Supporting Information

Title: Synthesis, Structural Characterization, and Theoretical Investigation of Compounds Containing an Al–O–M–O–Al (M = Ti, Zr) Core

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Complete Reference (23):

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Vreven, Jr. T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03, Revision C.02*, Gaussian, Inc., Wallingford CT, **2004**.

Table S1. Crystal Data and Structure Refinement for **7**

Identification code	**7**
Empirical formula	$C_{64}H_{100}Al_2N_6O_2Ti$
Formula weight	1087.36
Temperature	133(2) K
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, $P2_1/c$
Unit cell dimensions	a = 22.6235(9) Å alpha = 90 deg. b = 17.1285(4) Å beta = 103.433(3)deg. c = 17.1933(5) Å gamma = 90 deg.
Volume	6480.2(4) $Å^3$
Z, Calculated density	4, 1.115 Mg/m^3
Absorption coefficient	0.204 mm^{-1}
F(000)	2360
Theta range for data collection	1.51 to 24.84 deg.
Index ranges	-26<=h<=26, -20<=k<=20, -20<=l<=20
Reflections collected / unique	98282 / 11152 [R(int) = 0.0826]
Observed reflections [I>2sigma(I)]	8232
Completeness to theta = 24.84	99.4%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11152 / 0 / 732
Goodness-of-fit on F^2	0.966

Final R indices [I>2sigma(I)]	$R_1 = 0.0395$, $wR_2 = 0.0910$
R indices (all data)	$R_1 = 0.0620$, $wR_2 = 0.0977$
Largest diff. peak and hole	0.342 and -0.353 e.Å $^{-3}$

Table S2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for **7** (U(eq) is Defined as one third of the Trace of the Orthogonalized Uij Tensor)

	x	y	z	U(eq)
Ti(1)	0.2374(1)	0.0166(1)	0.0686(1)	0.02276(9)
Al(1)	0.3138(1)	-0.1076(1)	0.2204(1)	0.02143(13)
Al(2)	0.2018(1)	0.2046(1)	0.1302(1)	0.02244(13)
O(1)	0.2811(1)	-0.0519(1)	0.1381(1)	0.0261(3)
O(2)	0.2217(1)	0.1124(1)	0.1032(1)	0.0261(3)
N(1)	0.4007(1)	-0.1093(1)	0.2427(1)	0.0236(3)
N(2)	0.3044(1)	-0.2189(1)	0.2022(1)	0.0231(3)
N(3)	0.2060(1)	0.2753(1)	0.0459(1)	0.0251(4)
N(4)	0.1146(1)	0.2080(1)	0.1128(1)	0.0241(3)
N(5)	0.2777(1)	0.0267(1)	-0.0178(1)	0.0327(4)
N(6)	0.1604(1)	-0.0293(1)	0.0220(1)	0.0291(4)
C(1)	0.4875(1)	-0.1518(1)	0.3509(1)	0.0347(5)
C(2)	0.4259(1)	-0.1647(1)	0.2955(1)	0.0251(4)
C(3)	0.3963(1)	-0.2345(1)	0.3036(1)	0.0261(4)
C(4)	0.3429(1)	-0.2643(1)	0.2536(1)	0.0257(4)
C(5)	0.3309(1)	-0.3505(1)	0.2591(1)	0.0338(5)
C(6)	0.4393(1)	-0.0487(1)	0.2219(1)	0.0257(4)
C(7)	0.4444(1)	0.0236(1)	0.2616(1)	0.0291(4)
C(8)	0.4782(1)	0.0823(1)	0.2360(1)	0.0367(5)
C(9)	0.5067(1)	0.0697(1)	0.1741(1)	0.0413(5)
C(10)	0.5033(1)	-0.0025(1)	0.1383(1)	0.0393(5)
C(11)	0.4699(1)	-0.0631(1)	0.1606(1)	0.0313(5)
C(12)	0.4157(1)	0.0397(1)	0.3317(1)	0.0332(5)
C(13)	0.4641(1)	0.0648(2)	0.4058(1)	0.0452(6)
C(14)	0.3653(1)	0.1006(1)	0.3105(1)	0.0392(5)
C(15)	0.4695(1)	-0.1426(1)	0.1214(1)	0.0421(6)
C(16)	0.5229(2)	-0.1924(2)	0.1646(2)	0.0635(8)
C(17)	0.4708(1)	-0.1379(2)	0.0325(2)	0.0492(6)
C(18)	0.2541(1)	-0.2548(1)	0.1454(1)	0.0258(4)
C(19)	0.2612(1)	-0.2687(1)	0.0673(1)	0.0310(5)
C(20)	0.2126(1)	-0.3014(1)	0.0120(1)	0.0402(5)
C(21)	0.1580(1)	-0.3168(1)	0.0317(1)	0.0430(6)
C(22)	0.1517(1)	-0.3023(1)	0.1081(1)	0.0366(5)
C(23)	0.1996(1)	-0.2720(1)	0.1670(1)	0.0297(5)
C(24)	0.3198(1)	-0.2492(1)	0.0432(1)	0.0350(5)
C(25)	0.3086(1)	-0.2181(2)	-0.0421(1)	0.0454(6)
C(26)	0.3631(1)	-0.3187(2)	0.0541(2)	0.0504(6)

C(27)	0.1898(1)	-0.2585(1)	0.2505(1)	0.0339(5)
C(28)	0.1699(1)	-0.3328(2)	0.2865(2)	0.0516(7)
C(29)	0.1436(1)	-0.1934(2)	0.2489(2)	0.0487(6)
C(30)	0.2890(1)	-0.0850(1)	0.3203(1)	0.0310(5)
C(31)	0.1775(1)	0.2958(2)	-0.1000(1)	0.0406(5)
C(32)	0.1645(1)	0.2661(1)	-0.0232(1)	0.0280(4)
C(33)	0.1089(1)	0.2287(1)	-0.0271(1)	0.0290(5)
C(34)	0.0829(1)	0.2082(1)	0.0362(1)	0.0261(4)
C(35)	0.0170(1)	0.1846(1)	0.0160(1)	0.0343(5)
C(36)	0.2544(1)	0.3312(1)	0.0489(1)	0.0304(5)
C(37)	0.2427(1)	0.4100(1)	0.0626(2)	0.0528(7)
C(38)	0.2890(2)	0.4640(2)	0.0645(2)	0.0636(8)
C(39)	0.3452(1)	0.4415(2)	0.0549(2)	0.0548(7)
C(40)	0.3561(1)	0.3642(2)	0.0427(1)	0.0422(6)
C(41)	0.3113(1)	0.3075(1)	0.0390(1)	0.0296(5)
C(42A)	0.1945(5)	0.4343(5)	0.1016(10)	0.042(3)
C(43A)	0.1471(5)	0.4617(6)	0.0303(11)	0.055(4)
C(44A)	0.2098(7)	0.4981(5)	0.1670(9)	0.058(3)
C(42B)	0.1745(4)	0.4382(3)	0.0606(6)	0.0386(17)
C(43B)	0.1404(3)	0.4791(4)	-0.0162(6)	0.0530(18)
C(44B)	0.1787(5)	0.4914(4)	0.1335(5)	0.0503(19)
C(45)	0.3257(1)	0.2232(1)	0.0242(1)	0.0318(5)
C(46)	0.3567(1)	0.2152(2)	-0.0457(2)	0.0458(6)
C(47)	0.3652(1)	0.1867(2)	0.0999(2)	0.0459(6)
C(48)	0.0806(1)	0.1985(1)	0.1744(1)	0.0258(4)
C(49)	0.0725(1)	0.1238(1)	0.2035(1)	0.0280(4)
C(50)	0.0375(1)	0.1161(2)	0.2605(1)	0.0369(5)
C(51)	0.0114(1)	0.1801(2)	0.2874(1)	0.0394(5)
C(52)	0.0206(1)	0.2532(2)	0.2595(1)	0.0356(5)
C(53)	0.0558(1)	0.2647(1)	0.2036(1)	0.0305(5)
C(54)	0.1020(1)	0.0522(1)	0.1771(1)	0.0295(4)
C(55)	0.0587(1)	-0.0175(1)	0.1588(1)	0.0383(5)
C(56)	0.1591(1)	0.0305(1)	0.2407(1)	0.0352(5)
C(57)	0.0660(1)	0.3470(1)	0.1777(1)	0.0398(5)
C(58)	0.0088(2)	0.3813(2)	0.1235(2)	0.0723(9)
C(59)	0.0883(1)	0.4003(2)	0.2499(2)	0.0553(7)
C(60)	0.2441(1)	0.2484(1)	0.2327(1)	0.0330(5)
C(61)	0.2449(1)	0.0560(2)	-0.0954(1)	0.0547(7)
C(62)	0.3355(1)	-0.0075(2)	-0.0203(2)	0.0501(6)
C(63)	0.1095(1)	0.0121(1)	-0.0278(1)	0.0383(5)
C(64)	0.1505(1)	-0.1133(1)	0.0164(1)	0.0358(5)

Table S3. Bond Lengths [pm] and Angles [deg] for **7**

Ti(1)-O(1)	179.8(1)
Ti(1)-O(2)	180.9(1)
Ti(1)-N(6)	191.0(2)
Ti(1)-N(5)	192.3(2)
Al(1)-O(1)	172.5(1)
Al(1)-N(1)	191.6(2)
Al(1)-N(2)	193.6(2)
Al(1)-C(30)	196.5(2)
Al(2)-O(2)	173.4(2)
Al(2)-N(3)	190.8(2)
Al(2)-N(4)	192.6(2)
Al(2)-C(60)	195.0(2)
N(1)-C(2)	134.5(2)
N(1)-C(6)	145.3(2)
N(2)-C(4)	133.7(2)
N(2)-C(18)	145.1(2)
N(3)-C(32)	134.1(2)
N(3)-C(36)	144.6(3)
N(4)-C(34)	134.5(2)
N(4)-C(48)	145.5(2)
N(5)-C(62)	144.3(3)
N(5)-C(61)	145.8(3)
N(6)-C(63)	145.0(3)
N(6)-C(64)	145.7(3)
C(1)-C(2)	151.0(3)
C(2)-C(3)	139.4(3)
C(3)-C(4)	140.6(3)
C(4)-C(5)	150.7(3)
C(6)-C(7)	140.5(3)
C(6)-C(11)	141.1(3)
C(7)-C(8)	139.6(3)
C(7)-C(12)	151.9(3)
C(8)-C(9)	138.4(3)
C(9)-C(10)	137.4(3)
C(10)-C(11)	139.1(3)
C(11)-C(15)	151.8(3)
C(12)-C(14)	152.6(3)
C(12)-C(13)	153.7(3)
C(15)-C(16)	152.4(4)
C(15)-C(17)	153.9(3)
C(18)-C(23)	139.9(3)
C(18)-C(19)	140.9(3)
C(19)-C(20)	139.3(3)

C(19)-C(24)	151.6(3)
C(20)-C(21)	137.9(3)
C(21)-C(22)	137.8(3)
C(22)-C(23)	140.0(3)
C(23)-C(27)	152.0(3)
C(24)-C(25)	152.5(3)
C(24)-C(26)	152.4(3)
C(27)-C(29)	152.5(3)
C(27)-C(28)	152.9(3)
C(31)-C(32)	150.6(3)
C(32)-C(33)	139.8(3)
C(33)-C(34)	139.9(3)
C(34)-C(35)	150.4(3)
C(36)-C(41)	139.7(3)
C(36)-C(37)	140.5(3)
C(37)-C(38)	139.3(4)
C(37)-C(42A)	146.7(8)
C(37)-C(42B)	161.0(8)
C(38)-C(39)	137.4(4)
C(39)-C(40)	137.2(4)
C(40)-C(41)	139.5(3)
C(41)-C(45)	151.4(3)
C(42A)-C(43A)	150.4(12)
C(42A)-C(44A)	154.8(11)
C(42B)-C(44B)	153.4(8)
C(42B)-C(43B)	153.4(7)
C(45)-C(47)	153.1(3)
C(45)-C(46)	153.2(3)
C(48)-C(49)	140.1(3)
C(48)-C(53)	140.9(3)
C(49)-C(50)	140.2(3)
C(49)-C(54)	151.5(3)
C(50)-C(51)	137.6(3)
C(51)-C(52)	137.4(3)
C(52)-C(53)	139.8(3)
C(53)-C(57)	151.1(3)
C(54)-C(55)	152.9(3)
C(54)-C(56)	153.3(3)
C(57)-C(58)	152.5(4)
C(57)-C(59)	153.0(3)

O(1)-Ti(1)-O(2)	119.58(6)
O(1)-Ti(1)-N(6)	108.55(7)
O(2)-Ti(1)-N(6)	106.35(7)
O(1)-Ti(1)-N(5)	106.61(7)
O(2)-Ti(1)-N(5)	109.64(7)

N(6)-Ti(1)-N(5)	105.24(7)
O(1)-Al(1)-N(1)	113.34(7)
O(1)-Al(1)-N(2)	113.68(7)
N(1)-Al(1)-N(2)	94.97(7)
O(1)-Al(1)-C(30)	116.96(8)
N(1)-Al(1)-C(30)	108.46(8)
N(2)-Al(1)-C(30)	107.08(8)
O(2)-Al(2)-N(3)	108.22(7)
O(2)-Al(2)-N(4)	107.85(7)
N(3)-Al(2)-N(4)	95.32(7)
O(2)-Al(2)-C(60)	119.24(8)
N(3)-Al(2)-C(60)	110.00(9)
N(4)-Al(2)-C(60)	113.49(8)
Al(1)-O(1)-Ti(1)	166.18(9)
Al(2)-O(2)-Ti(1)	175.58(8)
C(2)-N(1)-C(6)	119.14(15)
C(2)-N(1)-Al(1)	113.48(13)
C(6)-N(1)-Al(1)	125.99(12)
C(4)-N(2)-C(18)	119.12(16)
C(4)-N(2)-Al(1)	115.83(13)
C(18)-N(2)-Al(1)	124.40(12)
C(32)-N(3)-C(36)	118.55(16)
C(32)-N(3)-Al(2)	116.73(13)
C(36)-N(3)-Al(2)	124.33(12)
C(34)-N(4)-C(48)	117.42(15)
C(34)-N(4)-Al(2)	116.52(13)
C(48)-N(4)-Al(2)	125.36(12)
C(62)-N(5)-C(61)	112.63(19)
C(62)-N(5)-Ti(1)	125.61(14)
C(61)-N(5)-Ti(1)	120.42(15)
C(63)-N(6)-C(64)	110.88(17)
C(63)-N(6)-Ti(1)	124.64(14)
C(64)-N(6)-Ti(1)	123.01(13)
N(1)-C(2)-C(3)	122.38(17)
N(1)-C(2)-C(1)	120.42(18)
C(3)-C(2)-C(1)	117.17(17)
C(2)-C(3)-C(4)	127.96(18)
N(2)-C(4)-C(3)	121.89(18)
N(2)-C(4)-C(5)	120.84(17)
C(3)-C(4)-C(5)	117.27(17)
C(7)-C(6)-C(11)	121.25(18)
C(7)-C(6)-N(1)	119.75(17)
C(11)-C(6)-N(1)	118.99(17)
C(8)-C(7)-C(6)	118.00(19)
C(8)-C(7)-C(12)	119.10(19)
C(6)-C(7)-C(12)	122.88(18)

C(9)-C(8)-C(7)	121.3(2)
C(10)-C(9)-C(8)	119.8(2)
C(9)-C(10)-C(11)	121.7(2)
C(10)-C(11)-C(6)	117.9(2)
C(10)-C(11)-C(15)	119.68(19)
C(6)-C(11)-C(15)	122.39(18)
C(7)-C(12)-C(14)	111.59(17)
C(7)-C(12)-C(13)	110.83(18)
C(14)-C(12)-C(13)	110.82(18)
C(11)-C(15)-C(16)	111.3(2)
C(11)-C(15)-C(17)	113.2(2)
C(16)-C(15)-C(17)	108.47(19)
C(23)-C(18)-C(19)	121.23(18)
C(23)-C(18)-N(2)	120.85(17)
C(19)-C(18)-N(2)	117.88(17)
C(20)-C(19)-C(18)	118.2(2)
C(20)-C(19)-C(24)	120.24(19)
C(18)-C(19)-C(24)	121.55(17)
C(21)-C(20)-C(19)	121.2(2)
C(22)-C(21)-C(20)	119.9(2)
C(21)-C(22)-C(23)	121.4(2)
C(22)-C(23)-C(18)	118.01(19)
C(22)-C(23)-C(27)	118.74(19)
C(18)-C(23)-C(27)	123.24(18)
C(19)-C(24)-C(25)	112.33(18)
C(19)-C(24)-C(26)	111.80(19)
C(25)-C(24)-C(26)	110.44(19)
C(23)-C(27)-C(29)	110.14(18)
C(23)-C(27)-C(28)	112.14(19)
C(29)-C(27)-C(28)	110.55(19)
N(3)-C(32)-C(33)	122.23(17)
N(3)-C(32)-C(31)	119.85(18)
C(33)-C(32)-C(31)	117.92(17)
C(34)-C(33)-C(32)	127.90(17)
N(4)-C(34)-C(33)	122.48(17)
N(4)-C(34)-C(35)	120.02(17)
C(33)-C(34)-C(35)	117.50(17)
C(41)-C(36)-C(37)	120.9(2)
C(41)-C(36)-N(3)	120.96(19)
C(37)-C(36)-N(3)	118.15(19)
C(38)-C(37)-C(36)	118.2(2)
C(38)-C(37)-C(42A)	115.8(4)
C(36)-C(37)-C(42A)	122.5(4)
C(38)-C(37)-C(42B)	120.9(3)
C(36)-C(37)-C(42B)	120.1(3)
C(42A)-C(37)-C(42B)	27.6(4)

C(39)-C(38)-C(37)	121.5(3)
C(40)-C(39)-C(38)	119.5(2)
C(39)-C(40)-C(41)	121.6(2)
C(40)-C(41)-C(36)	118.2(2)
C(40)-C(41)-C(45)	119.22(19)
C(36)-C(41)-C(45)	122.55(18)
C(37)-C(42A)-C(43A)	100.3(8)
C(37)-C(42A)-C(44A)	118.0(6)
C(43A)-C(42A)-C(44A)	111.7(7)
C(44B)-C(42B)-C(43B)	110.8(5)
C(44B)-C(42B)-C(37)	106.5(5)
C(43B)-C(42B)-C(37)	116.3(4)
C(41)-C(45)-C(47)	110.60(18)
C(41)-C(45)-C(46)	111.91(17)
C(47)-C(45)-C(46)	110.33(19)
C(49)-C(48)-C(53)	120.82(18)
C(49)-C(48)-N(4)	119.80(17)
C(53)-C(48)-N(4)	119.38(18)
C(50)-C(49)-C(48)	118.55(19)
C(50)-C(49)-C(54)	119.48(19)
C(48)-C(49)-C(54)	121.94(17)
C(51)-C(50)-C(49)	121.1(2)
C(50)-C(51)-C(52)	119.8(2)
C(51)-C(52)-C(53)	121.7(2)
C(52)-C(53)-C(48)	118.0(2)
C(52)-C(53)-C(57)	118.97(19)
C(48)-C(53)-C(57)	123.07(18)
C(49)-C(54)-C(55)	112.85(17)
C(49)-C(54)-C(56)	109.79(17)
C(55)-C(54)-C(56)	110.54(18)
C(53)-C(57)-C(58)	111.9(2)
C(53)-C(57)-C(59)	111.2(2)
C(58)-C(57)-C(59)	109.8(2)

Symmetry transformations used to generate equivalent atoms.

Table S4. Anisotropic Displacement Parameters ($Å^2$) for **7**

	U11	U22	U33	U23	U13	U12
Ti(1)	0.02455(18)	0.02144(19)	0.02128(16)	0.00158(14)	0.00326(13)	0.00217(14)
Al(1)	0.0219(3)	0.0202(3)	0.0214(3)	0.0005(2)	0.0033(2)	0.0009(2)
Al(2)	0.0227(3)	0.0229(3)	0.0212(3)	-0.0005(2)	0.0042(2)	0.0001(2)
O(1)	0.0263(7)	0.0242(8)	0.0270(7)	0.0018(6)	0.0045(5)	0.0010(6)
O(2)	0.0265(7)	0.0250(8)	0.0266(7)	0.0018(6)	0.0056(5)	0.0011(6)
N(1)	0.0252(8)	0.0205(9)	0.0244(8)	0.0010(7)	0.0044(6)	0.0001(7)
N(2)	0.0223(8)	0.0231(9)	0.0236(8)	0.0011(7)	0.0044(6)	-0.0002(6)
N(3)	0.0254(8)	0.0224(9)	0.0280(8)	-0.0001(7)	0.0073(7)	0.0008(7)
N(4)	0.0238(8)	0.0259(9)	0.0227(8)	-0.0002(7)	0.0055(6)	0.0022(7)
N(5)	0.0376(10)	0.0334(11)	0.0280(8)	0.0031(8)	0.0092(7)	0.0022(8)
N(6)	0.0301(9)	0.0252(10)	0.0285(8)	-0.0001(7)	-0.0001(7)	0.0025(7)
C(1)	0.0281(11)	0.0324(13)	0.0377(11)	0.0019(9)	-0.0045(9)	0.0021(9)
C(2)	0.0250(10)	0.0248(11)	0.0246(9)	-0.0007(8)	0.0038(8)	0.0040(8)
C(3)	0.0283(10)	0.0238(11)	0.0250(9)	0.0047(8)	0.0039(8)	0.0052(8)
C(4)	0.0286(10)	0.0237(11)	0.0259(9)	0.0027(8)	0.0084(8)	0.0028(8)
C(5)	0.0352(11)	0.0229(11)	0.0413(11)	0.0055(9)	0.0048(9)	0.0002(9)
C(6)	0.0204(9)	0.0222(11)	0.0321(10)	0.0043(8)	0.0013(8)	0.0003(8)
C(7)	0.0267(10)	0.0255(11)	0.0312(10)	0.0007(9)	-0.0013(8)	0.0006(8)
C(8)	0.0343(11)	0.0234(12)	0.0479(13)	0.0008(10)	0.0004(10)	-0.0060(9)
C(9)	0.0329(12)	0.0344(14)	0.0563(14)	0.0088(11)	0.0095(10)	-0.0087(10)
C(10)	0.0321(11)	0.0357(14)	0.0540(13)	0.0044(11)	0.0179(10)	-0.0043(9)
C(11)	0.0247(10)	0.0298(12)	0.0401(11)	0.0021(9)	0.0091(9)	0.0002(9)
C(12)	0.0398(12)	0.0250(12)	0.0304(10)	-0.0020(9)	-0.0008(9)	0.0006(9)
C(13)	0.0545(15)	0.0369(14)	0.0363(12)	-0.0028(10)	-0.0058(11)	-0.0002(11)
C(14)	0.0445(13)	0.0330(13)	0.0383(12)	-0.0032(10)	0.0058(10)	0.0042(10)
C(15)	0.0440(13)	0.0362(14)	0.0550(14)	-0.0077(11)	0.0296(11)	-0.0061(10)
C(16)	0.100(2)	0.0429(17)	0.0603(17)	0.0123(13)	0.0457(16)	0.0285(16)
C(17)	0.0457(14)	0.0534(17)	0.0526(14)	-0.0084(12)	0.0197(11)	0.0028(12)
C(18)	0.0261(10)	0.0188(11)	0.0304(10)	0.0004(8)	0.0022(8)	0.0005(8)
C(19)	0.0360(11)	0.0235(11)	0.0322(11)	-0.0049(8)	0.0048(9)	-0.0010(9)
C(20)	0.0465(13)	0.0357(13)	0.0343(11)	-0.0087(10)	0.0008(10)	-0.0035(11)
C(21)	0.0395(13)	0.0341(14)	0.0477(14)	-0.0066(11)	-0.0057(10)	-0.0088(10)
C(22)	0.0294(11)	0.0275(12)	0.0501(13)	0.0024(10)	0.0035(9)	-0.0056(9)
C(23)	0.0294(11)	0.0216(11)	0.0364(11)	0.0035(8)	0.0040(9)	0.0005(8)
C(24)	0.0400(12)	0.0369(13)	0.0286(10)	-0.0075(9)	0.0091(9)	-0.0052(10)
C(25)	0.0549(15)	0.0462(16)	0.0361(12)	-0.0019(11)	0.0128(11)	-0.0035(12)
C(26)	0.0476(14)	0.0542(17)	0.0528(14)	0.0094(12)	0.0183(12)	0.0089(12)
C(27)	0.0298(11)	0.0342(13)	0.0385(11)	0.0044(10)	0.0097(9)	-0.0026(9)
C(28)	0.0509(15)	0.0529(17)	0.0533(15)	0.0144(13)	0.0168(12)	-0.0123(12)
C(29)	0.0325(12)	0.0499(16)	0.0651(16)	-0.0087(13)	0.0143(11)	-0.0006(11)

C(30) 0.0311(11) 0.0309(12) 0.0302(10) 0.0000(9) 0.0054(8) 0.0030(9)
C(31) 0.0406(12) 0.0535(15) 0.0298(11) 0.0133(10) 0.0123(9) 0.0064(11)
C(32) 0.0341(11) 0.0255(11) 0.0249(10) 0.0025(8) 0.0082(8) 0.0070(9)
C(33) 0.0312(11) 0.0329(12) 0.0206(9) -0.0012(8) 0.0012(8) 0.0013(9)
C(34) 0.0270(10) 0.0232(11) 0.0262(10) -0.0019(8) 0.0022(8) 0.0034(8)
C(35) 0.0273(11) 0.0425(14) 0.0298(10) -0.0014(9) -0.0003(8) -0.0019(9)
C(36) 0.0372(11) 0.0249(11) 0.0302(10) 0.0019(9) 0.0101(9) -0.0058(9)
C(37) 0.0669(17) 0.0275(13) 0.0778(18) -0.0068(12) 0.0452(15) -0.0075(12)
C(38) 0.088(2) 0.0278(15) 0.090(2) -0.0137(14) 0.0519(18) -0.0177(14)
C(39) 0.0598(17) 0.0416(16) 0.0659(17) -0.0035(13) 0.0206(14) -0.0246(13)
C(40) 0.0351(12) 0.0417(15) 0.0485(13) 0.0058(11) 0.0069(10) -0.0096(10)
C(41) 0.0305(11) 0.0299(12) 0.0260(10) 0.0053(8) 0.0015(8) -0.0026(9)
C(42A) 0.051(5) 0.027(4) 0.053(7) -0.004(4) 0.020(5) -0.005(4)
C(43A) 0.052(6) 0.038(6) 0.073(10) -0.010(6) 0.012(6) 0.005(4)
C(44A) 0.071(7) 0.041(5) 0.073(7) -0.017(4) 0.036(6) -0.005(5)
C(42B) 0.051(4) 0.025(3) 0.042(5) -0.001(3) 0.015(3) 0.004(3)
C(43B) 0.058(3) 0.042(3) 0.054(4) -0.003(3) 0.003(3) 0.015(2)
C(44B) 0.071(5) 0.030(3) 0.057(4) -0.003(3) 0.028(3) 0.008(3)
C(45) 0.0263(10) 0.0305(12) 0.0387(11) 0.0081(9) 0.0080(9) 0.0010(8)
C(46) 0.0455(14) 0.0410(15) 0.0572(15) 0.0088(12) 0.0248(12) 0.0039(11)
C(47) 0.0341(12) 0.0443(15) 0.0546(14) 0.0189(12) 0.0007(10) 0.0008(10)
C(48) 0.0183(9) 0.0348(12) 0.0236(9) -0.0007(8) 0.0036(7) -0.0004(8)
C(49) 0.0223(10) 0.0348(12) 0.0263(9) 0.0009(9) 0.0047(8) 0.0009(8)
C(50) 0.0315(11) 0.0452(14) 0.0359(11) 0.0052(10) 0.0116(9) -0.0015(10)
C(51) 0.0285(11) 0.0593(17) 0.0339(11) -0.0018(11) 0.0141(9) 0.0001(10)
C(52) 0.0267(10) 0.0480(15) 0.0336(11) -0.0070(10) 0.0102(9) 0.0045(10)
C(53) 0.0231(10) 0.0370(13) 0.0301(10) -0.0026(9) 0.0037(8) 0.0041(9)
C(54) 0.0287(10) 0.0307(12) 0.0297(10) 0.0038(9) 0.0080(8) 0.0002(9)
C(55) 0.0345(11) 0.0384(13) 0.0411(12) -0.0006(10) 0.0072(9) -0.0052(10)
C(56) 0.0307(11) 0.0369(13) 0.0375(11) 0.0038(10) 0.0069(9) 0.0018(9)
C(57) 0.0442(13) 0.0330(13) 0.0463(13) -0.0031(10) 0.0189(10) 0.0054(10)
C(58) 0.097(2) 0.0436(18) 0.0635(18) 0.0020(14) -0.0078(17) 0.0136(16)
C(59) 0.0511(15) 0.0446(16) 0.0690(17) -0.0152(13) 0.0117(13) -0.0043(12)
C(60) 0.0322(11) 0.0376(13) 0.0286(10) -0.0033(9) 0.0060(8) -0.0015(9)
C(61) 0.0641(17) 0.0678(19) 0.0304(12) 0.0103(12) 0.0071(11) -0.0099(14)
C(62) 0.0638(16) 0.0356(14) 0.0629(16) 0.0082(12) 0.0394(13) 0.0128(12)
C(63) 0.0352(12) 0.0369(13) 0.0358(11) -0.0009(10) -0.0060(9) 0.0043(10)
C(64) 0.0363(12) 0.0282(12) 0.0394(12) -0.0073(10) 0.0019(9) -0.0022(9)

Table S5. Crystal Data and Structure Refinement for **8**

Identification code	**8**
Empirical formula	$C_{64}H_{100}Al_2N_6O_2Zr$
Formula weight	1130.68
Temperature	133(2) K
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, $P2_1/c$
Unit cell dimensions	a = 22.6139(9) Å alpha = 90 deg. b = 17.1826(8) Å beta = 102.419(3) deg. c = 17.2375(6) Å gamma = 90 deg.
Volume	6541.2(5) $Å^3$
Z, Calculated density	4, 1.148 Mg/m^3
Absorption coefficient	0.239 mm^{-1}
F(000)	2432
Theta range for data collection	1.50 to 24.90 deg.
Index ranges	-26<=h<=26, -20<=k<=19, -20<=l<=20
Reflections collected / unique	66342 / 11255 [R(int) = 0.1005]
Observed reflections [I>2sigma(I)]	8169
Completeness to theta = 24.90	98.8%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11255 / 0 / 732
Goodness-of-fit on F^2	0.967

Final R indices [I>2sigma(I)]	$R_1 = 0.0373$, $wR_2 = 0.0744$
R indices (all data)	$R_1 = 0.0647$, $wR_2 = 0.0810$
Largest diff. peak and hole	0.243 and -0.321 e.$Å^{-3}$

Table S6. Atomic Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for **8** (U(eq) is Defined as one third of the Trace of the Orthogonalized Uij Tensor.)

	x	y	z	U(eq)
Zr(1)	0.2399(1)	0.0173(1)	0.0660(1)	0.02156(6)
Al(1)	0.3160(1)	-0.1099(1)	0.2245(1)	0.02100(15)
Al(2)	0.2013(1)	0.2097(1)	0.1318(1)	0.02235(15)
O(1)	0.2855(1)	-0.0552(1)	0.1424(1)	0.0256(4)
O(2)	0.2235(1)	0.1193(1)	0.1055(1)	0.0254(4)
N(1)	0.4026(1)	-0.1117(1)	0.2470(1)	0.0227(4)
N(2)	0.3065(1)	-0.2202(1)	0.2059(1)	0.0226(4)
N(3)	0.2041(1)	0.2795(1)	0.0467(1)	0.0246(4)
N(4)	0.1143(1)	0.2090(1)	0.1151(1)	0.0238(4)
N(5)	0.2846(1)	0.0287(1)	-0.0265(1)	0.0317(5)
N(6)	0.1576(1)	-0.0314(1)	0.0151(1)	0.0288(5)
C(1)	0.4876(1)	-0.1538(2)	0.3544(2)	0.0334(6)
C(2)	0.4271(1)	-0.1672(1)	0.2990(1)	0.0240(5)
C(3)	0.3975(1)	-0.2371(1)	0.3058(1)	0.0255(5)
C(4)	0.3447(1)	-0.2658(1)	0.2553(1)	0.0250(5)
C(5)	0.3330(1)	-0.3519(1)	0.2592(2)	0.0330(6)
C(6)	0.4408(1)	-0.0511(1)	0.2254(1)	0.0244(5)
C(7)	0.4436(1)	0.0215(2)	0.2621(1)	0.0285(5)
C(8)	0.4759(1)	0.0806(2)	0.2342(2)	0.0374(6)
C(9)	0.5050(1)	0.0678(2)	0.1726(2)	0.0412(7)
C(10)	0.5043(1)	-0.0049(2)	0.1397(2)	0.0408(7)
C(11)	0.4723(1)	-0.0658(2)	0.1645(2)	0.0321(6)
C(12)	0.4145(1)	0.0381(1)	0.3320(2)	0.0316(6)
C(13)	0.4621(1)	0.0643(2)	0.4056(2)	0.0459(7)
C(14)	0.3635(1)	0.0984(2)	0.3110(2)	0.0389(7)
C(15)	0.4745(1)	-0.1456(2)	0.1273(2)	0.0438(7)
C(16)	0.5296(2)	-0.1914(2)	0.1700(2)	0.0675(11)
C(17)	0.4743(1)	-0.1427(2)	0.0382(2)	0.0495(8)
C(18)	0.2564(1)	-0.2540(1)	0.1490(1)	0.0255(5)
C(19)	0.2634(1)	-0.2658(1)	0.0702(2)	0.0300(6)
C(20)	0.2148(1)	-0.2969(2)	0.0149(2)	0.0375(6)
C(21)	0.1604(1)	-0.3126(2)	0.0356(2)	0.0420(7)
C(22)	0.1538(1)	-0.2998(2)	0.1124(2)	0.0366(6)
C(23)	0.2013(1)	-0.2714(2)	0.1708(2)	0.0302(6)
C(24)	0.3220(1)	-0.2457(2)	0.0455(2)	0.0326(6)
C(25)	0.3113(1)	-0.2107(2)	-0.0375(2)	0.0436(7)
C(26)	0.3637(1)	-0.3167(2)	0.0515(2)	0.0465(7)

C(27)	0.1920(1)	-0.2598(2)	0.2552(2)	0.0354(6)
C(28)	0.1729(2)	-0.3353(2)	0.2901(2)	0.0543(8)
C(29)	0.1450(1)	-0.1959(2)	0.2560(2)	0.0529(8)
C(30)	0.2889(1)	-0.0876(2)	0.3238(1)	0.0299(6)
C(31)	0.1764(1)	0.2980(2)	-0.0988(2)	0.0375(6)
C(32)	0.1639(1)	0.2684(1)	-0.0218(1)	0.0273(5)
C(33)	0.1091(1)	0.2285(2)	-0.0250(1)	0.0292(6)
C(34)	0.0833(1)	0.2076(1)	0.0393(1)	0.0270(5)
C(35)	0.0178(1)	0.1819(2)	0.0201(2)	0.0346(6)
C(36)	0.2515(1)	0.3367(2)	0.0486(1)	0.0297(6)
C(37)	0.2378(2)	0.4148(2)	0.0598(2)	0.0481(7)
C(38)	0.2834(2)	0.4694(2)	0.0628(2)	0.0587(9)
C(39)	0.3410(2)	0.4483(2)	0.0566(2)	0.0555(9)
C(40)	0.3538(1)	0.3715(2)	0.0461(2)	0.0430(7)
C(41)	0.3092(1)	0.3137(2)	0.0412(1)	0.0303(6)
C(42A)	0.1916(11)	0.4398(10)	0.0979(18)	0.043(5)
C(43A)	0.1434(10)	0.4664(11)	0.028(2)	0.062(9)
C(44A)	0.2044(15)	0.5012(9)	0.1659(16)	0.061(6)
C(42B)	0.1710(4)	0.4408(4)	0.0604(7)	0.0418(18)
C(43B)	0.1390(4)	0.4837(5)	-0.0154(5)	0.0575(19)
C(44B)	0.1734(5)	0.4920(4)	0.1339(5)	0.050(2)
C(45)	0.3252(1)	0.2307(2)	0.0271(2)	0.0312(6)
C(46)	0.3572(1)	0.2238(2)	-0.0426(2)	0.0468(7)
C(47)	0.3638(1)	0.1945(2)	0.1024(2)	0.0477(8)
C(48)	0.0805(1)	0.1977(2)	0.1776(1)	0.0275(5)
C(49)	0.0732(1)	0.1230(2)	0.2060(1)	0.0289(5)
C(50)	0.0386(1)	0.1138(2)	0.2639(2)	0.0366(6)
C(51)	0.0120(1)	0.1770(2)	0.2918(2)	0.0412(7)
C(52)	0.0207(1)	0.2499(2)	0.2652(2)	0.0371(6)
C(53)	0.0556(1)	0.2625(2)	0.2081(1)	0.0313(6)
C(54)	0.1028(1)	0.0523(2)	0.1780(2)	0.0291(5)
C(55)	0.0605(1)	-0.0177(2)	0.1613(2)	0.0409(6)
C(56)	0.1604(1)	0.0315(2)	0.2397(2)	0.0355(6)
C(57)	0.0655(1)	0.3452(2)	0.1830(2)	0.0398(7)
C(58)	0.0093(2)	0.3781(2)	0.1279(2)	0.0699(11)
C(59)	0.0853(2)	0.3982(2)	0.2556(2)	0.0540(8)
C(60)	0.2419(1)	0.2549(2)	0.2334(2)	0.0334(6)
C(61)	0.2534(2)	0.0560(2)	-0.1043(2)	0.0627(10)
C(62)	0.3448(1)	0.0001(2)	-0.0266(2)	0.0502(8)
C(63)	0.1066(1)	0.0087(2)	-0.0345(2)	0.0408(7)
C(64)	0.1459(1)	-0.1144(2)	0.0155(2)	0.0343(6)

Table S7. Bond Lengths [pm] and Angles [deg] for **8**

Zr(1)-O(1)	194.1(2)
Zr(1)-O(2)	194.4(2)
Zr(1)-N(6)	205.7(2)
Zr(1)-N(5)	207.2(2)
Al(1)-O(1)	171.6(2)
Al(1)-N(1)	191.3(2)
Al(1)-N(2)	192.6(2)
Al(1)-C(30)	197.4(2)
Al(2)-O(2)	172.3(2)
Al(2)-N(3)	190.7(2)
Al(2)-N(4)	192.6(2)
Al(2)-C(60)	195.5(3)
N(1)-C(2)	134.4(3)
N(1)-C(6)	145.2(3)
N(2)-C(4)	133.1(3)
N(2)-C(18)	145.1(3)
N(3)-C(32)	134.1(3)
N(3)-C(36)	144.9(3)
N(4)-C(34)	134.4(3)
N(4)-C(48)	146.2(3)
N(5)-C(62)	145.0(3)
N(5)-C(61)	145.2(4)
N(6)-C(64)	145.0(3)
N(6)-C(63)	145.3(3)
C(1)-C(2)	150.8(3)
C(2)-C(3)	139.2(3)
C(3)-C(4)	140.7(3)
C(4)-C(5)	150.7(3)
C(6)-C(7)	139.4(3)
C(6)-C(11)	141.3(3)
C(7)-C(8)	139.5(4)
C(7)-C(12)	151.9(3)
C(8)-C(9)	138.2(4)
C(9)-C(10)	137.1(4)
C(10)-C(11)	139.1(4)
C(11)-C(15)	151.9(4)
C(12)-C(14)	153.3(4)
C(12)-C(13)	154.5(4)
C(15)-C(16)	152.3(5)
C(15)-C(17)	153.5(4)
C(18)-C(23)	140.9(3)
C(18)-C(19)	141.4(4)

C(19)-C(20)	139.5(4)
C(19)-C(24)	151.7(4)
C(20)-C(21)	138.1(4)
C(21)-C(22)	138.2(4)
C(22)-C(23)	139.3(4)
C(23)-C(27)	152.8(4)
C(24)-C(25)	152.3(4)
C(24)-C(26)	153.0(4)
C(27)-C(29)	153.0(4)
C(27)-C(28)	153.1(4)
C(31)-C(32)	150.4(3)
C(32)-C(33)	140.7(3)
C(33)-C(34)	140.5(3)
C(34)-C(35)	151.3(3)
C(36)-C(41)	139.7(4)
C(36)-C(37)	139.9(4)
C(37)-C(38)	138.8(4)
C(37)-C(42A)	141.5(18)
C(37)-C(42B)	157.8(9)
C(38)-C(39)	137.8(5)
C(39)-C(40)	137.0(4)
C(40)-C(41)	140.4(4)
C(41)-C(45)	150.5(4)
C(42A)-C(43A)	151(2)
C(42A)-C(44A)	156(2)
C(42B)-C(44B)	153.4(9)
C(42B)-C(43B)	153.9(8)
C(45)-C(47)	153.2(4)
C(45)-C(46)	153.4(4)
C(48)-C(49)	139.5(4)
C(48)-C(53)	140.1(3)
C(49)-C(50)	140.5(3)
C(49)-C(54)	151.5(4)
C(50)-C(51)	137.6(4)
C(51)-C(52)	136.3(4)
C(52)-C(53)	140.4(4)
C(53)-C(57)	151.5(4)
C(54)-C(55)	152.3(4)
C(54)-C(56)	153.7(3)
C(57)-C(58)	152.2(4)
C(57)-C(59)	153.3(4)

O(1)-Zr(1)-O(2)	117.05(7)
O(1)-Zr(1)-N(6)	109.09(7)
O(2)-Zr(1)-N(6)	107.07(7)
O(1)-Zr(1)-N(5)	107.87(7)

O(2)-Zr(1)-N(5)	110.21(8)
N(6)-Zr(1)-N(5)	104.88(8)
O(1)-Al(1)-N(1)	112.86(8)
O(1)-Al(1)-N(2)	112.98(8)
N(1)-Al(1)-N(2)	95.20(9)
O(1)-Al(1)-C(30)	117.65(10)
N(1)-Al(1)-C(30)	108.81(10)
N(2)-Al(1)-C(30)	106.92(10)
O(2)-Al(2)-N(3)	107.74(8)
O(2)-Al(2)-N(4)	107.56(9)
N(3)-Al(2)-N(4)	95.20(9)
O(2)-Al(2)-C(60)	119.15(10)
N(3)-Al(2)-C(60)	110.60(11)
N(4)-Al(2)-C(60)	113.83(10)
Al(1)-O(1)-Zr(1)	166.50(10)
Al(2)-O(2)-Zr(1)	173.21(10)
C(2)-N(1)-C(6)	119.86(19)
C(2)-N(1)-Al(1)	113.79(15)
C(6)-N(1)-Al(1)	125.16(15)
C(4)-N(2)-C(18)	120.1(2)
C(4)-N(2)-Al(1)	116.04(16)
C(18)-N(2)-Al(1)	123.38(15)
C(32)-N(3)-C(36)	118.3(2)
C(32)-N(3)-Al(2)	117.35(16)
C(36)-N(3)-Al(2)	123.82(15)
C(34)-N(4)-C(48)	117.87(19)
C(34)-N(4)-Al(2)	116.62(15)
C(48)-N(4)-Al(2)	124.76(15)
C(62)-N(5)-C(61)	112.1(2)
C(62)-N(5)-Zr(1)	125.74(18)
C(61)-N(5)-Zr(1)	121.42(19)
C(64)-N(6)-C(63)	110.3(2)
C(64)-N(6)-Zr(1)	123.23(16)
C(63)-N(6)-Zr(1)	126.00(17)
N(1)-C(2)-C(3)	122.2(2)
N(1)-C(2)-C(1)	120.1(2)
C(3)-C(2)-C(1)	117.7(2)
C(2)-C(3)-C(4)	127.5(2)
N(2)-C(4)-C(3)	122.5(2)
N(2)-C(4)-C(5)	120.7(2)
C(3)-C(4)-C(5)	116.7(2)
C(7)-C(6)-C(11)	121.1(2)
C(7)-C(6)-N(1)	119.9(2)
C(11)-C(6)-N(1)	119.0(2)
C(6)-C(7)-C(8)	118.1(2)
C(6)-C(7)-C(12)	122.9(2)

C(8)-C(7)-C(12)	119.0(2)
C(9)-C(8)-C(7)	121.3(3)
C(10)-C(9)-C(8)	119.9(3)
C(9)-C(10)-C(11)	121.3(3)
C(10)-C(11)-C(6)	118.2(2)
C(10)-C(11)-C(15)	118.8(2)
C(6)-C(11)-C(15)	123.0(2)
C(7)-C(12)-C(14)	111.8(2)
C(7)-C(12)-C(13)	111.2(2)
C(14)-C(12)-C(13)	110.7(2)
C(11)-C(15)-C(16)	111.1(3)
C(11)-C(15)-C(17)	113.6(2)
C(16)-C(15)-C(17)	109.1(2)
C(23)-C(18)-C(19)	120.8(2)
C(23)-C(18)-N(2)	120.7(2)
C(19)-C(18)-N(2)	118.4(2)
C(20)-C(19)-C(18)	118.5(2)
C(20)-C(19)-C(24)	120.1(2)
C(18)-C(19)-C(24)	121.4(2)
C(21)-C(20)-C(19)	120.8(3)
C(20)-C(21)-C(22)	120.1(2)
C(21)-C(22)-C(23)	121.5(3)
C(22)-C(23)-C(18)	118.1(2)
C(22)-C(23)-C(27)	119.4(2)
C(18)-C(23)-C(27)	122.6(2)
C(19)-C(24)-C(25)	112.5(2)
C(19)-C(24)-C(26)	111.3(2)
C(25)-C(24)-C(26)	110.4(2)
C(23)-C(27)-C(29)	109.9(2)
C(23)-C(27)-C(28)	111.8(2)
C(29)-C(27)-C(28)	110.5(2)
N(3)-C(32)-C(33)	121.9(2)
N(3)-C(32)-C(31)	120.5(2)
C(33)-C(32)-C(31)	117.5(2)
C(34)-C(33)-C(32)	127.2(2)
N(4)-C(34)-C(33)	123.0(2)
N(4)-C(34)-C(35)	120.0(2)
C(33)-C(34)-C(35)	117.0(2)
C(41)-C(36)-C(37)	121.5(2)
C(41)-C(36)-N(3)	120.5(2)
C(37)-C(36)-N(3)	118.0(2)
C(38)-C(37)-C(36)	118.0(3)
C(38)-C(37)-C(42A)	113.2(8)
C(36)-C(37)-C(42A)	124.2(7)
C(38)-C(37)-C(42B)	120.9(4)
C(36)-C(37)-C(42B)	120.8(4)

C(42A)-C(37)-C(42B)	26.8(10)
C(39)-C(38)-C(37)	121.7(3)
C(40)-C(39)-C(38)	119.6(3)
C(39)-C(40)-C(41)	121.3(3)
C(36)-C(41)-C(40)	117.9(2)
C(36)-C(41)-C(45)	122.9(2)
C(40)-C(41)-C(45)	119.2(2)
C(37)-C(42A)-C(43A)	101.6(15)
C(37)-C(42A)-C(44A)	121.3(13)
C(43A)-C(42A)-C(44A)	112.3(14)
C(44B)-C(42B)-C(43B)	110.7(6)
C(44B)-C(42B)-C(37)	107.7(6)
C(43B)-C(42B)-C(37)	114.0(5)
C(41)-C(45)-C(47)	111.1(2)
C(41)-C(45)-C(46)	111.7(2)
C(47)-C(45)-C(46)	110.6(2)
C(49)-C(48)-C(53)	120.9(2)
C(49)-C(48)-N(4)	120.1(2)
C(53)-C(48)-N(4)	119.1(2)
C(48)-C(49)-C(50)	118.6(2)
C(48)-C(49)-C(54)	122.2(2)
C(50)-C(49)-C(54)	119.3(2)
C(51)-C(50)-C(49)	120.8(3)
C(52)-C(51)-C(50)	120.0(2)
C(51)-C(52)-C(53)	121.5(3)
C(48)-C(53)-C(52)	118.1(3)
C(48)-C(53)-C(57)	122.9(2)
C(52)-C(53)-C(57)	119.0(2)
C(49)-C(54)-C(55)	113.0(2)
C(49)-C(54)-C(56)	109.4(2)
C(55)-C(54)-C(56)	110.6(2)
C(53)-C(57)-C(58)	111.8(3)
C(53)-C(57)-C(59)	111.0(2)
C(58)-C(57)-C(59)	110.4(3)

Symmetry transformations used to generate equivalent atoms.

Table S8. Anisotropic Displacement parameters ($Å^2$) for **8**

	U11	U22	U33	U23	U13	U12
Zr(1)	0.02186(11)	0.02069(11)	0.02199(11)	0.00214(10)	0.00441(8)	0.00176(11)
Al(1)	0.0198(3)	0.0208(4)	0.0224(3)	0.0005(3)	0.0046(3)	0.0016(3)
Al(2)	0.0215(4)	0.0234(4)	0.0224(3)	-0.0003(3)	0.0052(3)	0.0002(3)
O(1)	0.0229(8)	0.0252(9)	0.0280(9)	0.0012(7)	0.0039(7)	0.0013(7)
O(2)	0.0218(8)	0.0261(9)	0.0290(9)	0.0020(7)	0.0067(7)	0.0004(7)
N(1)	0.0203(10)	0.0202(11)	0.0277(10)	0.0013(8)	0.0057(8)	0.0003(8)
N(2)	0.0216(10)	0.0225(11)	0.0235(10)	0.0025(8)	0.0041(8)	0.0001(8)
N(3)	0.0248(11)	0.0234(11)	0.0259(10)	-0.0010(8)	0.0066(8)	0.0015(8)
N(4)	0.0218(10)	0.0272(11)	0.0230(10)	0.0007(8)	0.0062(8)	0.0015(8)
N(5)	0.0346(12)	0.0331(13)	0.0297(11)	0.0024(9)	0.0121(9)	0.0020(10)
N(6)	0.0275(11)	0.0262(13)	0.0303(11)	-0.0002(9)	0.0007(8)	0.0004(9)
C(1)	0.0255(13)	0.0319(15)	0.0380(15)	0.0039(11)	-0.0035(11)	0.0018(11)
C(2)	0.0225(12)	0.0223(13)	0.0270(12)	-0.0017(10)	0.0049(9)	0.0048(10)
C(3)	0.0256(13)	0.0249(14)	0.0260(12)	0.0049(10)	0.0057(10)	0.0053(10)
C(4)	0.0261(13)	0.0247(13)	0.0257(12)	0.0018(10)	0.0088(10)	0.0024(10)
C(5)	0.0362(15)	0.0229(14)	0.0380(14)	0.0049(11)	0.0040(11)	-0.0009(11)
C(6)	0.0183(12)	0.0215(13)	0.0318(13)	0.0031(10)	0.0020(10)	-0.0022(10)
C(7)	0.0221(12)	0.0264(13)	0.0331(13)	-0.0007(11)	-0.0027(10)	-0.0005(11)
C(8)	0.0367(15)	0.0248(15)	0.0481(16)	-0.0013(12)	0.0032(12)	-0.0061(12)
C(9)	0.0338(15)	0.0325(17)	0.0571(18)	0.0090(13)	0.0090(13)	-0.0078(12)
C(10)	0.0293(14)	0.0378(19)	0.0595(18)	0.0054(13)	0.0190(13)	-0.0037(11)
C(11)	0.0231(13)	0.0294(15)	0.0450(15)	0.0032(12)	0.0101(11)	0.0017(11)
C(12)	0.0386(15)	0.0221(14)	0.0318(13)	-0.0023(10)	0.0025(11)	0.0009(10)
C(13)	0.0528(18)	0.0379(18)	0.0398(16)	-0.0045(13)	-0.0058(14)	0.0013(14)
C(14)	0.0422(16)	0.0311(16)	0.0423(16)	-0.0037(12)	0.0067(13)	0.0043(12)
C(15)	0.0449(17)	0.0339(16)	0.064(2)	-0.0060(14)	0.0362(15)	-0.0059(13)
C(16)	0.107(3)	0.049(2)	0.060(2)	0.0148(17)	0.047(2)	0.038(2)
C(17)	0.0424(17)	0.052(2)	0.059(2)	-0.0129(15)	0.0204(15)	0.0046(14)
C(18)	0.0252(13)	0.0187(13)	0.0303(12)	0.0011(10)	0.0006(10)	-0.0009(10)
C(19)	0.0341(14)	0.0214(14)	0.0317(14)	-0.0042(10)	0.0014(11)	-0.0036(10)
C(20)	0.0448(17)	0.0330(16)	0.0319(14)	-0.0057(12)	0.0022(12)	-0.0034(13)
C(21)	0.0402(17)	0.0320(17)	0.0454(17)	-0.0015(12)	-0.0097(13)	-0.0078(12)
C(22)	0.0273(14)	0.0281(15)	0.0511(17)	0.0026(12)	0.0012(12)	-0.0079(11)
C(23)	0.0267(13)	0.0229(14)	0.0397(15)	0.0050(11)	0.0044(11)	0.0000(10)
C(24)	0.0402(16)	0.0303(15)	0.0293(13)	-0.0070(11)	0.0118(11)	-0.0044(12)
C(25)	0.0513(18)	0.0434(18)	0.0385(16)	-0.0016(13)	0.0148(13)	-0.0023(14)
C(26)	0.0474(18)	0.0468(19)	0.0493(18)	0.0072(14)	0.0190(14)	0.0073(14)

C(27) 0.0279(14) 0.0373(16) 0.0424(16) 0.0040(12) 0.0108(12) -0.0047(11)
C(28) 0.053(2) 0.055(2) 0.058(2) 0.0146(16) 0.0173(16) -0.0155(16)
C(29) 0.0306(16) 0.060(2) 0.069(2) -0.0120(17) 0.0129(14) -0.0002(14)
C(30) 0.0261(13) 0.0333(15) 0.0302(13) 0.0006(10) 0.0060(10) 0.0023(11)
C(31) 0.0388(16) 0.0468(18) 0.0290(14) 0.0065(12) 0.0120(11) 0.0040(13)
C(32) 0.0314(14) 0.0224(14) 0.0284(13) -0.0001(10) 0.0072(10) 0.0057(10)
C(33) 0.0283(13) 0.0331(15) 0.0248(12) -0.0025(10) 0.0027(10) 0.0009(11)
C(34) 0.0267(13) 0.0257(14) 0.0281(13) -0.0012(10) 0.0048(10) 0.0019(10)
C(35) 0.0246(13) 0.0451(17) 0.0311(14) -0.0015(12) -0.0004(10) -0.0017(12)
C(36) 0.0356(15) 0.0266(14) 0.0278(13) 0.0011(10) 0.0085(10) -0.0063(11)
C(37) 0.0612(19) 0.0253(15) 0.067(2) -0.0035(14) 0.0340(16) -0.0047(14)
C(38) 0.079(3) 0.0275(19) 0.080(2) -0.0086(15) 0.042(2) -0.0142(16)
C(39) 0.061(2) 0.0367(19) 0.070(2) -0.0035(16) 0.0175(17) -0.0249(16)
C(40) 0.0339(16) 0.0384(18) 0.0541(18) 0.0061(14) 0.0035(13) -0.0103(13)
C(41) 0.0326(14) 0.0279(14) 0.0290(13) 0.0073(10) 0.0031(10) -0.0036(11)
C(42A) 0.050(12) 0.019(7) 0.066(14) -0.006(8) 0.024(10) -0.008(7)
C(43A) 0.035(10) 0.035(12) 0.12(3) -0.017(13) 0.031(15) -0.005(7)
C(44A) 0.074(14) 0.037(9) 0.077(13) -0.021(7) 0.029(11) -0.010(8)
C(42B) 0.042(5) 0.027(3) 0.058(5) -0.007(4) 0.014(4) 0.005(3)
C(43B) 0.060(4) 0.051(4) 0.058(4) 0.000(3) 0.006(3) 0.015(3)
C(44B) 0.067(5) 0.032(3) 0.056(4) -0.002(3) 0.024(3) 0.007(3)
C(45) 0.0228(13) 0.0280(15) 0.0438(15) 0.0100(11) 0.0097(11) -0.0001(10)
C(46) 0.0465(18) 0.0409(18) 0.0599(19) 0.0071(14) 0.0265(15) 0.0030(14)
C(47) 0.0319(16) 0.0449(19) 0.062(2) 0.0203(15) 0.0008(14) -0.0013(13)
C(48) 0.0176(12) 0.0382(16) 0.0263(12) -0.0022(11) 0.0042(9) 0.0013(10)
C(49) 0.0206(12) 0.0391(16) 0.0266(12) 0.0012(11) 0.0042(10) 0.0004(11)
C(50) 0.0298(14) 0.0474(18) 0.0354(14) 0.0051(12) 0.0131(11) -0.0013(12)
C(51) 0.0297(15) 0.061(2) 0.0375(15) -0.0017(14) 0.0164(12) 0.0021(13)
C(52) 0.0250(14) 0.0547(19) 0.0324(14) -0.0067(13) 0.0079(11) 0.0065(12)
C(53) 0.0215(13) 0.0428(16) 0.0283(13) -0.0062(11) 0.0027(10) 0.0039(11)
C(54) 0.0252(13) 0.0335(15) 0.0303(13) 0.0036(11) 0.0099(10) -0.0010(11)
C(55) 0.0367(15) 0.0403(16) 0.0471(16) -0.0009(14) 0.0126(12) -0.0039(14)
C(56) 0.0302(14) 0.0393(17) 0.0374(14) 0.0052(12) 0.0080(11) 0.0041(12)
C(57) 0.0380(16) 0.0363(17) 0.0498(17) -0.0058(13) 0.0201(13) 0.0064(12)
C(58) 0.090(3) 0.047(2) 0.062(2) 0.0007(17) -0.007(2) 0.0128(19)
C(59) 0.0482(19) 0.046(2) 0.070(2) -0.0161(16) 0.0160(16) 0.0010(15)
C(60) 0.0307(14) 0.0398(16) 0.0294(13) -0.0038(11) 0.0056(11) -0.0015(12)
C(61) 0.064(2) 0.088(3) 0.0341(17) 0.0161(17) 0.0063(15) -0.020(2)
C(62) 0.0553(19) 0.036(2) 0.071(2) 0.0045(14) 0.0396(17) 0.0093(13)
C(63) 0.0368(15) 0.0388(17) 0.0403(15) 0.0020(12) -0.0060(12) 0.0029(12)
C(64) 0.0337(14) 0.0284(15) 0.0395(15) -0.0053(11) 0.0047(11) -0.0041(11)

Table S9. Calculated Atomic Coordinates for **7**

Ti	-0.31570400	0.24385300	-1.26499500
Al	-3.01533100	0.22740800	1.02384300
Al	2.93733600	0.07302600	0.22892600
O	-1.80634800	0.10740500	-0.24946000
O	1.32132900	0.15151800	-0.48309600
N	-3.72270000	-1.49914900	1.63283800
N	-4.75899500	0.94053500	0.41511000
N	4.09198500	-0.94422300	-0.97532000
N	3.82371600	1.79209100	-0.08743900
N	-0.45601600	-1.12245500	-2.61827000
N	-0.34322800	1.88179700	-2.26912900
C	-5.21863100	-2.46476800	3.36937600
H	-4.99956500	-3.47759700	3.02630800
H	-6.27193000	-2.40333000	3.65284400
H	-4.61291900	-2.29252400	4.26829100
C	-4.87050700	-1.41323200	2.33300800
C	-5.79217400	-0.36558700	2.17595500
H	-6.67403300	-0.41579100	2.80516100
C	-5.81470700	0.63757000	1.18177100
C	-7.13078100	1.37704500	1.03535300
H	-7.31255900	1.69783000	0.00798200
H	-7.12156400	2.27611800	1.66295200
H	-7.96018900	0.74782200	1.36759800
C	-3.03309100	-2.77478400	1.61899600
C	-2.01074600	-3.05103100	2.55685200
C	-1.38242900	-4.30418400	2.51540100
H	-0.59167100	-4.52374500	3.22884500
C	-1.75725600	-5.27260900	1.59196400
H	-1.26333600	-6.24184700	1.58160100
C	-2.77166500	-4.99396000	0.67926500
H	-3.06073400	-5.75647000	-0.03864600
C	-3.42375800	-3.75409100	0.66505700
C	-1.57394100	-2.05121200	3.62369900
H	-2.24689400	-1.19089200	3.57426400
C	-1.67557300	-2.63416400	5.04803700
H	-2.67809100	-3.02255600	5.26228400
H	-1.44623400	-1.85970600	5.79011700
H	-0.96500800	-3.45516400	5.20266800
C	-0.14581300	-1.53900800	3.35796000
H	-0.05530100	-1.08368000	2.36655400
H	0.58448800	-2.35516500	3.41648700
H	0.13948700	-0.78721100	4.10415100

C	-4.54897100	-3.51261800	-0.34442800
H	-4.59071600	-2.43370600	-0.52859700
C	-5.92873100	-3.94278600	0.20233900
H	-6.23898700	-3.35285600	1.06817100
H	-5.91602400	-5.00013400	0.49680600
H	-6.69777100	-3.82049900	-0.57076500
C	-4.31622500	-4.21368600	-1.69663800
H	-3.30866100	-4.04209600	-2.08451600
H	-5.03566900	-3.84230500	-2.43630300
H	-4.46922600	-5.29763400	-1.62380600
C	-4.92791700	1.91137400	-0.64989200
C	-5.16037900	1.44340100	-1.96904800
C	-5.35847600	2.38207900	-2.98928200
H	-5.54993000	2.03653600	-4.00113800
C	-5.30959100	3.75016100	-2.73649000
H	-5.46403300	4.46285100	-3.54375400
C	-5.05796700	4.19648800	-1.44470600
H	-5.01224700	5.26539500	-1.24953700
C	-4.86822600	3.30207500	-0.38086300
C	-5.23619000	-0.04623500	-2.29356300
H	-4.63936500	-0.57061800	-1.54031300
C	-4.64121200	-0.39487500	-3.66914100
H	-3.62912800	0.00757600	-3.78202400
H	-5.25573900	-0.01449400	-4.49461200
H	-4.58867000	-1.48330100	-3.78606300
C	-6.68470800	-0.56843500	-2.19592200
H	-7.10081800	-0.43988500	-1.19162100
H	-6.72740900	-1.63731200	-2.44014000
H	-7.33712300	-0.03757600	-2.90105400
C	-4.60286200	3.88705700	1.00563900
H	-4.52580400	3.05959400	1.71721200
C	-5.73814400	4.81962300	1.47829000
H	-6.71912000	4.33404100	1.44497300
H	-5.80009400	5.72072000	0.85618300
H	-5.55609300	5.14581900	2.50956400
C	-3.26464200	4.65256700	1.03630400
H	-2.43378300	4.02596100	0.70102200
H	-3.04201200	4.99741000	2.05363100
H	-3.29913600	5.53549200	0.38579800
C	-2.47009800	1.28641700	2.60311500
H	-1.49890800	0.96455500	2.99972400
H	-3.19404800	1.21614300	3.42830600
H	-2.36098500	2.35281700	2.37168500
C	4.77360000	-1.19592600	-3.34620900
H	5.40774500	-2.04240500	-3.07609100
H	5.27570100	-0.59892700	-4.11153500

H	3.85518600	-1.61149000	-3.78309900
C	4.39904200	-0.35423000	-2.14343800
C	4.36944000	1.04174200	-2.32495100
H	4.61529100	1.39324500	-3.32107500
C	4.24012400	2.04450700	-1.33644200
C	4.59353800	3.45749700	-1.75281400
H	5.28575100	3.92053900	-1.04361100
H	3.69331100	4.08332200	-1.76926100
H	5.04359400	3.47048900	-2.74802500
C	4.54178900	-2.29794300	-0.71269400
C	5.89913300	-2.52045100	-0.35279700
C	6.31167200	-3.82492400	-0.05135800
H	7.35100600	-4.00391900	0.21393700
C	5.42228100	-4.89394600	-0.07250000
H	5.76074600	-5.89676600	0.17931700
C	4.09935700	-4.66520300	-0.42857700
H	3.40396200	-5.50062200	-0.46033000
C	3.63869100	-3.38535000	-0.77113800
C	6.94630400	-1.40935500	-0.28519400
H	6.43282500	-0.44973300	-0.39606200
C	7.97951600	-1.52043500	-1.42608100
H	7.51026700	-1.46476000	-2.41362200
H	8.52657600	-2.46994500	-1.37130900
H	8.71408900	-0.70805700	-1.35886200
C	7.66998000	-1.39853300	1.07489500
H	8.35238400	-0.54250700	1.13735300
H	8.27260500	-2.30284700	1.22028300
H	6.95936900	-1.33554300	1.90528500
C	2.19537500	-3.24784200	-1.24028400
H	2.01528900	-2.20930300	-1.53204900
C	1.94588300	-4.13501600	-2.47756700
H	2.63757200	-3.89273100	-3.29360400
H	0.92452100	-3.99883900	-2.84659600
H	2.07268600	-5.19945000	-2.24479200
C	1.19634700	-3.58466100	-0.11838300
H	1.34865100	-2.94391300	0.75593300
H	1.29453600	-4.62724500	0.20975000
H	0.16724600	-3.43799400	-0.46190800
C	3.89997300	2.85261200	0.90516500
C	2.81545500	3.74705400	1.07760000
C	2.93501100	4.78187300	2.01525500
H	2.10229100	5.46736900	2.15219800
C	4.09041600	4.95038200	2.76879900
H	4.17010800	5.76901700	3.48093300
C	5.13770100	4.04919200	2.61365200
H	6.03535600	4.16956800	3.21477600

C	5.06217400	2.98289800	1.70678800
C	1.50131100	3.60135300	0.32376400
H	1.62847100	2.84950600	-0.45735000
C	1.04771900	4.90891300	-0.35194500
H	1.81721100	5.31504500	-1.02009100
H	0.80513100	5.68822700	0.38114700
H	0.14524600	4.72619400	-0.94587100
C	0.40729900	3.07781100	1.27201900
H	0.71003700	2.14368500	1.75506800
H	-0.50995200	2.87493700	0.71117500
H	0.17957000	3.80719100	2.05995900
C	6.24058100	2.01600200	1.63260500
H	5.91948800	1.14491400	1.05336900
C	7.44820900	2.64624600	0.90881300
H	7.20395700	2.92671500	-0.12193600
H	8.29078100	1.94440300	0.87267800
H	7.78963800	3.55020200	1.42879600
C	6.65072100	1.51951500	3.03366900
H	5.79956800	1.07760300	3.56329800
H	7.04569000	2.33168400	3.65531900
H	7.43664200	0.76125300	2.95705700
C	3.12599600	-0.50101000	2.09987700
H	2.82474300	-1.54673600	2.24533700
H	2.51280900	0.10301000	2.78208900
H	4.16528300	-0.42147900	2.44837400
C	0.26270400	-1.06540500	-3.87844800
H	0.72887100	-2.03474400	-4.12635300
H	1.06187500	-0.31681400	-3.84420800
H	-0.40317600	-0.80275400	-4.72205500
C	-1.47412100	-2.15470100	-2.61797200
H	-1.03990500	-3.16439100	-2.73325600
H	-2.19319900	-2.02299000	-3.44681600
H	-2.03111400	-2.13571000	-1.67795900
C	0.78605600	2.34799800	-3.05556100
H	0.95008200	3.43182800	-2.92167900
H	0.62884600	2.18035700	-4.13752800
H	1.70554400	1.82937800	-2.76600500
C	-1.57054900	2.57042600	-2.63562300
H	-1.47011500	3.66287700	-2.50655300
H	-2.40659800	2.23651200	-2.01703800
H	-1.84021100	2.39487500	-3.69340600

Table S10. Calculated Atomic Coordinates for **8**

Zr	-0.30722700	0.09814700	-1.30216200
Al	-3.10685300	0.22268800	1.10095100
Al	3.07208500	0.03640500	0.30473900
O	-1.93656900	0.02175600	-0.18773000
O	1.46061800	0.02828800	-0.40533700
N	-3.86941000	-1.45735000	1.74530600
N	-4.83314400	0.98213700	0.50299700
N	4.29120300	-0.94486700	-0.86706300
N	3.87410000	1.79435000	-0.04280900
N	-0.45410600	-1.44831000	-2.70801400
N	-0.29609400	1.79888800	-2.51100400
C	-5.37900100	-2.36982700	3.49494100
H	-5.10340700	-3.38328600	3.19874800
H	-6.44555800	-2.34074600	3.73084600
H	-4.82118900	-2.14229900	4.41360100
C	-5.01694600	-1.34007500	2.44281900
C	-5.91225300	-0.27560000	2.26850000
H	-6.80459700	-0.29889700	2.88561700
C	-5.90841200	0.70176600	1.24445500
C	-7.24378400	1.38354300	1.01297800
H	-7.18641800	2.21584100	0.31289500
H	-7.64299600	1.74398500	1.96758800
H	-7.96182800	0.65174000	0.62326100
C	-3.22811800	-2.75162200	1.66450700
C	-2.10469200	-3.04970500	2.47178700
C	-1.47405500	-4.29209700	2.31532300
H	-0.60581900	-4.52569900	2.92722100
C	-1.94440300	-5.23555200	1.40816200
H	-1.44310500	-6.19532600	1.30413900
C	-3.07385300	-4.94756100	0.64672300
H	-3.45429600	-5.69661700	-0.04381300
C	-3.73568700	-3.71711400	0.75318400
C	-1.58393200	-2.09346000	3.54053700
H	-2.23116300	-1.21211400	3.54453200
C	-1.66133700	-2.72096800	4.94782200
H	-2.67683500	-3.05840000	5.18633300
H	-1.35934400	-1.98936600	5.70733500
H	-0.99525000	-3.58738500	5.04157900
C	-0.15030500	-1.61905300	3.24009500
H	-0.07853500	-1.13832900	2.25891800
H	0.55810600	-2.45636100	3.25238200
H	0.18319900	-0.89710200	3.99547100
C	-5.00648100	-3.49799600	-0.07167200

H	-5.28571000	-2.44346600	0.01446800
C	-6.18144100	-4.34053000	0.47129800
H	-6.40868700	-4.11133600	1.51695600
H	-5.95650600	-5.41262500	0.40796500
H	-7.08896500	-4.15521500	-0.11696600
C	-4.80869300	-3.80174600	-1.56814400
H	-4.00155900	-3.20328400	-1.99734200
H	-5.73010100	-3.58053000	-2.12127000
H	-4.57405300	-4.85867400	-1.74366600
C	-4.93392600	1.95522100	-0.56710300
C	-5.15115200	1.51030500	-1.89406300
C	-5.25847800	2.46699200	-2.91269700
H	-5.43898900	2.13693900	-3.93266000
C	-5.14287300	3.82763500	-2.64721100
H	-5.23013600	4.55366200	-3.45255500
C	-4.91772500	4.25116400	-1.34143400
H	-4.83124800	5.31516700	-1.13358100
C	-4.81081300	3.33999600	-0.28134300
C	-5.32301500	0.03654700	-2.25163100
H	-5.03656200	-0.55497800	-1.37689700
C	-4.41443000	-0.39413800	-3.41848900
H	-3.35757900	-0.22192100	-3.18952400
H	-4.65456300	0.14373700	-4.34369400
H	-4.54682900	-1.46263100	-3.62262800
C	-6.79894700	-0.27995100	-2.57236000
H	-7.46141700	-0.01838400	-1.73950400
H	-6.92896300	-1.34819700	-2.78544000
H	-7.13905300	0.27985300	-3.45277400
C	-4.59969200	3.89392200	1.12791600
H	-4.48589100	3.04939500	1.81269400
C	-5.80655500	4.72930100	1.60588100
H	-6.73868900	4.15529900	1.59256000
H	-5.95285300	5.61345500	0.97319100
H	-5.64251500	5.08031500	2.63219600
C	-3.31478500	4.74045900	1.21946300
H	-2.43892300	4.18266200	0.87578200
H	-3.13541600	5.04901800	2.25668600
H	-3.38998800	5.65154100	0.61282700
C	-2.48197900	1.29622600	2.64227700
H	-1.52075500	0.93345300	3.02900600
H	-3.18902200	1.28758300	3.48491000
H	-2.31984100	2.34875400	2.37896300
C	5.06388800	-1.20904000	-3.20657800
H	5.85104600	-1.90926000	-2.91746100
H	5.42417400	-0.58738100	-4.02950900
H	4.22253000	-1.81353900	-3.56954900

C	4.60076900	-0.36246600	-2.03872700
C	4.51249800	1.02625300	-2.24969700
H	4.77380600	1.37022400	-3.24423200
C	4.31178500	2.04067600	-1.28482800
C	4.62338200	3.45804800	-1.71992100
H	5.25357000	3.96950600	-0.98656100
H	3.69958900	4.04223000	-1.80474100
H	5.12711900	3.46648200	-2.68908600
C	4.78321600	-2.28079100	-0.58993900
C	6.13227800	-2.45071800	-0.17623000
C	6.59156200	-3.74170200	0.11511000
H	7.62577100	-3.87908400	0.42203800
C	5.75437600	-4.84917600	0.03111100
H	6.12843200	-5.84185700	0.27236900
C	4.43639100	-4.67090500	-0.36965000
H	3.78061300	-5.53506200	-0.44473800
C	3.93125900	-3.40483400	-0.70005800
C	7.11981500	-1.29377800	-0.03101800
H	6.57237400	-0.35801400	-0.17736800
C	8.24004100	-1.34856700	-1.09107600
H	7.84431500	-1.30557900	-2.11123500
H	8.82635000	-2.27147100	-1.00077100
H	8.92855900	-0.50344600	-0.96550100
C	7.73679500	-1.26095000	1.38064300
H	8.38279700	-0.38246300	1.49571600
H	8.35589700	-2.14561100	1.57113300
H	6.96272000	-1.22438700	2.15416600
C	2.49342900	-3.31707800	-1.19758600
H	2.28202300	-2.28221900	-1.48149500
C	2.29125300	-4.19665400	-2.44791600
H	2.99713700	-3.93330000	-3.24505500
H	1.27696000	-4.07310100	-2.83944000
H	2.43236100	-5.26108700	-2.22348400
C	1.49190800	-3.70181700	-0.09185600
H	1.59756400	-3.05185600	0.78292600
H	1.63968500	-4.73759000	0.24011900
H	0.46239400	-3.61245300	-0.45399300
C	3.86104200	2.87881200	0.92532300
C	2.74458100	3.74611600	1.01054900
C	2.77498400	4.79788400	1.93656600
H	1.91786700	5.46303700	2.00728500
C	3.87347700	5.00963200	2.76083100
H	3.88345400	5.83968300	3.46401000
C	4.95484600	4.13899300	2.68581100
H	5.80884700	4.29653700	3.33952500
C	4.96828400	3.05855400	1.79279800

C	1.48800000	3.56182600	0.16981700
H	1.68528100	2.80261000	-0.59046200
C	1.05608200	4.85146500	-0.55339800
H	1.86261300	5.26855500	-1.16852700
H	0.74415300	5.63228200	0.15077800
H	0.20365600	4.64235600	-1.20894000
C	0.34130100	3.03107700	1.04993100
H	0.61480700	2.09086500	1.53834600
H	-0.55038900	2.84641200	0.44024700
H	0.07363500	3.75129800	1.83317400
C	6.18248600	2.13425300	1.79469500
H	5.91635200	1.23782300	1.22678400
C	7.39329000	2.79016800	1.09938800
H	7.17895300	3.03184700	0.05228100
H	8.26236800	2.12054300	1.11627300
H	7.67960200	3.72091200	1.60519300
C	6.55599500	1.68883700	3.22257400
H	5.69944300	1.23700400	3.73454500
H	6.90785600	2.52820400	3.83374800
H	7.36433800	0.95110000	3.19366100
C	3.26348100	-0.49564700	2.18936100
H	2.89647200	-1.51471900	2.37024700
H	2.69491500	0.16525500	2.85823500
H	4.30819300	-0.47248300	2.52925200
C	0.15168900	-1.39493800	-4.02823600
H	0.74898000	-2.29750800	-4.24884700
H	0.81946300	-0.52989100	-4.11966600
H	-0.60768800	-1.30966000	-4.82867400
C	-1.33744400	-2.59173800	-2.56810300
H	-0.80617700	-3.55287100	-2.69099900
H	-2.14536900	-2.58017400	-3.32368900
H	-1.80607300	-2.60235100	-1.57768600
C	0.85013100	2.21570800	-3.30150100
H	1.07703000	3.28836800	-3.16299200
H	0.68118600	2.06330900	-4.38422900
H	1.74816300	1.65111000	-3.02159600
C	-1.49053900	2.55608700	-2.85138500
H	-1.35358400	3.63960300	-2.68176600
H	-2.34439200	2.23422500	-2.24682100
H	-1.76850200	2.43139700	-3.91405900