

Supporting information

Solubility Studies. Saturated solutions were prepared by stirring approximately 100 mg of the borate complexes in 10 mL of *n*-hexanes for at least 2 hours at 25 °C. The mixture was allowed to settle until the solution was completely clear upon visible inspection. A sample of 2.0(1) mL was taken while ensuring that no precipitated material was sampled. The solvent was removed *in vacuo* and the residue was kept under vacuum (0.1 mbar) for 1 h upon which the weight was constant within ± 1 mg. The weight of the residue was determined. When the amount of residue was < 5 mg a second sample was taken and analyzed by ICP/AAS analyses for boron (accurate down to 10 mass ppm) and rhodium (accurate down to 1 mass ppm). Furthermore, the solubility of the rhodium complexes was checked visually. Only **4b** resulted in significant orange coloring of the hexanes layer. All other rhodium compounds gave clear colorless hexanes layers.

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2a

: Jun 27 11:53:43 2000

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S U P P L E M E N T A R Y M A T E R I A L

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B E L O N G I N G T O T H E P A P E R

Increasing the Lipophilic Character of Tetraphenylborate
Anions through Alkyl- and Perfluoroalkylsilyl Substituents.

b y

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Compound 2a

C o n t e n t s

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Table S1 - Crystal Data and Details of the Structure Determination
for: 2a

Crystal Data	
Empirical Formula	C36 H52 B Si4, C20 H40 Na O8
Formula Weight	1039.46
Crystal System	Monoclinic
Space group	P21/c (No. 14)
a, b, c [Angstrom]	13.540(2) 20.606(3) 27.693(3)
alpha, beta, gamma [deg]	90 118.86(2) 90
V [Ang**3]	6767(2)
Z	4
D(calc) [g/cm**3]	1.020
F(000)	2256
Mu(MoKa) [/mm]	0.137
Crystal Size [mm]	0.3 x 0.3 x 0.4

Data Collection	
Temperature (K)	150
Radiation [Angstrom]	MoKa (graphite monochromator) 0.71073
Theta Min-Max [Deg]	1.3, 25.3
Dataset	-16: 16 ; -16: 24 ; -33: 29
Tot., Uniq. Data, R(int)	44964, 12222, 0.043

Refinement	
Npar	631
wR2, R1, S	0.2304, 0.0793 [for 9530 F > 4 sigma(F)], 1.069
w [sigma**2(F)+(0.1202P)**2+6.41P]**-1, P=(Max(Fo**2,0)+2Fc**2)/3	
Max. and Av. Shift/Error	0.006, 0.000
Min. and Max. resd. dens. [e/Ang^3]	-0.48, 0.96

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Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: 2a

Atom	x	y	z	U(eq) [Ang ²]
Si1	0.10522(7)	0.43526(5)	-0.09153(3)	0.0449(3)
Si2	0.90935(7)	0.31288(5)	0.22475(4)	0.0459(3)
Si3	0.36099(11)	0.52153(6)	0.33942(5)	0.0608(4)
Si4	0.15587(9)	0.07388(5)	0.16802(5)	0.0560(3)
C1	0.3193(2)	0.37093(13)	0.09607(11)	0.0293(8)
C2	0.3326(3)	0.34442(15)	0.05349(12)	0.0409(10)
C3	0.2723(3)	0.36441(15)	-0.00091(12)	0.0406(10)
C4	0.1925(2)	0.41380(14)	-0.01696(11)	0.0347(8)
C5	0.1805(3)	0.44257(15)	0.02530(12)	0.0409(9)
C6	0.2419(3)	0.42214(14)	0.07980(12)	0.0369(9)
C7	0.1979(3)	0.4633(2)	-0.12005(14)	0.0594(13)
C8	0.0314(4)	0.3600(3)	-0.13002(17)	0.0812(18)
C9	0.0007(4)	0.4988(3)	-0.09962(17)	0.0914(18)
C10	0.5209(2)	0.33069(13)	0.17155(10)	0.0295(8)
C11	0.5764(2)	0.27088(14)	0.18174(12)	0.0364(9)
C12	0.6889(3)	0.26549(14)	0.19441(13)	0.0395(9)
C13	0.7541(2)	0.31919(14)	0.19826(12)	0.0346(8)
C14	0.6983(2)	0.37917(14)	0.18601(12)	0.0361(9)
C15	0.5861(2)	0.38373(14)	0.17258(12)	0.0349(9)
C16	0.9460(4)	0.2340(2)	0.2055(2)	0.0780(16)
C17	0.9603(3)	0.3803(2)	0.1988(2)	0.0742(18)
C18	0.9793(4)	0.3188(3)	0.30236(19)	0.090(2)
C19	0.3843(2)	0.38739(13)	0.20546(11)	0.0297(8)
C20	0.4781(2)	0.41591(15)	0.24975(12)	0.0368(9)
C21	0.4699(3)	0.45452(16)	0.28860(13)	0.0439(10)
C22	0.3673(3)	0.46808(15)	0.28644(12)	0.0402(9)

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Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: 2a

Atom	x	y	z	U(eq) [Ang ²]
C23	0.2733(3)	0.43969(17)	0.24287(13)	0.0441(10)
C24	0.2817(2)	0.40047(16)	0.20446(12)	0.0401(9)
C25	0.4526(6)	0.5927(2)	0.3509(2)	0.102(3)
C26	0.4188(9)	0.4798(3)	0.4067(3)	0.163(5)
C27	0.2148(6)	0.5505(6)	0.3139(5)	0.247(6)
C28	0.3330(2)	0.26958(13)	0.16042(11)	0.0315(8)
C29	0.3547(6)	0.2397(3)	0.20757(16)	0.127(2)
C30	0.3057(6)	0.1808(3)	0.21014(17)	0.121(2)
C31	0.2306(3)	0.14930(14)	0.16603(13)	0.0427(9)
C32	0.2239(6)	0.1741(2)	0.11888(19)	0.109(2)
C33	0.2721(5)	0.2327(2)	0.11633(17)	0.095(2)
C34	0.1642(8)	0.0647(3)	0.2387(3)	0.153(4)
C35	0.0037(4)	0.0839(3)	0.1222(3)	0.100(2)
C36	0.2047(7)	0.0044(3)	0.1481(5)	0.226(7)
B	0.3901(3)	0.34005(15)	0.15899(12)	0.0293(9)
Na	0.64584(12)	0.20487(8)	0.43415(7)	0.0677(6)
O1	0.5745(2)	0.12538(13)	0.48781(10)	0.0572(9)
O2	0.6132(2)	0.07786(11)	0.40487(10)	0.0538(8)
O3	0.6377(2)	0.16326(13)	0.33721(11)	0.0655(10)
O4	0.7282(3)	0.28125(12)	0.38246(10)	0.0674(10)
O5	0.6868(2)	0.33734(14)	0.46275(11)	0.0651(9)
O6	0.6402(2)	0.25207(14)	0.52706(11)	0.0621(9)
O7	0.8271(3)	0.1813(2)	0.49635(15)	0.1049(16)
O8	0.4636(2)	0.24004(14)	0.38610(13)	0.0725(10)
C37	0.6098(3)	0.06064(19)	0.48731(17)	0.0631(14)
C38	0.5649(3)	0.03907(18)	0.42967(17)	0.0578(11)

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Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued) for: 2a

Atom	x	y	z	U(eq) [Ång ²]
C39	0.5733(4)	0.06150(19)	0.34879(16)	0.0628(14)
C40	0.6447(4)	0.09477(18)	0.32967(17)	0.0635(14)
C41	0.6994(4)	0.1979(2)	0.31802(19)	0.0733(16)
C42	0.6869(4)	0.26881(19)	0.32573(15)	0.0651(14)
C43	0.7377(4)	0.3482(2)	0.39267(18)	0.0734(16)
C44	0.7730(4)	0.3606(2)	0.45204(18)	0.0676(16)
C45	0.7036(5)	0.3546(3)	0.5150(2)	0.0865(17)
C46	0.6191(5)	0.3192(2)	0.5254(2)	0.0847(17)
C47	0.5675(3)	0.2141(2)	0.53900(16)	0.0643(14)
C48	0.5975(3)	0.1455(2)	0.54128(15)	0.0633(14)
C49	0.9086(5)	0.1658(4)	0.4784(2)	0.115(3)
C50	1.0091(5)	0.2026(3)	0.5143(3)	0.101(3)
C51	1.0090(5)	0.1973(4)	0.5709(3)	0.110(3)
C52	0.8888(4)	0.1920(4)	0.5529(2)	0.109(3)
C53	0.4226(4)	0.2982(2)	0.3561(2)	0.0759(16)
C54	0.2971(4)	0.2968(3)	0.3320(3)	0.108(2)
C55	0.2709(4)	0.2345(3)	0.3478(3)	0.116(3)
C56	0.3730(3)	0.1962(2)	0.37073(18)	0.0698(16)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

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Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters for: 2a

Atom	x	y	z	U(iso) [Ång ²]
H2	0.38500	0.31130	0.06200	0.0490
H3	0.28550	0.34440	-0.02730	0.0490
H5	0.12980	0.47660	0.01690	0.0490
H6	0.23100	0.44330	0.10650	0.0440
H7A	0.25120	0.42980	-0.11520	0.0890
H7B	0.23750	0.50170	-0.10100	0.0890
H7C	0.15260	0.47270	-0.15860	0.0890
H8A	0.08630	0.32760	-0.12550	0.1210
H8B	-0.01380	0.36990	-0.16850	0.1210
H8C	-0.01600	0.34380	-0.11580	0.1210
H9A	-0.04370	0.50970	-0.13790	0.1370
H9B	0.03960	0.53670	-0.07920	0.1370
H9C	-0.04770	0.48270	-0.08600	0.1370
H11	0.53670	0.23330	0.18000	0.0440
H12	0.72150	0.22450	0.20050	0.0470
H14	0.73750	0.41660	0.18700	0.0430
H15	0.55210	0.42440	0.16370	0.0420
H16A	0.91880	0.19940	0.21910	0.1170
H16B	1.02640	0.23070	0.22130	0.1170
H16C	0.91170	0.23110	0.16610	0.1170
H17A	1.04020	0.37600	0.21280	0.1110
H17B	0.94480	0.42090	0.21090	0.1110
H17C	0.92260	0.37920	0.15930	0.1110
H18A	0.95330	0.28400	0.31640	0.1350
H18B	0.96050	0.35960	0.31260	0.1350
H18C	1.05960	0.31570	0.31750	0.1350

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Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters (continued)
for: 2a

Atom	x	y	z	U(iso) [Ang ²]
H20	0.54900	0.40860	0.25320	0.0440
H21	0.53550	0.47200	0.31720	0.0530
H23	0.20250	0.44730	0.23950	0.0530
H24	0.21620	0.38190	0.17670	0.0480
H25A	0.52850	0.57850	0.36300	0.1540
H25B	0.45110	0.62020	0.37850	0.1540
H25C	0.42590	0.61660	0.31710	0.1540
H26A	0.49480	0.46640	0.41820	0.2440
H26B	0.37350	0.44240	0.40320	0.2440
H26C	0.41800	0.50880	0.43360	0.2440
H27A	0.16600	0.51410	0.30780	0.3700
H27B	0.19040	0.57370	0.27990	0.3700
H27C	0.21220	0.57890	0.34080	0.3700
H29	0.40530	0.25940	0.24060	0.1530
H30	0.32710	0.16290	0.24460	0.1460
H32	0.18480	0.15040	0.08650	0.1310
H33	0.26130	0.24690	0.08220	0.1140
H34A	0.13610	0.10330	0.24710	0.2290
H34B	0.24130	0.05790	0.26620	0.2290
H34C	0.11960	0.02810	0.23800	0.2290
H35A	-0.02250	0.12130	0.13330	0.1490
H35B	-0.03530	0.04600	0.12430	0.1490
H35C	-0.01060	0.08950	0.08500	0.1490
H36A	0.28420	-0.00060	0.17220	0.3350
H36B	0.19070	0.00970	0.11090	0.3350
H36C	0.16570	-0.03330	0.15040	0.3350

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Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters (continued)
for: 2a

Atom	x	y	z	U(iso) [Ang ²]
H37A	0.58220	0.03240	0.50630	0.0750
H37B	0.69150	0.05840	0.50630	0.0750
H38A	0.58370	-0.00620	0.42870	0.0690
H38B	0.48350	0.04340	0.41000	0.0690
H39A	0.49540	0.07510	0.32680	0.0760
H39B	0.57700	0.01490	0.34500	0.0760
H40A	0.72220	0.08020	0.35080	0.0760
H40B	0.61840	0.08520	0.29110	0.0760
H41A	0.67190	0.18850	0.27930	0.0890
H41B	0.77820	0.18550	0.33830	0.0890
H42A	0.72900	0.29400	0.31220	0.0780
H42B	0.60820	0.28120	0.30510	0.0780
H43A	0.66580	0.36910	0.36950	0.0880
H43B	0.79300	0.36650	0.38380	0.0880
H44A	0.84330	0.33830	0.47540	0.0810
H44B	0.78440	0.40670	0.45980	0.0810
H45A	0.69430	0.40110	0.51670	0.1030
H45B	0.77940	0.34310	0.54280	0.1030
H46A	0.62520	0.33320	0.56020	0.1020
H46B	0.54340	0.32870	0.49630	0.1020
H47A	0.48990	0.22060	0.51070	0.0770
H47B	0.57430	0.22740	0.57410	0.0770
H48A	0.67690	0.13940	0.56720	0.0760
H48B	0.55390	0.11970	0.55360	0.0760
H49A	0.88050	0.17830	0.44020	0.1380
H49B	0.92470	0.11960	0.48200	0.1380

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Table S4 - (An)isotropic Displacement Parameters for: 2a

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Si1	0.0408(5)	0.0617(6)	0.0288(4)	0.0071(4)	0.0140(4)	0.0171(4)
Si2	0.0296(4)	0.0451(5)	0.0606(6)	0.0084(4)	0.0174(4)	0.0086(4)
Si3	0.0801(8)	0.0592(7)	0.0591(6)	-0.0099(5)	0.0462(6)	0.0070(5)
Si4	0.0480(6)	0.0329(5)	0.0684(7)	0.0081(4)	0.0132(5)	-0.0081(4)
C1	0.0269(13)	0.0291(14)	0.0321(14)	0.0016(11)	0.0143(11)	0.0002(11)
C2	0.0432(17)	0.0411(17)	0.0400(16)	0.0075(13)	0.0213(14)	0.0185(14)
C3	0.0457(17)	0.0475(18)	0.0315(15)	0.0000(13)	0.0210(13)	0.0143(14)
C4	0.0321(14)	0.0388(16)	0.0316(14)	0.0030(12)	0.0140(12)	0.0043(12)
C5	0.0482(18)	0.0343(16)	0.0347(15)	0.0056(12)	0.0157(14)	0.0163(13)
C6	0.0435(16)	0.0336(15)	0.0315(14)	-0.0031(12)	0.0165(13)	0.0048(13)
C7	0.073(3)	0.069(2)	0.0403(18)	0.0109(17)	0.0305(18)	0.014(2)
C8	0.071(3)	0.110(4)	0.044(2)	-0.013(2)	0.013(2)	-0.023(3)
C9	0.090(3)	0.136(4)	0.047(2)	0.034(3)	0.032(2)	0.075(3)
C10	0.0305(14)	0.0310(14)	0.0236(12)	0.0040(11)	0.0103(11)	0.0037(11)
C11	0.0340(15)	0.0298(15)	0.0415(16)	0.0070(12)	0.0151(13)	0.0029(12)
C12	0.0384(16)	0.0293(15)	0.0490(17)	0.0104(13)	0.0197(14)	0.0102(12)
C13	0.0296(14)	0.0351(15)	0.0357(15)	0.0071(12)	0.0130(12)	0.0066(12)
C14	0.0321(15)	0.0306(15)	0.0434(16)	0.0046(12)	0.0164(13)	0.0000(12)
C15	0.0329(15)	0.0266(14)	0.0417(16)	0.0053(12)	0.0152(13)	0.0056(11)
C16	0.057(2)	0.057(2)	0.130(4)	-0.003(2)	0.053(3)	0.0126(19)
C17	0.049(2)	0.067(3)	0.111(4)	0.012(2)	0.042(2)	-0.0033(19)
C18	0.045(2)	0.136(5)	0.064(3)	0.010(3)	0.006(2)	0.023(3)
C19	0.0268(13)	0.0325(14)	0.0278(13)	0.0042(11)	0.0117(11)	0.0001(11)
C20	0.0272(14)	0.0430(17)	0.0340(15)	-0.0029(12)	0.0099(12)	0.0041(12)
C21	0.0378(16)	0.0493(19)	0.0383(16)	-0.0074(14)	0.0134(14)	0.0013(14)
C22	0.0472(17)	0.0388(16)	0.0390(16)	0.0028(13)	0.0242(14)	0.0052(14)

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Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters (continued) for: 2a

Atom	x	y	z	U(iso) [Ang^2]
H50A	1.00310	0.24740	0.50230	0.1210
H50B	1.07630	0.18330	0.51630	0.1210
H51A	1.04960	0.15910	0.59140	0.1320
H51B	1.04150	0.23560	0.59340	0.1320
H52A	0.87610	0.15650	0.57220	0.1310
H52B	0.86290	0.23170	0.56200	0.1310
H53A	0.44310	0.30090	0.32710	0.0910
H53B	0.45400	0.33540	0.38020	0.0910
H54A	0.27190	0.33210	0.34650	0.1290
H54B	0.26060	0.30070	0.29220	0.1290
H55A	0.24590	0.24050	0.37490	0.1400
H55B	0.21150	0.21280	0.31590	0.1400
H56A	0.38150	0.17220	0.40260	0.0840
H56B	0.37070	0.16560	0.34360	0.0840

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The Temperature Factor has the Form of $\text{Exp}(-T)$ Where
 $T = 8 * (\pi^2) * U * (\sin(\theta) / \lambda)^2$ for Isotropic Atoms

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Table S4 - (An)isotropic Displacement Parameters (continued)
for: 2a

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
C33	0.0358(16)	0.057(2)	0.0464(18)	0.0041(15)	0.0254(14)	0.0054(14)
C4	0.0311(15)	0.0527(19)	0.0350(15)	-0.0016(14)	0.0147(12)	-0.0045(13)
C5	0.180(6)	0.056(3)	0.101(4)	-0.026(3)	0.092(4)	-0.013(3)
C6	0.380(13)	0.068(3)	0.097(4)	0.000(3)	0.160(7)	0.001(5)
C7	0.100(5)	0.354(15)	0.258(11)	-0.210(11)	0.064(6)	0.038(7)
C8	0.0273(13)	0.0315(14)	0.0310(14)	0.0025(11)	0.0104(11)	0.0019(11)
C9	0.181(6)	0.120(4)	0.031(2)	0.005(2)	0.012(3)	-0.112(4)
C10	0.173(6)	0.111(4)	0.037(2)	0.011(2)	0.017(3)	-0.098(4)
C11	0.0414(17)	0.0304(15)	0.0424(17)	0.0049(13)	0.0092(14)	-0.0001(13)
C12	0.172(6)	0.071(3)	0.055(3)	-0.013(2)	0.031(3)	-0.075(4)
C13	0.162(5)	0.058(3)	0.045(2)	-0.0066(19)	0.035(3)	-0.055(3)
C14	0.220(9)	0.117(5)	0.096(4)	0.014(4)	0.055(5)	-0.092(6)
C15	0.059(3)	0.077(3)	0.161(6)	0.008(3)	0.051(3)	-0.005(2)
C16	0.173(7)	0.043(3)	0.57(2)	-0.064(6)	0.266(11)	-0.026(4)
C17	0.0272(15)	0.0290(15)	0.0280(15)	0.0028(12)	0.0103(12)	0.0013(12)
C18	0.0477(8)	0.0783(11)	0.0713(10)	0.0162(8)	0.0241(7)	0.0052(7)
C19	0.0580(15)	0.0659(16)	0.0500(14)	0.0145(12)	0.0280(12)	0.0107(12)
C20	0.0612(15)	0.0432(13)	0.0548(14)	0.0032(11)	0.0263(12)	-0.0053(11)
C21	0.0853(19)	0.0559(16)	0.0565(15)	-0.0010(12)	0.0352(15)	-0.0094(14)
C22	0.096(2)	0.0481(15)	0.0469(14)	0.0080(11)	0.0255(14)	-0.0098(14)
C23	0.0598(16)	0.0662(17)	0.0623(16)	-0.0137(13)	0.0240(13)	-0.0141(13)
C24	0.0553(15)	0.0813(19)	0.0569(15)	-0.0129(13)	0.0328(13)	-0.0057(13)
C25	0.066(2)	0.172(4)	0.076(2)	0.000(2)	0.0338(18)	0.021(2)
C26	0.0421(14)	0.0642(17)	0.096(2)	0.0212(15)	0.0213(14)	0.0022(12)
C27	0.060(2)	0.060(2)	0.071(3)	0.022(2)	0.033(2)	0.0030(19)
C28	0.059(2)	0.0441(19)	0.071(2)	0.0093(17)	0.032(2)	-0.0028(17)

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Table S4 - (An)isotropic Displacement Parameters (continued)
for: 2a

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
C39	0.075(3)	0.045(2)	0.060(2)	-0.0044(17)	0.026(2)	-0.0060(18)
C40	0.089(3)	0.047(2)	0.054(2)	-0.0068(17)	0.034(2)	-0.008(2)
C41	0.085(3)	0.076(3)	0.061(2)	0.008(2)	0.037(2)	-0.003(2)
C42	0.089(3)	0.057(2)	0.046(2)	0.0117(17)	0.030(2)	-0.004(2)
C43	0.090(3)	0.052(2)	0.069(3)	0.004(2)	0.031(2)	-0.018(2)
C44	0.072(3)	0.054(2)	0.072(3)	-0.0106(19)	0.031(2)	-0.026(2)
C45	0.094(3)	0.085(3)	0.090(3)	-0.040(3)	0.052(3)	-0.028(3)
C46	0.092(3)	0.091(3)	0.090(3)	-0.042(3)	0.059(3)	-0.016(3)
C47	0.054(2)	0.037(3)	0.052(2)	-0.008(2)	0.0335(18)	-0.004(2)
C48	0.056(2)	0.038(3)	0.0440(19)	0.013(2)	0.0306(18)	-0.002(2)
C49	0.078(4)	0.194(7)	0.080(4)	-0.001(4)	0.044(3)	0.031(4)
C50	0.092(4)	0.105(4)	0.135(5)	0.039(4)	0.077(4)	0.036(3)
C51	0.088(4)	0.150(6)	0.093(4)	0.009(4)	0.045(3)	0.023(4)
C52	0.070(3)	0.195(7)	0.059(3)	0.033(3)	0.029(2)	0.028(4)
C53	0.061(2)	0.065(3)	0.086(3)	0.022(2)	0.023(2)	-0.005(2)
C54	0.062(3)	0.080(3)	0.173(6)	0.058(4)	0.050(3)	0.020(3)
C55	0.051(3)	0.085(4)	0.187(7)	0.032(4)	0.037(3)	0.004(2)
C56	0.057(2)	0.064(3)	0.068(3)	0.016(2)	0.014(2)	-0.0062(19)

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The Temperature Factor has the Form of $\text{Exp}(-T)$ Where

$$T = 8 * (\pi^2) * U * (\sin(\theta) / \lambda)^2 \quad \text{for Isotropic Atoms}$$

$$T = 2 * (\pi^2) * \sum_i \sum_j h(i) * h(j) * U(i, j) * \text{Astar}(i) * \text{Astar}(j), \quad \text{for Anisotropic Atoms. Astar}(i) \text{ are Reciprocal Axial Lengths and } h(i) \text{ are the Reflection Indices.}$$

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Table S5 - Bond Distances (Angstrom)
for: 2a

Si1	-C4	1.871(3)	O4	-C42	1.414(4)
Si1	-C7	1.868(4)	O5	-C44	1.419(6)
Si1	-C8	1.874(6)	O5	-C45	1.398(6)
Si1	-C9	1.860(6)	O6	-C46	1.409(5)
Si2	-C13	1.867(3)	O6	-C47	1.416(5)
Si2	-C16	1.851(5)	O7	-C52	1.391(6)
Si2	-C17	1.844(5)	O7	-C49	1.448(8)
Si2	-C18	1.888(5)	O8	-C53	1.410(5)
Si3	-C22	1.869(4)	O8	-C56	1.414(5)
Si3	-C25	1.847(6)	C1	-C2	1.388(4)
Si3	-C26	1.848(7)	C1	-C6	1.400(4)
Si3	-C27	1.850(11)	C1	-B	1.658(4)
Si4	-C31	1.870(4)	C2	-C3	1.385(4)
Si4	-C34	1.915(8)	C3	-C4	1.392(5)
Si4	-C35	1.837(7)	C4	-C5	1.390(4)
Si4	-C36	1.773(9)	C5	-C6	1.391(4)
Na	-O2	2.712(3)	C10	-B	1.643(5)
Na	-O4	2.704(4)	C10	-C15	1.397(4)
Na	-O1	2.685(3)	C10	-C11	1.399(4)
Na	-O8	2.284(4)	C11	-C12	1.393(5)
Na	-O7	2.268(5)	C12	-C13	1.387(5)
O1	-C48	1.420(5)	C13	-C14	1.402(4)
O1	-C37	1.419(5)	C14	-C15	1.382(4)
O2	-C39	1.417(5)	C19	-B	1.647(4)
O2	-C38	1.404(5)	C19	-C20	1.400(4)
O3	-C40	1.436(5)	C19	-C24	1.402(4)
O3	-C41	1.385(6)	C20	-C21	1.385(5)
O4	-C43	1.402(5)	C21	-C22	1.390(6)

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Table S5 - Bond Distances (Angstrom)
for: 2a

C22	-C23	1.391(5)	C16	-H16B	0.9599
C23	-C24	1.384(5)	C17	-H17A	0.9611
C28	-C33	1.333(5)	C17	-H17B	0.9613
C28	-B	1.655(4)	C17	-H17C	0.9584
C28	-C29	1.342(6)	C18	-H18A	0.9599
C29	-C30	1.401(10)	C18	-H18C	0.9602
C30	-C31	1.322(6)	C18	-H18B	0.9601
C31	-C32	1.364(6)	C20	-H20	0.9300
C32	-C33	1.390(7)	C21	-H21	0.9311
C2	-H2	0.9291	C23	-H23	0.9305
C3	-H3	0.9285	C24	-H24	0.9305
C5	-H5	0.9289	C25	-H25A	0.9600
C6	-H6	0.9295	C25	-H25B	0.9595
C7	-H7C	0.9599	C25	-H25C	0.9606
C7	-H7A	0.9601	C26	-H26B	0.9603
C7	-H7B	0.9586	C26	-H26C	0.9591
C8	-H8C	0.9604	C26	-H26A	0.9593
C8	-H8B	0.9603	C27	-H27A	0.9591
C8	-H8A	0.9613	C27	-H27B	0.9612
C9	-H9C	0.9594	C27	-H27C	0.9612
C9	-H9A	0.9594	C29	-H29	0.9305
C9	-H9B	0.9590	C30	-H30	0.9294
C11	-H11	0.9305	C32	-H32	0.9298
C12	-H12	0.9300	C33	-H33	0.9311
C14	-H14	0.9291	C34	-H34B	0.9602
C15	-H15	0.9303	C34	-H34A	0.9576
C16	-H16C	0.9595	C34	-H34C	0.9605
C16	-H16A	0.9590	C35	-H35B	0.9601

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Table S5 - Bond Distances (Angstrom) (continued)
for: 2a

C35	-H35A	0.9589	C42	-H42B	0.9692
C35	-H35C	0.9589	C43	-H43A	0.9705
C36	-H36C	0.9586	C43	-H43B	0.9699
C36	-H36A	0.9598	C44	-H44A	0.9702
C36	-H36B	0.9595	C44	-H44B	0.9697
C37	-C38	1.476(6)	C45	-H45A	0.9705
C39	-C40	1.476(8)	C45	-H45B	0.9693
C41	-C42	1.498(6)	C46	-H46A	0.9705
C43	-C44	1.496(6)	C46	-H46B	0.9700
C45	-C46	1.497(10)	C47	-H47A	0.9702
C47	-C48	1.464(6)	C47	-H47B	0.9706
C49	-C50	1.452(10)	C48	-H48A	0.9705
C50	-C51	1.572(11)	C48	-H48B	0.9706
C51	-C52	1.458(10)	C49	-H49A	0.9704
C53	-C54	1.496(9)	C49	-H49B	0.9710
C54	-C55	1.454(9)	C50	-H50A	0.9712
C55	-C56	1.446(8)	C50	-H50B	0.9698
C37	-H37A	0.9719	C51	-H51A	0.9710
C37	-H37B	0.9700	C51	-H51B	0.9696
C38	-H38A	0.9707	C52	-H52A	0.9691
C38	-H38B	0.9695	C52	-H52B	0.9701
C39	-H39A	0.9705	C53	-H53A	0.9697
C39	-H39B	0.9699	C53	-H53B	0.9695
C40	-H40A	0.9700	C54	-H54A	0.9690
C40	-H40B	0.9692	C54	-H54B	0.9694
C41	-H41A	0.9698	C55	-H55A	0.9687
C41	-H41B	0.9699	C55	-H55B	0.9702
C42	-H42A	0.9700	C56	-H56A	0.9689

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Table S5 - Bond Distances (Angstrom) (continued)
for: 2a

C56	-H56B	0.9698
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Table S6 - Bond Angles
for: 2a

				(Degrees)	(continued)	
	C2	-C3	-C4	121.6(3)	C29	-C28
	Si1	-C4	-C5	124.1(2)	C28	-C29
	Si1	-C4	-C3	120.3(2)	C29	-C30
	C3	-C4	-C5	115.6(3)	Si4	-C30
	C4	-C5	-C6	122.2(3)	Si4	-C31
	C1	-C6	-C5	122.7(3)	C30	-C31
	C11	-C10	-B	124.4(3)	C31	-C32
	C15	-C10	-B	121.2(2)	C28	-C33
	C11	-C10	-C15	114.4(3)	C1	-C2
	C10	-C11	-C12	122.4(3)	C3	-C2
	C11	-C12	-C13	122.3(3)	C2	-C3
	Si2	-C13	-C12	121.9(2)	C4	-C3
	Si2	-C13	-C14	122.0(2)	C6	-C5
	C12	-C13	-C14	115.8(3)	C4	-C5
	C13	-C14	-C15	121.3(3)	C1	-C6
	C10	-C15	-C14	123.7(3)	C5	-C6
	C24	-C19	-B	121.3(3)	Si1	-C7
	C20	-C19	-B	124.6(3)	H7A	-C7
	C20	-C19	-C24	114.1(3)	H7A	-C7
	C19	-C20	-C21	122.9(3)	Si1	-C7
	C20	-C21	-C22	122.4(3)	Si1	-C7
	Si3	-C22	-C23	124.0(3)	H7B	-C7
	Si3	-C22	-C21	120.5(3)	Si1	-C8
	C21	-C22	-C23	115.5(3)	Si1	-C8
	C22	-C23	-C24	122.1(4)	Si1	-C8
	C19	-C24	-C23	123.1(3)	H8A	-C8
	C33	-C28	-B	124.6(3)	H8B	-C8
	C29	-C28	-C33	112.2(4)	H8A	-C8

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Table S6 - Bond Angles
for: 2a

	-Si1	-C7	110.15(15)	O1	-Na	-O8	86.55(12)
	-Si1	-C8	108.15(18)	O2	-Na	-O4	116.92(11)
	-Si1	-C9	109.74(16)	O2	-Na	-O7	88.90(13)
	-Si1	-C8	107.4(2)	O2	-Na	-O8	99.07(11)
	-Si1	-C9	111.0(2)	O1	-Na	-O2	61.74(9)
	-Si1	-C9	110.4(3)	O4	-Na	-O7	87.43(14)
	-Si2	-C16	110.8(2)	Na	-O1	-C48	116.3(2)
	-Si2	-C17	110.88(18)	C37	-O1	-C48	112.3(3)
	-Si2	-C18	107.1(2)	Na	-O1	-C37	110.8(2)
	-Si2	-C17	110.3(2)	Na	-O2	-C39	118.6(2)
	-Si2	-C18	109.1(2)	C38	-O2	-C39	112.3(3)
	-Si2	-C18	108.6(2)	Na	-O2	-C38	116.8(2)
	-Si3	-C25	108.8(2)	C40	-O3	-C41	110.9(4)
	-Si3	-C26	111.1(3)	Na	-O4	-C42	116.1(3)
	-Si3	-C27	109.6(4)	Na	-O4	-C43	119.2(3)
	-Si3	-C26	105.9(3)	C42	-O4	-C43	110.6(3)
	-Si3	-C27	108.4(4)	C44	-O5	-C45	113.0(4)
	-Si3	-C27	112.9(5)	C46	-O6	-C47	113.4(4)
	-Si4	-C34	110.3(3)	Na	-O7	-C49	120.7(3)
	-Si4	-C35	109.2(2)	C49	-O7	-C52	106.2(4)
	-Si4	-C36	111.9(4)	Na	-O7	-C52	131.5(4)
	-Si4	-C35	102.1(4)	Na	-O8	-C56	120.6(2)
	-Si4	-C36	113.0(4)	C53	-O8	-C56	109.1(4)
	-Si4	-C36	109.8(4)	Na	-O8	-C53	128.3(3)
	-Na	-O8	96.46(12)	C2	-C1	-C6	114.0(3)
	-Na	-O8	168.29(16)	C2	-C1	-B	119.7(3)
	-Na	-O4	176.91(13)	C6	-C1	-B	126.2(3)
	-Na	-O7	89.74(13)	C1	-C2	-C3	123.8(3)

Table S6 - Bond Angles
for: 2a[illegible]

Table S6 - Bond Angles
for: 2a

Table S6 - Bond Angles for: 2a			(Degrees)	(continued)			
Si13	-C27	-H27B	109.46	O1	-C37	-C38	109.2(3)
H27A	-C27	-H27C	109.44	O2	-C38	-C37	108.2(3)
C28	-C29	-H29	117.90	O2	-C39	-C40	108.3(4)
C30	-C29	-H29	118.03	O3	-C40	-C39	107.7(4)
C31	-C30	-H30	118.25	O3	-C41	-C42	108.5(4)
C29	-C30	-H30	118.38	O4	-C42	-C41	108.9(3)
C31	-C32	-H32	118.05	O4	-C43	-C44	109.8(3)
C33	-C32	-H32	118.02	O5	-C44	-C43	108.3(4)
C32	-C33	-H33	118.48	O5	-C45	-C46	108.5(4)
C28	-C33	-H33	118.38	O6	-C46	-C45	108.8(5)
Si14	-C34	-H34B	109.28	O6	-C47	-C48	109.5(4)
H34A	-C34	-H34C	109.72	O1	-C48	-C47	108.7(3)
H34B	-C34	-H34C	109.49	O7	-C49	-C50	105.5(5)
Si14	-C34	-H34A	109.39	C49	-C50	-C51	101.2(6)
Si14	-C34	-H34C	109.31	C50	-C51	-C52	101.7(6)
H34A	-C34	-H34B	109.63	O7	-C52	-C51	111.2(5)
Si14	-C35	-H35C	109.46	O8	-C53	-C54	106.6(4)
Si14	-C35	-H35B	109.45	C53	-C54	-C55	105.8(5)
H35A	-C35	-H35B	109.57	C54	-C55	-C56	107.1(5)
Si14	-C35	-H35A	109.52	O8	-C56	-C55	106.9(4)
H35B	-C35	-H35C	109.34	C38	-C37	-H37A	109.86
H35A	-C35	-H35C	109.49	O1	-C37	-H37B	109.92
H36A	-C36	-H36B	109.44	O1	-C37	-H37A	109.77
H36A	-C36	-H36C	109.62	C38	-C37	-H37B	109.80
Si14	-C36	-H36A	109.38	H37A	-C37	-H37B	108.29
Si14	-C36	-H36B	109.39	O2	-C38	-H38A	110.07
H36B	-C36	-H36C	109.51	C37	-C38	-H38A	110.04
Si14	-C36	-H36C	109.49	C37	-C38	-H38B	110.06

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Table S6 - Bond Angles
for: 2a

			(Degrees)	(continued)	
A	-C38	-H38B	108.37	C43	-C44
					-H44A
	-C38	-H38B	110.14	O5	-C44
	-C39	-H39B	109.99	H44A	-C44
	-C39	-H39A	110.02	C43	-C44
	-C39	-H39A	110.06	O5	-C45
A	-C39	-H39B	108.38	O5	-C45
	-C39	-H39B	110.12	C46	-C45
	-C40	-H40B	110.19	H45A	-C45
	-C40	-H40A	110.18	C46	-C45
A	-C40	-H40B	108.47	C45	-C46
	-C40	-H40B	110.18	C45	-C46
	-C40	-H40A	110.15	H46A	-C46
	-C41	-H41A	109.91	O6	-C46
	-C41	-H41A	110.05	O6	-C46
	-C41	-H41B	110.05	C48	-C47
A	-C41	-H41B	108.40	O6	-C47
	-C41	-H41B	109.92	O6	-C47
	-C42	-H42B	109.87	H47A	-C47
	-C42	-H42A	109.82	C48	-C47
	-C42	-H42A	109.95	O1	-C48
A	-C42	-H42B	108.37	O1	-C48
	-C42	-H42B	109.91	C47	-C48
	-C43	-H43B	109.62	H48A	-C48
A	-C43	-H43B	108.10	C47	-C48
	-C43	-H43A	109.71	C50	-C49
	-C43	-H43A	109.77	H49A	-C49
	-C43	-H43B	109.78	C50	-C49
	-C44	-H44B	110.09	O7	-C49

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Table S6 - Bond Angles
for: 2a

			(Degrees)	(continued)	
O7	-C49	-H49B	110.58	C53	-C54
C49	-C50	-H50A	111.47	C55	-C54
C49	-C50	-H50B	111.61	C53	-C54
C51	-C50	-H50A	111.53	H54A	-C54
C51	-C50	-H50B	111.53	C55	-C54
H50A	-C50	-H50B	109.30	C54	-C55
C50	-C51	-H51B	111.45	H55A	-C55
C52	-C51	-H51A	111.26	C56	-C55
C50	-C51	-H51A	111.51	C54	-C55
H51A	-C51	-H51B	109.32	C56	-C55
C52	-C51	-H51B	111.48	H56A	-C56
O7	-C52	-H52A	109.34	C55	-C56
C51	-C52	-H52B	109.38	O8	-C56
H52A	-C52	-H52B	108.10	O8	-C56
O7	-C52	-H52B	109.27	C55	-C56
C51	-C52	-H52A	109.51	C19	-B
O8	-C53	-H53A	110.36	C10	-B
C54	-C53	-H53B	110.40	C10	-B
O8	-C53	-H53B	110.44	C1	-B
C54	-C53	-H53A	110.43	C1	-B
H53A	-C53	-H53B	108.61	C1	-B

110.58 -H54B
110.62 -H54A
110.60 -H54A
108.70 -H54B
110.53 -H54B
110.34 -H55A
108.55 -H55B
110.18 -H55B
110.38 -H55B
110.31 -H55A
108.61 -H56B
110.39 -H56B
110.33 -H56B
110.34 -H56A
110.29 -H56A
107.6(3) -C28
111.1(2) -C28
110.9(2) -C19
106.6(3) -C10
111.9(2) -C19
108.8(2) -C28

4a

: Jun 27 12:02:09 2000

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S U P P L E M E N T A R Y M A T E R I A L

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B E L O N G I N G T O T H E P A P E R

Increasing the Lipophilic Character of Tetraphenylborate
Anions through Alkyl- and Perfluoroalkylsilyl Substituents.

b y

Joep van den Broeke, Martin Lutz, Huub Kooijman,
Anthony L. Spek, Berth-Jan Deelman, and Gerard van Koten

Compound 4a

C o n t e n t s

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Table S1 - Crystal Data and Details of the Structure Determination
for: 4a

Table S2 - Final Coordinates and Equivalent Isotropic Displacement
Parameters of the non-Hydrogen atoms
for: 4a

Table S3 - Hydrogen Atom Positions and Isotropic Displacement
Parameters
for: 4a

Table S4 - (An)isotropic Displacement Parameters
for: 4a

Table S5 - Bond Distances (Angstrom)
for: 4a

Table S6 - Bond Angles (Degrees)
for: 4a

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Table S1 - Crystal Data and Details of the Structure Determination
for: 4a

Crystal Data	
Empirical Formula	C52 H48 P4 Rh, C36 H52 B Si4
Formula Weight	1507.64
Crystal System	Monoclinic
Space group	P21 (No. 4)
a, b, c [Angstrom]	14.7259(2) 20.1809(2) 16.4196(2)
alpha, beta, gamma [deg]	90 96.5775(4) 90
V [Ang**3]	4847.49(10)
Z	2
D(calc) [g/cm**3]	1.033
F(000)	1588
Mu(MoKa) [/mm]	0.328
Crystal Size [mm]	0.25 x 0.25 x 0.63
Data Collection	
Temperature (K)	150
Radiation [Angstrom]	MoKa (graphite monochromator) 0.71073
Theta Min-Max [Deg]	1.3, 27.5
Dataset	-19: 18 ; -26: 26 ; 0: 21
Tot., Uniq. Data, R(int)	96384, 22082, 0.076
Refinement	
Npar	992
wR2, R1, S	0.0880, 0.0348 [for 19688 F > 4 sigma(F)], 1.039
w	[sigma**2(F)+(0.0511P)**2]**-1, P=(Max(Fo**2,0)+2Fc**2)/3
Max. and Av. Shift/Error	0.013, 0.001
Min. and Max. resd. dens. [e/Ang^3]	-0.35, 0.39

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Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms
for: 4a

Atom	x	y	z	U(eq) [Ang ²]
Rh	0.28853(1)	0.65540(1)	0.32427(1)	0.0311(1)
P1	0.32214(4)	0.54723(3)	0.29588(3)	0.0301(2)
P2	0.14072(4)	0.61694(3)	0.31548(4)	0.0357(2)
P3	0.25929(5)	0.76630(3)	0.31240(4)	0.0446(2)
P4	0.43275(4)	0.69026(3)	0.37372(4)	0.0348(2)
C1	0.21971(16)	0.49524(12)	0.30474(16)	0.0413(8)
C2	0.13597(16)	0.53440(12)	0.26729(16)	0.0422(8)
C3	0.3524(2)	0.81270(12)	0.37173(16)	0.0500(9)
C4	0.4427(2)	0.78032(12)	0.35885(15)	0.0447(8)
C5	0.41459(16)	0.49712(11)	0.34692(13)	0.0353(7)
C6	0.49888(17)	0.49394(12)	0.31642(16)	0.0433(8)
C7	0.5687(2)	0.45540(16)	0.3541(2)	0.0629(10)
C8	0.5543(2)	0.41862(15)	0.42376(19)	0.0673(11)
C9	0.4732(3)	0.42205(15)	0.45487(16)	0.0629(12)
C10	0.4021(2)	0.46116(12)	0.41735(14)	0.0457(8)
C11	0.33469(16)	0.53742(12)	0.18738(13)	0.0384(7)
C12	0.3265(2)	0.59215(16)	0.13563(16)	0.0593(10)
C13	0.3294(3)	0.5829(2)	0.05170(18)	0.0831(15)
C14	0.3398(3)	0.5213(2)	0.01961(18)	0.0833(15)
C15	0.3504(3)	0.4675(2)	0.0701(2)	0.0729(13)
C16	0.3462(2)	0.47415(15)	0.15484(17)	0.0525(9)
C17	0.10962(16)	0.59809(12)	0.41802(15)	0.0392(7)
C18	0.0327(2)	0.56007(15)	0.42743(19)	0.0566(9)
C19	0.0114(2)	0.54468(17)	0.5060(2)	0.0625(10)
C20	0.0636(2)	0.56668(16)	0.57303(19)	0.0623(11)
C21	0.1404(2)	0.60506(16)	0.56502(18)	0.0603(10)

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Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms
for: 4a

Atom	x	y	z	U(eq) [Ang ²]
C22	0.1627(2)	0.62099(13)	0.48706(15)	0.0475(8)
C23	0.03764(15)	0.65749(16)	0.26575(15)	0.0474(7)
C24	-0.0187(2)	0.69305(16)	0.3106(2)	0.0620(10)
C25	-0.0967(2)	0.7244(2)	0.2722(3)	0.0857(15)
C26	-0.1169(2)	0.7205(2)	0.1890(3)	0.0847(15)
C27	-0.0615(2)	0.6856(2)	0.1438(2)	0.0789(13)
C28	0.01632(17)	0.65373(19)	0.18090(16)	0.0581(8)
*C29A	0.1686(4)	0.8093(3)	0.3582(5)	0.053(2)
*C30A	0.1590(5)	0.8036(3)	0.4405(5)	0.070(3)
*C31A	0.0860(5)	0.8344(3)	0.4712(6)	0.059(4)
*C32A	0.0232(6)	0.8705(4)	0.4199(7)	0.111(5)
*C33A	0.0326(4)	0.8762(3)	0.3386(7)	0.089(4)
*C34A	0.1057(4)	0.8460(3)	0.3070(6)	0.067(3)
*C35A	0.2633(6)	0.7958(5)	0.2128(5)	0.0322(19)
*C36A	0.3136(8)	0.8489(5)	0.1878(5)	0.032(2)
*C37A	0.3070(7)	0.8665(5)	0.1059(6)	0.043(2)
*C38A	0.2500(6)	0.8315(4)	0.0486(5)	0.059(3)
*C39A	0.2008(6)	0.7799(4)	0.0728(5)	0.071(3)
*C40A	0.2072(5)	0.7612(4)	0.1539(5)	0.054(2)
C41	0.44775(16)	0.68008(12)	0.48518(14)	0.0382(6)
C42	0.4074(2)	0.62604(12)	0.51940(16)	0.0472(8)
C43	0.4150(2)	0.61669(14)	0.60336(17)	0.0532(9)
C44	0.46463(19)	0.6617(2)	0.65470(15)	0.0659(9)
C45	0.5050(3)	0.7145(2)	0.62239(18)	0.0779(13)
C46	0.4973(2)	0.72433(16)	0.53675(16)	0.0560(9)
C47	0.54017(16)	0.66034(15)	0.34063(17)	0.0500(8)

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Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued) for: 4a

Atom	x	y	z	U(eq) [Å ²]
C48	0.60830(19)	0.63184(15)	0.3932(2)	0.0627(10)
C49	0.6904(2)	0.61230(18)	0.3648(4)	0.0902(16)
C50	0.7035(3)	0.6212(2)	0.2840(4)	0.102(2)
C51	0.6354(3)	0.6496(3)	0.2304(3)	0.1016(17)
C52	0.5520(2)	0.66877(15)	0.2578(2)	0.0676(11)
C34B	0.0916(4)	0.8368(4)	0.2564(5)	0.059(3)
C35B	0.2697(9)	0.7840(6)	0.1986(6)	0.040(3)
C29B	0.1452(5)	0.8055(3)	0.3202(4)	0.036(2)
C30B	0.1176(5)	0.8068(3)	0.3981(4)	0.051(2)
C31B	0.0371(5)	0.8387(3)	0.4125(5)	0.064(3)
C32B	-0.0157(5)	0.8695(3)	0.3479(5)	0.069(3)
C33B	0.0116(5)	0.8678(4)	0.2720(5)	0.076(3)
C37B	0.3238(8)	0.8561(6)	0.0976(8)	0.053(3)
C38B	0.2856(7)	0.8151(5)	0.0355(6)	0.071(4)
C36B	0.3160(10)	0.8407(7)	0.1786(8)	0.057(4)
C40B	0.2322(7)	0.7433(5)	0.1354(5)	0.056(3)
C39B	0.2404(7)	0.7599(5)	0.0552(5)	0.076(4)
Si1	0.82950(5)	0.80541(3)	0.56678(4)	0.0409(2)
Si2	0.25536(6)	1.03968(4)	0.29564(8)	0.0725(4)
Si3	0.62311(6)	0.72067(4)	-0.05365(5)	0.0604(3)
Si4	0.91380(5)	1.18041(4)	0.15956(5)	0.0503(2)
C53	0.70066(13)	0.90326(10)	0.31616(12)	0.0298(6)
C54	0.69449(16)	0.83541(12)	0.33243(14)	0.0376(7)
C55	0.73142(17)	0.80752(12)	0.40615(14)	0.0402(7)
C56	0.77902(15)	0.84505(11)	0.46922(13)	0.0350(7)

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Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued) for: 4a

Atom	x	y	z	U(eq) [Å ²]
C57	0.78492(15)	0.91359(11)	0.45365(12)	0.0349(6)
C58	0.74758(15)	0.94087(11)	0.38053(13)	0.0344(6)
C59	0.8761(3)	0.72271(15)	0.53999(18)	0.0668(10)
C60	0.92254(19)	0.85813(15)	0.62069(16)	0.0517(9)
C61	0.7404(2)	0.79683(15)	0.63700(17)	0.0548(9)
C62	0.54954(14)	0.96324(11)	0.24771(13)	0.0322(6)
C63	0.51746(16)	0.95969(11)	0.32483(14)	0.0389(7)
C64	0.43094(17)	0.98194(12)	0.33848(17)	0.0438(8)
C65	0.37034(16)	1.00846(11)	0.27625(19)	0.0465(8)
C66	0.40198(16)	1.01232(12)	0.19962(18)	0.0458(8)
C67	0.48826(16)	0.99050(12)	0.18462(15)	0.0401(7)
C68	0.1692(3)	1.0135(2)	0.2084(4)	0.111(2)
C69	0.2575(3)	1.1299(2)	0.2961(5)	0.140(3)
C70	0.2211(3)	1.0033(3)	0.3902(4)	0.140(3)
C71	0.64387(14)	0.88411(11)	0.15667(13)	0.0330(6)
C72	0.56399(18)	0.84635(15)	0.13612(17)	0.0517(9)
C73	0.5569(2)	0.79888(15)	0.07531(18)	0.0566(9)
C74	0.62973(17)	0.78304(12)	0.03116(13)	0.0417(7)
C75	0.70968(18)	0.81833(13)	0.05285(15)	0.0463(8)
C76	0.71526(17)	0.86698(13)	0.11318(14)	0.0426(7)
C77	0.5179(3)	0.6717(2)	-0.0560(3)	0.1133(19)
C78	0.7271(3)	0.6674(2)	-0.0380(3)	0.1126(17)
C79	0.6207(3)	0.7644(2)	-0.1548(2)	0.1002(18)
C80	0.71625(15)	1.00289(11)	0.21238(12)	0.0320(6)
C81	0.81144(15)	0.99521(12)	0.21100(14)	0.0371(7)
C82	0.86867(16)	1.04753(12)	0.19491(14)	0.0390(7)

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Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued)
for: 4a

Atom	x	y	z	U(eq) [Ang ²]
C83	0.83513(16)	1.11120(11)	0.17961(13)	0.0380(7)
C84	0.74144(17)	1.11999(12)	0.18215(14)	0.0401(7)
C85	0.68369(16)	1.06713(11)	0.19755(13)	0.0362(6)
C86	1.0037(3)	1.1874(2)	0.2493(3)	0.1014(17)
C87	0.9675(3)	1.1614(2)	0.0651(2)	0.0840(14)
C88	0.8522(3)	1.26130(17)	0.1494(2)	0.0750(13)
B	0.65235(15)	0.93895(12)	0.23267(14)	0.0299(6)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Starred Atom sites have a S.O.F less than 1.0

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Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters
for: 4a

Atom	x	y	z	U(iso) [Ang ²]
H1B	0.21450	0.48520	0.36300	0.0500
H1A	0.22440	0.45290	0.27500	0.0500
H13	0.32400	0.62020	0.01620	0.0990
H14	0.33970	0.51590	-0.03790	0.1000
H15	0.36080	0.42520	0.04780	0.0870
H2A	0.07920	0.51120	0.27760	0.0510
H2B	0.13670	0.53870	0.20730	0.0510
H3A	0.35200	0.85940	0.35310	0.0600
H3B	0.34400	0.81220	0.43070	0.0600
H4A	0.49230	0.79840	0.39850	0.0540
H4B	0.45780	0.78970	0.30270	0.0540
H6	0.50840	0.51870	0.26890	0.0520
H7	0.62610	0.45380	0.33300	0.0760
H8	0.60170	0.39110	0.44930	0.0810
H9	0.46450	0.39760	0.50280	0.0760
H10	0.34540	0.46330	0.43970	0.0550
H12	0.31910	0.63530	0.15710	0.0710
*H31A	0.07910	0.83080	0.52780	0.1180
*H32A	-0.02680	0.89130	0.44150	0.1330
*H33A	-0.01080	0.90090	0.30360	0.1070
*H34A	0.11260	0.85040	0.25040	0.0810
*H36A	0.35270	0.87310	0.22710	0.0380
*H37A	0.34160	0.90280	0.08910	0.0520
*H38A	0.24540	0.84350	-0.00770	0.0710
*H39A	0.16120	0.75630	0.03320	0.0850
*H40A	0.17300	0.72430	0.16950	0.0650

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Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters (continued)
for: 4a

Atom	x	y	z	U(iso) [Ång ²]
H42	0.37390	0.59490	0.48440	0.0570
H43	0.38650	0.57970	0.62570	0.0640
H44	0.47030	0.65560	0.71240	0.0790
H45	0.53890	0.74510	0.65780	0.0930
H46	0.52620	0.76130	0.51470	0.0670
H48	0.59980	0.62530	0.44910	0.0750
H49	0.73730	0.59280	0.40170	0.1080
H50	0.75930	0.60780	0.26510	0.1220
H51	0.64490	0.65630	0.17470	0.1220
H52	0.50440	0.68710	0.22060	0.0810
H16	0.35100	0.43630	0.18950	0.0630
H18	-0.00530	0.54460	0.38060	0.0680
H19	-0.04080	0.51830	0.51210	0.0750
H20	0.04800	0.55600	0.62600	0.0750
H21	0.17760	0.62040	0.61240	0.0720
H22	0.21470	0.64770	0.48140	0.0570
H24	-0.00440	0.69630	0.36840	0.0740
H25	-0.13560	0.74850	0.30390	0.1030
H26	-0.16960	0.74220	0.16280	0.1020
H27	-0.07610	0.68280	0.08600	0.0950
H28	0.05460	0.62960	0.14870	0.0700
*H30A	0.20190	0.77880	0.47570	0.0840
*H30B	0.15390	0.78570	0.44210	0.0610
*H31B	0.01850	0.83930	0.46610	0.0770
*H32B	-0.07060	0.89170	0.35700	0.0820
*H33B	-0.02530	0.88850	0.22810	0.0910

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Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters (continued)
for: 4a

Atom	x	y	z	U(iso) [Ång ²]
*H34B	0.10960	0.83680	0.20270	0.0700
*H36B	0.34240	0.86920	0.22090	0.0680
*H37B	0.35560	0.89500	0.08470	0.0630
*H38B	0.29100	0.82550	-0.02010	0.0840
*H39B	0.21370	0.73190	0.01250	0.0910
*H40B	0.20090	0.70400	0.14740	0.0670
H54	0.66390	0.80740	0.29160	0.0450
H55	0.72420	0.76130	0.41420	0.0480
H57	0.81540	0.94160	0.49460	0.0420
H58	0.75360	0.98730	0.37290	0.0410
H59A	0.92280	0.72900	0.50270	0.1000
H59B	0.82640	0.69530	0.51320	0.1000
H59C	0.90330	0.70060	0.59010	0.1000
H60A	0.97130	0.86380	0.58540	0.0780
H60B	0.94740	0.83650	0.67190	0.0780
H60C	0.89760	0.90160	0.63290	0.0780
H61A	0.76680	0.77590	0.68820	0.0820
H61B	0.69040	0.76930	0.61110	0.0820
H61C	0.71670	0.84070	0.64890	0.0820
H63	0.55620	0.94140	0.36940	0.0470
H64	0.41300	0.97880	0.39210	0.0530
H66	0.36280	1.03070	0.15540	0.0550
H67	0.50600	0.99410	0.13090	0.0480
H68A	0.18610	1.03190	0.15710	0.1670
H68B	0.10860	1.02990	0.21780	0.1670

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Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters (continued)
for: 4a

Atom	x	y	z	U(iso) [Ang ²]
H68C	0.16780	0.96500	0.20500	0.1670
H69A	0.27990	1.14590	0.24570	0.2110
H69B	0.29820	1.14550	0.34360	0.2110
H69C	0.19570	1.14690	0.29920	0.2110
H70A	0.22150	0.95490	0.38600	0.2090
H70B	0.15950	1.01850	0.39800	0.2090
H70C	0.26410	1.01730	0.43700	0.2090
H72	0.51290	0.85390	0.16540	0.0620
H73	0.50050	0.77610	0.06300	0.0680
H75	0.76190	0.80900	0.02580	0.0560
H76	0.77160	0.88980	0.12520	0.0510
H77A	0.51550	0.63920	-0.10060	0.1700
H77B	0.46480	0.70120	-0.06510	0.1700
H77C	0.51710	0.64860	-0.00360	0.1700
H78A	0.72470	0.63420	-0.08180	0.1690
H78B	0.72940	0.64500	0.01520	0.1690
H78C	0.78170	0.69490	-0.03920	0.1690
H79A	0.61710	0.73160	-0.19910	0.1500
H79B	0.67650	0.79070	-0.15550	0.1500
H79C	0.56720	0.79360	-0.16270	0.1500
H81	0.83760	0.95260	0.22150	0.0450
H82	0.93220	1.03940	0.19440	0.0470
H84	0.71600	1.16300	0.17320	0.0480
H85	0.62020	1.07550	0.19790	0.0430
H86A	1.04530	1.22390	0.24010	0.1520
H86B	1.03830	1.14590	0.25580	0.1520

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Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters (continued)
for: 4a

Atom	x	y	z	U(iso) [Ang ²]
H86C	0.97470	1.19610	0.29900	0.1520
H87A	0.92000	1.15800	0.01830	0.1260
H87B	1.00060	1.11930	0.07210	0.1260
H87C	1.01030	1.19690	0.05500	0.1260
H88A	0.80240	1.25860	0.10450	0.1130
H88B	0.89490	1.29640	0.13760	0.1130
H88C	0.82700	1.27140	0.20070	0.1130

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The Temperature Factor has the Form of $\text{Exp}(-T)$ Where
 $T = 8 * (\pi^2) * U * (\sin(\text{Theta}) / \text{Lambda})^2$ for Isotropic Atoms

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Table S4 - (An)isotropic Displacement Parameters
for: 4a

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
C1	0.0350(1)	0.0278(1)	0.0317(1)	0.0029(1)	0.0086(1)	0.0001(1)
C2	0.0338(3)	0.0313(3)	0.0255(2)	0.0001(2)	0.0053(2)	-0.0015(2)
C3	0.0346(3)	0.0386(3)	0.0352(3)	0.0047(2)	0.0094(2)	0.0011(2)
C4	0.0489(3)	0.0317(3)	0.0568(4)	0.0103(3)	0.0216(3)	0.0068(3)
C5	0.0413(3)	0.0289(3)	0.0347(3)	-0.0006(2)	0.0062(2)	-0.0043(2)
C6	0.0428(13)	0.0316(12)	0.0504(14)	-0.0023(10)	0.0095(10)	-0.0071(10)
C7	0.0359(12)	0.0452(14)	0.0456(13)	-0.0029(11)	0.0050(10)	-0.0065(10)
C8	0.081(2)	0.0302(12)	0.0413(13)	-0.0007(10)	0.0175(13)	0.0007(12)
C9	0.0642(16)	0.0324(12)	0.0355(12)	-0.0007(9)	-0.0024(11)	-0.0056(11)
C10	0.0460(13)	0.0289(11)	0.0299(10)	-0.0029(8)	-0.0004(9)	0.0016(9)
C11	0.0436(13)	0.0410(13)	0.0443(13)	-0.0010(10)	0.0001(10)	0.0053(10)
C12	0.0540(16)	0.0649(19)	0.0691(19)	-0.0015(15)	0.0035(14)	0.0173(14)
C13	0.083(2)	0.0552(18)	0.0578(18)	-0.0034(14)	-0.0176(17)	0.0302(16)
C14	0.103(3)	0.0513(17)	0.0326(13)	0.0027(11)	0.0001(14)	0.0291(16)
C15	0.0698(17)	0.0346(12)	0.0330(11)	-0.0013(9)	0.0073(11)	0.0090(11)
C16	0.0411(12)	0.0469(13)	0.0269(10)	-0.0034(9)	0.0029(9)	-0.0063(10)
C17	0.075(2)	0.0655(18)	0.0366(14)	0.0058(12)	0.0026(13)	-0.0183(15)
C18	0.127(3)	0.091(3)	0.0298(14)	0.0113(16)	0.0025(17)	-0.030(2)
C19	0.110(3)	0.111(3)	0.0300(14)	-0.0123(17)	0.0132(16)	-0.027(2)
C20	0.080(2)	0.096(3)	0.0432(16)	-0.0328(18)	0.0096(15)	-0.0036(19)
C21	0.0628(17)	0.0572(16)	0.0362(13)	-0.0128(12)	0.0006(12)	-0.0017(13)
C22	0.0432(12)	0.0387(13)	0.0375(12)	0.0079(9)	0.0130(10)	0.0047(9)
C23	0.0524(15)	0.0650(18)	0.0551(16)	0.0125(13)	0.0184(13)	-0.0033(13)
C24	0.0581(17)	0.0702(19)	0.0638(18)	0.0151(15)	0.0274(15)	-0.0038(15)
C25	0.077(2)	0.0642(19)	0.0510(16)	0.0190(14)	0.0301(15)	0.0175(15)
C26	0.076(2)	0.0673(19)	0.0390(14)	-0.0005(12)	0.0130(13)	0.0101(15)

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Table S4 - (An)isotropic Displacement Parameters (continued)
for: 4a

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
C27	0.0581(15)	0.0459(14)	0.0399(13)	0.0015(11)	0.0111(11)	0.0012(12)
C28	0.0373(10)	0.0518(13)	0.0542(13)	0.0185(15)	0.0096(9)	0.0031(13)
C29	0.0554(16)	0.0674(19)	0.0675(18)	0.0244(15)	0.0257(14)	0.0161(14)
C30	0.0552(19)	0.086(3)	0.123(3)	0.041(2)	0.041(2)	0.0268(18)
C31	0.0452(17)	0.108(3)	0.100(3)	0.057(2)	0.0042(18)	0.0095(18)
C32	0.0455(16)	0.114(3)	0.074(2)	0.035(2)	-0.0065(15)	-0.0015(18)
C33	0.0457(12)	0.0754(18)	0.0530(13)	0.0139(17)	0.0052(11)	-0.0004(16)
C34	0.045(3)	0.036(3)	0.082(5)	0.004(3)	0.022(4)	0.003(2)
C35	0.074(5)	0.065(4)	0.076(5)	-0.001(4)	0.032(4)	0.011(3)
C36	0.113(7)	0.077(5)	0.116(8)	0.007(5)	0.058(6)	0.040(5)
C37	0.089(6)	0.062(5)	0.199(14)	-0.010(7)	0.089(8)	0.014(5)
C38	0.051(4)	0.050(4)	0.170(11)	0.015(5)	0.029(6)	0.002(3)
C39	0.046(3)	0.049(4)	0.109(7)	0.016(4)	0.016(4)	0.000(3)
C40	0.024(3)	0.026(4)	0.045(3)	-0.002(2)	-0.003(3)	0.000(3)
C41	0.040(5)	0.024(3)	0.032(3)	0.007(3)	0.009(3)	0.000(3)
C42	0.047(5)	0.040(3)	0.044(4)	0.004(3)	0.008(3)	-0.009(3)
C43	0.078(6)	0.057(4)	0.036(4)	0.011(3)	-0.022(4)	-0.019(4)
C44	0.076(6)	0.071(5)	0.060(5)	0.008(4)	-0.020(4)	-0.028(4)
C45	0.057(4)	0.051(4)	0.049(4)	0.011(3)	-0.019(3)	-0.033(4)
C46	0.0393(11)	0.0379(11)	0.0374(11)	0.0024(9)	0.0038(9)	0.0021(9)
C47	0.0622(16)	0.0336(12)	0.0454(13)	0.0020(10)	0.0047(12)	-0.0021(11)
C48	0.0633(17)	0.0468(15)	0.0491(15)	0.0177(12)	0.0041(13)	0.0012(13)
C49	0.0599(15)	0.100(2)	0.0350(12)	0.0135(16)	-0.0072(11)	-0.0142(19)
C50	0.080(2)	0.106(3)	0.0425(14)	0.0110(16)	-0.0154(15)	-0.048(2)
C51	0.0559(16)	0.0721(19)	0.0384(13)	0.0072(12)	-0.0015(12)	-0.0230(14)
C52	0.0434(12)	0.0395(13)	0.0705(15)	-0.0099(14)	0.0214(11)	-0.0131(12)

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Table S4 - (An)isotropic Displacement Parameters (continued)
for: 4a

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
C57	0.0456(15)	0.0557(17)	0.088(2)	-0.0189(15)	0.0126(15)	-0.0032(12)
C58	0.0481(18)	0.064(2)	0.160(4)	-0.029(2)	0.019(2)	-0.0003(16)
C59	0.073(3)	0.074(3)	0.171(5)	-0.023(3)	0.064(3)	-0.005(2)
C60	0.114(3)	0.091(3)	0.117(3)	-0.019(3)	0.087(3)	-0.017(3)
C61	0.0732(19)	0.061(2)	0.0755(19)	-0.0126(15)	0.0386(16)	-0.0128(15)
C62	0.054(4)	0.070(5)	0.055(4)	0.026(4)	0.020(3)	0.023(3)
C63	0.049(5)	0.024(4)	0.048(5)	0.005(3)	0.008(3)	0.006(3)
C64	0.043(4)	0.028(3)	0.041(4)	0.009(3)	0.018(3)	0.008(3)
C65	0.060(4)	0.050(4)	0.045(4)	0.001(3)	0.016(3)	0.003(3)
C66	0.069(5)	0.057(5)	0.075(5)	-0.004(4)	0.042(4)	0.006(4)
C67	0.067(5)	0.060(4)	0.086(6)	0.008(4)	0.039(5)	0.018(4)
C68	0.067(5)	0.079(5)	0.086(6)	0.029(5)	0.026(4)	0.028(4)
C69	0.042(5)	0.061(7)	0.053(6)	0.015(5)	-0.004(4)	-0.019(5)
C70	0.073(7)	0.096(8)	0.041(4)	0.025(5)	-0.001(4)	-0.034(6)
C71	0.046(7)	0.051(7)	0.072(9)	-0.007(5)	-0.002(6)	-0.014(5)
C72	0.070(6)	0.057(5)	0.041(4)	0.004(3)	0.007(3)	-0.012(4)
C73	0.096(8)	0.085(7)	0.041(4)	0.007(4)	-0.012(4)	-0.035(6)
C74	0.0491(4)	0.0404(3)	0.0320(3)	0.0057(3)	0.0000(3)	0.0053(3)
C75	0.0379(4)	0.0456(5)	0.1392(9)	0.0018(5)	0.0330(5)	0.0031(3)
C76	0.0649(5)	0.0621(5)	0.0504(4)	-0.0255(4)	-0.0101(4)	0.0089(4)
C77	0.0529(4)	0.0448(4)	0.0512(4)	0.0073(3)	-0.0030(3)	-0.0102(3)
C78	0.0282(9)	0.0334(11)	0.0275(10)	0.0001(8)	0.0025(8)	0.0028(8)
C79	0.0378(12)	0.0384(12)	0.0354(11)	-0.0005(9)	-0.0009(9)	0.0000(9)
C80	0.0443(13)	0.0360(12)	0.0395(12)	0.0071(10)	0.0014(10)	0.0017(10)
C81	0.0331(11)	0.0365(12)	0.0349(11)	0.0061(9)	0.0011(9)	0.0029(9)

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Table S4 - (An)isotropic Displacement Parameters (continued)
for: 4a

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
C57	0.0384(11)	0.0408(12)	0.0246(10)	-0.0026(8)	0.0001(8)	0.0005(9)
C58	0.0398(11)	0.0325(11)	0.0302(10)	-0.0009(8)	0.0008(9)	0.0054(9)
C59	0.094(2)	0.0535(17)	0.0494(15)	-0.0003(13)	-0.0075(16)	0.0244(16)
C60	0.0497(15)	0.0612(17)	0.0419(13)	0.0029(12)	-0.0053(11)	0.0018(12)
C61	0.0639(18)	0.0520(16)	0.0500(15)	0.0139(12)	0.0131(13)	-0.0029(13)
C62	0.0300(10)	0.0316(11)	0.0349(11)	-0.0003(8)	0.0033(8)	0.0027(8)
C63	0.0431(12)	0.0365(12)	0.0382(12)	-0.0006(9)	0.0096(10)	0.0027(10)
C64	0.0421(13)	0.0374(13)	0.0554(15)	-0.0050(11)	0.0206(11)	-0.0027(10)
C65	0.0338(12)	0.0278(12)	0.0799(18)	-0.0062(12)	0.0153(12)	-0.0003(9)
C66	0.0327(11)	0.0371(13)	0.0661(16)	0.0095(11)	-0.0004(11)	0.0043(9)
C67	0.0343(11)	0.0410(13)	0.0442(13)	0.0017(10)	0.0011(10)	0.0004(9)
C68	0.0458(19)	0.079(3)	0.206(6)	-0.001(3)	0.003(3)	0.0104(17)
C69	0.077(3)	0.058(2)	0.296(9)	-0.037(4)	0.065(4)	0.007(2)
C70	0.094(3)	0.153(5)	0.194(6)	0.011(4)	0.113(4)	0.016(3)
C71	0.0338(10)	0.0352(11)	0.0290(10)	0.0040(8)	-0.0003(8)	0.0021(8)
C72	0.0416(14)	0.0563(16)	0.0579(16)	-0.0190(13)	0.0089(12)	-0.0073(11)
C73	0.0509(15)	0.0570(17)	0.0612(17)	-0.0222(14)	0.0037(13)	-0.0137(13)
C74	0.0518(14)	0.0415(13)	0.0296(11)	-0.0051(9)	-0.0054(10)	0.0075(10)
C75	0.0489(14)	0.0517(15)	0.0402(12)	-0.0107(11)	0.0130(11)	0.0033(11)
C76	0.0409(12)	0.0518(14)	0.0366(12)	-0.0085(10)	0.0107(10)	-0.0046(10)
C77	0.109(3)	0.098(3)	0.130(4)	-0.065(3)	0.001(3)	-0.032(3)
C78	0.119(3)	0.099(3)	0.108(3)	-0.062(3)	-0.038(3)	0.060(3)
C79	0.129(4)	0.123(3)	0.0447(18)	-0.027(2)	-0.007(2)	0.035(3)
C80	0.0368(11)	0.0334(11)	0.0248(10)	-0.0022(8)	-0.0009(8)	0.0015(9)
C81	0.0373(11)	0.0380(12)	0.0352(11)	0.0022(9)	0.0011(9)	0.0017(9)
C82	0.0334(11)	0.0457(13)	0.0372(11)	0.0008(10)	0.0008(9)	0.0001(10)

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Table S4 - (An)isotropic Displacement Parameters (continued)
for: 4a

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
3	0.0438(12)	0.0397(13)	0.0284(10)	0.0027(9)	-0.0044(9)	-0.0089(10)
4	0.0473(13)	0.0322(12)	0.0388(12)	-0.0016(9)	-0.0035(10)	0.0024(10)
5	0.0345(11)	0.0399(12)	0.0329(10)	-0.0040(9)	-0.0015(9)	0.0058(9)
6	0.090(3)	0.087(3)	0.114(3)	0.023(2)	-0.045(2)	-0.046(2)
7	0.083(2)	0.075(2)	0.103(3)	0.016(2)	0.049(2)	0.002(2)
8	0.107(3)	0.0517(18)	0.070(2)	0.0091(16)	0.026(2)	0.0006(18)
	0.0279(10)	0.0330(12)	0.0290(11)	-0.0004(9)	0.0043(9)	0.0024(9)

=====
 The Temperature Factor has the Form of $\text{Exp}(-T)$ Where
 $T = 8 * (\pi^2) * U * (\sin(\theta) / \lambda)^2$ for Isotropic Atoms
 $T = 2 * (\pi^2) * \sum h(i) * h(j) * U(i,j) * \text{Astar}(i) * \text{Astar}(j)$, for
 Anisotropic Atoms. $\text{Astar}(i)$ are Reciprocal Axial Lengths and
 $h(i)$ are the Reflection Indices.

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Table S5 - Bond Distances (Angstrom)
for: 4a

Rh	-P1	2.2979(6)	Si3	-C74	1.871(2)
Rh	-P2	2.2997(6)	Si3	-C79	1.877(4)
Rh	-P3	2.2833(6)	Si4	-C83	1.868(2)
Rh	-P4	2.2956(6)	Si4	-C86	1.870(5)
P1	-C1	1.857(2)	Si4	-C87	1.860(4)
P1	-C5	1.821(2)	Si4	-C88	1.866(4)
P1	-C11	1.823(2)	C1	-C2	1.533(3)
P2	-C2	1.842(3)	C3	-C4	1.518(4)
P2	-C17	1.835(3)	C5	-C6	1.392(3)
P2	-C23	1.832(3)	C5	-C10	1.395(3)
P3	-C3	1.844(3)	C6	-C7	1.378(4)
P3	-C29A	1.825(6)	C7	-C8	1.400(4)
P3	-C35A	1.748(8)	C8	-C9	1.353(5)
P3	-C29B	1.875(7)	C9	-C10	1.397(5)
P3	-C35B	1.926(10)	C11	-C12	1.390(4)
P4	-C4	1.842(3)	C11	-C16	1.402(4)
P4	-C41	1.830(2)	C12	-C13	1.396(4)
P4	-C47	1.833(3)	C13	-C14	1.366(6)
Si1	-C61	1.851(3)	C14	-C15	1.364(5)
Si1	-C56	1.867(2)	C15	-C16	1.406(4)
Si1	-C59	1.876(3)	C17	-C18	1.391(4)
Si1	-C60	1.875(3)	C17	-C22	1.381(4)
Si2	-C69	1.821(4)	C18	-C19	1.397(4)
Si2	-C68	1.877(6)	C19	-C20	1.344(4)
Si2	-C70	1.839(6)	C20	-C21	1.389(4)
Si2	-C65	1.868(3)	C21	-C22	1.395(4)
Si3	-C78	1.865(4)	C23	-C28	1.395(4)
Si3	-C77	1.834(4)	C23	-C24	1.373(4)

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Table S5 - Bond Distances (Angstrom) (continued)
for: 4a

C24	-C25	1.397(5)	C41	-C42	1.391(4)
C25	-C26	1.367(7)	C41	-C46	1.380(4)
C26	-C27	1.361(5)	C42	-C43	1.383(4)
C27	-C28	1.392(4)	C43	-C44	1.389(4)
C29A	-C30A	1.380(11)	C44	-C45	1.357(5)
C29A	-C34A	1.391(10)	C45	-C46	1.412(4)
C29B	-C34B	1.389(10)	C47	-C48	1.373(4)
C29B	-C30B	1.386(9)	C47	-C52	1.401(4)
C30A	-C31A	1.386(10)	C48	-C49	1.401(5)
C30B	-C31B	1.393(10)	C49	-C50	1.374(9)
C31A	-C32A	1.385(13)	C50	-C51	1.381(7)
C31B	-C32B	1.388(11)	C51	-C52	1.410(6)
C32A	-C33A	1.363(16)	C1	-H1B	0.9894
C32B	-C33B	1.353(11)	C1	-H1A	0.9905
C33A	-C34A	1.388(10)	C2	-H2A	0.9895
C33B	-C34B	1.383(10)	C2	-H2B	0.9901
C35A	-C36A	1.386(12)	C3	-H3A	0.9907
C35A	-C36A	1.391(14)	C3	-H3B	0.9901
C35B	-C36B	1.390(19)	C4	-H4B	0.9911
C35B	-C40B	1.388(14)	C4	-H4A	0.9907
C36A	-C37A	1.383(13)	C6	-H6	0.9504
C36B	-C37B	1.383(18)	C7	-H7	0.9501
C37A	-C38A	1.381(13)	C8	-H8	0.9510
C37B	-C38B	1.382(16)	C9	-H9	0.9499
C38A	-C39A	1.354(12)	C10	-H10	0.9507
C38B	-C39B	1.356(14)	C12	-H12	0.9504
C39A	-C40A	1.377(12)	C13	-H13	0.9498
C39B	-C40B	1.377(12)	C14	-H14	0.9504

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Table S5 - Bond Distances (Angstrom) (continued)
for: 4a

C15	-H15	0.9482	C39A	-H39A	0.9502
C16	-H16	0.9503	C39B	-H39B	0.9499
C18	-H18	0.9504	C40A	-H40A	0.9504
C19	-H19	0.9497	C40B	-H40B	0.9493
C20	-H20	0.9495	C42	-H42	0.9506
C21	-H21	0.9505	C43	-H43	0.9504
C22	-H22	0.9497	C44	-H44	0.9495
C24	-H24	0.9506	C45	-H45	0.9498
C25	-H25	0.9507	C46	-H46	0.9509
C26	-H26	0.9501	C48	-H48	0.9497
C27	-H27	0.9505	C49	-H49	0.9503
C28	-H28	0.9501	C50	-H50	0.9503
C30A	-H30A	0.9487	C51	-H51	0.9506
C30B	-H30B	0.9490	C52	-H52	0.9504
C31A	-H31A	0.9492	C53	-C54	1.400(3)
C31B	-H31B	0.9513	C53	-C58	1.415(3)
C32A	-H32A	0.9508	C53	-B	1.637(3)
C32B	-H32B	0.9510	C54	-C55	1.388(3)
C33A	-H33A	0.9503	C55	-C56	1.404(3)
C33B	-H33B	0.9485	C56	-C57	1.411(3)
C34A	-H34A	0.9505	C57	-C58	1.377(3)
C34B	-H34B	0.9493	C62	-C63	1.403(3)
C36A	-H36A	0.9494	C62	-C67	1.406(3)
C36B	-H36B	0.9500	C62	-B	1.637(3)
C37A	-H37A	0.9511	C63	-C64	1.393(3)
C37B	-H37B	0.9503	C64	-C65	1.385(4)
C38A	-H38A	0.9505	C65	-C66	1.393(4)
C38B	-H38B	0.9489	C66	-C67	1.393(3)

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Table S5 - Bond Distances (Angstrom) (continued)
for: 4a

C71	-C72	1.410(3)	C64	-H64	0.9499
C71	-C76	1.381(3)	C66	-H66	0.9496
C71	-B	1.662(3)	C67	-H67	0.9510
C72	-C73	1.379(4)	C68	-H68A	0.9784
C73	-C74	1.399(4)	C68	-H68B	0.9804
C74	-C75	1.387(4)	C68	-H68C	0.9804
C75	-C76	1.390(4)	C69	-H69A	0.9800
C80	-C81	1.413(3)	C69	-H69B	0.9796
C80	-C85	1.394(3)	C69	-H69C	0.9793
C80	-B	1.653(3)	C70	-H70A	0.9792
C81	-C82	1.395(3)	C70	-H70B	0.9798
C82	-C83	1.389(3)	C70	-H70C	0.9797
C83	-C84	1.396(3)	C72	-H72	0.9504
C84	-C85	1.405(3)	C73	-H73	0.9505
C54	-H54	0.9501	C75	-H75	0.9499
C55	-H55	0.9498	C76	-H76	0.9497
C57	-H57	0.9508	C77	-H77A	0.9807
C58	-H58	0.9508	C77	-H77B	0.9805
C59	-H59A	0.9800	C77	-H77C	0.9798
C59	-H59B	0.9805	C78	-H78A	0.9806
C59	-H59C	0.9803	C78	-H78B	0.9807
C60	-H60A	0.9797	C78	-H78C	0.9790
C60	-H60B	0.9803	C79	-H79A	0.9804
C60	-H60C	0.9806	C79	-H79B	0.9794
C61	-H61A	0.9805	C79	-H79C	0.9805
C61	-H61B	0.9798	C81	-H81	0.9499
C61	-H61C	0.9795	C82	-H82	0.9508
C63	-H63	0.9495	C84	-H84	0.9501

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Table S5 - Bond Distances (Angstrom) (continued)
for: 4a

C85	-H85	0.9507	C87	-H87B	0.9797
C86	-H86A	0.9808	C87	-H87C	0.9808
C86	-H86B	0.9798	C88	-H88A	0.9800
C86	-H86C	0.9793	C88	-H88B	0.9811
C87	-H87A	0.9805	C88	-H88C	0.9800

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Table S6 - Bond Angles (Degrees) (continued)
for: 4a

C87	-Si4	-C88	110.78(17)	C19	-C20	-C21	120.1(3)
C86	-Si4	-C87	110.02(19)	C20	-C21	-C22	119.7(3)
C83	-Si4	-C86	108.36(15)	C17	-C22	-C21	120.4(3)
P1	-C1	-C2	107.50(16)	P2	-C23	-C24	121.0(2)
P2	-C2	-C1	107.74(17)	P2	-C23	-C28	120.1(2)
P3	-C3	-C4	108.54(17)	C24	-C23	-C28	118.9(3)
P4	-C4	-C3	108.79(18)	C23	-C24	-C25	120.7(3)
P1	-C5	-C6	120.69(17)	C24	-C25	-C26	119.9(3)
C6	-C5	-C10	118.8(2)	C25	-C26	-C27	120.0(3)
P1	-C5	-C10	120.51(19)	C26	-C27	-C28	121.0(3)
C5	-C6	-C7	121.0(2)	C23	-C28	-C27	119.5(3)
C6	-C7	-C8	119.4(3)	C30A	-C29A	-C34A	120.0(6)
C7	-C8	-C9	120.3(3)	P3	-C29A	-C34A	118.2(6)
C8	-C9	-C10	120.8(3)	P3	-C29A	-C30A	121.7(5)
C5	-C10	-C9	119.7(3)	P3	-C29B	-C30B	115.5(5)
P1	-C11	-C16	120.11(19)	P3	-C29B	-C34B	125.2(5)
P1	-C11	-C12	119.98(19)	C30B	-C29B	-C34B	119.1(7)
C12	-C11	-C16	119.8(2)	C29A	-C30A	-C31A	119.3(7)
C11	-C12	-C13	119.1(3)	C29B	-C30B	-C31B	120.7(6)
C12	-C13	-C14	121.3(3)	C30A	-C31A	-C32A	120.4(9)
C13	-C14	-C15	120.0(3)	C30B	-C31B	-C32B	119.4(7)
C14	-C15	-C16	120.7(3)	C31A	-C32A	-C33A	120.3(8)
C11	-C16	-C15	119.0(3)	C31B	-C32B	-C33B	119.5(7)
P2	-C17	-C22	120.44(19)	C32A	-C33A	-C34A	119.9(8)
P2	-C17	-C18	120.5(2)	C32B	-C33B	-C34B	122.1(7)
C18	-C17	-C22	119.0(2)	C29A	-C34A	-C33A	119.9(9)
C17	-C18	-C19	119.8(3)	C29B	-C34B	-C33B	119.2(7)
C18	-C19	-C20	121.0(3)	P3	-C35A	-C40A	113.6(7)

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Table S6 - Bond Angles (Degrees)
for: 4a

-Rh	-P2	83.74(2)	C29B	-P3	-C35B	99.2(4)
-Rh	-P3	163.09(2)	Rh	-P4	-C4	109.87(9)
-Rh	-P4	98.68(2)	Rh	-P4	-C41	108.67(8)
-Rh	-P3	99.07(2)	Rh	-P4	-C47	126.10(9)
-Rh	-P4	162.99(2)	C4	-P4	-C41	103.95(11)
-Rh	-P4	83.54(2)	C4	-P4	-C47	101.61(13)
-P1	-C1	108.97(8)	C41	-P4	-C47	104.48(12)
-P1	-C5	126.95(7)	C56	-Si1	-C60	111.07(11)
-P1	-C11	110.47(8)	C56	-Si1	-C61	109.48(12)
-P1	-C5	102.79(11)	C59	-Si1	-C60	110.39(16)
-P1	-C11	100.92(11)	C59	-Si1	-C61	111.54(15)
-P1	-C11	103.61(11)	C60	-Si1	-C61	106.90(13)
-P2	-C2	108.74(8)	C56	-Si1	-C59	107.48(12)
-P2	-C17	110.26(8)	C65	-Si2	-C68	108.76(18)
-P2	-C23	127.38(10)	C65	-Si2	-C69	108.81(17)
-P2	-C17	101.86(11)	C68	-Si2	-C69	107.1(3)
-P2	-C23	102.93(12)	C68	-Si2	-C70	107.8(2)
-P2	-C23	102.74(11)	C69	-Si2	-C70	113.7(3)
-P3	-C3	109.34(8)	C65	-Si2	-C70	110.54(19)
-P3	-C29A	124.8(2)	C74	-Si3	-C78	108.26(17)
-P3	-C35A	112.8(3)	C74	-Si3	-C79	109.65(14)
-P3	-C29B	124.72(19)	C74	-Si3	-C77	110.48(17)
-P3	-C35B	103.3(4)	C78	-Si3	-C79	109.0(2)
-P3	-C29A	94.3(2)	C77	-Si3	-C79	107.7(2)
-P3	-C35A	102.6(3)	C77	-Si3	-C78	111.75(19)
-P3	-C29B	111.6(2)	C83	-Si4	-C87	108.92(15)
-P3	-C35B	106.3(4)	C83	-Si4	-C88	111.41(15)
-P3	-C35A	109.2(4)	C86	-Si4	-C88	107.31(17)

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Table S6 - Bond Angles
for: 4a

				(Degrees)	(continued)	
C7	-C8	-H8		119.85	C24	-C25
C8	-C9	-H9		119.65	C25	-C26
C10	-C9	-H9		119.57	C27	-C26
C5	-C10	-H10		120.09	C26	-C27
C9	-C10	-H10		120.17	C28	-C27
C11	-C12	-H12		120.45	C27	-C28
C13	-C12	-H12		120.42	C23	-C28
C12	-C13	-H13		119.34	C29A	-C30A
C14	-C13	-H13		119.33	C31A	-C30A
C15	-C14	-H14		119.97	C31B	-C30B
C13	-C14	-H14		120.02	C29B	-C30B
C14	-C15	-H15		119.62	C32A	-C31A
C16	-C15	-H15		119.69	C30A	-C31A
C15	-C16	-H16		120.47	C32B	-C31B
C11	-C16	-H16		120.52	C30B	-C31B
C17	-C18	-H18		120.18	C33A	-C32A
C19	-C18	-H18		120.03	C31A	-C32A
C18	-C19	-H19		119.47	C31B	-C32B
C20	-C19	-H19		119.53	C33B	-C32B
C19	-C20	-H20		119.97	C32A	-C33A
C21	-C20	-H20		119.88	C34A	-C33A
C20	-C21	-H21		120.21	C32B	-C33B
C22	-C21	-H21		120.12	C34B	-C33B
C21	-C22	-H22		119.85	C33A	-C34A
C17	-C22	-H22		119.78	C29A	-C34A
C23	-C24	-H24		119.55	C29B	-C34B
C25	-C24	-H24		119.74	C33B	-C34B
C26	-C25	-H25		120.06	C35A	-C36A

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Table S6 - Bond Angles
for: 4a

				(Degrees)	(continued)	
-C35A	-C36A			119.8(4)	-C51	
-C35A	-C40A			120.4(4)	-C52	
-C35B	-C36B			119.1(3)	-C51	
-C35B	-C40B			110.22	-H1A	
-C35B	-C40B			110.21	-H1B	
-C36A	-C37A			110.19	-H1B	
-C36B	-C37B			110.20	-H1A	
-C37A	-C38A			108.51	-H1B	
-C37B	-C38B			110.12	-H2A	
-C38A	-C39A			110.22	-H2A	
-C38B	-C39B			110.11	-H2B	
-C39A	-C40A			108.50	-H2B	
-C39B	-C40B			110.14	-H2B	
-C40A	-C39A			110.01	-H3A	
-C40B	-C39B			108.34	-H3B	
-C41	-C46			109.96	-H3B	
-C41	-C46			110.05	-H3B	
-C41	-C42			109.93	-H3A	
-C42	-C43			109.93	-H4B	
-C43	-C44			109.97	-H4A	
-C44	-C45			108.29	-H4B	
-C45	-C46			109.97	-H4B	
-C45	-C45			109.89	-H4A	
-C47	-C52			119.52	-H6	
-C47	-C48			119.51	-H6	
-C47	-C52			120.31	-H7	
-C48	-C49			120.28	-H7	
-C49	-C50			119.88	-H8	

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Table S6 - Bond Angles
for: 4a

		(Degrees)	(continued)			
-C36A	-H36A	119.88	C41	-C46	-H46	120.15
-C36B	-H36B	119.75	C49	-C48	-H48	119.79
-C36B	-H36B	119.66	C47	-C48	-H48	119.89
-C37A	-H37A	120.02	C50	-C49	-H49	119.84
-C37A	-H37A	119.96	C48	-C49	-H49	119.74
-C37B	-H37B	119.97	C49	-C50	-H50	120.02
-C37B	-H37B	119.81	C51	-C50	-H50	120.13
-C38A	-H38A	120.15	C52	-C51	-H51	119.85
-C38A	-H38A	120.03	C50	-C51	-H51	119.74
-C38B	-H38B	120.37	C51	-C52	-H52	120.47
-C38B	-H38B	120.59	C47	-C52	-H52	120.43
-C39A	-H39A	119.46	C54	-C53	-C58	114.76(19)
-C39A	-H39A	119.54	C54	-C53	-B	123.95(18)
-C39B	-H39B	119.06	C58	-C53	-B	121.16(18)
-C39B	-H39B	119.13	C53	-C54	-C55	122.4(2)
-C40A	-H40A	119.72	C54	-C55	-C56	122.5(2)
-C40A	-H40A	119.89	Si1	-C56	-C55	121.18(17)
-C40B	-H40B	120.03	Si1	-C56	-C57	123.28(16)
-C40B	-H40B	119.96	C55	-C56	-C57	115.53(19)
-C42	-H42	119.31	C56	-C57	-C58	121.5(2)
-C42	-H42	119.36	C53	-C58	-C57	123.3(2)
-C43	-H43	120.19	C63	-C62	-C67	115.5(2)
-C43	-H43	120.29	C63	-C62	-B	122.26(19)
-C44	-H44	120.06	C67	-C62	-B	122.20(19)
-C44	-H44	119.96	C62	-C63	-C64	122.5(2)
-C45	-H45	119.61	C63	-C64	-C65	122.0(2)
-C45	-H45	119.67	Si2	-C65	-C64	121.6(2)
-C46	-H46	120.07	Si2	-C65	-C66	122.6(2)

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Table S6 - Bond Angles
for: 4a

		(Degrees)	(continued)			
C64	-C65	-C66	115.7(2)	C56	-C57	-H57
C65	-C66	-C67	123.2(2)	C53	-C58	-H58
C62	-C67	-C66	121.0(2)	C57	-C58	-H58
C72	-C71	-C76	113.9(2)	Si1	-C59	-H59C
C72	-C71	-B	121.91(19)	H59A	-C59	-H59B
C76	-C71	-B	123.98(19)	Si1	-C59	-H59B
C71	-C72	-C73	122.7(2)	H59B	-C59	-H59C
C72	-C73	-C74	122.4(3)	H59A	-C59	-H59C
Si3	-C74	-C73	124.2(2)	Si1	-C59	-H59A
Si3	-C74	-C75	120.45(19)	Si1	-C60	-H60A
C73	-C74	-C75	115.4(2)	Si1	-C60	-H60C
C74	-C75	-C76	121.6(2)	H60A	-C60	-H60B
C71	-C76	-C75	124.0(2)	H60A	-C60	-H60C
C81	-C80	-C85	114.9(2)	H60B	-C60	-H60C
C81	-C80	-B	120.41(19)	Si1	-C60	-H60B
C85	-C80	-B	124.66(19)	Si1	-C61	-H61A
C80	-C81	-C82	122.8(2)	Si1	-C61	-H61B
C81	-C82	-C83	121.6(2)	H61B	-C61	-H61C
Si4	-C83	-C82	120.58(18)	H61A	-C61	-H61C
Si4	-C83	-C84	123.04(17)	Si1	-C61	-H61C
C82	-C83	-C84	116.4(2)	H61A	-C61	-H61B
C83	-C84	-C85	122.0(2)	C64	-C63	-H63
C80	-C85	-C84	122.3(2)	C62	-C63	-H63
C55	-C54	-H54	118.74	C63	-C64	-H64
C53	-C54	-H54	118.89	C65	-C64	-H64
C54	-C55	-H55	118.73	C65	-C66	-H66
C56	-C55	-H55	118.79	C67	-C66	-H66
C58	-C57	-H57	119.21	C66	-C67	-H67

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Table S6 - Bond Angles
for: 4a

		(Degrees)	(continued)	
	-H67	119.48	Si3	-C77
2	-C67			
2	-H68A	109.50	Si3	-C77
2	-H68C	109.41	H77A	-C77
2	-H68B	109.47	H77B	-C77
2	-H68B	109.43	H77A	-C77
2	-H68C	109.41	Si3	-C78
2	-H69B	109.61	Si3	-C78
2	-H69C	109.47	H78A	-C78
2	-H69C	109.56	Si3	-C78
2	-H69C	109.46	H78B	-C78
2	-H69C	109.48	H78A	-C78
2	-H69B	109.39	Si3	-C79
2	-H69A	109.47	Si3	-C79
2	-H70B	109.45	H79A	-C79
2	-H70C	109.38	H79B	-C79
2	-H70B	109.55	H79A	-C79
2	-H70C	109.53	Si3	-C79
2	-H70C	109.39	C82	-C81
2	-H70A	109.53	C80	-C81
2	-H72	118.65	C81	-C82
2	-H72	118.62	C83	-C82
2	-H73	118.80	C85	-C84
2	-H73	118.85	C83	-C84
2	-H75	119.22	C80	-C85
2	-H75	119.14	C84	-C85
2	-H76	118.00	H86A	-C86
2	-H76	118.03	H86A	-C86
2	-H77B	109.45	Si4	-C86

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Table S6 - Bond Angles
for: 4a

		(Degrees)	(continued)	
	-H86A	109.49	Si4	-C88
	-H86B	109.50	H88B	-C88
	-H86C	109.48	H88A	-C88
	-H87A	109.56	H88A	-C88
	-H87B	109.54	C53	-B
	-H87B	109.39	C53	-B
	-H87C	109.46	C71	-B
	-H87C	109.43	C62	-B
	-H87C	109.46	C62	-B
	-H88B	109.47	C53	-B
	-H88C	109.47		

Si4	-C86	109.45	-H77C	109.45
Si4	-C86	109.52	-H77A	109.52
H86B	-C86	109.54	-H77C	109.54
Si4	-C87	109.46	-H77C	109.46
Si4	-C87	109.41	-H77B	109.41
H87A	-C87	109.44	-H78A	109.44
H87A	-C87	109.50	-H78C	109.50
H87B	-C87	109.45	-H78B	109.45
Si4	-C87	109.42	-H78B	109.42
Si4	-C88	109.55	-H78C	109.55
Si4	-C88	109.47	-H78C	109.47
		109.53	-H79B	109.53
		109.45	-H79C	109.45
		109.47	-H79C	109.47
		109.59	-H79C	109.59
		109.35	-H79B	109.35
		109.44	-H79A	109.44
		118.58	-H81	118.58
		118.61	-H81	118.61
		119.17	-H82	119.17
		119.20	-H82	119.20
		119.04	-H84	119.04
		119.00	-H84	119.00
		118.88	-H85	118.88
		118.82	-H85	118.82
		109.43	-H86B	109.43
		109.48	-H86C	109.48
		109.46	-H86C	109.46