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Table S1. Crystal data and structure refinement for $(Me_5CpMoCl)_2B_3H_7$.

Molecule	$(Me_5CpMoCl)_2B_3H_7$
Empirical formula	$C_{20}\ H_{37}\ B_3\ Cl_2\ Mo_2$
Formula weight	572.71
Crystal system	Tetragonal
Space group	$P4_32_12$
Unit cell dimensions	a = 8.5231(13) Å
	b = 8.5231(13) Å
	c = 32.956(7) Å
Volume	2394.0(7) $Å^3$
Z	4
Density (calculated)	1.589 Mg/m^3
F(000)	1160
Wavelength	0.71073 Å
Absorption coefficient	1.275 mm^{-1}
Crystal size	0.40 x 0.33 x 0.02 mm
Temperature	293(2) K
Diffractometer	Enraf-Nonius CAD4
Theta range for data collection	2.47 to 24.96°
Index ranges	$0 \le h \le 10,\ 0 \le k \le 10,\ 0 \le l \le 39$
Scan method	ω
Scan rate	1.37 - 8.24 °/min (in ω)
Scan width	0.75° + 0.35°tanθ (in ω)
Total data collected	2422
Unique data	2099 [R(int) = 0.0497]
Unique observed data [$I>2\sigma(I)$]	1826
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.9954 and 0.8225
Refinement method	Full-matrix on F^2 (SHELXL-93)
Weighting scheme	sigma weight
Data / restraints / parameters	2099 / 0 / 137
Goodness-of-fit on F^2	1.143
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0420, wR_2 = 0.0944

Table S1. continued Page 2.

R indices (all data)	R_1 = 0.0542, wR_2 = 0.1053
Absolute structure parameter	-0.08(14)
Largest diff. peak and hole	0.934 and -0.472 e·Å^{-3}

Table S2. Atomic coordinates and equivalent isotropic displacement parameters U_{eq} for $(Me_5CpMoCl)_2B_3H_7$.

	x	y	z	U_{eq}(Å^2)
Mo	0.05861(7)	0.22025(7)	0.96350(2)	0.0313(2)
C(1)	-0.0994(9)	0.1169(8)	0.9136(2)	0.044(2)
C(2)	-0.2030(9)	0.1754(10)	0.9438(2)	0.046(2)
C(3)	-0.1816(8)	0.3388(9)	0.9460(2)	0.041(2)
C(4)	-0.0708(9)	0.3844(8)	0.9166(2)	0.042(2)
C(5)	-0.0184(9)	0.2467(9)	0.8966(2)	0.044(2)
C(6)	-0.0919(12)	-0.0499(10)	0.8984(3)	0.068(3)
C(7)	-0.3308(10)	0.0865(12)	0.9643(3)	0.069(3)
C(8)	-0.2773(12)	0.4466(13)	0.9723(3)	0.075(3)
C(9)	-0.0258(12)	0.5499(10)	0.9065(3)	0.068(3)
C(10)	0.0889(12)	0.2437(13)	0.8608(2)	0.075(3)
Cl	0.2775(3)	0.3975(3)	0.95349(6)	0.0614(6)
B(1)	0.0163(9)	0.0163(9)	1.0000	0.033(2)
B(2)	0.1976(12)	-0.0075(11)	0.9704(2)	0.045(2)

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$.

Table S3. Bond lengths (Å) for $(Me_5CpMoCl)_2B_3H_7$.

Mo-B(1)	2.144(8)	C(6)-H(6B)	0.96
Mo-B(2)#1	2.257(8)	C(6)-H(6C)	0.96
Mo-B(2)	2.286(8)	C(7)-H(7A)	0.96
Mo-C(1)	2.302(7)	C(7)-H(7B)	0.96
Mo-C(5)	2.312(7)	C(7)-H(7C)	0.96
Mo-C(2)	2.353(8)	C(8)-H(8A)	0.96
Mo-C(3)	2.355(6)	C(8)-H(8B)	0.96
Mo-C(4)	2.358(7)	C(8)-H(8C)	0.96
Mo-Cl	2.423(2)	C(9)-H(9A)	0.96
Mo-Mo#1	3.0958(12)	C(9)-H(9B)	0.96
Mo-H(3)	1.74(6)	C(9)-H(9C)	0.96
C(1)-C(5)	1.419(10)	C(10)-H(10A)	0.96
C(1)-C(2)	1.423(11)	C(10)-H(10B)	0.96
C(1)-C(6)	1.509(10)	C(10)-H(10C)	0.96
C(2)-C(3)	1.406(11)	B(1)-B(2)#1	1.838(11)
C(2)-C(7)	1.488(11)	B(1)-B(2)	1.838(11)
C(3)-C(4)	1.408(11)	B(1)-Mo#1	2.144(8)
C(3)-C(8)	1.504(11)	B(1)-H(1)	1.06(14)
C(4)-C(5)	1.420(10)	B(2)-Mo#1	2.257(8)
C(4)-C(9)	1.499(11)	B(2)-H(2)	1.27(5)
C(5)-C(10)	1.491(10)	B(2)-H(3)	1.26(6)
C(6)-H(6A)	0.96	B(2)-H(4)	1.06(7)

Symmetry transformations used to generate equivalent atoms:

#1 y,x,-z+2

Table S4. Bond angles (deg) for $(Me_5CpMoCl)_2B_3H_7$.

B(1)-Mo-B(2)#1	49.3(3)	C(3)-Mo-Cl	111.6(2)
B(1)-Mo-B(2)	48.9(3)	C(4)-Mo-Cl	84.3(2)
B(2)#1-Mo-B(2)	87.7(3)	B(1)-Mo-Mo#1	43.8(2)
B(1)-Mo-C(1)	89.6(3)	B(2)#1-Mo-Mo#1	47.4(2)
B(2)#1-Mo-C(1)	120.7(3)	B(2)-Mo-Mo#1	46.6(2)
B(2)-Mo-C(1)	92.9(3)	C(1)-Mo-Mo#1	130.2(2)
B(1)-Mo-C(5)	124.5(3)	C(5)-Mo-Mo#1	155.6(2)
B(2)#1-Mo-C(5)	149.1(3)	C(2)-Mo-Mo#1	124.3(2)
B(2)-Mo-C(5)	109.0(3)	C(3)-Mo-Mo#1	140.2(2)
C(1)-Mo-C(5)	35.8(3)	C(4)-Mo-Mo#1	168.9(2)
B(1)-Mo-C(2)	82.1(3)	Cl-Mo-Mo#1	92.33(5)
B(2)#1-Mo-C(2)	90.9(3)	B(1)-Mo-H(3)	81(2)
B(2)-Mo-C(2)	112.4(3)	B(2)#1-Mo-H(3)	120(2)
C(1)-Mo-C(2)	35.6(3)	B(2)-Mo-H(3)	33(2)
C(5)-Mo-C(2)	59.0(3)	C(1)-Mo-H(3)	84(2)
B(1)-Mo-C(3)	109.8(3)	C(5)-Mo-H(3)	83(2)
B(2)#1-Mo-C(3)	93.2(3)	C(2)-Mo-H(3)	117(2)
B(2)-Mo-C(3)	147.1(4)	C(3)-Mo-H(3)	140(2)
C(1)-Mo-C(3)	58.7(3)	C(4)-Mo-H(3)	116(2)
C(5)-Mo-C(3)	58.6(3)	Cl-Mo-H(3)	78(2)
C(2)-Mo-C(3)	34.8(3)	Mo#1-Mo-H(3)	74(2)
B(1)-Mo-C(4)	140.3(3)	C(5)-C(1)-C(2)	107.8(6)
B(2)#1-Mo-C(4)	124.5(3)	C(5)-C(1)-C(6)	125.7(8)
B(2)-Mo-C(4)	144.3(3)	C(2)-C(1)-C(6)	126.1(8)
C(1)-Mo-C(4)	59.0(3)	C(5)-C(1)-Mo	72.5(4)
C(5)-Mo-C(4)	35.4(3)	C(2)-C(1)-Mo	74.2(4)
C(2)-Mo-C(4)	58.2(3)	C(6)-C(1)-Mo	125.0(6)
C(3)-Mo-C(4)	34.8(3)	C(3)-C(2)-C(1)	107.6(7)
B(1)-Mo-Cl	135.3(2)	C(3)-C(2)-C(7)	125.1(8)
B(2)#1-Mo-Cl	112.1(3)	C(1)-C(2)-C(7)	126.5(8)
B(2)-Mo-Cl	98.3(3)	C(3)-C(2)-Mo	72.7(4)
C(1)-Mo-Cl	126.3(2)	C(1)-C(2)-Mo	70.2(4)
C(5)-Mo-Cl	91.6(2)	C(7)-C(2)-Mo	130.6(5)
C(2)-Mo-Cl	142.5(2)	C(2)-C(3)-C(4)	109.0(7)

Table S4. continued Page 2.

C(2)-C(3)-C(8)	124.4(9)	H(8A)-C(8)-H(8C)	109.5
C(4)-C(3)-C(8)	126.3(8)	H(8B)-C(8)-H(8C)	109.5
C(2)-C(3)-Mo	72.6(4)	C(4)-C(9)-H(9A)	109.5(5)
C(4)-C(3)-Mo	72.8(4)	C(4)-C(9)-H(9B)	109.5(5)
C(8)-C(3)-Mo	126.4(5)	H(9A)-C(9)-H(9B)	109.5
C(3)-C(4)-C(5)	107.6(6)	C(4)-C(9)-H(9C)	109.5(5)
C(3)-C(4)-C(9)	125.8(8)	H(9A)-C(9)-H(9C)	109.5
C(5)-C(4)-C(9)	126.4(7)	H(9B)-C(9)-H(9C)	109.5
C(3)-C(4)-Mo	72.5(4)	C(5)-C(10)-H(10A)	109.5(5)
C(5)-C(4)-Mo	70.5(4)	C(5)-C(10)-H(10B)	109.5(5)
C(9)-C(4)-Mo	125.8(5)	H(10A)-C(10)-H(10B)	109.5
C(1)-C(5)-C(4)	107.9(6)	C(5)-C(10)-H(10C)	109.5(5)
C(1)-C(5)-C(10)	126.6(8)	H(10A)-C(10)-H(10C)	109.5
C(4)-C(5)-C(10)	125.1(7)	H(10B)-C(10)-H(10C)	109.5
C(1)-C(5)-Mo	71.7(4)	B(2)#1-B(1)-B(2)	117.8(9)
C(4)-C(5)-Mo	74.1(4)	B(2)#1-B(1)-Mo#1	69.6(4)
C(10)-C(5)-Mo	125.3(6)	B(2)-B(1)-Mo#1	68.5(4)
C(1)-C(6)-H(6A)	109.5(5)	B(2)#1-B(1)-Mo	68.5(4)
C(1)-C(6)-H(6B)	109.5(5)	B(2)-B(1)-Mo	69.6(4)
H(6A)-C(6)-H(6B)	109.5	Mo#1-B(1)-Mo	92.4(4)
C(1)-C(6)-H(6C)	109.5(4)	B(2)#1-B(1)-H(1)	121.1(4)
H(6A)-C(6)-H(6C)	109.5	B(2)-B(1)-H(1)	121.1(4)
H(6B)-C(6)-H(6C)	109.5	Mo#1-B(1)-H(1)	133.8(2)
C(2)-C(7)-H(7A)	109.5(5)	Mo-B(1)-H(1)	133.8(2)
C(2)-C(7)-H(7B)	109.5(5)	B(1)-B(2)-Mo#1	62.2(3)
H(7A)-C(7)-H(7B)	109.5	B(1)-B(2)-Mo	61.5(3)
C(2)-C(7)-H(7C)	109.5(5)	Mo#1-B(2)-Mo	85.9(3)
H(7A)-C(7)-H(7C)	109.5	B(1)-B(2)-H(2)	115(3)
H(7B)-C(7)-H(7C)	109.5	Mo#1-B(2)-H(2)	130(2)
C(3)-C(8)-H(8A)	109.5(6)	Mo-B(2)-H(2)	140(2)
C(3)-C(8)-H(8B)	109.5(4)	B(1)-B(2)-H(3)	108(3)
H(8A)-C(8)-H(8B)	109.5	Mo#1-B(2)-H(3)	121(3)
C(3)-C(8)-H(8C)	109.5(5)	Mo-B(2)-H(3)	49(3)

Table S4. continued Page 3.

H(2)-B(2)-H(3)	108(4)	Mo-B(2)-H(4)	106(4)
B(1)-B(2)-H(4)	108(4)	H(2)-B(2)-H(4)	112(5)
Mo#1-B(2)-H(4)	46(4)	H(3)-B(2)-H(4)	106(5)

Symmetry transformations used to generate equivalent atoms:

#1 y,x,-z+2

Table S5. Anisotropic displacement parameters ($Å^2$) for $(Me_5CpMoCl)_2B_3H_7$.

	U11	U22	U33	U23	U13	U12
Mo	0.0296(3)	0.0297(3)	0.0345(3)	0.0010(3)	-0.0023(2)	0.0000(2)
C(1)	0.052(5)	0.033(4)	0.047(4)	-0.003(3)	-0.025(4)	0.000(3)
C(2)	0.034(4)	0.056(5)	0.049(4)	0.005(4)	-0.012(4)	-0.004(4)
C(3)	0.033(4)	0.047(4)	0.044(4)	-0.006(3)	-0.015(3)	0.014(3)
C(4)	0.042(4)	0.039(4)	0.044(4)	0.006(3)	-0.016(3)	0.000(3)
C(5)	0.040(4)	0.051(5)	0.040(3)	0.002(3)	-0.002(3)	0.006(3)
C(6)	0.089(7)	0.033(4)	0.082(6)	-0.013(4)	-0.045(5)	0.005(4)
C(7)	0.038(4)	0.087(7)	0.082(6)	0.025(6)	-0.012(5)	-0.017(4)
C(8)	0.063(6)	0.087(8)	0.075(5)	-0.027(6)	-0.021(5)	0.033(5)
C(9)	0.073(7)	0.034(4)	0.097(7)	0.016(5)	-0.026(5)	0.000(4)
C(10)	0.076(7)	0.105(9)	0.044(4)	0.001(5)	0.001(4)	0.013(5)
Cl	0.0506(11)	0.0667(14)	0.0669(12)	0.0261(10)	-0.0155(10)	-0.0248(10)
B(1)	0.034(4)	0.034(4)	0.031(5)	0.004(3)	-0.004(3)	-0.008(5)
B(2)	0.054(5)	0.040(5)	0.040(4)	-0.002(3)	-0.015(4)	0.016(4)

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

Table S6. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for $(Me_5CpMoCl)_2B_3H_7$.

	x	y	z	$U_{iso}(Å^2)$
H(6A)	-0.1571(12)	-0.1153(10)	0.9150(3)	0.102
H(6B)	0.0145(12)	-0.0866(10)	0.8996(3)	0.102
H(6C)	-0.1283(12)	-0.0538(10)	0.8708(3)	0.102
H(7A)	-0.3204(10)	-0.0231(12)	0.9582(3)	0.103
H(7B)	-0.4306(10)	0.1236(12)	0.9548(3)	0.103
H(7C)	-0.3238(10)	0.1019(12)	0.9931(3)	0.103
H(8A)	-0.2416(12)	0.5525(13)	0.9688(3)	0.113
H(8B)	-0.2655(12)	0.4166(13)	1.0003(3)	0.113
H(8C)	-0.3858(12)	0.4394(13)	0.9648(3)	0.113
H(9A)	0.0520(12)	0.5493(10)	0.8854(3)	0.103
H(9B)	0.0161(12)	0.6001(10)	0.9302(3)	0.103
H(9C)	-0.1168(12)	0.6061(10)	0.8974(3)	0.103
H(10A)	0.1279(12)	0.3475(13)	0.8558(2)	0.113
H(10B)	0.0326(12)	0.2071(13)	0.8375(2)	0.113
H(10C)	0.1752(12)	0.1744(13)	0.8663(2)	0.113
H(1)	-0.0716(119)	-0.0716(119)	1.0000	0.078(39)
H(2)	0.2143(63)	-0.1405(59)	0.9534(15)	0.010(13)
H(3)	0.1994(79)	0.0954(79)	0.9430(18)	0.035(17)
H(4)	0.2943(88)	0.0191(94)	0.9896(21)	0.052(20)

Table S7. Selected torsion angles for $(Me_5CpMoCl)_2BH_3$.

-167.97	(0.44)	B1 - Mo - C1 - C5	142.97	(0.46)	B1 - Mo - C2 - C3
151.78	(0.47)	B2_$2 - Mo - C1 - C5	94.32	(0.49)	B2_$2 - Mo - C2 - C3
-119.16	(0.49)	B2 - Mo - C1 - C5	-177.78	(0.46)	B2 - Mo - C2 - C3
0.00	(0.00)	C5 - Mo - C1 - C5	-116.65	(0.64)	C1 - Mo - C2 - C3
115.01	(0.62)	C2 - Mo - C1 - C5	-78.41	(0.49)	C5 - Mo - C2 - C3
78.40	(0.47)	C3 - Mo - C1 - C5	0.00	(0.00)	C3 - Mo - C2 - C3
37.54	(0.43)	C4 - Mo - C1 - C5	-36.70	(0.43)	C4 - Mo - C2 - C3
-16.72	(0.53)	C1 - Mo - C1 - C5	-35.37	(0.64)	C1 - Mo - C2 - C3
-150.08	(0.36)	Mo_$2 - Mo - C1 - C5	130.37	(0.40)	Mo_$2 - Mo - C2 - C3
77.02	(0.42)	B1 - Mo - C1 - C2	-100.37	(0.42)	B1 - Mo - C2 - C1
36.77	(0.53)	B2_$2 - Mo - C1 - C2	-149.03	(0.47)	B2_$2 - Mo - C2 - C1
125.83	(0.47)	B2 - Mo - C1 - C2	-61.13	(0.49)	B2 - Mo - C2 - C1
-115.01	(0.62)	C5 - Mo - C1 - C2	0.00	(0.01)	C1 - Mo - C2 - C1
0.00	(0.01)	C2 - Mo - C1 - C2	38.24	(0.41)	C5 - Mo - C2 - C1
-36.61	(0.45)	C3 - Mo - C1 - C2	116.65	(0.64)	C3 - Mo - C2 - C1
-77.47	(0.47)	C4 - Mo - C1 - C2	79.95	(0.46)	C4 - Mo - C2 - C1
-131.73	(0.40)	C1 - Mo - C1 - C2	81.28	(0.53)	C1 - Mo - C2 - C1
94.90	(0.43)	Mo_$2 - Mo - C1 - C2	-112.98	(0.39)	Mo_$2 - Mo - C2 - C1
-46.29	(0.76)	B1 - Mo - C1 - C6	21.22	(0.81)	B1 - Mo - C2 - C7
-86.54	(0.82)	B2_$2 - Mo - C1 - C6	-27.44	(0.85)	B2_$2 - Mo - C2 - C7
2.52	(0.78)	B2 - Mo - C1 - C6	60.46	(0.90)	B2 - Mo - C2 - C7
121.68	(0.98)	C5 - Mo - C1 - C6	121.59	(1.03)	C1 - Mo - C2 - C7
-123.31	(0.95)	C2 - Mo - C1 - C6	159.83	(0.95)	C5 - Mo - C2 - C7
-159.92	(0.87)	C3 - Mo - C1 - C6	-121.76	(1.04)	C3 - Mo - C2 - C7
159.22	(0.89)	C4 - Mo - C1 - C6	-158.46	(0.94)	C4 - Mo - C2 - C7
104.96	(0.73)	C1 - Mo - C1 - C6	-157.13	(0.68)	C1 - Mo - C2 - C7
-28.40	(0.88)	Mo_$2 - Mo - C1 - C6	8.61	(0.93)	Mo_$2 - Mo - C2 - C7
-1.68	(0.80)	C5 - C1 - C2 - C3	2.19	(0.81)	C1 - C2 - C3 - C4
-174.42	(0.67)	C6 - C1 - C2 - C3	-167.95	(0.68)	C7 - C2 - C3 - C4
63.52	(0.50)	Mo - C1 - C2 - C3	64.12	(0.49)	Mo - C2 - C3 - C4
168.28	(0.73)	C5 - C1 - C2 - C7	175.53	(0.66)	C1 - C2 - C3 - C8
-4.46	(1.19)	C6 - C1 - C2 - C7	5.39	(1.18)	C7 - C2 - C3 - C8
-126.52	(0.77)	Mo - C1 - C2 - C7	-122.54	(0.69)	Mo - C2 - C3 - C8
-65.20	(0.48)	C5 - C1 - C2 - Mo	-61.93	(0.50)	C1 - C2 - C3 - Mo
122.06	(0.71)	C6 - C1 - C2 - Mo	127.93	(0.75)	C7 - C2 - C3 - Mo
0.00	(0.00)	Mo - C1 - C2 - Mo	0.00	(0.00)	Mo - C2 - C3 - Mo

Table S7. continued Page 2.

-39.34	(0.50)	B1 - Mo - C3 - C2	
-86.95	(0.51)	B2_$2 - Mo - C3 - C2	
3.78	(0.79)	B2 - Mo - C3 - C2	
37.48	(0.44)	C1 - Mo - C3 - C2	
79.70	(0.49)	C5 - Mo - C3 - C2	
0.00	(0.00)	C2 - Mo - C3 - C2	
117.03	(0.63)	C4 - Mo - C3 - C2	
157.72	(0.41)	C1 - Mo - C3 - C2	
-79.34	(0.50)	Mo_$2 - Mo - C3 - C2	
-156.38	(0.40)	B1 - Mo - C3 - C4	
156.02	(0.48)	B2_$2 - Mo - C3 - C4	
-113.26	(0.62)	B2 - Mo - C3 - C4	
-79.56	(0.48)	C1 - Mo - C3 - C4	
-37.34	(0.40)	C5 - Mo - C3 - C4	
-117.03	(0.63)	C2 - Mo - C3 - C4	
0.00	(0.01)	C4 - Mo - C3 - C4	
40.69	(0.45)	C1 - Mo - C3 - C4	
163.63	(0.32)	Mo_$2 - Mo - C3 - C4	
80.90	(0.86)	B1 - Mo - C3 - C8	
33.30	(0.93)	B2_$2 - Mo - C3 - C8	
124.02	(0.84)	B2 - Mo - C3 - C8	
157.72	(0.96)	C1 - Mo - C3 - C8	
-160.06	(0.95)	C5 - Mo - C3 - C8	
120.24	(1.05)	C2 - Mo - C3 - C8	
-122.73	(1.05)	C4 - Mo - C3 - C8	
-82.04	(0.86)	C1 - Mo - C3 - C8	
40.90	(1.00)	Mo_$2 - Mo - C3 - C8	
-1.84	(0.81)	C2 - C3 - C4 - C5	
-175.02	(0.69)	C8 - C3 - C4 - C5	
62.15	(0.48)	Mo - C3 - C4 - C5	
174.16	(0.73)	C2 - C3 - C4 - C9	
0.97	(1.21)	C8 - C3 - C4 - C9	
-121.85	(0.77)	Mo - C3 - C4 - C9	
-63.99	(0.50)	C2 - C3 - C4 - Mo	
122.83	(0.72)	C8 - C3 - C4 - Mo	
0.00	(0.01)	Mo - C3 - C4 - Mo	
36.20	(0.56)	B1 - Mo - C4 - C3	
-29.48	(0.59)	B2_$2 - Mo - C4 - C3	
121.23	(0.64)	B2 - Mo - C4 - C3	
78.63	(0.50)	C1 - Mo - C4 - C3	
116.65	(0.62)	C5 - Mo - C4 - C3	
36.70	(0.44)	C2 - Mo - C4 - C3	
0.00	(0.01)	C3 - Mo - C4 - C3	
-142.48	(0.43)	C1 - Mo - C4 - C3	
-69.63	(1.16)	Mo_$2 - Mo - C4 - C3	
-80.45	(0.51)	B1 - Mo - C4 - C5	
-146.13	(0.47)	B2_$2 - Mo - C4 - C5	
4.58	(0.79)	B2 - Mo - C4 - C5	
-38.02	(0.43)	C1 - Mo - C4 - C5	
0.00	(0.01)	C5 - Mo - C4 - C5	
-79.95	(0.47)	C2 - Mo - C4 - C5	
-116.65	(0.62)	C3 - Mo - C4 - C5	
100.86	(0.41)	C1 - Mo - C4 - C5	
173.72	(0.81)	Mo_$2 - Mo - C4 - C5	
158.11	(0.61)	B1 - Mo - C4 - C9	
92.43	(0.81)	B2_$2 - Mo - C4 - C9	
-116.86	(0.84)	B2 - Mo - C4 - C9	
-159.46	(0.87)	C1 - Mo - C4 - C9	
-121.44	(0.93)	C5 - Mo - C4 - C9	
158.61	(0.85)	C2 - Mo - C4 - C9	
121.91	(0.92)	C3 - Mo - C4 - C9	
-20.57	(0.72)	C1 - Mo - C4 - C9	
52.28	(1.50)	Mo_$2 - Mo - C4 - C9	
0.56	(0.79)	C2 - C1 - C5 - C4	
173.34	(0.68)	C6 - C1 - C5 - C4	
-65.77	(0.49)	Mo - C1 - C5 - C4	
-172.85	(0.74)	C2 - C1 - C5 - C10	
-0.07	(1.21)	C6 - C1 - C5 - C10	
120.82	(0.79)	Mo - C1 - C5 - C10	
66.33	(0.49)	C2 - C1 - C5 - Mo	
-120.89	(0.72)	C6 - C1 - C5 - Mo	
0.00		Mo - C1 - C5 - Mo	

0.77	(0.79)	C3 - C4 - C5 - C1
-175.19	(0.74)	C9 - C4 - C5 - C1
64.18	(0.48)	Mo - C4 - C5 - C1
174.31	(0.72)	C3 - C4 - C5 - C10
-1.66	(1.24)	C9 - C4 - C5 - C10
-122.28	(0.78)	Mo - C4 - C5 - C10
-63.41	(0.47)	C3 - C4 - C5 - Mo
120.62	(0.78)	C9 - C4 - C5 - Mo
0.00	(0.01)	Mo - C4 - C5 - Mo
14.65	(0.54)	B1 - Mo - C5 - C1
-52.22	(0.83)	B2_$2 - Mo - C5 - C1
67.27	(0.52)	B2 - Mo - C5 - C1
0.00	(0.00)	C1 - Mo - C5 - C1
-37.97	(0.44)	C2 - Mo - C5 - C1
-78.87	(0.49)	C3 - Mo - C5 - C1
-115.55	(0.64)	C4 - Mo - C5 - C1
166.58	(0.44)	C1 - Mo - C5 - C1
67.37	(0.65)	Mo_$2 - Mo - C5 - C1
130.20	(0.40)	B1 - Mo - C5 - C4
63.33	(0.76)	B2_$2 - Mo - C5 - C4
-177.18	(0.49)	B2 - Mo - C5 - C4
115.55	(0.64)	C1 - Mo - C5 - C4
77.58	(0.48)	C2 - Mo - C5 - C4
36.68	(0.44)	C3 - Mo - C5 - C4
0.00	(0.01)	C4 - Mo - C5 - C4
-77.86	(0.42)	C1 - Mo - C5 - C4
-177.07	(0.37)	Mo_$2 - Mo - C5 - C4
-107.73	(0.71)	B1 - Mo - C5 - C10
-174.60	(0.73)	B2_$2 - Mo - C5 - C10
-55.11	(0.81)	B2 - Mo - C5 - C10
-122.38	(0.94)	C1 - Mo - C5 - C10
-160.35	(0.85)	C2 - Mo - C5 - C10
158.75	(0.83)	C3 - Mo - C5 - C10
122.07	(0.90)	C4 - Mo - C5 - C10
44.20	(0.73)	C1 - Mo - C5 - C10
-55.01	(0.93)	Mo_$2 - Mo - C5 - C10

0.00	(0.01)	B2_$2 - Mo - B1 - B2_$2
132.93	(0.61)	B2 - Mo - B1 - B2_$2
-132.89	(0.40)	C1 - Mo - B1 - B2_$2
-141.40	(0.38)	C5 - Mo - B1 - B2_$2
-97.99	(0.40)	C2 - Mo - B1 - B2_$2
-76.58	(0.41)	C3 - Mo - B1 - B2_$2
-97.56	(0.48)	C4 - Mo - B1 - B2_$2
80.58	(0.33)	C1 - Mo - B1 - B2_$2
66.91	(0.35)	Mo_$2 - Mo - B1 - B2_$2
-132.93	(0.61)	B2_$2 - Mo - B1 - B2
0.00	(0.01)	B2 - Mo - B1 - B2
94.18	(0.41)	C1 - Mo - B1 - B2
85.67	(0.47)	C5 - Mo - B1 - B2
129.08	(0.41)	C2 - Mo - B1 - B2
150.48	(0.38)	C3 - Mo - B1 - B2
129.51	(0.43)	C4 - Mo - B1 - B2
-52.35	(0.40)	C1 - Mo - B1 - B2
-66.02	(0.35)	Mo_$2 - Mo - B1 - B2
-66.91	(0.35)	B2_$2 - Mo - B1 - Mo_$2
66.02	(0.35)	B2 - Mo - B1 - Mo_$2
160.19	(0.21)	C1 - Mo - B1 - Mo_$2
151.68	(0.25)	C5 - Mo - B1 - Mo_$2
-164.90	(0.20)	C2 - Mo - B1 - Mo_$2
-143.50	(0.19)	C3 - Mo - B1 - Mo_$2
-164.47	(0.30)	C4 - Mo - B1 - Mo_$2
13.67	(0.10)	C1 - Mo - B1 - Mo_$2
0.00		Mo_$2 - Mo - B1 - Mo_$2
50.85	(0.18)	B2_$2 - B1 - B2 - Mo_$2
0.00	(0.01)	Mo_$2 - B1 - B2 - Mo_$2
101.23	(0.31)	Mo - B1 - B2 - Mo_$2
-50.38	(0.17)	B2_$2 - B1 - B2 - Mo
-101.23	(0.31)	Mo_$2 - B1 - B2 - Mo
0.00	(0.01)	Mo - B1 - B2 - Mo
0.00	(0.01)	B1 - Mo - B2 - B1
33.74	(0.48)	B2_$2 - Mo - B2 - B1
-86.93	(0.40)	C1 - Mo - B2 - B1

Table S7. continued Page 4.

-119.65	(0.37)	C5 - Mo - B2 - B1	-147.34	(0.33)	C1 - Mo - B2 - Mo_$2
-56.26	(0.42)	C2 - Mo - B2 - B1	179.94	(0.25)	C5 - Mo - B2 - Mo_$2
-58.59	(0.62)	C3 - Mo - B2 - B1	-116.68	(0.30)	C2 - Mo - B2 - Mo_$2
-122.45	(0.51)	C4 - Mo - B2 - B1	-119.00	(0.44)	C3 - Mo - B2 - Mo_$2
145.78	(0.33)	C1 - Mo - B2 - B1	177.14	(0.35)	C4 - Mo - B2 - Mo_$2
60.41	(0.35)	Mo_$2 - Mo - B2 - B1	85.36	(0.27)	C1 - Mo - B2 - Mo_$2
-60.41	(0.34)	B1 - Mo - B2 - Mo_$2	0.00	(0.01)	Mo_$2 - Mo - B2 - Mo_$2
-26.67	(0.50)	B2_$2 - Mo - B2 - Mo_$2			