Table 1 Refined Positional Parameters for Compound 1

Atom	x	y	z	Ueq, Å^2
N13	0.8442(4)	-0.0467(3)	0.8024(3)	0.0686(13)
N16	0.8498(4)	-0.0481(3)	0.5570(3)	0.0698(13)
C5	0.7646(4)	0.1543(3)	0.7747(4)	0.0565(12)
C6	0.8265(2)	0.1495(2)	0.6821(5)	0.0603(9)
C9	0.6437(2)	0.0443(2)	0.6781(4)	0.0466(7)
C12	0.9349(3)	0.1478(3)	0.7125(5)	0.093(2)
C14	0.8718(3)	-0.0804(3)	0.8730(4)	0.0573(13)
C15	0.8972(4)	-0.1223(3)	0.9665(4)	0.071(2)
C17	0.8723(5)	-0.0799(3)	0.4865(4)	0.069(2)
C18	0.9103(5)	-0.1223(5)	0.3979(4)	0.103(2)
B1	0.6519(3)	0.2011(3)	0.7502(3)	0.0444(11)
B2	0.7567(3)	0.2339(2)	0.6905(4)	0.0492(9)
B3	0.6596(4)	0.1988(3)	0.6127(4)	0.0540(14)
B4	0.5819(2)	0.1325(2)	0.6766(4)	0.0467(8)
B7	0.7712(4)	0.1598(3)	0.5881(4)	0.0481(12)
B8	0.6603(4)	0.0960(4)	0.5815(3)	0.0478(12)
B10	0.6597(4)	0.0896(3)	0.7760(4)	0.0465(11)
Li1	0.7953(4)	0.0116(3)	0.6755(9)	0.0603(14)
H1	0.622(2)	0.245(2)	0.813(2)	0.029(8)
H2	0.789(3)	0.295(2)	0.659(4)	0.086(14)
H3	0.620(4)	0.245(3)	0.577(4)	0.08(2)
H4	0.505(3)	0.135(2)	0.686(5)	0.070(9)
H5	0.800(2)	0.165(2)	0.849(2)	0.031(9)
H7	0.822(4)	0.178(4)	0.531(4)	0.10(2)
H8	0.638(4)	0.076(3)	0.518(4)	0.07(2)
H9	0.609(2)	-0.005(2)	0.660(2)	0.040(9)
H10	0.643(2)	0.071(2)	0.858(3)	0.028(9)
H12a	0.9573	0.0938	0.7066	0.118
H12b	0.9717	0.1792	0.6555	0.118
H12c	0.9404	0.1743	0.7679	0.118
H15c	0.9648	-0.1167	0.9691	0.093
H15a	0.8786	-0.1774	0.9542	0.093
H15b	0.8633	-0.0956	1.0132	0.093
H18c	0.8602	-0.1612	0.3658	0.134
H18a	0.9654	-0.1563	0.4076	0.134
H18b	0.9258	-0.0864	0.3387	0.134

$U_{eq}=\frac{1}{3}[U_{11}(aa^*)^2+U_{22}(bb^*)^2+U_{33}(cc^*)^2+2U_{12}aa^*bb^*cos\gamma+2U_{13}aa^*cc^*cos\beta+2U_{23}bb^*cc^*cos$

Table 2. Refined Thermal Parameters (U's) for Compound 1

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N13	0.081(3)	0.059(3)	0.066(3)	-0.008(2)	-0.020(2)	0.028(2)
N16	0.085(4)	0.057(3)	0.067(3)	0.003(2)	-0.005(2)	0.012(2)
C5	0.061(3)	0.049(2)	0.060(3)	-0.006(2)	-0.009(2)	-0.004(2)
C6	0.043(2)	0.048(2)	0.090(2)	-0.024(3)	-0.007(3)	-0.0056(13)
C9	0.050(2)	0.0363(14)	0.053(2)	-0.010(2)	0.018(2)	-0.0064(12)
C12	0.044(2)	0.093(3)	0.141(6)	-0.019(3)	-0.001(2)	-0.010(2)
C14	0.053(3)	0.048(3)	0.071(3)	-0.010(2)	-0.024(2)	0.020(2)
C15	0.093(4)	0.051(3)	0.070(3)	-0.015(2)	-0.031(3)	0.017(3)
C17	0.093(4)	0.058(3)	0.056(3)	0.012(3)	0.005(3)	0.001(3)
C18	0.123(6)	0.125(6)	0.061(3)	-0.002(3)	0.033(3)	0.035(5)
B1	0.048(3)	0.046(3)	0.039(2)	-0.005(2)	-0.005(2)	0.012(2)
B2	0.062(2)	0.037(2)	0.049(2)	-0.006(2)	-0.006(2)	-0.005(2)
B3	0.070(3)	0.036(3)	0.056(3)	0.004(2)	-0.015(2)	0.006(2)
B4	0.042(2)	0.049(2)	0.049(2)	-0.007(3)	0.006(2)	0.0043(13)
B7	0.075(3)	0.033(2)	0.037(2)	0.000(2)	0.019(2)	0.001(2)
B8	0.054(3)	0.062(3)	0.027(2)	-0.002(2)	0.003(2)	0.004(2)
B10	0.049(3)	0.031(2)	0.059(3)	0.007(2)	0.006(2)	-0.005(2)
Li1	0.063(3)	0.048(3)	0.069(3)	-0.015(5)	-0.006(5)	0.013(2)

The form of the anisotropic displacement parameter is:
$\exp[-2\pi^2(a^{*2}U_{11}h^2+b^{*2}U_{22}k^2+c^{*2}U_{33}l^2+ 2b^*c^*U_{23}kl+2a^*c^*U_{13}hl+2a^*b^*U_{12}hk)]$.

Table 3. Bond Distances (Å) in Compound 1

N13-C14	1.147(6)	N13-Li1	2.040(11)	N16-C17	1.111(7)
N16-Li1	1.989(10)	C5-C6	1.495(7)	C5-B2	1.706(7)
C5-B1	1.755(7)	C5-B10	1.782(7)	C5-Li1	2.689(8)
C5-H5	1.11(3)	C6-B7	1.468(8)	C6-C12	1.544(5)
C6-B2	1.672(4)	C6-Li1	2.272(6)	C9-B10	1.505(7)
C9-B8	1.545(7)	C9-B4	1.661(4)	C9-Li1	2.151(6)
C9-H9	0.97(3)	B1-B2	1.727(7)	B1-B4	1.763(7)
B1-B3	1.825(5)	B1-B10	1.839(7)	B1-H1	1.17(3)
B2-B3	1.780(7)	B2-B7	1.821(7)	B2-H2	1.16(4)
B3-B7	1.692(8)	B3-B8	1.713(8)	B3-B4	1.735(7)
B3-H3	1.03(5)	B4-B8	1.760(6)	B4-B10	1.832(7)
B4-H4	1.07(3)	B7-B8	1.844(8)	B7-Li1	2.682(9)
B7-H7	1.07(6)	B8-Li1	2.619(9)	B8-H8	0.95(5)
B10-Li1	2.616(9)	B10-H10	1.15(4)		

Table 4. Bond Angles (°) in Compound 1

C14-N13-Li1	179.1(5)	C17-N16-Li1	173.5(5)	C6-C5-B2	62.6(3)
C6-C5-B1	112.0(4)	B2-C5-B1	59.8(3)	C6-C5-B10	116.0(4)
B2-C5-B10	113.4(4)	B1-C5-B10	62.6(3)	C6-C5-Li1	57.6(3)
B2-C5-Li1	109.8(4)	B1-C5-Li1	114.8(3)	B10-C5-Li1	68.2(3)
C6-C5-H5	119(2)	B2-C5-H5	119(2)	B1-C5-H5	119(2)
B10-C5-H5	116(2)	Li1-C5-H5	119(2)	B7-C6-C5	113.3(3)
B7-C6-C12	136.2(5)	C5-C6-C12	109.7(5)	B7-C6-B2	70.5(3)
C5-C6-B2	64.9(3)	C12-C6-B2	123.5(3)	B7-C6-Li1	88.9(4)
C5-C6-Li1	88.6(4)	C12-C6-Li1	100.0(3)	B2-C6-Li1	134.0(2)
B10-C9-B8	115.3(3)	B10-C9-B4	70.5(3)	B8-C9-B4	66.5(3)
B10-C9-Li1	89.6(4)	B8-C9-Li1	88.7(4)	B4-C9-Li1	135.0(2)
B10-C9-H9	134(2)	B8-C9-H9	108(2)	B4-C9-H9	117(2)
Li1-C9-H9	106(2)	N13-C14-C15	174.4(6)	N16-C17-C18	175.0(7)
B2-B1-C5	58.7(3)	B2-B1-B4	113.3(3)	C5-B1-B4	108.2(3)
B2-B1-B3	60.1(3)	C5-B1-B3	97.1(4)	B4-B1-B3	57.8(3)
B2-B1-B10	109.7(3)	C5-B1-B10	59.4(3)	B4-B1-B10	61.1(3)
B3-B1-B10	99.3(4)	B2-B1-H1	116(2)	C5-B1-H1	116(2)
B4-B1-H1	126(2)	B3-B1-H1	138(2)	B10-B1-H1	119(2)
C6-B2-C5	52.5(3)	C6-B2-B1	105.0(3)	C5-B2-B1	61.5(3)
C6-B2-B3	97.6(3)	C5-B2-B3	100.7(3)	B1-B2-B3	62.7(2)
C6-B2-B7	49.5(3)	C5-B2-B7	89.1(2)	B1-B2-B7	103.4(3)
B3-B2-B7	56.0(3)	C6-B2-H2	117(2)	C5-B2-H2	148(2)
B1-B2-H2	138(2)	B3-B2-H2	111(2)	B7-B2-H2	105(2)
B7-B3-B8	65.6(3)	B7-B3-B4	115.0(4)	B8-B3-B4	61.4(3)
B7-B3-B2	63.2(3)	B8-B3-B2	116.4(4)	B4-B3-B2	112.1(4)
B7-B3-B1	104.6(4)	B8-B3-B1	105.1(4)	B4-B3-B1	59.3(3)
B2-B3-B1	57.2(3)	B7-B3-H3	131(3)	B8-B3-H3	126(3)
B4-B3-H3	110(3)	B2-B3-H3	115(3)	B1-B3-H3	114(3)
C9-B4-B3	102.8(3)	C9-B4-B8	53.6(3)	B3-B4-B8	58.7(3)
C9-B4-B1	104.7(3)	B3-B4-B1	62.9(2)	B8-B4-B1	105.8(3)
C9-B4-B10	50.7(3)	B3-B4-B10	103.0(3)	B8-B4-B10	91.7(2)
B1-B4-B10	61.5(3)	C9-B4-H4	123(2)	B3-B4-H4	130(2)
B8-B4-H4	135(3)	B1-B4-H4	117(3)	B10-B4-H4	121(3)
C6-B7-B3	110.4(4)	C6-B7-B2	60.0(3)	B3-B7-B2	60.8(3)
C6-B7-B8	113.9(4)	B3-B7-B8	57.8(3)	B2-B7-B8	108.2(3)
C6-B7-Li1	57.9(3)	B3-B7-Li1	111.2(3)	B2-B7-Li1	106.3(3)
B8-B7-Li1	67.8(3)	C6-B7-H7	107(3)	B3-B7-H7	129(3)
B2-B7-H7	115(3)	B8-B7-H7	132(3)	Li1-B7-H7	118(3)
C9-B8-B3	108.9(4)	C9-B8-B4	59.9(2)	B3-B8-B4	59.9(3)
C9-B8-B7	112.6(4)	B3-B8-B7	56.6(3)	B4-B8-B7	106.6(3)
C9-B8-Li1	55.2(3)	B3-B8-Li1	113.2(3)	B4-B8-Li1	105.6(3)
B7-B8-Li1	71.5(3)	C9-B8-H8	121(3)	B3-B8-H8	122(3)
B4-B8-H8	123(3)	B7-B8-H8	120(3)	Li1-B8-H8	118(3)
C9-B10-C5	113.3(4)	C9-B10-B1	108.0(4)	C5-B10-B1	58.0(3)
C9-B10-B4	58.7(3)	C5-B10-B4	104.1(3)	B1-B10-B4	57.4(2)
C9-B10-Li1	55.3(3)	C5-B10-Li1	72.6(3)	B1-B10-Li1	114.9(3)
B4-B10-Li1	103.5(3)	C9-B10-H10	131(2)	C5-B10-H10	109(2)
B1-B10-H10	115(2)	B4-B10-H10	132(2)	Li1-B10-H10	119(2)
N16-Li1-N13	107.5(2)	N16-Li1-C9	119.8(5)	N13-Li1-C9	114.8(5)
N16-Li1-C6	115.8(5)	N13-Li1-C6	111.1(4)	C9-Li1-C6	86.6(2)
N16-Li1-B10	154.7(4)	N13-Li1-B10	92.3(4)	C9-Li1-B10	35.1(2)
C6-Li1-B10	69.0(2)	N16-Li1-B8	98.3(5)	N13-Li1-B8	150.0(4)
C9-Li1-B8	36.1(2)	C6-Li1-B8	69.0(2)	B10-Li1-B8	59.0(2)
N16-Li1-B7	98.0(4)	N13-Li1-B7	144.0(4)	C9-Li1-B7	70.6(2)
C6-Li1-B7	33.2(2)	B10-Li1-B7	72.6(2)	B8-Li1-B7	40.7(2)

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N16-Li1-C5	149.5(4)	N13-Li1-C5	92.7(4)	C9-Li1-C5	68.2(2)
C6-Li1-C5	33.8(2)	B10-Li1-C5	39.2(2)	B8-Li1-C5	71.0(2)
B7-Li1-C5	54.88(14)				

Table 5. Refined Positional Parameters for Compound 2

Atom	x	y	z	Ueq, Å^2
V1	0.25953(7)	0.02259(14)	0.29985(10)	0.0349(4)
C2	0.3692(4)	-0.0742(9)	0.3445(6)	0.039(2)
C3	0.2676(4)	0.2465(9)	0.2245(6)	0.041(2)
C4	0.3826(4)	0.1063(9)	0.3943(6)	0.041(2)
B5	0.3577(5)	-0.0608(11)	0.2159(7)	0.040(2)
B6	0.3007(5)	0.1243(11)	0.1492(6)	0.039(2)
B7	0.3283(5)	0.2811(10)	0.3381(7)	0.042(2)
B8	0.4397(5)	0.0307(12)	0.3129(8)	0.046(2)
B9	0.3492(5)	0.3196(11)	0.2069(7)	0.045(2)
B10	0.4214(6)	0.2490(11)	0.3189(8)	0.048(2)
B11	0.4020(6)	0.1370(12)	0.1878(8)	0.048(2)
C12	0.3935(5)	-0.2343(11)	0.4149(7)	0.052(2)
C2'	0.1839(5)	-0.1365(10)	0.1951(6)	0.045(2)
C3'	0.2101(5)	0.0510(10)	0.4255(6)	0.046(2)
C4'	0.1274(4)	0.0042(10)	0.2068(6)	0.044(2)
B5'	0.2006(5)	-0.2578(12)	0.2974(8)	0.047(2)
B6'	0.2157(6)	-0.1487(12)	0.4305(8)	0.049(2)
B7'	0.1419(5)	0.1175(12)	0.3282(8)	0.045(2)
B8'	0.1053(6)	-0.2144(13)	0.2188(9)	0.054(2)
B9'	0.1287(6)	-0.0364(14)	0.4275(9)	0.056(2)
B10'	0.0735(6)	-0.0508(14)	0.2922(8)	0.054(2)
B11'	0.1247(5)	-0.2353(12)	0.3613(9)	0.050(2)
C12'	0.0898(6)	0.1051(14)	0.1031(8)	0.068(3)
H3	0.2307	0.3288	0.1946	0.052
H4	0.4001	0.1123	0.4836	0.051
H5	0.3559	-0.1780	0.1676	0.050

H6	0.2684	0.1024	0.0640	0.048
H7	0.3169	0.3761	0.3954	0.052
H8	0.4990	-0.0144	0.3350	0.057
H9	0.3551	0.4415	0.1669	0.056
H10	0.4692	0.3357	0.3542	0.060
H11	0.4349	0.1421	0.1269	0.060
H12a	0.4477	-0.2464	0.4318	0.069
H12b	0.3698	-0.3331	0.3753	0.069
H12c	0.3782	-0.2237	0.4807	0.069
H2'	0.2015	-0.1622	0.1202	0.056
H3'	0.2309	0.1388	0.4843	0.058
H5'	0.2316	-0.3782	0.2976	0.059
H6'	0.2544	-0.2125	0.5009	0.062
H7'	0.1260	0.2536	0.3224	0.056
H8'	0.0652	-0.3004	0.1637	0.067
H9'	0.1010	-0.0184	0.4933	0.070
H10'	0.0122	-0.0258	0.2736	0.067
H11'	0.1007	-0.3456	0.3945	0.062
H12d	0.1283	0.1499	0.0717	0.090
H12e	0.0607	0.1980	0.1204	0.090
H12f	0.0567	0.0312	0.0511	0.090

$U_{eq}=^{1}/_{3}[U_{11}(aa^*)^2+U_{22}(bb^*)^2+U_{33}(cc^*)^2+2U_{12}aa^*bb^*cos\gamma+2U_{13}aa^*cc^*cos\beta+2U_{23}bb^*cc^*cos\alpha]$

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Table 6. Refined Thermal Parameters (U's) for Compound 2

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
V1	0.0388(8)	0.0302(6)	0.0354(7)	0.0020(5)	0.0095(5)	0.0013(5)
C2	0.038(4)	0.033(4)	0.045(4)	0.002(3)	0.009(3)	-0.001(3)
C3	0.048(5)	0.037(4)	0.037(4)	0.005(3)	0.009(3)	0.003(3)
C4	0.044(5)	0.038(4)	0.037(4)	0.000(3)	0.004(3)	-0.004(3)
B5	0.040(5)	0.044(5)	0.038(4)	-0.004(4)	0.015(3)	0.001(4)
B6	0.043(5)	0.046(5)	0.030(4)	0.006(3)	0.013(3)	0.000(4)
B7	0.044(5)	0.029(4)	0.050(5)	-0.002(3)	0.011(4)	-0.001(3)
B8	0.042(6)	0.046(5)	0.051(5)	0.003(4)	0.014(4)	0.001(4)
B9	0.050(6)	0.042(5)	0.045(5)	0.009(4)	0.015(4)	-0.002(4)
B10	0.052(6)	0.038(5)	0.058(6)	0.001(4)	0.022(4)	-0.007(4)
B11	0.051(6)	0.044(5)	0.046(5)	0.005(4)	0.011(4)	-0.002(4)
C12	0.041(5)	0.049(5)	0.060(5)	0.015(4)	0.002(4)	0.004(3)
C2'	0.047(5)	0.043(4)	0.046(4)	-0.010(3)	0.015(3)	-0.004(3)
C3'	0.049(5)	0.049(4)	0.045(4)	-0.006(3)	0.021(4)	-0.006(4)
C4'	0.033(4)	0.042(4)	0.052(4)	0.000(3)	0.003(3)	0.002(3)
B5'	0.044(6)	0.040(5)	0.059(6)	-0.002(4)	0.014(4)	-0.003(4)
B6'	0.048(6)	0.052(5)	0.050(5)	0.010(4)	0.016(4)	-0.003(4)
B7'	0.025(5)	0.052(5)	0.057(5)	-0.002(4)	0.012(4)	0.002(4)
B8'	0.047(6)	0.052(5)	0.071(7)	-0.012(5)	0.032(5)	-0.012(4)
B9'	0.056(7)	0.061(6)	0.056(6)	-0.003(5)	0.026(5)	-0.005(5)
B10'	0.045(6)	0.058(6)	0.059(6)	-0.001(5)	0.017(4)	-0.001(4)
B11'	0.038(5)	0.049(5)	0.066(6)	0.007(4)	0.020(4)	-0.006(4)
C12'	0.058(6)	0.074(6)	0.067(6)	0.005(5)	0.008(5)	0.006(5)

The form of the anisotropic displacement parameter is:
$\exp[-2\pi^2(a^{*2}U_{11}h^2+b^{*2}U_{22}k^2+c^{*2}U_{33}l^2+ 2b^*c^*U_{23}kl+2a^*c^*U_{13}hl+2a^*b^*U_{12}hk)]$.

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Table 7. Bond Distances (Å) in Compound 2

V1-C3	2.024(7)	V1-C3'	2.051(7)	V1-C2'	2.064(8)
V1-C2	2.073(8)	V1-C4	2.343(8)	V1-B7	2.363(8)
V1-B6	2.380(8)	V1-B7'	2.390(9)	V1-C4'	2.391(8)
V1-B5	2.411(8)	V1-B6'	2.434(9)	V1-B5'	2.442(9)
C2-C12	1.536(10)	C2-C4	1.542(10)	C2-B5	1.601(11)
C2-B8	1.665(11)	C3-B6	1.585(11)	C3-B7	1.594(11)
C3-B9	1.665(12)	C4-B7	1.730(11)	C4-B10	1.743(11)
C4-B8	1.758(12)	B5-B8	1.815(13)	B5-B11	1.827(13)
B5-B6	1.854(12)	B6-B11	1.786(13)	B6-B9	1.821(13)
B7-B10	1.798(13)	B7-B9	1.837(12)	B8-B10	1.747(13)
B8-B11	1.767(13)	B9-B10	1.754(14)	B9-B11	1.778(13)
B10-B11	1.836(13)	C2'-C4'	1.544(11)	C2'-B5'	1.576(12)
C2'-B8'	1.661(12)	C3'-B6'	1.568(12)	C3'-B7'	1.592(12)
C3'-B9'	1.642(13)	C4'-C12'	1.536(12)	C4'-B10'	1.707(13)
C4'-B7'	1.742(12)	C4'-B8'	1.775(12)	B5'-B8'	1.793(14)
B5'-B11'	1.795(13)	B5'-B6'	1.854(14)	B6'-B11'	1.794(14)
B6'-B9'	1.81(2)	B7'-B10'	1.789(14)	B7'-B9'	1.809(14)
B8'-B11'	1.76(2)	B8'-B10'	1.773(14)	B9'-B10'	1.75(2)
B9'-B11'	1.764(14)	B10'-B11'	1.815(14)		

Table 8. Bond Angles (°) in Compound 2

C3-V1-C3'	112.3(3)	C3-V1-C2'	109.7(3)	C3'-V1-C2'	102.3(3)
C3-V1-C2	105.0(3)	C3'-V1-C2	114.8(3)	C2'-V1-C2	112.8(3)
C3-V1-C4	79.6(3)	C3'-V1-C4	97.5(3)	C2'-V1-C4	152.4(3)
C2-V1-C4	40.3(3)	C3-V1-B7	41.7(3)	C3'-V1-B7	93.8(3)
C2'-V1-B7	151.3(3)	C2-V1-B7	80.5(3)	C4-V1-B7	43.1(3)
C3-V1-B6	41.2(3)	C3'-V1-B6	153.4(3)	C2'-V1-B6	88.9(3)
C2-V1-B6	81.6(3)	C4-V1-B6	81.6(3)	B7-V1-B6	67.3(3)
C3-V1-B7'	89.2(3)	C3'-V1-B7'	41.1(3)	C2'-V1-B7'	79.2(3)
C2-V1-B7'	155.9(3)	C4-V1-B7'	127.8(3)	B7-V1-B7'	98.8(3)
B6-V1-B7'	120.6(3)	C3-V1-C4'	90.5(3)	C3'-V1-C4'	78.3(3)
C2'-V1-C4'	39.7(3)	C2-V1-C4'	152.4(3)	C4-V1-C4'	167.0(3)
B7-V1-C4'	124.3(3)	B6-V1-C4'	96.5(3)	B7'-V1-C4'	42.7(3)
C3-V1-B5	82.3(3)	C3'-V1-B5	155.7(3)	C2'-V1-B5	89.8(3)
C2-V1-B5	41.0(3)	C4-V1-B5	65.1(3)	B7-V1-B5	84.6(3)
B6-V1-B5	45.5(3)	B7'-V1-B5	163.0(3)	C4'-V1-B5	122.3(3)
C3-V1-B6'	151.8(3)	C3'-V1-B6'	39.8(3)	C2'-V1-B6'	79.9(3)
C2-V1-B6'	94.6(3)	C4-V1-B6'	104.4(3)	B7-V1-B6'	125.8(3)
B6-V1-B6'	165.8(3)	B7'-V1-B6'	66.1(3)	C4'-V1-B6'	80.4(3)
B5-V1-B6'	125.0(3)	C3-V1-B5'	149.4(3)	C3'-V1-B5'	79.8(3)
C2'-V1-B5'	39.8(3)	C2-V1-B5'	93.7(3)	C4-V1-B5'	128.1(3)
B7-V1-B5'	168.8(3)	B6-V1-B5'	121.6(3)	B7'-V1-B5'	82.6(3)
C4'-V1-B5'	63.7(3)	B5-V1-B5'	97.4(3)	B6'-V1-B5'	44.7(3)
C12-C2-C4	121.2(6)	C12-C2-B5	126.1(7)	C4-C2-B5	108.9(6)
C12-C2-B8	115.0(6)	C4-C2-B8	66.3(5)	B5-C2-B8	67.5(5)
C12-C2-V1	124.5(5)	C4-C2-V1	79.3(4)	B5-C2-V1	80.9(4)
B8-C2-V1	120.3(5)	B6-C3-B7	111.6(6)	B6-C3-B9	68.1(5)
B7-C3-B9	68.6(5)	B6-C3-V1	81.5(4)	B7-C3-V1	80.6(4)
B9-C3-V1	122.9(5)	C2-C4-B7	123.0(6)	C2-C4-B10	113.9(6)

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B7-C4-B10	62.4(5)	C2-C4-B8	60.2(5)	B7-C4-B8	112.7(6)
B10-C4-B8	59.9(5)	C2-C4-V1	60.4(4)	B7-C4-V1	69.1(4)
B10-C4-V1	111.8(5)	B8-C4-V1	103.9(5)	C2-B5-B8	57.9(5)
C2-B5-B11	108.2(6)	B8-B5-B11	58.0(5)	C2-B5-B6	115.2(6)
B8-B5-B6	105.3(6)	B11-B5-B6	58.0(5)	C2-B5-V1	58.1(4)
B8-B5-V1	99.6(5)	B11-B5-V1	106.1(5)	B6-B5-V1	66.4(4)
C3-B6-B11	109.5(6)	C3-B6-B9	58.1(5)	B11-B6-B9	59.1(5)
C3-B6-B5	116.9(6)	B11-B6-B5	60.2(5)	B9-B6-B5	108.6(6)
C3-B6-V1	57.3(3)	B11-B6-V1	108.8(5)	B9-B6-V1	100.3(4)
B5-B6-V1	68.1(3)	C3-B7-C4	115.1(6)	C3-B7-B10	107.8(6)
C4-B7-B10	59.2(5)	C3-B7-B9	57.5(5)	C4-B7-B9	105.8(6)
B10-B7-B9	57.7(5)	C3-B7-V1	57.7(4)	C4-B7-V1	67.8(4)
B10-B7-V1	108.8(5)	B9-B7-V1	100.4(5)	C2-B8-B10	107.6(6)
C2-B8-C4	53.5(4)	B10-B8-C4	59.6(5)	C2-B8-B11	108.2(7)
B10-B8-B11	63.0(6)	C4-B8-B11	103.0(6)	C2-B8-B5	54.6(5)
B10-B8-B5	106.5(7)	C4-B8-B5	91.4(6)	B11-B8-B5	61.3(5)
C3-B9-B10	106.7(6)	C3-B9-B11	106.2(6)	B10-B9-B11	62.7(5)
C3-B9-B6	53.9(4)	B10-B9-B6	104.1(6)	B11-B9-B6	59.5(5)
C3-B9-B7	53.9(4)	B10-B9-B7	60.0(5)	B11-B9-B7	104.2(6)
B6-B9-B7	91.9(5)	C4-B10-B8	60.5(5)	C4-B10-B9	108.9(6)
B8-B10-B9	112.6(7)	C4-B10-B7	58.5(5)	B8-B10-B7	110.0(6)
B9-B10-B7	62.3(5)	C4-B10-B11	100.8(6)	B8-B10-B11	59.0(5)
B9-B10-B11	59.3(5)	B7-B10-B11	103.4(7)	B8-B11-B9	110.5(6)
B8-B11-B6	110.4(6)	B9-B11-B6	61.5(5)	B8-B11-B5	60.7(5)
B9-B11-B5	111.7(6)	B6-B11-B5	61.7(5)	B8-B11-B10	58.0(5)
B9-B11-B10	58.0(5)	B6-B11-B10	102.2(6)	B5-B11-B10	102.4(6)
C4'-C2'-B5'	109.6(6)	C4'-C2'-B8'	67.2(6)	B5'-C2'-B8'	67.2(6)
C4'-C2'-V1	81.6(4)	B5'-C2'-V1	83.1(5)	B8'-C2'-V1	124.4(5)
B6'-C3'-B7'	112.7(7)	B6'-C3'-B9'	68.5(6)	B7'-C3'-B9'	68.0(6)

B6'-C3'-V1	83.4(5)	B7'-C3'-V1	80.9(5)	B9'-C3'-V1	123.8(6)
C12'-C4'-C2'	116.1(7)	C12'-C4'-B10'	118.5(7)	C2'-C4'-B10'	113.3(6)
C12'-C4'-B7'	115.5(7)	C2'-C4'-B7'	120.2(6)	B10'-C4'-B7'	62.5(5)
C12'-C4'-B8'	120.7(7)	C2'-C4'-B8'	59.6(5)	B10'-C4'-B8'	61.2(5)
B7'-C4'-B8'	113.5(6)	C12'-C4'-V1	123.8(6)	C2'-C4'-V1	58.6(4)
B10'-C4'-V1	112.1(5)	B7'-C4'-V1	68.6(4)	B8'-C4'-V1	103.8(5)
C2'-B5'-B8'	58.6(5)	C2'-B5'-B11'	108.4(7)	B8'-B5'-B11'	58.9(5)
C2'-B5'-B6'	115.4(6)	B8'-B5'-B6'	108.0(6)	B11'-B5'-B6'	58.9(5)
C2'-B5'-V1	57.0(4)	B8'-B5'-V1	101.3(5)	B11'-B5'-V1	107.3(5)
B6'-B5'-V1	67.4(4)	C3'-B6'-B11'	108.3(7)	C3'-B6'-B9'	57.7(6)
B11'-B6'-B9'	58.7(6)	C3'-B6'-B5'	115.5(7)	B11'-B6'-B5'	58.9(5)
B9'-B6'-B5'	106.8(7)	C3'-B6'-V1	56.8(4)	B11'-B6'-V1	107.6(5)
B9'-B6'-V1	99.5(5)	B5'-B6'-V1	67.9(4)	C3'-B7'-C4'	115.3(6)
C3'-B7'-B10'	107.8(7)	C4'-B7'-B10'	57.8(5)	C3'-B7'-B9'	57.3(5)
C4'-B7'-B9'	105.4(6)	B10'-B7'-B9'	58.4(6)	C3'-B7'-V1	57.9(4)
C4'-B7'-V1	68.7(4)	B10'-B7'-V1	109.0(5)	B9'-B7'-V1	101.0(5)
C2'-B8'-B11'	106.0(7)	C2'-B8'-B10'	104.6(7)	B11'-B8'-B10'	61.8(6)
C2'-B8'-C4'	53.3(5)	B11'-B8'-C4'	101.0(6)	B10'-B8'-C4'	57.5(5)
C2'-B8'-B5'	54.1(5)	B11'-B8'-B5'	60.6(6)	B10'-B8'-B5'	104.3(7)
C4'-B8'-B5'	91.2(6)	C3'-B9'-B10'	107.2(7)	C3'-B9'-B11'	106.5(7)
B10'-B9'-B11'	62.1(6)	C3'-B9'-B6'	53.8(5)	B10'-B9'-B6'	105.1(7)
B11'-B9'-B6'	60.3(6)	C3'-B9'-B7'	54.7(5)	B10'-B9'-B7'	60.2(6)
B11'-B9'-B7'	104.4(7)	B6'-B9'-B7'	93.4(6)	C4'-B10'-B9'	109.5(7)
C4'-B10'-B8'	61.3(5)	B9'-B10'-B8'	112.5(8)	C4'-B10'-B7'	59.7(5)
B9'-B10'-B7'	61.4(6)	B8'-B10'-B7'	111.3(7)	C4'-B10'-B11'	101.6(6)
B9'-B10'-B11'	59.2(6)	B8'-B10'-B11'	58.9(6)	B7'-B10'-B11'	103.2(7)
B9'-B11'-B8'	112.5(7)	B9'-B11'-B6'	61.1(6)	B8'-B11'-B6'	112.1(6)
B9'-B11'-B5'	111.4(6)	B8'-B11'-B5'	60.5(5)	B6'-B11'-B5'	62.2(5)
B9'-B11'-B10'	58.7(6)	B8'-B11'-B10'	59.4(6)	B6'-B11'-B10'	103.1(6)

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B5'-B11'-B10' 102.6(6)

Table 9. Refined Positional Parameters for Compound 3

Atom	x	y	z	Ueq, Å^2
V1	0.34524(5)	0.12926(2)	0.06497(4)	0.0240(2)
C2	0.5082(3)	0.06519(10)	0.1674(3)	0.0322(6)
C3	0.4055(3)	0.19087(10)	0.2142(3)	0.0291(5)
C4	0.4182(3)	0.07638(10)	0.2819(3)	0.0329(6)
B5	0.6591(4)	0.10971(12)	0.1740(3)	0.0327(6)
B6	0.6031(4)	0.18216(12)	0.2044(3)	0.0314(6)
B7	0.3486(4)	0.14362(12)	0.3054(3)	0.0313(6)
B8	0.6571(4)	0.06961(13)	0.3311(3)	0.0381(7)
B9	0.5558(4)	0.18385(12)	0.3761(3)	0.0353(6)
B10	0.5539(4)	0.11352(13)	0.4249(3)	0.0376(7)
B11	0.7251(4)	0.13928(13)	0.3530(3)	0.0370(7)
C12	0.3045(5)	0.03033(13)	0.3144(4)	0.0476(7)
C2'	0.0820(3)	0.10580(10)	0.0042(3)	0.0312(5)
C3'	0.3825(3)	0.15295(10)	-0.1236(3)	0.0310(5)
C5'	0.0536(3)	0.16363(10)	-0.0623(3)	0.0299(5)
B4'	0.1481(4)	0.06348(12)	-0.0924(3)	0.0355(7)
B6'	0.2195(4)	0.19248(11)	-0.1234(3)	0.0301(6)
B7'	0.3184(4)	0.09105(12)	-0.1691(3)	0.0345(6)
B8'	-0.0546(4)	0.10526(13)	-0.1646(3)	0.0380(7)
B9'	0.2184(4)	0.15094(13)	-0.2806(3)	0.0376(7)
B10'	0.0835(4)	0.09243(13)	-0.2719(3)	0.0391(7)
B11'	0.0149(4)	0.16255(12)	-0.2447(3)	0.0369(7)
C12'	-0.0510(4)	0.20514(12)	-0.0035(4)	0.0401(6)
H2	0.491(4)	0.0311(11)	0.124(3)	0.038(7)
H3	0.337(4)	0.2230(11)	0.190(3)	0.040(8)
H5	0.754(4)	0.1022(11)	0.115(3)	0.039(7)

H6	0.671(4)	0.2159(12)	0.165(3)	0.042(8)
H7	0.229(4)	0.1441(11)	0.340(3)	0.038(7)
H8	0.729(4)	0.0326(11)	0.378(3)	0.037(7)
H9	0.575(4)	0.2169(11)	0.449(3)	0.043(8)
H10	0.561(4)	0.0997(11)	0.533(3)	0.040(7)
H11	0.860(4)	0.1478(11)	0.412(3)	0.041(7)
H12a	-0.055(5)	0.240(2)	-0.045(4)	0.079(12)
H12b	0.003(6)	0.212(2)	0.100(5)	0.091(13)
H12c	-0.169(6)	0.193(2)	-0.015(5)	0.093(14)
H2'	0.035(4)	0.0971(12)	0.074(3)	0.040(8)
H3'	0.489(4)	0.1671(12)	-0.120(3)	0.044(8)
H4'	0.148(3)	0.0180(11)	-0.071(3)	0.038(7)
H6'	0.223(3)	0.2375(10)	-0.112(3)	0.030(6)
H7'	0.405(4)	0.0618(11)	-0.194(3)	0.038(7)
H8'	-0.195(4)	0.0948(12)	-0.182(3)	0.044(8)
H9'	0.242(4)	0.1660(11)	-0.379(3)	0.044(8)
H10'	0.030(4)	0.0668(11)	-0.364(3)	0.041(8)
H11'	-0.086(4)	0.1873(11)	-0.307(3)	0.037(7)
H12d	0.251(5)	0.039(2)	0.391(5)	0.089(13)
H12e	0.379(5)	-0.005(2)	0.340(4)	0.080(12)
H12f	0.197(6)	0.024(2)	0.232(5)	0.089(13)

$$U_{eq}={}^{1}/_{3}[U_{11}(aa^*)^2+U_{22}(bb^*)^2+U_{33}(cc^*)^2+2U_{12}aa^*bb^*cos\gamma+2U_{13}aa^*cc^*cos\beta+2U_{23}bb^*cc^*cos\alpha]$$

Table 10. Refined Thermal Parameters (U's) for Compound 3

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
V1	0.0259(2)	0.0215(2)	0.0247(2)	0.0004(2)	0.0079(2)	0.0007(2)
C2	0.0380(14)	0.0231(12)	0.0304(13)	-0.0009(10)	0.0036(11)	0.0032(10)
C3	0.0330(13)	0.0252(12)	0.0287(12)	-0.0010(10)	0.0091(10)	0.0012(10)
C4	0.0381(14)	0.0296(12)	0.0289(13)	0.0057(10)	0.0075(11)	-0.0018(10)
B5	0.0258(14)	0.035(2)	0.036(2)	0.0036(12)	0.0076(12)	0.0058(11)
B6	0.0299(14)	0.0289(14)	0.034(2)	-0.0016(11)	0.0073(12)	-0.0038(11)
B7	0.037(2)	0.034(2)	0.0236(13)	-0.0029(11)	0.0114(12)	-0.0019(12)
B8	0.039(2)	0.033(2)	0.036(2)	0.0038(13)	0.0030(13)	0.0054(13)
B9	0.039(2)	0.033(2)	0.030(2)	-0.0066(12)	0.0057(12)	-0.0040(12)
B10	0.043(2)	0.038(2)	0.027(2)	0.0035(12)	0.0040(12)	-0.0015(13)
B11	0.033(2)	0.037(2)	0.035(2)	0.0000(12)	0.0015(13)	-0.0007(12)
C12	0.056(2)	0.038(2)	0.049(2)	0.0123(14)	0.016(2)	-0.0101(14)
C2'	0.0308(13)	0.0281(12)	0.0333(13)	0.0035(10)	0.0080(11)	-0.0033(10)
C3'	0.0326(13)	0.0311(13)	0.0306(13)	0.0001(10)	0.0117(11)	0.0015(11)
C5'	0.0247(11)	0.0282(12)	0.0349(13)	0.0015(10)	0.0068(10)	0.0017(9)
B4'	0.039(2)	0.0248(14)	0.036(2)	-0.0049(12)	0.0017(13)	-0.0037(12)
B6'	0.036(2)	0.0240(13)	0.0296(14)	0.0063(11)	0.0098(12)	0.0029(11)
B7'	0.045(2)	0.0282(14)	0.030(2)	-0.0049(11)	0.0125(13)	0.0066(12)
B8'	0.032(2)	0.034(2)	0.040(2)	-0.0017(13)	0.0008(13)	-0.0042(12)
B9'	0.049(2)	0.037(2)	0.0261(14)	0.0016(12)	0.0093(13)	0.0044(13)
B10'	0.047(2)	0.034(2)	0.029(2)	-0.0042(12)	0.0006(13)	0.0015(13)
B11'	0.039(2)	0.034(2)	0.031(2)	-0.0007(12)	0.0006(13)	0.0032(13)
C12'	0.035(2)	0.039(2)	0.051(2)	0.0020(13)	0.0185(13)	0.0082(12)

The form of the anisotropic displacement parameter is:
$\exp[-2\pi^2(a^{*2}U_{11}h^2+b^{*2}U_{22}k^2+c^{*2}U_{33}l^2+ 2b^*c^*U_{23}kl+2a^*c^*U_{13}hl+2a^*b^*U_{12}hk)]$.

Table 11. Bond Distances (Å) in Compound 3

V1-C3	2.028(2)	V1-C2'	2.031(2)	V1-C3'	2.036(3)
V1-C2	2.048(2)	V1-B6'	2.352(3)	V1-B7	2.368(3)
V1-C5'	2.373(2)	V1-C4	2.383(2)	V1-B5	2.391(3)
V1-B4'	2.398(3)	V1-B6	2.409(3)	V1-B7'	2.414(3)
C2-C4	1.520(4)	C2-B5	1.577(4)	C2-B8	1.660(4)
C2-H2	0.91(3)	C3-B6	1.589(4)	C3-B7	1.591(4)
C3-B9	1.657(4)	C3-H3	0.93(3)	C4-C12	1.513(4)
C4-B10	1.717(4)	C4-B7	1.743(4)	C4-B8	1.781(4)
B5-B11	1.808(4)	B5-B8	1.817(4)	B5-B6	1.842(4)
B5-H5	1.09(3)	B6-B11	1.792(4)	B6-B9	1.829(4)
B6-H6	1.10(3)	B7-B10	1.812(4)	B7-B9	1.823(4)
B7-H7	1.09(3)	B8-B11	1.749(4)	B8-B10	1.752(4)
B8-H8	1.08(3)	B9-B10	1.758(4)	B9-B11	1.769(4)
B9-H9	1.05(3)	B10-B11	1.803(5)	B10-H10	1.09(3)
B11-H11	1.05(3)	C12-H12d	0.98(4)	C12-H12e	1.01(4)
C12-H12f	0.98(4)	C2'-C5'	1.521(3)	C2'-B4'	1.581(4)
C2'-B8'	1.661(4)	C2'-H2'	0.89(3)	C3'-B7'	1.588(4)
C3'-B6'	1.588(4)	C3'-B9'	1.663(4)	C3'-H3'	0.89(3)
C5'-C12'	1.512(3)	C5'-B11'	1.713(4)	C5'-B6'	1.732(4)
C5'-B8'	1.776(4)	B4'-B10'	1.806(4)	B4'-B8'	1.819(4)
B4'-B7'	1.841(4)	B4'-H4'	1.11(3)	B6'-B11'	1.812(4)
B6'-B9'	1.830(4)	B6'-H6'	1.09(2)	B7'-B10'	1.793(4)
B7'-B9'	1.826(4)	B7'-H7'	1.06(3)	B8'-B10'	1.750(5)
B8'-B11'	1.752(4)	B8'-H8'	1.09(3)	B9'-B11'	1.753(5)
B9'-B10'	1.775(5)	B9'-H9'	1.10(3)	B10'-B11'	1.813(4)
B10'-H10'	1.06(3)	B11'-H11'	1.02(3)	C12'-H12a	0.93(4)
C12'-H12b	0.98(4)	C12'-H12c	0.93(4)		

Table 12. Bond Angles (°) in Compound 3

C3-V1-C2'	113.47(10)	C3-V1-C3'	112.38(10)	C2'-V1-C3'	103.36(11)
C3-V1-C2	103.23(10)	C2'-V1-C2	110.50(10)	C3'-V1-C2	114.22(10)
C3-V1-B6'	92.15(10)	C2'-V1-B6'	79.34(10)	C3'-V1-B6'	41.65(10)
C2-V1-B6'	155.72(10)	C3-V1-B7	41.54(10)	C2'-V1-B7	91.51(11)
C3'-V1-B7	153.92(10)	C2-V1-B7	79.17(10)	B6'-V1-B7	123.75(10)
C3-V1-C5'	95.21(9)	C2'-V1-C5'	39.45(9)	C3'-V1-C5'	79.26(9)
C2-V1-C5'	149.81(9)	B6'-V1-C5'	43.00(9)	B7-V1-C5'	100.37(9)
C3-V1-C4	79.19(9)	C2'-V1-C4	92.85(9)	C3'-V1-C4	153.25(10)
C2-V1-C4	39.21(9)	B6'-V1-C4	165.05(10)	B7-V1-C4	43.04(9)
C5'-V1-C4	125.05(9)	C3-V1-B5	81.30(10)	C2'-V1-B5	151.19(10)
C3'-V1-B5	92.41(10)	C2-V1-B5	40.70(10)	B6'-V1-B5	126.42(10)
B7-V1-B5	83.96(10)	C5'-V1-B5	169.04(9)	C4-V1-B5	64.70(10)
C3-V1-B4'	154.24(11)	C2'-V1-B4'	40.78(10)	C3'-V1-B4'	81.25(11)
C2-V1-B4'	89.60(10)	B6'-V1-B4'	84.09(10)	B7-V1-B4'	122.59(11)
C5'-V1-B4'	64.94(9)	C4-V1-B4'	98.38(10)	B5-V1-B4'	121.18(10)
C3-V1-B6	40.84(9)	C2'-V1-B6	154.27(10)	C3'-V1-B6	91.94(10)
C2-V1-B6	80.78(10)	B6'-V1-B6	99.88(10)	B7-V1-B6	67.30(10)
C5'-V1-B6	127.33(9)	C4-V1-B6	81.60(9)	B5-V1-B6	45.12(10)
B4'-V1-B6	164.80(10)	C3-V1-B7'	153.09(10)	C2'-V1-B7'	80.66(11)
C3'-V1-B7'	40.71(10)	C2-V1-B7'	91.94(10)	B6'-V1-B7'	67.17(10)
B7-V1-B7'	165.36(10)	C5'-V1-B7'	81.45(10)	C4-V1-B7'	124.50(9)
B5-V1-B7'	96.92(10)	B4'-V1-B7'	45.00(11)	B6-V1-B7'	123.10(10)
C4-C2-B5	111.2(2)	C4-C2-B8	67.9(2)	B5-C2-B8	68.2(2)
C4-C2-V1	82.41(14)	B5-C2-V1	81.42(14)	B8-C2-V1	124.3(2)
C4-C2-H2	118(2)	B5-C2-H2	129(2)	B8-C2-H2	117(2)
V1-C2-H2	118(2)	B6-C3-B7	112.7(2)	B6-C3-B9	68.6(2)
B7-C3-B9	68.3(2)	B6-C3-V1	82.58(14)	B7-C3-V1	80.78(14)
B9-C3-V1	123.2(2)	B6-C3-H3	126(2)	B7-C3-H3	120(2)

B9-C3-H3	121(2)	V1-C3-H3	116(2)	C12-C4-C2	117.5(2)
C12-C4-B10	117.5(2)	C2-C4-B10	112.5(2)	C12-C4-B7	115.0(2)
C2-C4-B7	119.7(2)	B10-C4-B7	63.1(2)	C12-C4-B8	120.6(2)
C2-C4-B8	59.8(2)	B10-C4-B8	60.1(2)	B7-C4-B8	113.1(2)
C12-C4-V1	125.8(2)	C2-C4-V1	58.38(12)	B10-C4-V1	111.2(2)
B7-C4-V1	68.01(12)	B8-C4-V1	103.1(2)	C2-B5-B11	106.8(2)
C2-B5-B8	58.1(2)	B11-B5-B8	57.7(2)	C2-B5-B6	115.9(2)
B11-B5-B6	58.8(2)	B8-B5-B6	107.5(2)	C2-B5-V1	57.88(12)
B11-B5-V1	107.2(2)	B8-B5-V1	101.7(2)	B6-B5-V1	67.96(12)
C2-B5-H5	119.4(14)	B11-B5-H5	122.9(14)	B8-B5-H5	123.1(14)
B6-B5-H5	118.5(14)	V1-B5-H5	124.8(14)	C3-B6-B11	107.8(2)
C3-B6-B9	57.5(2)	B11-B6-B9	58.5(2)	C3-B6-B5	114.7(2)
B11-B6-B5	59.6(2)	B9-B6-B5	107.2(2)	C3-B6-V1	56.58(12)
B11-B6-V1	107.0(2)	B9-B6-V1	99.1(2)	B5-B6-V1	66.91(12)
C3-B6-H6	120.3(14)	B11-B6-H6	121.0(14)	B9-B6-H6	124.0(14)
B5-B6-H6	118.5(14)	V1-B6-H6	126.8(14)	C3-B7-C4	115.8(2)
C3-B7-B10	107.5(2)	C4-B7-B10	57.7(2)	C3-B7-B9	57.6(2)
C4-B7-B9	105.4(2)	B10-B7-B9	57.8(2)	C3-B7-V1	57.69(12)
C4-B7-V1	68.94(12)	B10-B7-V1	108.3(2)	B9-B7-V1	100.7(2)
C3-B7-H7	125.9(14)	C4-B7-H7	112.5(14)	B10-B7-H7	118.2(14)
B9-B7-H7	128.4(14)	V1-B7-H7	125(2)	C2-B8-B11	105.8(2)
C2-B8-B10	104.2(2)	B11-B8-B10	62.0(2)	C2-B8-C4	52.3(2)
B11-B8-C4	101.4(2)	B10-B8-C4	58.1(2)	C2-B8-B5	53.7(2)
B11-B8-B5	60.9(2)	B10-B8-B5	104.5(2)	C4-B8-B5	90.5(2)
C2-B8-H8	118.3(14)	B11-B8-H8	130.0(14)	B10-B8-H8	122.4(14)
C4-B8-H8	123.4(14)	B5-B8-H8	131.4(14)	C3-B9-B10	107.1(2)
C3-B9-B11	105.8(2)	B10-B9-B11	61.5(2)	C3-B9-B7	54.1(2)
B10-B9-B7	60.7(2)	B11-B9-B7	103.8(2)	C3-B9-B6	53.9(2)
B10-B9-B6	104.4(2)	B11-B9-B6	59.7(2)	B7-B9-B6	92.9(2)

C3-B9-H9	119(2)	B10-B9-H9	124(2)	B11-B9-H9	127(2)
B7-B9-H9	125(2)	B6-B9-H9	128(2)	C4-B10-B8	61.8(2)
C4-B10-B9	109.5(2)	B8-B10-B9	113.1(2)	C4-B10-B11	101.7(2)
B8-B10-B11	58.9(2)	B9-B10-B11	59.6(2)	C4-B10-B7	59.1(2)
B8-B10-B7	111.2(2)	B9-B10-B7	61.4(2)	B11-B10-B7	103.0(2)
C4-B10-H10	117.3(14)	B8-B10-H10	115.6(14)	B9-B10-H10	123.6(14)
B11-B10-H10	131.7(14)	B7-B10-H10	120.6(14)	B8-B11-B9	112.7(2)
B8-B11-B6	112.8(2)	B9-B11-B6	61.8(2)	B8-B11-B10	59.1(2)
B9-B11-B10	58.9(2)	B6-B11-B10	104.1(2)	B8-B11-B5	61.4(2)
B9-B11-B5	111.3(2)	B6-B11-B5	61.5(2)	B10-B11-B5	102.8(2)
B8-B11-H11	118(2)	B9-B11-H11	118(2)	B6-B11-H11	121(2)
B10-B11-H11	126(2)	B5-B11-H11	123(2)	C4-C12-H12d	115(2)
C4-C12-H12e	110(2)	H12d-C12-H12e	109(3)	C4-C12-H12f	110(2)
H12d-C12-H12f	102(3)	H12e-C12-H12f	111(3)	C5'-C2'-B4'	111.3(2)
C5'-C2'-B8'	67.7(2)	B4'-C2'-B8'	68.2(2)	C5'-C2'-V1	82.53(14)
B4'-C2'-V1	82.2(2)	B8'-C2'-V1	124.6(2)	C5'-C2'-H2'	120(2)
B4'-C2'-H2'	126(2)	B8'-C2'-H2'	118(2)	V1-C2'-H2'	118(2)
B7'-C3'-B6'	112.3(2)	B7'-C3'-B9'	68.3(2)	B6'-C3'-B9'	68.5(2)
B7'-C3'-V1	82.5(2)	B6'-C3'-V1	79.90(14)	B9'-C3'-V1	122.7(2)
B7'-C3'-H3'	125(2)	B6'-C3'-H3'	121(2)	B9'-C3'-H3'	119(2)
V1-C3'-H3'	118(2)	C12'-C5'-C2'	117.7(2)	C12'-C5'-B11'	117.8(2)
C2'-C5'-B11'	112.7(2)	C12'-C5'-B6'	114.7(2)	C2'-C5'-B6'	119.3(2)
B11'-C5'-B6'	63.5(2)	C12'-C5'-B8'	121.2(2)	C2'-C5'-B8'	59.9(2)
B11'-C5'-B8'	60.2(2)	B6'-C5'-B8'	113.3(2)	C12'-C5'-V1	125.0(2)
C2'-C5'-V1	58.02(12)	B11'-C5'-V1	111.6(2)	B6'-C5'-V1	67.83(12)
B8'-C5'-V1	103.22(14)	C2'-B4'-B10'	106.8(2)	C2'-B4'-B8'	58.0(2)
B10'-B4'-B8'	57.7(2)	C2'-B4'-B7'	115.1(2)	B10'-B4'-B7'	58.9(2)
B8'-B4'-B7'	107.1(2)	C2'-B4'-V1	57.03(12)	B10'-B4'-V1	107.3(2)
B8'-B4'-V1	100.9(2)	B7'-B4'-V1	67.96(13)	C2'-B4'-H4'	120.1(13)

B10'-B4'-H4'	122.8(13)	B8'-B4'-H4'	124.2(13)	B7'-B4'-H4'	118.2(13)
V1-B4'-H4'	124.6(13)	C3'-B6'-C5'	116.5(2)	C3'-B6'-B11'	107.6(2)
C5'-B6'-B11'	57.8(2)	C3'-B6'-B9'	57.7(2)	C5'-B6'-B9'	105.3(2)
B11'-B6'-B9'	57.5(2)	C3'-B6'-V1	58.45(12)	C5'-B6'-V1	69.16(12)
B11'-B6'-V1	108.8(2)	B9'-B6'-V1	101.3(2)	C3'-B6'-H6'	127.1(13)
C5'-B6'-H6'	110.9(13)	B11'-B6'-H6'	116.7(13)	B9'-B6'-H6'	128.7(13)
V1-B6'-H6'	124.8(13)	C3'-B7'-B10'	108.5(2)	C3'-B7'-B9'	57.8(2)
B10'-B7'-B9'	58.7(2)	C3'-B7'-B4'	115.3(2)	B10'-B7'-B4'	59.6(2)
B9'-B7'-B4'	107.4(2)	C3'-B7'-V1	56.74(12)	B10'-B7'-V1	107.1(2)
B9'-B7'-V1	99.2(2)	B4'-B7'-V1	67.04(13)	C3'-B7'-H7'	121.3(14)
B10'-B7'-H7'	120(2)	B9'-B7'-H7'	125(2)	B4'-B7'-H7'	116.8(14)
V1-B7'-H7'	127(2)	C2'-B8'-B10'	105.9(2)	C2'-B8'-B11'	104.2(2)
B10'-B8'-B11'	62.3(2)	C2'-B8'-C5'	52.40(14)	B10'-B8'-C5'	101.8(2)
B11'-B8'-C5'	58.1(2)	C2'-B8'-B4'	53.8(2)	B10'-B8'-B4'	60.8(2)
B11'-B8'-B4'	104.7(2)	C5'-B8'-B4'	90.9(2)	C2'-B8'-H8'	117(2)
B10'-B8'-H8'	130(2)	B11'-B8'-H8'	124(2)	C5'-B8'-H8'	123(2)
B4'-B8'-H8'	130(2)	C3'-B9'-B11'	107.1(2)	C3'-B9'-B10'	106.0(2)
B11'-B9'-B10'	61.8(2)	C3'-B9'-B7'	53.9(2)	B11'-B9'-B7'	104.5(2)
B10'-B9'-B7'	59.7(2)	C3'-B9'-B6'	53.8(2)	B11'-B9'-B6'	60.7(2)
B10'-B9'-B6'	103.8(2)	B7'-B9'-B6'	92.3(2)	C3'-B9'-H9'	120(2)
B11'-B9'-H9'	122(2)	B10'-B9'-H9'	124.8(14)	B7'-B9'-H9'	129(2)
B6'-B9'-H9'	126.7(14)	B8'-B10'-B9'	112.0(2)	B8'-B10'-B7'	112.4(2)
B9'-B10'-B7'	61.6(2)	B8'-B10'-B4'	61.5(2)	B9'-B10'-B4'	111.3(2)
B7'-B10'-B4'	61.5(2)	B8'-B10'-B11'	58.9(2)	B9'-B10'-B11'	58.5(2)
B7'-B10'-B11'	103.4(2)	B4'-B10'-B11'	102.8(2)	B8'-B10'-H10'	117(2)
B9'-B10'-H10'	120(2)	B7'-B10'-H10'	122(2)	B4'-B10'-H10'	121(2)
B11'-B10'-H10'	127(2)	C5'-B11'-B8'	61.6(2)	C5'-B11'-B9'	109.6(2)
B8'-B11'-B9'	113.0(2)	C5'-B11'-B6'	58.8(2)	B8'-B11'-B6'	110.6(2)
B9'-B11'-B6'	61.8(2)	C5'-B11'-B10'	101.7(2)	B8'-B11'-B10'	58.8(2)

B9'-B11'-B10'	59.7(2)	B6'-B11'-B10'	103.0(2)	C5'-B11'-H11'	118(2)
B8'-B11'-H11'	116(2)	B9'-B11'-H11'	123(2)	B6'-B11'-H11'	121(2)
B10'-B11'-H11'	131(2)	C5'-C12'-H12a	112(2)	C5'-C12'-H12b	113(2)
H12a-C12'-H12b	104(3)	C5'-C12'-H12c	112(3)	H12a-C12'-H12c	109(3)
H12b-C12'-H12c	106(3)				

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Table 13. Refined Positional Parameters for Compound 4

Atom	x	y	z	Ueq, Å^2
V1	0.24439(2)	-0.02204(5)	0.48295(3)	0.0257(2)
C2	0.13298(14)	0.0714(3)	0.4499(2)	0.0311(5)
C3	0.2355(2)	-0.2341(3)	0.3897(2)	0.0330(6)
C4	0.12025(14)	-0.1124(3)	0.4805(2)	0.0293(5)
B5	0.1435(2)	0.0715(4)	0.3281(2)	0.0337(6)
B6	0.2008(2)	-0.1031(4)	0.2929(2)	0.0361(7)
B7	0.1759(2)	-0.2794(4)	0.4592(2)	0.0321(6)
B8	0.0599(2)	-0.0260(4)	0.3584(3)	0.0362(7)
B9	0.1529(2)	-0.3021(4)	0.3089(3)	0.0384(7)
B10	0.0804(2)	-0.2436(4)	0.3696(3)	0.0369(7)
B11	0.0980(2)	-0.1195(4)	0.2584(2)	0.0390(7)
C12	0.1081(2)	0.2196(4)	0.5094(3)	0.0430(7)
C2'	0.2948(2)	-0.0722(4)	0.6472(2)	0.0349(6)
C3'	0.3212(2)	0.1441(3)	0.4466(2)	0.0372(6)
B4'	0.2859(2)	0.1249(4)	0.6583(3)	0.0389(7)
C5'	0.36368(14)	-0.1172(3)	0.6062(2)	0.0337(6)
B6'	0.3775(2)	-0.0109(4)	0.4912(3)	0.0354(7)
B7'	0.3029(2)	0.2509(4)	0.5431(3)	0.0396(7)
B8'	0.3751(2)	0.0153(4)	0.7236(3)	0.0429(8)
B9'	0.4010(2)	0.2070(4)	0.5377(3)	0.0437(8)
B10'	0.3791(2)	0.2153(4)	0.6663(3)	0.0447(8)
B11'	0.4318(2)	0.0395(4)	0.6304(3)	0.0404(7)
C12'	0.3927(2)	-0.2989(4)	0.6201(3)	0.0531(9)
H3	0.280(2)	-0.294(4)	0.396(2)	0.035(7)
H4	0.100(2)	-0.125(3)	0.540(2)	0.031(7)
H5	0.141(2)	0.192(4)	0.286(2)	0.040(7)

H6	0.232(2)	-0.073(4)	0.226(3)	0.051(9)
H7	0.182(2)	-0.375(4)	0.519(2)	0.048(8)
H8	0.003(2)	0.021(3)	0.350(2)	0.031(7)
H9	0.149(2)	-0.419(4)	0.261(3)	0.050(8)
H10	0.032(2)	-0.328(4)	0.372(2)	0.040(7)
H11	0.060(2)	-0.116(4)	0.175(2)	0.043(8)
H12a	0.056(3)	0.239(5)	0.485(3)	0.085(13)
H12b	0.120(2)	0.203(6)	0.584(4)	0.091(14)
H12c	0.141(3)	0.314(7)	0.506(4)	0.12(2)
H2'	0.269(2)	-0.160(4)	0.675(2)	0.043(8)
H3'	0.311(2)	0.182(4)	0.375(3)	0.061(10)
H4'	0.248(2)	0.180(4)	0.703(2)	0.048(8)
H6'	0.4047(14)	-0.088(3)	0.443(2)	0.030(7)
H7'	0.276(2)	0.380(4)	0.529(2)	0.046(8)
H8'	0.400(2)	-0.031(4)	0.804(3)	0.045(8)
H9'	0.440(2)	0.290(4)	0.511(2)	0.047(8)
H10'	0.404(2)	0.320(4)	0.725(3)	0.056(9)
H11'	0.490(2)	0.002(4)	0.659(3)	0.046(8)
H12a'	0.354(3)	-0.372(6)	0.585(4)	0.095(14)
H12b'	0.405(3)	-0.331(6)	0.697(4)	0.10(2)
H12c'	0.443(3)	-0.308(7)	0.595(4)	0.13(2)

$U_{eq}=1/3[U_{11}(aa^*)^2+U_{22}(bb^*)^2+U_{33}(cc^*)^2+2U_{12}aa^*bb^*cos\gamma+2U_{13}aa^*cc^*cos\beta+2U_{23}bb^*cc^*cos\alpha]$

Table 14. Refined Thermal Parameters (U's) for Compound 4

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
V1	0.0255(3)	0.0241(2)	0.0271(2)	-0.0002(2)	0.0063(2)	0.0006(2)
C2	0.0289(12)	0.0283(12)	0.0345(13)	-0.0003(10)	0.0059(11)	0.0020(10)
C3	0.0301(13)	0.0330(13)	0.0340(13)	-0.0059(10)	0.0055(11)	0.0038(10)
C4	0.0262(12)	0.0332(13)	0.0302(13)	-0.0014(10)	0.0106(11)	-0.0040(10)
B5	0.030(2)	0.035(2)	0.034(2)	0.0046(12)	0.0053(13)	0.0035(12)
B6	0.040(2)	0.038(2)	0.0277(14)	-0.0042(12)	0.0048(13)	0.0017(13)
B7	0.035(2)	0.0258(14)	0.0332(14)	-0.0012(11)	0.0045(13)	-0.0011(11)
B8	0.0272(14)	0.040(2)	0.037(2)	-0.0001(13)	0.0014(13)	0.0031(12)
B9	0.039(2)	0.039(2)	0.034(2)	-0.0096(13)	0.0041(14)	-0.0020(13)
B10	0.035(2)	0.036(2)	0.038(2)	-0.0057(12)	0.0059(13)	-0.0049(12)
B11	0.035(2)	0.048(2)	0.029(2)	-0.0042(13)	0.0008(13)	0.0010(13)
C12	0.033(2)	0.040(2)	0.056(2)	-0.0118(13)	0.013(2)	0.0065(12)
C2'	0.0349(14)	0.0370(14)	0.0296(13)	0.0007(11)	0.0032(11)	-0.0070(11)
C3'	0.0322(13)	0.0385(14)	0.040(2)	0.0112(12)	0.0075(12)	-0.0022(11)
B4'	0.037(2)	0.041(2)	0.035(2)	-0.0128(13)	0.0039(14)	-0.0049(13)
C5'	0.0277(12)	0.0298(13)	0.0387(14)	0.0047(10)	0.0006(11)	0.0006(10)
B6'	0.0254(14)	0.042(2)	0.042(2)	0.0012(13)	0.0146(13)	-0.0007(12)
B7'	0.034(2)	0.0250(14)	0.055(2)	-0.0025(13)	0.005(2)	-0.0045(12)
B8'	0.040(2)	0.048(2)	0.035(2)	-0.0016(14)	0.001(2)	-0.0069(14)
B9'	0.031(2)	0.038(2)	0.059(2)	0.006(2)	0.006(2)	-0.0078(13)
B10'	0.035(2)	0.039(2)	0.054(2)	-0.010(2)	0.003(2)	-0.0077(13)
B11'	0.028(2)	0.038(2)	0.051(2)	0.0027(14)	0.003(2)	-0.0040(12)
C12'	0.043(2)	0.033(2)	0.071(2)	0.009(2)	-0.005(2)	0.0046(13)

The form of the anisotropic displacement parameter is:
$\exp[-2\pi^2(a^{*2}U_{11}h^2+b^{*2}U_{22}k^2+c^{*2}U_{33}l^2+ 2b^*c^*U_{23}kl+2a^*c^*U_{13}hl+2a^*b^*U_{12}hk)]$.

Table 15. Bond Distances (Å) in Compound 4

V1-C3	2.022(2)	V1-C3'	2.043(3)	V1-C2'	2.053(3)
V1-C2	2.070(2)	V1-C4	2.337(2)	V1-B7	2.351(3)
V1-B6'	2.370(3)	V1-B6	2.387(3)	V1-B5	2.389(3)
V1-C5'	2.401(2)	V1-B4'	2.419(3)	V1-B7'	2.424(3)
C2-C12	1.518(4)	C2-C4	1.533(3)	C2-B5	1.591(4)
C2-B8	1.680(4)	C3-B6	1.588(4)	C3-B7	1.596(4)
C3-B9	1.646(4)	C3-H3	0.91(3)	C4-B7	1.718(4)
C4-B10	1.726(4)	C4-B8	1.758(4)	C4-H4	0.92(3)
B5-B8	1.819(4)	B5-B11	1.821(4)	B5-B6	1.844(4)
B5-H5	1.09(3)	B6-B11	1.787(4)	B6-B9	1.827(4)
B6-H6	1.16(3)	B7-B10	1.802(4)	B7-B9	1.827(4)
B7-H7	1.05(3)	B8-B11	1.748(4)	B8-B10	1.752(4)
B8-H8	1.07(3)	B9-B10	1.741(4)	B9-B11	1.764(4)
B9-H9	1.09(3)	B10-B11	1.801(4)	B10-H10	1.10(3)
B11-H11	1.08(3)	C12-H12A	0.92(4)	C12-H12B	0.91(4)
C12-H12C	0.96(5)	C2'-C5'	1.507(4)	C2'-B4'	1.573(4)
C2'-B8'	1.652(4)	C2'-H2'	0.95(3)	C3'-B7'	1.582(4)
C3'-B6'	1.589(4)	C3'-B9'	1.651(4)	C3'-H3'	0.92(3)
B4'-B10'	1.799(5)	B4'-B8'	1.811(5)	B4'-B7'	1.846(5)
B4'-H4'	1.09(3)	C5'-C12'	1.518(4)	C5'-B11'	1.709(4)
C5'-B6'	1.744(4)	C5'-B8'	1.772(4)	B6'-B11'	1.800(5)
B6'-B9'	1.826(4)	B6'-H6'	1.07(3)	B7'-B10'	1.789(5)
B7'-B9'	1.819(5)	B7'-H7'	1.12(3)	B8'-B10'	1.742(5)
B8'-B11'	1.760(5)	B8'-H8'	1.05(3)	B9'-B11'	1.748(5)
B9'-B10'	1.764(5)	B9'-H9'	1.07(3)	B10'-B11'	1.805(5)
B10'-H10'	1.11(3)	B11'-H11'	1.05(3)	C12'-H12a'	0.91(4)
C12'-H12b'	0.96(5)	C12'-H12c'	1.05(5)		

Table 16. Bond Angles (°) in Compound 4

C3-V1-C3'	110.66(11)	C3-V1-C2'	111.46(11)	C3'-V1-C2'	101.90(11)
C3-V1-C2	104.95(10)	C3'-V1-C2	113.84(10)	C2'-V1-C2	114.23(11)
C3-V1-C4	79.32(10)	C3'-V1-C4	153.44(10)	C2'-V1-C4	96.62(10)
C2-V1-C4	40.13(9)	C3-V1-B7	41.97(11)	C3'-V1-B7	152.63(11)
C2'-V1-B7	92.00(10)	C2-V1-B7	80.53(10)	C4-V1-B7	42.98(9)
C3-V1-B6'	88.66(11)	C3'-V1-B6'	41.37(10)	C2'-V1-B6'	78.28(11)
C2-V1-B6'	155.21(10)	C4-V1-B6'	164.29(10)	B7-V1-B6'	121.78(11)
C3-V1-B6	41.18(10)	C3'-V1-B6	90.44(11)	C2'-V1-B6	152.58(11)
C2-V1-B6	81.76(10)	C4-V1-B6	81.41(10)	B7-V1-B6	67.85(11)
B6'-V1-B6	96.23(11)	C3-V1-B5	82.00(10)	C3'-V1-B5	91.81(11)
C2'-V1-B5	155.25(11)	C2-V1-B5	41.02(10)	C4-V1-B5	64.54(10)
B7-V1-B5	84.62(10)	B6'-V1-B5	124.09(11)	B6-V1-B5	45.41(10)
C3-V1-C5'	91.79(10)	C3'-V1-C5'	78.67(10)	C2'-V1-C5'	38.57(10)
C2-V1-C5'	152.72(10)	C4-V1-C5'	126.71(9)	B7-V1-C5'	99.13(9)
B6'-V1-C5'	42.87(10)	B6-V1-C5'	123.68(10)	B5-V1-C5'	166.06(10)
C3-V1-B4'	151.52(11)	C3'-V1-B4'	80.53(12)	C2'-V1-B4'	40.14(11)
C2-V1-B4'	93.17(10)	C4-V1-B4'	102.51(10)	B7-V1-B4'	123.42(11)
B6'-V1-B4'	83.28(11)	B6-V1-B4'	166.90(11)	B5-V1-B4'	124.86(11)
C5'-V1-B4'	64.01(10)	C3-V1-B7'	150.89(12)	C3'-V1-B7'	40.35(12)
C2'-V1-B7'	79.75(11)	C2-V1-B7'	93.53(10)	C4-V1-B7'	127.41(10)
B7-V1-B7'	166.92(11)	B6'-V1-B7'	66.75(11)	B6-V1-B7'	123.11(12)
B5-V1-B7'	98.60(11)	C5'-V1-B7'	80.79(10)	B4'-V1-B7'	44.82(12)
C12-C2-C4	121.4(2)	C12-C2-B5	126.9(2)	C4-C2-B5	107.8(2)
C12-C2-B8	114.1(2)	C4-C2-B8	66.2(2)	B5-C2-B8	67.5(2)
C12-C2-V1	125.0(2)	C4-C2-V1	79.37(14)	B5-C2-V1	80.3(2)
B8-C2-V1	120.7(2)	B6-C3-B7	112.3(2)	B6-C3-B9	68.8(2)
B7-C3-B9	68.6(2)	B6-C3-V1	81.8(2)	B7-C3-V1	80.1(2)
B9-C3-V1	122.9(2)	B6-C3-H3	124(2)	B7-C3-H3	123(2)

B9-C3-H3	120(2)	V1-C3-H3	117(2)	C2-C4-B7	123.6(2)
C2-C4-B10	115.0(2)	B7-C4-B10	63.1(2)	C2-C4-B8	60.9(2)
B7-C4-B8	114.2(2)	B10-C4-B8	60.4(2)	C2-C4-V1	60.50(12)
B7-C4-V1	68.93(13)	B10-C4-V1	112.3(2)	B8-C4-V1	104.8(2)
C2-C4-H4	115(2)	B7-C4-H4	115(2)	B10-C4-H4	115(2)
B8-C4-H4	118(2)	V1-C4-H4	127(2)	C2-B5-B8	58.6(2)
C2-B5-B11	107.8(2)	B8-B5-B11	57.4(2)	C2-B5-B6	116.7(2)
B8-B5-B6	106.4(2)	B11-B5-B6	58.4(2)	C2-B5-V1	58.66(12)
B8-B5-V1	100.9(2)	B11-B5-V1	106.2(2)	B6-B5-V1	67.24(12)
C2-B5-H5	118(2)	B8-B5-H5	124(2)	B11-B5-H5	122.6(14)
B6-B5-H5	119(2)	V1-B5-H5	125.8(14)	C3-B6-B11	107.8(2)
C3-B6-B9	57.1(2)	B11-B6-B9	58.4(2)	C3-B6-B5	115.6(2)
B11-B6-B5	60.2(2)	B9-B6-B5	107.7(2)	C3-B6-V1	56.98(13)
B11-B6-V1	107.5(2)	B9-B6-V1	99.1(2)	B5-B6-V1	67.35(13)
C3-B6-H6	122(2)	B11-B6-H6	121(2)	B9-B6-H6	126(2)
B5-B6-H6	116(2)	V1-B6-H6	126(2)	C3-B7-C4	114.8(2)
C3-B7-B10	107.0(2)	C4-B7-B10	58.7(2)	C3-B7-B9	57.0(2)
C4-B7-B9	104.9(2)	B10-B7-B9	57.3(2)	C3-B7-V1	57.91(13)
C4-B7-V1	68.09(12)	B10-B7-V1	108.8(2)	B9-B7-V1	100.4(2)
C3-B7-H7	127(2)	C4-B7-H7	113(2)	B10-B7-H7	117(2)
B9-B7-H7	128(2)	V1-B7-H7	125(2)	C2-B8-B11	107.3(2)
C2-B8-B10	106.5(2)	B11-B8-B10	61.9(2)	C2-B8-C4	52.89(14)
B11-B8-C4	101.1(2)	B10-B8-C4	58.9(2)	C2-B8-B5	53.9(2)
B11-B8-B5	61.4(2)	B10-B8-B5	105.2(2)	C4-B8-B5	89.7(2)
C2-B8-H8	117.2(14)	B11-B8-H8	129.3(14)	B10-B8-H8	121.5(14)
C4-B8-H8	124(2)	B5-B8-H8	131.4(14)	C3-B9-B10	107.6(2)
C3-B9-B11	106.3(2)	B10-B9-B11	61.8(2)	C3-B9-B6	54.1(2)
B10-B9-B6	104.6(2)	B11-B9-B6	59.7(2)	C3-B9-B7	54.4(2)
B10-B9-B7	60.6(2)	B11-B9-B7	103.8(2)	B6-B9-B7	92.7(2)

C3-B9-H9	122(2)	B10-B9-H9	122(2)	B11-B9-H9	123(2)
B6-B9-H9	128(2)	B7-B9-H9	128(2)	C4-B10-B9	108.3(2)
C4-B10-B8	60.7(2)	B9-B10-B8	113.0(2)	C4-B10-B11	100.2(2)
B9-B10-B11	59.7(2)	B8-B10-B11	58.9(2)	C4-B10-B7	58.2(2)
B9-B10-B7	62.0(2)	B8-B10-B7	110.4(2)	B11-B10-B7	103.3(2)
C4-B10-H10	119.9(14)	B9-B10-H10	123(2)	B8-B10-H10	117(2)
B11-B10-H10	131.1(14)	B7-B10-H10	120.7(14)	B8-B11-B9	112.1(2)
B8-B11-B6	112.2(2)	B9-B11-B6	61.9(2)	B8-B11-B10	59.2(2)
B9-B11-B10	58.5(2)	B6-B11-B10	103.8(2)	B8-B11-B5	61.3(2)
B9-B11-B5	111.5(2)	B6-B11-B5	61.5(2)	B10-B11-B5	103.2(2)
B8-B11-H11	115(2)	B9-B11-H11	121(2)	B6-B11-H11	125(2)
B10-B11-H11	125(2)	B5-B11-H11	122(2)	C2-C12-H12a	112(3)
C2-C12-H12b	112(3)	H12a-C12-H12b	107(4)	C2-C12-H12c	107(3)
H12a-C12-H12c	117(4)	H12b-C12-H12c	101(4)	C5'-C2'-B4'	112.1(2)
C5'-C2'-B8'	68.0(2)	B4'-C2'-B8'	68.3(2)	C5'-C2'-V1	83.3(2)
B4'-C2'-V1	82.5(2)	B8'-C2'-V1	125.5(2)	C5'-C2'-H2'	119(2)
B4'-C2'-H2'	128(2)	B8'-C2'-H2'	122(2)	V1-C2'-H2'	113(2)
B7'-C3'-B6'	112.6(2)	B7'-C3'-B9'	68.4(2)	B6'-C3'-B9'	68.6(2)
B7'-C3'-V1	82.9(2)	B6'-C3'-V1	80.4(2)	B9'-C3'-V1	123.5(2)
B7'-C3'-H3'	123(2)	B6'-C3'-H3'	122(2)	B9'-C3'-H3'	119(2)
V1-C3'-H3'	117(2)	C2'-B4'-B10'	106.3(2)	C2'-B4'-B8'	57.9(2)
B10'-B4'-B8'	57.7(2)	C2'-B4'-B7'	114.9(2)	B10'-B4'-B7'	58.8(2)
B8'-B4'-B7'	107.3(2)	C2'-B4'-V1	57.32(13)	B10'-B4'-V1	107.1(2)
B8'-B4'-V1	101.6(2)	B7'-B4'-V1	67.75(13)	C2'-B4'-H4'	122(2)
B10'-B4'-H4'	122(2)	B8'-B4'-H4'	124(2)	B7'-B4'-H4'	117(2)
V1-B4'-H4'	125(2)	C2'-C5'-C12'	118.1(3)	C2'-C5'-B11'	112.7(2)
C12'-C5'-B11'	117.0(2)	C2'-C5'-B6'	118.9(2)	C12'-C5'-B6'	115.3(3)
B11'-C5'-B6'	62.8(2)	C2'-C5'-B8'	59.9(2)	C12'-C5'-B8'	120.1(2)
B11'-C5'-B8'	60.7(2)	B6'-C5'-B8'	113.2(2)	C2'-C5'-V1	58.14(12)

C12'-C5'-V1	126.1(2)	B11'-C5'-V1	111.2(2)	B6'-C5'-V1	67.64(12)
B8'-C5'-V1	103.5(2)	C3'-B6'-C5'	116.2(2)	C3'-B6'-B11'	107.4(2)
C5'-B6'-B11'	57.7(2)	C3'-B6'-B9'	57.3(2)	C5'-B6'-B9'	105.1(2)
B11'-B6'-B9'	57.6(2)	C3'-B6'-V1	58.21(13)	C5'-B6'-V1	69.50(13)
B11'-B6'-V1	109.1(2)	B9'-B6'-V1	101.1(2)	C3'-B6'-H6'	125.7(14)
C5'-B6'-H6'	112.8(14)	B11'-B6'-H6'	117.8(13)	B9'-B6'-H6'	127.9(14)
V1-B6'-H6'	124.6(14)	C3'-B7'-B10'	108.0(2)	C3'-B7'-B9'	57.6(2)
B10'-B7'-B9'	58.5(2)	C3'-B7'-B4'	115.2(2)	B10'-B7'-B4'	59.3(2)
B9'-B7'-B4'	107.1(2)	C3'-B7'-V1	56.76(13)	B10'-B7'-V1	107.2(2)
B9'-B7'-V1	99.4(2)	B4'-B7'-V1	67.43(13)	C3'-B7'-H7'	122(2)
B10'-B7'-H7'	118(2)	B9'-B7'-H7'	123(2)	B4'-B7'-H7'	117(2)
V1-B7'-H7'	129(2)	C2'-B8'-B10'	105.4(2)	C2'-B8'-B11'	103.5(2)
B10'-B8'-B11'	62.1(2)	C2'-B8'-C5'	52.1(2)	B10'-B8'-C5'	101.5(2)
B11'-B8'-C5'	57.9(2)	C2'-B8'-B4'	53.8(2)	B10'-B8'-B4'	60.8(2)
B11'-B8'-B4'	104.5(2)	C5'-B8'-B4'	90.9(2)	C2'-B8'-H8'	119(2)
B10'-B8'-H8'	131(2)	B11'-B8'-H8'	120(2)	C5'-B8'-H8'	121(2)
B4'-B8'-H8'	134(2)	C3'-B9'-B11'	107.1(2)	C3'-B9'-B10'	106.1(2)
B11'-B9'-B10'	61.9(2)	C3'-B9'-B7'	54.0(2)	B11'-B9'-B7'	104.8(2)
B10'-B9'-B7'	59.9(2)	C3'-B9'-B6'	54.1(2)	B11'-B9'-B6'	60.4(2)
B10'-B9'-B6'	103.7(2)	B7'-B9'-B6'	92.7(2)	C3'-B9'-H9'	119(2)
B11'-B9'-H9'	124(2)	B10'-B9'-H9'	126(2)	B7'-B9'-H9'	128(2)
B6'-B9'-H9'	126(2)	B8'-B10'-B9'	112.9(2)	B8'-B10'-B7'	113.0(2)
B9'-B10'-B7'	61.6(2)	B8'-B10'-B4'	61.5(2)	B9'-B10'-B4'	111.7(2)
B7'-B10'-B4'	61.9(2)	B8'-B10'-B11'	59.4(2)	B9'-B10'-B11'	58.6(2)
B7'-B10'-B11'	103.7(2)	B4'-B10'-B11'	103.1(2)	B8'-B10'-H10'	117(2)
B9'-B10'-H10'	119(2)	B7'-B10'-H10'	122(2)	B4'-B10'-H10'	122(2)
B11'-B10'-H10'	126(2)	C5'-B11'-B9'	110.2(2)	C5'-B11'-B8'	61.4(2)
B9'-B11'-B8'	112.8(2)	C5'-B11'-B6'	59.5(2)	B9'-B11'-B6'	62.0(2)
B8'-B11'-B6'	111.1(2)	C5'-B11'-B10'	101.4(2)	B9'-B11'-B10'	59.5(2)

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B8'-B11'-B10'	58.5(2)	B6'-B11'-B10'	103.1(2)	C5'-B11'-H11'	117(2)
B9'-B11'-H11'	123(2)	B8'-B11'-H11'	116(2)	B6'-B11'-H11'	120(2)
B10'-B11'-H11'	132(2)	C5'-C12'-H12a'	110(3)	C5'-C12'-H12b'	110(3)
H12a'-C12'-H12b'	105(4)	C5'-C12'-H12c'	110(3)	H12a'-C12'-H12c'	114(4)
H12b'-C12'-H12c'	108(4)				

Table 17. Refined Positional Parameters for Compound 5

Atom	x	y	z	Ueq, Å^2
V1	0.61496(10)	0.2500	0.2500	0.0405(4)
C2	0.5288(4)	0.1660(5)	0.3794(6)	0.048(2)
C3	0.7046(5)	0.3429(6)	0.3629(7)	0.055(2)
C4	0.5127(5)	0.2772(5)	0.4305(6)	0.052(2)
C12	0.4396(5)	0.0995(6)	0.3335(8)	0.057(2)
B5	0.6374(6)	0.1276(6)	0.4225(7)	0.047(2)
B6	0.7387(6)	0.2280(6)	0.4122(7)	0.051(2)
B7	0.5983(7)	0.3780(8)	0.4157(10)	0.068(3)
B8	0.5468(6)	0.1755(7)	0.5381(8)	0.058(2)
B9	0.7035(7)	0.3358(8)	0.5177(9)	0.070(3)
B10	0.5813(6)	0.3083(8)	0.5652(9)	0.065(2)
B11	0.6739(7)	0.2031(8)	0.5587(8)	0.069(3)
H3	0.745(4)	0.382(4)	0.317(5)	0.04(2)
H4	0.445(5)	0.304(5)	0.430(5)	0.05(2)
H5	0.662(4)	0.043(4)	0.412(5)	0.05(2)
H6	0.818(5)	0.201(5)	0.390(6)	0.06(2)
H7	0.568(5)	0.456(5)	0.403(6)	0.07(2)
H8	0.488(5)	0.132(5)	0.606(6)	0.09(2)
H9	0.748(5)	0.383(5)	0.575(6)	0.07(2)
H10	0.539(5)	0.345(5)	0.640(7)	0.08(2)
H11	0.709(4)	0.170(4)	0.643(5)	0.05(2)
H12c	0.396(5)	0.079(5)	0.403(6)	0.07(2)
H12b	0.464(5)	0.034(5)	0.285(6)	0.08(2)
H12a	0.392(6)	0.144(6)	0.272(8)	0.11(3)

$U_{eq}=1/3[U_{11}(aa^*)^2+U_{22}(bb^*)^2+U_{33}(cc^*)^2+2U_{12}aa^*bb^*cos\gamma+2U_{13}aa^*cc^*cos\beta+2U_{23}bb^*cc^*cos$

Table 18. Refined Thermal Parameters (U's) for Compound 5

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
V1	0.0324(7)	0.0408(7)	0.0482(8)	0.0071(8)	0.000	0.000
C2	0.038(3)	0.053(4)	0.054(4)	0.016(3)	0.009(3)	0.008(3)
C3	0.051(4)	0.053(4)	0.062(5)	0.009(4)	-0.007(4)	-0.005(3)
C4	0.041(3)	0.058(5)	0.057(4)	0.008(3)	0.004(3)	0.019(3)
C12	0.046(4)	0.056(4)	0.069(5)	0.016(4)	0.015(4)	-0.012(4)
B5	0.049(4)	0.050(4)	0.043(4)	0.018(4)	0.009(4)	0.014(4)
B6	0.042(4)	0.057(5)	0.053(4)	0.010(4)	-0.005(4)	0.009(3)
B7	0.056(5)	0.064(6)	0.084(7)	-0.001(5)	-0.014(5)	0.013(5)
B8	0.049(5)	0.076(6)	0.048(5)	0.022(4)	-0.004(4)	0.018(4)
B9	0.063(6)	0.085(7)	0.060(6)	0.004(5)	-0.012(5)	0.003(5)
B10	0.052(5)	0.086(6)	0.055(6)	0.010(5)	-0.008(4)	0.019(5)
B11	0.063(5)	0.096(7)	0.047(5)	0.015(5)	0.000(4)	0.025(5)

The form of the anisotropic displacement parameter is:
$exp[-2\pi^2(a^{*2}U_{11}h^2+b^{*2}U_{22}k^2+c^{*2}U_{33}l^2+2b^*c^*U_{23}kl+2a^*c^*U_{13}hl+2a^*b^*U_{12}hk)]$.

Table 19. Bond Distances (Å) in Compound 5

V1-C3	2.042(7)	V1-C3'	2.042(7)	V1-C2	2.063(6)
V1-C2'	2.063(6)	V1-C4'	2.352(7)	V1-C4	2.352(7)
V1-B7	2.375(10)	V1-B7'	2.375(10)	V1-B6'	2.379(7)
V1-B6	2.379(7)	V1-B5'	2.391(7)	V1-B5	2.391(7)
C2-C4	1.509(9)	C2-C12	1.524(9)	C2-B5	1.584(9)
C2-B8	1.685(10)	C3-B7	1.575(11)	C3-B6	1.596(10)
C3-B9	1.625(12)	C3-H3	0.88(5)	C4-B7	1.705(12)
C4-B10	1.724(11)	C4-B8	1.761(10)	C4-H4	0.95(6)
C12-H12c	0.96(7)	C12-H12b	1.02(7)	C12-H12a	1.06(8)
B5-B11	1.781(12)	B5-B8	1.809(11)	B5-B6	1.844(11)
B5-H5	1.12(5)	B6-B11	1.787(11)	B6-B9	1.807(12)
B6-H6	1.13(6)	B7-B10	1.809(13)	B7-B9	1.835(12)
B7-H7	1.06(6)	B8-B11	1.733(12)	B8-B10	1.750(13)
B8-H8	1.19(7)	B9-B10	1.729(13)	B9-B11	1.762(14)
B9-H9	1.03(6)	B10-B11	1.803(11)	B10-H10	1.06(7)
B11-H11	1.08(5)				

Table 20. Bond Angles (°) in Compound 5

C3-V1-C3'	108.9(4)	C3-V1-C2	103.4(3)	C3'-V1-C2	114.3(3)
C3-V1-C2'	114.3(3)	C3'-V1-C2'	103.4(3)	C2-V1-C2'	112.8(3)
C3-V1-C4'	152.1(2)	C3'-V1-C4'	77.6(3)	C2-V1-C4'	97.8(2)
C2'-V1-C4'	39.3(2)	C3-V1-C4	77.6(3)	C3'-V1-C4	152.1(2)
C2-V1-C4	39.3(2)	C2'-V1-C4	97.8(2)	C4'-V1-C4	109.7(3)
C3-V1-B7	40.9(3)	C3'-V1-B7	149.7(3)	C2-V1-B7	79.2(3)
C2'-V1-B7	94.9(3)	C4'-V1-B7	129.3(3)	C4-V1-B7	42.3(3)
C3-V1-B7'	149.7(3)	C3'-V1-B7'	40.9(3)	C2-V1-B7'	94.9(3)
C2'-V1-B7'	79.2(3)	C4'-V1-B7'	42.3(3)	C4-V1-B7'	129.3(3)
B7-V1-B7'	169.3(4)	C3-V1-B6'	87.0(3)	C3'-V1-B6'	41.5(3)
C2-V1-B6'	155.7(3)	C2'-V1-B6'	81.5(3)	C4'-V1-B6'	80.7(2)
C4-V1-B6'	162.8(2)	B7-V1-B6'	120.6(3)	B7'-V1-B6'	67.6(3)
C3-V1-B6	41.5(3)	C3'-V1-B6	87.0(3)	C2-V1-B6	81.5(3)
C2'-V1-B6	155.7(3)	C4'-V1-B6	162.9(2)	C4-V1-B6	80.7(2)
B7-V1-B6	67.6(3)	B7'-V1-B6	120.6(3)	B6'-V1-B6	92.8(4)
C3-V1-B5'	90.0(3)	C3'-V1-B5'	81.7(3)	C2-V1-B5'	153.4(3)
C2'-V1-B5'	40.8(2)	C4'-V1-B5'	63.6(2)	C4-V1-B5'	126.0(3)
B7-V1-B5'	97.5(3)	B7'-V1-B5'	83.8(3)	B6'-V1-B5'	45.5(3)
B6-V1-B5'	122.0(3)	C3-V1-B5	81.7(3)	C3'-V1-B5	90.0(3)
C2-V1-B5	40.8(2)	C2'-V1-B5	153.4(3)	C4'-V1-B5	126.0(3)
C4-V1-B5	63.6(2)	B7-V1-B5	83.8(3)	B7'-V1-B5	97.5(3)
B6'-V1-B5	122.0(3)	B6-V1-B5	45.5(3)	B5'-V1-B5	165.7(4)
C4-C2-C12	120.5(6)	C4-C2-B5	107.9(6)	C12-C2-B5	129.0(6)
C4-C2-B8	66.7(5)	C12-C2-B8	117.4(6)	B5-C2-B8	67.1(4)
C4-C2-V1	80.8(4)	C12-C2-V1	120.0(5)	B5-C2-V1	80.8(3)
B8-C2-V1	122.3(5)	B7-C3-B6	113.0(6)	B7-C3-B9	70.0(6)
B6-C3-B9	68.2(5)	B7-C3-V1	81.0(5)	B6-C3-V1	80.6(4)
B9-C3-V1	122.8(6)	B7-C3-H3	126(4)	B6-C3-H3	121(4)
B9-C3-H3	126(4)	V1-C3-H3	111(4)	C2-C4-B7	124.0(6)
C2-C4-B10	115.2(5)	B7-C4-B10	63.7(5)	C2-C4-B8	61.5(4)
B7-C4-B8	115.1(6)	B10-C4-B8	60.3(5)	C2-C4-V1	60.0(3)
B7-C4-V1	69.6(4)	B10-C4-V1	112.9(4)	B8-C4-V1	105.2(4)
C2-C4-H4	117(4)	B7-C4-H4	111(4)	B10-C4-H4	115(4)
B8-C4-H4	120(4)	V1-C4-H4	126(4)	C2-C12-H12c	112(4)
C2-C12-H12b	111(4)	H12c-C12-H12b	111(5)	C2-C12-H12a	112(4)
H12c-C12-H12a	104(6)	H12b-C12-H12a	108(6)	C2-B5-B11	108.3(6)

C2-B5-B8	59.1(4)	B11-B5-B8	57.7(5)	C2-B5-B6	115.9(5)
B11-B5-B6	59.1(5)	B8-B5-B6	107.2(6)	C2-B5-V1	58.4(3)
B11-B5-V1	107.4(5)	B8-B5-V1	102.2(4)	B6-B5-V1	66.9(3)
C2-B5-H5	122(3)	B11-B5-H5	120(3)	B8-B5-H5	125(3)
B6-B5-H5	116(3)	V1-B5-H5	125(3)	C3-B6-B11	107.4(6)

C3-B6-B9	56.6(5)	B11-B6-B9	58.7(5)	C3-B6-B5	115.4(5)
B11-B6-B5	58.7(5)	B9-B6-B5	106.7(5)	C3-B6-V1	57.9(3)
B11-B6-V1	107.7(4)	B9-B6-V1	100.0(4)	B5-B6-V1	67.6(3)
C3-B6-H6	118(3)	B11-B6-H6	125(3)	B9-B6-H6	126(3)
B5-B6-H6	119(3)	V1-B6-H6	122(3)	C3-B7-C4	114.8(7)
C3-B7-B10	106.3(6)	C4-B7-B10	58.7(5)	C3-B7-B9	56.3(5)
C4-B7-B9	103.8(6)	B10-B7-B9	56.7(5)	C3-B7-V1	58.1(4)
C4-B7-V1	68.2(4)	B10-B7-V1	108.6(6)	B9-B7-V1	99.3(5)
C3-B7-H7	123(4)	C4-B7-H7	116(3)	B10-B7-H7	121(4)
B9-B7-H7	129(4)	V1-B7-H7	124(4)	C2-B8-B11	106.0(6)
C2-B8-B10	105.4(6)	B11-B8-B10	62.3(5)	C2-B8-C4	51.9(4)
B11-B8-C4	100.6(6)	B10-B8-C4	58.8(5)	C2-B8-B5	53.8(4)
B11-B8-B5	60.3(5)	B10-B8-B5	104.6(6)	C4-B8-B5	88.9(5)
C2-B8-H8	118(3)	B11-B8-H8	131(3)	B10-B8-H8	121(3)
C4-B8-H8	123(3)	B5-B8-H8	133(3)	C3-B9-B10	107.9(7)
C3-B9-B11	107.3(7)	B10-B9-B11	62.2(5)	C3-B9-B6	55.1(5)
B10-B9-B6	105.6(7)	B11-B9-B6	60.1(5)	C3-B9-B7	53.7(5)
B10-B9-B7	60.9(5)	B11-B9-B7	104.2(7)	B6-B9-B7	93.1(6)
C3-B9-H9	123(4)	B10-B9-H9	119(4)	B11-B9-H9	122(4)
B6-B9-H9	129(4)	B7-B9-H9	128(4)	C4-B10-B9	107.6(7)
C4-B10-B8	60.9(5)	B9-B10-B8	112.8(7)	C4-B10-B11	99.3(6)
B9-B10-B11	59.8(5)	B8-B10-B11	58.4(5)	C4-B10-B7	57.7(4)
B9-B10-B7	62.4(5)	B8-B10-B7	110.6(7)	B11-B10-B7	103.6(7)
C4-B10-H10	115(4)	B9-B10-H10	128(4)	B8-B10-H10	113(4)
B11-B10-H10	134(4)	B7-B10-H10	120(4)	B8-B11-B9	112.0(6)
B8-B11-B5	61.9(5)	B9-B11-B5	111.5(6)	B8-B11-B6	113.2(6)
B9-B11-B6	61.2(5)	B5-B11-B6	62.2(4)	B8-B11-B10	59.3(5)
B9-B11-B10	58.0(5)	B5-B11-B10	103.6(6)	B6-B11-B10	103.4(6)
B8-B11-H11	116(3)	B9-B11-H11	118(3)	B5-B11-H11	125(3)
B6-B11-H11	124(3)	B10-B11-H11	123(3)		

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Figure Captions

SM 1. Cyclic voltammogram of oxidation of 0.5 mM **7** in THF / 0.1 M [NBu4][PF6], 250 μm Pt electrode, scan rate 0.2 V/s, ambient temperature.

SM 2. Cyclic voltammogram of oxidation waves of 0.5 mM **2** in THF / 0.1 M [NBu4][PF6], 250 μm Pt electrode, ambient temperature.

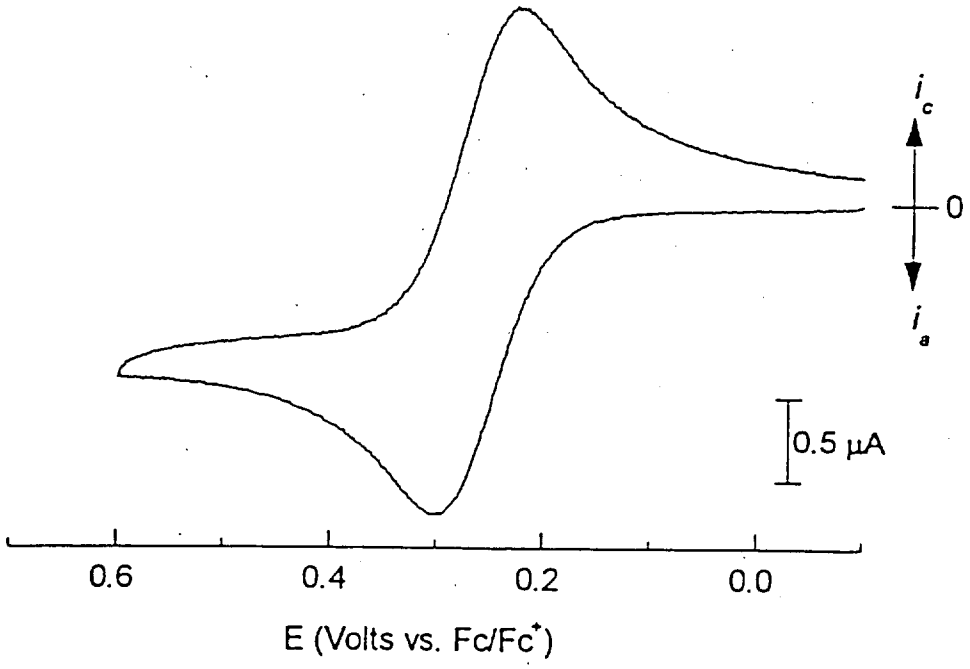

FIGURE SM 1

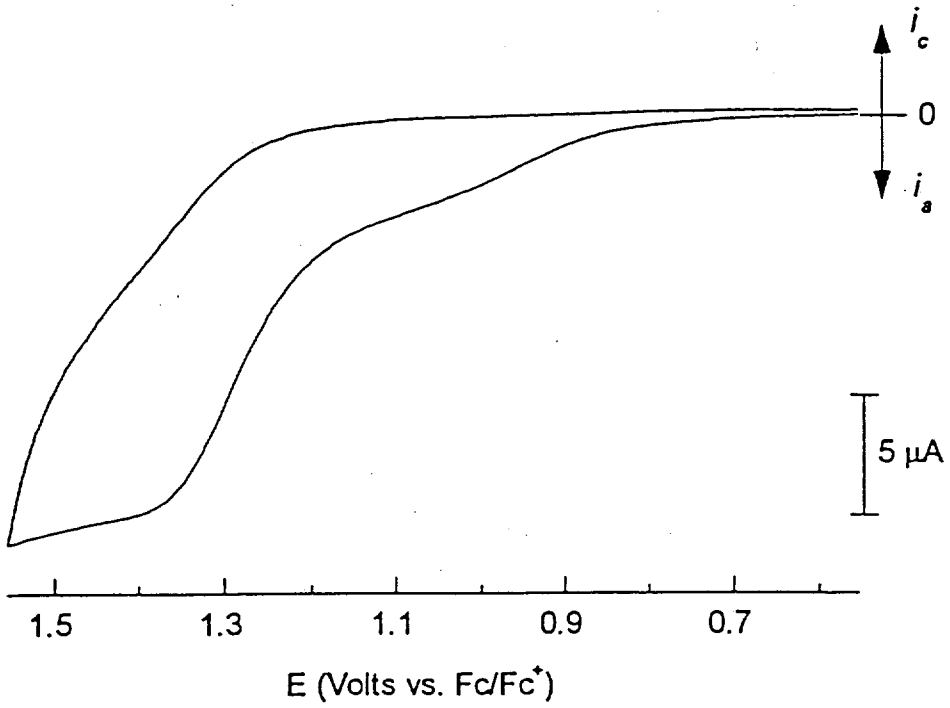

FIGURE SM 2