32
3	10.441	8.4662	17	18	23.055	3.8546	2
4	11.615	7.6130	27	19	23.482	3.7855	22
5	12.944	6.8338	19	20	24.247	3.6678	9
6	14.600	6.0623	10	21	25.167	3.5357	3
7	14.857	5.9581	33	22	26.040	3.4192	13
8	15.288	5.7908	33	23	26.430	3.3696	1
9	17.990	4.9267	23	24	27.191	3.2769	3
10	18.558	4.7773	23	25	27.490	3.2420	9
11	19.233	4.6111	2	26	28.378	3.1425	3
12	20.566	4.3152	20	27	28.669	3.1113	3
13	20.982	4.2305	2	28	29.117	3.0645	6
14	21.593	4.1121	12	29	29.439	3.0316	5
15	21.892	4.0567	13	30	29.660	3.0095	3

Tc 18



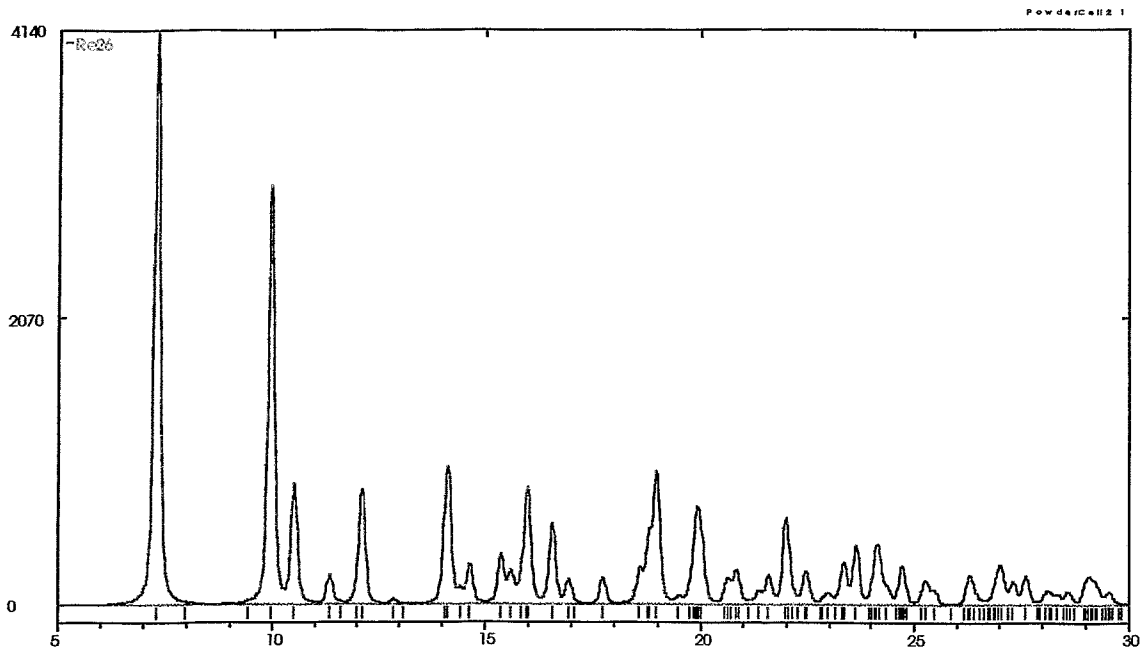
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	7.975	11.0779	7	19	19.291	4.5974	10
2	9.403	9.3981	34	21	19.949	4.4472	33
3	9.937	8.8944	100	23	20.803	4.2665	8
4	10.588	8.3484	22	26	22.088	4.0212	23
5	11.564	7.6462	7	28	22.875	3.8846	5
6	12.140	7.2849	30	29	23.247	3.8231	14
7	12.884	6.8656	21	30	23.762	3.7415	22
9	14.325	6.1780	51	31	24.052	3.6971	26
11	15.380	5.7565	7	32	24.461	3.6362	26
12	15.537	5.6985	12	33	24.981	3.5616	8
13	15.950	5.5522	27	35	25.906	3.4365	7
15	16.996	5.2127	9	36	26.215	3.3967	5
16	17.673	5.0145	12	37	26.878	3.3144	22
17	18.640	4.7566	22	42	28.839	3.0934	5
18	18.892	4.6935	47	43	29.272	3.0485	12

Re 18a



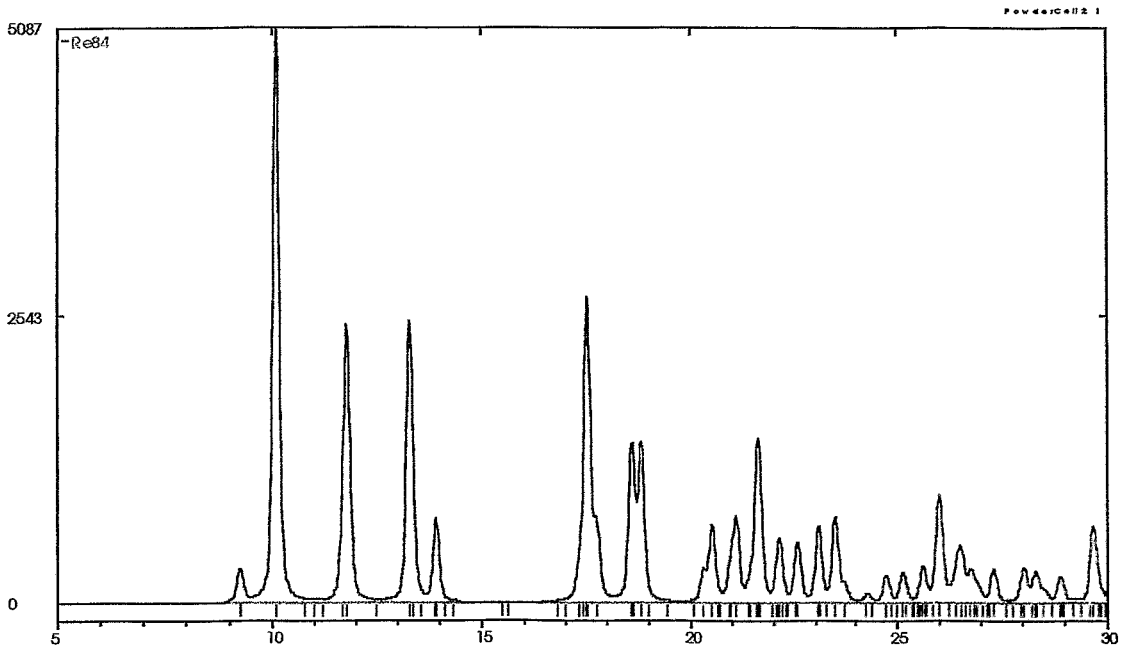
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	9.719	9.0928	17	17	21.777	4.0778	10
2	10.678	8.2782	12	18	22.087	4.0213	27
3	11.834	7.4722	10	19	22.362	3.9724	6
4	12.410	7.1267	100	21	23.030	3.8588	5
5	12.580	7.0308	67	22	23.234	3.8253	3
7	14.849	5.9612	38	23	23.788	3.7375	27
8	16.266	5.4450	57	24	24.220	3.6718	14
9	16.540	5.3553	7	25	24.980	3.5618	4
10	17.753	4.9922	8	26	25.078	3.5481	5
11	19.032	4.6593	4	27	25.321	3.5146	14
12	19.560	4.5347	15	30	27.554	3.2346	4
13	20.107	4.4127	7	31	28.154	3.1670	19
14	20.440	4.3415	15	32	28.529	3.1262	13
15	21.156	4.1961	6	33	28.768	3.1008	11
16	21.418	4.1454	29	34	29.474	3.0281	14

Re 18b



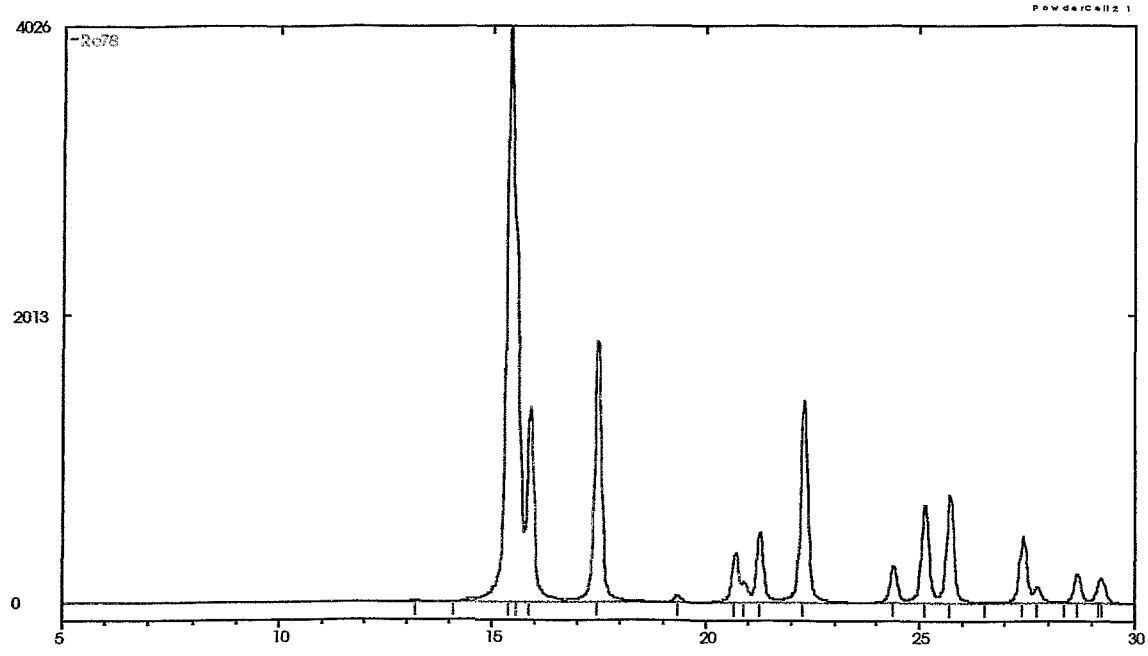
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	7.305	12.0918	100	17	18.969	4.6746	23
2	9.981	8.8553	73	18	19.938	4.4496	17
3	10.534	8.3913	21	19	20.675	4.2926	5
4	11.374	7.7735	5	20	20.854	4.2562	6
5	12.119	7.2970	20	22	21.601	4.1107	5
7	14.134	6.2611	24	23	22.006	4.0359	15
8	14.643	6.0445	7	24	22.476	3.9526	6
9	15.375	5.7583	9	26	23.354	3.8060	7
10	15.601	5.6754	6	27	23.641	3.7604	10
11	15.984	5.5403	20	28	24.152	3.6819	11
12	16.562	5.3484	14	29	24.720	3.5987	7
13	16.938	5.2304	4	32	26.295	3.3866	5
14	17.742	4.9953	5	33	27.006	3.2990	7
15	18.600	4.7666	6	35	27.610	3.2282	5
16	18.816	4.7124	13	38	29.088	3.0674	5

Re 19



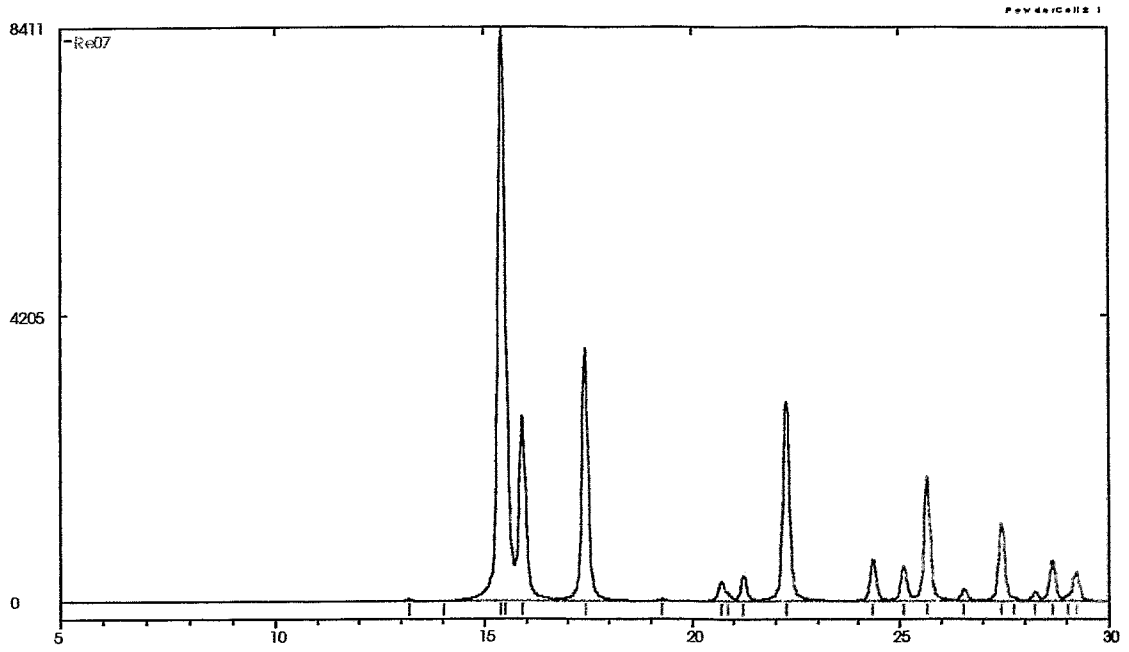
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	9.265	9.5380	6	16	23.087	3.8493	13
2	10.110	8.7426	100	17	23.494	3.7835	15
3	11.792	7.4986	49	18	23.698	3.7515	4
4	13.284	6.6597	49	19	24.292	3.6610	2
5	13.915	6.3591	15	20	24.738	3.5960	5
6	17.535	5.0537	53	21	25.129	3.5410	5
7	17.730	4.9984	15	22	25.608	3.4758	6
8	18.608	4.7645	28	23	26.000	3.4244	19
9	18.820	4.7114	28	24	26.487	3.3624	10
10	20.300	4.3711	6	25	26.760	3.3287	6
11	20.523	4.3242	14	26	27.297	3.2645	6
12	21.092	4.2086	15	27	28.025	3.1812	6
13	21.654	4.1008	29	28	28.306	3.1503	5
14	22.143	4.0113	11	29	28.916	3.0853	5
15	22.585	3.9338	10	30	29.686	3.0070	13

Tc 20



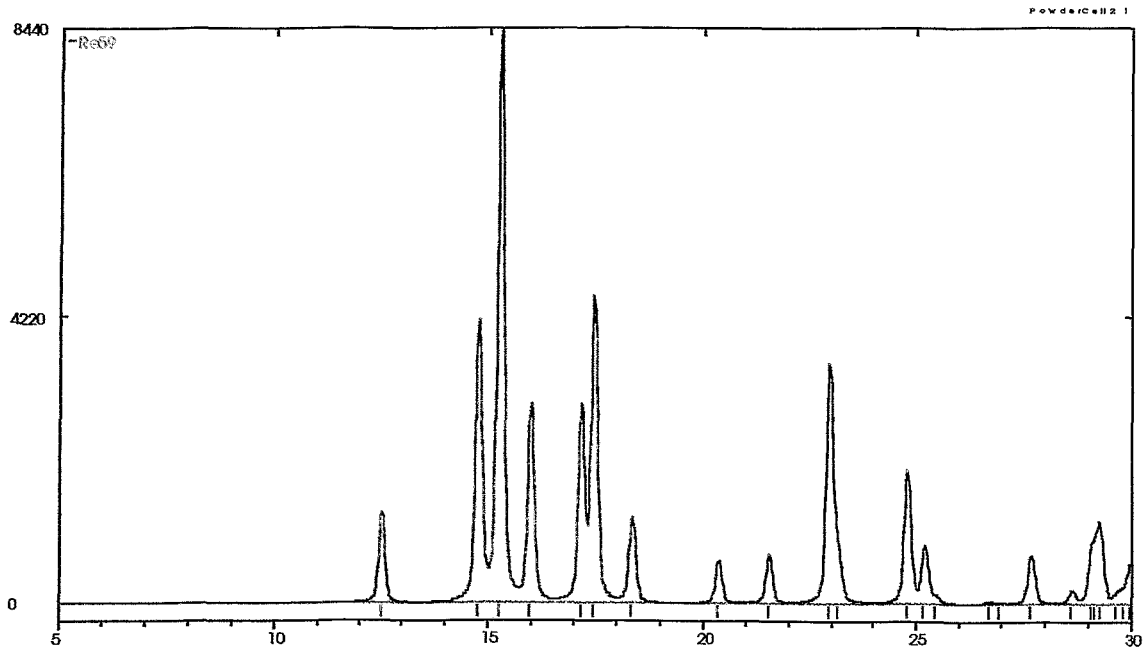
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
2	15.429	5.7383	100	17	29.225	3.0533	4
3	15.524	5.7036	70				
4	15.897	5.5704	34				
5	17.496	5.0649	45				
6	19.347	4.5843	1				
7	20.715	4.2845	9				
8	20.925	4.2419	4				
9	21.293	4.1694	12				
10	22.308	3.9819	35				
11	24.410	3.6436	6				
12	25.124	3.5417	17				
13	25.711	3.4621	19				
14	27.421	3.2500	11				
15	27.739	3.2135	3				
16	28.670	3.1112	5				

Re 20a



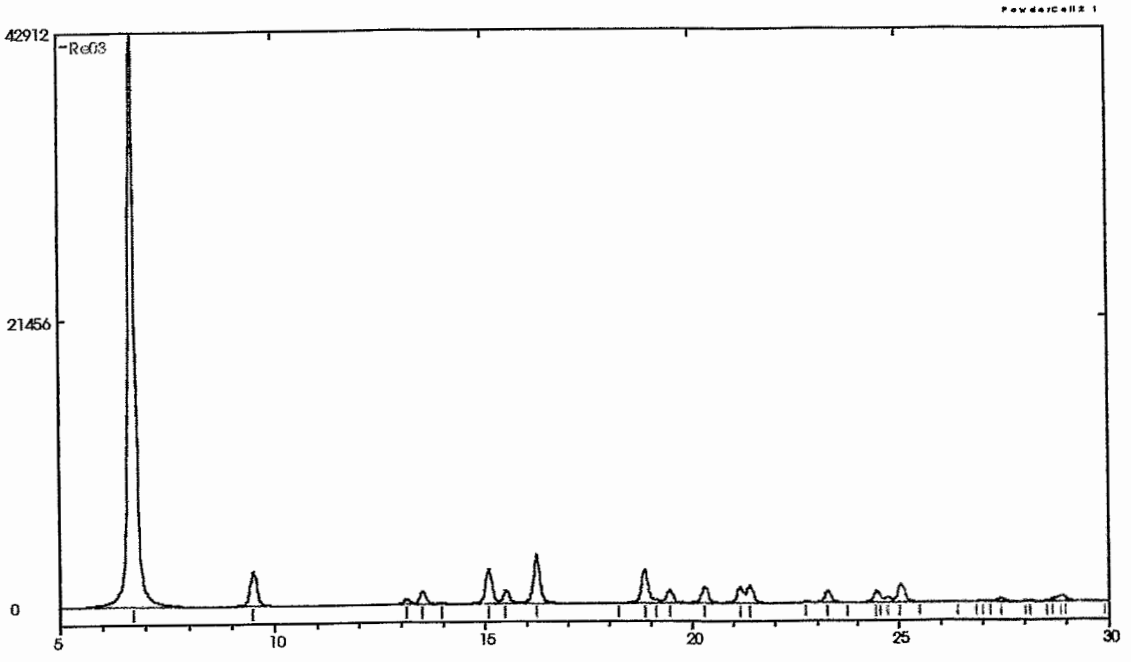
-N-	2 theta	---d---	I_{rel}
1	15.425	5.7399	100
2	15.909	5.5664	32
3	17.434	5.0826	44
4	20.713	4.2848	3
5	20.900	4.2469	1
6	21.259	4.1761	5
7	22.275	3.9878	35
8	24.360	3.6510	7
9	25.093	3.5460	6
10	25.656	3.4694	22
11	26.538	3.3561	2
12	27.439	3.2479	14
13	28.242	3.1573	2
14	28.657	3.1126	7
15	29.231	3.0527	5

Re 20b



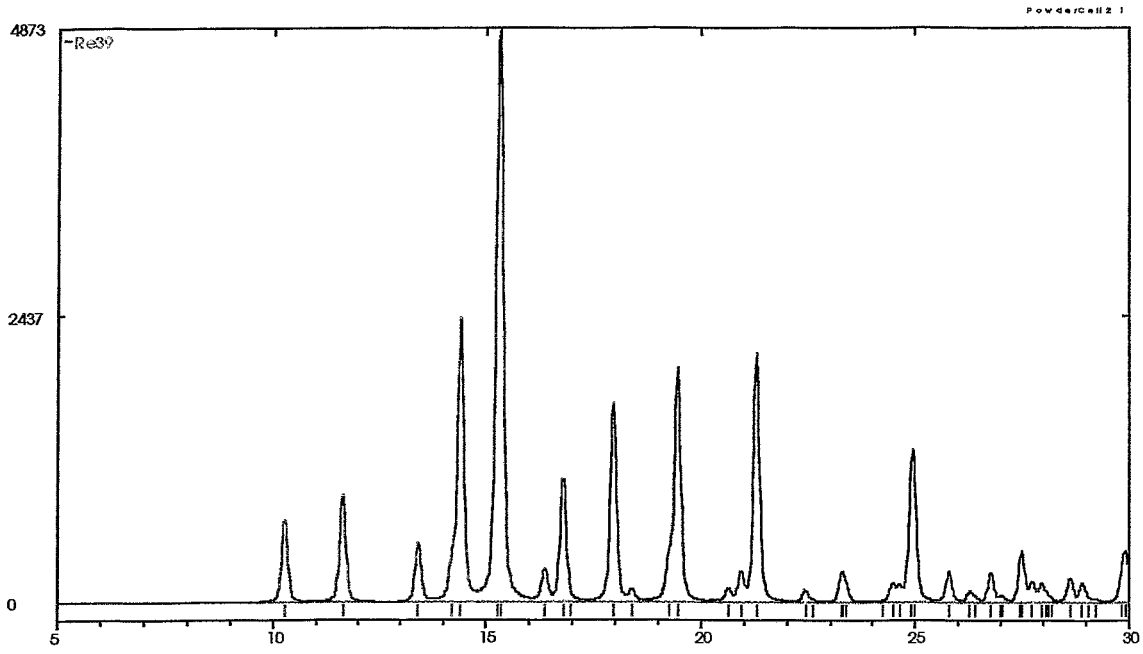
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	12.519	7.0651	16	16	28.635	3.1149	2
2	14.776	5.9904	49	17	29.095	3.0667	11
3	15.269	5.7982	100	18	29.232	3.0526	14
4	15.993	5.5372	35				
5	17.184	5.1560	35				
6	17.482	5.0688	54				
7	18.360	4.8283	15				
8	20.353	4.3598	7				
9	21.558	4.1187	9				
10	22.974	3.8680	42				
11	23.142	3.8404	12				
12	24.787	3.5890	23				
13	25.196	3.5317	10				
14	26.708	3.3351	1				
15	27.683	3.2198	8				

Re 21



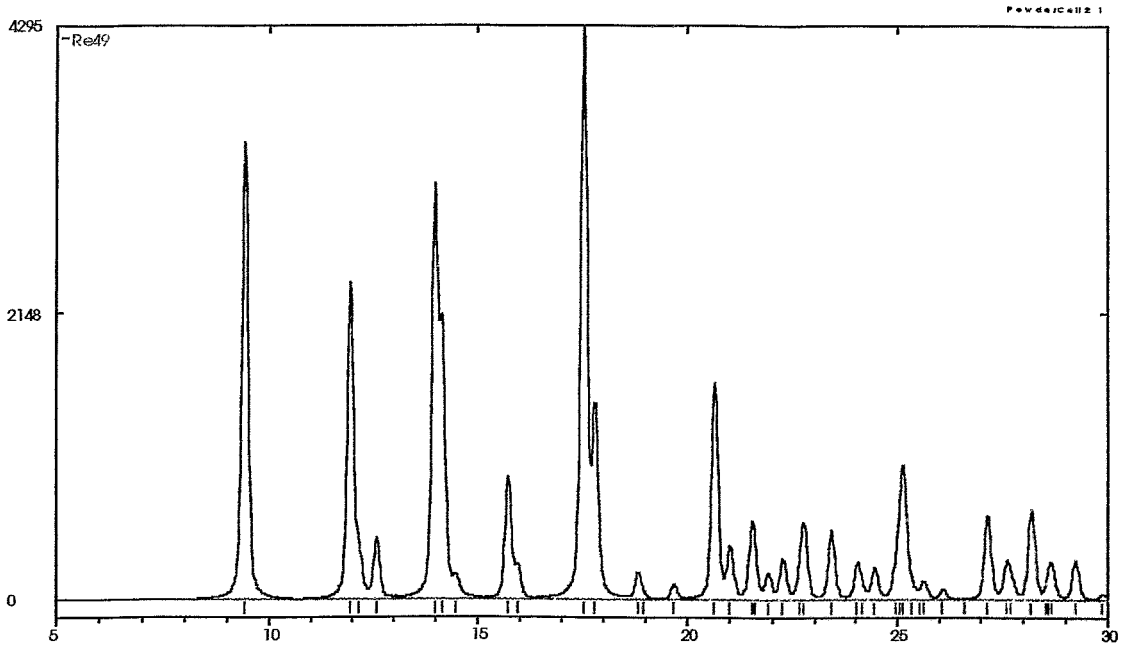
-N-	2 theta	—d—	I_{rel}
1	6.733	13.1177	100
2	9.535	9.2680	9
3	13.121	6.7420	2
4	13.493	6.5569	5
5	13.959	6.3394	1
6	15.109	5.8591	14
7	15.525	5.7029	5
8	16.250	5.4501	21
9	18.871	4.6988	17
10	19.473	4.5549	7
11	20.307	4.3696	9
12	21.193	4.1889	9
13	21.418	4.1454	10
14	22.779	3.9007	1
15	23.280	3.8178	7
16	24.467	3.6352	7
17	24.736	3.5964	4
18	25.054	3.5515	12
19	27.426	3.2494	3
20	28.075	3.1757	1
21	28.665	3.1117	2
22	28.894	3.0876	5

Re 22



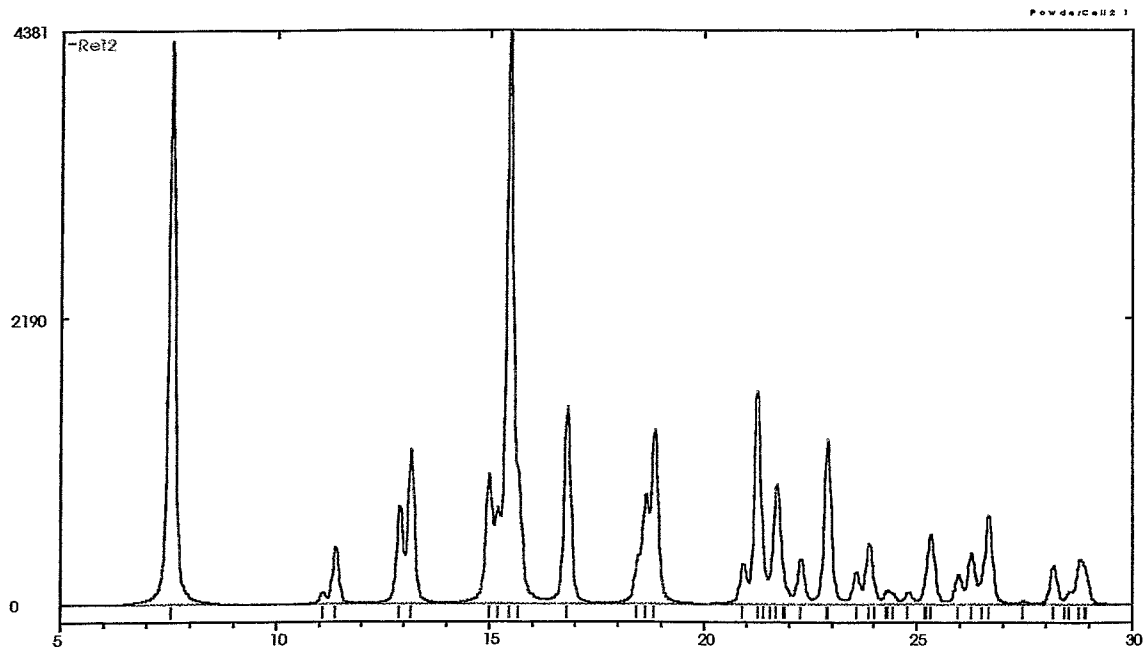
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	10.273	8.6038	14	16	22.427	3.9612	2
2	11.633	7.6008	19	17	23.286	3.8169	5
3	13.399	6.6028	10	18	24.482	3.6330	3
4	14.180	6.2409	10	19	24.650	3.6087	3
5	14.410	6.1417	50	20	24.947	3.5664	27
6	15.318	5.7795	100	21	25.779	3.4531	5
7	16.367	5.4114	6	22	26.270	3.3898	2
8	16.786	5.2773	21	23	26.755	3.3293	5
9	17.963	4.9342	35	24	27.002	3.2995	1
10	18.390	4.8204	2	25	27.488	3.2423	9
11	19.260	4.6047	10	26	27.738	3.2136	4
12	19.461	4.5575	41	27	27.971	3.1873	3
13	20.636	4.3008	3	28	28.630	3.1154	4
14	20.929	4.2411	5	29	28.911	3.0858	3
15	21.302	4.1677	43	31	29.917	2.9843	9

Re 23



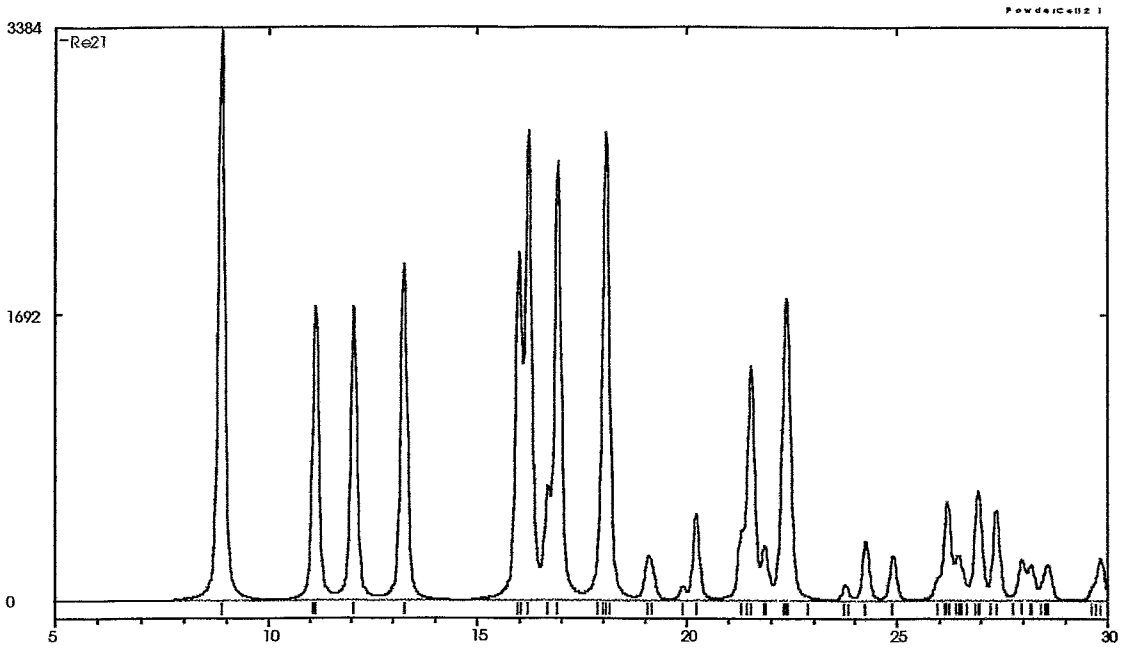
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	9.447	9.3543	80	16	21.924	4.0509	5
2	11.959	7.3947	55	17	22.275	3.9877	7
3	12.583	7.0294	11	18	22.751	3.9054	14
4	14.010	6.3161	73	19	23.420	3.7954	12
5	14.125	6.2650	49	20	24.058	3.6962	7
6	14.520	6.0955	5	21	24.478	3.6336	6
7	15.733	5.6281	21	22	25.134	3.5403	23
8	16.020	5.5280	5	23	25.628	3.4732	3
9	17.546	5.0504	100	24	26.077	3.4144	2
10	17.820	4.9734	34	25	27.151	3.2817	15
11	18.850	4.7039	5	26	27.633	3.2255	7
12	19.689	4.5054	3	27	28.191	3.1630	16
13	20.671	4.2934	38	28	28.656	3.1127	7
14	21.036	4.2198	9	29	29.241	3.0517	7
15	21.563	4.1179	14	30	29.899	2.9861	1

Re 24



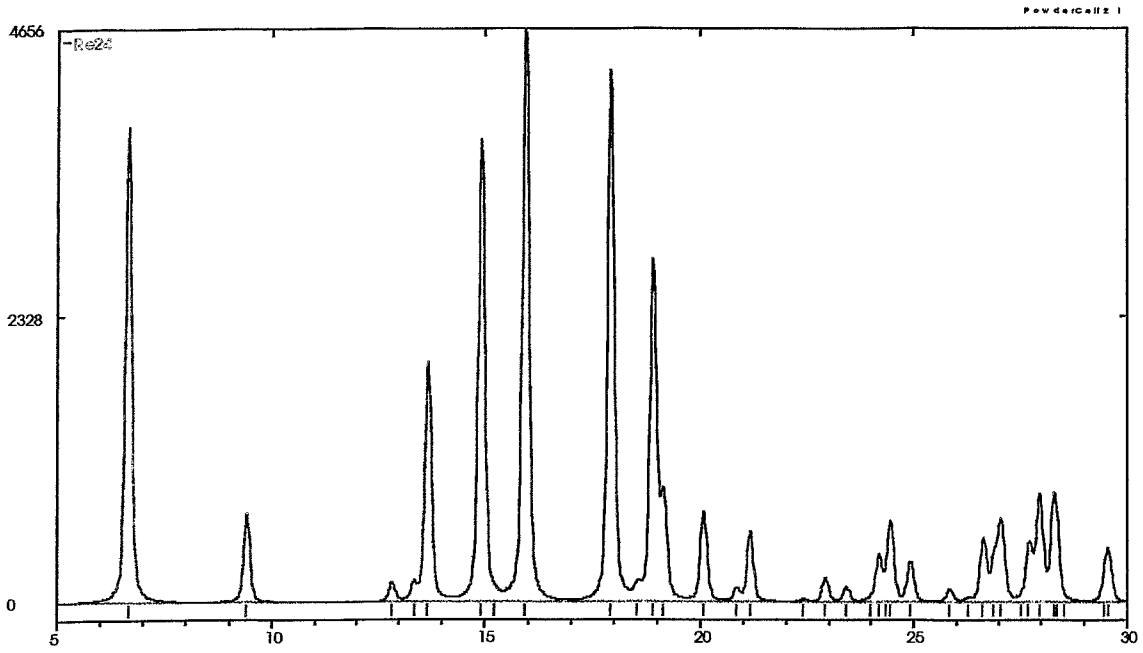
-N-	2 theta	---d---	I_{rel}	-N-	2 theta	---d---	I_{rel}
1	7.586	11.6448	98	16	22.915	3.8779	29
2	11.094	7.9691	2	17	23.595	3.7675	6
3	11.405	7.7525	10	18	23.895	3.7210	11
4	12.908	6.8527	17	19	24.351	3.6523	2
5	13.177	6.7138	27	20	24.801	3.5870	2
6	15.006	5.8993	23	21	25.328	3.5137	12
7	15.198	5.8250	17	22	25.958	3.4297	5
8	15.479	5.7199	100	23	26.265	3.3904	9
9	16.825	5.2653	34	24	26.661	3.3409	16
10	18.660	4.7514	19	25	28.177	3.1645	7
11	18.863	4.7007	31	26	28.828	3.0945	8
12	20.933	4.2404	7				
13	21.284	4.1713	37				
14	21.745	4.0837	21				
15	22.284	3.9862	8				

Re 25



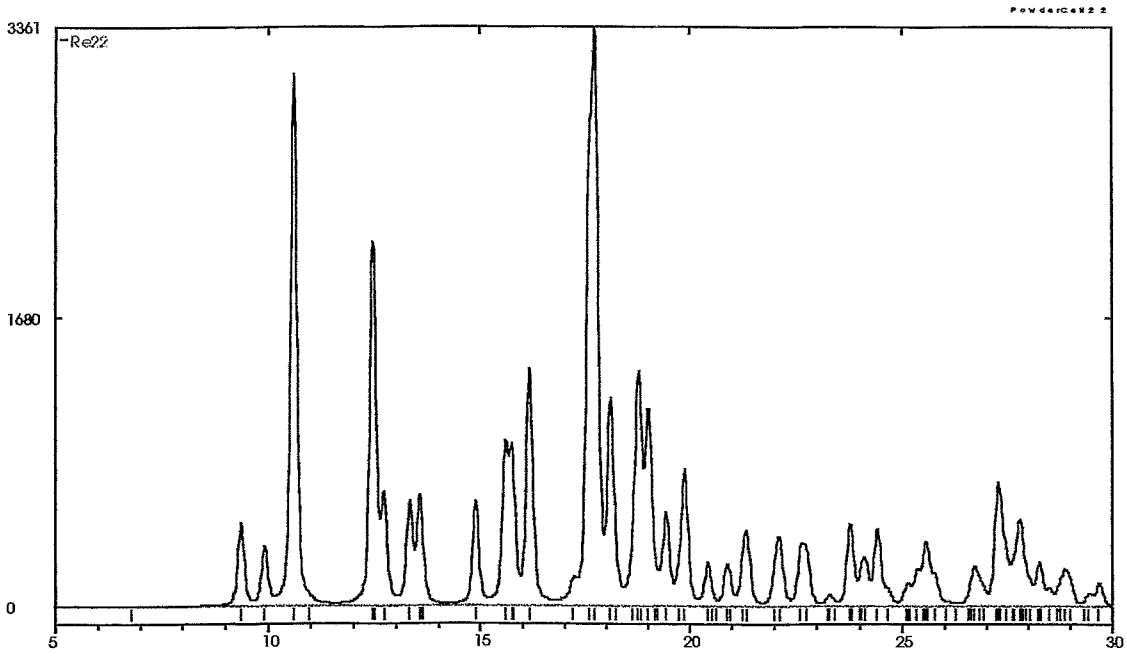
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	8.901	9.9264	100	16	22.383	3.9688	53
2	11.152	7.9274	52	17	23.782	3.7384	3
3	12.075	7.3236	52	18	24.264	3.6652	10
4	13.241	6.6810	59	19	24.911	3.5715	8
5	16.008	5.5320	61	20	25.963	3.4291	4
6	16.224	5.4588	82	21	26.181	3.4010	17
7	16.660	5.3170	20	22	26.459	3.3659	8
8	16.925	5.2343	77	23	26.928	3.3084	19
9	18.085	4.9013	82	24	27.367	3.2563	16
10	19.108	4.6410	8	25	27.977	3.1866	7
11	19.919	4.4539	3	26	28.186	3.1635	6
12	20.248	4.3823	15	27	28.582	3.1206	6
13	21.280	4.1720	12	28	29.849	2.9909	7
14	21.557	4.1189	41				
15	21.883	4.0584	10				

Re 26



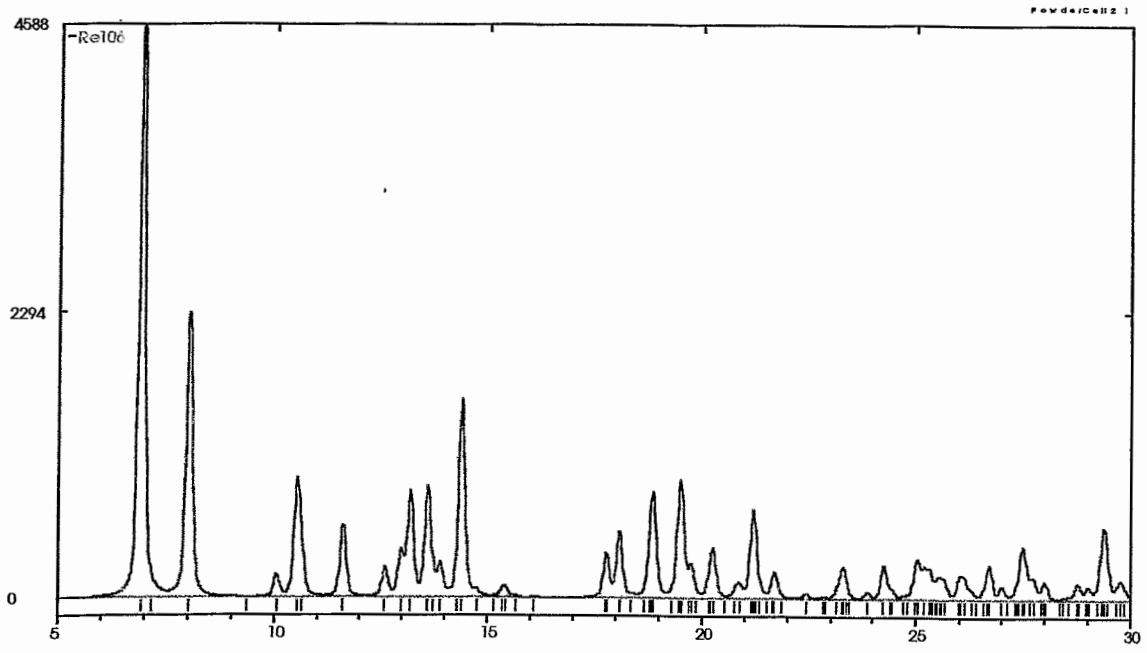
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	6.667	13.2470	83	16	22.922	3.8766	4
2	9.438	9.3636	16	17	23.423	3.7948	3
3	12.829	6.8947	3	18	24.189	3.6764	8
4	13.360	6.6220	4	19	24.458	3.6366	14
5	13.675	6.4704	42	20	24.931	3.5687	7
6	14.929	5.9293	81	21	25.824	3.4473	2
7	15.955	5.5502	100	22	26.633	3.3443	11
8	17.941	4.9402	93	23	26.867	3.3158	9
9	18.560	4.7768	4	24	27.028	3.2963	15
10	18.927	4.6849	60	25	27.732	3.2143	11
11	19.200	4.6190	18	26	27.973	3.1871	19
12	20.083	4.4178	16	27	28.302	3.1508	19
13	20.855	4.2559	3	28	29.547	3.0208	10
14	21.180	4.1914	12				
15	22.424	3.9616	1				

Re 26a



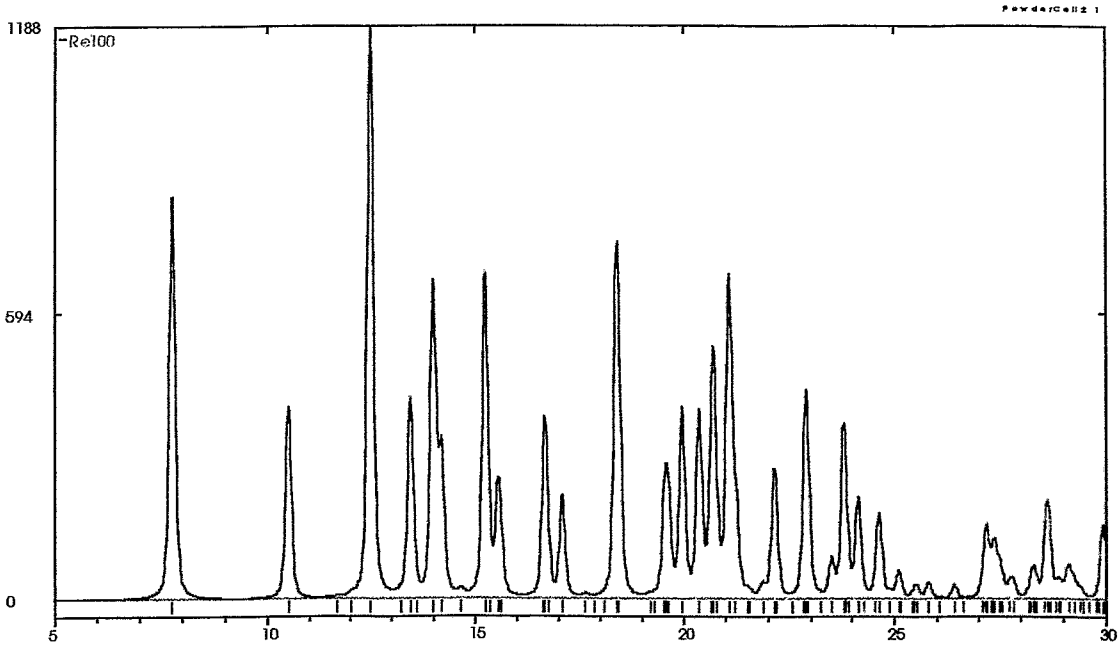
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	9.359	9.4419	14	17	19.007	4.6655	34
2	9.908	8.9201	11	18	19.428	4.5652	16
3	10.588	8.3484	92	19	19.881	4.4623	24
4	12.486	7.0833	63	20	20.435	4.3424	8
5	12.732	6.9470	20	22	21.338	4.1608	13
6	13.339	6.6325	18	23	22.107	4.0177	12
7	13.580	6.5153	19	24	22.649	3.9228	11
8	14.910	5.9371	18	25	22.712	3.9120	11
9	15.631	5.6646	29	27	23.787	3.7376	14
10	15.757	5.6197	28	28	24.122	3.6865	9
11	16.181	5.4732	41	29	24.437	3.6397	14
13	17.638	5.0244	84	33	25.583	3.4792	11
14	17.741	4.9953	100	36	27.306	3.2634	21
15	18.120	4.8918	36	37	27.813	3.2050	15
16	18.789	4.7192	41	38	28.280	3.1532	8

Re 26b



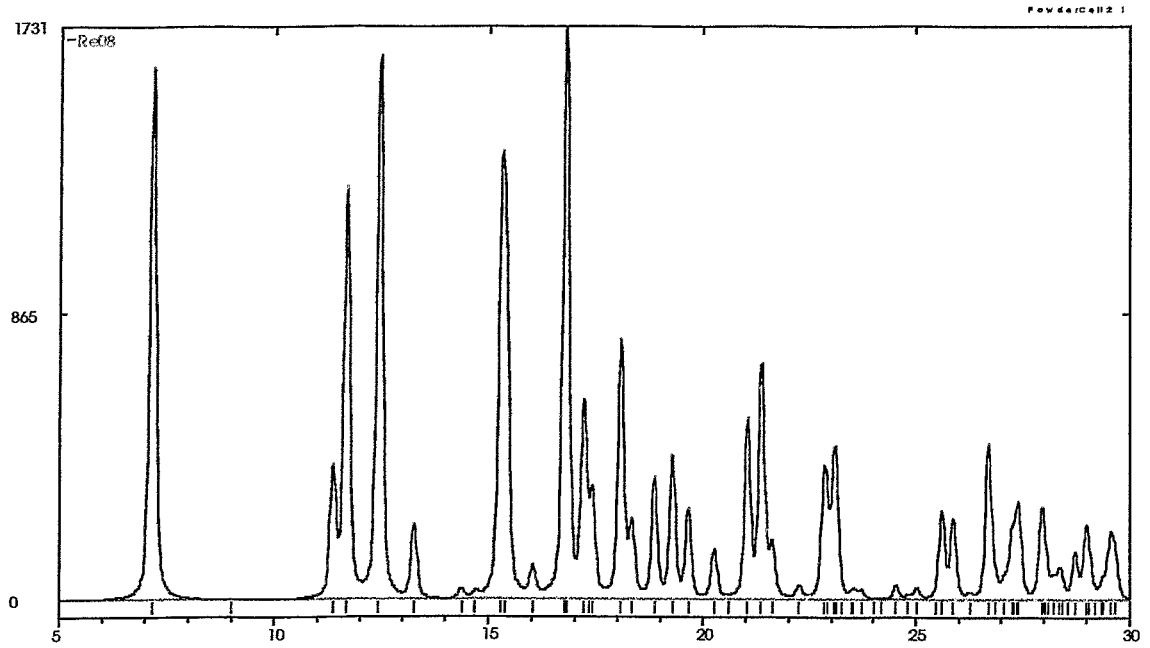
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	6.929	12.7478	100	18	19.754	4.4906	6
2	8.032	10.9989	50	19	20.253	4.3811	9
3	10.073	8.7744	4	21	21.229	4.1819	16
4	10.550	8.3786	21	22	21.725	4.0874	5
5	11.626	7.6056	13	25	23.301	3.8145	6
6	12.605	7.0169	5	27	24.270	3.6644	6
7	12.986	6.8119	8	29	25.040	3.5534	7
8	13.191	6.7066	19	30	25.201	3.5310	6
9	13.600	6.5059	20	31	25.540	3.4849	4
10	13.890	6.3705	6	32	26.038	3.4194	4
11	14.399	6.1465	35	34	26.701	3.3360	6
14	17.788	4.9823	8	36	27.493	3.2416	9
15	18.087	4.9006	12	37	27.720	3.2156	4
16	18.870	4.6989	19	41	29.390	3.0366	13
17	19.512	4.5459	21	42	29.774	2.9983	3

Re 27



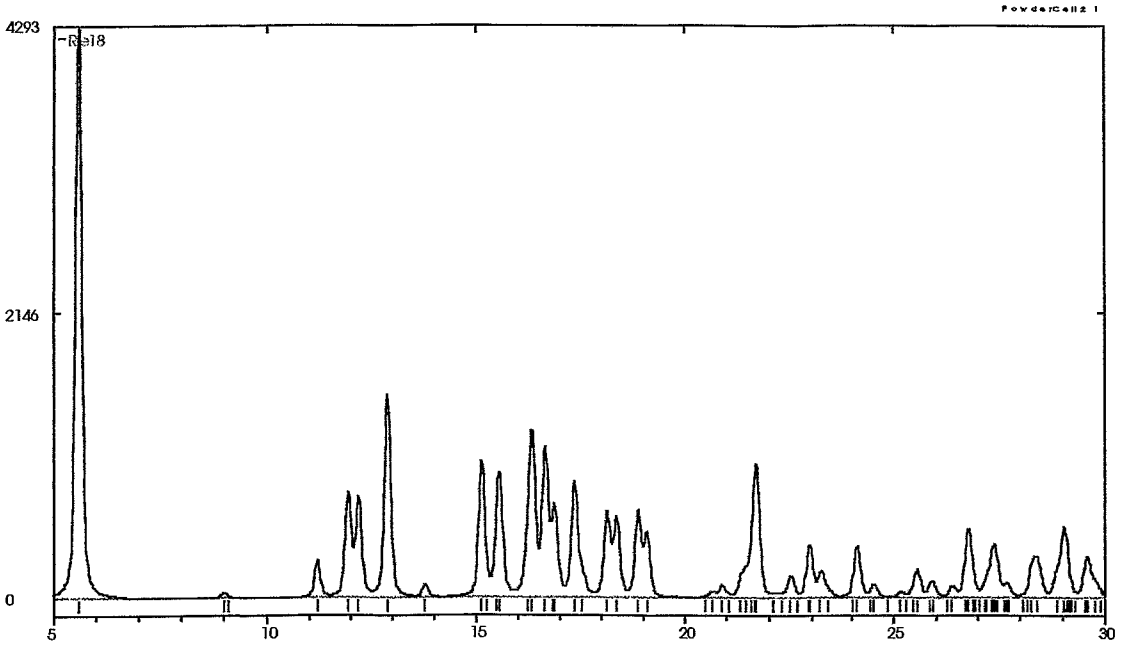
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	7.794	11.3337	70	17	21.100	4.2071	57
2	10.511	8.4097	34	18	21.234	4.1810	24
3	12.491	7.0808	100	20	22.174	4.0057	23
4	13.446	6.5799	35	21	22.913	3.8781	37
5	14.004	6.3187	56	22	23.520	3.7794	7
6	14.200	6.2321	28	23	23.816	3.7331	31
8	15.250	5.8053	57	24	24.151	3.6820	18
9	15.567	5.6880	21	25	24.646	3.6092	15
10	16.681	5.3104	32	30	27.186	3.2776	13
11	17.089	5.1844	18	31	27.372	3.2557	11
12	18.413	4.8145	63	32	27.500	3.2408	8
13	19.592	4.5275	24	34	28.295	3.1516	6
14	19.973	4.4420	34	35	28.628	3.1156	17
15	20.388	4.3523	33	37	29.130	3.0631	6
16	20.721	4.2832	44	39	29.924	2.9836	13

Re 28



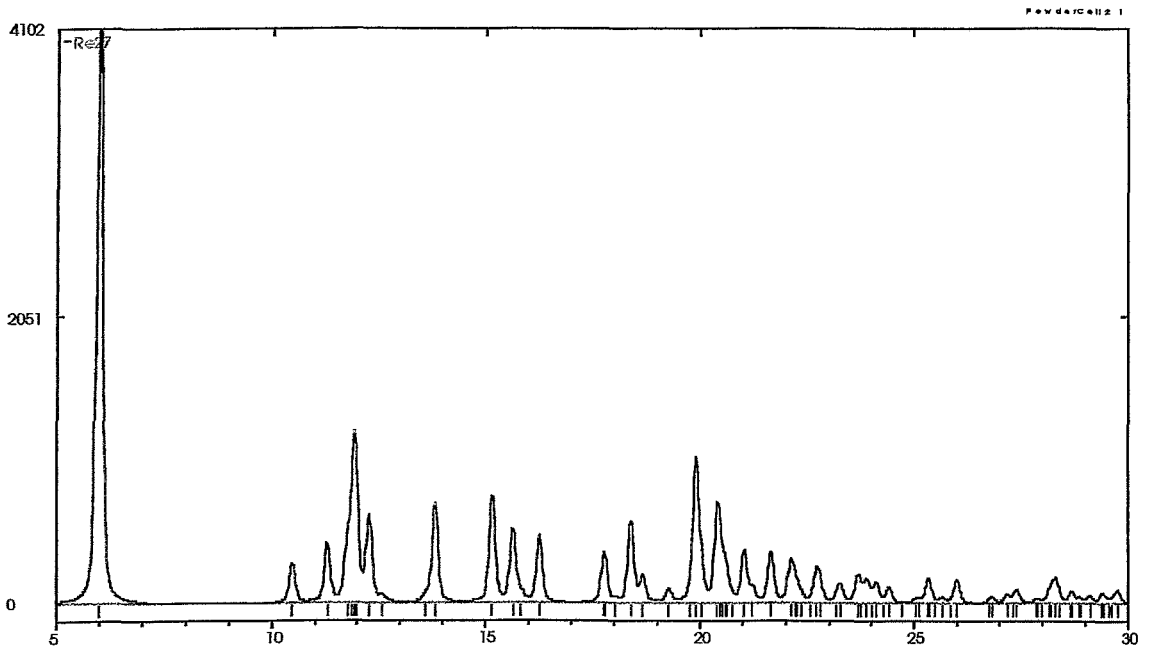
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	7.172	12.3150	93	18	20.274	4.3767	9
2	11.373	7.7738	24	19	21.058	4.2154	32
3	11.683	7.5683	72	20	21.386	4.1516	41
4	12.431	7.1149	95	21	21.641	4.1032	10
5	13.249	6.6771	13	23	22.858	3.8874	23
8	15.323	5.7777	78	24	23.090	3.8489	27
9	16.016	5.5293	6	29	25.587	3.4786	16
10	16.779	5.2795	100	30	25.852	3.4435	14
11	17.209	5.1487	35	31	26.692	3.3371	27
12	17.390	5.0955	20	32	27.280	3.2665	14
13	18.082	4.9018	46	33	27.393	3.2532	17
14	18.337	4.8343	14	34	27.957	3.1888	16
15	18.866	4.7000	21	36	28.734	3.1044	8
16	19.293	4.5969	25	37	29.005	3.0760	13
17	19.658	4.5123	16	38	29.581	3.0174	12

Re 29



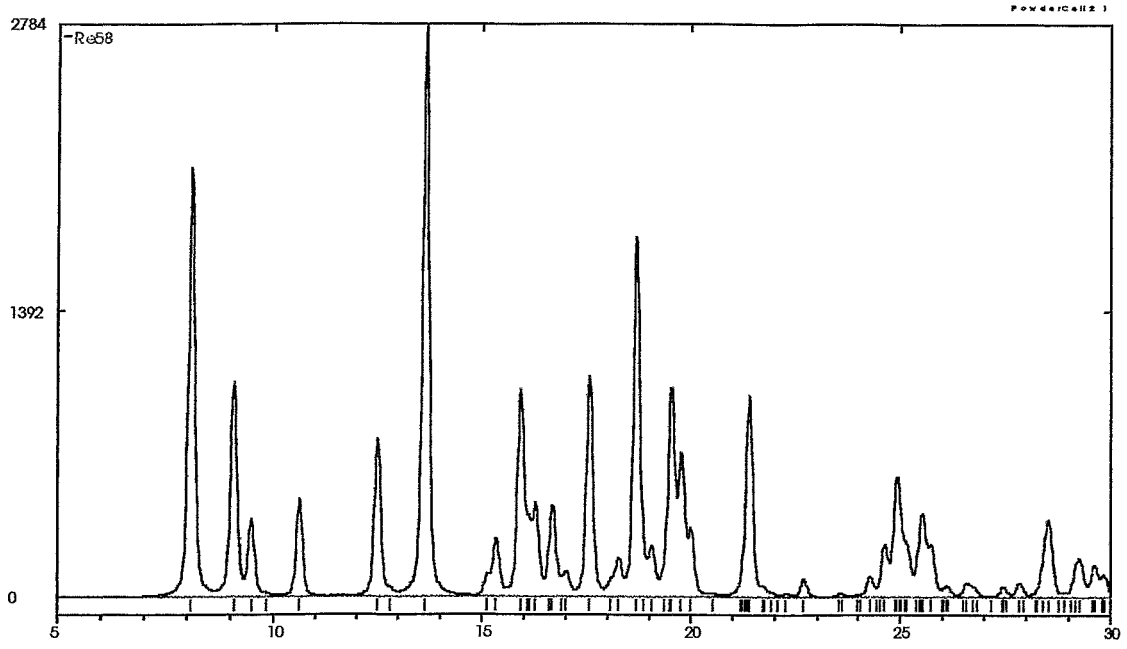
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	5.600	15.7687	100	17	19.100	4.6430	11
3	11.208	7.8881	7	20	21.420	4.1450	5
4	11.948	7.4015	19	21	21.716	4.0892	24
5	12.195	7.2519	18	22	22.531	3.9431	4
6	12.891	6.8621	36	23	22.969	3.8689	9
7	13.769	6.4261	2	24	23.236	3.8250	5
8	15.150	5.8433	24	25	24.126	3.6859	9
9	15.565	5.6886	22	28	25.548	3.4838	5
10	16.345	5.4188	29	29	25.895	3.4380	3
11	16.664	5.3156	26	31	26.774	3.3271	12
12	16.880	5.2482	16	32	27.389	3.2537	9
13	17.372	5.1006	20	33	27.700	3.2179	3
14	18.146	4.8848	15	34	28.359	3.1446	7
15	18.361	4.8280	14	35	29.052	3.0712	12
16	18.895	4.6929	15	36	29.597	3.0158	7

Re 30



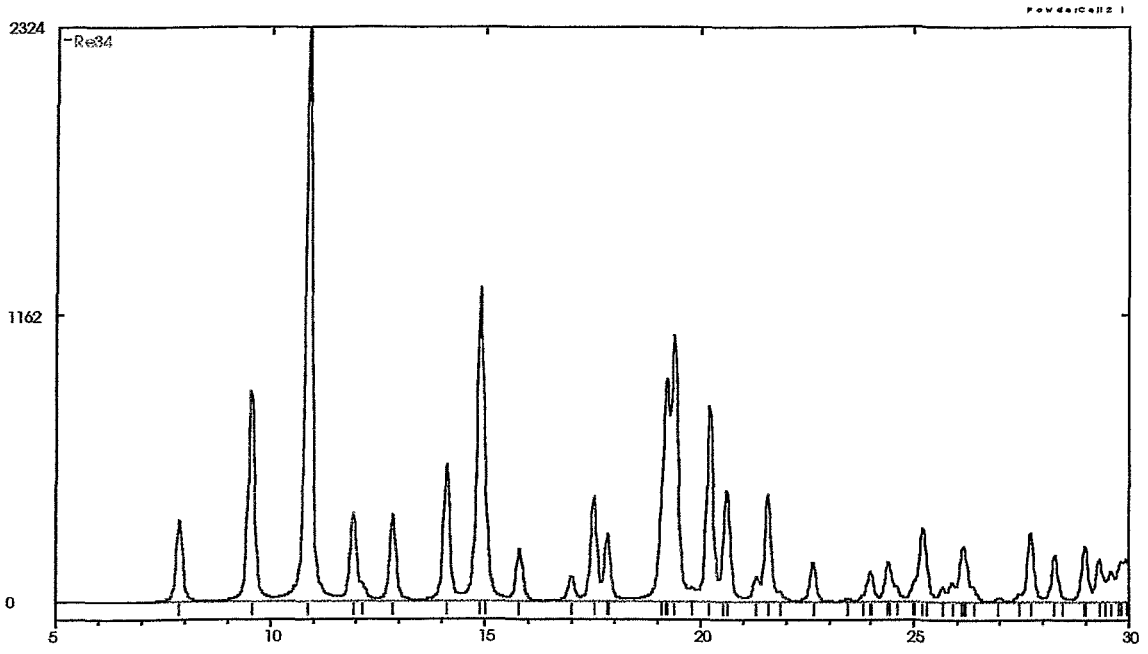
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	5.986	14.7523	100	19	20.620	4.3040	9
2	10.483	8.4318	7	20	21.051	4.2168	9
3	11.303	7.8222	10	21	21.260	4.1758	3
4	11.780	7.5064	14	22	21.682	4.0956	9
5	11.951	7.3996	30	23	22.148	4.0103	8
6	12.280	7.2020	15	24	22.739	3.9075	6
9	13.825	6.4002	17	25	23.260	3.8211	3
10	15.171	5.8353	18	26	23.693	3.7523	5
11	15.651	5.6573	13	27	23.887	3.7222	4
12	16.260	5.4468	12	28	24.114	3.6877	4
13	17.773	4.9866	9	29	24.410	3.6437	3
14	18.399	4.8183	14	30	25.330	3.5134	4
15	18.666	4.7498	5	32	25.991	3.4254	4
17	19.919	4.4538	26	37	28.173	3.1650	3
18	20.432	4.3432	18	38	28.293	3.1518	4

Re 31



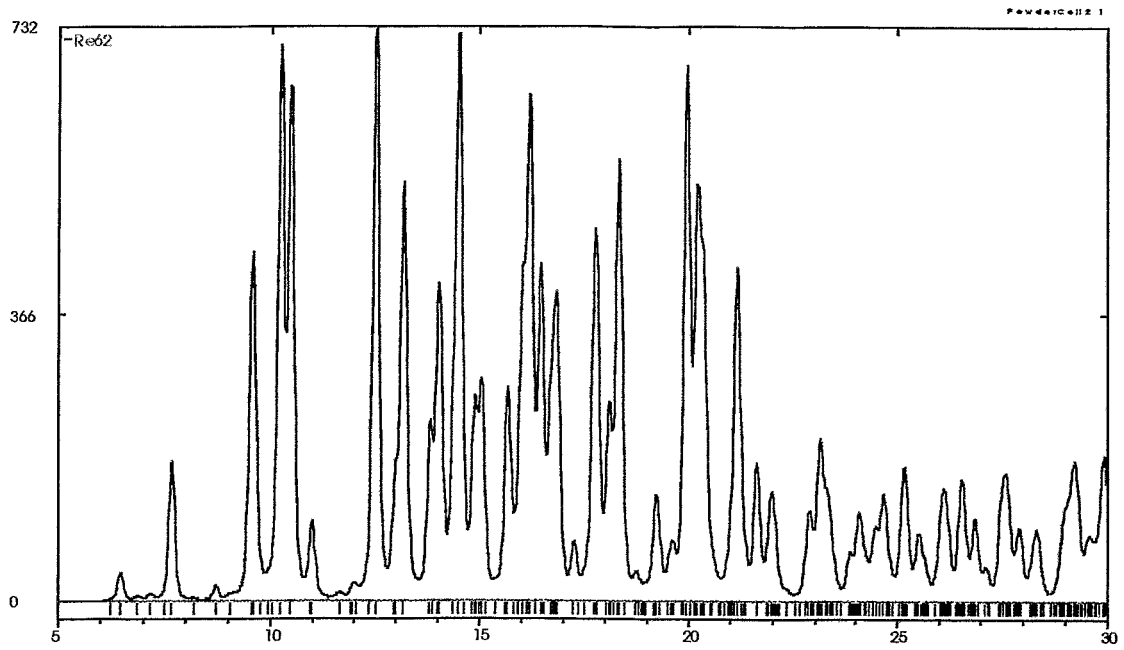
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	8.130	10.8664	75	16	19.077	4.6484	9
2	9.116	9.6936	38	17	19.542	4.5388	37
3	9.507	9.2949	14	18	19.793	4.4818	25
4	10.626	8.3188	17	19	20.020	4.4316	12
5	12.490	7.0812	28	20	21.420	4.1450	35
6	13.630	6.4915	100	24	24.289	3.6616	4
7	15.120	5.8549	4	25	24.648	3.6089	9
8	15.355	5.7659	10	26	24.934	3.5683	21
9	15.920	5.5625	36	27	25.158	3.5369	10
10	16.268	5.4441	16	28	25.523	3.4872	15
11	16.688	5.3081	16	29	25.720	3.4609	9
12	16.997	5.2125	5	34	28.518	3.1274	14
13	17.568	5.0442	39	35	29.241	3.0518	7
14	18.264	4.8536	7	36	29.622	3.0133	6
15	18.712	4.7383	63	37	29.820	2.9938	4

Re 32



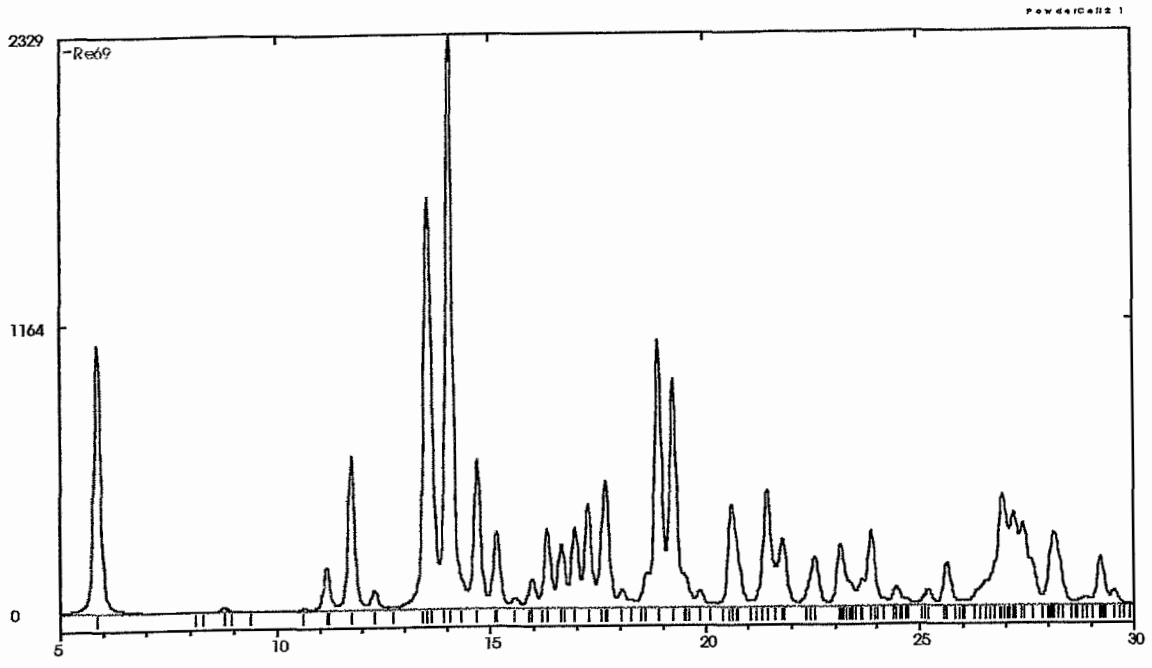
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	7.889	11.1983	14	18	21.332	4.1620	4
2	9.565	9.2389	37	19	21.592	4.1123	19
3	10.892	8.1162	100	21	22.628	3.9263	7
4	11.947	7.4016	15	22	23.992	3.7061	5
6	12.851	6.8831	15	23	24.408	3.6439	7
7	14.115	6.2693	24	25	25.000	3.5590	4
8	14.900	5.9408	55	26	25.206	3.5304	13
9	15.814	5.5996	9	29	26.137	3.4066	10
10	16.986	5.2158	4	33	27.715	3.2161	12
11	17.517	5.0588	18	34	28.270	3.1543	8
12	17.838	4.9684	12	35	28.984	3.0782	10
13	19.228	4.6122	39	36	29.321	3.0435	7
14	19.416	4.5680	46	37	29.589	3.0166	5
16	20.224	4.3873	34	38	29.828	2.9930	7
17	20.629	4.3021	19	39	29.937	2.9824	7

Re 33



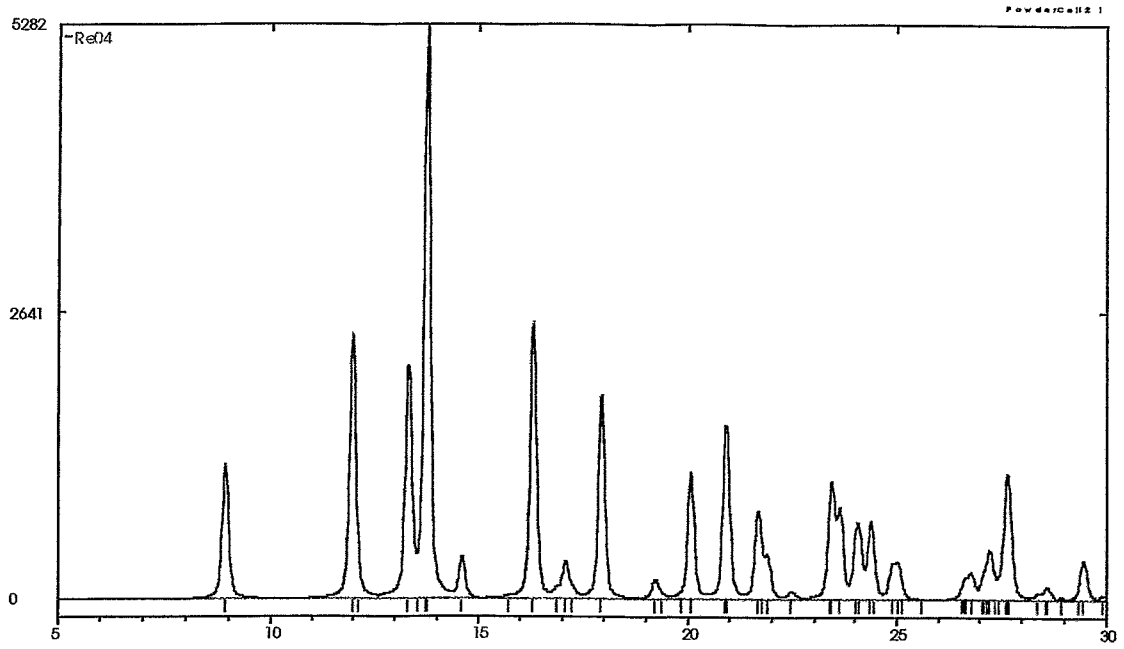
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
4	7.684	11.4966	24	23	16.479	5.3749	59
6	9.600	9.2054	61	24	16.738	5.2925	45
7	10.244	8.6280	97	25	16.813	5.2691	54
8	10.502	8.4167	90	27	17.771	4.9870	65
12	12.511	7.0692	100	28	18.100	4.8971	35
13	13.004	6.8025	24	29	18.332	4.8356	77
14	13.171	6.7165	73	33	19.970	4.4425	93
15	13.840	6.3934	32	34	20.255	4.3808	72
16	14.039	6.3034	56	35	20.328	4.3652	64
17	14.509	6.1001	99	36	21.181	4.1912	58
18	14.908	5.9376	36	37	21.655	4.1006	24
19	15.046	5.8837	38	40	23.144	3.8399	29
20	15.697	5.6409	37	46	25.167	3.5357	24
21	16.063	5.5131	59	52	27.569	3.2329	22
22	16.180	5.4736	88	56	29.218	3.0540	24

Re 34



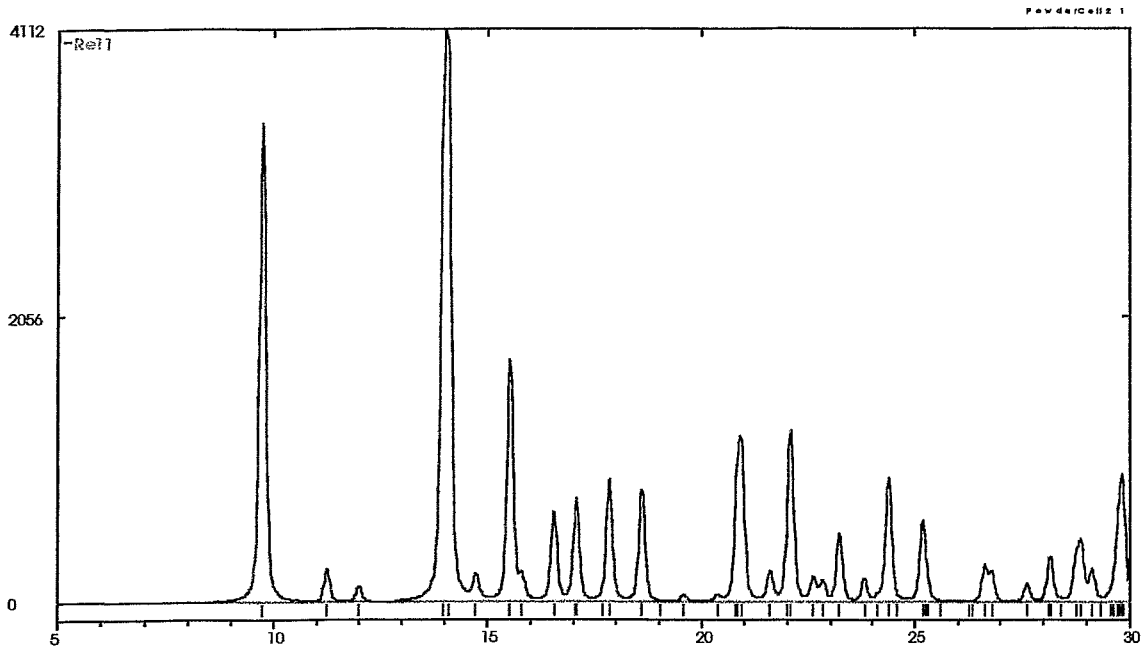
-N-	2 theta	---d---	I_{rel}	-N-	2 theta	---d---	I_{rel}
1	5.865	15.0558	47	20	19.251	4.6067	40
3	11.174	7.9119	7	21	19.531	4.5414	6
4	11.760	7.5191	27	23	20.644	4.2989	18
6	13.555	6.5271	72	24	21.478	4.1340	20
7	14.062	6.2927	100	25	21.824	4.0692	12
8	14.709	6.0178	26	26	22.554	3.9391	9
9	15.163	5.8384	13	27	23.148	3.8394	11
11	15.970	5.5450	5	29	23.876	3.7239	13
12	16.338	5.4212	14	32	25.630	3.4729	7
13	16.640	5.3232	11	33	26.940	3.3069	19
14	16.957	5.2245	14	34	27.178	3.2785	16
15	17.271	5.1304	18	35	27.416	3.2505	14
16	17.672	5.0148	22	36	27.640	3.2247	8
18	18.600	4.7666	6	37	28.149	3.1676	13
19	18.909	4.6894	47	38	29.230	3.0528	8

Re 35



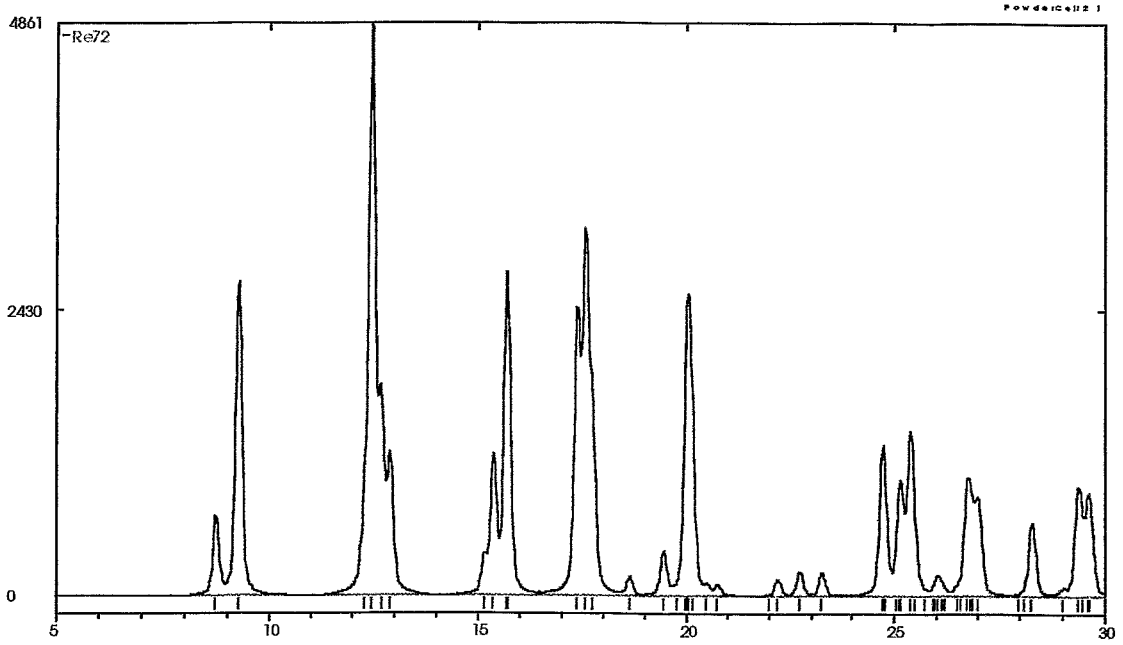
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	8.942	9.8812	23	16	23.413	3.7964	21
2	11.983	7.3798	46	17	23.612	3.7650	17
3	13.302	6.6506	41	18	24.048	3.6976	14
4	13.742	6.4386	100	19	24.368	3.6498	14
5	14.593	6.0652	7	20	24.882	3.5755	6
6	16.304	5.4323	49	21	25.004	3.5584	6
7	16.885	5.2468	2	22	26.630	3.3446	4
8	17.066	5.1914	7	23	26.777	3.3267	5
9	17.937	4.9412	36	24	27.100	3.2877	6
10	19.221	4.6140	4	25	27.235	3.2718	9
11	20.061	4.4227	23	26	27.651	3.2235	23
12	20.913	4.2444	31	27	28.385	3.1417	1
13	21.680	4.0958	16	28	28.575	3.1213	2
14	21.893	4.0565	8	29	29.433	3.0322	8
15	22.456	3.9560	1	30	29.907	2.9853	1

Re 36



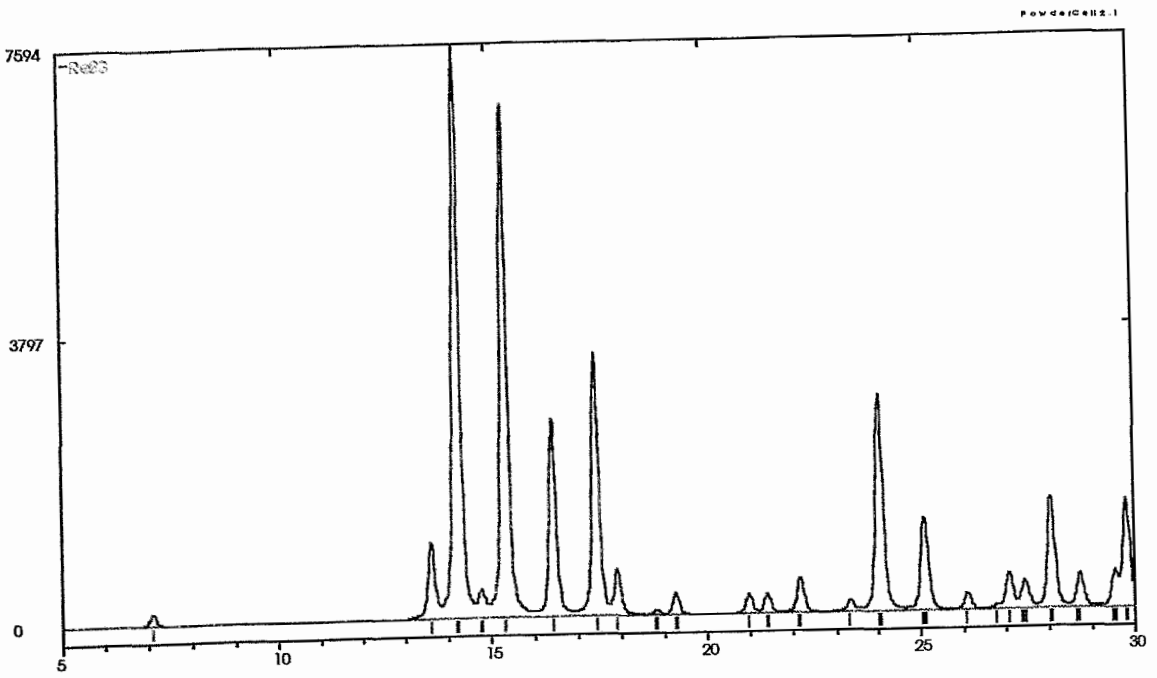
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	11.255	7.8553	6	16	22.627	3.9265	4
2	11.998	7.3703	3	17	22.833	3.8917	4
3	14.019	6.3124	100	18	23.220	3.8277	12
4	14.739	6.0053	5	19	23.806	3.7346	4
5	15.532	5.7005	42	20	24.392	3.6463	22
6	15.785	5.6096	5	21	25.181	3.5338	14
7	16.552	5.3515	16	22	26.624	3.3455	6
8	17.066	5.1914	18	23	26.782	3.3260	5
9	17.848	4.9658	21	24	27.623	3.2267	3
10	18.607	4.7647	20	25	28.150	3.1674	8
11	19.577	4.5308	1	26	28.757	3.1019	9
12	20.374	4.3554	1	27	28.865	3.0906	11
13	20.913	4.2443	29	28	29.132	3.0629	6
14	21.616	4.1079	5	29	29.825	2.9932	22
15	22.091	4.0206	30				

Re 37



-N-	2 theta	---d---	I_{rel}	-N-	2 theta	---d---	I_{rel}
1	8.768	10.0775	14	16	20.766	4.2740	2
2	9.291	9.5112	55	17	22.234	3.9951	3
3	12.471	7.0922	100	18	22.747	3.9062	4
4	12.661	6.9859	37	19	23.270	3.8196	4
5	12.888	6.8634	25	20	24.740	3.5958	26
6	15.178	5.8328	7	21	25.151	3.5379	20
7	15.393	5.7518	25	22	25.389	3.5053	29
8	15.713	5.6353	57	23	26.032	3.4202	4
9	17.393	5.0945	51	24	26.760	3.3287	21
10	17.584	5.0398	64	25	26.989	3.3010	17
11	17.740	4.9957	39	26	28.287	3.1524	13
12	18.649	4.7542	3	27	29.037	3.0727	2
13	19.459	4.5580	8	28	29.385	3.0371	19
14	20.048	4.4255	53	29	29.615	3.0140	18
15	20.483	4.3324	2				

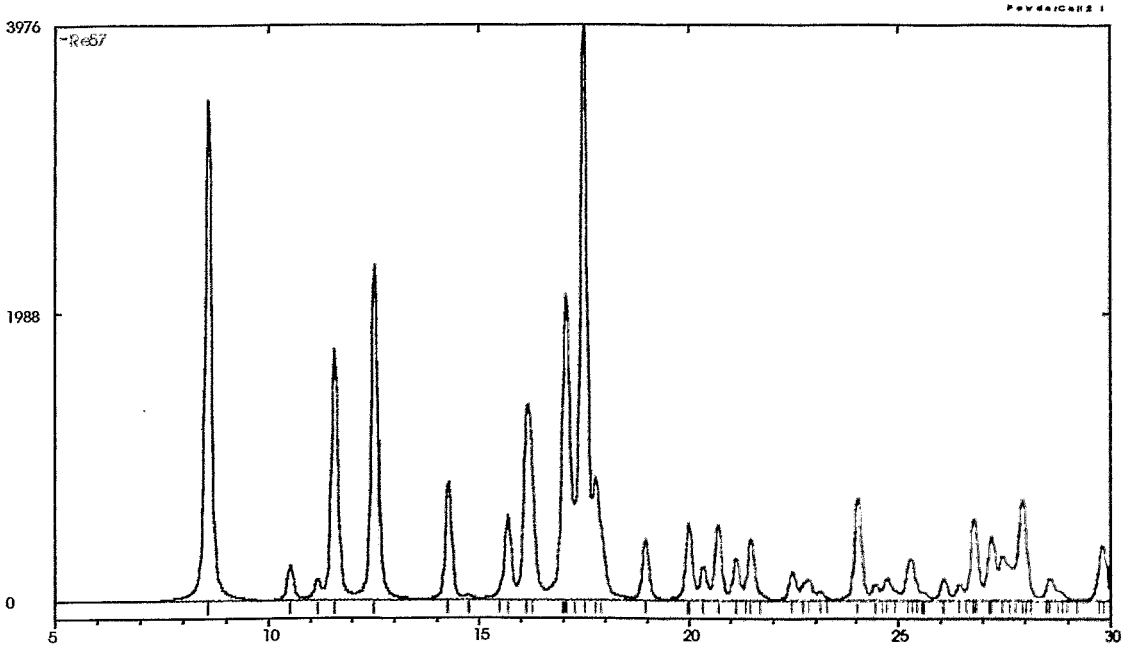
Re 38



-N-	2 theta	—d—	I_{rel}
1	7.105	12.4315	2
2	13.609	6.5015	13
3	14.229	6.2194	100
4	14.793	5.9837	5
5	15.351	5.7672	89
6	16.446	5.3856	35
7	17.426	5.0849	46
8	17.917	4.9468	8
9	18.829	4.7092	1
10	19.274	4.6014	4
11	20.987	4.2294	3
12	21.422	4.1446	3
13	22.191	4.0026	6
14	23.344	3.8076	2
15	24.047	3.6979	38

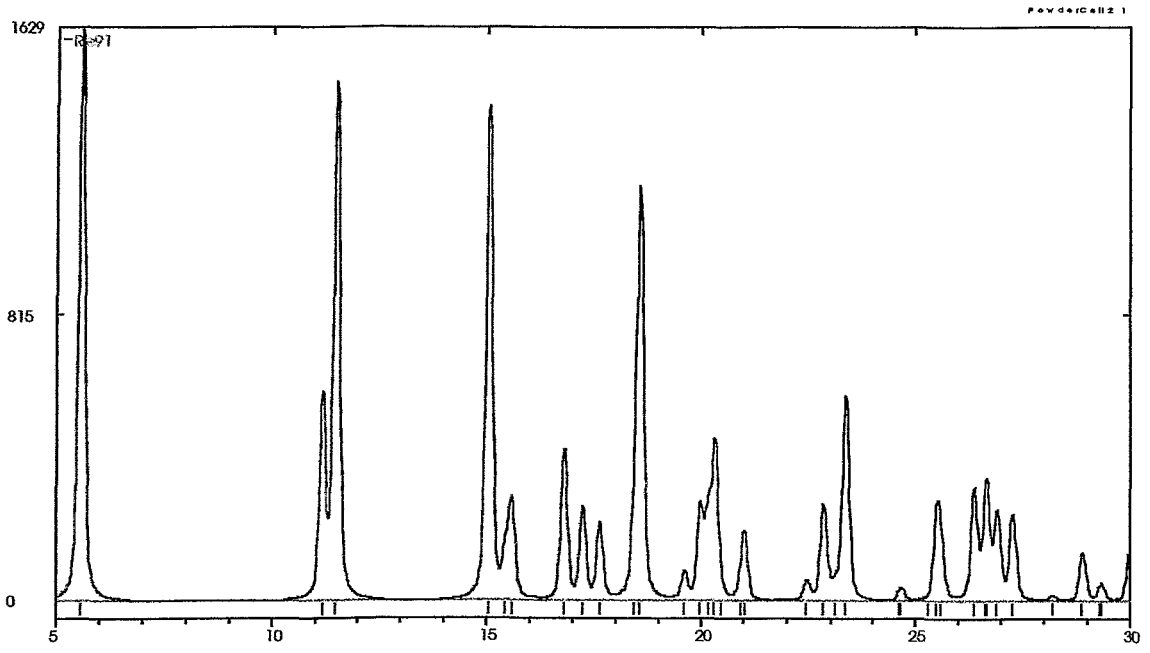
-N-	2 theta	—d—	I_{rel}
16	25.106	3.5442	16
17	26.095	3.4121	3
18	27.069	3.2915	6
19	27.439	3.2479	5
20	28.062	3.1772	19
21	28.729	3.1049	6
22	29.567	3.0188	6
23	29.826	2.9932	19

Re 39



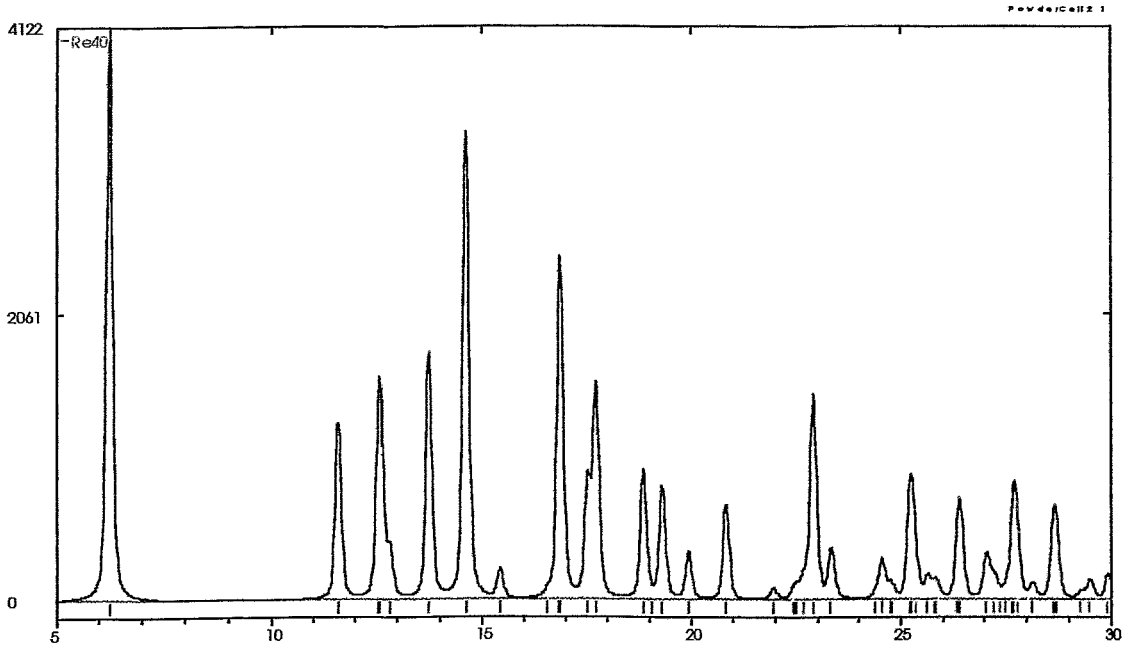
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	8.623	10.2463	87	17	21.150	4.1973	7
2	10.537	8.3892	6	18	21.505	4.1288	11
3	11.195	7.8972	4	19	22.475	3.9527	5
4	11.593	7.6273	44	20	22.822	3.8935	4
5	12.549	7.0481	58	22	24.042	3.6986	18
6	14.276	6.1990	21	24	24.748	3.5946	4
8	15.693	5.6425	15	25	25.291	3.5186	7
9	16.190	5.4703	34	26	26.067	3.4156	4
10	17.077	5.1882	53	27	26.452	3.3668	3
11	17.508	5.0614	100	28	26.783	3.3259	14
12	17.820	4.9734	20	29	27.202	3.2756	11
13	18.978	4.6726	11	30	27.498	3.2411	8
14	20.004	4.4351	14	31	27.939	3.1909	18
15	20.347	4.3610	6	32	28.577	3.1210	4
16	20.702	4.2870	13	34	29.809	2.9948	10

Tc 40



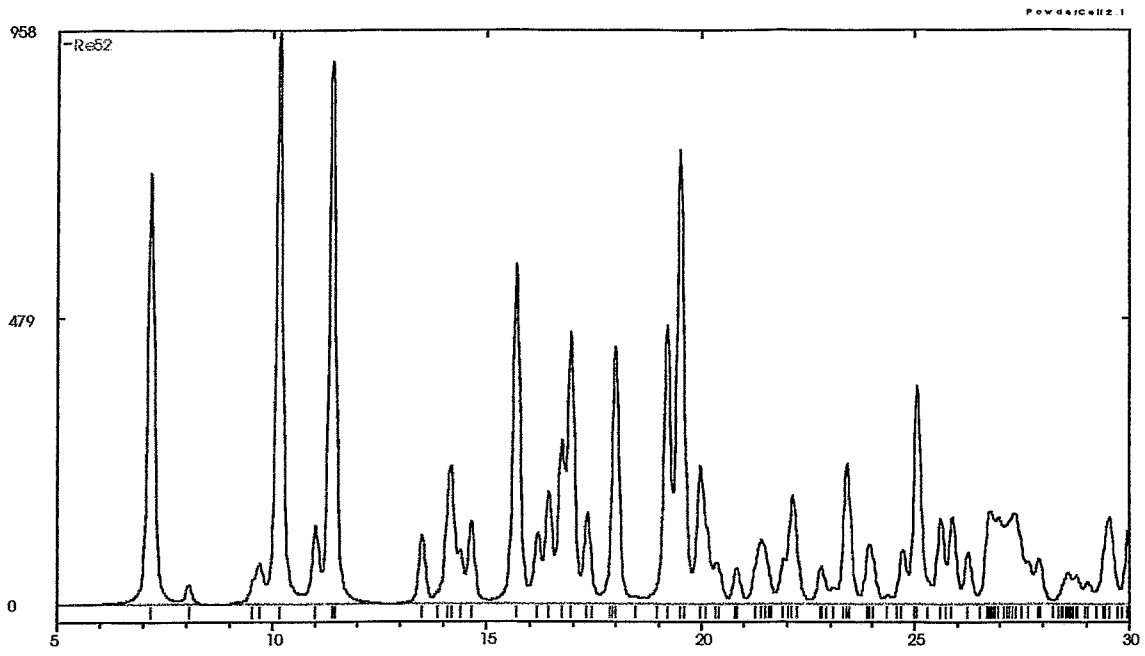
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	5.592	15.7923	100	16	22.486	3.9508	4
2	11.196	7.8966	37	17	22.865	3.8863	17
3	11.506	7.6847	91	18	23.377	3.8022	36
4	15.055	5.8801	86	19	24.669	3.6059	2
5	15.438	5.7351	11	20	25.532	3.4859	18
6	15.570	5.6866	18	21	26.369	3.3772	20
7	16.805	5.2715	26	22	26.656	3.3415	21
8	17.236	5.1405	16	23	26.908	3.3108	16
9	17.635	5.0252	14	24	27.277	3.2668	15
10	18.573	4.7734	72	25	28.204	3.1615	1
11	19.629	4.5190	5	26	28.905	3.0864	8
12	20.020	4.4315	17	27	29.335	3.0422	3
13	20.173	4.3983	18				
14	20.325	4.3657	28				
15	21.032	4.2205	12				

Re 40



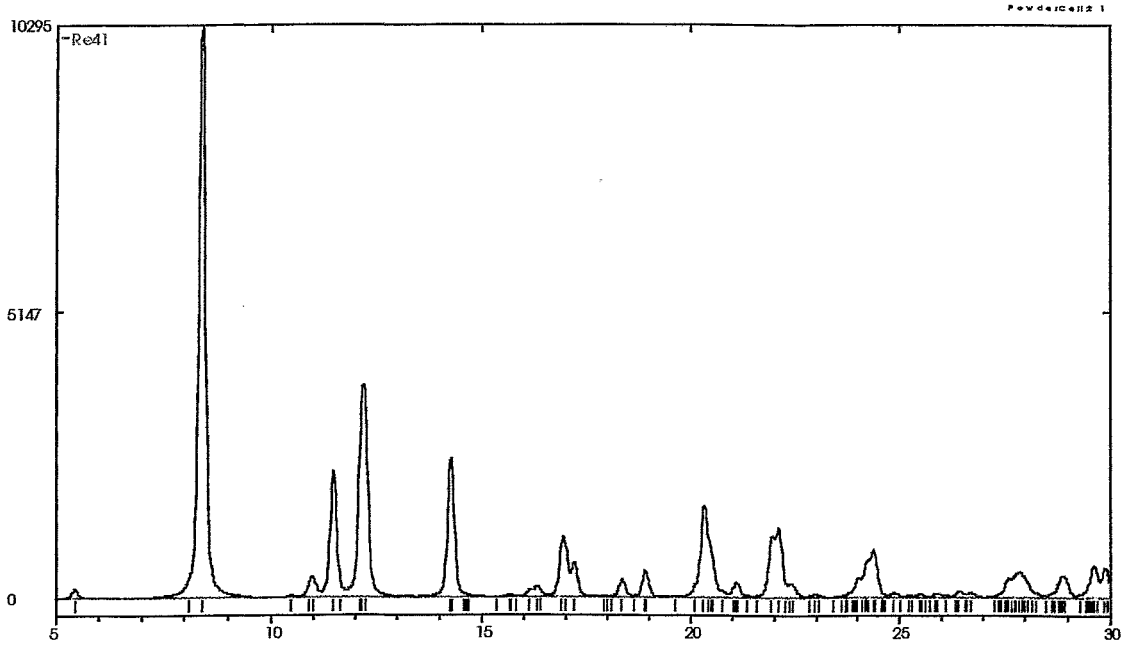
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	6.274	14.0767	100	17	22.916	3.8776	36
2	11.604	7.6195	31	18	23.343	3.8077	9
3	12.594	7.0228	39	19	24.560	3.6217	7
4	12.792	6.9145	10	20	24.764	3.5923	3
5	13.731	6.4438	43	21	25.248	3.5245	22
6	14.637	6.0471	82	22	25.649	3.4703	4
7	15.428	5.7386	5	23	25.812	3.4489	4
8	16.880	5.2481	60	24	26.403	3.3729	18
9	17.560	5.0465	23	25	27.073	3.2909	8
10	17.732	4.9979	38	26	27.225	3.2729	5
11	18.875	4.6977	23	27	27.727	3.2148	21
12	19.321	4.5902	20	28	28.137	3.1689	3
13	19.945	4.4481	8	29	28.671	3.1111	17
14	20.845	4.2581	17	30	29.494	3.0261	3
16	22.480	3.9519	3	31	29.956	2.9804	4

Tc 41



-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	7.194	12.2785	75	18	19.218	4.6146	49
4	10.175	8.6867	100	19	19.511	4.5460	79
5	11.027	8.0172	14	20	19.984	4.4394	24
6	11.415	7.7454	95	23	21.435	4.1421	11
7	13.495	6.5560	12	25	22.155	4.0092	19
8	14.168	6.2461	24	27	23.402	3.7983	25
9	14.399	6.1463	9	28	23.948	3.7128	10
10	14.662	6.0370	14	29	24.731	3.5970	9
11	15.696	5.6415	59	30	25.056	3.5512	38
12	16.189	5.4707	12	31	25.601	3.4767	15
13	16.432	5.3903	20	32	25.876	3.4404	15
14	16.740	5.2918	29	34	26.777	3.3267	16
15	16.944	5.2287	48	35	26.980	3.3021	15
16	17.333	5.1120	16	36	27.329	3.2607	16
17	18.007	4.9221	45	42	29.526	3.0229	15

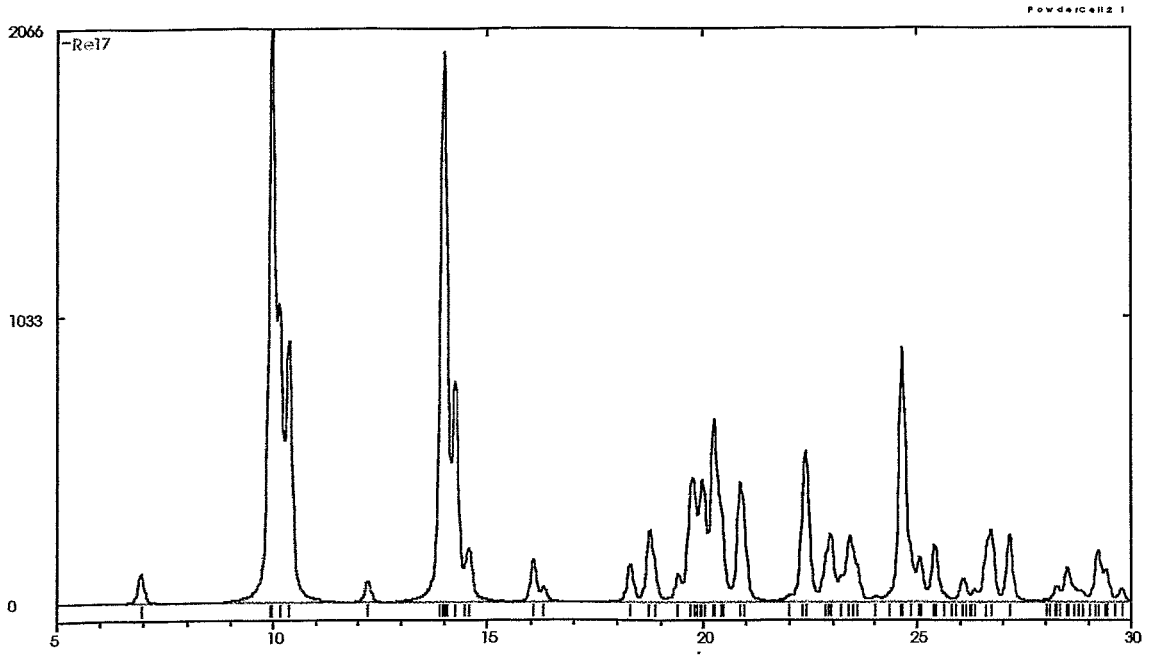
Re41



-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	5.457	16.1829	2	17	22.110	4.0172	12
2	8.432	10.4776	100	18	22.440	3.9588	3
3	10.992	8.0429	4	19	22.976	3.8678	1
4	11.488	7.6967	22	20	24.020	3.7019	3
5	12.211	7.2423	37	21	24.217	3.6722	6
6	14.270	6.2018	24	22	24.368	3.6499	8
8	16.328	5.4244	2	23	24.880	3.5759	1
9	16.956	5.2247	11	25	25.881	3.4398	1
10	17.213	5.1476	6	26	26.432	3.3693	1
11	18.352	4.8305	3	27	26.684	3.3380	1
12	18.928	4.6846	5	28	27.660	3.2224	3
13	20.348	4.3609	16	29	27.865	3.1992	5
14	20.527	4.3233	8	30	28.893	3.0876	4
15	21.111	4.2050	3	31	29.633	3.0122	6
16	21.966	4.0432	11	32	29.898	2.9861	5

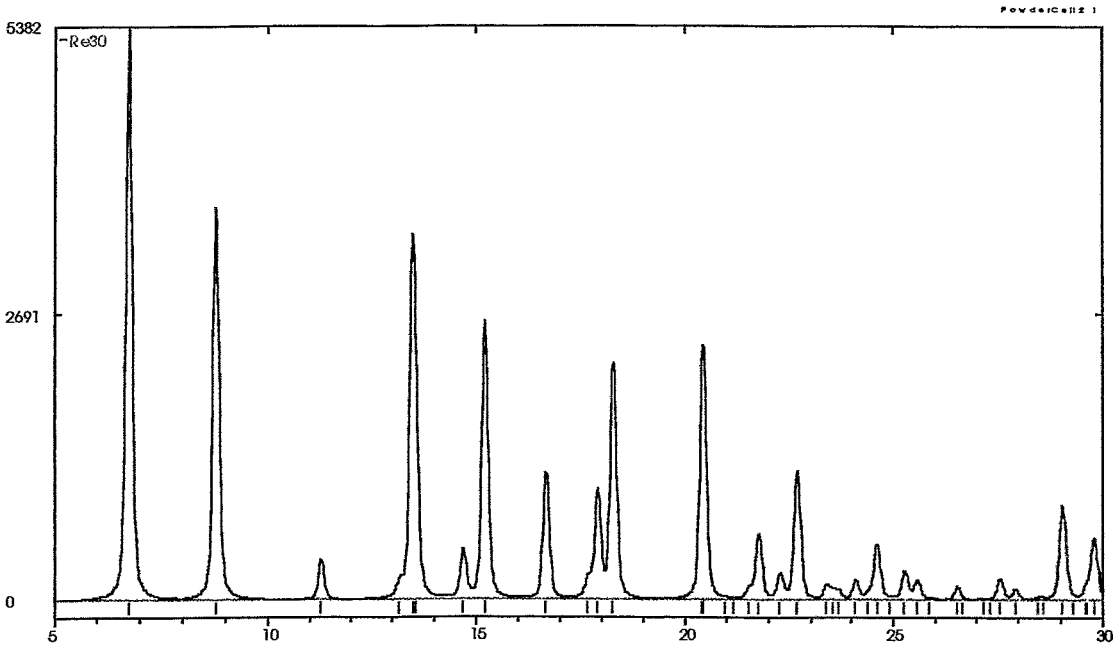
File: Re41.raw

Re 42



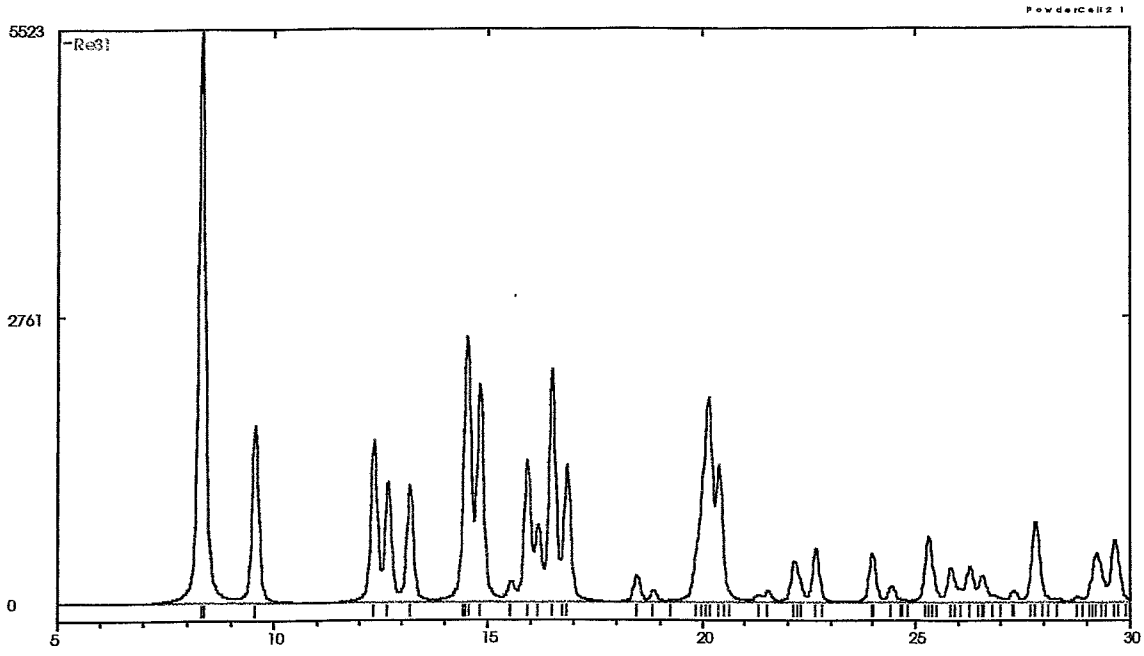
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	6.956	12.6971	5	18	20.888	4.2494	21
2	9.986	8.8503	100	19	22.408	3.9644	26
3	10.180	8.6823	52	20	22.960	3.8703	12
4	10.395	8.5032	46	21	23.412	3.7966	12
6	13.990	6.3253	96	22	23.600	3.7668	6
7	14.258	6.2067	39	24	24.663	3.6068	45
8	14.587	6.0677	9	25	25.066	3.5497	8
9	16.060	5.5141	7	26	25.406	3.5030	10
11	18.313	4.8406	7	27	26.062	3.4164	4
12	18.753	4.7280	13	29	26.598	3.3487	10
13	19.427	4.5655	5	30	26.708	3.3351	13
14	19.763	4.4886	22	31	27.151	3.2816	12
15	19.995	4.4370	22	33	28.504	3.1289	6
16	20.266	4.3783	32	34	29.234	3.0525	9
17	20.440	4.3415	18	35	29.400	3.0356	6

Re 43



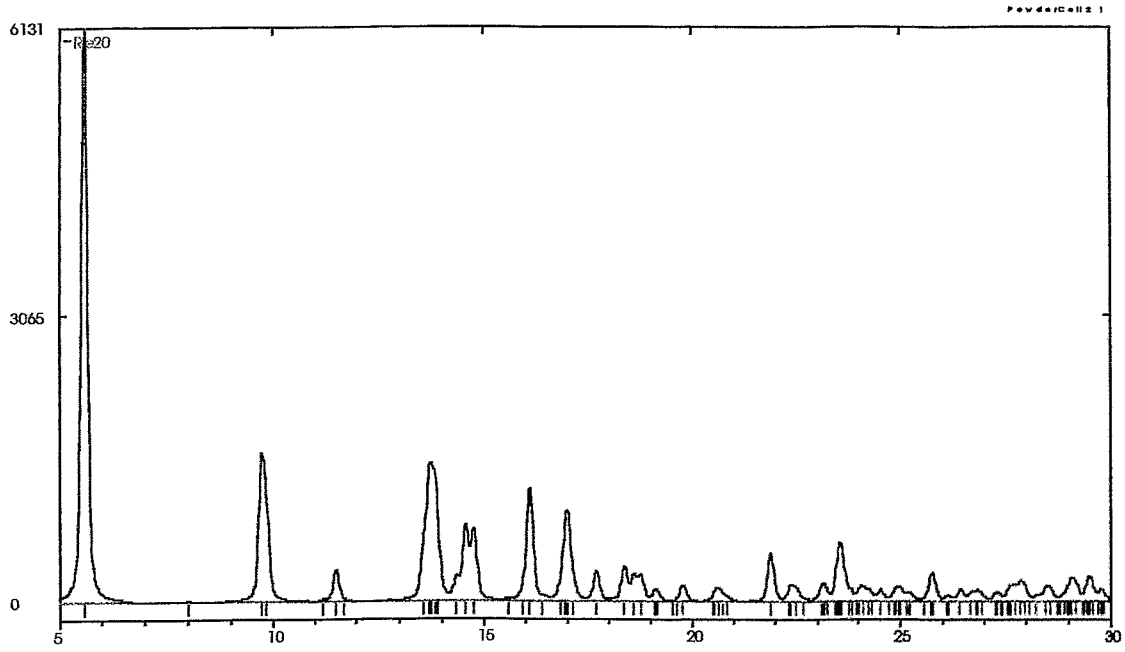
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	6.771	13.0443	100	16	23.429	3.7939	3
2	8.820	10.0175	69	17	23.640	3.7605	2
3	11.291	7.8306	7	18	24.108	3.6886	3
4	13.140	6.7324	4	19	24.624	3.6125	10
5	13.500	6.5537	64	20	25.281	3.5200	5
6	14.703	6.0200	9	21	25.560	3.4822	3
7	15.238	5.8099	49	22	26.544	3.3553	2
8	16.689	5.3078	22	23	27.562	3.2337	4
9	17.729	4.9989	5	24	27.940	3.1908	2
10	17.926	4.9443	19	25	29.049	3.0714	16
11	18.295	4.8455	41	26	29.807	2.9950	11
12	20.455	4.3384	45				
13	21.797	4.0741	12				
14	22.315	3.9807	5				
15	22.702	3.9138	23				

Re 44



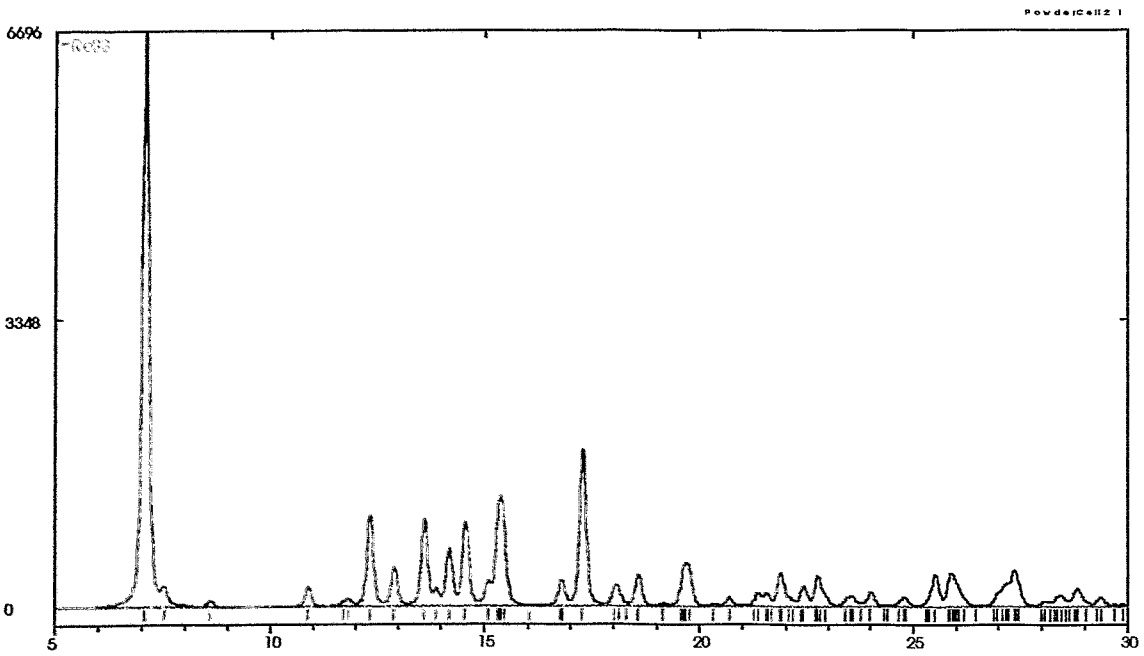
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	8.351	10.5794	100	16	20.394	4.3511	24
2	9.602	9.2037	31	17	21.336	4.1611	1
3	12.348	7.1622	29	18	21.577	4.1152	2
4	12.673	6.9796	21	19	22.193	4.0023	7
5	13.184	6.7099	21	20	22.672	3.9189	9
6	14.535	6.0892	47	21	23.989	3.7066	9
7	14.830	5.9686	38	22	24.458	3.6366	3
8	15.553	5.6930	4	23	25.313	3.5157	12
9	15.939	5.5557	25	24	25.830	3.4465	6
10	16.176	5.4752	14	25	26.263	3.3906	6
11	16.508	5.3657	41	26	26.563	3.3529	5
12	16.855	5.2561	24	27	27.292	3.2650	2
13	18.479	4.7976	5	28	27.808	3.2056	14
14	18.869	4.6992	2	29	29.239	3.0519	9
15	20.153	4.4027	36	30	29.653	3.0103	11

Re 45



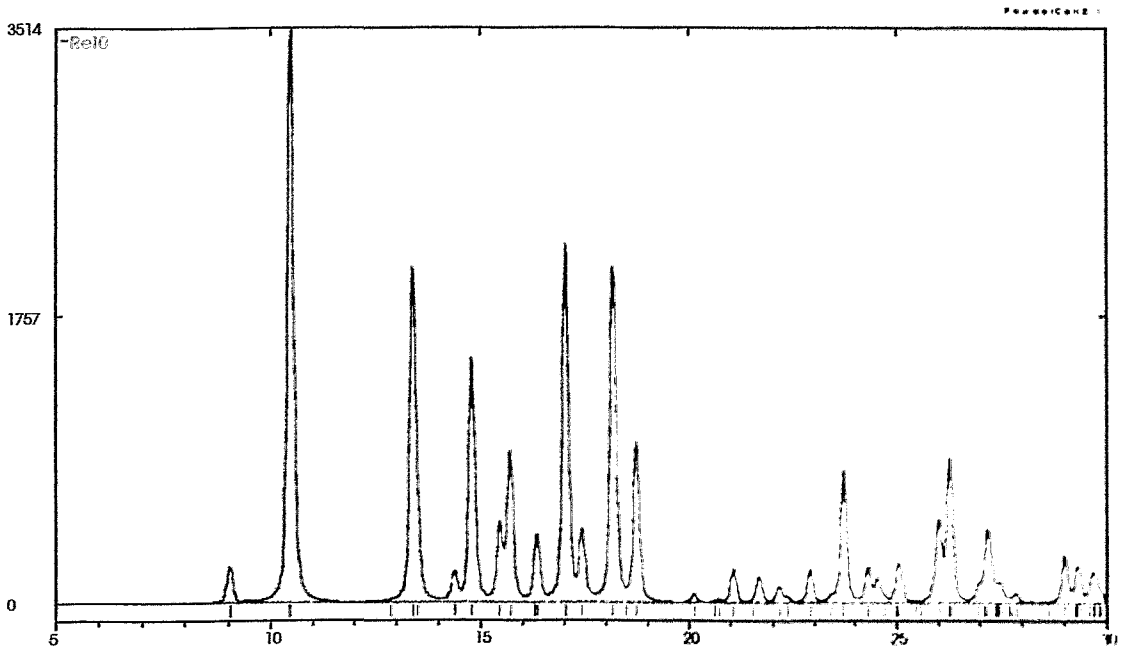
-N-	2 theta	---d---	I_{rel}	-N-	2 theta	---d---	I_{rel}
1	5.598	15.7753	100	16	19.779	4.4851	3
2	9.778	9.0383	26	17	20.630	4.3020	2
3	11.527	7.6705	5	18	21.909	4.0536	8
4	13.727	6.4459	24	19	22.428	3.9609	3
5	13.815	6.4049	23	20	23.153	3.8385	3
6	14.320	6.1802	4	21	23.566	3.7722	10
7	14.580	6.0707	13	22	24.083	3.6923	3
8	14.768	5.9937	13	24	24.951	3.5658	3
9	16.104	5.4995	20	26	25.744	3.4577	5
10	16.987	5.2153	16	31	27.676	3.2207	3
11	17.706	5.0051	5	32	27.890	3.1964	4
12	18.380	4.8232	6	33	28.515	3.1278	3
13	18.618	4.7620	5	34	29.098	3.0664	4
14	18.775	4.7224	5	35	29.489	3.0266	4
15	19.131	4.6355	2	36	29.769	2.9988	2

Re 46



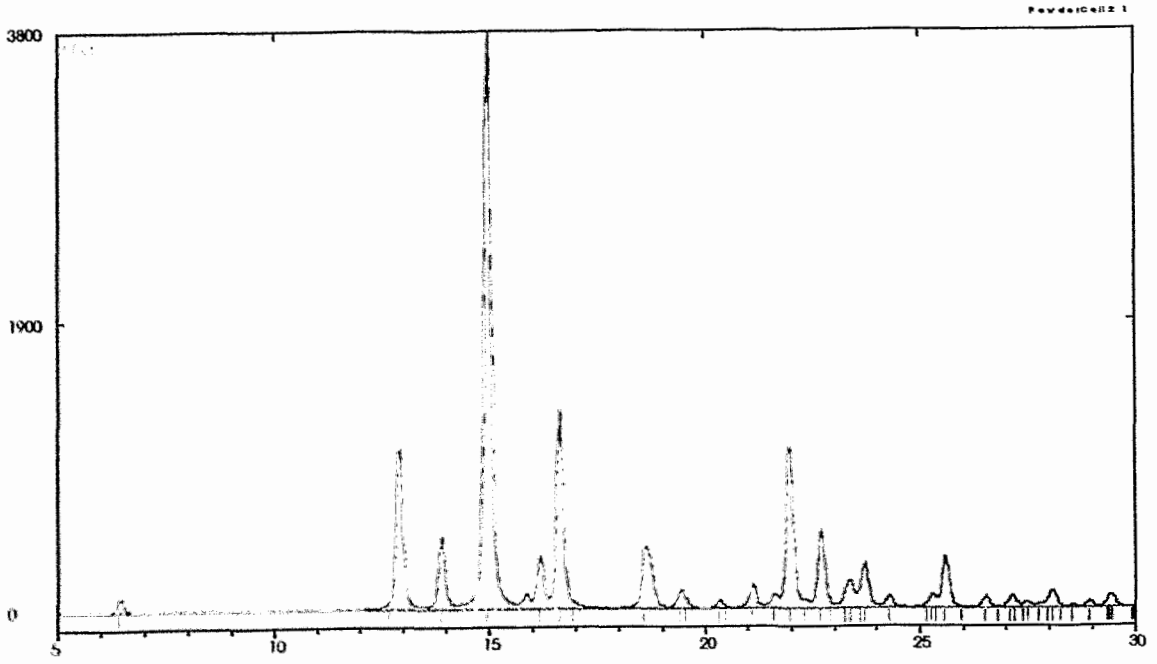
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	7.083	12.4705	100	19	21.379	4.1529	2
2	7.499	11.7787	4	20	21.566	4.1172	2
4	10.893	8.1158	3	21	21.905	4.0544	6
6	12.336	7.1693	16	22	22.427	3.9611	4
7	12.892	6.8611	7	23	22.777	3.9010	5
8	13.609	6.5014	15	24	23.544	3.7756	2
9	14.198	6.2330	10	25	24.009	3.7035	2
10	14.587	6.0678	15	26	24.783	3.5897	2
11	15.080	5.8704	4	27	25.510	3.4889	6
12	15.385	5.7548	19	28	25.891	3.4385	6
13	16.789	5.2764	5	29	27.140	3.2830	4
14	17.288	5.1253	27	30	27.376	3.2552	6
15	18.076	4.9037	4	31	28.425	3.1375	2
16	18.584	4.7705	6	32	28.833	3.0940	3
17	19.703	4.5021	8	33	29.379	3.0377	2

Re 47



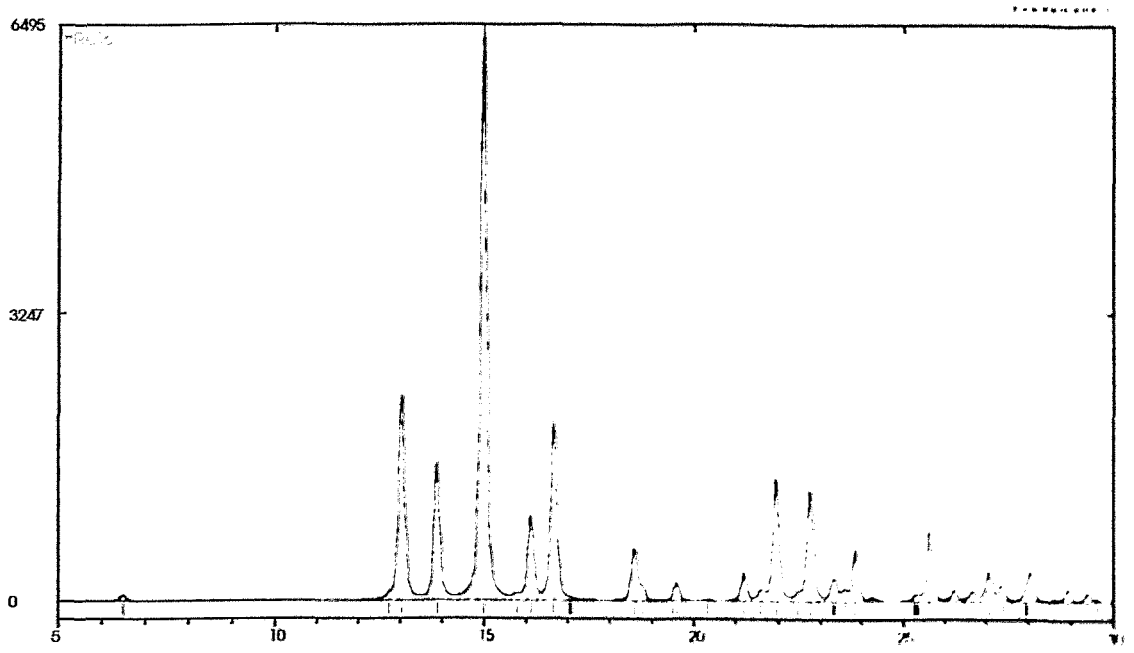
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	9.063	9.7495	6	19	22.906	3.8794	6
2	10.493	8.4242	100	21	23.726	3.7472	23
3	13.387	6.6085	58	22	24.309	3.6586	6
4	14.393	6.1489	5	23	24.540	3.6247	4
5	14.807	5.9778	43	24	25.048	3.5522	7
6	15.478	5.7204	14	25	26.005	3.4237	15
7	15.712	5.6355	27	26	26.263	3.3906	26
8	16.353	5.4161	12	27	26.960	3.3045	4
9	17.042	5.1988	62	28	27.174	3.2790	13
10	17.430	5.0839	13	29	27.473	3.2440	4
11	18.182	4.8751	59	30	27.854	3.2004	2
12	18.732	4.7333	28	31	29.010	3.0755	8
15	21.079	4.2113	6	32	29.309	3.0448	6
16	21.693	4.0934	5	33	29.693	3.0063	5
17	22.168	4.0069	3	34	29.880	2.9879	2

Tc 48



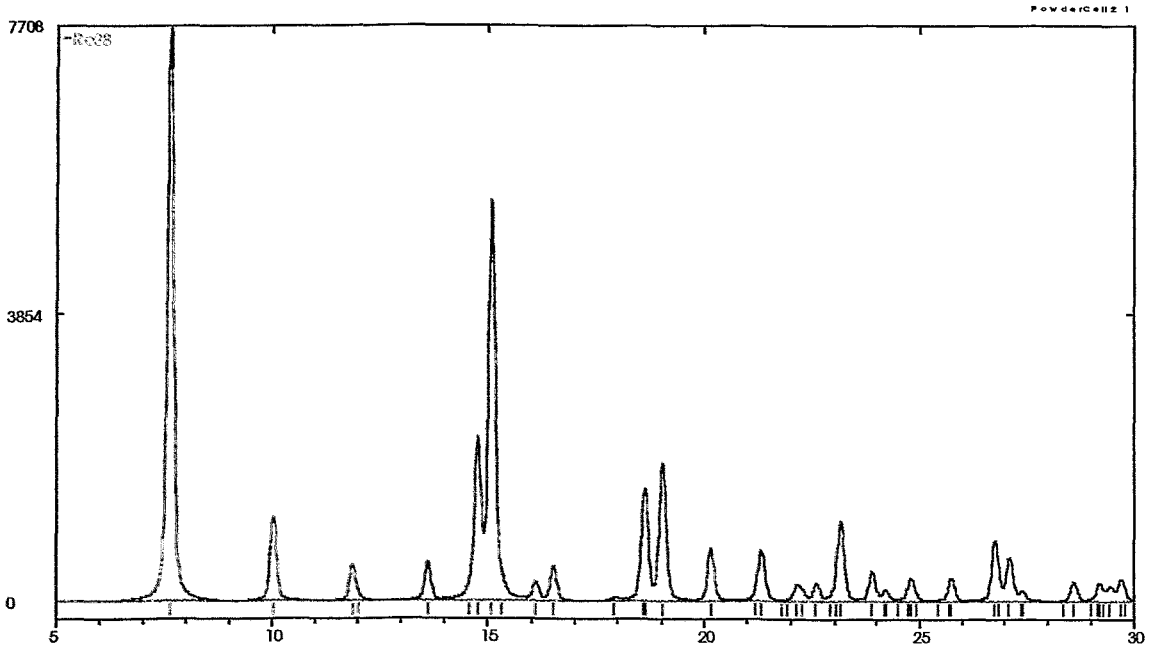
-N-	2 theta	—d—	I_{rel}
1	6.448	13.6968	2
2	12.908	6.8529	28
3	13.889	6.3707	13
4	14.982	5.9086	100
5	15.843	5.5893	3
6	16.174	5.4757	9
7	16.644	5.3222	34
8	18.611	4.7637	11
9	18.717	4.7370	9
10	19.426	4.5658	3
11	20.358	4.3587	1
12	21.120	4.2032	4
13	21.630	4.1053	2
14	21.982	4.0402	28
15	22.340	3.9763	2
16	22.701	3.9139	14
17	23.281	3.8178	4
18	23.363	3.8044	5
19	23.718	3.7483	8
20	24.289	3.6616	2
21	25.280	3.5202	2
22	25.571	3.4807	9
23	26.512	3.3593	2
24	27.133	3.2838	2
25	27.491	3.2419	1
26	28.072	3.1760	3
27	28.939	3.0828	1
28	29.438	3.0317	2

Re 48



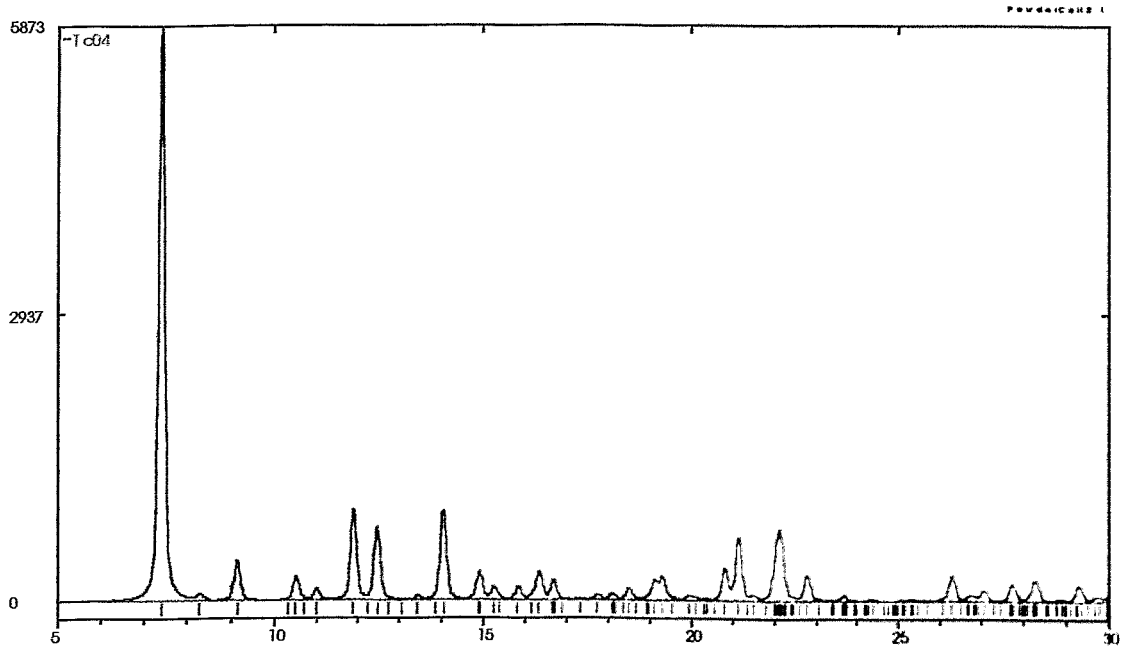
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	6.504	13.5785	1	16	23.864	3.7258	9
2	13.030	6.7890	36	17	24.276	3.6634	1
3	13.877	6.3764	24	18	25.327	3.5138	1
4	14.990	5.9056	100	19	25.623	3.4738	12
5	16.122	5.4931	15	20	26.229	3.3949	2
6	16.674	5.3126	31	21	26.670	3.3398	2
7	18.592	4.7685	9	22	27.060	3.2925	5
8	18.800	4.7163	3	23	27.370	3.2559	3
9	19.590	4.5279	3	24	28.048	3.1787	5
10	21.218	4.1839	5	25	28.628	3.1156	1
11	21.630	4.1052	2	26	28.927	3.0841	2
12	21.970	4.0424	21	27	29.396	3.0359	2
13	22.774	3.9015	19				
14	23.348	3.8068	4				
15	23.586	3.7690	2				

Re 49



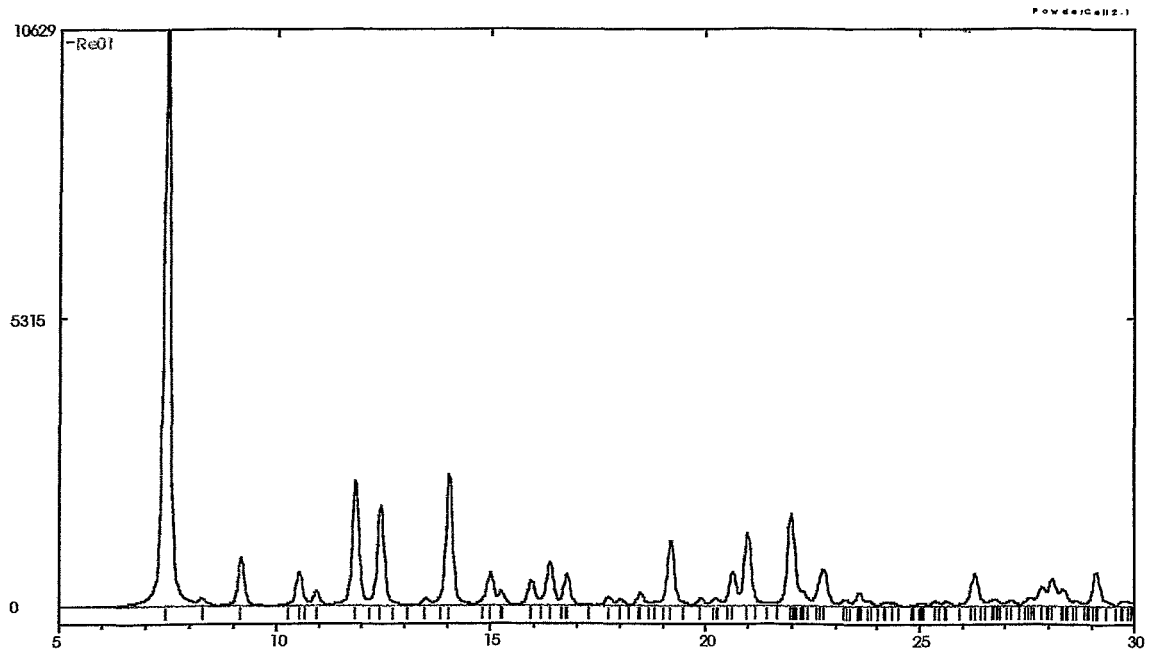
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	7.653	11.5429	100	16	23.153	3.8385	14
2	10.057	8.7880	15	17	23.906	3.7193	5
3	11.896	7.4332	6	18	24.224	3.6712	2
4	13.617	6.4975	7	19	24.797	3.5876	4
5	14.777	5.9899	29	20	25.741	3.4581	4
6	15.114	5.8572	70	21	26.783	3.3260	11
7	16.103	5.4997	3	22	27.130	3.2842	8
8	16.518	5.3622	6	23	27.398	3.2527	2
9	17.966	4.9335	1	24	28.605	3.1181	3
10	18.623	4.7607	20	25	29.229	3.0529	3
11	19.052	4.6546	24	26	29.457	3.0298	3
12	20.172	4.3985	9	27	29.719	3.0037	4
13	21.351	4.1582	9				
14	22.189	4.0030	3				
15	22.608	3.9298	3				

Tc 50



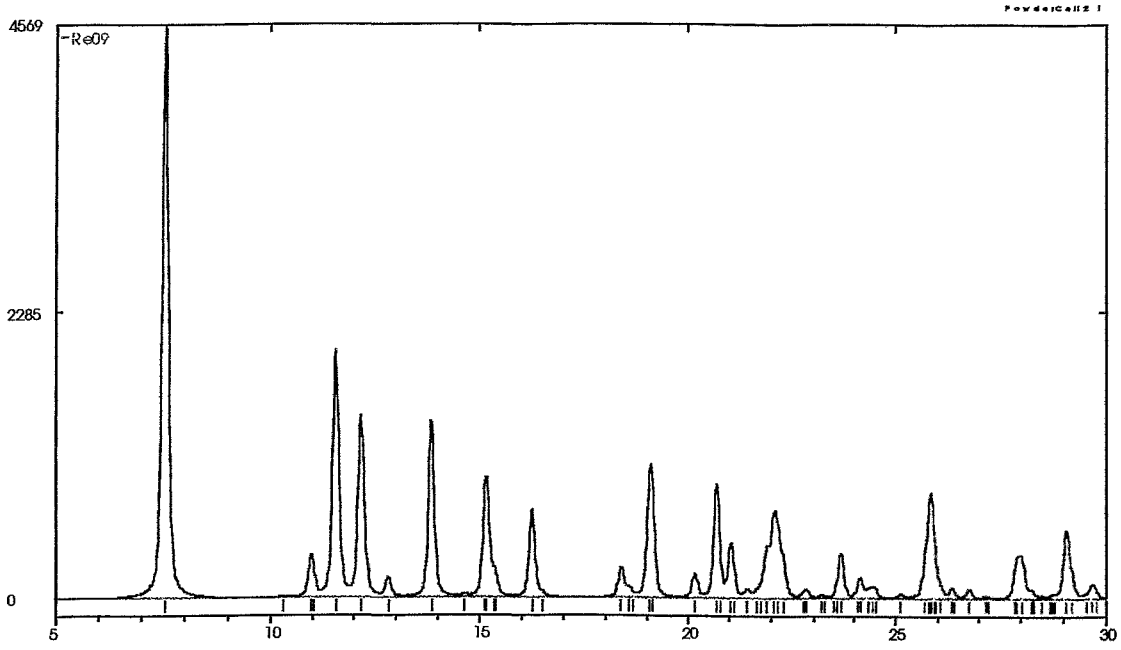
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	7.438	11.8763	100	18	18.508	4.7901	2
2	8.326	10.6107	1	19	19.127	4.6365	4
3	9.177	9.6291	7	20	19.295	4.5965	4
4	10.532	8.3926	4	22	20.828	4.2615	6
5	11.016	8.0254	2	23	21.157	4.1959	11
6	11.918	7.4195	16	24	21.525	4.1251	1
7	12.480	7.0869	13	25	22.128	4.0139	13
9	14.052	6.2973	15	26	22.798	3.8975	5
10	14.913	5.9356	5	27	23.694	3.7520	1
11	15.279	5.7944	2	30	26.291	3.3870	5
12	15.844	5.5890	2	31	26.755	3.3294	1
13	16.343	5.4193	5	32	27.066	3.2918	2
14	16.690	5.3076	3	33	27.745	3.2127	3
16	17.763	4.9893	1	34	28.265	3.1548	4
17	18.115	4.8930	1	35	29.306	3.0451	3

Re 50



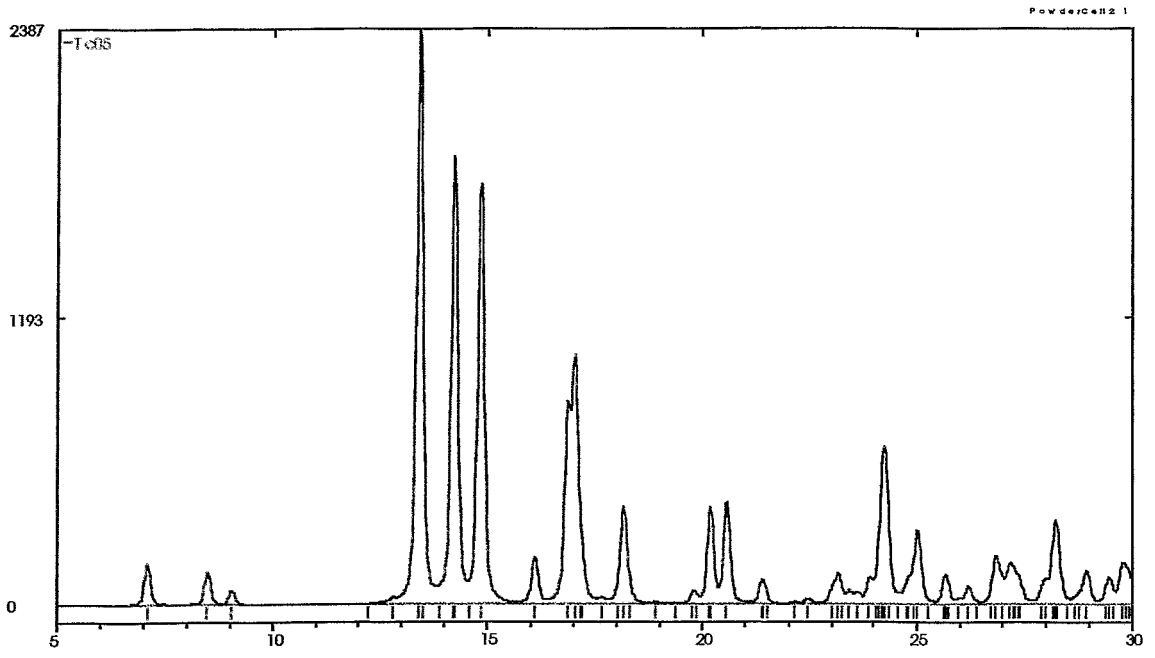
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	7.492	11.7910	100	19	20.255	4.3807	4
2	9.207	9.5980	10	20	20.663	4.2950	16
3	10.550	8.3784	8	21	21.005	4.2259	35
4	10.957	8.0682	4	22	22.010	4.0353	46
5	11.862	7.4545	34	23	22.738	3.9076	19
6	12.441	7.1090	29	24	23.247	3.8232	4
8	14.038	6.3038	42	25	23.575	3.7707	7
9	15.007	5.8987	11	30	26.284	3.3879	19
10	15.275	5.7958	5	31	26.749	3.3301	4
11	15.948	5.5526	9	33	27.588	3.2307	5
12	16.367	5.4114	16	34	27.838	3.2022	12
13	16.760	5.2854	12	35	28.085	3.1747	17
14	17.735	4.9971	3	36	28.338	3.1469	11
16	18.475	4.7986	5	37	29.109	3.0652	22
17	19.191	4.6211	29	38	29.765	2.9991	4

Re 51



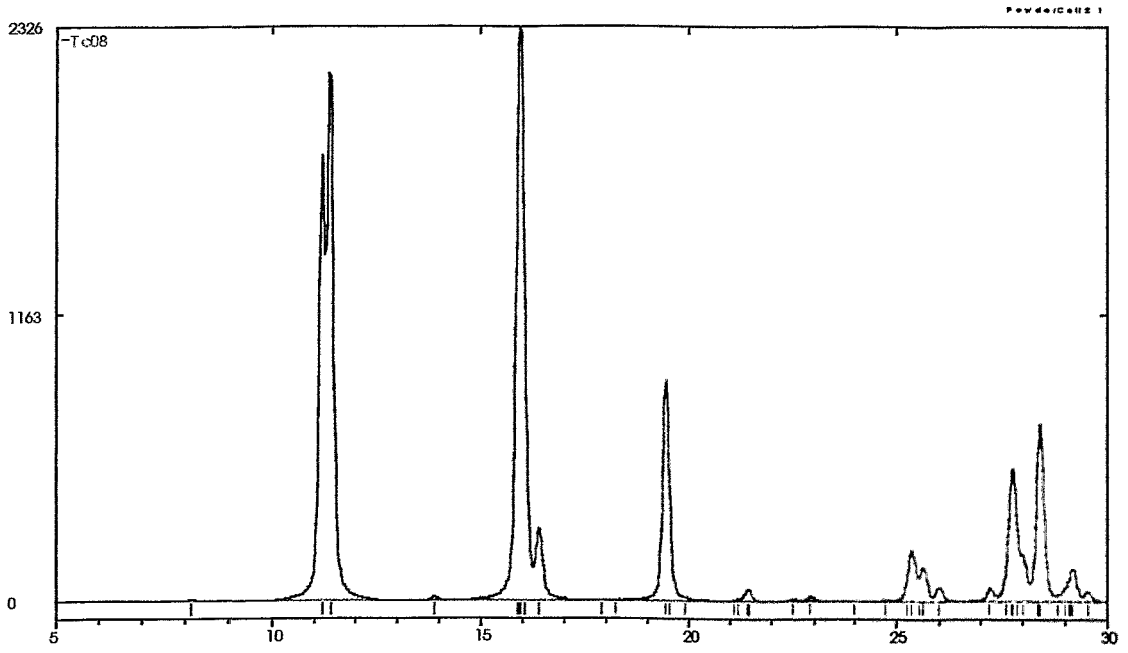
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	7.566	11.6744	100	16	21.446	4.1401	2
2	10.986	8.0471	7	17	21.945	4.0470	9
3	11.576	7.6383	43	18	22.108	4.0175	15
4	12.185	7.2579	32	19	22.320	3.9799	8
5	12.805	6.9076	4	20	22.828	3.8923	2
6	13.850	6.3889	31	21	23.682	3.7539	8
7	15.172	5.8348	21	22	24.152	3.6819	4
8	15.400	5.7491	5	23	24.462	3.6360	2
9	16.247	5.4511	15	25	25.836	3.4457	18
10	18.384	4.8221	5	26	26.345	3.3803	2
11	18.580	4.7717	2	27	26.765	3.3282	2
12	19.106	4.6414	23	28	27.928	3.1921	8
13	20.176	4.3977	4	29	27.991	3.1850	8
14	20.713	4.2848	20	31	29.071	3.0691	12
15	21.058	4.2154	10	32	29.675	3.0081	3

Tc 52



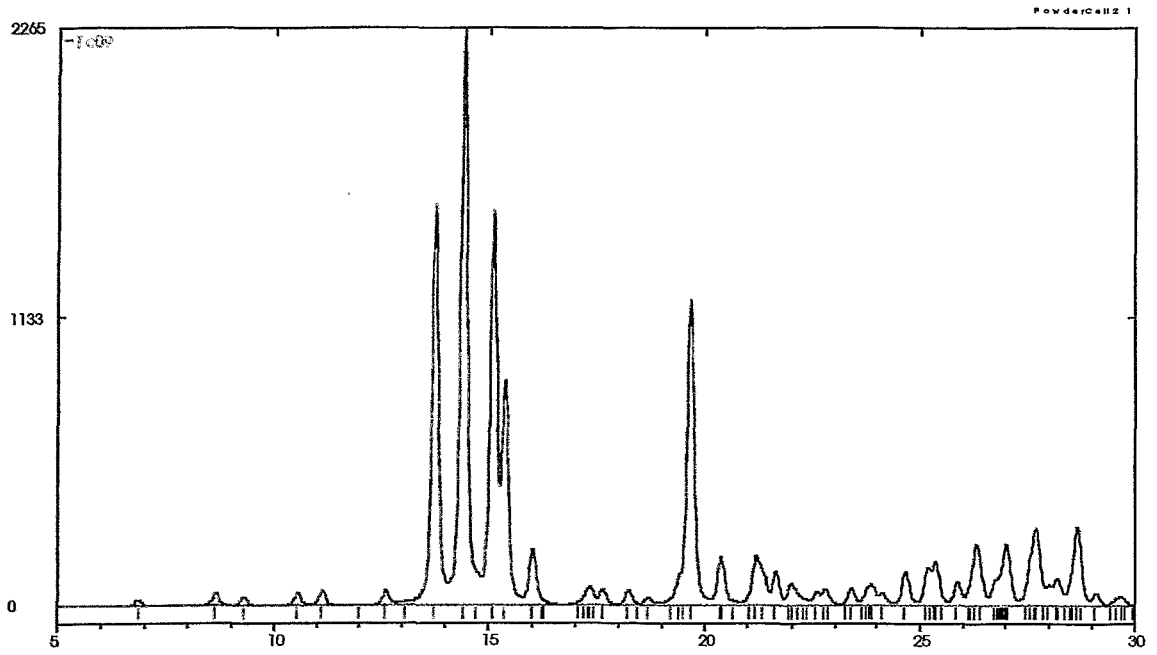
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	7.108	12.4264	7	16	22.464	3.9546	1
2	8.490	10.4062	6	17	23.153	3.8385	5
3	9.050	9.7636	3	18	23.920	3.7171	5
4	13.412	6.5964	100	19	24.249	3.6675	28
5	14.234	6.2172	78	20	24.770	3.5915	4
6	14.854	5.9593	73	21	25.017	3.5566	13
7	16.089	5.5043	8	22	25.660	3.4689	5
8	16.883	5.2473	35	23	26.199	3.3987	3
9	17.030	5.2024	43	24	26.856	3.3171	8
10	17.662	5.0176	1	25	27.203	3.2755	7
11	18.173	4.8777	17	26	27.960	3.1885	4
12	19.824	4.4750	2	27	28.235	3.1581	15
13	20.213	4.3897	17	28	28.946	3.0821	6
14	20.587	4.3108	18	29	29.468	3.0287	5
15	21.425	4.1441	4	30	29.816	2.9941	7

Tc 53



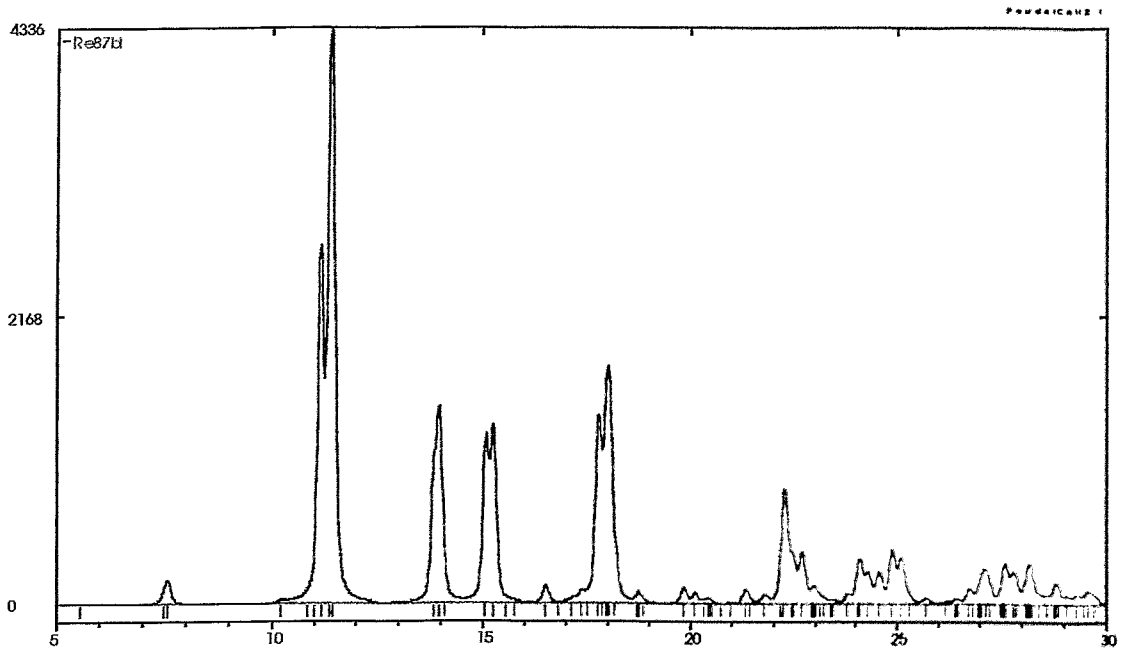
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	11.222	7.8783	78	16	29.186	3.0573	6
2	11.412	7.7474	92	17	29.529	3.0226	2
3	13.899	6.3664	1				
4	15.964	5.5471	100				
5	16.411	5.3973	13				
6	19.454	4.5592	39				
7	21.453	4.1387	2				
8	22.937	3.8742	1				
9	25.361	3.5091	9				
10	25.629	3.4730	6				
11	26.002	3.4240	3				
12	27.226	3.2728	2				
13	27.756	3.2115	23				
14	28.000	3.1841	8				
15	28.412	3.1389	31				

Tc 54



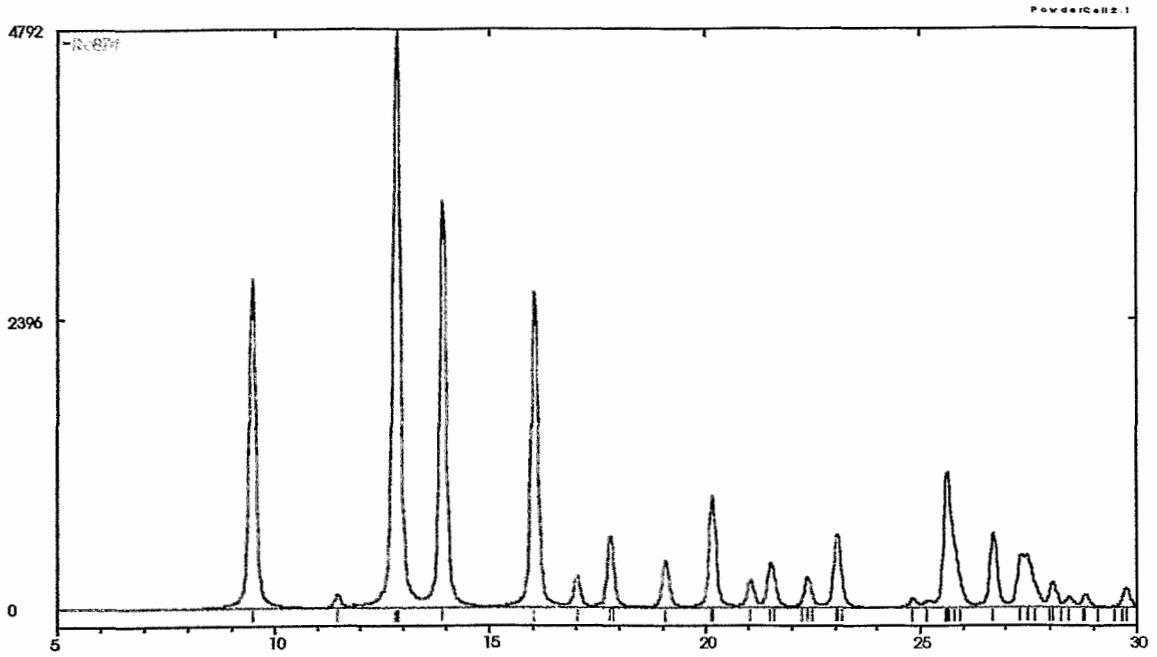
-N-	2 theta	---d---	I_{rel}	-N-	2 theta	---d---	I_{rel}
7	13.749	6.4357	70	25	23.388	3.8005	3
8	14.423	6.1364	100	26	23.756	3.7425	3
9	15.105	5.8607	68	27	23.870	3.7248	4
10	15.369	5.7606	39	29	24.647	3.6091	6
11	16.014	5.5301	10	30	25.170	3.5353	7
12	17.332	5.1123	3	31	25.345	3.5113	8
13	17.636	5.0249	3	32	25.851	3.4437	4
16	19.400	4.5718	5	33	26.306	3.3851	11
17	19.669	4.5098	53	34	26.780	3.3263	5
18	20.387	4.3526	8	35	27.008	3.2988	11
19	21.212	4.1852	9	36	27.561	3.2337	9
20	21.340	4.1604	6	37	27.690	3.2191	13
21	21.639	4.1036	6	38	27.995	3.1846	4
22	21.997	4.0375	4	39	28.179	3.1643	5
24	22.772	3.9018	3	40	28.650	3.1133	14

Re 55



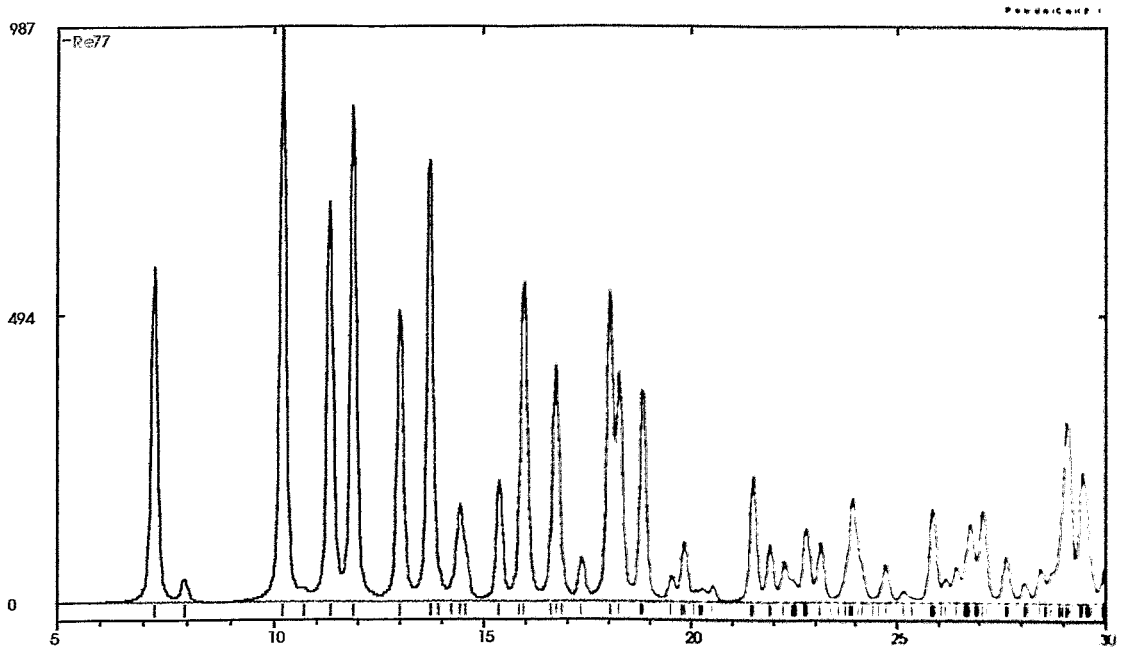
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	7.593	11.6342	4	17	22.482	3.9516	9
2	11.187	7.9032	62	18	22.689	3.9160	9
3	11.437	7.7308	100	19	23.000	3.8637	3
4	13.865	6.3818	27	21	24.110	3.6883	8
5	13.950	6.3431	34	22	24.300	3.6599	6
6	15.095	5.8645	29	23	24.572	3.6200	6
7	15.251	5.8048	31	24	24.883	3.5754	10
8	16.513	5.3642	3	25	25.080	3.5478	8
9	17.816	4.9745	33	27	26.745	3.3306	3
10	18.014	4.9204	41	28	27.118	3.2856	6
11	18.776	4.7224	2	29	27.603	3.2290	7
12	19.856	4.4678	3	30	27.800	3.2065	6
13	20.129	4.4078	2	31	28.176	3.1646	7
14	21.357	4.1571	2	32	28.811	3.0962	4
16	22.280	3.9870	20	33	29.586	3.0169	2

Re 56



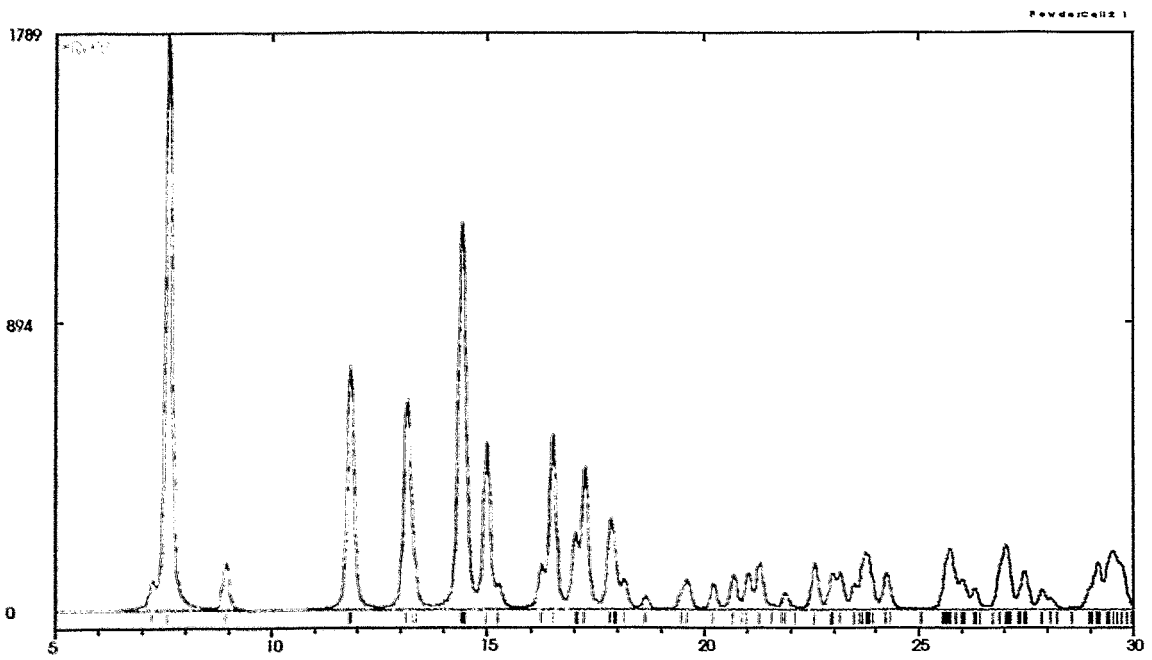
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	9.514	9.2885	57	16	25.637	3.4720	23
2	11.498	7.6901	2	17	25.811	3.4490	10
3	12.848	6.8848	100	18	26.727	3.3327	13
4	13.929	6.3529	70	19	27.372	3.2557	9
5	16.045	5.5193	55	20	27.505	3.2403	9
6	17.023	5.2044	5	21	28.068	3.1765	4
7	17.808	4.9768	12	22	28.457	3.1340	2
8	19.082	4.6473	8	23	28.837	3.0935	2
9	20.177	4.3976	19	24	29.765	2.9991	3
10	21.075	4.2120	5				
11	21.553	4.1196	8				
12	22.392	3.9672	5				
13	23.070	3.8522	13				
14	24.839	3.5817	2				
15	25.185	3.5332	1				

Tc 57



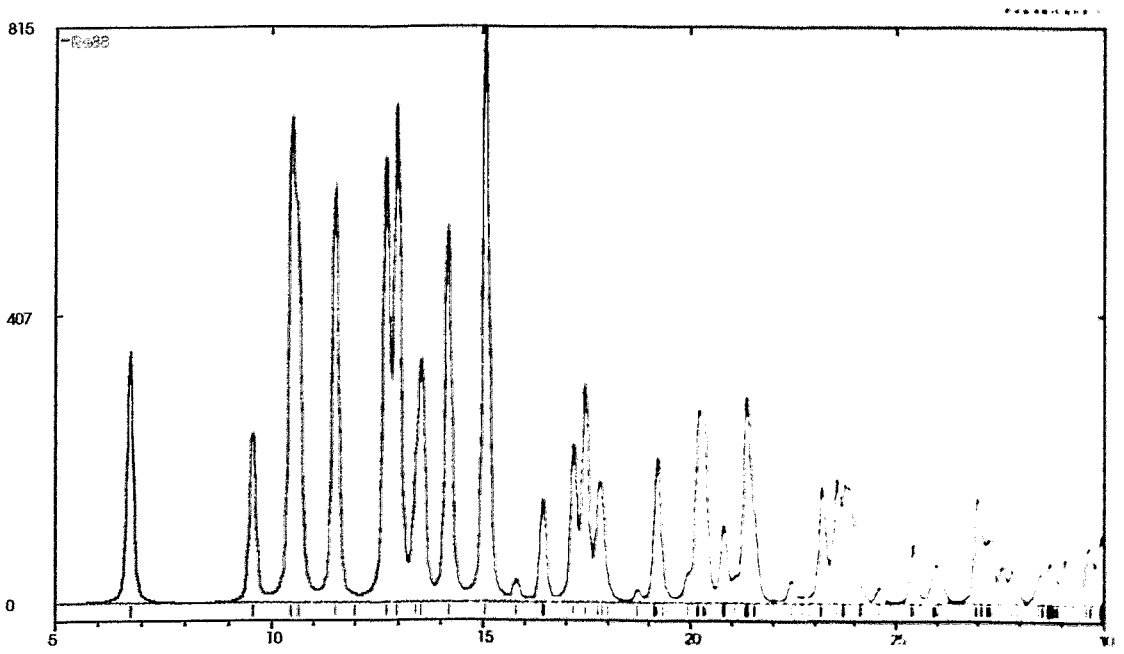
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	7.273	12.1447	58	18	19.845	4.4703	11
3	10.235	8.6361	100	21	21.528	4.1245	22
4	11.355	7.7866	69	22	21.937	4.0484	10
5	11.903	7.4292	86	23	22.288	3.9855	7
6	13.002	6.8035	51	25	22.804	3.8965	13
7	13.716	6.4508	77	26	23.149	3.8392	11
8	14.447	6.1261	17	27	23.937	3.7145	18
9	14.562	6.0779	10	28	24.106	3.6888	8
10	15.387	5.7538	21	29	24.726	3.5977	7
11	15.975	5.5434	56	31	25.852	3.4436	17
12	16.736	5.2930	41	34	26.770	3.3275	14
13	17.355	5.1057	8	35	27.068	3.2915	16
14	18.039	4.9136	54	36	27.641	3.2247	8
15	18.247	4.8579	40	39	29.093	3.0669	32
16	18.835	4.7076	37	40	29.469	3.0286	23

Tc 58



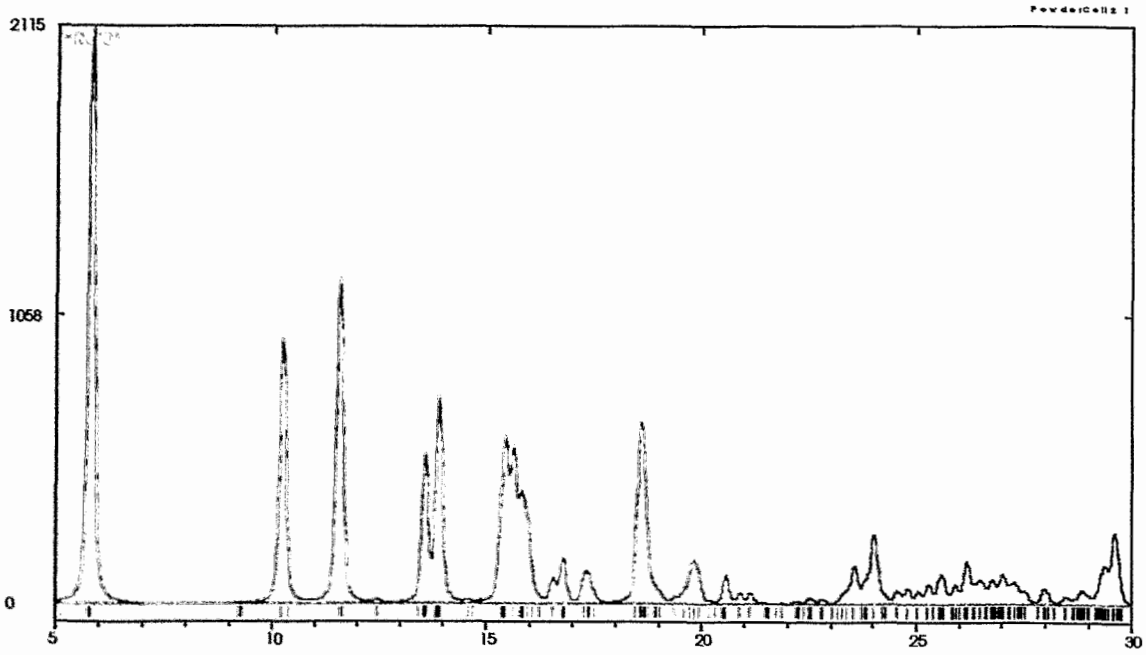
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
2	7.626	11.5827	100	21	21.306	4.1668	8
3	8.959	9.8631	8	23	22.567	3.9369	8
4	11.849	7.4628	42	24	22.982	3.8668	6
5	13.137	6.7340	36	25	23.157	3.8378	6
6	14.430	6.1335	67	27	23.761	3.7417	10
7	15.010	5.8976	29	28	23.858	3.7266	8
9	16.254	5.4489	8	29	24.244	3.6683	6
10	16.502	5.3675	30	30	25.711	3.4621	11
11	17.036	5.2005	13	31	26.008	3.4233	5
12	17.252	5.1358	25	33	26.910	3.3105	8
13	17.865	4.9610	16	34	27.036	3.2953	11
14	18.160	4.8810	5	35	27.464	3.2450	7
17	19.608	4.5238	5	39	29.170	3.0590	8
19	20.701	4.2874	6	40	29.523	3.0232	10
20	21.038	4.2195	6	41	29.720	3.0036	8

Tc 59



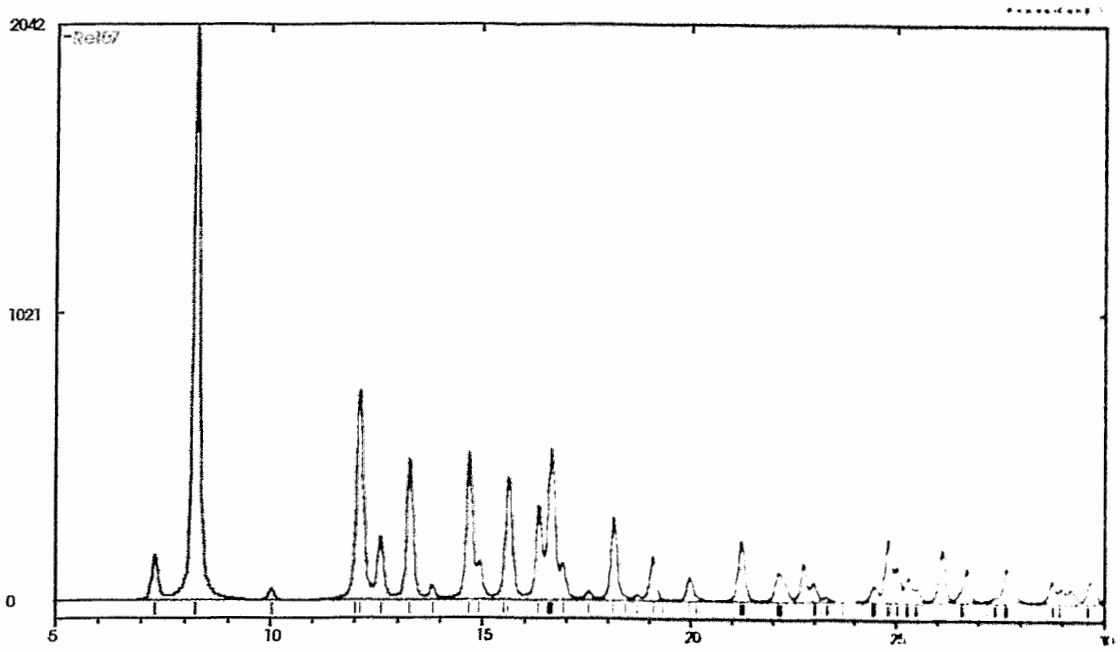
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	6.762	13.0608	44	18	19.230	4.6119	26
2	9.582	9.2231	30	20	20.226	4.3869	33
3	10.536	8.3897	84	21	20.314	4.3681	32
4	10.615	8.3278	70	22	20.826	4.2619	14
5	11.540	7.6620	73	23	21.397	4.1495	36
6	12.737	6.9444	77	24	21.540	4.1221	17
7	12.966	6.8226	87	26	23.196	3.8315	21
8	13.433	6.5863	29	27	23.582	3.7697	22
9	13.532	6.5384	42	28	23.768	3.7405	21
10	14.194	6.2347	66	29	23.872	3.7245	20
11	15.083	5.8693	100	31	25.428	3.5001	10
13	16.450	5.3844	18	33	26.990	3.3009	19
14	17.193	5.1535	28	34	27.246	3.2705	11
15	17.471	5.0718	38	39	29.106	3.0656	8
16	17.827	4.9714	21	40	29.647	3.0108	10

Tc 60



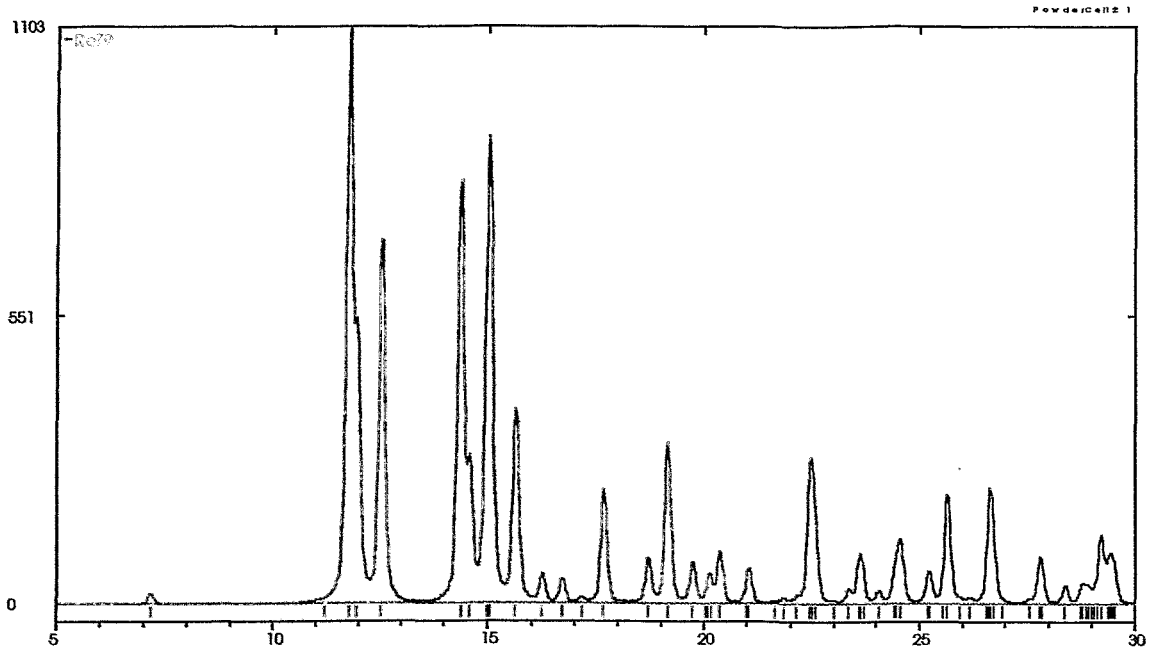
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	5.811	15.1979	100	23	24.030	3.7004	12
2	10.258	8.6168	46	24	24.575	3.6196	2
3	11.598	7.6238	56	25	24.798	3.5875	3
5	13.566	6.5221	26	27	25.300	3.5174	3
6	13.906	6.3632	36	28	25.571	3.4807	5
7	15.445	5.7326	29	29	25.917	3.4350	3
8	15.602	5.6750	28	30	26.178	3.4014	7
9	15.860	5.5834	19	31	26.496	3.3614	4
10	16.560	5.3489	5	32	26.780	3.3263	4
11	16.780	5.2792	8	33	27.044	3.2945	5
12	17.337	5.1109	6	34	27.260	3.2688	4
13	18.603	4.7659	31	36	27.995	3.1846	3
15	19.840	4.4713	8	38	28.861	3.0910	2
16	20.582	4.3119	5	39	29.384	3.0371	7
22	23.575	3.7708	7	40	29.622	3.0134	12

Tc 61



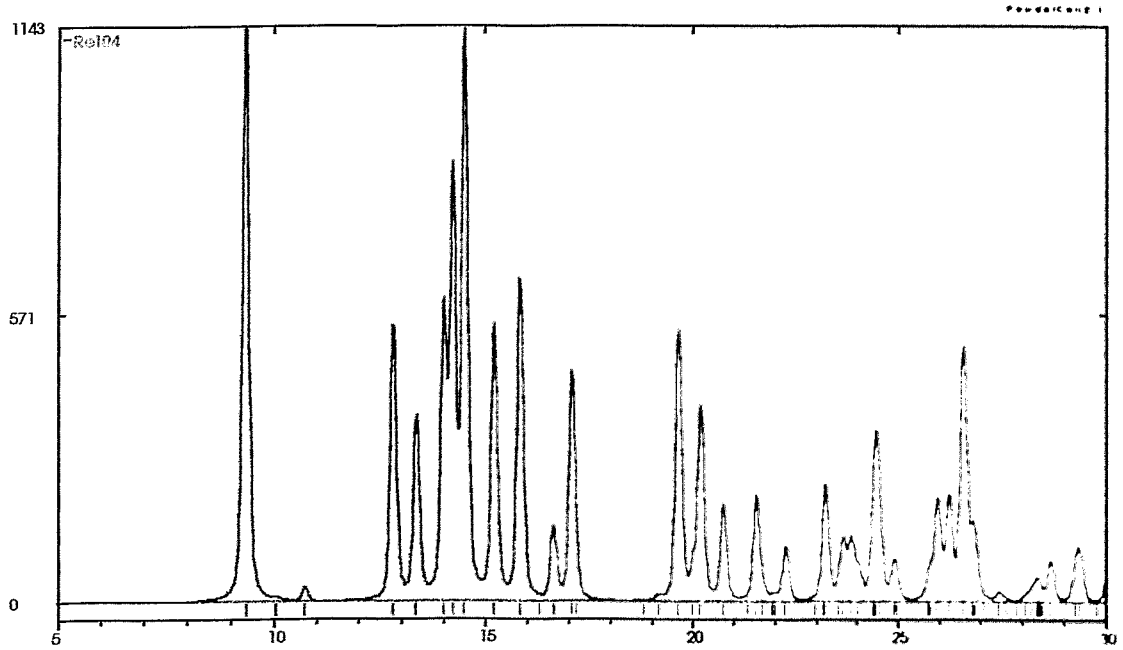
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	7.333	12.0456	8	20	22.156	4.0089	5
2	8.283	10.6654	100	21	22.340	3.9763	3
4	12.126	7.2929	36	22	22.756	3.9045	7
5	12.570	7.0365	11	23	22.996	3.8644	3
6	13.269	6.6672	25	25	24.469	3.6350	3
8	14.700	6.0212	26	26	24.810	3.5857	11
9	14.931	5.9285	7	27	25.034	3.5542	6
10	15.644	5.6600	22	28	25.295	3.5182	4
11	16.351	5.4169	16	30	26.106	3.4106	9
12	16.653	5.3193	27	31	26.712	3.3346	6
13	16.914	5.2379	6	33	27.672	3.2211	6
15	18.148	4.8844	15	34	27.793	3.2073	3
17	19.103	4.6422	8	35	28.758	3.1019	4
18	19.990	4.4382	4	36	28.995	3.0771	3
19	21.240	4.1797	11	38	29.687	3.0069	4

Tc 62



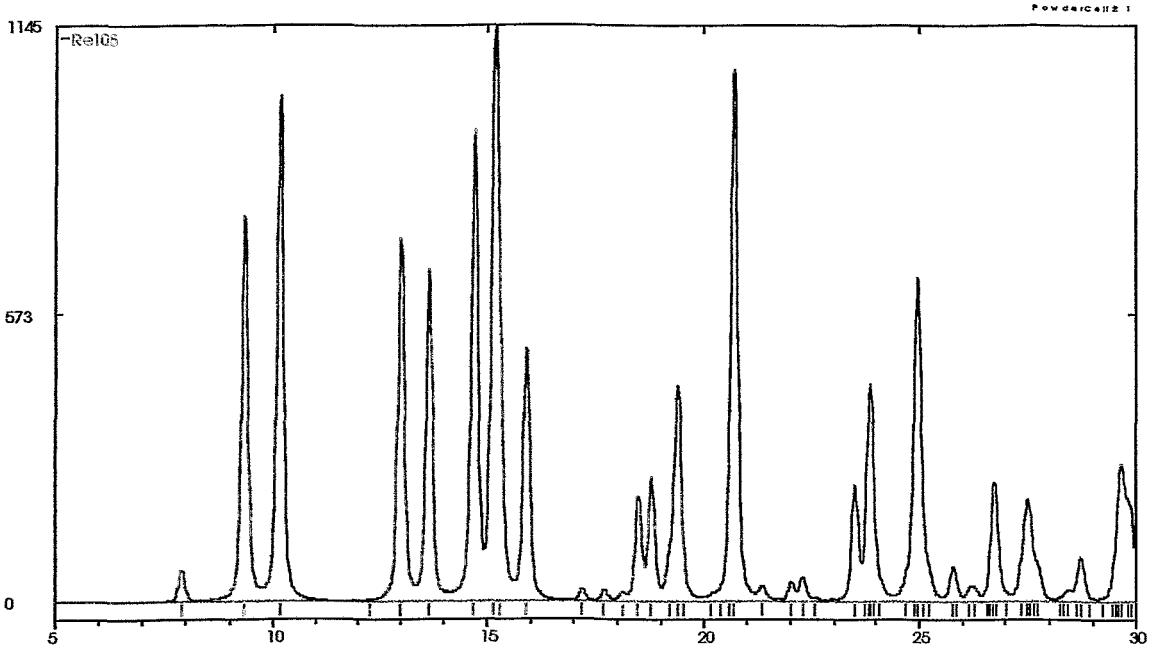
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
2	11.769	7.5131	100	18	21.051	4.2169	6
3	11.960	7.3938	50	21	22.485	3.9511	25
4	12.533	7.0572	63	22	23.369	3.8035	3
5	14.375	6.1565	74	23	23.629	3.7623	9
6	14.600	6.0623	26	24	24.053	3.6969	2
7	15.028	5.8904	81	25	24.460	3.6363	9
8	15.635	5.6633	34	26	24.541	3.6245	11
9	16.241	5.4531	5	27	25.209	3.5299	6
10	16.705	5.3028	4	28	25.627	3.4732	19
12	17.674	5.0141	20	31	26.648	3.3425	20
13	18.699	4.7415	8	33	27.800	3.2065	8
14	19.160	4.6286	28	34	28.364	3.1441	3
15	19.739	4.4941	7	35	28.777	3.0998	4
16	20.135	4.4065	5	36	29.225	3.0533	12
17	20.380	4.3542	9	37	29.445	3.0310	9

Tc 63



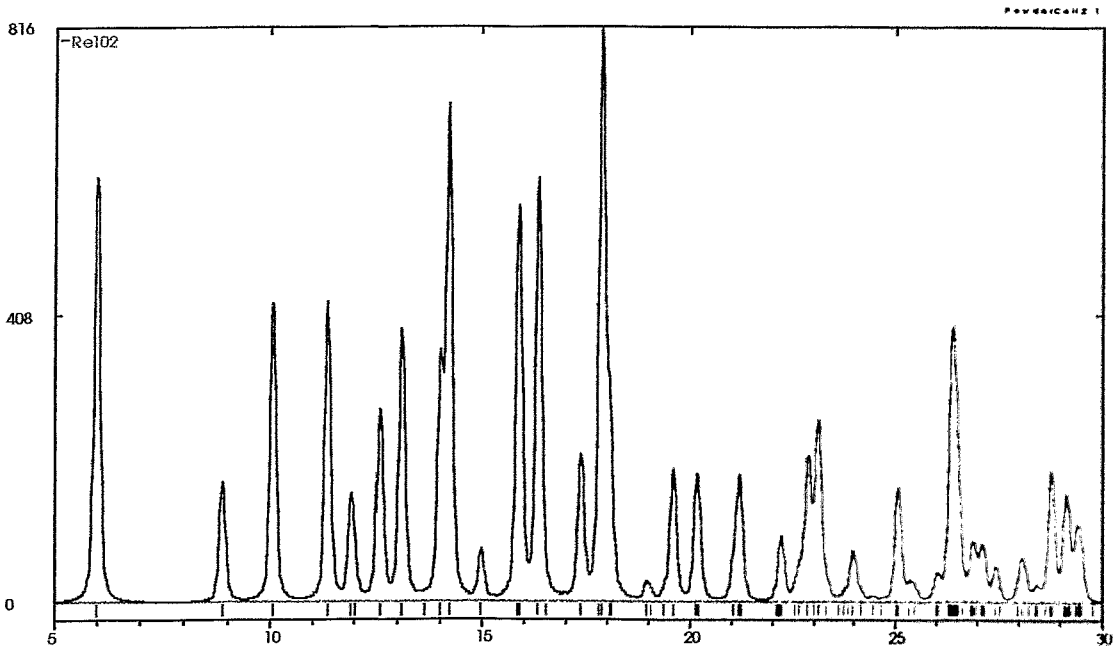
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	9.363	9.4384	100	16	22.275	3.9879	10
2	10.729	8.2395	2	17	23.234	3.8253	20
3	12.817	6.9014	48	18	23.664	3.7568	11
4	13.347	6.6285	33	19	23.866	3.7254	12
5	14.020	6.3116	53	20	24.473	3.6344	30
6	14.241	6.2143	77	21	24.915	3.5708	7
7	14.519	6.0960	100	22	25.731	3.4595	6
8	15.222	5.8159	48	23	25.945	3.4315	18
9	15.848	5.5877	56	24	26.217	3.3964	19
10	16.627	5.3274	13	25	26.573	3.3518	45
11	17.086	5.1855	40	26	26.860	3.3166	14
12	19.662	4.5115	47	27	27.455	3.2460	2
13	20.206	4.3913	34	28	28.358	3.1446	4
14	20.753	4.2768	17	29	28.688	3.1093	7
15	21.571	4.1164	19	30	29.349	3.0408	10

Tc 64



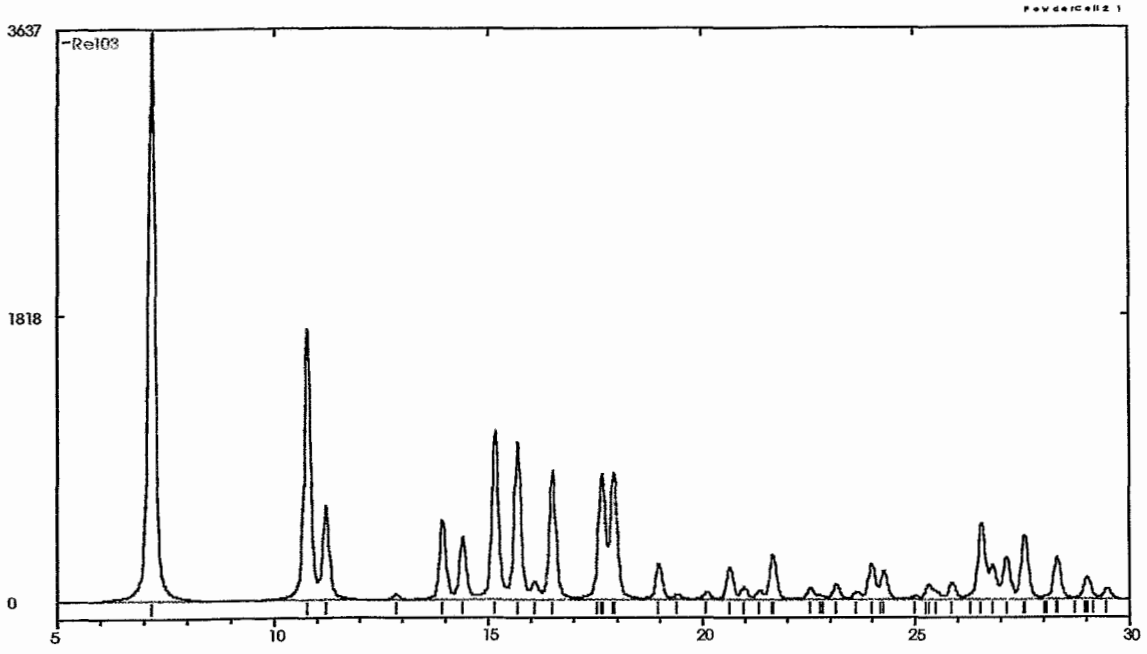
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	7.931	11.1388	6	16	20.727	4.2821	92
2	9.375	9.4257	67	17	21.364	4.1557	3
3	10.172	8.6889	88	18	22.054	4.0272	3
4	13.003	6.8031	63	19	22.305	3.9825	4
5	13.656	6.4790	58	20	23.523	3.7789	20
6	14.719	6.0135	82	21	23.889	3.7219	38
7	15.185	5.8302	100	22	24.969	3.5634	56
8	15.915	5.5642	44	23	25.776	3.4535	6
9	17.205	5.1497	2	24	26.232	3.3945	3
10	17.718	5.0018	2	25	26.767	3.3279	21
11	18.140	4.8864	2	26	27.515	3.2391	18
12	18.487	4.7955	18	27	27.723	3.2153	7
13	18.797	4.7171	22	28	28.440	3.1358	2
14	19.212	4.6162	10	29	28.729	3.1050	8
15	19.419	4.5674	38	30	29.687	3.0069	24

Tc 65



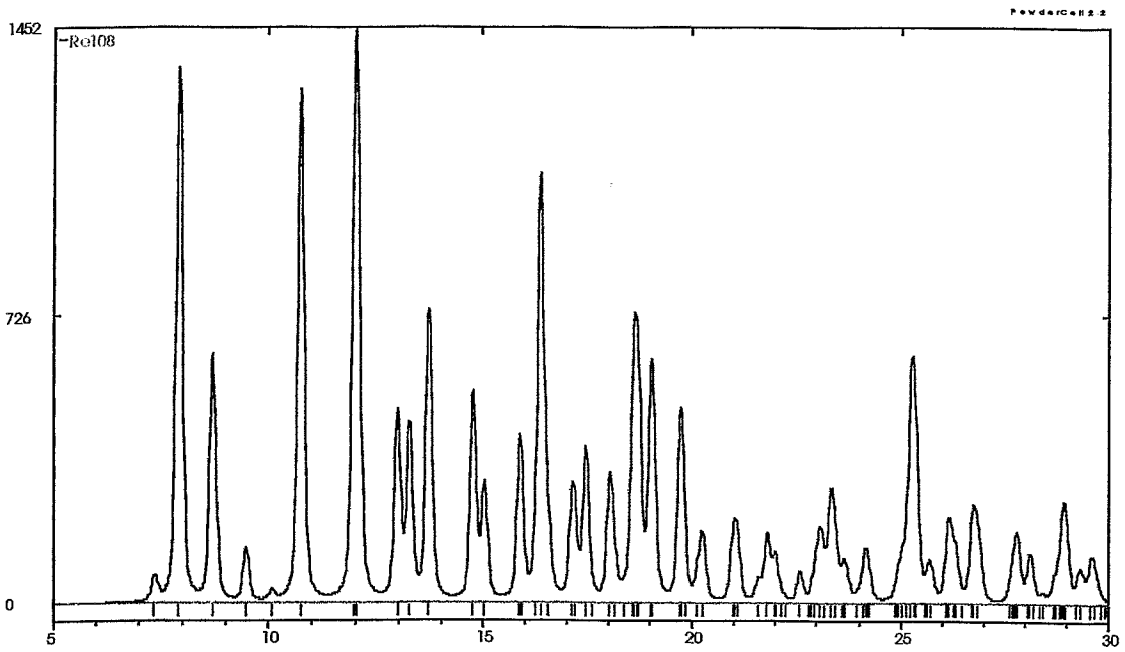
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	6.001	14.7165	74	17	20.178	4.3973	22
2	8.903	9.9243	21	18	21.198	4.1879	22
3	10.081	8.7677	52	19	22.220	3.9975	11
4	11.380	7.7692	52	20	22.877	3.8842	25
5	11.944	7.4040	19	21	23.102	3.8468	32
6	12.585	7.0282	34	22	23.972	3.7091	9
7	13.095	6.7556	48	24	25.054	3.5514	20
8	14.020	6.3117	44	27	26.393	3.3741	48
9	14.212	6.2268	87	28	26.897	3.3121	11
10	14.989	5.9057	9	29	27.103	3.2874	10
11	15.887	5.5738	69	30	27.428	3.2492	6
12	16.359	5.4143	74	31	28.077	3.1755	8
13	17.368	5.1019	26	33	28.792	3.0982	23
14	17.887	4.9550	100	34	29.148	3.0612	19
16	19.610	4.5232	23	35	29.434	3.0322	14

Tc 66



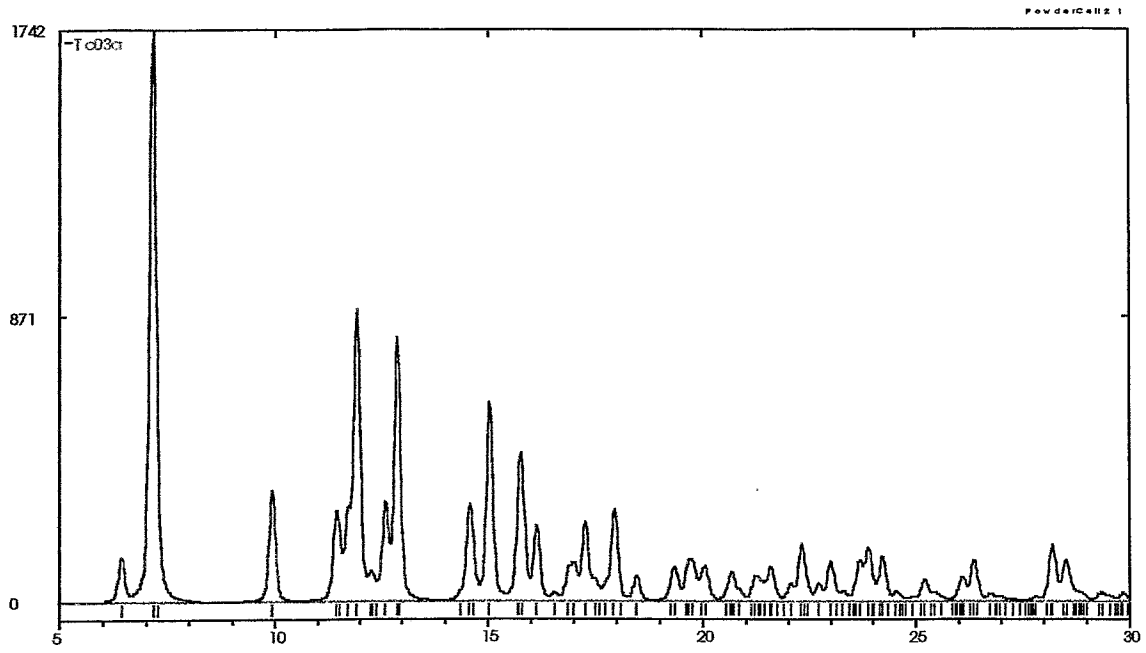
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	7.187	12.2907	100	19	21.687	4.0946	8
2	10.797	8.1874	48	20	22.573	3.9358	2
3	11.233	7.8709	16	21	23.171	3.8356	3
5	13.946	6.3453	14	23	23.983	3.7075	6
6	14.407	6.1430	11	24	24.273	3.6639	5
7	15.175	5.8338	30	26	25.326	3.5139	3
8	15.709	5.6367	28	27	25.476	3.4935	2
9	16.095	5.5022	3	28	25.877	3.4403	3
10	16.522	5.3612	23	29	26.556	3.3539	13
11	17.665	5.0168	22	30	26.820	3.3214	6
12	17.937	4.9412	22	31	27.128	3.2845	7
13	18.992	4.6690	6	32	27.559	3.2341	11
16	20.657	4.2964	6	33	28.332	3.1475	7
17	20.998	4.2273	2	34	29.030	3.0735	4
18	21.368	4.1550	2	35	29.490	3.0265	2

Re 67



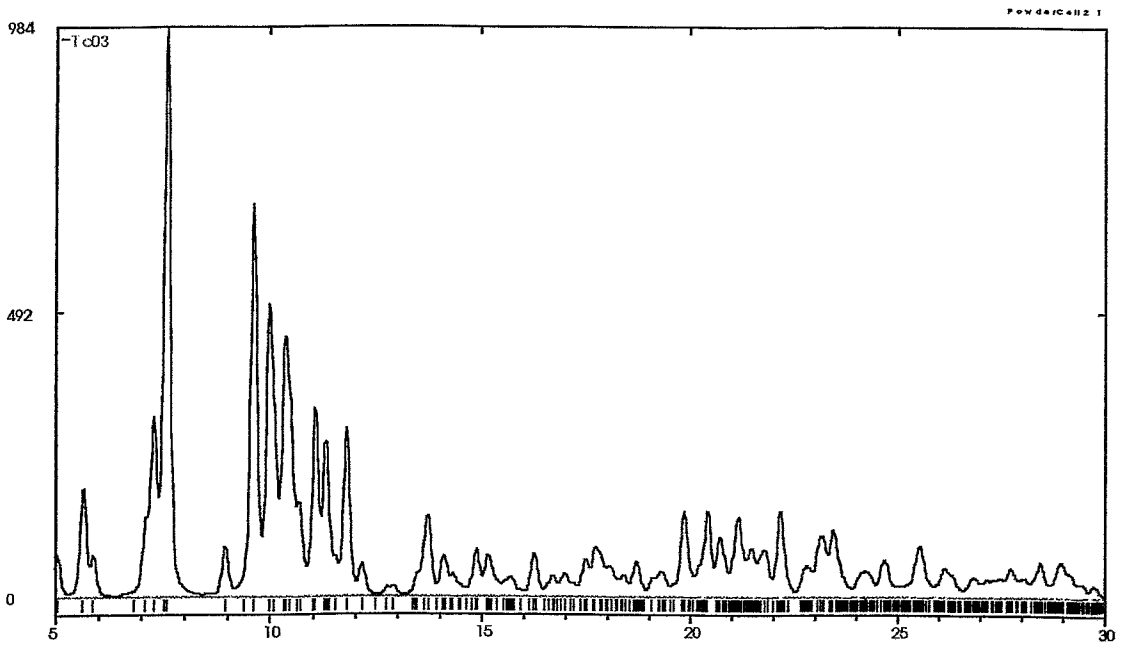
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
2	7.936	11.1315	93	18	18.678	4.7469	51
3	8.713	10.1411	43	19	19.059	4.6528	42
4	9.491	9.3106	10	20	19.760	4.4893	34
6	10.753	8.2207	89	21	20.251	4.3815	12
7	12.036	7.3471	100	22	21.041	4.2188	15
8	13.012	6.7982	34	24	21.813	4.0711	12
9	13.292	6.6556	32	27	23.094	3.8482	13
10	13.732	6.4435	51	28	23.367	3.8038	20
11	14.792	5.9839	37	30	24.172	3.6789	10
12	15.059	5.8785	21	32	25.298	3.5178	43
13	15.912	5.5651	29	34	26.186	3.4004	15
14	16.411	5.3973	75	35	26.320	3.3834	12
15	17.176	5.1585	21	36	26.789	3.3252	17
16	17.479	5.0696	27	37	27.809	3.2055	12
17	18.068	4.9056	23	39	28.944	3.0824	18

Tc 68



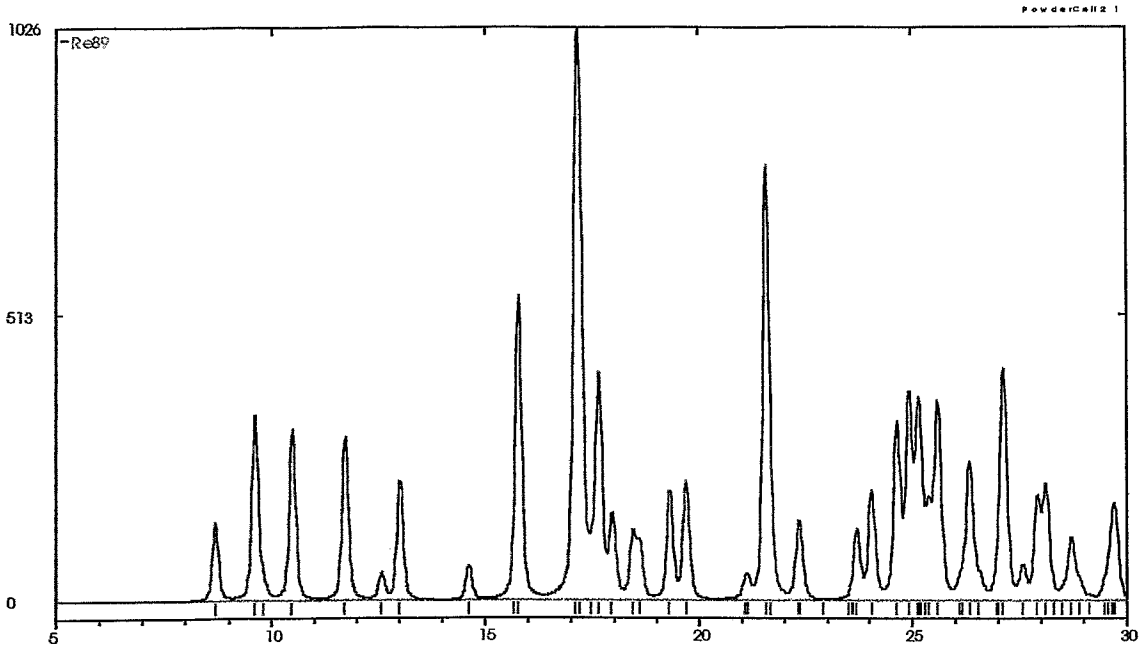
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	6.428	13.7394	8	17	17.965	4.9335	16
2	7.172	12.3149	100	19	19.370	4.5787	6
3	9.951	8.8818	20	20	19.727	4.4967	8
4	11.462	7.7141	16	21	20.060	4.4229	6
5	11.750	7.5253	17	22	20.663	4.2950	5
6	11.936	7.4087	51	23	21.270	4.1740	5
7	12.262	7.2124	5	24	21.595	4.1119	6
8	12.614	7.0119	18	26	22.354	3.9739	10
9	12.889	6.8627	46	28	23.022	3.8601	7
10	14.597	6.0635	17	29	23.698	3.7515	7
11	15.049	5.8824	35	30	23.883	3.7229	9
12	15.773	5.6141	26	31	24.229	3.6704	8
13	16.150	5.4839	13	34	26.345	3.3803	7
15	16.971	5.2203	7	37	28.207	3.1612	10
16	17.267	5.1315	14	38	28.519	3.1273	7

Tc 69



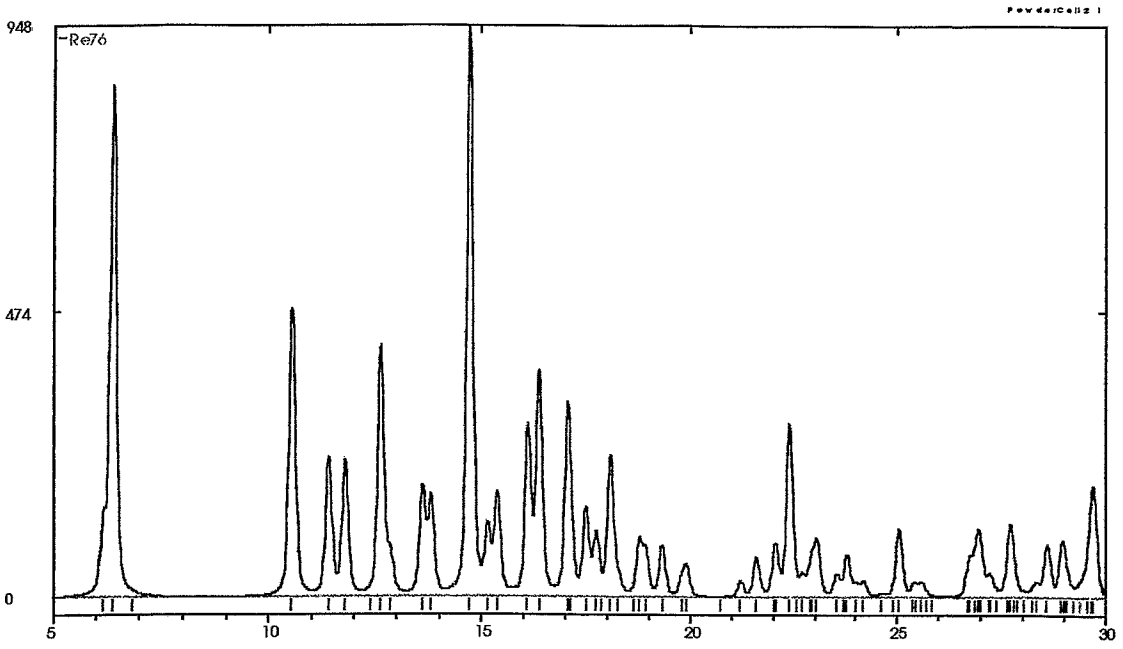
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	5.056	17.4645	8	19	14.094	6.2789	7
2	5.643	15.6492	19	21	14.883	5.9475	8
3	5.900	14.9676	7	22	15.163	5.8383	7
4	7.134	12.3809	14	24	16.258	5.4474	8
5	7.308	12.0871	32	28	17.754	4.9917	9
6	7.603	11.6179	100	34	19.868	4.4651	15
7	8.966	9.8545	9	35	20.420	4.3457	15
8	9.650	9.1580	69	36	20.733	4.2807	11
9	10.024	8.8167	51	37	21.173	4.1928	14
10	10.411	8.4901	45	38	21.493	4.1310	9
11	10.720	8.2461	17	39	21.787	4.0761	8
12	11.068	7.9875	33	40	22.185	4.0038	15
13	11.304	7.8211	27	42	23.161	3.8373	11
14	11.797	7.4959	30	43	23.449	3.7907	12
18	13.709	6.4543	14	46	25.530	3.4863	9

Tc 70



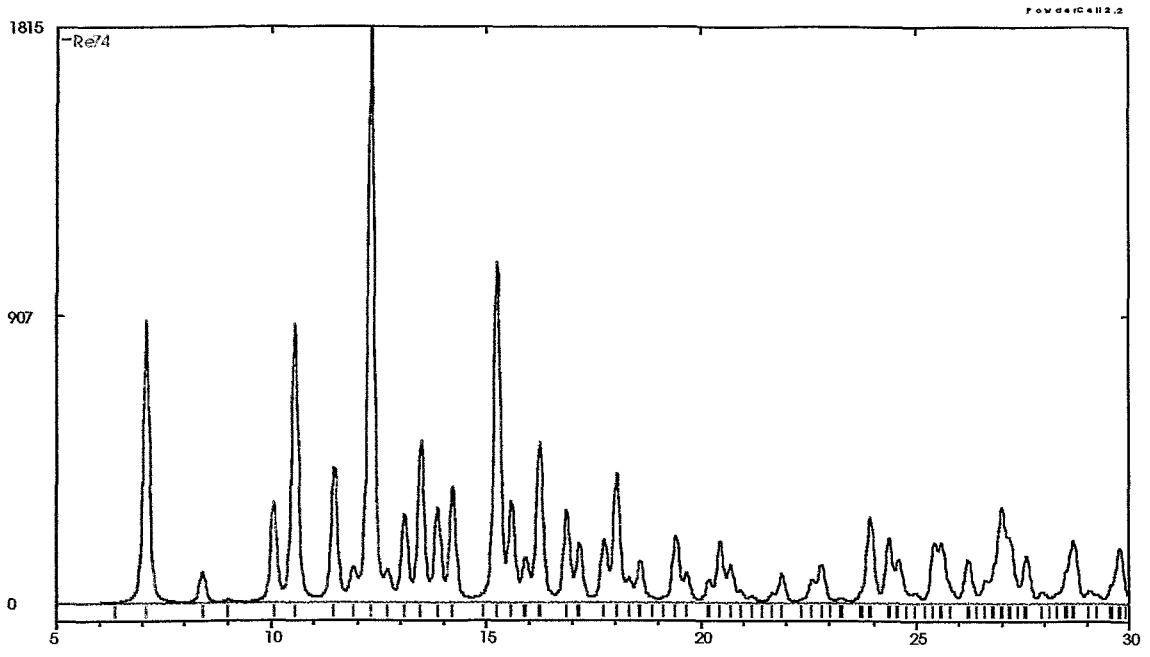
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	8.701	10.1542	14	18	22.376	3.9700	14
2	9.623	9.1832	33	19	23.704	3.7505	13
3	10.509	8.4112	30	20	24.052	3.6971	19
4	11.737	7.5341	29	21	24.659	3.6073	31
6	13.016	6.7960	21	22	24.928	3.5690	37
7	14.633	6.0487	6	23	25.143	3.5391	36
8	15.790	5.6080	53	24	25.388	3.5054	18
9	17.163	5.1622	100	25	25.601	3.4768	35
10	17.655	5.0195	40	26	26.326	3.3827	24
11	17.953	4.9369	15	28	27.121	3.2852	41
12	18.482	4.7968	12	29	27.574	3.2323	6
13	18.573	4.7734	11	30	27.924	3.1926	19
14	19.338	4.5862	19	31	28.106	3.1723	21
15	19.718	4.4987	21	32	28.712	3.1067	11
17	21.595	4.1119	76	34	29.720	3.0036	17

Tc 71



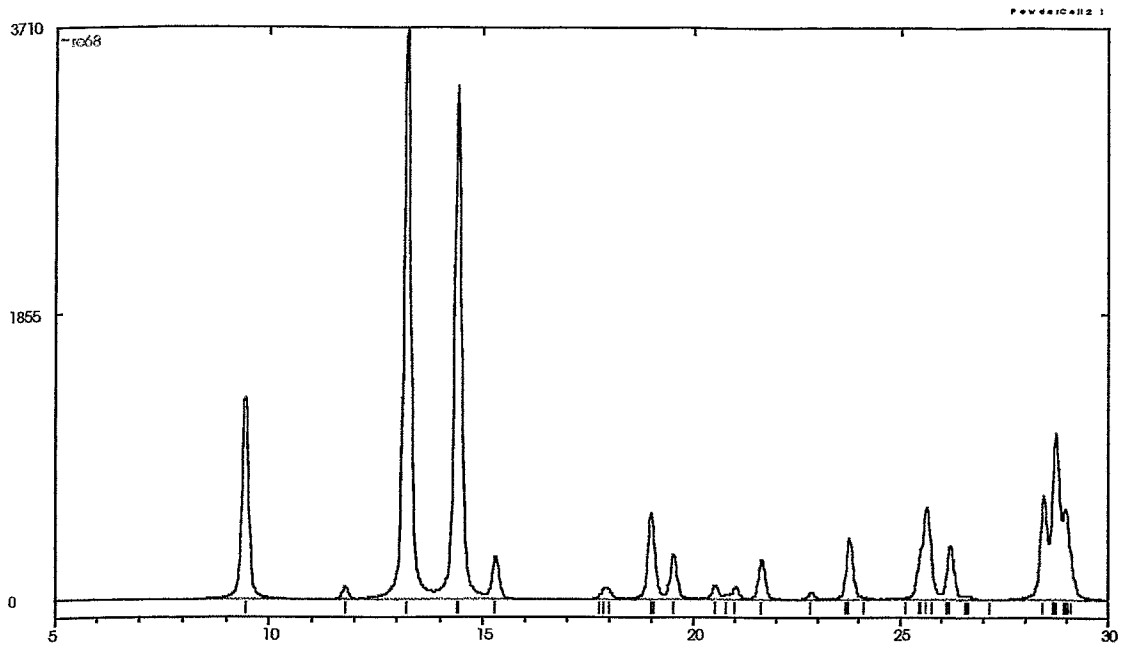
-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	6.205	14.2335	16	16	17.514	5.0596	16
2	6.418	13.7599	90	17	17.741	4.9953	12
3	10.565	8.3667	51	18	18.091	4.8996	25
4	11.438	7.7300	25	19	18.796	4.7174	11
5	11.811	7.4869	24	20	18.918	4.6872	9
6	12.629	7.0035	44	21	19.339	4.5862	9
7	12.832	6.8931	9	25	22.081	4.0223	10
8	13.605	6.5034	20	26	22.417	3.9629	30
9	13.795	6.4144	18	27	23.041	3.8570	10
10	14.745	6.0031	100	31	25.061	3.5505	12
11	15.160	5.8396	13	34	26.947	3.3060	12
12	15.399	5.7496	19	36	27.711	3.2167	13
13	16.132	5.4899	30	37	28.585	3.1202	9
14	16.388	5.4046	40	38	28.971	3.0795	10
15	17.088	5.1848	34	39	29.709	3.0047	20

Re 71



-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	7.106	12.4294	49	20	17.755	4.9915	11
4	10.052	8.7929	18	21	18.048	4.9111	23
5	10.553	8.3765	49	24	19.426	4.5658	12
6	11.470	7.7084	23	27	20.455	4.3384	11
8	12.332	7.1714	100	36	23.948	3.7129	15
10	13.120	6.7425	15	37	24.372	3.6493	11
11	13.503	6.5523	28	38	24.607	3.6149	8
12	13.881	6.3747	17	40	25.451	3.4969	11
13	14.234	6.2174	20	41	25.618	3.4745	11
14	15.278	5.7946	59	42	26.225	3.3954	8
15	15.626	5.6663	18	44	27.007	3.2988	17
16	15.948	5.5529	8	45	27.200	3.2759	12
17	16.266	5.4449	28	46	27.588	3.2306	8
18	16.887	5.2460	16	49	28.702	3.1078	11
19	17.178	5.1577	10	51	29.793	2.9964	10

Tc 72



-N-	2 theta	—d—	I_{rel}	-N-	2 theta	—d—	I_{rel}
1	9.465	9.3364	35	16	26.214	3.3968	9
2	11.794	7.4973	2	17	26.589	3.3498	1
3	13.229	6.6874	100	18	28.433	3.1366	18
4	14.425	6.1353	90	19	28.736	3.1041	29
5	15.307	5.7837	8	20	28.980	3.0786	16
6	17.930	4.9432	2				
7	19.006	4.6658	15				
8	19.541	4.5391	8				
9	20.545	4.3196	3				
10	21.026	4.2217	2				
11	21.673	4.0971	7				
12	22.866	3.8861	1				
13	23.790	3.7372	11				
14	25.491	3.4915	9				
15	25.646	3.4708	16				