

there appear to be no significant differences in the structure of the anion in the [PtH(PPh₃)₃]⁺ salt. A view of the anion is shown in Fig. 2.

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Bis(bis- η -cyclopentadienylmolybdenumdi- μ -oxo)phosphorus Hexafluorophosphate

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Abstract. [(C₂H₅)₂MoO₂Mo(C₂H₅)₂](PF₆)₂, C₂₀H₂₀O₄F₁₂P₃Mo₂, $M_r = 837.2$. Monoclinic, $C2/c$, $a = 17.079$ (9), $b = 23.619$ (13), $c = 12.399$ (7) Å, $\beta = 117.02$ (2)°, $U = 4455.7$ Å³, $D_c = 2.50$ g cm⁻³ for $Z = 8$. Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å, $\mu = 14$ cm⁻¹. The structure of the cation is as would be expected from the known structures of bent $d^2(\eta\text{-C}_5\text{H}_5)_2\text{MX}_2$ systems. The anions have near-spherical symmetry and show considerable apparent distortion.

Introduction. Needle crystals from the reaction of ($\eta\text{-C}_5\text{H}_5$)₂MoCl₂ and Na₂HPO₄ in an aqueous medium were supplied by Dr M. L. H. Green and Mr C. Rañao. They were sensitive to air and moisture and were mounted for X-ray examination in nitrogen-filled capillary tubes. It was not possible to measure their density. After survey photography by oscillation and Weissenberg techniques, the selected crystal was set up on a Hilger & Watts PDP8-controlled four-circle diffractometer and cell parameters and orientation matrix were obtained by a least-squares fit to the setting angles of 20 reflexions.

The intensities of each independent reflexion with $\sin \theta/\lambda < 0.59$ were measured by an $\omega/2\theta$ scan with ordinate analysis (Watson, Shotton, Cox & Muirhead, 1970). Mo $K\alpha$ radiation was used with a graphite

monochromator. Reflexions with $I < 4\sigma(I)$, where $\sigma(I)$ is the standard deviation derived from counting statistics, or whose apparent centre was more than 0.14° from the predicted position, were not included in subsequent calculations. Lorentz and polarization corrections, and an empirical absorption correction (North, Phillips & Mathews, 1968), were applied, leading to a set of 3495 independent observed structure amplitudes.

The structure was solved by Patterson and Fourier techniques. Refinement was by least squares with a large-block approximation to the normal matrix: one block was calculated from the derivatives of the positional parameters, and one from those of the corresponding anisotropic temperature factors and the scale factor. Difference syntheses permitted the location of the H atoms in their expected positions. They were positioned geometrically ($\text{C-H} = 1.0$ Å; $U_{\text{iso}} = 0.05$) and included in the structure factor calculations, being readjusted after each cycle. Four low-angle reflexions, 150, $\bar{3}11$, 221, $\bar{1}32$, were given zero weight in the last cycles because of suspected extinction effects. Each reflexion was assigned a weight according to $\omega = 1/\sum_{r=1}^n A_r T_r^*(X)$ where n is the number of coefficients, A_r , for a Chebyshev series; T_r^* is the polynomial function and X is $F_o/F_o(\text{max})$. Five coefficients, A_r , were used with values 145.74, 193.82, 94.01, 40.75 and 18.23 (Rollett, 1965) and the final R was 0.041 for 3491 reflexions. All calculations were

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Table 1. Fractional atomic coordinates ($\times 10^4$) and anisotropic temperature factors ($\times 10^2$) for the non-hydrogen atoms

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₂₃	<i>U</i> ₁₃	<i>U</i> ₁₂
Mo(1)	1913.3 (3)	3951.0 (2)	3312.8 (4)	3.47 (2)	3.59 (3)	5.51 (3)	-1.09 (2)	2.29 (2)	-0.55 (2)
Mo(2)	1099.7 (3)	1969.5 (2)	769.4 (4)	5.04 (3)	3.28 (2)	4.37 (3)	-0.43 (2)	2.68 (2)	0.10 (2)
P(1)	1638.3 (9)	2923.1 (6)	2169 (1)	4.20 (7)	3.66 (7)	5.48 (8)	-0.86 (6)	2.39 (6)	-0.03 (5)
O(1)	2500 (2)	3186 (2)	3112 (4)	3.6 (2)	4.9 (2)	7.6 (3)	-1.5 (2)	1.7 (2)	0.6 (2)
O(2)	970 (2)	3384 (1)	2087 (3)	3.6 (2)	4.1 (2)	5.5 (2)	-1.3 (2)	1.6 (2)	-0.2 (1)
O(3)	1613 (3)	2801 (1)	939 (4)	6.1 (2)	3.5 (2)	6.3 (2)	-0.3 (2)	3.9 (2)	-0.6 (2)
O(4)	1424 (3)	2334 (2)	2492 (3)	6.2 (2)	4.3 (2)	4.5 (2)	-0.5 (2)	3.0 (2)	0.3 (2)
C(11)	2875 (5)	4642 (3)	3270 (8)	7.4 (5)	6.6 (4)	11.1 (6)	-1.9 (4)	6.4 (4)	-2.6 (4)
C(12)	2063 (5)	4890 (3)	3011 (8)	8.9 (5)	3.7 (3)	14.0 (7)	-1.2 (4)	8.1 (5)	-1.5 (3)
C(13)	1409 (5)	4659 (3)	1926 (8)	7.3 (5)	6.1 (4)	10.0 (6)	2.9 (4)	4.5 (4)	-0.1 (4)
C(14)	1862 (6)	4270 (3)	1520 (7)	12.4 (7)	6.9 (5)	7.4 (5)	0.2 (4)	6.2 (5)	-1.9 (5)
C(15)	2747 (5)	4270 (3)	2359 (8)	8.5 (5)	7.5 (5)	11.1 (6)	0.2 (4)	7.2 (5)	-0.9 (4)
C(21)	2562 (4)	3798 (4)	5337 (6)	4.8 (3)	10.0 (6)	5.1 (4)	-0.5 (4)	1.7 (3)	0.9 (4)
C(22)	2232 (5)	4348 (3)	5167 (7)	6.7 (4)	8.3 (5)	7.3 (4)	-3.4 (4)	3.7 (4)	-2.4 (4)
C(23)	1313 (5)	4339 (3)	4521 (6)	6.5 (4)	8.7 (5)	7.3 (4)	-1.1 (4)	4.6 (4)	0.8 (4)
C(24)	1061 (4)	3782 (3)	4322 (6)	4.0 (3)	10.2 (5)	5.3 (3)	-1.3 (4)	2.0 (3)	-2.1 (4)
C(25)	1825 (5)	3440 (3)	4804 (6)	9.8 (6)	6.3 (4)	6.5 (4)	-0.2 (3)	4.8 (4)	-0.9 (4)
C(31)	1505 (6)	1137 (3)	278 (8)	9.3 (6)	5.4 (4)	10.2 (6)	-3.5 (4)	2.9 (5)	1.9 (4)
C(32)	1840 (5)	1156 (3)	1565 (7)	8.4 (5)	4.2 (3)	8.1 (5)	1.0 (3)	4.3 (4)	1.9 (3)
C(33)	2480 (4)	1578 (3)	1932 (6)	6.3 (4)	6.1 (4)	7.1 (4)	0.2 (3)	3.6 (3)	1.0 (3)
C(34)	2525 (5)	1812 (3)	945 (8)	7.8 (5)	7.4 (5)	11.3 (6)	2.2 (4)	6.9 (5)	3.3 (4)
C(35)	1919 (6)	1565 (4)	-81 (7)	11.1 (7)	9.2 (6)	7.3 (5)	0.2 (4)	5.9 (5)	3.0 (5)
C(41)	-195 (5)	2484 (4)	-206 (9)	5.3 (4)	8.6 (5)	10.6 (7)	0.1 (5)	2.6 (4)	1.4 (4)
C(42)	-286 (5)	2171 (5)	600 (7)	5.4 (4)	18 (1)	6.3 (4)	0.0 (6)	2.9 (4)	2.2 (5)
C(43)	-246 (5)	1605 (5)	328 (14)	5.1 (5)	13.1 (9)	26 (2)	13 (1)	4.5 (7)	-0.5 (5)
C(44)	-150 (5)	1631 (5)	-753 (12)	5.9 (5)	10.0 (7)	19 (1)	-9.9 (8)	0.0 (6)	-1.4 (5)
C(45)	-101 (5)	2182 (5)	-999 (7)	7.1 (5)	15.5 (9)	5.1 (4)	-0.4 (5)	1.8 (4)	0.4 (6)
P(2)	0	60.5 (9)	2500	4.4 (1)	4.4 (1)	5.0 (1)	0	2.64 (9)	0
F(1)	-96 (5)	52 (3)	3686 (5)	18.9 (6)	18.0 (6)	9.7 (4)	0.6 (4)	10.6 (4)	0.8 (5)
F(2)	971 (4)	47 (5)	3298 (7)	6.4 (3)	36 (1)	16.2 (7)	-7.0 (8)	3.2 (4)	-5.4 (6)
F(3)	0	-580 (3)	2500	33 (2)	5.4 (4)	9.3 (6)	0	3.2 (7)	0
F(4)	0	697 (3)	2500	48 (2)	5.4 (5)	17 (1)	0	18 (1)	0
P(3)	5000	1029 (1)	2500	5.0 (1)	5.0 (1)	6.7 (1)	0	2.6 (1)	0
F(5)	4540 (5)	1029 (3)	3342 (6)	15.4 (6)	16.6 (6)	13.6 (5)	-0.7 (4)	10.5 (5)	0.0 (5)
F(6)	4081 (4)	973 (4)	1454 (6)	10.5 (5)	32 (1)	9.9 (4)	-2.4 (6)	1.6 (4)	3.5 (6)
F(7)	5000	370 (4)	2500	16.8 (9)	7.7 (5)	38 (2)	0	18 (1)	0
F(8)	5000	1652 (4)	2500	45 (2)	5.4 (5)	42 (2)	0	35 (2)	0

performed on the Oxford University ICL 1906A computer with the Oxford package of crystallographic programs (Carruthers & Rollett, 1973). Complex neutral-atom scattering factors were taken from *International Tables for X-ray Crystallography* (1962).

The final atomic parameters are given in Tables 1 and 2.* Table 3 lists interatomic distances and interbond angles for the non-hydrogen atoms.

Discussion. The structure consists of discrete organometallic cations and hexafluorophosphate anions.

The structure of the cation, projected onto the Mo(1)O(1)O(2)P(1) plane in Fig. 1, is as would be expected from the known structures of bent d^2 (η -

Table 2. Fractional atomic coordinates ($\times 10^4$) for the hydrogen atoms

	<i>x</i>	<i>y</i>	<i>z</i>
H(11)	3447	4724	3995
H(12)	1961	5184	3515
H(13)	766	4747	1524
H(14)	1590	4038	763
H(15)	3216	4035	2304
H(21)	3194	3682	5752
H(22)	2598	4698	5464
H(23)	916	4676	4255
H(24)	441	3642	3906
H(25)	1839	3017	4771
H(31)	1052	865	-279
H(32)	1657	921	2082
H(33)	2854	1695	2792
H(34)	2940	2118	979
H(35)	1792	1666	-929
H(41)	-194	2909	-206
H(42)	-372	2324	1292
H(43)	-269	1267	802
H(44)	-135	1300	-1242
H(45)	-10	2328	-1690

*A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32007 (31 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 3. *Interatomic distances (Å) and bond angles (°)*

Cation			
Mo(1)—O(1)	2.137 (4)	Mo(2)—O(3)	2.122 (3)
Mo(1)—O(2)	2.116 (3)	Mo(2)—O(4)	2.129 (3)
Mo(1)—C(11)	2.332 (6)	Mo(2)—C(31)	2.259 (6)
Mo(1)—C(12)	2.280 (6)	Mo(2)—C(32)	2.265 (6)
Mo(1)—C(13)	2.268 (7)	Mo(2)—C(33)	2.324 (6)
Mo(1)—C(14)	2.310 (7)	Mo(2)—C(34)	2.372 (6)
Mo(1)—C(15)	2.350 (7)	Mo(2)—C(35)	2.308 (6)
Mo(1)—C(21)	2.265 (7)	Mo(2)—C(41)	2.324 (7)
Mo(1)—C(22)	2.307 (6)	Mo(2)—C(42)	2.328 (7)
Mo(1)—C(23)	2.351 (6)	Mo(2)—C(43)	2.277 (8)
Mo(1)—C(24)	2.345 (6)	Mo(2)—C(44)	2.257 (8)
Mo(1)—C(25)	2.271 (7)	Mo(2)—C(45)	2.276 (8)
P(1)—O(1)	1.535 (4)	P(1)—O(3)	1.533 (4)
P(1)—O(2)	1.548 (4)	P(1)—O(4)	1.537 (4)
C(11)—C(12)	1.40 (1)	C(31)—C(32)	1.43 (1)
C(12)—C(13)	1.41 (1)	C(32)—C(33)	1.39 (1)
C(13)—C(14)	1.43 (1)	C(33)—C(34)	1.38 (1)
C(14)—C(15)	1.39 (1)	C(34)—C(35)	1.35 (1)
C(15)—C(11)	1.37 (1)	C(35)—C(31)	1.42 (1)
C(21)—C(22)	1.39 (1)	C(41)—C(42)	1.31 (1)
C(22)—C(23)	1.40 (1)	C(42)—C(43)	1.39 (2)
C(23)—C(24)	1.37 (1)	C(43)—C(44)	1.42 (2)
C(24)—C(25)	1.42 (1)	C(44)—C(45)	1.35 (2)
C(25)—C(21)	1.41 (1)	C(45)—C(41)	1.28 (1)
O(1)—Mo(1)—O(2)	68.0 (1)	O(3)—Mo(2)—O(4)	67.6 (1)
O(1)—P(1)—O(2)	100.9 (2)	O(2)—P(1)—O(3)	112.4 (2)
O(1)—P(1)—O(3)	114.7 (2)	O(2)—P(1)—O(4)	113.5 (2)
O(1)—P(1)—O(4)	115.3 (2)	O(3)—P(1)—O(4)	100.7 (2)
Mo(1)—O(1)—P(1)	95.3 (2)	Mo(2)—O(3)—P(1)	95.5 (2)
Mo(1)—O(2)—P(1)	95.8 (2)	Mo(2)—O(4)—P(1)	95.1 (2)
C(15)—C(11)—C(12)	108.0 (7)	C(35)—C(31)—C(32)	108.8 (7)
C(11)—C(12)—C(13)	109.3 (7)	C(31)—C(32)—C(33)	104.2 (7)
C(12)—C(13)—C(14)	105.2 (7)	C(32)—C(33)—C(34)	110.4 (7)
C(13)—C(14)—C(15)	108.4 (7)	C(33)—C(34)—C(35)	109.7 (7)
C(14)—C(15)—C(11)	109.2 (7)	C(34)—C(35)—C(31)	106.8 (7)
C(25)—C(21)—C(22)	105.9 (6)	C(45)—C(41)—C(42)	111.8 (9)
C(21)—C(22)—C(23)	110.1 (6)	C(41)—C(42)—C(43)	108.9 (9)
C(22)—C(23)—C(24)	107.2 (7)	C(42)—C(43)—C(44)	103.0 (7)
C(23)—C(24)—C(25)	108.5 (6)	C(43)—C(44)—C(45)	107.6 (8)
C(24)—C(25)—C(21)	108.2 (6)	C(44)—C(45)—C(41)	108.7 (9)
Anion I			
P(2)—F(1)	1.553 (5)	P(2)—F(3)	1.514 (7)
P(2)—F(2)	1.496 (6)	P(2)—F(4)	1.504 (8)
F(1)—P(2)—F(1')	178.5 (6)	F(2)—P(2)—F(2')	177.6 (9)
F(1)—P(2)—F(2)	86.3 (4)	F(2)—P(2)—F(3)	88.8 (4)
F(1)—P(2)—F(2')	93.7 (4)	F(2)—P(2)—F(4)	91.2 (4)
F(1)—P(2)—F(3)	89.3 (3)	F(3)—P(2)—F(4)	180.0
F(1)—P(2)—F(4)	90.7 (3)		
Anion II			
P(3)—F(5)	1.565 (5)	P(3)—F(7)	1.556 (9)
P(3)—F(6)	1.521 (6)	P(3)—F(8)	1.471 (9)
F(5)—P(3)—F(5')	180.0 (6)	F(6)—P(3)—F(6')	170.0 (8)
F(5)—P(3)—F(6)	86.2 (4)	F(6)—P(3)—F(7)	85.0 (4)
F(5)—P(3)—F(6')	93.8 (4)	F(6)—P(3)—F(8)	95.0 (4)
F(5)—P(3)—F(7)	90.0 (3)	F(7)—P(3)—F(8)	180.0
F(5)—P(3)—F(8)	90.0 (3)		

C₅H₅)₂MX₂ systems (Prout, Cameron, Forder, Critchley, Denton & Rees, 1974).

Projections on to the Mo(1)O(1)O(2) and Mo(2)O(3)O(4) planes (Fig. 2) show that the cyclo-

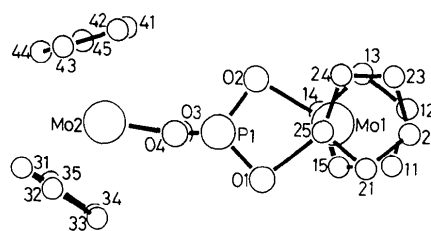


Fig. 1. The cation projected on to the plane through Mo(1)O(1)O(2)P(1). For clarity, the carbon atoms are labelled by their serial number only.

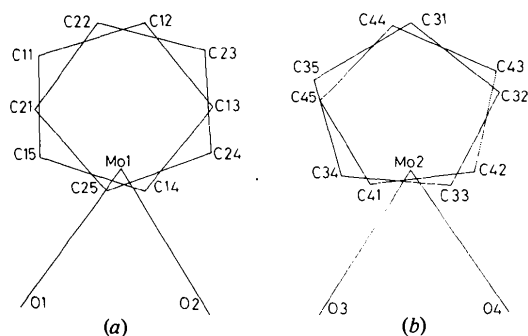


Fig. 2. Projections of the (η -C₅H₅)₂MoO₂ moieties on to (a) the Mo(1)O(1)O(2) plane and (b) the Mo(2)O(3)O(4) plane.

pentadienyl rings adopt a staggered configuration at Mo(1) and an eclipsed configuration at Mo(2). This provides further confirmation for the belief (Prout, Allison, Delbaere & Gore, 1972) that the choice of conformation can be attributed to crystal-packing effects.

The MoO₂PO₂Mo bridging system can be compared to phosphate structures such as calcium bis-(dihydrogenphosphate) monohydrate (Dickens & Bowen, 1971) and calcium hydrogenphosphate dihydrate (Jones & Smith, 1962) in which chains of alternating Ca ions and phosphate groups are present. The mean P—O length of 1.538 (7) Å obtained here is intermediate between the values obtained in Ca(H₂PO₄)₂·H₂O, 1.496 (1) Å for the oxo bridges and 1.571 (2), 1.578 (2) Å for the hydroxo bridges.

The anions lie on mirror planes and, as is usual with ions having near-spherical symmetry, they have large temperature factors and show considerable apparent distortion.

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(1R,2S)-2-[(S)-(p-Chlorophenyl)sulfinyl]-N,N,3,3-tetramethylcyclopropylamine

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Abstract. C₁₃H₁₈NOSCl, orthorhombic, *P*2₁2₁2₁, *a* = 10.526 (1), *b* = 11.130 (1), *c* = 11.993 (2) Å, *Z* = 4, *D*_c = 1.28 g cm⁻³. Positional and thermal parameters for all atoms were refined. The final agreement index *R* was 0.037 for 1192 reflexions. The O atom of the sulfinyl group and the dimethylamino group are *syn* related.

Introduction. Reactions of some isomeric aminocyclopropyl sulfoxides were studied because the ring openings of the cyclopropanes proceed *via* zwitterionic intermediates and because of the interesting stereochemistry of the reactions (Rynbrandt, Dutton & Chidester, 1976). This crystal structure was determined as part of the study in order to establish the configuration at the S atom relative to the configuration at C(1) and C(2).

The crystals, which were small clear prisms, were supplied by Dr R. H. Rynbrandt. The racemic mixture crystallized from diethyl ether as an equal mixture of (+) and (−) crystals instead of the usual (±) crystals. Face development was not good enough to permit separation into two types under the microscope. One crystal was selected at random. Precession photographs of the crystal, 0.15 × 0.15 × 0.3 mm, showed that the unit cell is orthorhombic; absence of reflections of type *h*00 for *h* odd, 0*k*0 for *k* odd, and 00*l* for *l* odd indicated the space group to be *P*2₁2₁2₁.

Intensity data for the 1192 reflections for which 2θ was less than 120° were measured using graphite-monochromated Cu *K*α radiation (λ = 1.5418 Å) on a Syntex P1̄ diffractometer controlled by an IBM 1800 computer. The θ–2θ scan technique was used with a scan range of approximately 3.2° and a variable scan

Table 1. Final atomic parameters, and standard deviations in parentheses

All values for anisotropic atoms have been multiplied by 10⁴. Coordinates of isotropic atoms have been multiplied by 10³. The form of the anisotropic temperature factors is exp(−*B*₁₁*h*² − *B*₂₂*k*² − *B*₃₃*l*² − *B*₁₂*hk* − *B*₁₃*hl* − *B*₂₃*kl*).

	x	y	z	B ₁₁	B ₂₂	B ₃₃	B ₁₂	B ₁₃	B ₂₃
Cl	772 (1)	8636 (1)	4979 (1)	92 (1)	197 (2)	123 (1)	21 (2)	18 (2)	67 (2)
S	5758 (1)	11048 (1)	3164 (1)	96 (1)	82 (1)	87 (1)	28 (2)	2 (1)	−3 (2)
O	6004 (2)	12060 (2)	3952 (2)	137 (3)	83 (2)	139 (2)	8 (5)	15 (4)	−94 (4)
N	8634 (2)	10962 (3)	2439 (2)	91 (2)	79 (3)	74 (2)	−12 (5)	1 (4)	−22 (5)
C(1)	8187 (2)	9927 (3)	3033 (2)	76 (3)	95 (3)	62 (2)	11 (6)	−20 (4)	14 (6)
C(2)	6838 (3)	9866 (3)	3448 (2)	81 (3)	78 (3)	55 (2)	18 (6)	−6 (4)	3 (5)
C(3)	7295 (3)	9058 (3)	2503 (2)	76 (3)	70 (3)	66 (2)	8 (6)	6 (4)	−1 (6)
C(4)	6840 (3)	9278 (3)	1330 (2)	108 (3)	100 (4)	64 (2)	4 (7)	1 (5)	−18 (6)
C(5)	7461 (3)	7746 (3)	2779 (3)	102 (3)	88 (4)	113 (3)	11 (7)	1 (6)	−4 (7)
C(6)	9080 (3)	11887 (3)	3227 (3)	118 (4)	108 (4)	117 (3)	−40 (8)	−11 (6)	−51 (7)
C(7)	9675 (3)	10607 (3)	1699 (3)	115 (4)	113 (4)	105 (3)	−39 (7)	36 (6)	2 (7)
C(8)	4369 (3)	10293 (3)	3684 (2)	85 (3)	77 (3)	66 (2)	34 (7)	−11 (5)	−14 (5)
C(9)	3974 (3)	9199 (3)	3301 (2)	95 (3)	112 (4)	93 (3)	22 (7)	27 (5)	−68 (6)
C(10)	2866 (3)	8680 (3)	3696 (3)	88 (3)	111 (4)	112 (3)	0 (7)	−11 (5)	−34 (7)
C(11)	2179 (3)	9283 (3)	4476 (2)	74 (3)	125 (4)	81 (2)	58 (7)	−16 (5)	34 (6)
C(12)	2542 (3)	10375 (3)	4880 (2)	111 (3)	129 (5)	70 (2)	62 (8)	27 (5)	−11 (6)
C(13)	3642 (3)	10873 (3)	4482 (2)	125 (4)	81 (4)	81 (2)	30 (7)	−3 (5)	−17 (6)

	x	y	z	B	x	y	z	B	
H(1)	874 (2)	962 (3)	350 (2)	4.3 (0.6)	H(6B)	839 (3)	1214 (3)	366 (2)	5.5 (0.7)
H(2)	668 (2)	951 (2)	415 (2)	2.3 (0.5)	H(6C)	984 (3)	1163 (3)	365 (3)	6.8 (0.9)
H(4A)	603 (2)	891 (3)	127 (2)	4.7 (0.6)	H(7A)	938 (3)	994 (3)	118 (2)	5.6 (0.7)
H(4B)	680 (2)	1008 (2)	113 (2)	3.3 (0.5)	H(7B)	985 (3)	1130 (3)	134 (2)	5.7 (0.8)
H(4C)	738 (2)	886 (3)	80 (2)	4.9 (0.6)	H(7C)	1045 (3)	1026 (3)	208 (2)	7.5 (0.8)
H(5A)	783 (2)	775 (3)	353 (2)	5.0 (0.7)	H(9)	438 (2)	885 (2)	277 (2)	3.2 (0.5)
H(5B)	804 (2)	741 (3)	227 (2)	4.9 (0.7)	H(10)	262 (3)	795 (3)	342 (2)	6.9 (0.8)
H(5C)	670 (2)	735 (2)	283 (2)	4.6 (0.7)	H(12)	205 (2)	1080 (3)	544 (2)	5.5 (0.7)
H(6A)	935 (3)	1254 (3)	286 (2)	6.9 (0.8)	H(13)	388 (2)	1159 (2)	467 (2)	4.4 (0.7)