

Heptacarbonyl- $1\kappa^3C,2\kappa^4C$ -(4-phenylpyridine- $1\kappa N$)di- μ -phenyltellurido- $1:2\kappa^4Te:Te$ -dirhenium(I)

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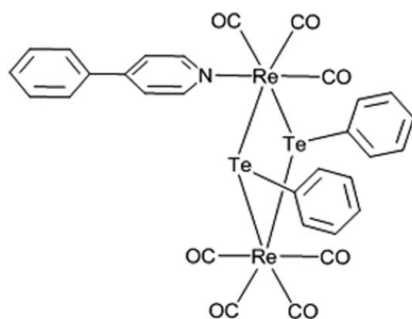
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Key indicators: single-crystal X-ray study; $T = 150$ K; mean $\sigma(C-C) = 0.020$ Å; R factor = 0.058; wR factor = 0.135; data-to-parameter ratio = 14.7.

In the title complex, $[Re_2(C_6H_5Te)_2(C_{11}H_9N)(CO)_7]$, two Re atoms are coordinated in slightly distorted octahedral coordination environments and are bridged by two Te atoms, which are coordinated in trigonal-pyramidal environments. The torsion angle for the Te—Re—Te—Re sequence of atoms is $17.06(3)^\circ$. The crystal structure is stabilized by weak C—H \cdots O and C—H $\cdots\pi$ interactions. In addition, there are Te \cdots Te distances [$4.0392(12)$ Å] and O \cdots O distances [$2.902(19)$ Å] which are shorter than the sum of the van der Waals radii for these atoms. A short intermolecular lone pair $\cdots\pi$ distance [C \equiv O \cdots Cg = $3.31(2)$ Å] is also observed.

Related literature

For the biological applications of Re and Te compounds, see: Begum *et al.* (2008); Atwood *et al.* (1983); Zhang & Leong (2000); Lima *et al.* (2009); Cunha *et al.* (2009); Kopf-Maier & Klapötke (1992). For a related structure, see Cecconi *et al.* (1998). For an example of a structure with weak Te \cdots Te contacts, see: Ritch & Chivers (2009). For details of electron lone pair interactions, see: Jain *et al.* (2009).



Experimental

Crystal data

$[Re_2(C_6H_5Te)_2(C_{11}H_9N)(CO)_7]$	$V = 3155.0(5)$ Å ³
$M_r = 1133.06$	$Z = 4$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 18.549(2)$ Å	$\mu = 9.53$ mm ⁻¹
$b = 12.3624(12)$ Å	$T = 150$ K
$c = 13.7768(11)$ Å	$0.23 \times 0.18 \times 0.15$ mm
$\beta = 92.927(9)^\circ$	

Data collection

Oxford Diffraction Xcalibur-S diffractometer	22729 measured reflections
Absorption correction: multi-scan (<i>CrysAlis PRO</i> ; Oxford Diffraction, 2009)	5553 independent reflections
$T_{min} = 0.218$, $T_{max} = 0.329$	4237 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.098$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.058$	12 restraints
$wR(F^2) = 0.135$	H-atom parameters constrained
$S = 1.03$	$\Delta\rho_{max} = 2.25$ e Å ⁻³
5553 reflections	$\Delta\rho_{min} = -3.27$ e Å ⁻³
379 parameters	

Table 1

Hydrogen-bond geometry (Å, °).

Cg is the centroid of the C14–C19 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C16—H16 \cdots O4 ⁱ	0.95	2.55	3.33 (2)	139
C11—H11 \cdots O4 ⁱⁱ	0.95	2.71	3.160 (18)	110
C17—H17 \cdots O1 ⁱⁱⁱ	0.95	2.46	3.271 (19)	144
C26—H26 \cdots O2 ^{iv}	0.95	2.71	3.34 (2)	124
C21—H21 \cdots O3 ^v	0.95	2.45	3.200 (16)	136
C29—H29 \cdots Cg ^{vi}	0.95	2.79	3.378 (15)	121

Symmetry codes: (i) $-x+1, -y, -z$; (ii) $-x+1, -y, -z+1$; (iii) $x, -y-\frac{1}{2}, z-\frac{1}{2}$; (iv) $x, y+1, z$; (v) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (vi) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2009); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5009).

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supplementary materials

Acta Cryst. (2010). E66, m518-m519 [doi:10.1107/S1600536810012389]

Heptacarbonyl-1 κ^3 C,2 κ^4 C-(4-phenylpyridine-1 κ N)di- μ -phenyltellurido-1:2 κ^4 Te:Te-dirhenium(I)

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Comment

Rhenium and tellurium compounds possess interesting and promising biological applications (Begum *et al.*, 2008; Atwood *et al.*, 1983; Zhang & Leong, 2000). Organic telluranes have been used as protease inhibitors and have applications in a wide range of disease models. Some tellurium derivatives also exhibit antioxidant as well as immunomodulatory effects (Cunha *et al.*, 2009). Recently, a novel organotellurium compound RT-01 was proven to act as antileishmanial agent for the disease Leishmaniasis (Lima *et al.*, 2009). Rhenium containing compounds are found to have anti tumor and cytostatic activity (Kopf-Maier & Klapotke, 1992). Considering the importance of the compounds, we have synthesized and undertaken the single crystal structure determination of title compound of which the molecular structure is shown in Fig. 1.

The Re₂Te₂ four-membered ring of atoms deviates significantly from planarity as described by the Te₂-Re₁-Te₁-Re₂ torsion angle of 17.06 (3)°. The Re-Te distances in the title compound can be compared with those in a related structure (Cecconi *et al.*, 1998). An intermolecular O₂...O₂(-x, -y, -z) = 2.902 (19) Å distance is less than the sum of the van der Waals radii for these atoms as is a short intermolecular Te...Te distance [Te₁...Te₂(x, 0.5-y, 0.5+z) = 4.0392 (12) Å]. The Te...Te contacts were also noticed in a Te structure reported by Ritch & Chivers (2009). A lone pair... π interaction as described by Jain, *et al.*, 2009 is also evident with O₃...Cg(C15-C28) = 3.31 (2) Å. Furthermore the crystal structure is stabilized by weak C-H...O (Fig 2.) and C—H... π interactions.

Experimental

A mixture of Re₂(CO)₁₀ (130 mg, 0.2 mmol) and diphenyl ditelluride (41 mg, 0.1 mmol), 4-phenylpyridine (93 mg, 0.6 mmol) were taken in a 50 ml two neck Schlenk flask and fitted with a reflux condenser. The system was evacuated and purged with N₂. Freshly distilled mesitylene (30 ml) was added under N₂ atmosphere. The reaction mixture was heated to 403K under N₂ for 6 h and allowed to cool to room temperature. The mesitylene was removed by vacuum distillation and the solid mixture was washed with hexane, chromatographed on silicagel using dichloromethane and hexane as eluent to obtain white color solid of mono substituted [Phpy(CO)₃Re(μ -TeC₆H₅)₂Re(CO)₄] (61 mg, 27% (based on Re₂(CO)₁₀) compound. Single crystals of the title compound were obtained by slow diffusion of hexane into a concentrated solution of the title compound in dichloromethane at 278K.

Refinement

The hydrogen atoms were placed in calculated positions (C-H = 0.95 Å) and included in the refinement in riding-model approximation with U_{iso}(H) = 1.2U_{eq}(C). Restraints were applied to the anisotropic displacement parameters of atoms C3 and C18 using the ISOR command in SHELXL-97 (Sheldrick, 2008). The need to restrain these parameters and the presence of some larger positive and lower negative density peaks in the difference Fourier may indicate the lowered precision of the structure.

Figures

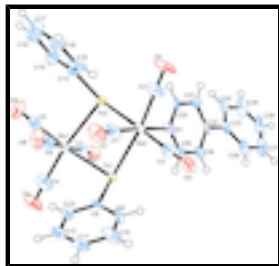


Fig. 1. : The molecular structure of title compound, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

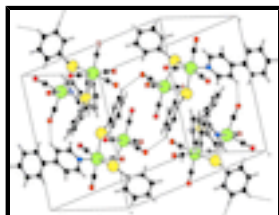


Fig. 2. : Part of the crystal structure of the title compound showing weak C-H...O interactions as dashed lines.

Heptacarbonyl-1 κ^3 C,2 κ^4 C-(4-phenylpyridine-1 κ N)di- μ -phenyltellurido-1:2 κ^4 Te:Te-dirhenium(I)

Crystal data

[Re₂(C₆H₅Te)₂(C₁₁H₉N)(CO)₇]

$M_r = 1133.06$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 18.549 (2) \text{ \AA}$

$b = 12.3624 (12) \text{ \AA}$

$c = 13.7768 (11) \text{ \AA}$

$\beta = 92.927 (9)^\circ$

$V = 3155.0 (5) \text{ \AA}^3$

$Z = 4$

$F(000) = 2064$

$D_x = 2.385 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 4169 reflections

$\theta = 3.0\text{--}32.8^\circ$

$\mu = 9.53 \text{ mm}^{-1}$

$T = 150 \text{ K}$

Plate, yellow

$0.23 \times 0.18 \times 0.15 \text{ mm}$

Data collection

Oxford Diffraction Xcalibur-S diffractometer

Radiation source: fine-focus sealed tube graphite

Detector resolution: 0 pixels mm^{-1}

ω scans

Absorption correction: multi-scan (*Crys.Alis Pro*; Oxford Diffraction, 2009)

$T_{\min} = 0.218$, $T_{\max} = 0.329$

22729 measured reflections

5553 independent reflections

4237 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.098$

$\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 3.0^\circ$

$h = -22 \rightarrow 22$

$k = -14 \rightarrow 14$

$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.058$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.135$	H-atom parameters constrained
$S = 1.03$	$w = 1/[\sigma^2(F_o^2) + (0.0776P)^2]$
5553 reflections	where $P = (F_o^2 + 2F_c^2)/3$
379 parameters	$(\Delta/\sigma)_{\max} < 0.001$
12 restraints	$\Delta\rho_{\max} = 2.25 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\min} = -3.27 \text{ e } \text{\AA}^{-3}$

Special details

Experimental. Mean plane calculation for molecule m1 = -0.11114(0.00018) m2 = 0.99346(0.00000) m3 = -0.02622(0.00031) D = 1.07228(0.00135) Atom d s/d/s (d/s)**2 Re1 * -0.1293 0.0005 -256.403 65742.445 Te1 * 0.2845 0.0008 379.024 143659.391 Re2 * -0.1290 0.0005 -255.731 65398.523 Te2 * 0.2873 0.0008 382.870 146589.250 ===== Sum((d/s)**2) for starred atoms 421389.625 Chi-squared at 95% for 1 degrees of freedom: 3.84 The group of atoms deviates significantly from planarity

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Re1	0.40209 (3)	0.14784 (4)	0.15533 (4)	0.02636 (17)
Re2	0.18223 (3)	0.11194 (4)	0.19775 (4)	0.02389 (16)
Te1	0.30828 (5)	0.16925 (6)	0.30588 (6)	0.0238 (2)
Te2	0.27148 (5)	0.15735 (6)	0.04687 (6)	0.0243 (2)
O1	0.2230 (6)	-0.1266 (8)	0.2217 (9)	0.054 (3)
O2	0.0593 (6)	0.0574 (9)	0.0498 (8)	0.059 (3)
O3	0.0858 (6)	0.0750 (11)	0.3700 (8)	0.059 (3)
O4	0.5334 (7)	0.1542 (11)	0.2999 (10)	0.070 (4)
O5	0.4940 (7)	0.1321 (9)	-0.0267 (9)	0.061 (3)
O6	0.3823 (6)	-0.1045 (8)	0.1626 (9)	0.050 (3)
O7	0.4133 (7)	0.3982 (8)	0.1504 (9)	0.056 (3)
N1	0.1553 (6)	0.2867 (8)	0.1910 (8)	0.027 (2)
C1	0.2085 (8)	-0.0355 (12)	0.2112 (10)	0.037 (4)
C2	0.1057 (8)	0.0777 (10)	0.1053 (10)	0.035 (3)

supplementary materials

C3	0.1248 (8)	0.0915 (11)	0.3036 (10)	0.036 (3)
C4	0.4859 (10)	0.1496 (12)	0.2468 (14)	0.054 (5)
C5	0.4597 (8)	0.1355 (12)	0.0427 (13)	0.043 (4)
C6	0.3904 (8)	-0.0134 (12)	0.1619 (10)	0.035 (3)
C7	0.4075 (8)	0.3054 (13)	0.1500 (11)	0.041 (4)
C8	0.3253 (7)	0.0368 (10)	0.4021 (9)	0.027 (3)
C9	0.2741 (7)	0.0131 (11)	0.4646 (10)	0.033 (3)
H9	0.2316	0.0561	0.4635	0.040*
C10	0.2808 (9)	-0.0711 (11)	0.5302 (12)	0.050 (4)
H10	0.2425	-0.0868	0.5713	0.060*
C11	0.3421 (9)	-0.1317 (11)	0.5362 (11)	0.039 (4)
H11	0.3477	-0.1889	0.5820	0.047*
C12	0.3957 (9)	-0.1080 (13)	0.4742 (11)	0.046 (4)
H12	0.4383	-0.1507	0.4770	0.055*
C13	0.3897 (8)	-0.0239 (13)	0.4079 (10)	0.043 (4)
H13	0.4281	-0.0076	0.3672	0.052*
C14	0.2771 (8)	0.0159 (11)	-0.0427 (10)	0.035 (4)
C15	0.3222 (8)	0.0223 (11)	-0.1190 (11)	0.042 (4)
H15	0.3506	0.0853	-0.1277	0.050*
C16	0.3259 (9)	-0.0641 (12)	-0.1833 (12)	0.056 (5)
H16	0.3559	-0.0597	-0.2370	0.067*
C17	0.2861 (10)	-0.1558 (12)	-0.1689 (13)	0.057 (5)
H17	0.2890	-0.2152	-0.2122	0.069*
C18	0.2416 (9)	-0.1620 (13)	-0.0915 (11)	0.046 (4)
H18	0.2149	-0.2264	-0.0819	0.055*
C19	0.2352 (8)	-0.0755 (10)	-0.0272 (10)	0.038 (4)
H19	0.2035	-0.0788	0.0248	0.045*
C20	0.1244 (6)	0.3322 (10)	0.1087 (10)	0.026 (3)
H20	0.1192	0.2883	0.0522	0.031*
C21	0.1002 (7)	0.4378 (11)	0.1022 (9)	0.029 (3)
H21	0.0786	0.4650	0.0431	0.034*
C22	0.1083 (7)	0.5032 (10)	0.1837 (10)	0.029 (3)
C23	0.0838 (7)	0.6196 (11)	0.1818 (11)	0.034 (3)
C24	0.0800 (8)	0.6762 (11)	0.0980 (12)	0.041 (4)
H24	0.0946	0.6434	0.0398	0.049*
C25	0.0545 (9)	0.7831 (12)	0.0961 (15)	0.055 (5)
H25	0.0525	0.8218	0.0364	0.066*
C26	0.0331 (9)	0.8316 (13)	0.1762 (16)	0.062 (5)
H26	0.0148	0.9034	0.1733	0.074*
C27	0.0379 (8)	0.7761 (11)	0.2643 (15)	0.051 (5)
H27	0.0245	0.8100	0.3226	0.061*
C28	0.0629 (7)	0.6686 (12)	0.2650 (13)	0.042 (4)
H28	0.0653	0.6293	0.3243	0.051*
C29	0.1396 (7)	0.4570 (11)	0.2687 (10)	0.035 (3)
H29	0.1453	0.4986	0.3266	0.042*
C30	0.1617 (7)	0.3514 (10)	0.2676 (10)	0.029 (3)
H30	0.1833	0.3225	0.3260	0.035*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Re1	0.0206 (3)	0.0269 (3)	0.0314 (3)	0.0006 (2)	-0.0005 (2)	-0.0038 (2)
Re2	0.0181 (3)	0.0254 (3)	0.0274 (3)	0.0002 (2)	-0.0063 (2)	0.0062 (2)
Te1	0.0187 (5)	0.0269 (4)	0.0250 (4)	0.0050 (3)	-0.0060 (4)	-0.0009 (3)
Te2	0.0294 (5)	0.0198 (4)	0.0231 (4)	0.0002 (3)	-0.0042 (4)	-0.0009 (3)
O1	0.056 (8)	0.029 (6)	0.077 (8)	0.001 (5)	-0.014 (7)	0.017 (5)
O2	0.053 (7)	0.054 (7)	0.065 (7)	-0.020 (6)	-0.042 (6)	0.011 (6)
O3	0.028 (6)	0.098 (10)	0.052 (7)	0.000 (6)	-0.002 (5)	0.028 (7)
O4	0.040 (8)	0.094 (10)	0.074 (9)	0.000 (7)	-0.033 (7)	0.002 (7)
O5	0.068 (9)	0.058 (8)	0.062 (8)	0.001 (6)	0.032 (7)	-0.010 (6)
O6	0.048 (7)	0.024 (6)	0.078 (8)	0.000 (5)	0.013 (6)	0.001 (5)
O7	0.069 (9)	0.027 (6)	0.070 (8)	-0.012 (5)	0.000 (7)	-0.003 (5)
N1	0.028 (6)	0.017 (5)	0.035 (6)	0.001 (5)	-0.007 (5)	0.002 (5)
C1	0.027 (8)	0.038 (9)	0.044 (9)	-0.007 (6)	-0.008 (7)	0.018 (7)
C2	0.040 (9)	0.020 (7)	0.044 (8)	-0.008 (6)	-0.011 (7)	0.020 (6)
C3	0.036 (3)	0.037 (3)	0.037 (3)	0.0004 (10)	0.0015 (10)	0.0002 (10)
C4	0.052 (12)	0.035 (9)	0.072 (12)	-0.001 (8)	-0.015 (10)	-0.002 (8)
C5	0.024 (8)	0.039 (9)	0.065 (11)	-0.003 (6)	-0.012 (8)	-0.007 (8)
C6	0.030 (9)	0.040 (9)	0.034 (8)	-0.005 (6)	-0.006 (7)	-0.004 (7)
C7	0.023 (8)	0.051 (10)	0.047 (9)	-0.010 (7)	-0.002 (7)	-0.022 (8)
C8	0.023 (7)	0.033 (7)	0.022 (6)	0.001 (6)	-0.013 (6)	-0.004 (6)
C9	0.009 (7)	0.036 (8)	0.054 (9)	0.007 (6)	0.001 (7)	0.005 (7)
C10	0.049 (10)	0.031 (8)	0.068 (11)	-0.014 (7)	-0.026 (9)	0.023 (8)
C11	0.050 (10)	0.030 (8)	0.035 (8)	0.000 (7)	-0.020 (8)	0.007 (6)
C12	0.044 (10)	0.054 (10)	0.038 (9)	0.021 (8)	-0.017 (8)	0.002 (7)
C13	0.036 (9)	0.058 (10)	0.037 (8)	0.009 (8)	0.009 (7)	0.002 (7)
C14	0.045 (10)	0.032 (8)	0.027 (7)	0.014 (7)	-0.015 (7)	-0.005 (6)
C15	0.041 (10)	0.029 (8)	0.054 (10)	0.002 (7)	-0.012 (8)	-0.003 (7)
C16	0.062 (12)	0.037 (9)	0.065 (11)	0.014 (8)	-0.027 (9)	-0.029 (8)
C17	0.070 (13)	0.036 (9)	0.064 (12)	0.018 (9)	-0.016 (10)	-0.026 (8)
C18	0.046 (4)	0.045 (4)	0.046 (4)	0.0000 (10)	0.0019 (10)	-0.0002 (10)
C19	0.054 (10)	0.022 (7)	0.034 (8)	-0.006 (7)	-0.028 (7)	0.006 (6)
C20	0.007 (6)	0.035 (7)	0.037 (8)	0.006 (5)	0.004 (6)	0.004 (6)
C21	0.025 (8)	0.041 (8)	0.020 (6)	-0.004 (6)	-0.002 (6)	0.002 (6)
C22	0.009 (7)	0.024 (6)	0.054 (9)	0.006 (5)	0.001 (6)	0.002 (6)
C23	0.011 (7)	0.043 (8)	0.047 (9)	-0.005 (6)	-0.001 (6)	0.000 (7)
C24	0.021 (8)	0.039 (8)	0.063 (10)	0.007 (6)	0.004 (7)	0.012 (8)
C25	0.040 (10)	0.035 (9)	0.092 (14)	0.002 (8)	0.019 (10)	0.013 (9)
C26	0.033 (10)	0.035 (9)	0.119 (17)	0.011 (7)	0.022 (11)	0.016 (11)
C27	0.030 (9)	0.027 (8)	0.097 (14)	0.003 (7)	0.012 (9)	-0.020 (9)
C28	0.013 (7)	0.049 (9)	0.066 (11)	-0.010 (6)	0.007 (7)	0.005 (8)
C29	0.021 (7)	0.037 (8)	0.046 (8)	0.010 (6)	-0.009 (7)	-0.006 (7)
C30	0.016 (7)	0.030 (7)	0.040 (8)	0.002 (5)	-0.002 (6)	-0.004 (6)

supplementary materials

Geometric parameters (Å, °)

Re1—C5	1.935 (18)	C13—H13	0.9500
Re1—C4	1.951 (18)	C14—C15	1.38 (2)
Re1—C7	1.951 (16)	C14—C19	1.39 (2)
Re1—C6	2.007 (15)	C15—C16	1.391 (19)
Re1—Te2	2.7832 (11)	C15—H15	0.9500
Re1—Te1	2.7872 (10)	C16—C17	1.37 (2)
Re2—C3	1.867 (15)	C16—H16	0.9500
Re2—C1	1.894 (15)	C17—C18	1.38 (2)
Re2—C2	1.906 (14)	C17—H17	0.9500
Re2—N1	2.218 (10)	C18—C19	1.40 (2)
Re2—Te2	2.7799 (11)	C18—H18	0.9500
Re2—Te1	2.7986 (10)	C19—H19	0.9500
Te1—C8	2.120 (13)	C20—C21	1.382 (18)
Te2—C14	2.145 (13)	C20—H20	0.9500
O1—C1	1.164 (16)	C21—C22	1.385 (18)
O2—C2	1.149 (16)	C21—H21	0.9500
O3—C3	1.212 (17)	C22—C29	1.402 (18)
O4—C4	1.117 (19)	C22—C23	1.509 (18)
O5—C5	1.175 (19)	C23—C24	1.35 (2)
O6—C6	1.136 (16)	C23—C28	1.37 (2)
O7—C7	1.152 (18)	C24—C25	1.40 (2)
N1—C30	1.325 (16)	C24—H24	0.9500
N1—C20	1.365 (16)	C25—C26	1.33 (2)
C8—C9	1.346 (18)	C25—H25	0.9500
C8—C13	1.410 (19)	C26—C27	1.39 (2)
C9—C10	1.380 (18)	C26—H26	0.9500
C9—H9	0.9500	C27—C28	1.41 (2)
C10—C11	1.36 (2)	C27—H27	0.9500
C10—H10	0.9500	C28—H28	0.9500
C11—C12	1.37 (2)	C29—C30	1.369 (18)
C11—H11	0.9500	C29—H29	0.9500
C12—C13	1.38 (2)	C30—H30	0.9500
C12—H12	0.9500		
C5—Re1—C4	93.7 (7)	C11—C12—C13	122.3 (14)
C5—Re1—C7	90.9 (6)	C11—C12—H12	118.9
C4—Re1—C7	88.4 (6)	C13—C12—H12	118.9
C5—Re1—C6	91.3 (6)	C12—C13—C8	118.4 (14)
C4—Re1—C6	93.8 (6)	C12—C13—H13	120.8
C7—Re1—C6	176.7 (6)	C8—C13—H13	120.8
C5—Re1—Te2	94.3 (4)	C15—C14—C19	121.9 (13)
C4—Re1—Te2	171.7 (6)	C15—C14—Te2	116.2 (11)
C7—Re1—Te2	89.0 (4)	C19—C14—Te2	121.9 (11)
C6—Re1—Te2	88.5 (4)	C14—C15—C16	119.5 (15)
C5—Re1—Te1	174.8 (4)	C14—C15—H15	120.3
C4—Re1—Te1	91.4 (6)	C16—C15—H15	120.3
C7—Re1—Te1	88.2 (4)	C17—C16—C15	119.9 (17)

C6—Re1—Te1	89.3 (4)	C17—C16—H16	120.1
Te2—Re1—Te1	80.57 (3)	C15—C16—H16	120.1
C3—Re2—C1	87.0 (6)	C16—C17—C18	120.3 (15)
C3—Re2—C2	93.2 (6)	C16—C17—H17	119.9
C1—Re2—C2	91.8 (6)	C18—C17—H17	119.9
C3—Re2—N1	91.6 (5)	C17—C18—C19	121.3 (15)
C1—Re2—N1	176.3 (5)	C17—C18—H18	119.4
C2—Re2—N1	91.7 (5)	C19—C18—H18	119.4
C3—Re2—Te2	175.5 (4)	C14—C19—C18	117.2 (15)
C1—Re2—Te2	96.2 (4)	C14—C19—H19	121.4
C2—Re2—Te2	89.8 (4)	C18—C19—H19	121.4
N1—Re2—Te2	85.1 (3)	N1—C20—C21	124.3 (12)
C3—Re2—Te1	96.5 (4)	N1—C20—H20	117.8
C1—Re2—Te1	89.3 (4)	C21—C20—H20	117.8
C2—Re2—Te1	170.3 (4)	C20—C21—C22	118.5 (12)
N1—Re2—Te1	87.5 (3)	C20—C21—H21	120.8
Te2—Re2—Te1	80.42 (3)	C22—C21—H21	120.8
C8—Te1—Re1	108.3 (4)	C21—C22—C29	117.6 (12)
C8—Te1—Re2	103.4 (3)	C21—C22—C23	121.5 (12)
Re1—Te1—Re2	96.67 (3)	C29—C22—C23	120.9 (12)
C14—Te2—Re2	108.3 (4)	C24—C23—C28	118.8 (14)
C14—Te2—Re1	102.0 (4)	C24—C23—C22	120.8 (14)
Re2—Te2—Re1	97.20 (3)	C28—C23—C22	120.4 (14)
C30—N1—C20	115.4 (11)	C23—C24—C25	120.6 (16)
C30—N1—Re2	123.0 (8)	C23—C24—H24	119.7
C20—N1—Re2	121.3 (8)	C25—C24—H24	119.7
O1—C1—Re2	177.8 (14)	C26—C25—C24	121.4 (17)
O2—C2—Re2	179.7 (16)	C26—C25—H25	119.3
O3—C3—Re2	177.2 (13)	C24—C25—H25	119.3
O4—C4—Re1	177.6 (15)	C25—C26—C27	119.4 (15)
O5—C5—Re1	177.4 (14)	C25—C26—H26	120.3
O6—C6—Re1	177.6 (13)	C27—C26—H26	120.3
O7—C7—Re1	176.7 (13)	C26—C27—C28	118.6 (16)
C9—C8—C13	118.1 (12)	C26—C27—H27	120.7
C9—C8—Te1	118.8 (9)	C28—C27—H27	120.7
C13—C8—Te1	123.0 (10)	C23—C28—C27	121.3 (16)
C8—C9—C10	122.7 (13)	C23—C28—H28	119.4
C8—C9—H9	118.6	C27—C28—H28	119.4
C10—C9—H9	118.6	C30—C29—C22	119.4 (13)
C11—C10—C9	120.1 (16)	C30—C29—H29	120.3
C11—C10—H10	119.9	C22—C29—H29	120.3
C9—C10—H10	119.9	N1—C30—C29	124.8 (13)
C10—C11—C12	118.3 (14)	N1—C30—H30	117.6
C10—C11—H11	120.9	C29—C30—H30	117.6
C12—C11—H11	120.9		
C5—Re1—Te1—C8	132 (5)	C7—Re1—C4—O4	19 (44)
C4—Re1—Te1—C8	-58.8 (6)	C6—Re1—C4—O4	-158 (44)
C7—Re1—Te1—C8	-147.2 (5)	Te2—Re1—C4—O4	-53 (46)
C6—Re1—Te1—C8	35.0 (5)	Te1—Re1—C4—O4	-69 (44)

supplementary materials

Te2—Re1—Te1—C8	123.5 (3)	C4—Re1—C5—O5	-110 (30)
C5—Re1—Te1—Re2	26 (5)	C7—Re1—C5—O5	-22 (30)
C4—Re1—Te1—Re2	-165.3 (5)	C6—Re1—C5—O5	156 (30)
C7—Re1—Te1—Re2	106.4 (4)	Te2—Re1—C5—O5	68 (30)
C6—Re1—Te1—Re2	-71.5 (4)	Te1—Re1—C5—O5	59 (32)
Te2—Re1—Te1—Re2	17.05 (3)	C5—Re1—C6—O6	-69 (33)
C3—Re2—Te1—C8	55.6 (6)	C4—Re1—C6—O6	-163 (33)
C1—Re2—Te1—C8	-31.3 (6)	C7—Re1—C6—O6	65 (38)
C2—Re2—Te1—C8	-128 (2)	Te2—Re1—C6—O6	25 (33)
N1—Re2—Te1—C8	146.9 (5)	Te1—Re1—C6—O6	106 (33)
Te2—Re2—Te1—C8	-127.7 (4)	C5—Re1—C7—O7	-101 (25)
C3—Re2—Te1—Re1	166.2 (4)	C4—Re1—C7—O7	-7(24)
C1—Re2—Te1—Re1	79.3 (4)	C6—Re1—C7—O7	125 (22)
C2—Re2—Te1—Re1	-17 (2)	Te2—Re1—C7—O7	165 (25)
N1—Re2—Te1—Re1	-102.5 (3)	Te1—Re1—C7—O7	85 (24)
Te2—Re2—Te1—Re1	-17.08 (3)	Re1—Te1—C8—C9	-162.0 (9)
C3—Re2—Te2—C14	169 (6)	Re2—Te1—C8—C9	-60.2 (10)
C1—Re2—Te2—C14	34.1 (6)	Re1—Te1—C8—C13	21.8 (12)
C2—Re2—Te2—C14	-57.7 (5)	Re2—Te1—C8—C13	123.6 (11)
N1—Re2—Te2—C14	-149.4 (5)	C13—C8—C9—C10	-3(2)
Te1—Re2—Te2—C14	122.3 (4)	Te1—C8—C9—C10	-179.6 (11)
C3—Re2—Te2—Re1	64 (6)	C8—C9—C10—C11	2(2)
C1—Re2—Te2—Re1	-71.1 (4)	C9—C10—C11—C12	-1(2)
C2—Re2—Te2—Re1	-162.9 (4)	C10—C11—C12—C13	1(2)
N1—Re2—Te2—Re1	105.4 (3)	C11—C12—C13—C8	-2(2)
Te1—Re2—Te2—Re1	17.13 (3)	C9—C8—C13—C12	3(2)
C5—Re1—Te2—C14	53.1 (6)	Te1—C8—C13—C12	179.1 (10)
C4—Re1—Te2—C14	-144 (3)	Re2—Te2—C14—C15	-177.0 (9)
C7—Re1—Te2—C14	144.0 (6)	Re1—Te2—C14—C15	-75.1 (10)
C6—Re1—Te2—C14	-38.1 (6)	Re2—Te2—C14—C19	5.7 (12)
Te1—Re1—Te2—C14	-127.7 (4)	Re1—Te2—C14—C19	107.6 (11)
C5—Re1—Te2—Re2	163.6 (4)	C19—C14—C15—C16	1(2)
C4—Re1—Te2—Re2	-34 (3)	Te2—C14—C15—C16	-176.7 (11)
C7—Re1—Te2—Re2	-105.5 (4)	C14—C15—C16—C17	-2(2)
C6—Re1—Te2—Re2	72.4 (4)	C15—C16—C17—C18	1(2)
Te1—Re1—Te2—Re2	-17.19 (3)	C16—C17—C18—C19	1(3)
C3—Re2—N1—C30	51.4 (11)	C15—C14—C19—C18	1(2)
C1—Re2—N1—C30	-16 (9)	Te2—C14—C19—C18	178.3 (10)
C2—Re2—N1—C30	144.6 (11)	C17—C18—C19—C14	-2(2)
Te2—Re2—N1—C30	-125.7 (10)	C30—N1—C20—C21	-0.4 (19)
Te1—Re2—N1—C30	-45.1 (10)	Re2—N1—C20—C21	173.8 (10)
C3—Re2—N1—C20	-122.5 (10)	N1—C20—C21—C22	1(2)
C1—Re2—N1—C20	170 (8)	C20—C21—C22—C29	-1.1 (18)
C2—Re2—N1—C20	-29.2 (11)	C20—C21—C22—C23	179.4 (12)
Te2—Re2—N1—C20	60.5 (9)	C21—C22—C23—C24	-26.1 (19)
Te1—Re2—N1—C20	141.1 (10)	C29—C22—C23—C24	154.5 (14)
C3—Re2—C1—O1	7(36)	C21—C22—C23—C28	151.8 (13)
C2—Re2—C1—O1	-86 (36)	C29—C22—C23—C28	-27.6 (19)
N1—Re2—C1—O1	75 (38)	C28—C23—C24—C25	0(2)

Te2—Re2—C1—O1	-176 (100)	C22—C23—C24—C25	177.5 (13)
Te1—Re2—C1—O1	104 (36)	C23—C24—C25—C26	0(2)
C3—Re2—C2—O2	58 (100)	C24—C25—C26—C27	2(3)
C1—Re2—C2—O2	145 (100)	C25—C26—C27—C28	-2(2)
N1—Re2—C2—O2	-34 (100)	C24—C23—C28—C27	0(2)
Te2—Re2—C2—O2	-119 (100)	C22—C23—C28—C27	-178.1 (13)
Te1—Re2—C2—O2	-119 (100)	C26—C27—C28—C23	1(2)
C1—Re2—C3—O3	-62 (27)	C21—C22—C29—C30	1.1 (19)
C2—Re2—C3—O3	30 (27)	C23—C22—C29—C30	-179.5 (12)
N1—Re2—C3—O3	122 (27)	C20—N1—C30—C29	0.4 (19)
Te2—Re2—C3—O3	163 (22)	Re2—N1—C30—C29	-173.7 (11)
Te1—Re2—C3—O3	-151 (27)	C22—C29—C30—N1	-1(2)
C5—Re1—C4—O4	110 (44)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C16—H16 \cdots O4 ⁱ	0.95	2.55	3.33 (2)	139
C11—H11 \cdots O4 ⁱⁱ	0.95	2.71	3.160 (18)	110
C17—H17 \cdots O1 ⁱⁱⁱ	0.95	2.46	3.271 (19)	144
C26—H26 \cdots O2 ^{iv}	0.95	2.71	3.34 (2)	124
C21—H21 \cdots O3 ^v	0.95	2.45	3.200 (16)	136
C29—H29 \cdots Cg ^{vi}	0.95	2.79	3.378 (15)	121

Symmetry codes: (i) $-x+1, -y, -z$; (ii) $-x+1, -y, -z+1$; (iii) $x, -y-1/2, z-1/2$; (iv) $x, y+1, z$; (v) $x, -y+1/2, z-1/2$; (vi) $x, -y+1/2, z+1/2$.

Fig. 1

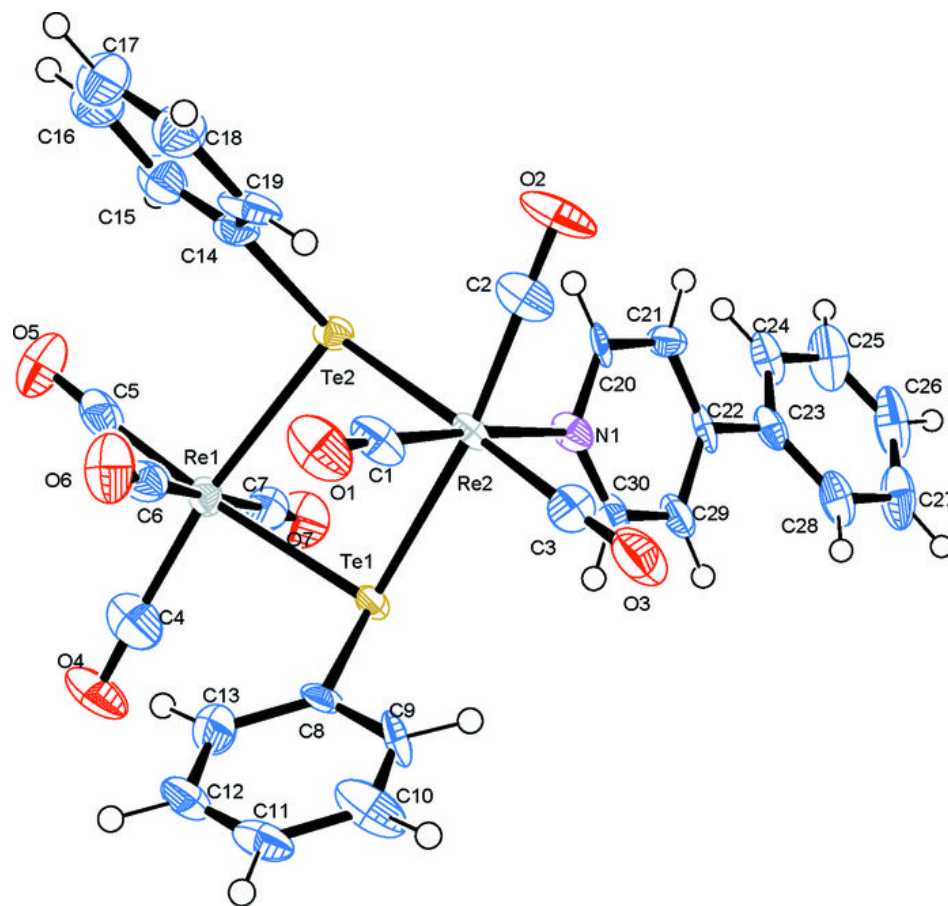


Fig. 2

