Electronic Supplementary Information for Dalton Transactions

Electronic Supporting Information

Activation of a bis(phenoxy-amine) precatalyst for olefin polymerisation: first evidence for an outer sphere ion pair with the methylborate counterion

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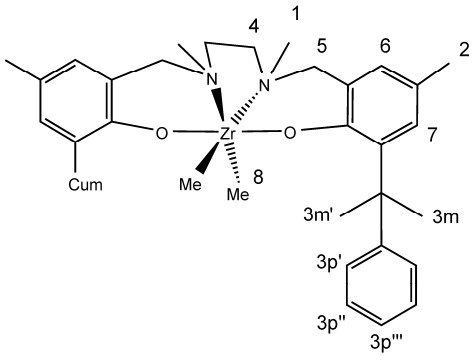
Experimental section. All manipulations of air-sensitive materials were performed with rigorous exclusion of oxygen and moisture in flamed Schlenk-type glassware on a dual-manifold Schlenk line, interfaced to a high-vacuum line (10^{-5} torr), or in a nitrogen-filled Vac-Atmosphere glove-box with a high-capacity recirculator (<1 ppm O_2 and H_2O). All solvents were freeze-pump-thaw degassed on the high-vacuum line, dried over Na/K alloy, and vacuum-transferred to a dry storage flask containing activated molecular sieves. $B(C_6F_5)_3$ was purified by sublimation (40-60 °C, 10^{-5} torr). NMR samples were prepared in oven-dried J-Young NMR tubes.

All NMR experiments were performed on a Bruker Avance DRX 400 instrument. Referencing by residual solvent signals is relative to TMS. Mixing time values for the Overhauser experiments were in the range 400-800 ms. The [ONNO] ligand was synthesized according to the literature.[1]

[1] Synthesis of 2-cumyl-4-methyl-phenol: J. Rosevear, J. F. K. Wilshire, *Aust. J. Chem.*, 1985, **38**, 1163; synthesis of the ligand: V. Busico, R. Cipullo, N. Friederichs, S. Ronca, G. Talarico, M. Togrou and B. Wang, *Macromol.*, 2004, **22** (37), 8201.

Synthesis of **1**: 564 mg (1.0 mmol) of the [ONNO] ligand were weighted in a Schlenk flask and dissolved in 20 mL of dry toluene. To this solution, 1.3 mL of a buthyl-lithium solution (1.6M in hexane, 2.1 mmol) were added at 0°C. The mixture was allowed to reach room temperature and stirred for 1 hour. Solid zirconium tetrachloride (233 mg, 1.1 mmol) was added and the resulting white suspension was stirred for 2 hours at 75 °C. A white precipitate formed. 0.85 mL of a methylmagnesium bromide solution (3M in diethyl ether, 2.5 mmol) were added. The obtained dark mixture was stirred overnight. The solvent was evaporated in vacuum, the resulting solid was dissolved in fresh toluene and the solid was filtered off through a little bed of celite. The filtrate, a colourless solution, was evaporated in vacuum to afford the desired compound, as a pale yellow powder (yield: 70%).



^{1}H NMR (C_6D_6, 296 K, *J* in Hertz, δ in ppm, the indexes "a" and "b" refer to the "in-plane" and "out-of-plane" protons, respectively): δ 7.60 (d, $^{3}J_{3p'\text{-}3p''}$ = 8.3, 3p'), 7.54 (s, 7), 7.27 (m, 3p''), 7.14 (t, $^{3}J_{3p''\text{-}3p'''}$ = 7.2, 3p'''), 6.64 (s, 6), 3.93 (d, $^{2}J_{5a\text{-}5b}$ = 13.6, 5b), 2.51 (d, $^{2}J_{4a\text{-}4b}$ = 9.3, 4a), 2.44 (s, 2), 2.40 (d, $^{2}J_{5a\text{-}5b}$ = 13.6, 5a), 2.24 (s, 3m), 1.89 (s, 3m'), 1.20 (s, 1), 0.83 (d, $^{2}J_{4a\text{-}4b}$ = 9.3, 4b), 0.46 (s, 8). ^{13}C NMR (C_6D_6, 296 K, *J* in Hertz, δ in ppm): δ 157.8, 152.1, 137.6, 129.7 (6), 129.0 (7), 127.1 (3p'), 125.5 (3p'''), 63.9 (5), 52.2 (4), 44.4 (1), 40.8 (8), 32.8 (3m'), 28.1 (3m''), 21.3 (2).

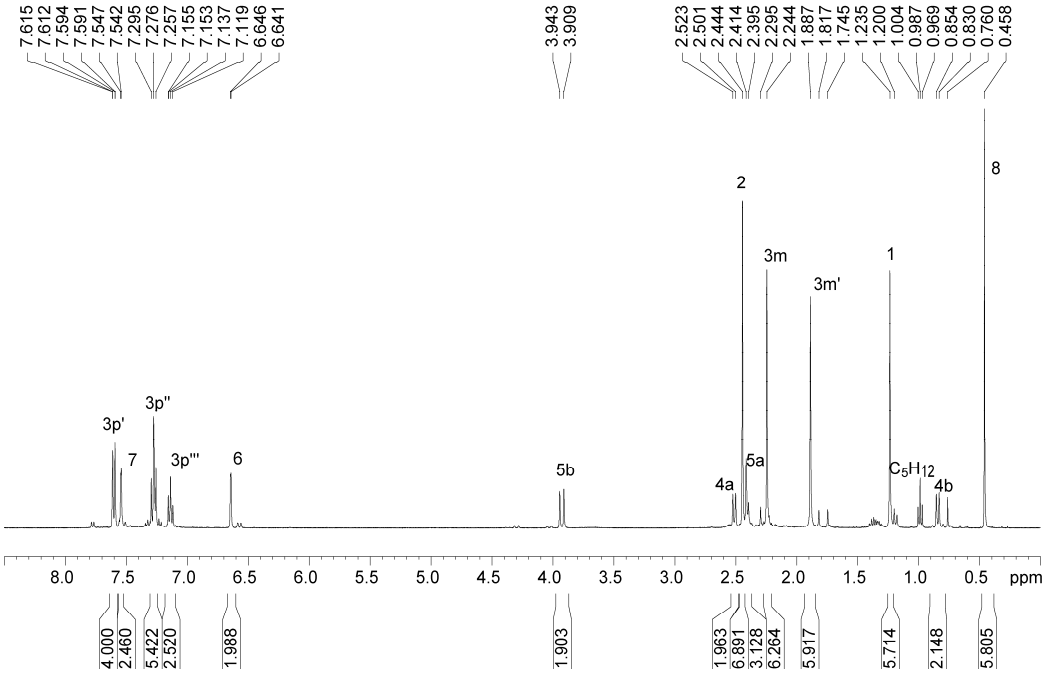


Figure S1. ^{1}H NMR spectrum (400.13 MHz, 296 K, in C_6D_6) of **1**.

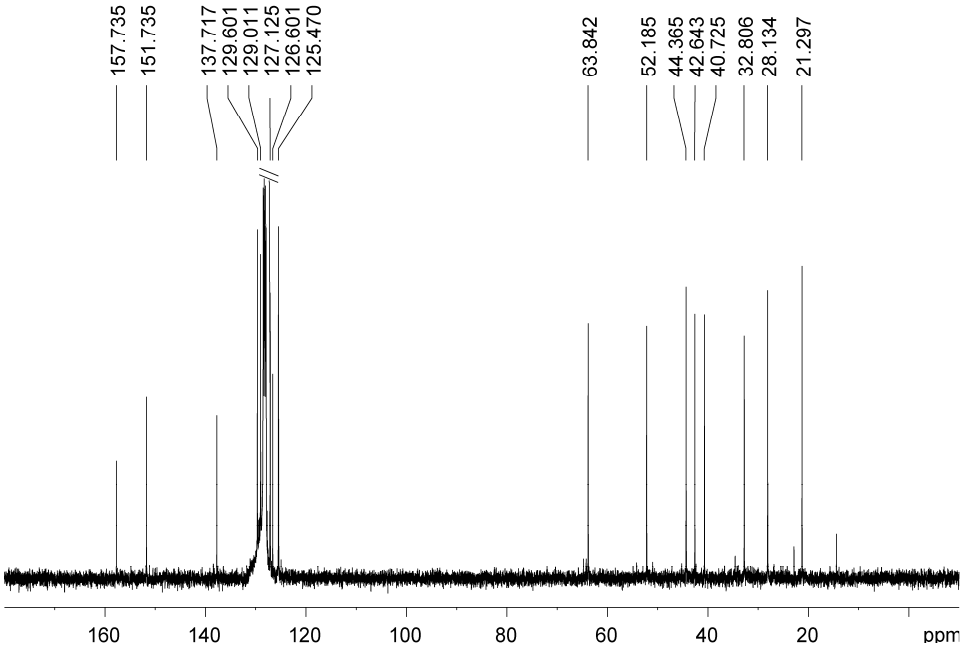
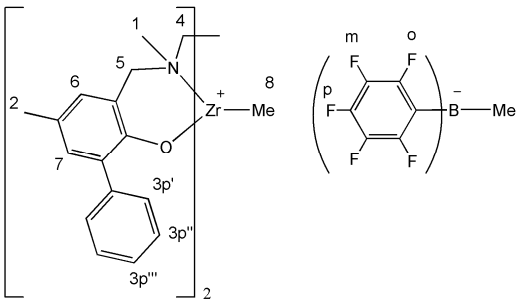


Figure S2. ^{13}C NMR spectrum (100.64 MHz, 296 K, in C_6D_6) of **1**.

Synthesis of **2**: 28 mg of **1** (41 μmol) and 25 mg of $B(C_6F_5)_3$ (49 μmol) were dissolved in dry benzene in an NMR tube having a PTFE valve. The tube was shaked and the solution turned to red. The formation of the desired product was immediate.



^{1}H NMR (C_6D_6, 296 K, *J* in Hertz, δ in ppm, underlined numbers refer to the "left" side of the cation): δ 7.53 (t, $^{3}J_{3p''\text{-}3p'''}$ = 7.5, 3p'''), 7.43 (s, 7), 7.38 (s, 7), 7.32 (t, $^{3}J_{3p''\text{-}3p'''}$ = 7.5, 3p'''), 7.24 (d, $^{3}J_{3p'\text{-}3p''}$ = 4.3, 3p'), 7.21 (d, $^{3}J_{3p'\text{-}3p''}$ = 4.3, 3p'), 7.11 (m, 3p''+3p''), 6.82 (s, 6), 6.74 (s, 6), 3.69 (d, $^{2}J_{5a\text{-}5b}$ = 14.5, 5b), 3.06 (d, $^{2}J_{5a\text{-}5b}$ = 14.5, 5a), 2.90 (d, $^{2}J_{5a\text{-}5b}$ = 14.5, 5a), 2.65 (d, $^{2}J_{5a\text{-}5b}$ = 14.5, 5b), 2.39 (s, 2), 2.37 (s, 2), 2.31 (m, 4a + 4a), 2.18 (m, 4b + 4b), 1.88 (s, 3m), 1.84 (s, 3m), 1.63 (m, 1 + 3m'), 1.46 (s, 8a + 1), -0.08 (s, 8). ^{19}F NMR (C_6D_6, 296 K, *J* in Hertz, δ in ppm): δ -132.09 (d, $^{3}J_{o\text{-}m}$ = 20.5, o), -164.13 (d, $^{3}J_{p\text{-}m}$ = 20.9, p), -166.74 (m, m).

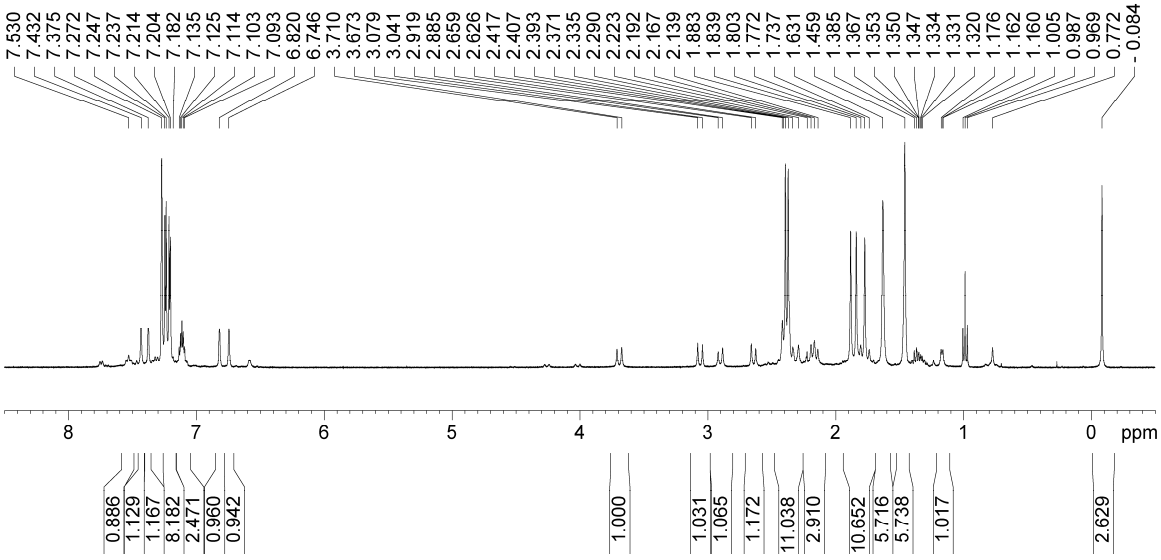


Figure S3. ^{1}H NMR spectrum (400.13 MHz, 296 K, in C_6D_6) of **2**.

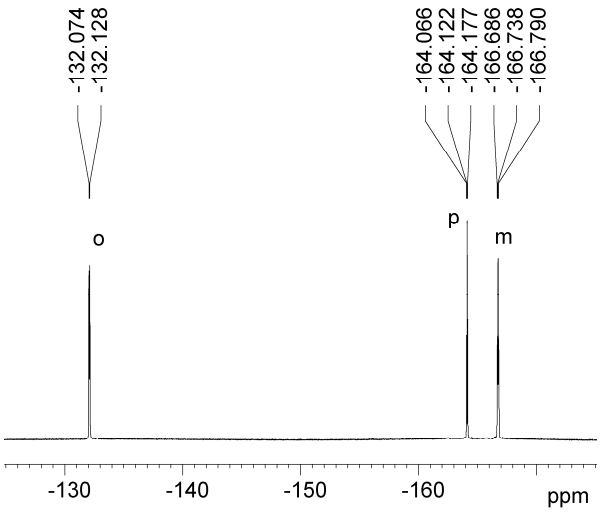


Figure S4. ^{19}F NMR spectrum (376.65 MHz, 296 K, in C_6D_6) of **2**.

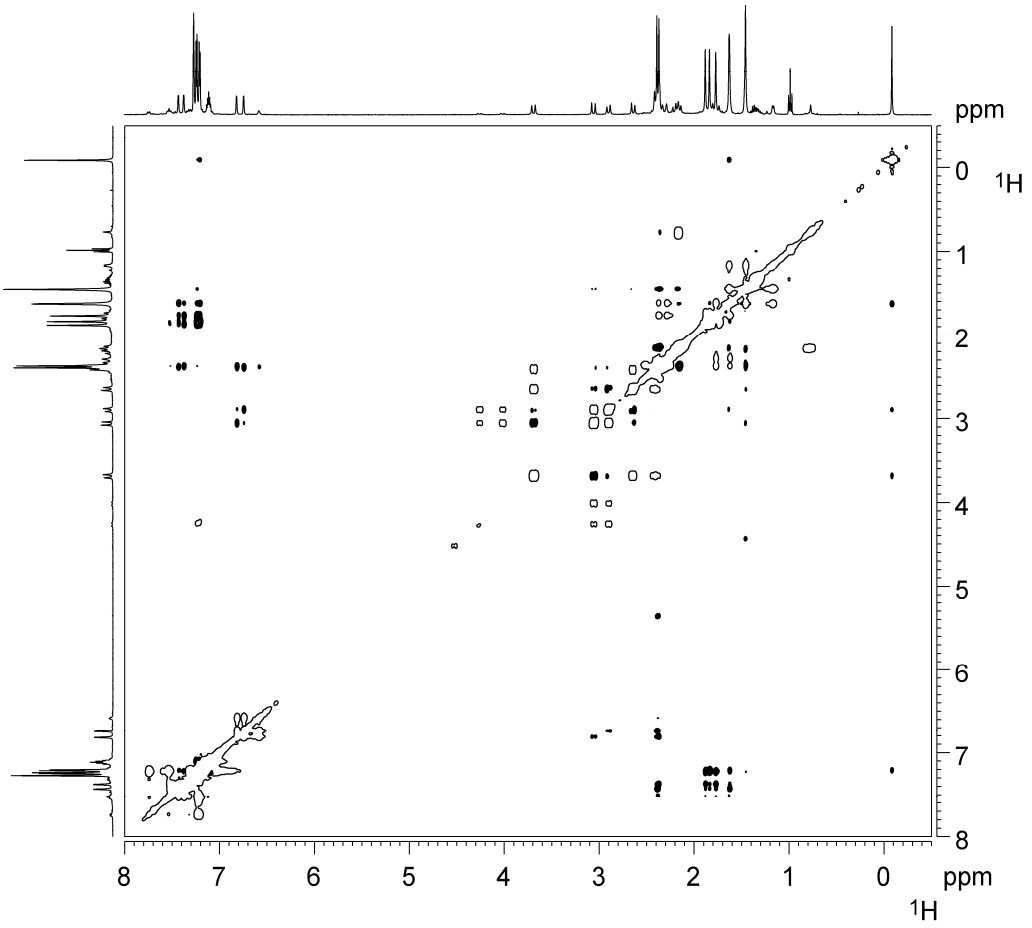


Figure S5. ^{1}H-NOESY spectrum of **2** (296 K, in C_6D_6).

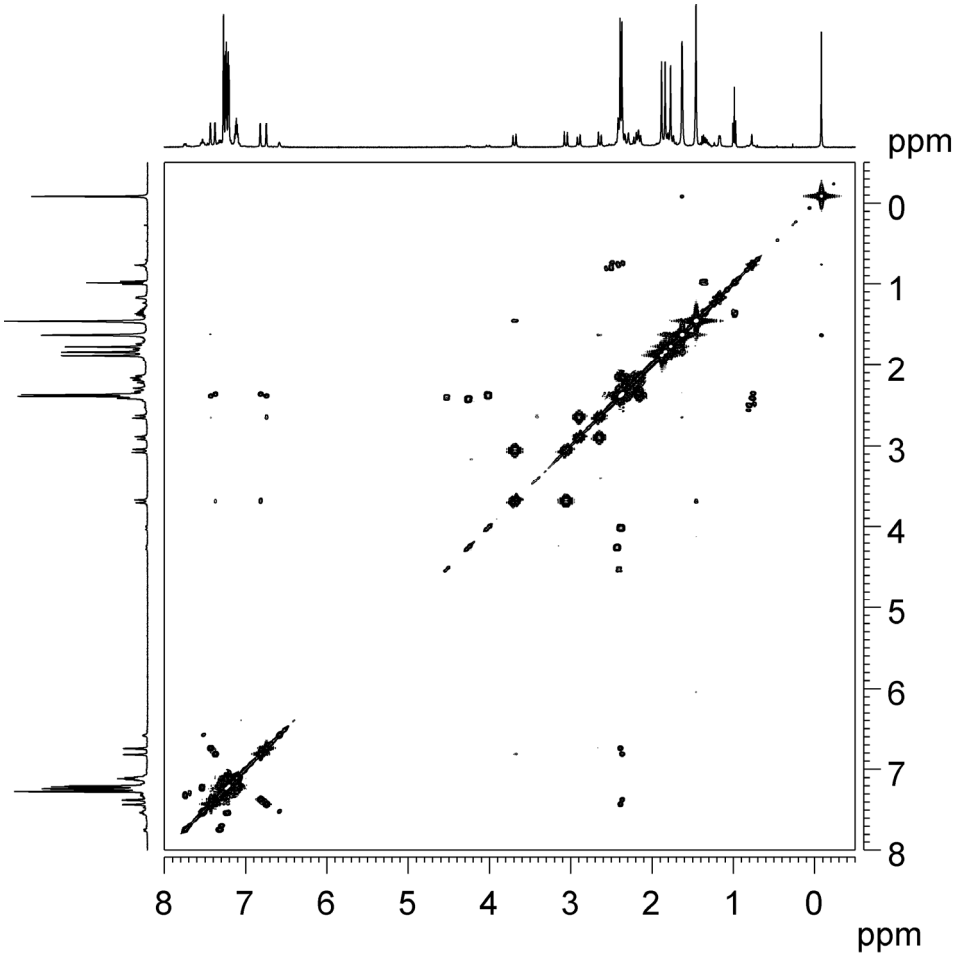


Figure S6. ^{1}H-COSY spectrum of **2** (296 K, in C_6D_6).

Computational Details. Density fuctional calculation were performed with the Turbomole program[2] (version 5.8) in combination with the OPTIMIZE routine of Baker and coworkers.[3] All geometries were fully optimized at the restricted RI[4]-BP86[5] level, using the SV(P)[6] basis set (small-core pseudopotential on Zr[7]). Thermal corrections (enthalpy and entropy) were calculated for the gas-phase , 300 K, 1 bar, using the standard formulas of statistical thermodynamics.[8]

Single-point solvent corrections were calculated using the conductor-like screening model (COSMO)[9] with $\varepsilon = 2$ to model an apolar solvent. Initial geometries and reasonable starting Hessians were obtained from PM3 computations with the Spartan package from Wavefunction Inc.[10]

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[2] (a) R. Ahlrichs, M. Bär, H.-P. Baron, R. Bauernschmitt, S. Böcker, M. Ehrig, K. Eichkorn, S. Elliott, F. Furche, F. Haase, M. Häser, C. Hättig, H. Horn, C. Huber, U. Huniar, M. Kattannek, A. Köhn, C. Kölmel, M. Kollwitz, K. May, C. Ochsenfeld, H. Ohm, A. Schäfer, U. Schneider, O. Treutler, K. Tsereteli, B. Unterreiner, M. von Arnim, F. Weigend, P. Weis, H. Weiss, *Turbomole* Version 5; Theoretical Chemistry Group, University of Karlsruhe, 2002. (b) O. Treutler, R. Ahlrichs, *J. Chem. Phys.* 1995, **102**, 346.

[3] (a) PQS, version 2.4; Parallel Quantum Solutions: Fayetteville, AK, 2001 (the Baker optimizer is available separately from PQS upon request). (b) Baker, J. J. Comput. Chem. 1986, 7 (4), 385–395.

[4] K. Eichhorn, O. Treutler, H. Öhm, M. Häser, R. Ahlrichs, *Chem. Phys. Lett.*, 1995, **242**, 652.

[5] A.D. Becke, *Phys. Rev. A* 1988, **38**, 3098; J.P. Perdew, *Phys. Rev. B* 1986, **33**, 8822; O. Treutler and R. Ahlrichs, *J. Chem. Phys.* 1995, **102**, 346.

[6] A. Schäfer, H. Horn, R. Ahlrichs, *J. Chem. Phys.* 1992, **97**, 2571.

[7] D. Andrae, U. Häussermann, M. Dolg, H. Stoll, H. Preuss, *Theor. Chim. Acta* 1990, **77**, 123.

[8] Frequencies below a threshold of 11 cm^{-1} were smoothly adjusted to a value remaining above 10 cm^{-1} to avoid artificial "blow-up" of the entropic correction for very low frequencies, for which the harmonic oscillator model is no longer appropriate.

[9] A. Schäfer, A. Klamt, D. Sattel, J. C. W. Lohrenz and F. Eckert, *Phys. Chem Chem. Phys.*, 2000, **2**, 2187.

[10] Y. Shao, L.F. Molnar, Y. Jung, J. Kussmann, C. Ochsenfeld, S.T. Brown, A.T.B. Gilbert, L.V. Slipchenko, S.V. Levchenko, D.P. O'Neill, R.A. DiStasio Jr., R.C. Lochan, T. Wang, G.J.O. Beran, N.A. Besley, J.M. Herbert, C.Y. Lin, T. Van Voorhis, S.H. Chien, A. Sodt, R.P. Steele, V.A. Rassolov, P.E. Maslen, P.P. Korambath, R.D. Adamson, B. Austin, J. Baker, E.F.C. Byrd, H. Dachsel, R.J. Doerksen, A. Dreuw, B.D. Dunietz, A.D. Dutoi, T.R. Furlani, S.R. Gwaltney, A.

Heyden, S. Hirata, C-P. Hsu, G. Kedziora, R.Z. Khalliulin, P. Klunzinger, A.M. Lee, M.S. Lee, W.Z. Liang, I. Lotan, N. Nair, B. Peters, E.I. Proynov, P.A. Pieniazek, Y.M. Rhee, J. Ritchie, E. Rosta, C.D. Sherrill, A.C. Simmonett, J.E. Subotnik, H.L. Woodcock III, W. Zhang, A.T. Bell, A.K. Chakraborty, D.M. Chipman, F.J. Keil, A.Warshel, W.J. Hehre, H.F. Schaefer, J. Kong, A.I. Krylov, P.M.W. Gill and M. Head-Gordon, *Phys. Chem. Chem. Phys.* 2006, **8**, 3172.

Coordinates of **2a**.

E = -4068.20996

$\Delta E_{gas\text{-}phase}$ = 0.0 Kcal/mol

ΔE_{COSMO} = 0.0 Kcal/mol

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Coordinates of **2b-C_6H_6**

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$\Delta E_{gas\text{-}phase}$ = 5.48 Kcal/mol

ΔE_{COSMO} = 4.48 Kcal/mol

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C 13.5200 0.3550 5.2810
C 13.0140 -0.9510 5.2230
C 12.4980 -1.4500 4.0080
C 10.6150 -0.4650 0.7670
C 10.1630 -0.6640 -0.5550
C 8.9820 -0.1130 -1.0800
C 8.1620 0.6760 -0.2580
C 8.5540 0.8950 1.0680
C 9.7490 0.3230 1.5450
F 12.5030 0.8170 -0.9480
F 14.7750 1.1090 -2.2810
F 16.9450 -0.5150 -1.7640
F 16.7410 -2.4510 0.1840
F 14.4820 -2.7570 1.5690
F 12.9730 1.4360 1.8650
F 13.9690 2.4060 4.1470
F 14.0090 0.8520 6.4310
F 13.0160 -1.7120 6.3290
F 12.0200 -2.7070 4.0710
F 10.8880 -1.4080 -1.4170
F 8.6360 -0.3130 -2.3680
F 7.0310 1.2230 -0.7380
F 7.8020 1.6850 1.8660

F 10.0270 0.6130 2.8430
C 11.5030 -2.8600 1.3130
H 11.2680 -3.1810 0.2730
H 10.5840 -3.0160 1.9200
H 12.2780 -3.5490 1.7060

Coordinates of **2c**

E = -4068.191281877

$\Delta E_{gas\text{-}phase}$ = 11.7 Kcal/mol

ΔE_{COSMO} = 9.79 Kcal/mol

Zr 17.3480 4.3990 6.2470
O 16.3210 5.5590 5.0110
O 18.6450 3.7000 7.6220
N 15.0290 4.2810 7.0980
N 17.1450 6.1070 8.0390
C 16.8440 2.3630 5.4310
H 16.1790 2.3810 4.5370
H 17.8710 2.0710 5.0800
C 14.7630 5.4920 7.9400
H 14.5530 6.3440 7.2640
H 13.8350 5.3360 8.5310
C 14.8170 3.0610 7.9290
H 14.8550 2.1600 7.2880
H 13.8260 3.1090 8.4370
H 15.6080 2.9740 8.7020
C 14.0270 4.2440 5.9670
H 13.0170 4.1170 6.4240
H 14.2470 3.3150 5.3970
C 13.9730 5.4230 5.0070
C 15.1660 5.9850 4.4750
C 15.1380 6.9290 3.4110
C 13.8650 7.3330 2.9550
H 13.7980 8.0730 2.1410
C 12.6600 6.8490 3.5030
C 12.7370 5.8830 4.5270
H 11.8060 5.4680 4.9520
C 16.4290 7.5580 2.7980
C 11.3230 7.3750 3.0300
C 15.9320 5.8080 8.8520
H 15.6790 6.6660 9.5110
H 16.1790 4.9530 9.5170
C 17.0330 7.4450 7.3930
H 17.9080 7.6010 6.7300
H 17.0150 8.2460 8.1660
H 16.1130 7.5300 6.7910
C 18.3690 6.1730 8.9120
H 18.2140 6.9920 9.6520
H 19.1990 6.4970 8.2410
C 18.8000 4.9250 9.6430
C 19.0550 3.7370 8.9120
C 19.7110 2.6310 9.5270
C 20.0130 2.7490 10.8980
H 20.5120 1.9100 11.4070
C 19.7060 3.8920 11.6680
C 19.1060 4.9820 11.0140
H 18.8820 5.9070 11.5740
C 20.0500 1.3600 8.7170
C 20.0400 3.9400 13.1430
H 16.5110 1.5450 6.1050
H 10.5280 6.6010 3.1040
H 11.3670 7.7230 1.9760
H 10.9920 8.2420 3.6480
H 21.1370 3.8630 13.3160
H 19.5670 3.0970 13.6960
H 19.6910 4.8850 13.6090
C 16.5690 8.9940 3.3670
H 17.4780 9.5000 2.9710
H 16.6050 9.0060 4.4760
H 15.6870 9.6010 3.0720
C 16.3190 7.6650 1.2510
H 17.2790 8.0320 0.8280
H 15.5300 8.3870 0.9530
H 16.0780 6.6910 0.7750
C 20.9600 0.3860 9.5140
H 20.4440 -0.0150 10.4140
H 21.9080 0.8690 9.8360
H 21.2270 -0.4770 8.8660
C 18.7280 0.6110 8.4130
H 18.1860 0.4170 9.3640
H 18.9170 -0.3750 7.9350
H 18.0680 1.2050 7.7490
C 17.6440 6.6730 3.1470
H 17.0170 5.0290 1.8560
C 17.7290 5.3580 2.6300
H 18.6290 3.3870 2.7900
C 18.6180 4.4210 3.1740
H 20.1850 4.0530 4.6650
C 19.4730 4.7840 4.2410
H 20.2600 6.4660 5.3870
C 19.5190 6.1420 4.6370
H 18.6650 8.1170 4.4280
C 18.6330 7.0760 4.0740

C 20.8390 1.7350 7.4410
H 19.8130 0.3630 6.0880
C 20.6170 1.1070 6.1970
H 21.2220 0.8920 4.1190
C 21.4140 1.4060 5.0760
H 23.0840 2.5760 4.2980
C 22.4550 2.3450 5.1740
H 23.5080 3.7120 6.5060
C 22.6900 2.9790 6.4080
H 22.0910 3.1790 8.4830
C 21.8930 2.6740 7.5230
B 13.1290 9.3580 11.2780
C 14.6920 9.8850 11.5990
C 15.8660 9.1120 11.6210
C 17.1560 9.6260 11.8370
C 17.3300 11.0010 12.0390
C 16.1970 11.8290 12.0220
C 14.9290 11.2640 11.7890
C 12.8370 9.9790 9.7520
C 13.6480 9.6000 8.6710
C 13.5530 10.1060 7.3690
C 12.5850 11.0840 7.0920
C 11.7440 11.5100 8.1300
C 11.8790 10.9560 9.4200
C 12.9800 7.6960 11.3300
C 13.3790 6.9860 12.4830
C 13.2180 5.6020 12.6680
C 12.6240 4.8390 11.6500
C 12.1860 5.4950 10.4930
C 12.3570 6.8860 10.3630
F 15.8390 7.7670 11.4000
F 18.2360 8.8100 11.8130
F 18.5530 11.5160 12.2380
F 16.3380 13.1530 12.1990
F 13.9130 12.1500 11.7230
F 14.6020 8.6400 8.8520
F 14.3670 9.6550 6.3840
F 12.4620 11.5930 5.8550
F 10.8110 12.4440 7.8840
F 11.0090 11.4300 10.3290
F 13.9850 7.6340 13.5010
F 13.6410 4.9990 13.7920
F 12.4860 3.5080 11.7740
F 11.6520 4.7700 9.4780
F 11.8930 7.3980 9.1960
C 12.0790 9.8900 12.4340
H 12.3580 9.4680 13.4250
H 11.0410 9.5540 12.2140
H 12.0510 10.9930 12.5390

Coordinates of **2d**

E = -4068.196754858

$\Delta E_{gas\text{-}phase}$ = 8.28 Kcal/mol

ΔE_{COSMO} = 6.10 Kcal/mol

Zr 12.8627 13.9963 -1.4133
O 14.4303 13.4882 -0.3338
O 10.9585 13.8618 -0.6955
N 14.4186 15.1631 -2.7996
N 12.5649 16.3541 -0.9345
C 12.7045 12.5375 -3.0782
H 13.6432 12.2175 -3.5835
H 12.3002 11.6363 -2.5485
C 14.6043 16.5660 -2.3081
H 15.2677 16.5283 -1.4184
H 15.1177 17.1764 -3.0797
C 13.9587 15.1997 -4.2248
H 13.9463 14.1780 -4.6442
H 14.6384 15.8419 -4.8237
H 12.9327 15.6168 -4.2916
C 15.7319 14.4146 -2.7460
H 16.4257 14.9073 -3.4636
H 15.5192 13.3962 -3.1396
C 16.4162 14.3100 -1.3958
C 15.7672 13.7576 -0.2574
C 16.4844 13.4963 0.9451
C 17.8441 13.8629 0.9713
H 18.4283 13.6806 1.8857
C 18.5096 14.4587 -0.1214
C 17.7762 14.6660 -1.3015
H 18.2724 15.1035 -2.1845
C 13.2581 17.1793 -1.9675
H 13.3861 18.2294 -1.6178
H 12.6092 17.2231 -2.8652
C 13.1415 16.6075 0.4118
H 12.6731 15.9282 1.1542
H 12.9538 17.6621 0.7237
H 14.2349 16.4276 0.4125
C 11.0920 16.6519 -0.9097
H 10.9431 17.7378 -1.1059
H 10.7480 16.4545 0.1284
C 10.2399 15.8264 -1.8503
C 10.0538 14.4419 -1.5455

C 8.9468 13.7285 -2.0998
C 8.2039 14.3986 -3.0945
H 7.3589 13.8744 -3.5646
C 8.4632 15.7180 -3.5282
C 9.4622 16.4381 -2.8508
H 9.6216 17.5058 -3.0827
H 11.9561 12.8137 -3.8560
C 15.7906 12.8426 2.1637
C 14.7692 13.8460 2.7578
H 15.2725 14.8158 2.9646
H 14.3567 13.4770 3.7218
H 13.9219 14.0296 2.0664
C 15.1433 11.4990 1.7525
C 14.1063 8.9246 1.1244
C 15.8695 10.5951 0.9445
C 13.8843 11.0849 2.2354
C 13.3709 9.8117 1.9267
C 15.3602 9.3251 0.6308
H 16.8569 10.8920 0.5528
H 13.2841 11.7541 2.8713
H 12.3870 9.5119 2.3248
H 15.9509 8.6413 -0.0014
H 13.7086 7.9237 0.8883
C 16.8017 12.5066 3.2942
H 17.2678 13.4237 3.7169
H 17.6073 11.8266 2.9443
H 16.2667 11.9884 4.1188
C 8.5087 12.3410 -1.5588
C 8.4255 12.4195 -0.0123
H 7.7124 13.2214 0.2786
H 9.4050 12.6448 0.4541
H 8.0424 11.4637 0.4066
C 7.0805 11.9659 -2.0451
H 6.3360 12.7337 -1.7389
H 6.7861 10.9983 -1.5848
H 7.0146 11.8326 -3.1448
C 9.4577 11.2238 -2.0542
C 11.0296 9.0689 -3.0498
C 10.1481 10.3616 -1.1773
C 9.5888 10.9909 -3.4429
C 10.3564 9.9260 -3.9377
C 10.9281 9.2979 -1.6688
H 10.0855 10.5106 -0.0892
H 9.0824 11.6604 -4.1588
H 10.4353 9.7698 -5.0263
H 11.4608 8.6442 -0.9586
H 11.6359 8.2321 -3.4338
C 19.9662 14.8528 -0.0160
H 20.5939 14.0037 0.3360
H 20.1104 15.6839 0.7117
H 20.3692 15.1908 -0.9935
C 7.6782 16.3480 -4.6552
H 8.3079 16.4338 -5.5685
H 7.3448 17.3767 -4.3958
H 6.7801 15.7485 -4.9156
B 15.1607 19.0040 -7.2184
C 15.3638 20.0237 -5.9050
C 14.7599 19.9057 -4.6429
C 14.9852 20.7758 -3.5635
C 15.8861 21.8390 -3.7094
C 16.5405 21.9989 -4.9403
C 16.2787 21.0951 -5.9875
C 16.5918 18.1423 -7.2879
C 17.0363 17.3987 -6.1832
C 18.2146 16.6434 -6.1349
C 19.0528 16.6217 -7.2593
C 18.6761 17.3585 -8.3915
C 17.4700 18.0903 -8.3873
C 13.8380 17.9932 -7.0762
C 12.5602 18.5234 -6.7954
C 11.3751 17.7685 -6.7732
C 11.4260 16.3978 -7.0717
C 12.6626 15.8188 -7.3819
C 13.8221 16.6204 -7.3852
F 13.9062 18.8759 -4.3651
F 14.3679 20.5787 -2.3736
F 16.1221 22.6815 -2.6915
F 17.4257 22.9953 -5.0985
F 16.9968 21.3010 -7.1108
F 16.2654 17.3337 -5.0524
F 18.5360 15.9203 -5.0360
F 20.1866 15.9051 -7.2514
F 19.4640 17.3497 -9.4777
F 17.1982 18.7365 -9.5359
F 12.4150 19.8354 -6.5054
F 10.1921 18.3393 -6.4658
F 10.3066 15.6483 -7.0511
F 12.7360 14.4997 -7.6473
F 14.9599 15.9530 -7.6948
C 14.8265 19.8828 -8.5756
H 13.9014 20.4817 -8.4183
H 14.6407 19.2192 -9.4498
H 15.6342 20.5862 -8.8613

Coordinates of **2b**

E = -4068.175314776

$\Delta E_{gas\text{-}phase}$ = 21.7 Kcal/mol

ΔE_{COSMO} = 17.6 Kcal/mol

Zr 10.9870 5.5720 0.8860
O 12.8080 5.6240 1.6870
O 9.6830 5.5620 -0.6370
N 10.4520 4.1490 2.6940
N 11.2870 3.2770 0.0670
C 10.0300 7.2140 2.0740
H 10.4700 7.4940 3.0570
H 10.3780 8.0090 1.3450
C 10.7110 2.6970 2.3800
H 11.7630 2.4760 2.6450
H 10.0860 2.0550 3.0340
C 9.0110 4.3060 3.0620
H 8.8110 5.3470 3.3740
H 8.7570 3.6090 3.8940
H 8.3670 4.0620 2.1910
C 11.3020 4.5760 3.8760
H 10.9710 3.9680 4.7480
H 11.0230 5.6300 4.0850
C 12.8100 4.4470 3.7490
C 13.5440 5.0680 2.6940
C 14.9690 5.0920 2.7050
C 15.6020 4.4620 3.7980
H 16.7010 4.4840 3.8440
C 14.9130 3.7910 4.8270
C 13.5090 3.8000 4.7850
H 12.9380 3.3060 5.5900
C 15.8150 5.8780 1.6610
C 15.6670 3.0630 5.9160
C 10.4540 2.3810 0.9150
H 10.6920 1.3110 0.7240
H 9.3900 2.5420 0.6370
C 12.7270 2.9000 0.1480
H 13.3200 3.5930 -0.4830
H 12.8780 1.8580 -0.2090
H 13.1090 2.9640 1.1830
C 10.9120 3.1910 -1.3900
H 11.1720 2.1680 -1.7450
H 11.6010 3.8940 -1.9160
C 9.4880 3.5010 -1.7770
C 8.9330 4.7700 -1.4630
C 7.6530 5.1500 -1.9610
C 6.9850 4.1980 -2.7640
H 6.0000 4.4680 -3.1740
C 7.4920 2.9190 -3.0620
C 8.7620 2.5860 -2.5550
H 9.1940 1.5970 -2.7810
C 7.0350 6.5590 -1.7390
C 6.7160 1.9320 -3.9050
H 8.9250 7.3190 2.1310
H 15.0330 2.8930 6.8120
H 16.5720 3.6250 6.2330
H 16.0110 2.0650 5.5570
H 5.6540 2.2360 -4.0160
H 6.7480 0.9160 -3.4560
H 7.1510 1.8460 -4.9280
C 15.5800 7.3850 1.9430
H 16.1320 8.0210 1.2160
H 15.8990 7.6660 2.9700
H 14.4990 7.6230 1.8490
C 15.4040 5.5950 0.1870
H 16.1040 6.1270 -0.4940
H 14.3760 5.9490 -0.0250
H 15.4640 4.5140 -0.0550
C 7.0710 6.9930 -0.2460
H 8.1120 7.1400 0.0960
H 6.5910 6.2410 0.4160
H 6.5190 7.9510 -0.1240
C 7.8920 7.5640 -2.5510
H 8.9450 7.5270 -2.2010
H 7.5260 8.6060 -2.4170
H 7.8890 7.3250 -3.6360
C 17.3110 5.4950 1.7620
H 16.9560 3.3990 1.2530
C 17.7150 4.1660 1.4820
H 19.3430 2.7430 1.3060
C 19.0640 3.7880 1.5220
H 21.1180 4.4390 1.8720
C 20.0560 4.7330 1.8400
H 20.4390 6.8070 2.3770
C 19.6760 6.0530 2.1220
H 18.0590 7.4720 2.3150
C 18.3190 6.4280 2.0840
C 5.5470 6.5960 -2.1660
H 5.7690 8.0240 -3.8030
C 5.0720 7.4080 -3.2160
H 3.3660 8.1010 -4.3700
C 3.7030 7.4540 -3.5440

H 1.7030 6.7190 -3.0850
C 2.7750 6.6840 -2.8280
H 2.5160 5.2470 -1.2090
C 3.2300 5.8640 -1.7800
H 4.9260 5.1610 -0.6410
C 4.5940 5.8250 -1.4560
B 11.2340 -2.8850 1.6980
C 12.7310 -2.2250 2.0850
C 13.2820 -1.0320 1.5850
C 14.5040 -0.4780 2.0060
C 15.2480 -1.1240 3.0020
C 14.7510 -2.3180 3.5450
C 13.5170 -2.8250 3.0930
C 10.3260 -2.5370 3.0580
C 10.1360 -1.2010 3.4460
C 9.4530 -0.7810 4.5930
C 8.9100 -1.7490 5.4520
C 9.0720 -3.1030 5.1250
C 9.7610 -3.4680 3.9490
C 10.5760 -2.2230 0.3170
C 11.3220 -2.2070 -0.8810
C 10.8340 -1.7430 -2.1130
C 9.5110 -1.2830 -2.1920
C 8.7120 -1.2950 -1.0420
C 9.2510 -1.7760 0.1690
F 12.6260 -0.2920 0.6440
F 14.9500 0.6900 1.4860
F 16.4080 -0.6030 3.4370
F 15.4380 -2.9460 4.5120
F 13.0940 -3.9380 3.7250
F 10.6190 -0.2000 2.6530
F 9.3010 0.5390 4.8750
F 8.2470 -1.3840 6.5610
F 8.5610 -4.0410 5.9390
F 9.8380 -4.7930 3.7250
F 12.6070 -2.6270 -0.8880
F 11.6100 -1.7320 -3.2110
F 9.0250 -0.8090 -3.3590
F 7.4420 -0.8490 -1.1080
F 8.3880 -1.7750 1.2120
C 11.3600 -4.4920 1.3540
H 12.0120 -4.6400 0.4650
H 10.3640 -4.9230 1.1030
H 11.7820 -5.0990 2.1810

Coordinates of **2e**

E = -4068.206678226

$\Delta E_{gas\text{-}phase}$ = 2.06 Kcal/mol

ΔE_{COSMO} = -0.87 Kcal/mol

Zr 0.1943 -0.4297 -0.6322
N -2.0919 0.0517 -0.1971
N 0.0684 1.9825 -0.6759
C -2.3611 1.3871 -0.8147
H -3.3839 1.7397 -0.5452
H -2.3314 1.2606 -1.9202
C -1.3331 2.4212 -0.3591
H -1.4132 2.5968 0.7323
H -1.5492 3.4019 -0.8404
O 2.0594 -0.0835 -0.1014
O -0.4334 -2.2525 -0.1522
C -2.8344 -1.0308 -0.9523
H -2.3973 -1.0591 -1.9801
H -3.8950 -0.7066 -1.0643
C -2.4886 0.0390 1.2382
H -1.9437 0.8213 1.7979
H -2.2506 -0.9479 1.6804
H -3.5839 0.2217 1.3338
C 1.0061 2.5015 0.4008
H 0.6562 2.0561 1.3564
H 0.8429 3.6002 0.4875
C 0.4857 2.5058 -2.0041
H 1.5067 2.1493 -2.2462
H 0.4972 3.6215 -1.9899
H -0.2154 2.1634 -2.7922
C 2.4835 2.2358 0.2179
C 5.2315 1.7497 0.1816
C 3.3936 3.3041 0.2960
C 2.9760 0.9065 0.0958
C 4.3717 0.6316 0.1223
C 4.7818 3.0826 0.2642
H 3.0065 4.3323 0.4000
H 6.3174 1.5683 0.1685
C -2.7971 -2.4029 -0.3150
C -2.7397 -4.9604 0.7874
C -3.9966 -3.0998 -0.0885
C -1.5530 -3.0013 0.0319
C -1.5015 -4.3188 0.5743
C -3.9897 -4.3893 0.4699
H -4.9566 -2.6217 -0.3503
C 0.4097 -0.7360 -2.8394
H 1.2910 -0.2002 -3.2610
H -0.4943 -0.4081 -3.4109
H 0.5451 -1.8234 -3.0494

C 4.9541 -0.8033 0.0047
C 4.8185 -1.2365 -1.4774
H 5.1859 -2.2757 -1.6279
H 5.3813 -0.5619 -2.1580
H 3.7502 -1.2102 -1.7804
C 4.1921 -1.8359 0.8880
H 4.7456 -2.7999 0.8828
H 3.1670 -2.0195 0.5122
H 4.1094 -1.4978 1.9424
C 5.7636 4.2284 0.3686
H 6.0842 4.3863 1.4246
H 5.3189 5.1836 0.0163
H 6.6829 4.0345 -0.2256
H -2.7292 -5.9669 1.2337
C -5.2715 -5.1540 0.7150
H -5.3842 -5.9957 -0.0068
H -6.1644 -4.5018 0.6097
H -5.2910 -5.5989 1.7343
C -0.1810 -5.0005 1.0250
C 0.2309 -4.3420 2.3660
H 1.1957 -4.7527 2.7355
H -0.5382 -4.4925 3.1532
H 0.3633 -3.2483 2.2353
C 0.9826 -4.8086 0.0069
H 1.8366 -5.4546 0.3050
H 1.3324 -3.7587 -0.0159
H 0.6855 -5.0966 -1.0246
C -0.3829 -6.5286 1.1671
C -0.6841 -9.3584 1.3270
C -0.7051 -7.3009 0.0249
C -0.2168 -7.2123 2.3891
C -0.3648 -8.6104 2.4695
C -0.8557 -8.6933 0.0996
H -0.8555 -6.8002 -0.9464
H 0.0327 -6.6592 3.3066
H -0.2271 -9.1146 3.4408
H -1.1086 -9.2646 -0.8094
H -0.7999 -10.4531 1.3900
C 6.4247 -0.8323 0.4846
C 9.0927 -0.9574 1.4794
C 6.7234 -0.5190 1.8330
C 7.4981 -1.2072 -0.3493
C 8.8169 -1.2704 0.1407
C 8.0350 -0.5781 2.3255
H 5.9133 -0.2078 2.5132
H 7.3207 -1.4596 -1.4056
H 9.6332 -1.5697 -0.5378
H 8.2326 -0.3260 3.3809
H 10.1247 -1.0071 1.8640
B -1.5754 3.0545 5.5488
C -2.9138 2.7798 4.5708
C -3.1119 3.2533 3.2603
C -4.2252 2.9355 2.4637
C -5.2119 2.0728 2.9574
C -5.0682 1.5592 4.2543
C -3.9304 1.9040 5.0092
C -0.7613 1.5936 5.4557
C -0.3534 1.1038 4.2081
C 0.2469 -0.1370 3.9771
C 0.4962 -0.9858 5.0640
C 0.1261 -0.5509 6.3459
C -0.4853 0.7108 6.5172
C -0.6359 4.3213 5.0292
C -1.2139 5.5824 4.7803
C -0.4858 6.7365 4.4474
C 0.9141 6.6633 4.3668
C 1.5467 5.4397 4.6256
C 0.7684 4.3146 4.9606
F -2.1877 4.0295 2.6349
F -4.3116 3.3871 1.1868
F -6.2597 1.7243 2.1901
F -5.9882 0.7115 4.7415
F -3.8432 1.2971 6.2104
F -0.5274 1.8803 3.0902
F 0.5998 -0.5146 2.7127
F 1.0720 -2.1847 4.8825
F 0.3631 -1.3438 7.4015
F -0.7902 1.0248 7.7868
F -2.5576 5.7356 4.8411
F -1.1078 7.9041 4.2079
F 1.6361 7.7493 4.0453
F 2.8885 5.3538 4.5590
F 1.4770 3.1888 5.2245
C -2.0320 3.4833 7.0733
H -2.6227 4.4261 7.0336
H -1.1412 3.6861 7.7095
H -2.6477 2.7265 7.6000

Coordinates of **2f**

E = -4068.203112508

$\Delta E_{gas\text{-}phase}$= 4.30 Kcal/mol

ΔE_{COSMO} = 2.40 Kcal/mol

Zr 0.3905 -0.4827 0.4661

N -1.9343 0.0492 -0.0086

N 0.4496 1.8395 -0.2296

C -1.9557 1.3778 -0.6961

H -2.9804 1.8174 -0.6557

H -1.7194 1.2169 -1.7692

C -0.9473 2.3430 -0.0668

H -1.1465 2.4595 1.0204

H -1.0497 3.3552 -0.5265

O 2.3528 -0.1679 0.5928

O -0.3299 -2.3241 0.4647

C -2.4479 -1.0299 -0.9426

H -1.7756 -1.0384 -1.8291

H -3.4508 -0.7099 -1.3095

C -2.7985 0.0905 1.2006

H -2.4739 0.8988 1.8837

H -2.7405 -0.8756 1.7369

H -3.8595 0.2683 0.9012

C 1.3710 2.4872 0.7826

H 1.0056 2.1808 1.7880

H 1.2377 3.5921 0.7068

C 0.9435 2.1539 -1.5970

H 1.9329 1.6860 -1.7608

H 1.0461 3.2583 -1.7163

H 0.2397 1.7768 -2.3606

C 2.8426 2.1605 0.6282

C 5.5710 1.6126 0.5082

C 3.7742 3.2107 0.5686

C 3.2952 0.8058 0.6045

C 4.6892 0.5120 0.5720

C 5.1557 2.9578 0.5005

H 3.4114 4.2534 0.5811

H 6.6521 1.4003 0.4661

C -2.5657 -2.4197 -0.3513

C -2.7798 -5.0568 0.5350

C -3.7753 -3.1201 -0.4918

C -1.4505 -3.0629 0.2626

C -1.5312 -4.4178 0.6881

C -3.9063 -4.4481 -0.0494

H -4.6340 -2.6198 -0.9733

C 0.0443 -0.1260 2.6722

H 1.0158 -0.2965 3.1950

H -0.6864 -0.8554 3.0909

H -0.2999 0.8940 2.9721

C 5.3081 -0.9099 0.5013

C 5.5559 -1.2105 -0.9999

H 5.9409 -2.2428 -1.1489

H 6.2728 -0.4919 -1.4533

H 4.5998 -1.1431 1.5583

C 4.4199 -2.0494 1.0752

H 5.0298 -2.9768 1.1359

H 3.5491 -2.2568 0.4240

H 4.0513 -1.8185 2.0974

C 6.1677 4.0803 0.4353

H 6.8237 4.0878 1.3355

H 5.6748 5.0735 0.3700

H 6.8360 3.9746 -0.4486

H -2.8723 -6.0997 0.8778

C -5.1909 -5.2188 -0.2550

H -5.1865 -5.7256 -1.2479

H -6.0813 -4.5536 -0.2290

H -5.3247 -6.0073 0.5162

C -0.3663 -5.1774 1.3779

C -0.4044 -4.7957 2.8799

H 0.4372 -5.2642 3.4366

H -1.3597 -5.1000 3.3601

H -0.3055 -3.6937 2.9888

C 1.0456 -4.8226 0.8227

H 1.7809 -5.5553 1.2201

H 1.3677 -3.8095 1.1315

H 1.0823 -4.8724 -0.2853

C -0.5250 -6.6997 1.1527

C -0.6793 -9.4946 0.6371

C -0.5583 -7.1994 -0.1719

C -0.5755 -7.6322 2.2086

C -0.6514 -9.0156 1.9550

C -0.6348 -8.5760 -0.4280

H -0.5454 -6.4940 -1.0192

H -0.5549 -7.2906 3.2546

H -0.6885 -9.7213 2.8020

H -0.6613 -8.9343 -1.4706

H -0.7376 -10.5776 0.4377

C 6.6152 -0.9339 1.3310

C 8.9468 -1.0579 2.9612

C 6.5789 -0.5568 2.6944

C 7.8472 -1.3750 0.8066

C 9.0011 -1.4359 1.6115

C 7.7249 -0.6164 3.5008

H 5.6317 -0.1978 3.1316

H 7.9236 -1.6818 -0.2474

H 9.9508 -1.7841 1.1718

H 7.6642 -0.3144 4.5599

H 9.8504 -1.1057 3.5913

B 0.8568 -1.6738 -4.0337

C -0.6043 -2.4312 -4.3201
C -1.5040 -2.1407 -5.3663
C -2.6955 -2.8541 -5.5991
C -3.0264 -3.9406 -4.7768
C -2.1531 -4.2946 -3.7378
C -0.9778 -3.5481 -3.5455
C 1.9983 -2.7915 -4.4770
C 2.0289 -3.2584 -5.8061
C 2.9322 -4.2188 -6.2865
C 3.8695 -4.7773 -5.4019
C 3.8786 -4.3576 -4.0642
C 2.9475 -3.3931 -3.6363
C 1.0253 -0.2299 -4.8433
C 0.0518 0.7760 -4.7193
C 0.1365 2.0590 -5.2773
C 1.2767 2.3998 -6.0215
C 2.2922 1.4456 -6.1748
C 2.1578 0.1759 -5.5760
F -1.2657 -1.1421 -6.2396
F -3.5091 -2.5127 -6.6105
F -4.1572 -4.6319 -4.9813
F -2.4439 -5.3470 -2.9518
F -0.1696 -3.9863 -2.5437
F 1.1709 -2.7428 -6.7133
F 2.9162 -4.6033 -7.5719
F 4.7475 -5.6923 -5.8357
F 4.7715 -4.8744 -3.2026
F 3.0351 -3.0613 -2.3206
F -1.0813 0.5414 -3.9819
F -0.8372 2.9667 -5.0780
F 1.3973 3.6190 -6.5641
F 3.3942 1.7584 -6.8709
F 3.2177 -0.6412 -5.7399
C 0.9866 -1.2376 -2.4195
H 0.1632 -0.5062 -2.2111
H 1.9603 -0.7384 -2.2276
H 0.8898 -2.1155 -1.7498

Coordinates of C_6H_6

E = -232.07658

H 0.0000 0.0000 -0.0470
C 0.0000 0.0000 1.0560
C 0.0000 0.0000 3.8680
C 0.0000 -1.2180 1.7590
C 0.0000 1.2180 1.7590
C 0.0000 1.2180 3.1650
C 0.0000 -1.2180 3.1650
H 0.0000 -2.1730 1.2070
H 0.0000 2.1730 1.2070
H 0.0000 2.1730 3.7170
H 0.0000 -2.1730 3.7170
H 0.0000 0.0000 4.9710

Coordinates of naked cation (**2c**$^+$)

E = -1821.37808

Zr 17.7940 4.1640 5.6030
O 16.6380 5.1820 4.3540
O 18.9750 3.6620 7.1450
N 15.4890 3.8840 6.5020
N 17.3740 6.0390 7.2730
C 17.4530 2.0760 4.8590
H 16.9160 2.0500 3.8830
H 18.5200 1.7820 4.6710
C 15.0750 5.1320 7.2140
H 14.7700 5.8710 6.4440
H 14.1710 4.9260 7.8350
C 15.4300 2.7390 7.4520
H 15.6440 1.7960 6.9160
H 14.4180 2.6670 7.9140
H 16.1840 2.8600 8.2560
C 14.5140 3.6090 5.3800
H 13.5170 3.4150 5.8430
H 14.8450 2.6500 4.9250
C 14.3410 4.6510 4.2820
C 15.4580 5.3340 3.7290
C 15.3490 6.1070 2.5390
C 14.0610 6.2280 1.9750
H 13.9320 6.8220 1.0570
C 12.9150 5.6250 2.5350
C 13.0800 4.8300 3.6890
H 12.2030 4.3150 4.1190
C 16.5720 6.8400 1.9000
C 11.5460 5.8280 1.9240
C 16.1870 5.6910 8.0900
H 15.8120 6.5850 8.6450
H 16.5070 4.9520 8.8560
C 17.1420 7.3100 6.5410
H 18.0220 7.5390 5.9080
H 16.9920 8.1520 7.2590
H 16.2590 7.2320 5.8800
C 18.5970 6.2400 8.1280
H 18.4410 7.1530 8.7500
H 19.4230 6.4800 7.4170

C 19.0190 5.0990 9.0210
C 19.3010 3.8340 8.4490
C 19.8980 2.7960 9.2230
C 20.1210 3.0700 10.5860
H 20.5710 2.2900 11.2190
C 19.8030 4.3030 11.1990
C 19.2610 5.3160 10.3900
H 19.0370 6.3040 10.8280
C 20.2780 1.4420 8.5840
C 20.0680 4.5200 12.6720
H 17.0330 1.2780 5.5100
H 10.9530 4.8870 1.9280
H 11.6140 6.1850 0.8750
H 10.9580 6.5840 2.4930
H 21.1550 4.4450 12.9040
H 19.5530 3.7560 13.2960
H 19.7230 5.5210 13.0080
C 16.5140 8.3250 2.3370
H 17.3550 8.9110 1.9040
H 16.5340 8.4380 3.4430
H 15.5670 8.7810 1.9800
C 16.5080 6.7950 0.3470
H 17.4360 7.2300 -0.0820
H 15.6560 7.3920 -0.0400
H 16.3970 5.7610 -0.0430
C 21.0780 0.5400 9.5620
H 20.4690 0.2510 10.4470
H 22.0100 1.0300 9.9180
H 21.3750 -0.3940 9.0390
C 18.9750 0.6840 8.2270
H 18.3370 0.5920 9.1320
H 19.1910 -0.3470 7.8730
H 18.3980 1.2100 7.4400
C 17.8720 6.1470 2.3600
H 17.4560 4.3000 1.2700
C 18.1080 4.7960 2.0070
H 19.2190 2.9720 2.4070
C 19.0820 4.0330 2.6680
H 20.6620 4.0250 4.1920
C 19.8750 4.6150 3.6890
H 20.4670 6.5070 4.6070
C 19.7700 6.0110 3.9100
H 18.7190 7.8420 3.4460
C 18.7990 6.7660 3.2300
C 21.1940 1.6830 7.3610
H 20.2700 0.2030 6.0460
C 21.0740 0.9470 6.1630
H 21.8740 0.5280 4.1850
C 21.9820 1.1300 5.1030
H 23.7510 2.1900 4.3930
C 23.0310 2.0570 5.2170
H 23.9940 3.5150 6.5210
C 23.1660 2.7950 6.4070
H 22.3850 3.1880 8.3900
C 22.2590 2.6070 7.4610

Coordinates of naked anion

($MeB(C_6F_5)_3^-$)

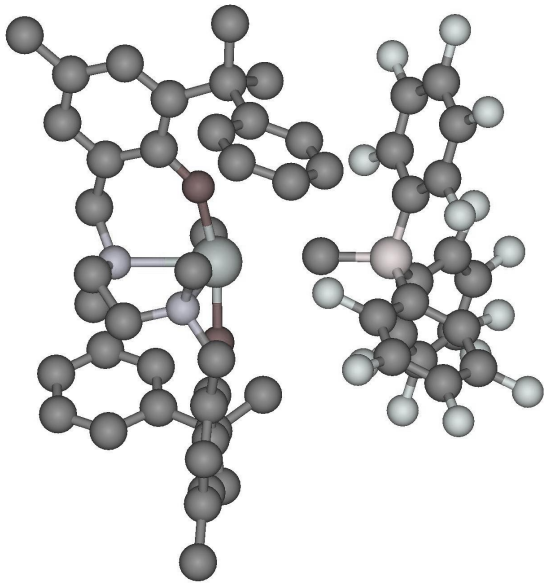
E = -2246.728780845

B 0.1560 6.0200 -0.6370
C -0.8030 4.9190 -1.4600
C -0.9180 3.5390 -1.2020
C -1.7460 2.6660 -1.9340
C -2.5490 3.1730 -2.9640
C -2.5060 4.5470 -3.2410
C -1.6560 5.3750 -2.4870
C -0.9500 6.9040 0.2490
C -1.8120 6.2500 1.1510
C -2.8360 6.8830 1.8730
C -3.0350 8.2620 1.7070
C -2.1970 8.9690 0.8340
C -1.1810 8.2860 0.1350
C 1.3200 5.3230 0.3300
C 2.2090 4.3600 -0.1890
C 3.3090 3.8350 0.5100
C 3.5780 4.2900 1.8100
C 2.7400 5.2610 2.3720
C 1.6510 5.7550 1.6280
F -0.2310 2.9520 -0.1990
F -1.7910 1.3500 -1.6420
F -3.3520 2.3580 -3.6740
F -3.2910 5.0580 -4.2120
F -1.7200 6.6910 -2.8000
F -1.6670 4.9250 1.3800
F -3.6250 6.1900 2.7190
F -4.0130 8.8980 2.3800
F -2.3710 10.2970 0.6750
F -0.4230 9.0670 -0.6660
F 2.0420 3.8820 -1.4450
F 4.1140 2.9090 -0.0510
F 4.6310 3.8070 2.4990
F 2.9920 5.7220 3.6150
F 0.9340 6.7190 2.2530

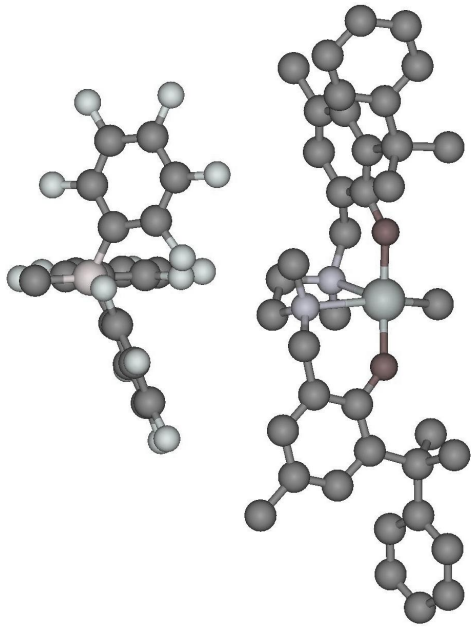
C 1.0430 6.9100 -1.7140 H 1.7080 7.6320 -1.1870

H 1.6990 6.2320 -2.3070 H 0.4290 7.4920 -2.4320

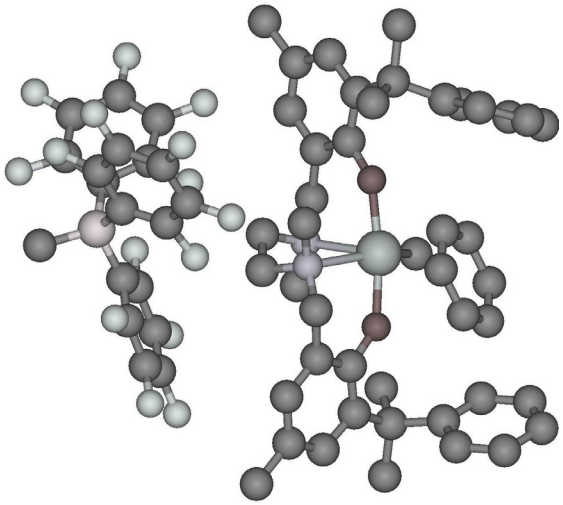
Structures of ion pairs



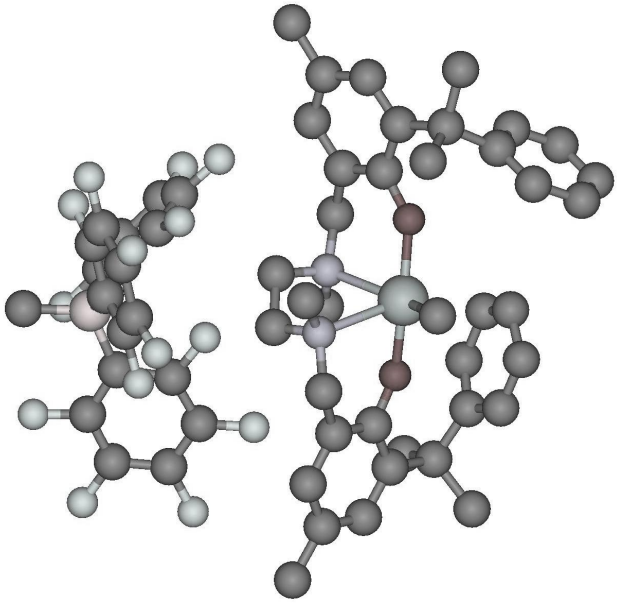
2a



2b



2b-C_6H_6



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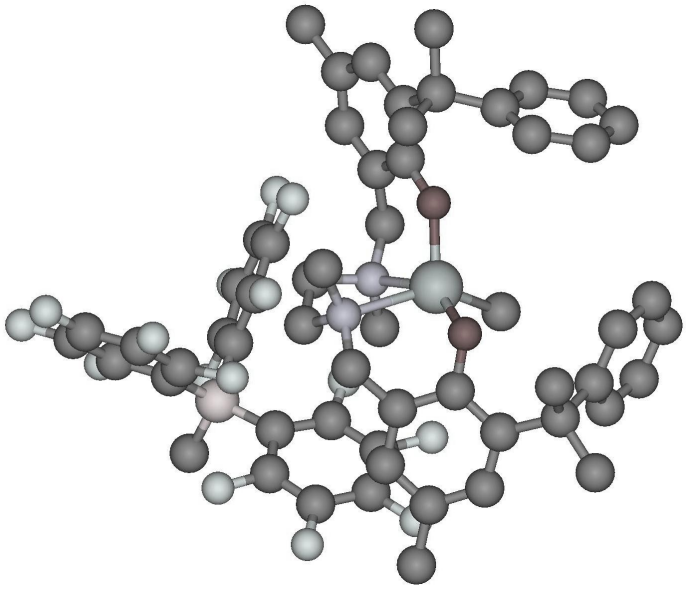

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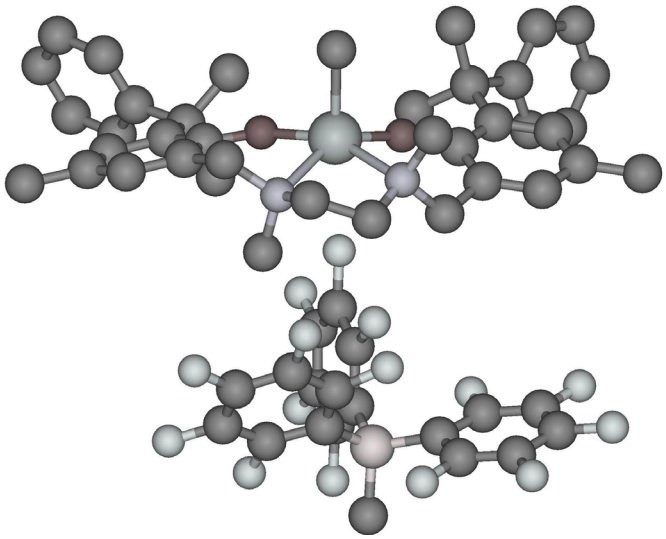
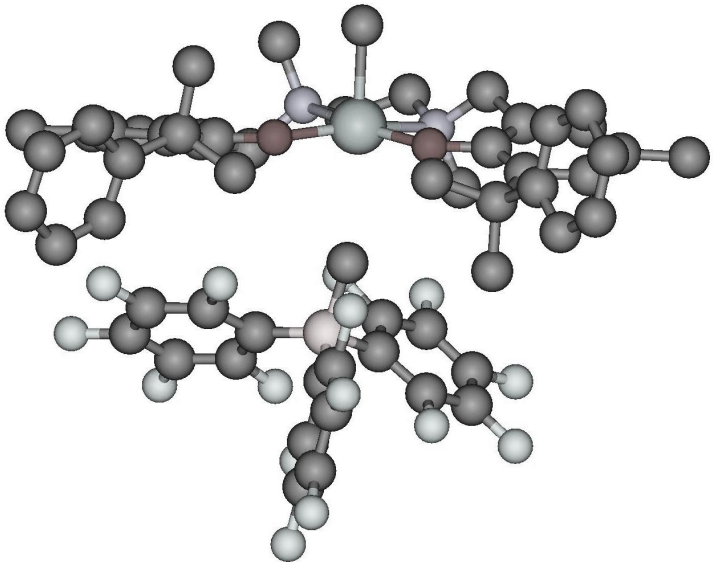


2e



2f