

C22	0.3337 (9)	0.0626 (8)	0.0876 (5)	4.00 (22)*
C23	0.393 (1)	0.0707 (9)	0.0327 (6)	5.57 (28)*
C24	0.341 (1)	0.0994 (9)	-0.0290 (6)	5.42 (26)*
C25	0.233 (1)	0.1225 (9)	-0.0375 (6)	4.78 (25)*
C26	0.1724 (9)	0.1171 (7)	0.0170 (5)	3.78 (21)*
C31	0.1095 (7)	-0.0578 (6)	0.1432 (4)	2.52 (16)*
C32	0.1110 (8)	-0.1084 (7)	0.0830 (5)	3.62 (19)*
C33	0.0887 (9)	-0.2036 (9)	0.0809 (6)	4.57 (24)*
C34	0.062 (1)	-0.2524 (9)	0.1361 (6)	5.10 (26)*
C35	0.057 (1)	-0.202 (1)	0.1959 (7)	6.01 (30)*
C36	0.0812 (9)	-0.1048 (9)	0.2000 (6)	4.65 (23)*
C41	0.4543 (8)	0.1532 (7)	0.3857 (5)	3.04 (18)*
C42	0.4760 (9)	0.1731 (7)	0.4539 (5)	3.52 (19)*
C43	0.5540 (9)	0.2427 (8)	0.4760 (6)	4.63 (24)*
C44	0.609 (1)	0.2863 (9)	0.4325 (6)	5.33 (27)*
C45	0.593 (1)	0.265 (1)	0.3641 (7)	6.92 (34)*
C46	0.512 (1)	0.197 (1)	0.3411 (6)	5.66 (29)*
C51	0.2725 (8)	0.0455 (7)	0.4230 (5)	3.11 (18)*
C52	0.188 (1)	0.1099 (9)	0.4283 (6)	4.90 (25)*
C53	0.126 (1)	0.101 (1)	0.4812 (6)	5.24 (25)*
C54	0.145 (1)	0.0262 (9)	0.5256 (6)	4.97 (25)*
C55	0.225 (1)	-0.0381 (9)	0.5202 (6)	4.69 (24)*
C56	0.2903 (8)	-0.0281 (7)	0.4687 (5)	3.38 (19)*
C61	0.4333 (8)	-0.0462 (7)	0.3506 (5)	3.23 (18)*
C62	0.374 (1)	-0.1254 (8)	0.3229 (5)	4.65 (24)*
C63	0.424 (1)	-0.2133 (9)	0.3200 (6)	5.11 (26)*
C64	0.534 (1)	-0.219 (1)	0.3430 (6)	5.93 (30)*
C65	0.593 (1)	-0.1430 (9)	0.3679 (6)	5.47 (28)*
C66	0.541 (1)	-0.0565 (9)	0.3733 (6)	4.83 (25)*

*Refined isotropically.

Table 2. Selected bond distances (Å) and angles (°)

Au1—P1	2.290 (2)	P2—C61	1.81 (1)
Au1—P2	2.300 (2)	N1—C1	1.14 (2)
Au1—N1	2.726 (11)	N2—C2	1.12 (2)
P1—C11	1.805 (9)	N3—C3	1.16 (2)
P1—C21	1.81 (1)	C1—C4	1.38 (2)
P1—C31	1.806 (9)	C2—C4	1.44 (2)
P2—C41	1.81 (1)	C3—C4	1.39 (2)
P2—C51	1.81 (1)		
P1—Au1—P2	161.23 (9)	C41—P2—C51	105.2 (4)
Au1—P1—C11	116.9 (3)	C41—P2—C61	106.4 (5)
Au1—P1—C21	113.0 (3)	C51—P2—C61	106.4 (5)
Au1—P1—C31	108.8 (3)	N1—C1—C4	177. (2)
C11—P1—C21	106.1 (4)	N2—C2—C4	177. (2)
C11—P1—C31	107.3 (4)	N3—C3—C4	179. (2)
C21—P1—C31	103.8 (5)	C1—C4—C2	120. (1)
Au1—P2—C41	116.8 (3)	C1—C4—C3	118. (1)
Au1—P2—C51	111.0 (3)	C2—C4—C3	122. (1)
Au1—P2—C61	110.3 (3)		

The title compound was synthesized by reacting 0.2008 g (0.27 mmol) Au(PPh₃)₂Cl with 0.2251 g (3.81 mmol) potassium tricyanomethanide (KTCM) in CH₂Cl₂ (DCM) overnight. 0.1884 g (0.23 mmol, yield 86%) ivory precipitate of Au(PPh₃)₂TCM was formed by adding a large amount of diethyl ether (Et₂O) to the reaction solution. Colorless crystals of Au(PPh₃)₂TCM were grown from DCM/Et₂O mixed solvents. The structure was solved by Patterson methods using *Personal SDP* (B. A. Frenz & Associates, Inc., 1989). H atoms were placed at idealized positions; these were included in the structure-factor calculations but not in the least-squares calculations. All calculations were carried out on a 80386-based IBM-compatible PC.

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55409 (31 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HA1016]

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Structure of the Tetrakis(2,2',5,5'-tetra-thiafulvalene) Hexatungstate Acetonitrile Solvate Salt (TTF)₄W₆O₁₉·0.5(CH₃CN)

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Abstract

The organic lattice is built from two different TTF chains which develop along the [010] direction. Each chain is formed by dimers separated by isolated molecules. Short intradimer S...S contacts [S1...S4 3.416 (7), S2...S3 3.411 (7), S11...S11 3.430 (7), S12...S12 3.446 (8), S13...S13 3.464 (9), S14...S14 3.338 (8) Å] and short anion-cation contacts [O2...S1 2.87 (1), O6...S4 2.86 (1), O16...S16 3.16 (2) Å] are observed.

Comment

The crystal structure represented in Fig. 2 is built from two discrete W₆O₁₉²⁻ units, two different organic chains and two isolated TTF molecules. The geometrical parameters of the two W₆O₁₉²⁻ units are very similar and compare well with those found in other radical cation salts containing W₆O₁₉²⁻, for example (TMTTF)₂W₆O₁₉ (Triki, Ouahab, Grandjean & Fabre, 1991) and (TTF)₃W₆O₁₉ (Triki,

Ouahab, Halet, Peña, Padiou, Grandjean, Garrigou-Lagrange & Delhaes, 1992). The organic lattice is built from six TTF molecules. The molecules (*A*, *C*) and (*D*, *E*) stack to form two different chains which develop along the [010] direction. The *B* and *F* molecules are orthogonal to these chains (see Fig. 2).

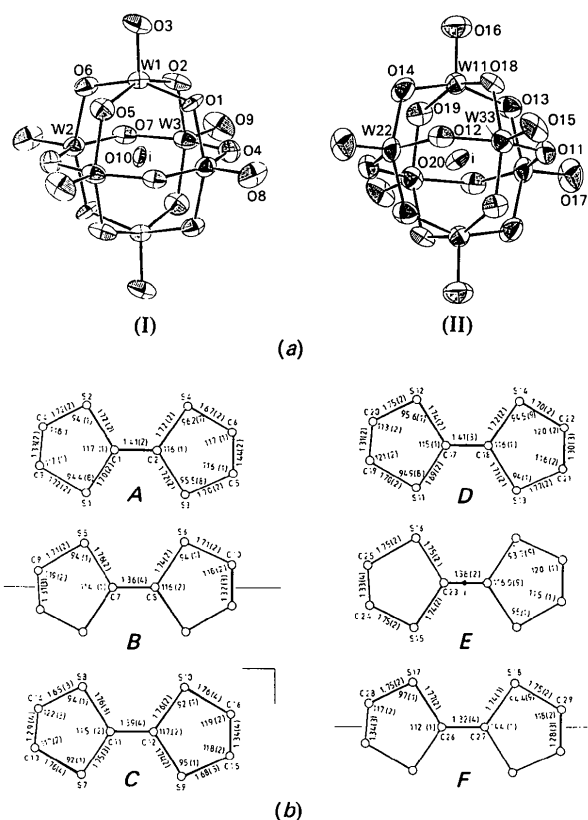


Fig. 1. (a) Atomic numbering for anions (I) and (II). (b) Bond distances (Å) and selected bond angles (°) for the TTF molecules.

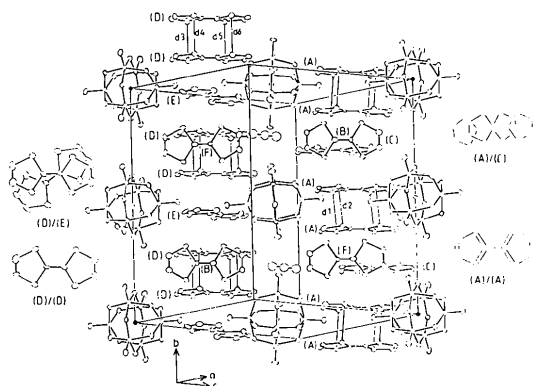


Fig. 2. Projection of the crystal structure showing the overlap between TTF molecules and the shortest contacts between heteroatoms [$d_1(S1^I-S4^{II}) = 3.416$ (7), $d_2(S2^I-S3^{II}) = 3.411$ (7), $d_3(S11^I-S11^{III}) = 3.430$ (7), $d_4(S12^I-S12^{III}) = 3.446$ (8), $d_5(S13^I-S13^{III}) = 3.464$ (9), $d_6(S14^I-S14^{III}) = 3.338$ (8) Å, symmetry code: (i) x, y, z ; (ii) $1-x, 1-y, -z$; (iii) $x, \frac{1}{2}-y, z$].

The organic stack is not regular; it can be described as being formed by dimers (*AA* and *DD*) separated by isolated molecules (*C* and *E* respectively). The intradimer overlaps are of the eclipsed type (*A/A* or *D/D*), while the overlaps between the dimer and the isolated TTF are of the ring-to-double-bond type (*A/C*) or a criss-cross like (*D/E*). The intradimer S...S contacts range between 3.33 and 3.47 Å. Short O...S anion-cation interactions are also observed [$O2\cdots S1 = 2.875$ (11), $O6\cdots S4 = 2.859$ (11) and $O16\cdots S16 = 3.157$ (13) Å, corresponding van der Waals distance 3.25 Å].

Experimental

Crystal data

[C₆S₄H₄]₄[W₆O₁₉].0.5C₂H₃N
 $M_r = 2262.50$
 Monoclinic
 $P2_1/m$
 $a = 14.399$ (6) Å
 $b = 20.51$ (2) Å
 $c = 16.817$ (5) Å
 $\beta = 100.75$ (3)°
 $V = 4879$ Å³
 $Z = 4$
 $D_x = 3.08$ Mg m⁻³

Mo $K\alpha$ radiation
 $\lambda = 0.71073$ Å
 Cell parameters from 25 reflections
 $\theta = 7.5-10^\circ$
 $\mu = 15.128$ mm⁻¹
 $T = 293$ K
 Needles
 $0.5 \times 0.16 \times 0.16$ mm
 Black

Data collection

Enraf-Nonius CAD-4 diffractometer
 $\theta-2\theta$ scans
 Absorption correction: empirical (DIFABS; Walker & Stuart, 1983)
 $T_{\min} = 0.797$, $T_{\max} = 1.250$
 8964 measured reflections
 8636 independent reflections

4010 observed reflections [$I \geq 3\sigma I$]
 $R_{\text{int}} = 0.058$
 $\theta_{\max} = 25^\circ$
 $h = -17 \rightarrow 17$
 $k = 0 \rightarrow 24$
 $l = 0 \rightarrow 20$
 3 standard reflections frequency: 60 min intensity variation: <4%

Refinement

Refinement on F
 Final $R = 0.033$
 $wR = 0.042$
 $S = 1.045$
 4010 reflections
 620 parameters
 H-atom parameters not refined
 $w = 4F_o^2/[\sigma(F)^2 + (0.06F_o)^2]$
 $(\Delta/\sigma)_{\max} = 0.01$

$\Delta\rho_{\max} = 1.461$ e Å⁻³
 $\Delta\rho_{\min} = -1.096$ e Å⁻³
 Extinction coefficient: $g = 1.517 \times 10^{-8}$
 Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. Fractional atomic coordinates and equivalent isotropic thermal parameters (Å²)

$$B_{\text{eq}} = (4/3)\sum_i \sum_j \beta_{ij} a_i a_j$$

Anion (I)	x	y	z	B_{eq}
W1	-0.12725 (4)	0.00241 (4)	0.06718 (4)	2.70 (1)
W2	0.07862 (5)	0.07584 (4)	0.09124 (4)	3.20 (2)
W3	-0.06758 (5)	0.08385 (4)	-0.08422 (4)	3.25 (2)

O1	-0.0410 (7)	0.0641 (6)	0.1262 (6)	3.1 (3)
O2	-0.1562 (7)	0.0704 (6)	-0.0140 (7)	3.9 (3)
O3	-0.2212 (7)	0.0029 (7)	0.1144 (6)	3.9 (3)
O4	0.0089 (8)	0.1281 (6)	0.0053 (7)	3.5 (3)
O5	-0.0473 (8)	-0.0654 (6)	0.1215 (6)	3.7 (3)
O6	-0.1663 (7)	-0.0586 (6)	-0.0194 (6)	3.1 (3)
O7	0.1173 (7)	-0.0070 (6)	0.1385 (6)	3.1 (2)
O8	0.1378 (8)	0.1291 (7)	0.1584 (7)	5.1 (3)
O9	-0.118 (1)	0.1458 (7)	-0.1471 (7)	5.5 (3)
O10	0.0	0.0	0.0	2.4 (3)

Anion (II)

W11	0.40848 (5)	0.49373 (4)	0.60004 (4)	3.32 (2)
W22	0.61658 (6)	0.55581 (4)	0.58820 (5)	3.62 (2)
W33	0.42695 (6)	0.59769 (4)	0.45608 (5)	3.47 (2)
O11	0.5336 (9)	0.6224 (6)	0.5356 (7)	4.1 (3)
O12	0.6513 (8)	0.4655 (7)	0.6054 (6)	4.1 (3)
O13	0.5206 (8)	0.5403 (7)	0.6509 (7)	4.1 (3)
O14	0.3339 (9)	0.4487 (7)	0.5110 (7)	4.5 (3)
O15	0.373 (1)	0.6688 (6)	0.4250 (8)	5.5 (4)
O16	0.3454 (9)	0.4899 (7)	0.6763 (7)	5.3 (4)
O17	0.6998 (9)	0.5963 (8)	0.6556 (9)	6.0 (4)
O18	0.3674 (8)	0.5733 (6)	0.5460 (6)	3.6 (3)
O19	0.4856 (8)	0.4171 (6)	0.6149 (7)	3.7 (3)
O20	0.5	0.5	0.5	2.9 (3)

TTF molecule A

S1	0.3585 (3)	0.5828 (2)	0.0391 (3)	3.3 (1)
S2	0.5471 (3)	0.5819 (3)	0.1395 (3)	3.7 (1)
S3	0.4484 (3)	0.5837 (3)	-0.1215 (3)	3.5 (1)
S4	0.6376 (3)	0.5831 (2)	-0.0226 (3)	3.0 (1)
C1	0.478 (1)	0.5835 (8)	0.044 (1)	3.0 (4)
C2	0.518 (1)	0.5835 (8)	-0.0263 (9)	2.6 (4)
C3	0.366 (1)	0.5835 (9)	0.142 (1)	3.7 (4)
C4	0.452 (1)	0.5833 (8)	0.188 (1)	3.5 (4)
C5	0.540 (1)	0.589 (1)	-0.172 (1)	4.6 (5)
C6	0.633 (1)	0.587 (1)	-0.122 (1)	3.7 (4)

TTF molecule B

S5	0.1827 (4)	0.3217 (3)	0.8155 (3)	4.5 (1)
S6	0.2940 (4)	0.3219 (3)	0.6645 (3)	4.1 (1)
C7	0.219 (2)	0.25	0.773 (1)	3.4 (6)
C8	0.263 (2)	0.25	0.708 (1)	3.8 (6)
C9	0.146 (2)	0.282 (1)	0.893 (1)	6.1 (6)
C10	0.349 (1)	0.282 (1)	0.596 (1)	4.8 (5)

TTF molecule C

S7	0.4083 (5)	0.75	-0.0455 (4)	4.0 (2)
S8	0.5938 (5)	0.75	0.0655 (5)	4.7 (2)
S9	0.2996 (5)	0.75	0.1044 (5)	4.2 (2)
S10	0.4835 (6)	0.75	0.2197 (5)	4.9 (2)
C11	0.470 (2)	0.75	0.054 (2)	3.7 (6)
C12	0.422 (2)	0.75	0.119 (1)	3.4 (6)
C13	0.514 (2)	0.75	-0.085 (2)	5.8 (9)
C14	0.592 (2)	0.75	-0.033 (2)	7 (1)
C15	0.295 (2)	0.75	0.204 (2)	5.1 (8)
C16	0.377 (2)	0.75	0.257 (1)	5.4 (8)

TTF molecule D

S11	0.0723 (3)	0.6664 (3)	0.6346 (3)	4.0 (1)
S12	-0.1173 (3)	0.6660 (3)	0.5400 (3)	4.3 (1)
S13	0.1592 (4)	0.6655 (3)	0.4704 (3)	4.7 (1)
S14	-0.0313 (4)	0.6686 (3)	0.3748 (3)	4.2 (1)
C17	0.004 (1)	0.667 (1)	0.541 (1)	3.6 (4)
C18	0.040 (1)	0.6663 (9)	0.469 (1)	3.4 (4)
C19	-0.020 (1)	0.665 (1)	0.685 (1)	3.7 (4)
C20	-0.107 (1)	0.667 (1)	0.645 (1)	4.7 (5)
C21	0.146 (1)	0.664 (1)	0.363 (1)	5.1 (5)
C22	0.060 (1)	0.665 (1)	0.323 (1)	5.2 (5)

TTF molecule E

S15	0.0688 (4)	0.5015 (3)	0.3945 (3)	4.9 (1)
S16	-0.1317 (4)	0.5045 (3)	0.4113 (3)	4.8 (1)
C23	-0.013 (1)	0.501 (1)	0.4584 (9)	3.4 (4)
C24	-0.018 (2)	0.504 (1)	0.307 (1)	5.4 (5)
C25	-0.109 (2)	0.506 (1)	0.313 (1)	5.7 (6)

TTF molecule F

S17	0.1997 (4)	0.6785 (3)	0.8302 (3)	4.2 (1)
S18	0.3382 (4)	0.6788 (3)	0.6969 (3)	4.7 (1)
C26	0.243 (2)	0.750	0.790 (1)	3.7 (6)
C27	0.300 (1)	0.750	0.737 (1)	2.3 (5)
C28	0.140 (1)	0.717 (1)	0.899 (1)	5.1 (5)
C29	0.419 (1)	0.719 (1)	0.648 (1)	6.1 (6)

Solvent (acetonitrile)

N1*	0.324 (3)	0.25	0.394 (2)	12 (1)
C30*	0.320 (3)	0.25	0.320 (3)	11 (1)
C31*	0.309 (4)	0.25	0.240 (3)	12 (1)

*Refined isotropically.

Table 2. Bond lengths (Å) and selected bond angles (°) in the $W_6O_{19}^{6-}$ units

W1—W2	2.382 (1)	W11—W22	3.296 (1)
W1—W3	3.290 (1)	W11—W33	3.274 (1)
W2—W3	3.294 (1)	W22—W33	3.297 (1)
W1—W2 ⁱ	3.295 (1)	W11—W22 ⁱⁱ	3.280 (1)
W1—W3 ⁱ	3.284 (1)	W11—W33 ⁱⁱ	3.295 (1)
W2—W3 ⁱ	3.280 (1)	W22—W33 ⁱⁱ	3.269 (1)
W1—O1	1.92 (1)	W11—O13	1.93 (1)
W1—O2	1.94 (1)	W11—O14	1.91 (1)
W1—O3	1.69 (1)	W11—O16	1.71 (1)
W1—O5	1.92 (1)	W11—O18	1.91 (1)
W1—O6	1.92 (1)	W11—O19	1.91 (1)
W1—O10	2.325 (1)	W11—O20	2.326 (1)
W2—O1	1.94 (1)	W22—O11	1.92 (1)
W2—O4	1.92 (1)	W22—O12	1.93 (1)
W2—O6	1.94 (1)	W22—O13	1.91 (1)
W2—O7	1.91 (1)	W22—O14	1.93 (1)
W2—O8	1.68 (1)	W22—O17	1.70 (1)
W2—O10	2.325 (1)	W22—O20	2.324 (1)
W3—O2	1.91 (1)	W33—O11	1.91 (1)
W3—O4	1.92 (1)	W33—O12	1.89 (1)
W3—O5	1.91 (1)	W33—O15	1.69 (1)
W3—O7	1.89 (1)	W33—O18	1.94 (1)
W3—O9	1.72 (1)	W33—O19	1.91 (1)
W3—O10	2.323 (1)	W33—O20	2.319 (1)
O1—W1—O2	85.6 (5)	O13—W11—O14	152.5 (5)
O1—W1—O3	104.5 (5)	O13—W11—O16	102.0 (5)
O1—W1—O5	87.6 (5)	O13—W11—O18	86.9 (5)
O1—W1—O6	153.1 (5)	O13—W11—O19	86.1 (5)
O2—W1—O3	103.9 (5)	O14—W11—O16	105.5 (6)
O2—W1—O5	152.1 (5)	O14—W11—O18	87.8 (5)
O2—W1—O6	86.6 (5)	O14—W11—O19	86.2 (5)
O3—W1—O5	104.0 (5)	O16—W11—O18	103.7 (6)
O3—W1—O6	102.3 (5)	O16—W11—O19	103.9 (6)
O5—W1—O6	87.4 (5)	O18—W11—O19	152.3 (5)
O1—W2—O4	85.9 (5)	O11—W22—O12	151.1 (5)
O1—W2—O6	152.5 (4)	O11—W22—O13	85.4 (5)
O1—W2—O7	88.3 (5)	O11—W22—O14	86.3 (5)
O1—W2—O8	104.2 (5)	O11—W22—O17	105.1 (6)
O4—W2—O6	86.7 (5)	O12—W22—O13	87.3 (5)
O4—W2—O7	151.3 (5)	O12—W22—O14	87.5 (5)
O4—W2—O8	105.7 (6)	O12—W22—O17	103.8 (6)
O6—W2—O7	85.6 (5)	O13—W22—O14	152.5 (5)
O6—W2—O8	103.3 (5)	O13—W22—O17	101.8 (6)
O7—W2—O8	103.0 (5)	O14—W22—O17	105.7 (6)
O2—W3—O4	86.2 (5)	O11—W33—O12	152.1 (5)
O2—W3—O5	153.0 (5)	O11—W33—O15	104.6 (6)
O2—W3—O7	86.7 (5)	O11—W33—O18	86.4 (5)
O2—W3—O9	103.4 (6)	O11—W33—O19	86.7 (5)
O4—W3—O5	86.9 (5)	O12—W33—O15	103.2 (6)
O4—W3—O7	151.8 (5)	O12—W33—O18	86.8 (5)
O4—W3—O9	104.3 (6)	O12—W33—O19	86.9 (5)
O5—W3—O7	87.1 (5)	O15—W33—O18	102.6 (6)
O5—W3—O9	103.7 (6)	O15—W33—O19	105.2 (6)
O7—W3—O9	103.8 (5)	O18—W33—O19	152.1 (5)

Symmetry code: (i) $-x, -y, -z$; (ii) $1-x, 1-y, 1-z$.

The structure was solved by direct methods and successive difference Fourier syntheses. The H atoms were placed at computed positions [$d(C-H) = 1.0 \text{ \AA}$; $B = 5.0 \text{ \AA}^2$]. The acetonitrile

trile molecule (N1, C30, C31) was refined isotropically; H atoms isotropic but not refined. All calculations were performed on a MicroVAX 3100 using *SDP* (B. A. Frenz & Associates, Inc., 1985).

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55449 (34 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: PA1021]

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Structure of Carbonylbis(diphenyldithiophosphinato)(triphenylphosphine)ruthenium Diethyl Ether Solvate, $[\text{Ru}(\text{CO})(\text{S}_2\text{PPh}_2)_2(\text{PPh}_3)] \cdot 0.25\text{Et}_2\text{O}$

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Abstract

Ruthenium is six coordinate; the principal distortion from octahedral geometry at the metal centre arises from the narrow bite angle of the chelating dithiolate ligand. The Ru–S distances vary by more than 0.11 Å; the bond *trans* to CO [2.5407 (11) Å] is significantly longer than that *trans* to PPh₃ [2.5205 (11) Å] and both are much longer than the other two mutually *trans* Ru–S distances [2.4295 (11), 2.4363 (10) Å]. These observations concur with the expected order of decreasing *trans* influence, CO > PPh₃ ≫ Ph₂PS₂[−].

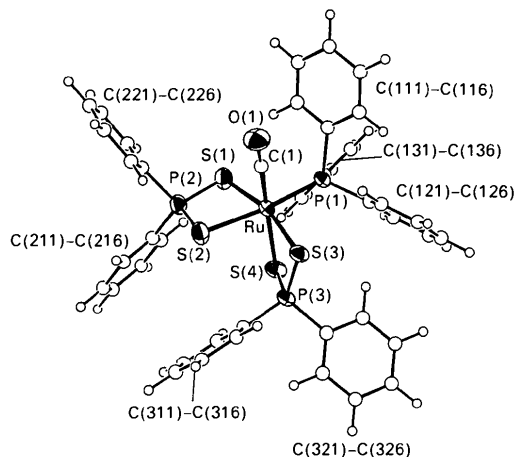
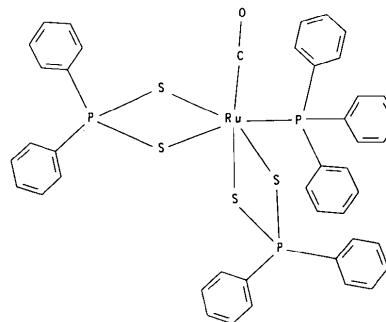


Fig. 1. View of the molecule showing the labelling of the non-H atoms. Thermal ellipsoids are drawn at the 30% probability level.

Comment

The proton-decoupled ³¹P NMR spectra of the complexes $[\text{Ru}(\text{S}_2\text{PR}_2)_2(\text{PPh}_3)(\text{CO})]$, $R = \text{Me}, \text{Ph}$ (Cole-Hamilton & Stephenson, 1974), OEt (McQueen, Schröder, Stephenson & Yellowlees, unpublished), show firstly that there are two magnetically inequivalent environments for the ³¹P nuclei of the dithiolate ligands and secondly that only one of these nuclei exhibits a ³ J_{PP} coupling to the coordinated PPh₃. Fig. 1 shows an Ru atom coordinated by two bidentate dithiolates in addition to the CO and PPh₃ ligands. We have used close analogues of the title compound in the preparation of tetracyanoethylene (tcne) complexes; in one there is an interesting intramolecular interaction between bound tcne and a phenyl ring in one S₂PPh₂[−] ligand and another has intermolecular stacking of bound tcne ligands (Blake, McQueen, Schröder, Stephenson & Yellowlees, 1988).



Experimental

Crystal data

$[\text{Ru}(\text{C}_{12}\text{H}_{10}\text{PS}_2)_2(\text{C}_{18}\text{H}_{15}\text{P})-$
 $(\text{CO})] \cdot 0.25\text{C}_4\text{H}_{10}\text{O}$
 $M_r = 908.5$

$D_x = 1.398 \text{ Mg m}^{-3}$
Mo $K\alpha$ radiation
 $\lambda = 0.71073 \text{ \AA}$