Electronic Supplementary Information for Dalton Transactions

Sample: SC0466

X-ray Structure Report

for

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Experimental

Data Collection

A yellow prism crystal of $C_{78}H_{76}MoNP_4Si$ having approximate dimensions of 0.16 x 0.08 x 0.06 mm was mounted on a glass fiber. All measurements were made on a Rigaku Saturn CCD area detector with graphite monochromated Mo-Kα radiation.

Indexing was performed from 10 images that were exposed for 60 seconds. The crystal-to-detector distance was 49.97 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive triclinic cell with dimensions:

a	= 12.916(3) Å	α	= 78.492(6)^o
b	= 13.954(3) Å	β	= 83.694(7)^o
c	= 18.290(4) Å	γ	= 86.519(7)^o
V	= 3207.8(13) Å^3		

For Z = 2 and F.W. = 1275.39, the calculated density is 1.320 g/cm^3. Based on a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

P-1 (#2)

The data were collected at a temperature of -160 $\pm$ 1^{o}C to a maximum 2θ value of 50.1^o. A total of 720 oscillation images were collected. A sweep of data was done using ω scans from -110.0 to 70.0^o in 0.5^o step, at χ=45.0^o and ϕ = 0.0^o. The exposure rate was 120.0 [sec./^{o}]. The detector swing angle was -20.25^o. A second sweep was performed using ω scans from -110.0 to 70.0^o in 0.5^o step, at χ=45.0^o and ϕ = 90.0^o. The exposure rate was 120.0 [sec./^{o}]. The detector swing angle was -20.25^o. The crystal-to-detector distance was 49.97 mm. Readout was performed in the 0.547 mm pixel mode.

Data Reduction

Of the 17709 reflections that were collected, 10486 were unique (R_{int} = 0.046); equivalent reflections were merged. Data were collected and processed using CrystalClear (Rigaku). Net intensities and sigmas were derived as follows:

$$F^2 = [\Sigma(P_i - mB_{ave})] \cdot \quad Lp^{-1}$$

where P_i is the value in counts of the i^{th} pixel
m is the number of pixels in the integration area
B_{ave} is the background average
Lp is the Lorentz and polarization factor

$$B_{ave} = \Sigma(B_j)/n$$

where n is the number of pixels in the background area
B_j is the value of the j^{th} pixel in counts

$$\sigma^2(F^2_{hkl}) = [(\Sigma P_i) + m((\Sigma(B_{ave} - B_j)^2)/(n-1))] \cdot \quad Lp \cdot \quad errmul + (erradd \cdot \quad F^2)^2$$

where erradd = 0.03
errmul = 2.70

The linear absorption coefficient, μ, for Mo-Kα radiation is 3.683 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.880 to 0.978. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[2] and expanded using Fourier techniques[3]. Some non-hydrogen atoms were refined anisotropically, while the rest were refined isotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[4] on F^2 was based on 10486 observed reflections and 762 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \; ||Fo| - |Fc|| \; / \; \Sigma \; |Fo| = 0.0625$$

$$wR2 = [\Sigma (w (Fo^2 - Fc^2)^2)/ \Sigma w(Fo^2)^2]^{1/2} = 0.1529$$

The standard deviation of an observation of unit weight[5] was 1.03. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.84 and -0.79 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[6]. Anomalous dispersion effects were included in Fcalc[7]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[8]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[9]. All calculations were performed using the CrystalStructure[10] crystallographic software package except for refinement, which was performed using SHELXL-97[11].

References

(1) CrystalClear: Rigaku Corporation, 1999. CrystalClear Software User's Guide, Molecular Structure Corporation, (c) 2000.J.W.Pflugrath (1999) Acta Cryst. D55, 1718-1725.

(2) SIR2002: Burla, M.C., Camalli, M., Carrozzini, B., Cascarano, G.L., Giacovazzo, C., Polidori, G., Spagna., R. (2003).

(3) DIRDIF99: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1999). The DIRDIF-99 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(4) Least Squares function minimized: (SHELXL97)

$\Sigma w(F_o^2-F_c^2)^2$ where w = Least Squares weights.

(5) Standard deviation of an observation of unit weight:

$$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$$

where: N_o = number of observations
N_v = number of variables

(6) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(7) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(8) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(9) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(10) CrystalStructure 3.8: Crystal Structure Analysis Package, Rigaku and Rigaku Americas (2000-2007). 9009 New Trails Dr. The Woodlands TX 77381 USA.

(11) SHELX97: Sheldrick, G.M. (1997).

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{78}H_{76}MoNP_4Si$
Formula Weight	1275.39
Crystal Color, Habit	yellow, prism
Crystal Dimensions	0.16 X 0.08 X 0.06 mm
Crystal System	triclinic
Lattice Type	Primitive
Indexing Images	10 images @ 60.0 seconds
Detector Position	49.97 mm
Pixel Size	0.137 mm
Lattice Parameters	a = 12.916(3) Å b = 13.954(3) Å c = 18.290(4) Å α = 78.492(6) ^{o} β = 83.694(7) ^{o} γ = 86.519(7) ^{o} V = 3207.8(13) Å^3
Space Group	P-1 (#2)
Z value	2
D_{calc}	1.320 g/cm^3
F_{000}	1334.00
μ(MoKα)	3.683 cm^{-1}

B. Intensity Measurements

Detector	Rigaku Saturn
Goniometer	Rigaku AFC10
Radiation	MoKα (λ = 0.71075 Å) graphite monochromated
Detector Aperture	70 mm x 70 mm
Data Images	720 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	-110.0 - 70.0^{o}
Exposure Rate	120.0 sec./^{o}
Detector Swing Angle	-20.25^{o}
ω oscillation Range (χ=45.0, ϕ=90.0)	-110.0 - 70.0^{o}
Exposure Rate	120.0 sec./^{o}
Detector Swing Angle	-20.25^{o}
Detector Position	49.97 mm
Pixel Size	0.137 mm
$2\theta_{max}$	50.1^{o}
No. of Reflections Measured	Total: 17709 Unique: 10486 (R_{int} = 0.046)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.880 - 0.978)

C. Structure Solution and Refinement

Structure Solution	Direct Methods
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma\ w\ (Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\ \sigma^2(Fo^2) + (0.0483 \cdot P)^2 + 9.2490 \cdot P\ ]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	50.1^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	10486
No. Variables	762
Reflection/Parameter Ratio	13.76
Residuals: R1 ($I>2.00\sigma(I)$)	0.0625
Residuals: R (All reflections)	0.0953
Residuals: wR2 (All reflections)	0.1529
Goodness of Fit Indicator	1.033
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	0.84 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.79 $e^-/Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
Mo(1)	0.26673(3)	0.26235(3)	0.28651(2)	1.332(10)	
P(1)	0.37234(10)	0.13693(9)	0.36297(7)	1.34(2)	
P(2)	0.12521(10)	0.15733(10)	0.36326(8)	1.59(2)	
P(3)	0.14970(10)	0.37909(10)	0.21495(7)	1.34(2)	
P(4)	0.24203(10)	0.39156(10)	0.36554(7)	1.44(2)	
Si(1)	0.38232(10)	0.35592(10)	0.17632(8)	1.45(2)	
N(1)	0.2762(3)	0.1489(3)	0.1501(2)	2.14(8)	
C(1)	0.2739(3)	0.1885(3)	0.2030(2)	1.71(9)	
C(2A)	0.2782(9)	0.0998(9)	0.0888(6)	2.7(2)	1/2
C(2B)	0.3127(9)	0.1542(8)	0.0696(6)	2.3(2)	1/2
C(3A)	0.3710(10)	0.1268(10)	0.0336(7)	3.5(2)	1/2
C(3B)	0.3654(9)	0.0560(9)	0.0589(7)	3.1(2)	1/2
C(4A)	0.3723(9)	0.0730(9)	-0.0329(6)	3.0(2)	1/2
C(4B)	0.2895(12)	-0.0202(11)	0.0706(9)	5.5(3)	1/2
C(5A)	0.2715(9)	0.0984(9)	-0.0686(7)	3.1(2)	1/2
C(5B)	0.1999(14)	0.0119(14)	0.0173(10)	6.3(4)	1/2
C(6A)	0.1731(11)	0.0780(11)	-0.0168(8)	4.0(2)	1/2
C(6B)	0.1517(14)	0.1076(13)	0.0371(11)	5.1(4)	1/2
C(7A)	0.1781(13)	0.1325(14)	0.0522(9)	4.5(3)	1/2
C(7B)	0.2245(9)	0.1842(9)	0.0193(7)	2.8(2)	1/2
C(8)	0.2895(3)	0.0650(3)	0.4417(2)	1.70(9)	
C(9)	0.1885(3)	0.0433(3)	0.4138(2)	1.77(9)	
C(10)	0.1442(3)	0.4967(3)	0.2457(2)	1.71(9)	
C(11)	0.1346(3)	0.4765(3)	0.3315(2)	1.72(9)	
C(12)	0.4405(3)	0.0345(3)	0.3241(2)	1.59(8)	
C(13)	0.5440(4)	0.0049(3)	0.3345(3)	1.94(9)	
C(14)	0.5926(4)	-0.0706(4)	0.3027(3)	2.16(10)	
C(15)	0.5400(4)	-0.1201(4)	0.2617(3)	2.59(10)	
C(16)	0.4381(4)	-0.0923(4)	0.2508(3)	2.33(10)	
C(17)	0.3888(4)	-0.0154(3)	0.2810(2)	1.70(9)	
C(18)	0.4799(3)	0.1710(3)	0.4093(2)	1.53(8)	
C(19)	0.5611(3)	0.2234(3)	0.3648(2)	1.74(9)	
C(20)	0.6440(4)	0.2508(4)	0.3970(3)	2.23(10)	
C(21)	0.6463(4)	0.2296(4)	0.4733(3)	2.37(10)	
C(22)	0.5658(4)	0.1788(4)	0.5181(3)	2.14(9)	
C(23)	0.4850(3)	0.1475(3)	0.4862(2)	1.58(8)	
C(24)	0.0274(3)	0.0973(3)	0.3231(3)	1.83(9)	

Table 1. Atomic coordinates and B_{iso}/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
C(25)	0.0601(4)	0.0522(3)	0.2625(3)	2.00(9)	
C(26)	-0.0079(4)	0.0031(4)	0.2311(3)	2.48(10)	
C(27)	-0.1117(4)	-0.0013(4)	0.2600(3)	3.04(12)	
C(28)	-0.1459(4)	0.0432(4)	0.3189(3)	3.04(12)	
C(29)	-0.0776(4)	0.0923(4)	0.3511(3)	2.53(10)	
C(30)	0.0420(3)	0.2021(4)	0.4391(2)	1.88(9)	
C(31)	0.0465(4)	0.1624(4)	0.5150(3)	2.29(10)	
C(32)	-0.0205(4)	0.1981(4)	0.5689(3)	2.67(11)	
C(33)	-0.0917(4)	0.2739(4)	0.5481(3)	2.82(11)	
C(34)	-0.0967(4)	0.3140(4)	0.4724(3)	2.34(10)	
C(35)	-0.0305(3)	0.2783(3)	0.4193(3)	1.98(9)	
C(36)	0.0103(3)	0.3589(3)	0.2109(2)	1.53(8)	
C(37)	-0.0714(4)	0.4174(4)	0.2357(2)	2.00(9)	
C(38)	-0.1746(4)	0.3966(4)	0.2302(3)	2.56(11)	
C(39)	-0.1959(4)	0.3187(4)	0.1992(3)	2.52(10)	
C(40)	-0.1156(4)	0.2614(4)	0.1738(3)	2.34(10)	
C(41)	-0.0126(3)	0.2806(4)	0.1794(2)	1.97(9)	
C(42)	0.1915(3)	0.4122(3)	0.1153(2)	1.67(9)	
C(43)	0.1264(4)	0.4561(4)	0.0602(3)	2.15(10)	
C(44)	0.1656(4)	0.4780(4)	-0.0143(3)	2.19(10)	
C(45)	0.2684(4)	0.4548(3)	-0.0349(2)	1.95(9)	
C(46)	0.3339(4)	0.4138(3)	0.0184(2)	1.82(9)	
C(47)	0.2979(3)	0.3924(3)	0.0953(2)	1.51(8)	
C(48)	0.3454(3)	0.4771(3)	0.3669(2)	1.67(9)	
C(49)	0.4364(3)	0.4399(3)	0.3993(2)	1.84(9)	
C(50)	0.5114(4)	0.5018(4)	0.4087(3)	2.42(10)	
C(51)	0.4980(4)	0.6018(4)	0.3872(3)	2.81(11)	
C(52)	0.4103(4)	0.6394(4)	0.3532(3)	2.62(10)	
C(53)	0.3349(4)	0.5779(3)	0.3425(2)	1.97(9)	
C(54)	0.2064(3)	0.3710(3)	0.4680(2)	1.59(8)	
C(55)	0.2640(4)	0.2997(3)	0.5133(3)	2.07(9)	
C(56)	0.2514(4)	0.2885(4)	0.5900(3)	2.31(10)	
C(57)	0.1810(4)	0.3480(4)	0.6246(3)	2.62(11)	
C(58)	0.1218(4)	0.4172(4)	0.5816(3)	2.89(12)	
C(59)	0.1346(4)	0.4294(4)	0.5038(3)	2.21(10)	
C(60)	0.4381(3)	0.4804(3)	0.1763(2)	1.60(9)	
C(61)	0.4026(4)	0.5671(3)	0.1331(3)	2.11(9)	

Table 1. Atomic coordinates and B_{iso}/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
C(62)	0.4516(4)	0.6553(4)	0.1277(3)	2.62(10)	
C(63)	0.5372(4)	0.6577(4)	0.1657(3)	2.55(11)	
C(64)	0.5727(4)	0.5727(4)	0.2111(3)	2.44(10)	
C(65)	0.5236(3)	0.4862(4)	0.2160(2)	1.93(9)	
C(66)	0.5034(3)	0.2911(3)	0.1377(2)	1.62(9)	
C(67)	0.5278(3)	0.1916(3)	0.1621(2)	1.77(9)	
C(68)	0.6150(4)	0.1444(4)	0.1323(3)	2.17(10)	
C(69)	0.6816(3)	0.1965(4)	0.0756(2)	2.03(9)	
C(70)	0.6612(3)	0.2947(4)	0.0508(3)	2.05(9)	
C(71)	0.5741(3)	0.3414(4)	0.0813(2)	1.97(9)	
C(72)	0.1102(5)	0.7626(4)	0.1805(3)	3.40(12)	
C(73)	0.0075(5)	0.7462(4)	0.2085(3)	3.62(13)	
C(74)	-0.0621(5)	0.7124(5)	0.1672(3)	4.17(14)	
C(75)	-0.0279(6)	0.6957(5)	0.0967(4)	4.40(15)	
C(76)	0.0731(6)	0.7123(5)	0.0673(4)	4.59(16)	
C(77)	0.1414(5)	0.7456(5)	0.1093(3)	4.15(14)	
C(78)	0.1853(5)	0.7963(5)	0.2248(4)	4.70(16)	

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
H(1A)	0.2795	0.0274	0.1076	3.23	1/2
H(1B)	0.3663	0.2051	0.0551	2.75	1/2
H(2A)	0.4355	0.1089	0.0587	4.17	1/2
H(2B)	0.4011	0.0631	0.0075	3.77	1/2
H(3A)	0.3688	0.1984	0.0146	4.17	1/2
H(3B)	0.4186	0.0368	0.0947	3.77	1/2
H(4A)	0.4323	0.0934	-0.0702	3.55	1/2
H(4B)	0.2590	-0.0324	0.1236	6.55	1/2
H(5A)	0.3795	0.0014	-0.0147	3.55	1/2
H(5B)	0.3246	-0.0818	0.0602	6.55	1/2
H(6A)	0.2703	0.1689	-0.0917	3.67	1/2
H(6B)	0.2289	0.0224	-0.0360	7.54	1/2
H(7A)	0.2713	0.0614	-0.1095	3.67	1/2
H(7B)	0.1471	-0.0387	0.0260	7.54	1/2
H(8A)	0.1674	0.0066	0.0017	4.82	1/2
H(8B)	0.0900	0.1278	0.0092	6.15	1/2
H(9A)	0.1114	0.1027	-0.0437	4.82	1/2
H(9B)	0.1280	0.0967	0.0914	6.15	1/2
H(10A)	0.1765	0.2042	0.0339	5.39	1/2
H(10B)	0.1900	0.2466	0.0284	3.32	1/2
H(11A)	0.1169	0.1162	0.0893	5.39	1/2
H(11B)	0.2523	0.1931	-0.0342	3.32	1/2
H(12)	0.3268	0.0030	0.4620	2.04	
H(13)	0.2740	0.1026	0.4825	2.04	
H(14)	0.1403	0.0128	0.4569	2.13	
H(15)	0.2033	-0.0038	0.3796	2.13	
H(16)	0.2082	0.5325	0.2255	2.06	
H(17)	0.0834	0.5373	0.2272	2.06	
H(18)	0.0668	0.4473	0.3515	2.06	
H(19)	0.1375	0.5386	0.3493	2.06	
H(20)	0.5817	0.0369	0.3638	2.33	
H(21)	0.6637	-0.0882	0.3094	2.59	
H(22)	0.5734	-0.1728	0.2412	3.11	
H(23)	0.4008	-0.1260	0.2224	2.80	
H(24)	0.3187	0.0034	0.2721	2.04	
H(25)	0.5592	0.2402	0.3120	2.09	
H(26)	0.6996	0.2844	0.3660	2.67	

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
H(27)	0.7026	0.2496	0.4953	2.84	
H(28)	0.5662	0.1654	0.5711	2.56	
H(29)	0.4325	0.1095	0.5172	1.90	
H(30)	0.1311	0.0552	0.2422	2.40	
H(31)	0.0163	-0.0274	0.1901	2.98	
H(32)	-0.1589	-0.0350	0.2388	3.64	
H(33)	-0.2173	0.0405	0.3381	3.65	
H(34)	-0.1026	0.1224	0.3922	3.04	
H(35)	0.0956	0.1106	0.5299	2.75	
H(36)	-0.0173	0.1702	0.6204	3.21	
H(37)	-0.1371	0.2985	0.5852	3.39	
H(38)	-0.1457	0.3659	0.4577	2.81	
H(39)	-0.0343	0.3063	0.3678	2.38	
H(40)	-0.0573	0.4718	0.2565	2.40	
H(41)	-0.2302	0.4365	0.2479	3.07	
H(42)	-0.2660	0.3049	0.1954	3.03	
H(43)	-0.1303	0.2080	0.1521	2.80	
H(44)	0.0424	0.2401	0.1616	2.36	
H(45)	0.0551	0.4707	0.0743	2.58	
H(46)	0.1217	0.5089	-0.0513	2.63	
H(47)	0.2944	0.4674	-0.0864	2.34	
H(48)	0.4049	0.3994	0.0030	2.18	
H(49)	0.4468	0.3711	0.4150	2.20	
H(50)	0.5730	0.4751	0.4303	2.91	
H(51)	0.5484	0.6442	0.3957	3.37	
H(52)	0.4012	0.7082	0.3368	3.14	
H(53)	0.2755	0.6050	0.3182	2.36	
H(54)	0.3129	0.2580	0.4907	2.48	
H(55)	0.2915	0.2394	0.6196	2.77	
H(56)	0.1737	0.3409	0.6776	3.14	
H(57)	0.0717	0.4571	0.6050	3.47	
H(58)	0.0936	0.4783	0.4746	2.66	
H(59)	0.3436	0.5665	0.1064	2.53	
H(60)	0.4257	0.7136	0.0977	3.14	
H(61)	0.5719	0.7171	0.1610	3.06	
H(62)	0.6306	0.5741	0.2386	2.93	
H(63)	0.5485	0.4286	0.2474	2.32	

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
H(64)	0.4826	0.1549	0.2007	2.12	
H(65)	0.6290	0.0767	0.1505	2.60	
H(66)	0.7410	0.1645	0.0542	2.43	
H(67)	0.7071	0.3308	0.0124	2.46	
H(68)	0.5618	0.4095	0.0635	2.36	
H(69)	-0.0161	0.7583	0.2570	4.35	
H(70)	-0.1322	0.7011	0.1874	5.00	
H(71)	-0.0746	0.6725	0.0682	5.28	
H(72)	0.0963	0.7012	0.0185	5.51	
H(73)	0.2113	0.7570	0.0887	4.97	
H(74)	0.2454	0.8234	0.1912	5.64	
H(75)	0.2089	0.7409	0.2620	5.64	
H(76)	0.1514	0.8469	0.2505	5.64	

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mo(1)	0.0130(2)	0.0177(2)	0.0190(2)	-0.00316(17)	0.00103(17)	-0.00218(18)
P(1)	0.0134(6)	0.0173(6)	0.0195(7)	-0.0015(5)	-0.0009(5)	-0.0023(5)
P(2)	0.0139(6)	0.0205(7)	0.0243(7)	-0.0049(5)	0.0021(5)	-0.0011(5)
P(3)	0.0139(6)	0.0177(6)	0.0187(7)	-0.0005(5)	-0.0005(5)	-0.0027(5)
P(4)	0.0147(6)	0.0190(6)	0.0207(7)	-0.0025(5)	0.0018(5)	-0.0048(5)
Si(1)	0.0143(6)	0.0197(7)	0.0193(7)	-0.0031(5)	0.0025(5)	-0.0011(6)
N(1)	0.029(2)	0.028(2)	0.027(2)	-0.001(2)	-0.002(2)	-0.012(2)
C(1)	0.014(2)	0.023(2)	0.024(2)	-0.000(2)	-0.002(2)	0.004(2)
C(8)	0.019(2)	0.019(2)	0.024(2)	0.000(2)	0.002(2)	-0.000(2)
C(9)	0.018(2)	0.021(2)	0.025(2)	-0.007(2)	0.006(2)	0.002(2)
C(10)	0.018(2)	0.022(2)	0.026(2)	-0.000(2)	-0.003(2)	-0.006(2)
C(11)	0.012(2)	0.024(2)	0.031(3)	0.000(2)	0.001(2)	-0.011(2)
C(12)	0.022(2)	0.015(2)	0.020(2)	-0.002(2)	0.002(2)	0.002(2)
C(13)	0.023(2)	0.018(2)	0.030(3)	-0.005(2)	-0.000(2)	0.000(2)
C(14)	0.020(2)	0.025(3)	0.034(3)	0.004(2)	0.003(2)	-0.002(2)
C(15)	0.037(3)	0.022(3)	0.039(3)	-0.001(2)	0.004(2)	-0.009(2)
C(16)	0.036(3)	0.025(3)	0.031(3)	-0.006(2)	-0.008(2)	-0.008(2)
C(17)	0.024(2)	0.018(2)	0.021(2)	0.000(2)	-0.004(2)	-0.000(2)
C(18)	0.019(2)	0.016(2)	0.023(2)	-0.002(2)	0.001(2)	-0.003(2)
C(19)	0.019(2)	0.024(2)	0.021(2)	-0.001(2)	-0.002(2)	0.001(2)
C(20)	0.018(2)	0.033(3)	0.033(3)	-0.011(2)	-0.004(2)	-0.002(2)
C(21)	0.022(2)	0.036(3)	0.034(3)	-0.010(2)	-0.007(2)	-0.006(2)
C(22)	0.031(3)	0.026(3)	0.025(3)	-0.003(2)	-0.006(2)	-0.002(2)
C(23)	0.018(2)	0.016(2)	0.023(2)	-0.001(2)	-0.000(2)	0.000(2)
C(24)	0.022(2)	0.020(2)	0.027(2)	-0.009(2)	-0.003(2)	-0.001(2)
C(25)	0.020(2)	0.025(2)	0.030(3)	-0.004(2)	-0.001(2)	-0.002(2)
C(26)	0.032(3)	0.034(3)	0.031(3)	-0.005(2)	-0.006(2)	-0.009(2)
C(27)	0.029(3)	0.048(4)	0.043(3)	-0.017(2)	-0.004(2)	-0.013(3)
C(28)	0.021(2)	0.049(4)	0.051(4)	-0.015(2)	0.001(2)	-0.020(3)
C(29)	0.023(2)	0.042(3)	0.033(3)	-0.016(2)	0.003(2)	-0.012(2)
C(30)	0.017(2)	0.031(3)	0.025(2)	-0.011(2)	-0.001(2)	-0.004(2)
C(31)	0.018(2)	0.036(3)	0.033(3)	-0.005(2)	-0.003(2)	-0.004(2)
C(32)	0.032(3)	0.046(3)	0.023(3)	-0.013(2)	0.004(2)	-0.006(2)
C(33)	0.023(3)	0.046(3)	0.041(3)	-0.010(2)	0.011(2)	-0.022(3)
C(34)	0.020(2)	0.030(3)	0.036(3)	-0.003(2)	0.001(2)	0.001(2)
C(35)	0.020(2)	0.026(3)	0.029(3)	-0.003(2)	0.003(2)	-0.007(2)
C(36)	0.013(2)	0.024(2)	0.019(2)	-0.001(2)	-0.005(2)	0.003(2)

Table 3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(37)	0.023(2)	0.024(2)	0.028(3)	0.003(2)	0.000(2)	-0.005(2)
C(38)	0.018(2)	0.046(3)	0.030(3)	0.006(2)	-0.000(2)	-0.002(2)
C(39)	0.017(2)	0.047(3)	0.030(3)	-0.007(2)	-0.003(2)	-0.001(2)
C(40)	0.029(3)	0.033(3)	0.026(3)	-0.012(2)	-0.005(2)	-0.002(2)
C(41)	0.017(2)	0.030(3)	0.026(2)	-0.002(2)	-0.004(2)	0.000(2)
C(42)	0.021(2)	0.020(2)	0.022(2)	-0.003(2)	-0.002(2)	-0.004(2)
C(43)	0.017(2)	0.035(3)	0.030(3)	-0.006(2)	-0.003(2)	-0.006(2)
C(44)	0.027(3)	0.029(3)	0.027(3)	-0.004(2)	-0.010(2)	0.002(2)
C(45)	0.032(3)	0.029(3)	0.014(2)	-0.005(2)	-0.006(2)	-0.001(2)
C(46)	0.022(2)	0.019(2)	0.025(2)	-0.005(2)	0.006(2)	-0.001(2)
C(47)	0.015(2)	0.016(2)	0.026(2)	-0.004(2)	0.003(2)	-0.004(2)
C(48)	0.020(2)	0.024(2)	0.020(2)	-0.008(2)	0.003(2)	-0.006(2)
C(49)	0.024(2)	0.023(2)	0.022(2)	-0.003(2)	0.001(2)	-0.002(2)
C(50)	0.026(2)	0.039(3)	0.029(3)	-0.013(2)	-0.000(2)	-0.007(2)
C(51)	0.040(3)	0.041(3)	0.029(3)	-0.022(2)	0.003(2)	-0.012(2)
C(52)	0.039(3)	0.026(3)	0.035(3)	-0.012(2)	-0.002(2)	-0.005(2)
C(53)	0.026(2)	0.023(2)	0.024(2)	-0.002(2)	0.002(2)	-0.004(2)
C(54)	0.017(2)	0.020(2)	0.024(2)	-0.005(2)	-0.002(2)	-0.003(2)
C(55)	0.024(2)	0.024(2)	0.030(3)	-0.003(2)	0.004(2)	-0.007(2)
C(56)	0.026(2)	0.029(3)	0.029(3)	-0.004(2)	-0.006(2)	0.004(2)
C(57)	0.030(3)	0.050(3)	0.019(2)	-0.009(2)	0.002(2)	-0.007(2)
C(58)	0.025(3)	0.059(4)	0.027(3)	0.005(2)	0.007(2)	-0.017(3)
C(59)	0.020(2)	0.036(3)	0.026(3)	0.008(2)	0.001(2)	-0.005(2)
C(60)	0.017(2)	0.024(2)	0.019(2)	-0.006(2)	0.007(2)	-0.004(2)
C(61)	0.030(3)	0.025(3)	0.025(3)	-0.003(2)	-0.004(2)	-0.001(2)
C(62)	0.043(3)	0.027(3)	0.029(3)	-0.008(2)	0.002(2)	-0.003(2)
C(63)	0.035(3)	0.030(3)	0.034(3)	-0.015(2)	0.008(2)	-0.014(2)
C(64)	0.023(2)	0.036(3)	0.036(3)	-0.011(2)	0.004(2)	-0.013(2)
C(65)	0.023(2)	0.025(3)	0.023(2)	-0.002(2)	0.001(2)	-0.000(2)
C(66)	0.015(2)	0.028(3)	0.020(2)	-0.004(2)	-0.003(2)	-0.007(2)
C(67)	0.015(2)	0.023(2)	0.025(2)	-0.002(2)	0.004(2)	0.001(2)
C(68)	0.027(2)	0.023(2)	0.029(3)	0.005(2)	-0.001(2)	-0.000(2)
C(69)	0.016(2)	0.035(3)	0.024(2)	0.007(2)	-0.000(2)	-0.006(2)
C(70)	0.019(2)	0.029(3)	0.026(3)	0.002(2)	0.002(2)	0.002(2)
C(71)	0.018(2)	0.028(3)	0.025(3)	-0.003(2)	-0.000(2)	0.001(2)
C(72)	0.040(3)	0.033(3)	0.053(4)	0.002(2)	0.005(3)	-0.008(3)
C(73)	0.045(3)	0.044(4)	0.046(4)	-0.008(3)	0.008(3)	-0.007(3)

Table 3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(74)	0.057(4)	0.056(4)	0.043(4)	-0.011(3)	0.001(3)	-0.005(3)
C(75)	0.066(5)	0.046(4)	0.058(4)	-0.001(3)	-0.008(4)	-0.015(3)
C(76)	0.063(5)	0.052(4)	0.058(4)	-0.003(3)	0.014(4)	-0.017(3)
C(77)	0.053(4)	0.055(4)	0.046(4)	0.002(3)	0.012(3)	-0.013(3)
C(78)	0.051(4)	0.062(5)	0.068(5)	0.005(3)	-0.016(4)	-0.016(4)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Mo(1)	P(1)	2.4559(12)	Mo(1)	P(2)	2.5297(13)
Mo(1)	P(3)	2.4364(13)	Mo(1)	P(4)	2.5120(15)
Mo(1)	Si(1)	2.5536(13)	Mo(1)	C(1)	1.996(5)
P(1)	C(8)	1.855(4)	P(1)	C(12)	1.855(5)
P(1)	C(18)	1.836(5)	P(2)	C(9)	1.864(4)
P(2)	C(24)	1.847(5)	P(2)	C(30)	1.845(5)
P(3)	C(10)	1.833(5)	P(3)	C(36)	1.851(4)
P(3)	C(42)	1.818(4)	P(4)	C(11)	1.848(4)
P(4)	C(48)	1.850(5)	P(4)	C(54)	1.848(5)
Si(1)	C(47)	1.905(5)	Si(1)	C(60)	1.920(5)
Si(1)	C(66)	1.898(5)	N(1)	C(1)	1.204(7)
N(1)	C(2A)	1.423(14)	N(1)	C(2B)	1.484(12)
C(2A)	C(3A)	1.495(16)	C(2A)	C(7A)	1.52(2)
C(2B)	C(3B)	1.530(18)	C(2B)	C(7B)	1.530(17)
C(3A)	C(4A)	1.55(2)	C(3B)	C(4B)	1.46(2)
C(4A)	C(5A)	1.512(17)	C(4B)	C(5B)	1.58(2)
C(5A)	C(6A)	1.505(17)	C(5B)	C(6B)	1.53(2)
C(6A)	C(7A)	1.61(2)	C(6B)	C(7B)	1.43(2)
C(8)	C(9)	1.521(7)	C(10)	C(11)	1.529(7)
C(12)	C(13)	1.398(7)	C(12)	C(17)	1.393(8)
C(13)	C(14)	1.387(7)	C(14)	C(15)	1.370(9)
C(15)	C(16)	1.374(8)	C(16)	C(17)	1.392(7)
C(18)	C(19)	1.402(6)	C(18)	C(23)	1.387(7)
C(19)	C(20)	1.386(8)	C(20)	C(21)	1.370(8)
C(21)	C(22)	1.389(7)	C(22)	C(23)	1.382(8)
C(24)	C(25)	1.396(8)	C(24)	C(29)	1.397(7)
C(25)	C(26)	1.382(8)	C(26)	C(27)	1.386(7)
C(27)	C(28)	1.367(9)	C(28)	C(29)	1.395(9)
C(30)	C(31)	1.394(7)	C(30)	C(35)	1.393(7)
C(31)	C(32)	1.387(8)	C(32)	C(33)	1.382(8)
C(33)	C(34)	1.392(8)	C(34)	C(35)	1.371(7)
C(36)	C(37)	1.388(7)	C(36)	C(41)	1.393(8)
C(37)	C(38)	1.399(7)	C(38)	C(39)	1.377(9)
C(39)	C(40)	1.369(8)	C(40)	C(41)	1.391(7)
C(42)	C(43)	1.405(7)	C(42)	C(47)	1.408(6)
C(43)	C(44)	1.382(7)	C(44)	C(45)	1.377(7)
C(45)	C(46)	1.376(7)	C(46)	C(47)	1.410(6)

Table 4. Bond lengths (Å) (continued)

atom	atom	distance	atom	atom	distance
C(48)	C(49)	1.400(7)	C(48)	C(53)	1.390(7)
C(49)	C(50)	1.383(8)	C(50)	C(51)	1.378(8)
C(51)	C(52)	1.377(8)	C(52)	C(53)	1.391(8)
C(54)	C(55)	1.396(6)	C(54)	C(59)	1.394(7)
C(55)	C(56)	1.372(7)	C(56)	C(57)	1.380(8)
C(57)	C(58)	1.370(8)	C(58)	C(59)	1.391(7)
C(60)	C(61)	1.390(6)	C(60)	C(65)	1.401(7)
C(61)	C(62)	1.399(8)	C(62)	C(63)	1.375(8)
C(63)	C(64)	1.390(7)	C(64)	C(65)	1.380(8)
C(66)	C(67)	1.398(7)	C(66)	C(71)	1.405(6)
C(67)	C(68)	1.385(7)	C(68)	C(69)	1.386(6)
C(69)	C(70)	1.374(7)	C(70)	C(71)	1.386(7)
C(72)	C(73)	1.383(8)	C(72)	C(77)	1.381(10)
C(72)	C(78)	1.484(11)	C(73)	C(74)	1.394(11)
C(74)	C(75)	1.376(10)	C(75)	C(76)	1.370(10)
C(76)	C(77)	1.386(11)			

Table 5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C(2A)	H(1A)	1.000	C(2B)	H(1B)	1.000
C(3A)	H(2A)	0.990	C(3A)	H(3A)	0.990
C(3B)	H(2B)	0.990	C(3B)	H(3B)	0.990
C(4A)	H(4A)	0.990	C(4A)	H(5A)	0.990
C(4B)	H(4B)	0.990	C(4B)	H(5B)	0.990
C(5A)	H(6A)	0.990	C(5A)	H(7A)	0.990
C(5B)	H(6B)	0.990	C(5B)	H(7B)	0.990
C(6A)	H(8A)	0.990	C(6A)	H(9A)	0.990
C(6B)	H(8B)	0.990	C(6B)	H(9B)	0.990
C(7A)	H(10A)	0.990	C(7A)	H(11A)	0.990
C(7B)	H(10B)	0.990	C(7B)	H(11B)	0.990
C(8)	H(12)	0.990	C(8)	H(13)	0.990
C(9)	H(14)	0.990	C(9)	H(15)	0.990
C(10)	H(16)	0.990	C(10)	H(17)	0.990
C(11)	H(18)	0.990	C(11)	H(19)	0.990
C(13)	H(20)	0.950	C(14)	H(21)	0.950
C(15)	H(22)	0.950	C(16)	H(23)	0.950
C(17)	H(24)	0.950	C(19)	H(25)	0.950
C(20)	H(26)	0.950	C(21)	H(27)	0.950
C(22)	H(28)	0.950	C(23)	H(29)	0.950
C(25)	H(30)	0.950	C(26)	H(31)	0.950
C(27)	H(32)	0.950	C(28)	H(33)	0.950
C(29)	H(34)	0.950	C(31)	H(35)	0.950
C(32)	H(36)	0.950	C(33)	H(37)	0.950
C(34)	H(38)	0.950	C(35)	H(39)	0.950
C(37)	H(40)	0.950	C(38)	H(41)	0.950
C(39)	H(42)	0.950	C(40)	H(43)	0.950
C(41)	H(44)	0.950	C(43)	H(45)	0.950
C(44)	H(46)	0.950	C(45)	H(47)	0.950
C(46)	H(48)	0.950	C(49)	H(49)	0.950
C(50)	H(50)	0.950	C(51)	H(51)	0.950
C(52)	H(52)	0.950	C(53)	H(53)	0.950
C(55)	H(54)	0.950	C(56)	H(55)	0.950
C(57)	H(56)	0.950	C(58)	H(57)	0.950
C(59)	H(58)	0.950	C(61)	H(59)	0.950
C(62)	H(60)	0.950	C(63)	H(61)	0.950
C(64)	H(62)	0.950	C(65)	H(63)	0.950

Table 5. Bond lengths involving hydrogens (Å) (continued)

atom	atom	distance	atom	atom	distance
C(67)	H(64)	0.950	C(68)	H(65)	0.950
C(69)	H(66)	0.950	C(70)	H(67)	0.950
C(71)	H(68)	0.950	C(73)	H(69)	0.950
C(74)	H(70)	0.950	C(75)	H(71)	0.950
C(76)	H(72)	0.950	C(77)	H(73)	0.950
C(78)	H(74)	0.980	C(78)	H(75)	0.980
C(78)	H(76)	0.980			

Table 6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
P(1)	Mo(1)	P(2)	79.45(4)	P(1)	Mo(1)	P(3)	175.37(4)
P(1)	Mo(1)	P(4)	101.40(4)	P(1)	Mo(1)	Si(1)	109.78(4)
P(1)	Mo(1)	C(1)	93.15(14)	P(2)	Mo(1)	P(3)	95.95(4)
P(2)	Mo(1)	P(4)	94.14(4)	P(2)	Mo(1)	Si(1)	162.45(5)
P(2)	Mo(1)	C(1)	92.49(14)	P(3)	Mo(1)	P(4)	79.31(4)
P(3)	Mo(1)	Si(1)	74.53(4)	P(3)	Mo(1)	C(1)	86.50(14)
P(4)	Mo(1)	Si(1)	98.41(4)	P(4)	Mo(1)	C(1)	164.88(14)
Si(1)	Mo(1)	C(1)	72.53(14)	Mo(1)	P(1)	C(8)	110.69(15)
Mo(1)	P(1)	C(12)	121.39(16)	Mo(1)	P(1)	C(18)	120.88(15)
C(8)	P(1)	C(12)	99.0(2)	C(8)	P(1)	C(18)	103.1(2)
C(12)	P(1)	C(18)	98.3(2)	Mo(1)	P(2)	C(9)	108.09(15)
Mo(1)	P(2)	C(24)	124.44(16)	Mo(1)	P(2)	C(30)	120.18(18)
C(9)	P(2)	C(24)	96.9(2)	C(9)	P(2)	C(30)	102.9(2)
C(24)	P(2)	C(30)	100.3(2)	Mo(1)	P(3)	C(10)	110.40(17)
Mo(1)	P(3)	C(36)	124.08(15)	Mo(1)	P(3)	C(42)	114.61(16)
C(10)	P(3)	C(36)	102.3(2)	C(10)	P(3)	C(42)	103.1(2)
C(36)	P(3)	C(42)	99.8(2)	Mo(1)	P(4)	C(11)	107.85(19)
Mo(1)	P(4)	C(48)	121.82(17)	Mo(1)	P(4)	C(54)	126.23(17)
C(11)	P(4)	C(48)	101.7(2)	C(11)	P(4)	C(54)	101.0(2)
C(48)	P(4)	C(54)	94.2(2)	Mo(1)	Si(1)	C(47)	106.64(14)
Mo(1)	Si(1)	C(60)	123.41(16)	Mo(1)	Si(1)	C(66)	118.81(15)
C(47)	Si(1)	C(60)	99.8(2)	C(47)	Si(1)	C(66)	105.8(2)
C(60)	Si(1)	C(66)	99.8(2)	C(1)	N(1)	C(2A)	178.5(6)
C(1)	N(1)	C(2B)	145.7(6)	Mo(1)	C(1)	N(1)	176.2(4)
N(1)	C(2A)	C(3A)	110.9(10)	N(1)	C(2A)	C(7A)	106.3(10)
C(3A)	C(2A)	C(7A)	110.2(10)	N(1)	C(2B)	C(3B)	109.4(8)
N(1)	C(2B)	C(7B)	112.2(8)	C(3B)	C(2B)	C(7B)	111.7(11)
C(2A)	C(3A)	C(4A)	110.5(11)	C(2B)	C(3B)	C(4B)	111.2(10)
C(3A)	C(4A)	C(5A)	108.6(10)	C(3B)	C(4B)	C(5B)	110.2(12)
C(4A)	C(5A)	C(6A)	115.8(10)	C(4B)	C(5B)	C(6B)	105.5(16)
C(5A)	C(6A)	C(7A)	107.8(12)	C(5B)	C(6B)	C(7B)	111.7(14)
C(2A)	C(7A)	C(6A)	109.3(13)	C(2B)	C(7B)	C(6B)	107.3(11)
P(1)	C(8)	C(9)	109.3(3)	P(2)	C(9)	C(8)	111.0(3)
P(3)	C(10)	C(11)	108.3(3)	P(4)	C(11)	C(10)	109.6(3)
P(1)	C(12)	C(13)	123.0(4)	P(1)	C(12)	C(17)	119.9(3)
C(13)	C(12)	C(17)	117.1(4)	C(12)	C(13)	C(14)	121.0(5)
C(13)	C(14)	C(15)	121.2(5)	C(14)	C(15)	C(16)	118.8(5)

Table 6. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(15)	C(16)	C(17)	120.8(5)	C(12)	C(17)	C(16)	121.2(4)
P(1)	C(18)	C(19)	118.4(3)	P(1)	C(18)	C(23)	123.4(3)
C(19)	C(18)	C(23)	118.2(4)	C(18)	C(19)	C(20)	120.7(4)
C(19)	C(20)	C(21)	120.4(4)	C(20)	C(21)	C(22)	119.5(5)
C(21)	C(22)	C(23)	120.4(5)	C(18)	C(23)	C(22)	120.7(4)
P(2)	C(24)	C(25)	118.6(3)	P(2)	C(24)	C(29)	123.7(4)
C(25)	C(24)	C(29)	117.7(5)	C(24)	C(25)	C(26)	121.8(4)
C(25)	C(26)	C(27)	119.5(5)	C(26)	C(27)	C(28)	119.8(6)
C(27)	C(28)	C(29)	121.0(5)	C(24)	C(29)	C(28)	120.1(5)
P(2)	C(30)	C(31)	123.5(3)	P(2)	C(30)	C(35)	118.2(3)
C(31)	C(30)	C(35)	118.3(4)	C(30)	C(31)	C(32)	120.3(4)
C(31)	C(32)	C(33)	120.5(5)	C(32)	C(33)	C(34)	119.6(5)
C(33)	C(34)	C(35)	119.8(5)	C(30)	C(35)	C(34)	121.5(4)
P(3)	C(36)	C(37)	124.3(4)	P(3)	C(36)	C(41)	117.1(3)
C(37)	C(36)	C(41)	118.6(4)	C(36)	C(37)	C(38)	120.3(5)
C(37)	C(38)	C(39)	120.3(5)	C(38)	C(39)	C(40)	119.7(5)
C(39)	C(40)	C(41)	120.8(5)	C(36)	C(41)	C(40)	120.3(4)
P(3)	C(42)	C(43)	124.7(3)	P(3)	C(42)	C(47)	115.0(3)
C(43)	C(42)	C(47)	120.3(4)	C(42)	C(43)	C(44)	120.3(4)
C(43)	C(44)	C(45)	119.8(4)	C(44)	C(45)	C(46)	120.7(4)
C(45)	C(46)	C(47)	121.4(4)	Si(1)	C(47)	C(42)	115.9(3)
Si(1)	C(47)	C(46)	126.2(3)	C(42)	C(47)	C(46)	117.4(4)
P(4)	C(48)	C(49)	118.5(3)	P(4)	C(48)	C(53)	123.7(3)
C(49)	C(48)	C(53)	117.7(5)	C(48)	C(49)	C(50)	120.8(4)
C(49)	C(50)	C(51)	120.9(5)	C(50)	C(51)	C(52)	119.0(5)
C(51)	C(52)	C(53)	120.7(5)	C(48)	C(53)	C(52)	120.9(4)
P(4)	C(54)	C(55)	117.9(3)	P(4)	C(54)	C(59)	124.4(3)
C(55)	C(54)	C(59)	117.2(4)	C(54)	C(55)	C(56)	121.3(5)
C(55)	C(56)	C(57)	120.7(4)	C(56)	C(57)	C(58)	119.2(5)
C(57)	C(58)	C(59)	120.4(5)	C(54)	C(59)	C(58)	121.0(4)
Si(1)	C(60)	C(61)	122.6(4)	Si(1)	C(60)	C(65)	120.5(3)
C(61)	C(60)	C(65)	116.7(4)	C(60)	C(61)	C(62)	121.7(5)
C(61)	C(62)	C(63)	120.0(5)	C(62)	C(63)	C(64)	119.5(5)
C(63)	C(64)	C(65)	119.9(5)	C(60)	C(65)	C(64)	122.1(4)
Si(1)	C(66)	C(67)	123.2(3)	Si(1)	C(66)	C(71)	121.1(3)
C(67)	C(66)	C(71)	115.8(4)	C(66)	C(67)	C(68)	122.8(4)
C(67)	C(68)	C(69)	119.6(4)	C(68)	C(69)	C(70)	119.5(4)

Table 6. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(69)	C(70)	C(71)	120.5(4)	C(66)	C(71)	C(70)	121.9(4)
C(73)	C(72)	C(77)	117.7(6)	C(73)	C(72)	C(78)	121.8(6)
C(77)	C(72)	C(78)	120.5(6)	C(72)	C(73)	C(74)	121.5(6)
C(73)	C(74)	C(75)	119.1(6)	C(74)	C(75)	C(76)	120.5(7)
C(75)	C(76)	C(77)	119.6(7)	C(72)	C(77)	C(76)	121.6(6)

Table 7. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	C(2A)	H(1A)	109.8	C(3A)	C(2A)	H(1A)	109.8
C(7A)	C(2A)	H(1A)	109.8	N(1)	C(2B)	H(1B)	107.8
C(3B)	C(2B)	H(1B)	107.8	C(7B)	C(2B)	H(1B)	107.8
C(2A)	C(3A)	H(2A)	109.6	C(2A)	C(3A)	H(3A)	109.6
C(4A)	C(3A)	H(2A)	109.6	C(4A)	C(3A)	H(3A)	109.6
H(2A)	C(3A)	H(3A)	108.1	C(2B)	C(3B)	H(2B)	109.4
C(2B)	C(3B)	H(3B)	109.4	C(4B)	C(3B)	H(2B)	109.4
C(4B)	C(3B)	H(3B)	109.4	H(2B)	C(3B)	H(3B)	108.0
C(3A)	C(4A)	H(4A)	110.0	C(3A)	C(4A)	H(5A)	110.0
C(5A)	C(4A)	H(4A)	110.0	C(5A)	C(4A)	H(5A)	110.0
H(4A)	C(4A)	H(5A)	108.4	C(3B)	C(4B)	H(4B)	109.6
C(3B)	C(4B)	H(5B)	109.6	C(5B)	C(4B)	H(4B)	109.6
C(5B)	C(4B)	H(5B)	109.6	H(4B)	C(4B)	H(5B)	108.1
C(4A)	C(5A)	H(6A)	108.3	C(4A)	C(5A)	H(7A)	108.3
C(6A)	C(5A)	H(6A)	108.3	C(6A)	C(5A)	H(7A)	108.3
H(6A)	C(5A)	H(7A)	107.4	C(4B)	C(5B)	H(6B)	110.6
C(4B)	C(5B)	H(7B)	110.6	C(6B)	C(5B)	H(6B)	110.6
C(6B)	C(5B)	H(7B)	110.6	H(6B)	C(5B)	H(7B)	108.7
C(5A)	C(6A)	H(8A)	110.2	C(5A)	C(6A)	H(9A)	110.2
C(7A)	C(6A)	H(8A)	110.2	C(7A)	C(6A)	H(9A)	110.2
H(8A)	C(6A)	H(9A)	108.5	C(5B)	C(6B)	H(8B)	109.3
C(5B)	C(6B)	H(9B)	109.3	C(7B)	C(6B)	H(8B)	109.3
C(7B)	C(6B)	H(9B)	109.3	H(8B)	C(6B)	H(9B)	108.0
C(2A)	C(7A)	H(10A)	109.8	C(2A)	C(7A)	H(11A)	109.8
C(6A)	C(7A)	H(10A)	109.8	C(6A)	C(7A)	H(11A)	109.8
H(10A)	C(7A)	H(11A)	108.3	C(2B)	C(7B)	H(10B)	110.3
C(2B)	C(7B)	H(11B)	110.3	C(6B)	C(7B)	H(10B)	110.3
C(6B)	C(7B)	H(11B)	110.3	H(10B)	C(7B)	H(11B)	108.5
P(1)	C(8)	H(12)	109.8	P(1)	C(8)	H(13)	109.8
C(9)	C(8)	H(12)	109.8	C(9)	C(8)	H(13)	109.8
H(12)	C(8)	H(13)	108.3	P(2)	C(9)	H(14)	109.4
P(2)	C(9)	H(15)	109.4	C(8)	C(9)	H(14)	109.4
C(8)	C(9)	H(15)	109.4	H(14)	C(9)	H(15)	108.0
P(3)	C(10)	H(16)	110.0	P(3)	C(10)	H(17)	110.0
C(11)	C(10)	H(16)	110.0	C(11)	C(10)	H(17)	110.0
H(16)	C(10)	H(17)	108.4	P(4)	C(11)	H(18)	109.8
P(4)	C(11)	H(19)	109.8	C(10)	C(11)	H(18)	109.7

Table 7. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(10)	C(11)	H(19)	109.7	H(18)	C(11)	H(19)	108.2
C(12)	C(13)	H(20)	119.5	C(14)	C(13)	H(20)	119.5
C(13)	C(14)	H(21)	119.4	C(15)	C(14)	H(21)	119.4
C(14)	C(15)	H(22)	120.6	C(16)	C(15)	H(22)	120.6
C(15)	C(16)	H(23)	119.6	C(17)	C(16)	H(23)	119.6
C(12)	C(17)	H(24)	119.4	C(16)	C(17)	H(24)	119.4
C(18)	C(19)	H(25)	119.7	C(20)	C(19)	H(25)	119.7
C(19)	C(20)	H(26)	119.8	C(21)	C(20)	H(26)	119.8
C(20)	C(21)	H(27)	120.3	C(22)	C(21)	H(27)	120.2
C(21)	C(22)	H(28)	119.8	C(23)	C(22)	H(28)	119.8
C(18)	C(23)	H(29)	119.7	C(22)	C(23)	H(29)	119.7
C(24)	C(25)	H(30)	119.1	C(26)	C(25)	H(30)	119.1
C(25)	C(26)	H(31)	120.2	C(27)	C(26)	H(31)	120.2
C(26)	C(27)	H(32)	120.1	C(28)	C(27)	H(32)	120.1
C(27)	C(28)	H(33)	119.5	C(29)	C(28)	H(33)	119.5
C(24)	C(29)	H(34)	119.9	C(28)	C(29)	H(34)	119.9
C(30)	C(31)	H(35)	119.8	C(32)	C(31)	H(35)	119.8
C(31)	C(32)	H(36)	119.8	C(33)	C(32)	H(36)	119.8
C(32)	C(33)	H(37)	120.2	C(34)	C(33)	H(37)	120.2
C(33)	C(34)	H(38)	120.1	C(35)	C(34)	H(38)	120.1
C(30)	C(35)	H(39)	119.2	C(34)	C(35)	H(39)	119.2
C(36)	C(37)	H(40)	119.9	C(38)	C(37)	H(40)	119.9
C(37)	C(38)	H(41)	119.8	C(39)	C(38)	H(41)	119.8
C(38)	C(39)	H(42)	120.2	C(40)	C(39)	H(42)	120.2
C(39)	C(40)	H(43)	119.6	C(41)	C(40)	H(43)	119.6
C(36)	C(41)	H(44)	119.8	C(40)	C(41)	H(44)	119.8
C(42)	C(43)	H(45)	119.9	C(44)	C(43)	H(45)	119.8
C(43)	C(44)	H(46)	120.1	C(45)	C(44)	H(46)	120.1
C(44)	C(45)	H(47)	119.7	C(46)	C(45)	H(47)	119.7
C(45)	C(46)	H(48)	119.3	C(47)	C(46)	H(48)	119.3
C(48)	C(49)	H(49)	119.6	C(50)	C(49)	H(49)	119.6
C(49)	C(50)	H(50)	119.6	C(51)	C(50)	H(50)	119.6
C(50)	C(51)	H(51)	120.5	C(52)	C(51)	H(51)	120.5
C(51)	C(52)	H(52)	119.6	C(53)	C(52)	H(52)	119.6
C(48)	C(53)	H(53)	119.6	C(52)	C(53)	H(53)	119.6
C(54)	C(55)	H(54)	119.3	C(56)	C(55)	H(54)	119.3
C(55)	C(56)	H(55)	119.6	C(57)	C(56)	H(55)	119.6

Table 7. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(56)	C(57)	H(56)	120.4	C(58)	C(57)	H(56)	120.4
C(57)	C(58)	H(57)	119.8	C(59)	C(58)	H(57)	119.8
C(54)	C(59)	H(58)	119.5	C(58)	C(59)	H(58)	119.5
C(60)	C(61)	H(59)	119.1	C(62)	C(61)	H(59)	119.1
C(61)	C(62)	H(60)	120.0	C(63)	C(62)	H(60)	120.0
C(62)	C(63)	H(61)	120.2	C(64)	C(63)	H(61)	120.2
C(63)	C(64)	H(62)	120.1	C(65)	C(64)	H(62)	120.1
C(60)	C(65)	H(63)	118.9	C(64)	C(65)	H(63)	118.9
C(66)	C(67)	H(64)	118.6	C(68)	C(67)	H(64)	118.6
C(67)	C(68)	H(65)	120.2	C(69)	C(68)	H(65)	120.2
C(68)	C(69)	H(66)	120.3	C(70)	C(69)	H(66)	120.3
C(69)	C(70)	H(67)	119.7	C(71)	C(70)	H(67)	119.7
C(66)	C(71)	H(68)	119.1	C(70)	C(71)	H(68)	119.1
C(72)	C(73)	H(69)	119.3	C(74)	C(73)	H(69)	119.2
C(73)	C(74)	H(70)	120.4	C(75)	C(74)	H(70)	120.4
C(74)	C(75)	H(71)	119.8	C(76)	C(75)	H(71)	119.8
C(75)	C(76)	H(72)	120.2	C(77)	C(76)	H(72)	120.2
C(72)	C(77)	H(73)	119.2	C(76)	C(77)	H(73)	119.2
C(72)	C(78)	H(74)	109.5	C(72)	C(78)	H(75)	109.5
C(72)	C(78)	H(76)	109.5	H(74)	C(78)	H(75)	109.5
H(74)	C(78)	H(76)	109.5	H(75)	C(78)	H(76)	109.5

Table 8. Torsion Angles(°)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
P(1)	Mo(1)	P(2)	C(9)	-10.26(19)	P(1)	Mo(1)	P(2)	C(24)	-122.4(2)
P(1)	Mo(1)	P(2)	C(30)	107.18(19)	P(2)	Mo(1)	P(1)	C(8)	-13.6(2)
P(2)	Mo(1)	P(1)	C(12)	101.63(19)	P(2)	Mo(1)	P(1)	C(18)	-134.15(19)
P(1)	Mo(1)	P(4)	C(11)	-164.29(15)	P(1)	Mo(1)	P(4)	C(48)	78.87(18)
P(1)	Mo(1)	P(4)	C(54)	-45.3(2)	P(4)	Mo(1)	P(1)	C(8)	78.5(2)
P(4)	Mo(1)	P(1)	C(12)	-166.24(18)	P(4)	Mo(1)	P(1)	C(18)	-42.01(19)
P(1)	Mo(1)	Si(1)	C(47)	147.78(17)	P(1)	Mo(1)	Si(1)	C(60)	-97.99(18)
P(1)	Mo(1)	Si(1)	C(66)	28.5(2)	Si(1)	Mo(1)	P(1)	C(8)	-178.1(2)
Si(1)	Mo(1)	P(1)	C(12)	-62.88(19)	Si(1)	Mo(1)	P(1)	C(18)	61.35(19)
C(1)	Mo(1)	P(1)	C(8)	-105.6(2)	C(1)	Mo(1)	P(1)	C(12)	9.7(2)
C(1)	Mo(1)	P(1)	C(18)	133.9(2)	P(2)	Mo(1)	P(3)	C(10)	107.80(16)
P(2)	Mo(1)	P(3)	C(36)	-13.9(2)	P(2)	Mo(1)	P(3)	C(42)	-136.4(2)
P(3)	Mo(1)	P(2)	C(9)	169.23(19)	P(3)	Mo(1)	P(2)	C(24)	57.1(2)
P(3)	Mo(1)	P(2)	C(30)	-73.33(19)	P(2)	Mo(1)	P(4)	C(11)	-84.23(16)
P(2)	Mo(1)	P(4)	C(48)	158.93(18)	P(2)	Mo(1)	P(4)	C(54)	34.8(2)
P(4)	Mo(1)	P(2)	C(9)	-111.11(19)	P(4)	Mo(1)	P(2)	C(24)	136.8(2)
P(4)	Mo(1)	P(2)	C(30)	6.33(19)	P(2)	Mo(1)	Si(1)	C(47)	28.4(2)
P(2)	Mo(1)	Si(1)	C(60)	142.6(2)	P(2)	Mo(1)	Si(1)	C(66)	-90.9(2)
Si(1)	Mo(1)	P(2)	C(9)	113.3(2)	Si(1)	Mo(1)	P(2)	C(24)	1.1(2)
Si(1)	Mo(1)	P(2)	C(30)	-129.3(2)	C(1)	Mo(1)	P(2)	C(9)	82.5(2)
C(1)	Mo(1)	P(2)	C(24)	-29.6(2)	C(1)	Mo(1)	P(2)	C(30)	-160.1(2)
P(3)	Mo(1)	P(4)	C(11)	11.05(15)	P(3)	Mo(1)	P(4)	C(48)	-105.79(18)
P(3)	Mo(1)	P(4)	C(54)	130.1(2)	P(4)	Mo(1)	P(3)	C(10)	14.69(16)
P(4)	Mo(1)	P(3)	C(36)	-107.0(2)	P(4)	Mo(1)	P(3)	C(42)	130.5(2)
P(3)	Mo(1)	Si(1)	C(47)	-30.43(17)	P(3)	Mo(1)	Si(1)	C(60)	83.79(18)
P(3)	Mo(1)	Si(1)	C(66)	-149.7(2)	Si(1)	Mo(1)	P(3)	C(10)	-87.23(16)
Si(1)	Mo(1)	P(3)	C(36)	151.0(2)	Si(1)	Mo(1)	P(3)	C(42)	28.6(2)
C(1)	Mo(1)	P(3)	C(10)	-160.1(2)	C(1)	Mo(1)	P(3)	C(36)	78.2(2)
C(1)	Mo(1)	P(3)	C(42)	-44.2(2)	P(4)	Mo(1)	Si(1)	C(47)	-106.81(17)
P(4)	Mo(1)	Si(1)	C(60)	7.41(18)	P(4)	Mo(1)	Si(1)	C(66)	133.9(2)
Si(1)	Mo(1)	P(4)	C(11)	83.46(16)	Si(1)	Mo(1)	P(4)	C(48)	-33.38(18)
Si(1)	Mo(1)	P(4)	C(54)	-157.5(2)	C(1)	Mo(1)	P(4)	C(11)	31.5(5)
C(1)	Mo(1)	P(4)	C(48)	-85.3(5)	C(1)	Mo(1)	P(4)	C(54)	150.6(5)
C(1)	Mo(1)	Si(1)	C(47)	60.8(2)	C(1)	Mo(1)	Si(1)	C(60)	175.0(2)
C(1)	Mo(1)	Si(1)	C(66)	-58.5(2)	Mo(1)	P(1)	C(8)	C(9)	41.5(3)
Mo(1)	P(1)	C(12)	C(13)	134.3(3)	Mo(1)	P(1)	C(12)	C(17)	-44.4(4)
Mo(1)	P(1)	C(18)	C(19)	-58.7(4)	Mo(1)	P(1)	C(18)	C(23)	121.5(3)

Table 8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle
C(8)	P(1)	C(12)	C(13)	-104.6(4)
C(12)	P(1)	C(8)	C(9)	-87.1(3)
C(8)	P(1)	C(18)	C(23)	-2.7(4)
C(12)	P(1)	C(18)	C(19)	75.8(4)
C(18)	P(1)	C(12)	C(13)	0.1(3)
Mo(1)	P(2)	C(9)	C(8)	38.9(3)
Mo(1)	P(2)	C(24)	C(29)	-139.3(3)
Mo(1)	P(2)	C(30)	C(35)	70.6(4)
C(9)	P(2)	C(24)	C(29)	103.2(4)
C(9)	P(2)	C(30)	C(31)	9.3(5)
C(30)	P(2)	C(9)	C(8)	-89.2(3)
C(24)	P(2)	C(30)	C(35)	-69.8(4)
C(30)	P(2)	C(24)	C(29)	-1.3(4)
Mo(1)	P(3)	C(36)	C(37)	118.3(3)
Mo(1)	P(3)	C(42)	C(43)	162.3(4)
C(10)	P(3)	C(36)	C(37)	-7.0(4)
C(36)	P(3)	C(10)	C(11)	89.7(3)
C(10)	P(3)	C(42)	C(47)	101.0(4)
C(36)	P(3)	C(42)	C(43)	27.4(5)
C(42)	P(3)	C(36)	C(37)	-112.8(4)
Mo(1)	P(4)	C(11)	C(10)	-41.2(3)
Mo(1)	P(4)	C(48)	C(53)	116.6(4)
Mo(1)	P(4)	C(54)	C(59)	-137.8(4)
C(11)	P(4)	C(48)	C(53)	-3.2(5)
C(11)	P(4)	C(54)	C(55)	172.3(4)
C(54)	P(4)	C(11)	C(10)	-175.2(3)
C(48)	P(4)	C(54)	C(59)	87.0(5)
C(54)	P(4)	C(48)	C(53)	-105.4(4)
Mo(1)	Si(1)	C(47)	C(46)	-156.4(4)
Mo(1)	Si(1)	C(60)	C(65)	76.9(4)
Mo(1)	Si(1)	C(66)	C(71)	-174.8(3)
C(47)	Si(1)	C(60)	C(65)	-165.6(4)
C(60)	Si(1)	C(47)	C(46)	74.2(4)
C(47)	Si(1)	C(66)	C(71)	65.5(5)
C(66)	Si(1)	C(47)	C(46)	-29.0(5)
C(60)	Si(1)	C(66)	C(71)	-37.7(5)
C(66)	Si(1)	C(60)	C(65)	-57.5(4)
C(8)	P(1)	C(12)	C(17)	76.7(4)
C(8)	P(1)	C(18)	C(19)	177.2(4)
C(18)	P(1)	C(8)	C(9)	172.1(3)
C(12)	P(1)	C(18)	C(23)	-104.0(4)
C(18)	P(1)	C(12)	C(17)	-178.6(3)
Mo(1)	P(2)	C(24)	C(25)	42.3(4)
Mo(1)	P(2)	C(30)	C(31)	-110.8(4)
C(9)	P(2)	C(24)	C(25)	-75.2(4)
C(24)	P(2)	C(9)	C(8)	168.6(3)
C(9)	P(2)	C(30)	C(35)	-169.4(4)
C(24)	P(2)	C(30)	C(31)	108.8(5)
C(30)	P(2)	C(24)	C(25)	-179.7(3)
Mo(1)	P(3)	C(10)	C(11)	-44.2(3)
Mo(1)	P(3)	C(36)	C(41)	-63.0(4)
Mo(1)	P(3)	C(42)	C(47)	-19.0(4)
C(10)	P(3)	C(36)	C(41)	171.7(3)
C(10)	P(3)	C(42)	C(43)	-77.8(5)
C(42)	P(3)	C(10)	C(11)	-167.1(3)
C(36)	P(3)	C(42)	C(47)	-153.8(4)
C(42)	P(3)	C(36)	C(41)	65.9(4)
Mo(1)	P(4)	C(48)	C(49)	-68.3(4)
Mo(1)	P(4)	C(54)	C(55)	50.3(5)
C(11)	P(4)	C(48)	C(49)	171.9(4)
C(48)	P(4)	C(11)	C(10)	88.1(3)
C(11)	P(4)	C(54)	C(59)	-15.8(5)
C(48)	P(4)	C(54)	C(55)	-84.9(4)
C(54)	P(4)	C(48)	C(49)	69.7(4)
Mo(1)	Si(1)	C(47)	C(42)	32.5(4)
Mo(1)	Si(1)	C(60)	C(61)	-108.5(4)
Mo(1)	Si(1)	C(66)	C(67)	6.0(5)
C(47)	Si(1)	C(60)	C(61)	9.1(4)
C(60)	Si(1)	C(47)	C(42)	-96.9(4)
C(47)	Si(1)	C(66)	C(67)	-113.7(4)
C(66)	Si(1)	C(47)	C(42)	159.9(3)
C(60)	Si(1)	C(66)	C(67)	143.1(4)
C(66)	Si(1)	C(60)	C(61)	117.1(4)
C(1)	N(1)	C(2B)	C(3B)	131.7(10)

Table 8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle
C(1)	N(1)	C(2B)	C(7B)	-103.9(12)
N(1)	C(2A)	C(7A)	C(6A)	-178.7(10)
C(7A)	C(2A)	C(3A)	C(4A)	-62.6(15)
N(1)	C(2B)	C(7B)	C(6B)	-65.2(14)
C(7B)	C(2B)	C(3B)	C(4B)	-55.2(13)
C(2B)	C(3B)	C(4B)	C(5B)	55.6(16)
C(3B)	C(4B)	C(5B)	C(6B)	-58.6(16)
C(4B)	C(5B)	C(6B)	C(7B)	65.0(17)
C(5B)	C(6B)	C(7B)	C(2B)	-64.8(17)
P(3)	C(10)	C(11)	P(4)	54.6(4)
P(1)	C(12)	C(17)	C(16)	179.8(3)
C(17)	C(12)	C(13)	C(14)	0.4(6)
C(13)	C(14)	C(15)	C(16)	1.6(7)
C(15)	C(16)	C(17)	C(12)	-1.1(7)
P(1)	C(18)	C(23)	C(22)	-177.3(4)
C(23)	C(18)	C(19)	C(20)	-0.1(6)
C(19)	C(20)	C(21)	C(22)	1.2(8)
C(21)	C(22)	C(23)	C(18)	-3.7(8)
P(2)	C(24)	C(29)	C(28)	-178.2(4)
C(29)	C(24)	C(25)	C(26)	-0.6(7)
C(25)	C(26)	C(27)	C(28)	0.2(6)
C(27)	C(28)	C(29)	C(24)	0.4(8)
P(2)	C(30)	C(35)	C(34)	178.5(4)
C(35)	C(30)	C(31)	C(32)	0.4(8)
C(31)	C(32)	C(33)	C(34)	0.5(9)
C(33)	C(34)	C(35)	C(30)	0.2(6)
P(3)	C(36)	C(41)	C(40)	-179.4(3)
C(41)	C(36)	C(37)	C(38)	1.1(7)
C(37)	C(38)	C(39)	C(40)	0.1(6)
C(39)	C(40)	C(41)	C(36)	-0.2(5)
P(3)	C(42)	C(47)	Si(1)	-10.1(5)
C(43)	C(42)	C(47)	Si(1)	168.7(4)
C(47)	C(42)	C(43)	C(44)	1.7(8)
C(43)	C(44)	C(45)	C(46)	-2.7(8)
C(45)	C(46)	C(47)	Si(1)	-169.1(4)
P(4)	C(48)	C(49)	C(50)	-173.3(4)
C(49)	C(48)	C(53)	C(52)	-2.9(7)
N(1)	C(2A)	C(3A)	C(4A)	-180.0(8)
C(3A)	C(2A)	C(7A)	C(6A)	61.1(16)
N(1)	C(2B)	C(3B)	C(4B)	69.6(13)
C(3B)	C(2B)	C(7B)	C(6B)	57.9(14)
C(2A)	C(3A)	C(4A)	C(5A)	57.2(12)
C(3A)	C(4A)	C(5A)	C(6A)	-55.5(15)
C(4A)	C(5A)	C(6A)	C(7A)	54.3(15)
C(5A)	C(6A)	C(7A)	C(2A)	-55.0(14)
P(1)	C(8)	C(9)	P(2)	-51.5(4)
P(1)	C(12)	C(13)	C(14)	-178.3(3)
C(13)	C(12)	C(17)	C(16)	1.0(6)
C(12)	C(13)	C(14)	C(15)	-1.7(7)
C(14)	C(15)	C(16)	C(17)	-0.2(6)
P(1)	C(18)	C(19)	C(20)	-180.0(3)
C(19)	C(18)	C(23)	C(22)	2.9(7)
C(18)	C(19)	C(20)	C(21)	-2.0(8)
C(20)	C(21)	C(22)	C(23)	1.6(8)
P(2)	C(24)	C(25)	C(26)	177.9(4)
C(25)	C(24)	C(29)	C(28)	0.2(6)
C(24)	C(25)	C(26)	C(27)	0.4(7)
C(26)	C(27)	C(28)	C(29)	-0.6(8)
P(2)	C(30)	C(31)	C(32)	-178.2(4)
C(31)	C(30)	C(35)	C(34)	-0.2(6)
C(30)	C(31)	C(32)	C(33)	-0.5(9)
C(32)	C(33)	C(34)	C(35)	-0.3(8)
P(3)	C(36)	C(37)	C(38)	179.8(3)
C(37)	C(36)	C(41)	C(40)	-0.6(7)
C(36)	C(37)	C(38)	C(39)	-0.9(7)
C(38)	C(39)	C(40)	C(41)	0.4(7)
P(3)	C(42)	C(43)	C(44)	-179.6(4)
P(3)	C(42)	C(47)	C(46)	178.0(4)
C(43)	C(42)	C(47)	C(46)	-3.2(7)
C(42)	C(43)	C(44)	C(45)	1.3(8)
C(44)	C(45)	C(46)	C(47)	1.1(8)
C(45)	C(46)	C(47)	C(42)	1.9(8)
P(4)	C(48)	C(53)	C(52)	172.2(4)
C(53)	C(48)	C(49)	C(50)	2.1(7)

Table 8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C(48)	C(49)	C(50)	C(51)	0.7(8)	C(49)	C(50)	C(51)	C(52)	-2.6(8)
C(50)	C(51)	C(52)	C(53)	1.8(8)	C(51)	C(52)	C(53)	C(48)	1.0(8)
P(4)	C(54)	C(55)	C(56)	171.6(4)	P(4)	C(54)	C(59)	C(58)	-171.5(4)
C(55)	C(54)	C(59)	C(58)	0.5(8)	C(59)	C(54)	C(55)	C(56)	-0.9(8)
C(54)	C(55)	C(56)	C(57)	-0.0(7)	C(55)	C(56)	C(57)	C(58)	1.5(9)
C(56)	C(57)	C(58)	C(59)	-1.9(9)	C(57)	C(58)	C(59)	C(54)	0.9(9)
Si(1)	C(60)	C(61)	C(62)	-173.1(4)	Si(1)	C(60)	C(65)	C(64)	173.0(4)
C(61)	C(60)	C(65)	C(64)	-1.9(7)	C(65)	C(60)	C(61)	C(62)	1.8(7)
C(60)	C(61)	C(62)	C(63)	0.1(6)	C(61)	C(62)	C(63)	C(64)	-1.9(8)
C(62)	C(63)	C(64)	C(65)	1.7(8)	C(63)	C(64)	C(65)	C(60)	0.2(6)
Si(1)	C(66)	C(67)	C(68)	178.4(4)	Si(1)	C(66)	C(71)	C(70)	-178.0(4)
C(67)	C(66)	C(71)	C(70)	1.3(8)	C(71)	C(66)	C(67)	C(68)	-0.9(8)
C(66)	C(67)	C(68)	C(69)	-0.3(8)	C(67)	C(68)	C(69)	C(70)	1.1(8)
C(68)	C(69)	C(70)	C(71)	-0.7(8)	C(69)	C(70)	C(71)	C(66)	-0.5(8)
C(73)	C(72)	C(77)	C(76)	-0.7(9)	C(77)	C(72)	C(73)	C(74)	0.9(9)
C(78)	C(72)	C(73)	C(74)	-178.5(6)	C(78)	C(72)	C(77)	C(76)	178.8(6)
C(72)	C(73)	C(74)	C(75)	-0.5(9)	C(73)	C(74)	C(75)	C(76)	-0.2(8)
C(74)	C(75)	C(76)	C(77)	0.4(9)	C(75)	C(76)	C(77)	C(72)	0.0(10)

The sign is positive if when looking from atom 2 to atom 3 a clock-wise motion of atom 1 would superimpose it on atom 4.

Table 9. Distances beyond the asymmetric unit out to 3.60 Å

atom	atom	distance	atom	atom	distance
C(13)	C(22)[1)]	3.562(6)	C(13)	C(23)[1)]	3.530(6)
C(21)	C(34)[2)]	3.586(7)	C(22)	C(13)[1)]	3.562(6)
C(23)	C(13)[1)]	3.530(6)	C(34)	C(21)[3)]	3.586(7)
C(39)	C(70)[3)]	3.525(8)	C(40)	C(69)[3)]	3.588(8)
C(45)	C(71)[4)]	3.507(7)	C(50)	C(50)[5)]	3.310(8)
C(69)	C(40)[2)]	3.588(8)	C(70)	C(39)[2)]	3.525(8)
C(71)	C(45)[4)]	3.507(7)			

Symmetry Operators:

(1) -X+1,-Y,-Z+1
(2) X+1,Y,Z
(3) X-1,Y,Z
(4) -X+1,-Y+1,-Z
(5) -X+1,-Y+1,-Z+1

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
C(3B)	H(2B)[1)]	3.566	C(3B)	H(4A)[1)]	3.241
C(3B)	H(5A)[1)]	3.392	C(4A)	H(2A)[1)]	3.504
C(4A)	H(2B)[1)]	3.414	C(4A)	H(3B)[1)]	3.230
C(4A)	H(5A)[1)]	3.458	C(4A)	H(61)[2)]	3.426
C(4A)	H(65)[1)]	3.286	C(4B)	H(66)[1)]	3.399
C(4B)	H(73)[3)]	3.269	C(4B)	H(74)[3)]	2.812
C(5A)	H(22)[1)]	3.551	C(5A)	H(61)[2)]	3.424
C(5A)	H(65)[1)]	3.244	C(5B)	H(66)[1)]	3.032
C(5B)	H(73)[3)]	3.536	C(6B)	H(71)[4)]	3.436
C(7A)	H(71)[4)]	3.442	C(7B)	H(71)[4)]	3.039
C(11)	H(57)[5)]	2.960	C(12)	H(28)[6)]	3.053
C(13)	H(28)[6)]	2.981	C(13)	H(29)[6)]	2.897
C(13)	H(33)[7)]	3.163	C(14)	H(28)[6)]	3.059
C(14)	H(29)[6)]	3.213	C(14)	H(32)[7)]	3.324
C(14)	H(33)[7)]	3.173	C(14)	H(55)[6)]	2.917
C(15)	H(4A)[1)]	3.428	C(15)	H(7A)[1)]	3.493
C(15)	H(28)[6)]	3.169	C(15)	H(52)[3)]	3.083
C(15)	H(55)[6)]	3.372	C(15)	H(61)[3)]	3.180
C(16)	H(4A)[1)]	3.538	C(16)	H(28)[6)]	3.208
C(16)	H(52)[3)]	2.949	C(16)	H(74)[3)]	3.198
C(17)	H(28)[6)]	3.158	C(21)	H(12)[6)]	3.237
C(21)	H(38)[7)]	3.339	C(22)	H(12)[6)]	2.794
C(22)	H(51)[8)]	3.371	C(22)	H(52)[8)]	3.422
C(23)	H(12)[6)]	3.211	C(23)	H(20)[6)]	3.439
C(25)	H(36)[9)]	3.437	C(25)	H(76)[3)]	3.070
C(26)	H(36)[9)]	3.287	C(26)	H(69)[3)]	3.360
C(26)	H(76)[3)]	2.901	C(27)	H(21)[10)]	3.182
C(27)	H(36)[9)]	3.374	C(27)	H(69)[3)]	3.512
C(28)	H(20)[10)]	3.527	C(28)	H(21)[10)]	3.195
C(28)	H(35)[9)]	3.246	C(29)	H(14)[9)]	3.550
C(29)	H(35)[9)]	3.212	C(31)	H(14)[9)]	3.464
C(32)	H(14)[9)]	3.542	C(32)	H(69)[5)]	3.446
C(32)	H(76)[5)]	3.499	C(33)	H(19)[5)]	3.498
C(33)	H(27)[10)]	2.984	C(33)	H(58)[5)]	3.398
C(34)	H(26)[10)]	3.530	C(34)	H(27)[10)]	2.756
C(34)	H(57)[5)]	3.246	C(34)	H(58)[5)]	3.237
C(35)	H(27)[10)]	3.586	C(37)	H(46)[4)]	3.445

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C(38)	H(26)[10)]	3.023	C(38)	H(46)[4)]	3.288
C(38)	H(47)[4)]	3.385	C(38)	H(62)[10)]	3.435
C(38)	H(63)[10)]	3.565	C(39)	H(26)[10)]	3.155
C(39)	H(46)[4)]	3.337	C(39)	H(47)[4)]	3.526
C(40)	H(46)[4)]	3.527	C(40)	H(66)[10)]	3.524
C(40)	H(72)[4)]	3.434	C(43)	H(45)[4)]	3.545
C(43)	H(46)[4)]	3.228	C(43)	H(71)[4)]	3.369
C(43)	H(72)	3.360	C(44)	H(45)[4)]	3.156
C(44)	H(67)[2)]	3.227	C(44)	H(71)[4)]	2.852
C(44)	H(72)	3.339	C(45)	H(67)[2)]	3.139
C(45)	H(68)[2)]	2.920	C(45)	H(71)[4)]	3.331
C(46)	H(67)[2)]	3.513	C(46)	H(68)[2)]	2.937
C(49)	H(50)[8)]	3.536	C(50)	H(50)[8)]	3.096
C(51)	H(28)[8)]	3.513	C(51)	H(50)[8)]	3.339
C(51)	H(55)[8)]	3.587	C(52)	H(27)[8)]	3.572
C(52)	H(28)[8)]	3.335	C(52)	H(75)	3.334
C(53)	H(37)[5)]	3.300	C(53)	H(75)	2.955
C(55)	H(51)[8)]	3.300	C(56)	H(21)[6)]	3.228
C(56)	H(51)[8)]	2.860	C(57)	H(51)[8)]	3.480
C(57)	H(69)[5)]	3.085	C(57)	H(70)[5)]	3.365
C(58)	H(18)[5)]	3.273	C(58)	H(19)[5)]	3.511
C(58)	H(38)[5)]	2.995	C(58)	H(58)[5)]	3.235
C(59)	H(38)[5)]	3.091	C(59)	H(57)[5)]	3.600
C(59)	H(58)[5)]	3.160	C(61)	H(48)[2)]	3.303
C(61)	H(67)[2)]	3.191	C(61)	H(68)[2)]	3.526
C(61)	H(73)	3.546	C(62)	H(48)[2)]	3.052
C(62)	H(67)[2)]	3.421	C(62)	H(73)	3.421
C(63)	H(4A)[2)]	3.586	C(63)	H(6A)[2)]	3.543
C(63)	H(22)[11)]	3.049	C(63)	H(47)[2)]	3.120
C(63)	H(48)[2)]	3.335	C(64)	H(41)[7)]	3.135
C(64)	H(47)[2)]	2.827	C(65)	H(41)[7)]	3.304
C(65)	H(47)[2)]	3.149	C(66)	H(42)[7)]	3.295
C(67)	H(42)[7)]	3.349	C(68)	H(5A)[1)]	3.234
C(68)	H(6B)[1)]	3.587	C(68)	H(7A)[1)]	3.226
C(68)	H(42)[7)]	3.248	C(68)	H(43)[7)]	3.533
C(69)	H(5A)[1)]	3.342	C(69)	H(5B)[1)]	3.222
C(69)	H(6B)[1)]	3.385	C(69)	H(7A)[1)]	3.554

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C(69)	H(42)[7)]	3.052	C(69)	H(43)[7)]	2.960
C(69)	H(60)[2)]	3.566	C(69)	H(72)[2)]	3.416
C(69)	H(73)[2)]	3.128	C(70)	H(42)[7)]	2.935
C(70)	H(43)[7)]	3.457	C(70)	H(47)[2)]	3.599
C(70)	H(59)[2)]	3.135	C(70)	H(60)[2)]	3.075
C(70)	H(72)[2)]	3.248	C(70)	H(73)[2)]	3.067
C(71)	H(42)[7)]	3.046	C(71)	H(47)[2)]	3.270
C(71)	H(59)[2)]	3.489	C(71)	H(60)[2)]	3.508
C(72)	H(4B)[11)]	3.464	C(72)	H(7B)[11)]	3.555
C(72)	H(16)	3.356	C(72)	H(17)	3.118
C(72)	H(31)[11)]	3.132	C(73)	H(17)	2.984
C(73)	H(31)[11)]	3.116	C(73)	H(36)[5)]	3.567
C(73)	H(56)[5)]	3.092	C(74)	H(6A)[4)]	3.353
C(74)	H(8B)[4)]	3.577	C(74)	H(9A)[4)]	3.155
C(74)	H(17)	3.087	C(74)	H(40)	3.428
C(74)	H(56)[5)]	3.013	C(75)	H(6A)[4)]	3.557
C(75)	H(8B)[4)]	2.942	C(75)	H(9A)[4)]	2.965
C(75)	H(10A)[4)]	3.270	C(75)	H(10B)[4)]	3.222
C(75)	H(11B)[4)]	3.404	C(75)	H(17)	3.303
C(75)	H(45)	3.343	C(75)	H(46)[4)]	3.448
C(76)	H(7B)[11)]	3.571	C(76)	H(8B)[4)]	3.194
C(76)	H(9A)[4)]	3.401	C(76)	H(17)	3.424
C(76)	H(45)	3.369	C(76)	H(66)[2)]	3.386
C(76)	H(67)[2)]	3.128	C(77)	H(4B)[11)]	3.599
C(77)	H(5B)[11)]	3.402	C(77)	H(7B)[11)]	3.092
C(77)	H(16)	3.416	C(77)	H(17)	3.326
C(77)	H(59)	3.508	C(77)	H(66)[2)]	3.250
C(77)	H(67)[2)]	3.108	C(78)	H(4B)[11)]	2.858
C(78)	H(5B)[11)]	3.512	C(78)	H(23)[11)]	3.040
C(78)	H(31)[11)]	3.201	C(78)	H(36)[5)]	3.464
C(78)	H(37)[5)]	3.465	C(78)	H(53)	3.104
H(1A)	H(74)[3)]	2.984	H(1A)	H(76)[3)]	3.584
H(2A)	C(4A)[1)]	3.504	H(2A)	H(2B)[1)]	3.414
H(2A)	H(4A)[1)]	3.191	H(2A)	H(5A)[1)]	2.890
H(2B)	C(3B)[1)]	3.566	H(2B)	C(4A)[1)]	3.414
H(2B)	H(2A)[1)]	3.414	H(2B)	H(2B)[1)]	3.031
H(2B)	H(3B)[1)]	3.247	H(2B)	H(4A)[1)]	3.112

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(2B)	H(5A)[1)]	2.929	H(3A)	H(60)[2)]	3.312
H(3A)	H(61)[2)]	3.217	H(3B)	C(4A)[1)]	3.230
H(3B)	H(2B)[1)]	3.247	H(3B)	H(4A)[1)]	2.630
H(3B)	H(5A)[1)]	2.920	H(4A)	C(3B)[1)]	3.241
H(4A)	C(15)[1)]	3.428	H(4A)	C(16)[1)]	3.538
H(4A)	C(63)[2)]	3.586	H(4A)	H(2A)[1)]	3.191
H(4A)	H(2B)[1)]	3.112	H(4A)	H(3B)[1)]	2.630
H(4A)	H(5A)[1)]	3.113	H(4A)	H(5B)[1)]	3.157
H(4A)	H(22)[1)]	3.110	H(4A)	H(23)[1)]	3.301
H(4A)	H(60)[2)]	3.275	H(4A)	H(61)[2)]	2.829
H(4A)	H(65)[1)]	3.209	H(4B)	C(72)[3)]	3.464
H(4B)	C(77)[3)]	3.599	H(4B)	C(78)[3)]	2.858
H(4B)	H(73)[3)]	3.237	H(4B)	H(74)[3)]	2.148
H(4B)	H(76)[3)]	2.858	H(5A)	C(3B)[1)]	3.392
H(5A)	C(4A)[1)]	3.458	H(5A)	C(68)[1)]	3.234
H(5A)	C(69)[1)]	3.342	H(5A)	H(2A)[1)]	2.890
H(5A)	H(2B)[1)]	2.929	H(5A)	H(3B)[1)]	2.920
H(5A)	H(4A)[1)]	3.113	H(5A)	H(5A)[1)]	3.214
H(5A)	H(65)[1)]	2.919	H(5A)	H(66)[1)]	3.107
H(5B)	C(69)[1)]	3.222	H(5B)	C(77)[3)]	3.402
H(5B)	C(78)[3)]	3.512	H(5B)	H(4A)[1)]	3.157
H(5B)	H(60)[3)]	3.047	H(5B)	H(66)[1)]	2.811
H(5B)	H(73)[3)]	2.690	H(5B)	H(74)[3)]	2.627
H(6A)	C(63)[2)]	3.543	H(6A)	C(74)[4)]	3.353
H(6A)	C(75)[4)]	3.557	H(6A)	H(22)[1)]	3.209
H(6A)	H(61)[2)]	2.705	H(6A)	H(70)[4)]	2.927
H(6A)	H(71)[4)]	3.306	H(6B)	C(68)[1)]	3.587
H(6B)	C(69)[1)]	3.385	H(6B)	H(65)[1)]	3.110
H(6B)	H(66)[1)]	2.695	H(7A)	C(15)[1)]	3.493
H(7A)	C(68)[1)]	3.226	H(7A)	C(69)[1)]	3.554
H(7A)	H(22)[1)]	3.172	H(7A)	H(32)[12)]	3.002
H(7A)	H(65)[1)]	2.450	H(7A)	H(66)[1)]	3.121
H(7B)	C(72)[3)]	3.555	H(7B)	C(76)[3)]	3.571
H(7B)	C(77)[3)]	3.092	H(7B)	H(8B)[12)]	3.543
H(7B)	H(9A)[12)]	3.473	H(7B)	H(66)[1)]	2.753
H(7B)	H(73)[3)]	2.958	H(7B)	H(74)[3)]	3.560
H(8A)	H(66)[1)]	2.918	H(8A)	H(73)[3)]	3.568

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(8B)	C(74)[4)]	3.577	H(8B)	C(75)[4)]	2.942
H(8B)	C(76)[4)]	3.194	H(8B)	H(7B)[12)]	3.543
H(8B)	H(71)[4)]	2.868	H(8B)	H(72)[4)]	3.290
H(9A)	C(74)[4)]	3.155	H(9A)	C(75)[4)]	2.965
H(9A)	C(76)[4)]	3.401	H(9A)	H(7B)[12)]	3.473
H(9A)	H(70)[4)]	3.397	H(9A)	H(71)[4)]	3.095
H(10A)	C(75)[4)]	3.270	H(10A)	H(71)[4)]	2.676
H(10B)	C(75)[4)]	3.222	H(10B)	H(71)[4)]	2.488
H(11B)	C(75)[4)]	3.404	H(11B)	H(61)[2)]	3.183
H(11B)	H(70)[4)]	3.387	H(11B)	H(71)[4)]	2.915
H(12)	C(21)[6)]	3.237	H(12)	C(22)[6)]	2.794
H(12)	C(23)[6)]	3.211	H(12)	H(20)[6)]	3.451
H(12)	H(27)[6)]	3.490	H(12)	H(28)[6)]	2.790
H(12)	H(29)[6)]	3.421	H(13)	H(33)[9)]	3.511
H(14)	C(29)[9)]	3.550	H(14)	C(31)[9)]	3.464
H(14)	C(32)[9)]	3.542	H(14)	H(34)[9)]	3.026
H(14)	H(35)[9)]	3.552	H(15)	H(36)[9)]	3.441
H(15)	H(76)[3)]	3.585	H(16)	C(72)	3.356
H(16)	C(77)	3.416	H(16)	H(73)	3.597
H(16)	H(75)	3.111	H(17)	C(72)	3.118
H(17)	C(73)	2.984	H(17)	C(74)	3.087
H(17)	C(75)	3.303	H(17)	C(76)	3.424
H(17)	C(77)	3.326	H(17)	H(57)[5)]	3.488
H(17)	H(69)	3.390	H(17)	H(70)	3.537
H(17)	H(75)	3.549	H(18)	C(58)[5)]	3.273
H(18)	H(57)[5)]	2.331	H(19)	C(33)[5)]	3.498
H(19)	C(58)[5)]	3.511	H(19)	H(37)[5)]	2.771
H(19)	H(57)[5)]	2.740	H(19)	H(75)	3.092
H(20)	C(23)[6)]	3.439	H(20)	C(28)[7)]	3.527
H(20)	H(12)[6)]	3.451	H(20)	H(28)[6)]	3.441
H(20)	H(29)[6)]	2.670	H(20)	H(33)[7)]	2.590
H(21)	C(27)[7)]	3.182	H(21)	C(28)[7)]	3.195
H(21)	C(56)[6)]	3.228	H(21)	H(28)[6)]	3.574
H(21)	H(29)[6)]	3.239	H(21)	H(32)[7)]	2.577
H(21)	H(33)[7)]	2.599	H(21)	H(55)[6)]	2.323
H(22)	C(5A)[1)]	3.551	H(22)	C(63)[3)]	3.049
H(22)	H(4A)[1)]	3.110	H(22)	H(6A)[1)]	3.209

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(22)	H(7A)[1)]	3.172	H(22)	H(51)[3)]	3.411
H(22)	H(52)[3)]	3.033	H(22)	H(55)[6)]	3.198
H(22)	H(61)[3)]	2.329	H(22)	H(62)[3)]	3.573
H(23)	C(78)[3)]	3.040	H(23)	H(4A)[1)]	3.301
H(23)	H(52)[3)]	2.793	H(23)	H(60)[3)]	3.479
H(23)	H(61)[3)]	3.285	H(23)	H(74)[3)]	2.332
H(23)	H(75)[3)]	3.122	H(23)	H(76)[3)]	3.239
H(24)	H(74)[3)]	3.387	H(24)	H(76)[3)]	3.271
H(25)	H(42)[7)]	2.979	H(26)	C(34)[7)]	3.530
H(26)	C(38)[7)]	3.023	H(26)	C(39)[7)]	3.155
H(26)	H(34)[7)]	3.317	H(26)	H(38)[7)]	3.141
H(26)	H(39)[7)]	3.473	H(26)	H(41)[7)]	2.822
H(26)	H(42)[7)]	3.062	H(27)	C(33)[7)]	2.984
H(27)	C(34)[7)]	2.756	H(27)	C(35)[7)]	3.586
H(27)	C(52)[8)]	3.572	H(27)	H(12)[6)]	3.490
H(27)	H(34)[7)]	3.575	H(27)	H(37)[7)]	2.970
H(27)	H(38)[7)]	2.567	H(27)	H(52)[8)]	3.361
H(28)	C(12)[6)]	3.053	H(28)	C(13)[6)]	2.981
H(28)	C(14)[6)]	3.059	H(28)	C(15)[6)]	3.169
H(28)	C(16)[6)]	3.208	H(28)	C(17)[6)]	3.158
H(28)	C(51)[8)]	3.513	H(28)	C(52)[8)]	3.335
H(28)	H(12)[6)]	2.790	H(28)	H(20)[6)]	3.441
H(28)	H(21)[6)]	3.574	H(28)	H(51)[8)]	3.096
H(28)	H(52)[8)]	2.749	H(29)	C(13)[6)]	2.897
H(29)	C(14)[6)]	3.213	H(29)	H(12)[6)]	3.421
H(29)	H(20)[6)]	2.670	H(29)	H(21)[6)]	3.239
H(29)	H(29)[6)]	3.559	H(30)	H(76)[3)]	2.878
H(31)	C(72)[3)]	3.132	H(31)	C(73)[3)]	3.116
H(31)	C(78)[3)]	3.201	H(31)	H(69)[3)]	3.031
H(31)	H(74)[3)]	3.512	H(31)	H(76)[3)]	2.572
H(32)	C(14)[10)]	3.324	H(32)	H(7A)[12)]	3.002
H(32)	H(21)[10)]	2.577	H(32)	H(65)[10)]	3.463
H(32)	H(69)[3)]	3.307	H(33)	C(13)[10)]	3.163
H(33)	C(14)[10)]	3.173	H(33)	H(13)[9)]	3.511
H(33)	H(20)[10)]	2.590	H(33)	H(21)[10)]	2.599
H(33)	H(35)[9)]	3.338	H(34)	H(14)[9)]	3.026
H(34)	H(26)[10)]	3.317	H(34)	H(27)[10)]	3.575

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(34)	H(35)[9)]	3.280	H(35)	C(28)[9)]	3.246
H(35)	C(29)[9)]	3.212	H(35)	H(14)[9)]	3.552
H(35)	H(33)[9)]	3.338	H(35)	H(34)[9)]	3.280
H(36)	C(25)[9)]	3.437	H(36)	C(26)[9)]	3.287
H(36)	C(27)[9)]	3.374	H(36)	C(73)[5)]	3.567
H(36)	C(78)[5)]	3.464	H(36)	H(15)[9)]	3.441
H(36)	H(69)[5)]	2.713	H(36)	H(75)[5)]	3.436
H(36)	H(76)[5)]	2.749	H(37)	C(53)[5)]	3.300
H(37)	C(78)[5)]	3.465	H(37)	H(19)[5)]	2.771
H(37)	H(27)[10)]	2.970	H(37)	H(52)[5)]	3.550
H(37)	H(53)[5)]	2.846	H(37)	H(58)[5)]	3.151
H(37)	H(75)[5)]	2.802	H(37)	H(76)[5)]	3.267
H(38)	C(21)[10)]	3.339	H(38)	C(58)[5)]	2.995
H(38)	C(59)[5)]	3.091	H(38)	H(26)[10)]	3.141
H(38)	H(27)[10)]	2.567	H(38)	H(57)[5)]	2.692
H(38)	H(58)[5)]	2.854	H(39)	H(26)[10)]	3.473
H(39)	H(57)[5)]	3.434	H(40)	C(74)	3.428
H(40)	H(56)[5)]	3.304	H(40)	H(57)[5)]	2.883
H(40)	H(70)	3.323	H(41)	C(64)[10)]	3.135
H(41)	C(65)[10)]	3.304	H(41)	H(26)[10)]	2.822
H(41)	H(47)[4)]	3.168	H(41)	H(62)[10)]	2.543
H(41)	H(63)[10)]	2.868	H(42)	C(66)[10)]	3.295
H(42)	C(67)[10)]	3.349	H(42)	C(68)[10)]	3.248
H(42)	C(69)[10)]	3.052	H(42)	C(70)[10)]	2.935
H(42)	C(71)[10)]	3.046	H(42)	H(25)[10)]	2.979
H(42)	H(26)[10)]	3.062	H(42)	H(47)[4)]	3.420
H(42)	H(63)[10)]	3.046	H(42)	H(66)[10)]	3.529
H(42)	H(67)[10)]	3.349	H(42)	H(68)[10)]	3.504
H(43)	C(68)[10)]	3.533	H(43)	C(69)[10)]	2.960
H(43)	C(70)[10)]	3.457	H(43)	H(66)[10)]	2.746
H(43)	H(67)[10)]	3.587	H(43)	H(72)[4)]	3.118
H(45)	C(43)[4)]	3.545	H(45)	C(44)[4)]	3.156
H(45)	C(75)	3.343	H(45)	C(76)	3.369
H(45)	H(45)[4)]	3.148	H(45)	H(46)[4)]	2.357
H(45)	H(71)	3.176	H(45)	H(71)[4)]	3.567
H(45)	H(72)	3.231	H(46)	C(37)[4)]	3.445
H(46)	C(38)[4)]	3.288	H(46)	C(39)[4)]	3.337

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(46)	C(40)[4)]	3.527	H(46)	C(43)[4)]	3.228
H(46)	C(75)[4)]	3.448	H(46)	H(45)[4)]	2.357
H(46)	H(46)[4)]	3.474	H(46)	H(67)[2)]	3.462
H(46)	H(71)[4)]	2.721	H(46)	H(72)	3.179
H(47)	C(38)[4)]	3.385	H(47)	C(39)[4)]	3.526
H(47)	C(63)[2)]	3.120	H(47)	C(64)[2)]	2.827
H(47)	C(65)[2)]	3.149	H(47)	C(70)[2)]	3.599
H(47)	C(71)[2)]	3.270	H(47)	H(41)[4)]	3.168
H(47)	H(42)[4)]	3.420	H(47)	H(61)[2)]	3.437
H(47)	H(62)[2)]	3.001	H(47)	H(63)[2)]	3.498
H(47)	H(67)[2)]	3.357	H(47)	H(68)[2)]	2.724
H(47)	H(71)[4)]	3.491	H(48)	C(61)[2)]	3.303
H(48)	C(62)[2)]	3.052	H(48)	C(63)[2)]	3.335
H(48)	H(60)[2)]	3.245	H(48)	H(68)[2)]	2.740
H(49)	H(51)[8)]	3.433	H(50)	C(49)[8)]	3.536
H(50)	C(50)[8)]	3.096	H(50)	C(51)[8)]	3.339
H(50)	H(50)[8)]	3.167	H(50)	H(51)[8)]	3.530
H(51)	C(22)[8)]	3.371	H(51)	C(55)[8)]	3.300
H(51)	C(56)[8)]	2.860	H(51)	C(57)[8)]	3.480
H(51)	H(22)[11)]	3.411	H(51)	H(28)[8)]	3.096
H(51)	H(49)[8)]	3.433	H(51)	H(50)[8)]	3.530
H(51)	H(54)[8)]	3.412	H(51)	H(55)[8)]	2.664
H(52)	C(15)[11)]	3.083	H(52)	C(16)[11)]	2.949
H(52)	C(22)[8)]	3.422	H(52)	H(22)[11)]	3.033
H(52)	H(23)[11)]	2.793	H(52)	H(27)[8)]	3.361
H(52)	H(28)[8)]	2.749	H(52)	H(37)[5)]	3.550
H(52)	H(74)	3.578	H(52)	H(75)	2.935
H(53)	C(78)	3.104	H(53)	H(37)[5)]	2.846
H(53)	H(74)	3.472	H(53)	H(75)	2.147
H(54)	H(51)[8)]	3.412	H(55)	C(14)[6)]	2.917
H(55)	C(15)[6)]	3.372	H(55)	C(51)[8)]	3.587
H(55)	H(21)[6)]	2.323	H(55)	H(22)[6)]	3.198
H(55)	H(51)[8)]	2.664	H(56)	C(73)[5)]	3.092
H(56)	C(74)[5)]	3.013	H(56)	H(40)[5)]	3.304
H(56)	H(62)[8)]	3.475	H(56)	H(69)[5)]	2.577
H(56)	H(70)[5)]	2.428	H(57)	C(11)[5)]	2.960
H(57)	C(34)[5)]	3.246	H(57)	C(59)[5)]	3.600

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(57)	H(17)[5)]	3.488	H(57)	H(18)[5)]	2.331
H(57)	H(19)[5)]	2.740	H(57)	H(38)[5)]	2.692
H(57)	H(39)[5)]	3.434	H(57)	H(40)[5)]	2.883
H(57)	H(58)[5)]	2.724	H(57)	H(69)[5)]	3.572
H(58)	C(33)[5)]	3.398	H(58)	C(34)[5)]	3.237
H(58)	C(58)[5)]	3.235	H(58)	C(59)[5)]	3.160
H(58)	H(37)[5)]	3.151	H(58)	H(38)[5)]	2.854
H(58)	H(57)[5)]	2.724	H(58)	H(58)[5)]	2.575
H(59)	C(70)[2)]	3.135	H(59)	C(71)[2)]	3.489
H(59)	C(77)	3.508	H(59)	H(67)[2)]	2.482
H(59)	H(68)[2)]	3.173	H(59)	H(73)	3.053
H(60)	C(69)[2)]	3.566	H(60)	C(70)[2)]	3.075
H(60)	C(71)[2)]	3.508	H(60)	H(3A)[2)]	3.312
H(60)	H(4A)[2)]	3.275	H(60)	H(5B)[11)]	3.047
H(60)	H(23)[11)]	3.479	H(60)	H(48)[2)]	3.245
H(60)	H(67)[2)]	2.960	H(60)	H(73)	2.814
H(60)	H(74)	3.229	H(61)	C(4A)[2)]	3.426
H(61)	C(5A)[2)]	3.424	H(61)	C(15)[11)]	3.180
H(61)	H(3A)[2)]	3.217	H(61)	H(4A)[2)]	2.829
H(61)	H(6A)[2)]	2.705	H(61)	H(11B)[2)]	3.183
H(61)	H(22)[11)]	2.329	H(61)	H(23)[11)]	3.285
H(61)	H(47)[2)]	3.437	H(62)	C(38)[7)]	3.435
H(62)	H(22)[11)]	3.573	H(62)	H(41)[7)]	2.543
H(62)	H(47)[2)]	3.001	H(62)	H(56)[8)]	3.475
H(62)	H(70)[7)]	3.574	H(63)	C(38)[7)]	3.565
H(63)	H(41)[7)]	2.868	H(63)	H(42)[7)]	3.046
H(63)	H(47)[2)]	3.498	H(65)	C(4A)[1)]	3.286
H(65)	C(5A)[1)]	3.244	H(65)	H(4A)[1)]	3.209
H(65)	H(5A)[1)]	2.919	H(65)	H(6B)[1)]	3.110
H(65)	H(7A)[1)]	2.450	H(65)	H(32)[7)]	3.463
H(66)	C(4B)[1)]	3.399	H(66)	C(5B)[1)]	3.032
H(66)	C(40)[7)]	3.524	H(66)	C(76)[2)]	3.386
H(66)	C(77)[2)]	3.250	H(66)	H(5A)[1)]	3.107
H(66)	H(5B)[1)]	2.811	H(66)	H(6B)[1)]	2.695
H(66)	H(7A)[1)]	3.121	H(66)	H(7B)[1)]	2.753
H(66)	H(8A)[1)]	2.918	H(66)	H(42)[7)]	3.529
H(66)	H(43)[7)]	2.746	H(66)	H(72)[2)]	2.928

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(66)	H(73)[2)]	2.644	H(67)	C(44)[2)]	3.227
H(67)	C(45)[2)]	3.139	H(67)	C(46)[2)]	3.513
H(67)	C(61)[2)]	3.191	H(67)	C(62)[2)]	3.421
H(67)	C(76)[2)]	3.128	H(67)	C(77)[2)]	3.108
H(67)	H(42)[7)]	3.349	H(67)	H(43)[7)]	3.587
H(67)	H(46)[2)]	3.462	H(67)	H(47)[2)]	3.357
H(67)	H(59)[2)]	2.482	H(67)	H(60)[2)]	2.960
H(67)	H(72)[2)]	2.572	H(67)	H(73)[2)]	2.519
H(68)	C(45)[2)]	2.920	H(68)	C(46)[2)]	2.937
H(68)	C(61)[2)]	3.526	H(68)	H(42)[7)]	3.504
H(68)	H(47)[2)]	2.724	H(68)	H(48)[2)]	2.740
H(68)	H(59)[2)]	3.173	H(68)	H(68)[2)]	3.509
H(69)	C(26)[11)]	3.360	H(69)	C(27)[11)]	3.512
H(69)	C(32)[5)]	3.446	H(69)	C(57)[5)]	3.085
H(69)	H(17)	3.390	H(69)	H(31)[11)]	3.031
H(69)	H(32)[11)]	3.307	H(69)	H(36)[5)]	2.713
H(69)	H(56)[5)]	2.577	H(69)	H(57)[5)]	3.572
H(70)	C(57)[5)]	3.365	H(70)	H(6A)[4)]	2.927
H(70)	H(9A)[4)]	3.397	H(70)	H(11B)[4)]	3.387
H(70)	H(17)	3.537	H(70)	H(40)	3.323
H(70)	H(56)[5)]	2.428	H(70)	H(62)[10)]	3.574
H(71)	C(6B)[4)]	3.436	H(71)	C(7A)[4)]	3.442
H(71)	C(7B)[4)]	3.039	H(71)	C(43)[4)]	3.369
H(71)	C(44)[4)]	2.852	H(71)	C(45)[4)]	3.331
H(71)	H(6A)[4)]	3.306	H(71)	H(8B)[4)]	2.868
H(71)	H(9A)[4)]	3.095	H(71)	H(10A)[4)]	2.676
H(71)	H(10B)[4)]	2.488	H(71)	H(11B)[4)]	2.915
H(71)	H(45)	3.176	H(71)	H(45)[4)]	3.567
H(71)	H(46)[4)]	2.721	H(71)	H(47)[4)]	3.491
H(72)	C(40)[4)]	3.434	H(72)	C(43)	3.360
H(72)	C(44)	3.339	H(72)	C(69)[2)]	3.416
H(72)	C(70)[2)]	3.248	H(72)	H(8B)[4)]	3.290
H(72)	H(43)[4)]	3.118	H(72)	H(45)	3.231
H(72)	H(46)	3.179	H(72)	H(66)[2)]	2.928
H(72)	H(67)[2)]	2.572	H(73)	C(4B)[11)]	3.269
H(73)	C(5B)[11)]	3.536	H(73)	C(61)	3.546
H(73)	C(62)	3.421	H(73)	C(69)[2)]	3.128

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(73)	C(70)[2)]	3.067	H(73)	H(4B)[11)]	3.237
H(73)	H(5B)[11)]	2.690	H(73)	H(7B)[11)]	2.958
H(73)	H(8A)[11)]	3.568	H(73)	H(16)	3.597
H(73)	H(59)	3.053	H(73)	H(60)	2.814
H(73)	H(66)[2)]	2.644	H(73)	H(67)[2)]	2.519
H(74)	C(4B)[11)]	2.812	H(74)	C(16)[11)]	3.198
H(74)	H(1A)[11)]	2.984	H(74)	H(4B)[11)]	2.148
H(74)	H(5B)[11)]	2.627	H(74)	H(7B)[11)]	3.560
H(74)	H(23)[11)]	2.332	H(74)	H(24)[11)]	3.387
H(74)	H(31)[11)]	3.512	H(74)	H(52)	3.578
H(74)	H(53)	3.472	H(74)	H(60)	3.229
H(75)	C(52)	3.334	H(75)	C(53)	2.955
H(75)	H(16)	3.111	H(75)	H(17)	3.549
H(75)	H(19)	3.092	H(75)	H(23)[11)]	3.122
H(75)	H(36)[5)]	3.436	H(75)	H(37)[5)]	2.802
H(75)	H(52)	2.935	H(75)	H(53)	2.147
H(76)	C(25)[11)]	3.070	H(76)	C(26)[11)]	2.901
H(76)	C(32)[5)]	3.499	H(76)	H(1A)[11)]	3.584
H(76)	H(4B)[11)]	2.858	H(76)	H(15)[11)]	3.585
H(76)	H(23)[11)]	3.239	H(76)	H(24)[11)]	3.271
H(76)	H(30)[11)]	2.878	H(76)	H(31)[11)]	2.572
H(76)	H(36)[5)]	2.749	H(76)	H(37)[5)]	3.267

Symmetry Operators:

(1) -X+1,-Y,-Z
(2) -X+1,-Y+1,-Z
(3) X,Y-1,Z
(4) -X,-Y+1,-Z
(5) -X,-Y+1,-Z+1
(6) -X+1,-Y,-Z+1
(7) X+1,Y,Z
(8) -X+1,-Y+1,-Z+1
(9) -X,-Y,-Z+1
(10) X-1,Y,Z
(11) X,Y+1,Z
(12) -X,-Y,-Z