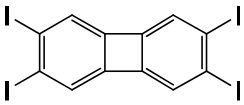
Reversible intercyclobutadiene haptotropism in cyclopentadienylcobalt linear [4]phenylene

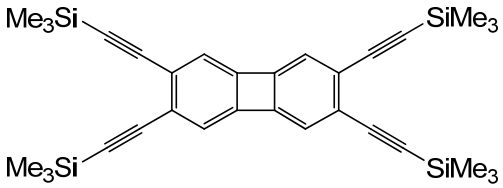
Thomas A. Albright, Sander Oldenhof, Oluwakemi A. Oloba, Robin Padilla and K. Peter C. Vollhardt*

Supporting Information

Experimental Procedures

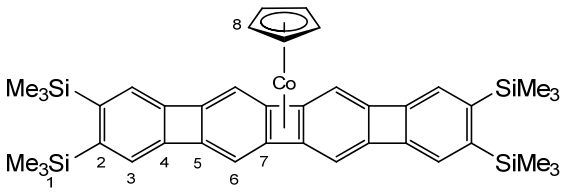


2,3,6,7-Tetraiodobiphenylene: To stirred $Hg(O_2CCF_3)_2$ (9.98 g, 23.4 mmol) in dry CH_2Cl_2 (200 mL) was added biphenylene (0.82 g, 5.39 mmol) in CH_2Cl_2 (10 mL). The mixture was completely shielded from light and stirred at RT for 3 d. A saturated solution of $CaCl_2$ in MeOH (5.20 g in 45 mL) was added and stirring continued for 3 h. A slurry formed, from which the solvent was decanted, followed by addition of dry CH_2Cl_2 (150 mL) and PyICl[1] (15.7 g, 6.50 mmol). The color changed from yellow-green to orange. After further stirring at RT for 42 h, the product was filtered off and the yellow solid washed with 1 M HCl (50 mL), H_2O (50 mL), MeOH (50 mL), and CH_2Cl_2 (50 mL) to give 2,3,6,7-tetraiodobiphenylene (1.09 g, 31%) as a bright yellow powder; m.p. >330 °C (decomp), sub. p. 200 °C (10 torr); ^{1}H NMR (400 MHz, CS_2/C_6D_6, 3:1): δ = 6.96 ppm (s); ^{13}C NMR (125 MHz, CS_2/C_6D_6, 3:1): δ = 150.5, 129.7, 109.1 ppm; IR (KBr): $\tilde{\nu}$ = 1403, 1218, 856, 801 cm^{-1}; MS (70 eV): *m*/*z* (%): 656 (80) [M^+], 402 (100), 328 (24), 148 (32), 127 (17). Anal. calcd for $C_{12}H_4I_4$: C, 21.98, H, 0.61; found: C, 22.48, H, 0.75.



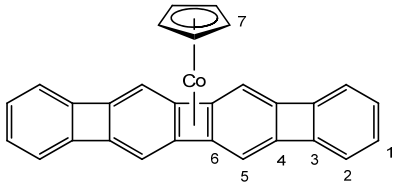
[1] H. A. Muathen, *J. Chem. Res. (M)*, 1994, 2201.

2,3,6,7-Tetrakis(trimethylsilylethynyl)biphenylene: A Schlenk flask was charged with 2,3,6,7-tetraiodobiphenylene (100 mg, 0.152 mmol), CuI (1.5 mg, 0.008 mmol), $Pd(PPh_3)_2Cl_2$ (5.6 mg, 0.008 mmol) degassed benzene (5 mL), and NEt_3 (5mL) to furnish a yellow suspension. After the addition of degassed trimethylsilylacetylene (760 mg, 1.1 mL, 7.7 mmol), the mixture was stirred at RT for 48 h, the dark brown solution filtered through a plug of silica, and the filtrate concentrated and subjected to column chromatography (silica gel), eluting with hexane/Et_2O (20 : 1) to give 2,3,6,7-tetrakis(trimethylsilylethynyl)biphenylene (76 mg, 93%) as yellow crystals; m.p. 246–247 °C (MeOH); ^{1}H NMR (400 MHz, $CDCl_3$) : δ = 6.74 (s, 4 H), 0.25 ppm (s, 36 H); ^{1}H NMR (300 MHz, C_6D_6): δ = 6.40 (s, 4 H), 0.29 ppm (s, 36 H); ^{13}C NMR (50 MHz, C_6D_6): δ = 148.6, 126.8, 103.6, 100.0, 0.015 ppm; UV/Vis (CH_3CN): λ_{max} (lgε) = 265 (4.39), 290 (4.63), 303 (4.88), 385 (3.45), 404 nm (3.64); IR (KBr): $\tilde{\nu}$ = 2960, 2155, 1300, 860, 840, 760 cm^{-1}; MS (EI) *m/z* (%): 536 (M^+, 21), 73 (100). Anal. calcd for $C_{32}H_{40}Si_4$: C, 71.57; H, 7.51; found: C, 71.28; H, 7.65.

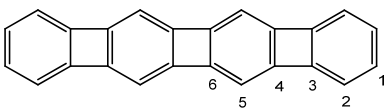


Linear [2,3,8,9-tetrakis(trimethylsilyl)[4]phenylene](cyclopentadienyl)cobalt (4): A Schlenk flask was charged with 2,3,6,7-tetrakis(trimethylsilylethynyl)biphenylene (300 mg, 0.558 mmol), 18-crown-6 (70.5 mg, 0.267 mmol), $KF{\cdot}2H_2O$ (489 mg, 5.19 mmol), and dry, degassed THF (25 mL). After stirring at RT for 3 h, the deep green mixture was filtered through a plug of silica using degassed THF and concentrated to approximately 15 mL (keeping exposure to light to a minimum). $CpCo(CO)_2$ (180 mg, 133 µL, 1.01 mmol) was added and the solution syringed into a boiling solution of degassed THF (150 mL) and bis(trimethylsilyl)acetylene (23 mL) over a period of 5 h, while irradiating with a projector lamp. The deep red reaction mixture was boiled and irradiated for an additional 14 h, the volatiles removed in vacuo, and the resulting black solid subjected to air free column chromatography (neutral alumina, activity III), eluting with hexane. The

first dark red fraction gave **4** (200 mg, 50%) as an air-sensitive deep-red solid; ^{1}H NMR (500 MHz, C_6D_6): δ = 7.45 (s, 4 H, H3), 6.72 (s, 4 H, H6), 4.60 (s, 5 H, H8), 0.33 ppm (s, 36 H, H1); ^{13}C NMR (150 MHz, C_6D_6): δ = 149.0 ($C5_q$), 148.0 ($C2_q$), 143.3 ($C4_q$), 125.2 (C3H), 114.9 (C6H), 80.1 (C8H), 74.1 ($C7_q$), 2.22 ppm ($C1H_3$); UV/Vis: (hexane): λ_{max} (relative intensity) = 281 (0.40), 356 (0.80), 487 sh nm (0.07); MS (EI) *m/z* (%): 712 (M^+, 10), 588 (30), 73 (100); HRMS (EI): calcd for $C_{41}H_{49}CoSi_4$: 712.2243; found: 712.2233. Anal. calcd for $C_{32}H_{40}Si_4$: C, 71.57; H, 7.51; found: C, 71.28; H, 7.65.

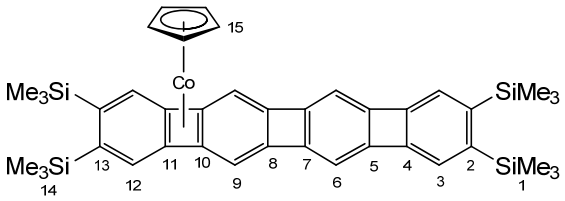


Linear [4]phenylene](cyclopentadienyl)cobalt (6): Under N_2, **4** (75 mg, 0.105 mmol) in THF/DMSO (3 : 1; 8 mL) was added to KO*t*-Bu (175 mg, 1.56 mmol) in *t*-BuOH (4 mL). The mixture was stirred at 85 °C for 16 h, cooled to RT, charged with degassed hexane (4 mL), and washed with degassed H_2O (3 x 5mL). Chromatography on an air free column of neutral alumina (activity III), eluting with toluene, provided **6** (31.2 mg, 70%) as an air-sensitive red solid; ^{1}H NMR (600 MHz, CS_2/C_6D_6, 3 : 1): δ = 6.78 (AA'm, 4 H, H1), 6.73 (BB'm, 4 H, H2), 6.52 (s, 4 H, H5), 4.39 ppm (s, 5 H, H7); ^{13}C NMR (150 MHz, C_6D_6): δ = 150.0 ($C4_q$), 142.6 ($C3_q$), 129.4 (C1H), 119.4 (C5H), 114.8 (C2H), 80.5 (C7H), 74.0 ppm ($C6_q$); UV/Vis: (THF): λ_{max} (relative intensity) = 303 (0.32), 337 (0.30), 350 (0.43), 386 (0.69), 512 (0.09), 548 nm (0.12); IR (neat) : $\tilde{\nu}$ = 2957, 2924, 2853, 1661, 1632, 1459, 1418, 1380, 1284, 1261, 1106, 1024, 802, 745 cm^{-1}; MS (EI) *m/z* (%): 424 (M^+, 100), 363 (38), 300 (100), 150 (22). HRMS (EI): calcd for $C_{29}H_{17}Co$: 424.0662; found: 424.0657.

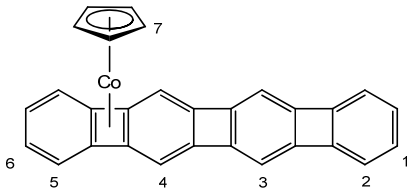


Linear [4]phenylene: Complex **6** (13 mg, 0.03 mmol) in toluene (1 mL) was heated to 95 °C for 90 h under a CO atmosphere. A precipitate formed that was triturated with a

few drops of degassed toluene to give highly insoluble linear [4]phenylene (9 mg, 100%): ^{1}H NMR (500 MHz, C_6D_6): δ = 6.45 (AA'm, 4 H, H1), 6.19 (BB'm, 4 H, H2), 5.76 ppm (s, 4 H, H5); UV/Vis: (DMSO): λ_{max} (relative intensity) = 302 (0.73), 314 (0.91), 458 (0.23), 487 nm (0.36); IR (film): 3069, 3045, 1645, 1436, 1409, 1277, 1180, 1148, 1105, 1077, 1013, 960, 916, 871, 849, 809, 744, 728 cm^{-1}; MS (EI) *m/z* (%): 300 (M^+, 100), 150 (16). HRMS (EI): calcd for $C_{24}H_{12}$: 300.0929; found: 300.0928.



Linear [2,3,8,9-tetrakis(trimethylsilyl)[4]phenylene](cyclopentadienyl)cobalt (5): A sample of **4** in C_6D_6 was irradiated in a Rayonet photochemical reactor fitted with 350 nm lamps for 3 h to reach the photostationary state of **5** : **4** = 2 : 1. Isomer **5**: ^{1}H NMR (500 MHz, C_6D_6): δ = 7.98 (s, 2 H, H12), 6.99 (s, 2 H, H3), 6.51 (s, 2 H, H9), 6.30 (s, 2 H, H6), 4.40 (s, 5 H, H15), 0.37 and 0.30 ppm (2 s, 36 H, H1 and H14); ^{13}C NMR (600 MHz, C_6D_6): δ = 154.0 ($C5_q$), 150.4 ($C8_q$), 149.9 ($C4_q$), 148.5 ($C2_q$), 141.3 ($C7_q$), 139.0 ($C13_q$), 135.8 (C12H), 122.3 (C3H), 112.3 and 110.9 ($C6/9_q$), 79.8 (C15H), 78.1 ($C11_q$), 72.5 ($C10_q$), 2.30 ($C14H_3$), 2.16 ppm ($C1H_3$); UV/Vis: (hexane): new λ_{max} = 411 nm.



Linear [4]phenylene](cyclopentadienyl)cobalt (7): A sample of **6** in THF-d_8 was irradiated in a Rayonet photochemical reactor fitted with 350 nm lamps for 3 h to reach the photostationary state of **7** : **6** = 2 : 1. Isomer **7**: ^{1}H NMR (400 MHz, THF-d_8): δ = 7.32 (AA'm, 2 H, H5), 6.93 (m, 4 H, H1 and H6), 6.49 (s, 2 H, H4), 6.44 (s, 2 H, H3), 6.41 (AA'm, 2 H, H2), 4.38 ppm (s, 5 H, H7); ^{1}H NMR (600 MHz, CS_2/C_6D_6): δ = 7.16 (m, 2

H, H5), 6.57 (m, 4 H, H1 and H6), 6.37 (AA'm, 2 H, H2), 6.32 (s, 2 H, H4), 6.20 (s, 2 H, H3), 4.27 ppm (s, 5 H, H7).

Computational Details

All calculations were performed using the *GAUSSIAN03*[2] program. GaussView 3.0[3] and ChemCraft[4] were employed to input structures as well as view output results. Optimized geometries were obtained at the hybrid density functional theory (DFT) using Becke's three-parameter exchange-correlation functional[5] containing the non-local gradient correction of Lee, Yang, and Parr[6] (B3LYP). For optimization purposes, a standard basis 3-21G[7] was used for hydrogen and carbon atoms. For cobalt, the LANL2DZ[8] basis set was applied, with the outermost d function released, yielding a triple-zeta d basis, along with the effective core potentials (ECP) to describe the core electrons. For the single point energy calculations, the basis sets were increased to 6-31G[9] for hydrogen, 6-311G*[10] for carbon, and the modified LANL2DZ basis as described above for cobalt with an added f-orbital coefficient.[11]

The potential energy surfaces were mapped through a scan calculation, a feature also available within the *GAUSSIAN03* program. Transition state structures were obtained in three different steps: (i) determination of initial and final products or the minimum

---

[2] Gaussian 03, Revision B.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, Gaussian, Inc., Pittsburgh PA, 2003.

[3] www.gaussian.com

[4] www.chemcraftprog.com

[5] A. D. Becke, *J. Chem. Phys.,* 1993, **98**, 5648.

[6] C. Lee, W. Yang and G. R. Parr, *Phys. Rev. B,* 1988, **37**, 785.

[7] J. S. Binkley, J. A. Pople and W. J. Hehre, *J. Am. Chem. Soc.,* 1980, **102**, 939 for hydrogen, and M. S. Gordon, J. S. Binkley, J. A. Pople, W. J. Pietro and W. J. Hehre, *J. Am. Chem. Soc*., 1983, **104**, 2797.

[8] P. J. Hay and W. R. Wadt, *J. Chem. Phys.,* 1985, **82**, 270.

[9] W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257.

[10] L. A. Curtiss, M. P. McGrath, J.-P. Blaudeau, N. E. Davis, R. C. Jr. Binning and L. Radom, *J. Chem. Phys.,* 1995, **103**, 6104.

[11] A. W. Ehlers, M. Böhme, S. Dapprich, A. Gobbi, A. Höllwarth, V. Jonas, K. F. Köhler, R. Stegmann, A. Veldkamp and G. Frenking, *Chem. Phys. Lett.,* 1993, **208**, 111.

closest to a TS, (ii) a linear QST2[12] search for an initial guess of a TS; and (iii) input of the results from (ii) into a QST3 search. Transition states and minima were confirmed by carrying out frequency calculations (using the same basis as that used for the optimizations).

Cartesian Coordinates and total energies (from the large basis set) of the stationary points

Structure **a**:

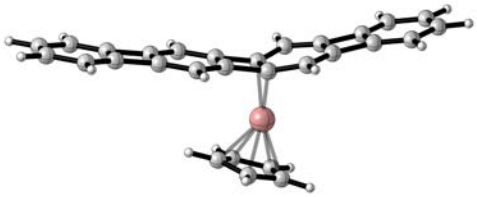
1	1	0	1.567125	2.963317	-1.683180
2	6	0	6.918081	-1.177404	.699259
3	6	0	5.721581	-1.054441	1.448014
4	6	0	4.559842	-.941787	.718079
5	6	0	3.058213	-.788634	.744855
6	6	0	1.946992	-.677504	1.519065
7	6	0	.743935	-.531129	.745587
8	6	0	-.742872	-.530950	.745654
9	6	0	-1.945912	-.678085	1.519118
10	6	0	-3.056977	-.789871	.744880
11	6	0	-4.558541	-.942943	.718087
12	6	0	-5.720256	-1.055735	1.448038
13	6	0	-6.916780	-1.178463	.699321
14	6	0	-6.916704	-1.181411	-.696685
15	6	0	-5.720124	-1.061918	-1.445814
16	6	0	-4.558457	-.946062	-.716258

[12] QST is a synchronous transit approach to the quadratic region around the transition state structure. For details, see: (*a*) J. B. Foresman and A. Frisch in *Exploring Chemistry with Electronic Structure Methods: A Guide to Using Gaussian*, Gaussian, Inc., Pittsburgh, PA, USA, 1996; (*b*) H. B. Schlegel in *Ab Initio Methods in Quantum Chemistry,* Part I, Wiley, Chichester, 1987.

17	6	0	-3.056963	-.793241	-.743644
18	6	0	-1.945767	-.684951	-1.518170
19	6	0	-.743022	-.533819	-.745363
20	6	0	.743881	-.534108	-.745347
21	6	0	1.946727	-.685242	-1.518043
22	6	0	3.058083	-.792218	-.743455
23	6	0	4.559666	-.945307	-.716217
24	6	0	5.721276	-1.061419	-1.445826
25	6	0	6.917923	-1.180735	-.696735
26	1	0	7.860966	-1.271751	1.225754
27	1	0	5.742667	-1.051266	2.530774
28	1	0	-1.946458	-.709584	2.601916
29	1	0	-5.741282	-1.052845	2.530803
30	1	0	-5.741056	-1.063547	-2.528580
31	1	0	-1.946000	-.721666	-2.600800
32	1	0	1.946924	-.722947	-2.600644
33	1	0	5.742145	-1.063375	-2.528591
34	1	0	7.860706	-1.277539	-1.222973
35	27	0	-.000459	1.218988	-.002421
36	6	0	-1.197695	2.953527	.232901
37	6	0	-.149880	2.972880	1.214492
38	6	0	1.101554	2.960665	.515809
39	6	0	.827280	2.972650	-.898366
40	6	0	-.592325	2.974802	-1.072980
41	1	0	-2.256847	2.922222	.436686
42	1	0	-.282242	2.967910	2.284937
43	1	0	2.081576	2.935471	.966292
44	1	0	1.947389	-.709520	2.601846
45	1	0	-1.120610	2.970594	-2.013359
46	1	0	-7.859535	-1.278067	-1.222889
47	1	0	-7.859652	-1.272956	1.225838

E_{TOT} = -1260.43836646

Structure *b*:

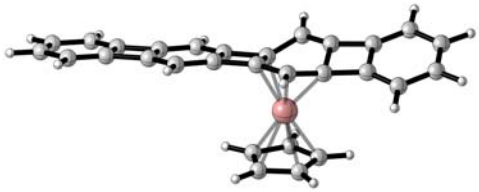


1	6	0	.000000	.000000	.000000
2	6	0	.000000	.000000	1.429093
3	6	0	1.229649	.000000	2.027783
4	6	0	2.037964	-.000517	3.325991
5	6	0	1.990112	.024199	4.717127
6	6	0	3.259766	.054854	5.298647
7	6	0	4.039757	.020785	6.614113
8	6	0	3.986480	.486243	7.974610
9	6	0	5.210706	.808690	8.484395
10	6	0	5.987461	1.268973	9.696267
11	6	0	5.952652	1.627572	11.023517
12	6	0	7.193663	2.001417	11.601778
13	6	0	8.378082	2.003508	10.866540
14	6	0	8.411411	1.631982	9.497195
15	6	0	7.207427	1.271163	8.938949
16	6	0	6.467177	.810980	7.704415
17	6	0	6.554261	.490908	6.380610
18	6	0	5.312543	.023052	5.824074
19	6	0	4.479698	.057028	4.541421
20	6	0	4.522028	.028763	3.145525
21	6	0	3.254183	.001689	2.571060
22	6	0	2.449462	.002247	1.270622
23	6	0	2.458580	.004545	-.096997
24	6	0	1.177892	.002177	-.731142
25	1	0	-.949681	-.000744	-.522737

26	1	0	-.931567	.001356	1.981194
27	1	0	1.070361	.033583	5.287983
28	1	0	3.057287	.558856	8.527639
29	1	0	5.043574	1.631735	11.612202
30	1	0	9.342299	1.639468	8.943679
31	1	0	7.461896	.566859	5.793297
32	1	0	5.441706	.041448	2.574616
33	1	0	3.366713	.009286	-.686834
34	1	0	1.130846	.003097	-1.814162
35	27	0	4.794945	-1.854510	6.405262
36	6	0	4.571065	-3.741074	7.427699
37	6	0	3.491351	-3.594109	6.529989
38	6	0	4.058475	-3.390980	5.212571
39	6	0	5.491106	-3.590660	5.290470
40	6	0	5.815024	-3.738869	6.656643
41	1	0	4.504721	-3.844521	8.499924
42	1	0	2.444167	-3.542281	6.781729
43	1	0	3.498911	-3.197357	4.310347
44	1	0	6.182371	-3.535806	4.464760
45	1	0	6.805042	-3.840437	7.074162
46	1	0	7.220254	2.294241	12.645243
47	1	0	9.300664	2.297952	11.353795

E_{TOT} = -1260.38446005

Structure **c**:



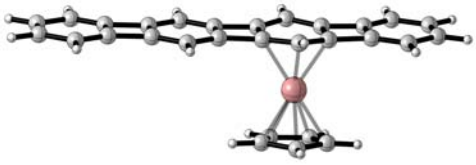
1	6	0	7.440907	-.240714	.714450
2	6	0	6.239769	-.097502	1.474210
3	6	0	5.072428	-.307358	.792783

4	6	0	3.543816	-.353727	.825781
5	6	0	2.398056	-.215810	1.602574
6	6	0	1.230677	-.454930	.875678
7	6	0	-.279848	-.484260	.926410
8	6	0	-1.495995	-.252571	1.599368
9	6	0	-2.578323	-.405113	.667038
10	6	0	-4.080162	-.581383	.693139
11	6	0	-5.271251	-.196266	1.271886
12	6	0	-6.437301	-.822181	.777231
13	6	0	-6.386540	-1.777858	-.244685
14	6	0	-5.168751	-2.173410	-.836878
15	6	0	-4.026348	-1.565340	-.348946
16	6	0	-2.546860	-1.441189	-.456709
17	6	0	-1.387290	-1.664134	-1.103514
18	6	0	-.326543	-.820068	-.531453
19	6	0	1.205106	-.796955	-.511141
20	6	0	2.358353	-.934656	-1.287699
21	6	0	3.522749	-.699591	-.563402
22	6	0	5.051593	-.651900	-.599797
23	6	0	6.196499	-.792155	-1.334639
24	6	0	7.420565	-.573370	-.631686
25	1	0	8.393241	-.084269	1.208086
26	1	0	6.278356	.161418	2.524907
27	1	0	2.409452	.032285	2.656014
28	1	0	-1.596041	.091408	2.620556
29	1	0	-5.331632	.543984	2.060985
30	1	0	-5.148640	-2.917660	-1.623520
31	1	0	-1.226143	-2.328973	-1.942608
32	1	0	2.345764	-1.200999	-2.336780
33	1	0	6.201838	-1.052686	-2.385671
34	1	0	8.356980	-.671245	-1.168809

35	27	0	-1.223236	.994218	-.048999
36	6	0	-1.975828	3.011595	.223177
37	6	0	-.551683	3.104078	.243354
38	6	0	-.059366	2.542871	-.971421
39	6	0	-1.195490	2.186513	-1.800057
40	6	0	-2.377626	2.473949	-1.058897
41	1	0	-2.645883	3.325757	1.008344
42	1	0	.051117	3.452681	1.067913
43	1	0	.977951	2.423398	-1.243114
44	1	0	-1.147539	1.766165	-2.792028
45	1	0	-3.392713	2.298141	-1.378863
46	1	0	-7.399399	-.555979	1.200078
47	1	0	-7.311215	-2.226701	-.589436

E_{TOT} = -1260.40940900

Structure *d*:



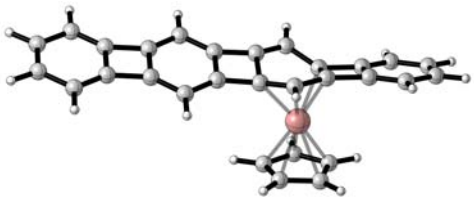
1	6	0	.000000	.000000	.000000
2	6	0	.000000	.000000	1.428203
3	6	0	1.230353	.000000	2.025168
4	6	0	2.036680	-.000128	3.324149
5	6	0	1.977659	.003634	4.717566
6	6	0	3.242892	.007577	5.299707
7	6	0	4.034253	-.011595	6.608411
8	6	0	3.957348	.107789	8.039866
9	6	0	5.301535	.010416	8.558199
10	6	0	6.164569	.079780	9.815724
11	6	0	6.217616	.106666	11.185175
12	6	0	7.521636	.163542	11.757081
13	6	0	8.672894	.192409	10.977667

14	6	0	8.609411	.168289	9.555969
15	6	0	7.351356	.114874	9.014035
16	6	0	6.512663	.090323	7.751670
17	6	0	6.552682	.142712	6.360749
18	6	0	5.262758	.034650	5.833837
19	6	0	4.458198	.010851	4.548797
20	6	0	4.517854	.002939	3.156020
21	6	0	3.253662	-.000862	2.572202
22	6	0	2.450136	.000108	1.270137
23	6	0	2.459807	.000807	-.097483
24	6	0	1.179069	.000551	-.730334
25	1	0	-.949135	-.000467	-.523297
26	1	0	-.930904	.000175	1.981224
27	1	0	1.054477	.006362	5.281673
28	1	0	3.081696	.393560	8.605828
29	1	0	5.337366	.089458	11.815723
30	1	0	9.513058	.199665	8.959595
31	1	0	7.454989	.201227	5.770144
32	1	0	5.441912	.007026	2.592962
33	1	0	3.367574	.001427	-.687582
34	1	0	1.131991	.000524	-1.813284
35	27	0	4.505270	-1.746035	7.704343
36	6	0	3.178051	-3.390925	8.515269
37	6	0	3.323013	-3.453242	7.098801
38	6	0	4.726035	-3.685676	6.786369
39	6	0	5.444288	-3.661224	8.005654
40	6	0	4.487155	-3.419270	9.076476
41	1	0	2.256725	-3.234784	9.054989
42	1	0	2.523907	-3.413397	6.373965
43	1	0	5.133755	-3.835147	5.798428
44	1	0	6.508607	-3.788306	8.131320

45	1	0	4.732947	-3.348520	10.125245
46	1	0	7.616289	.186463	12.836980
47	1	0	9.641524	.237463	11.461250

E_{TOT} = -1260.38786622

Structure **e**:

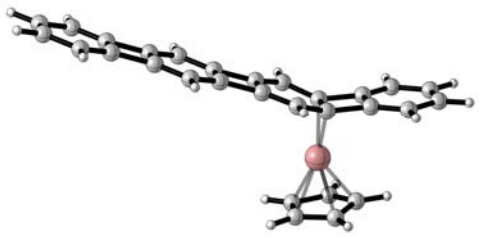


1	6	0	.000000	.000000	.000000
2	6	0	.000000	.000000	1.425298
3	6	0	1.231925	.000000	2.024745
4	6	0	2.032198	.000284	3.322612
5	6	0	1.982872	-.000138	4.704720
6	6	0	3.258541	.002277	5.290792
7	6	0	4.011204	-.000659	6.595287
8	6	0	3.928761	.598404	7.896627
9	6	0	5.164923	.426711	8.557675
10	6	0	6.017590	.498402	9.805879
11	6	0	6.114794	.916088	11.108833
12	6	0	7.340871	.621497	11.767119
13	6	0	8.375433	-.046135	11.119447
14	6	0	8.266919	-.470988	9.765891
15	6	0	7.080473	-.189199	9.134720
16	6	0	6.255616	-.308081	7.848941
17	6	0	6.475741	-.187253	6.400648
18	6	0	5.298663	-.008063	5.769859
19	6	0	4.477613	.010888	4.536717
20	6	0	4.518167	.004232	3.128397
21	6	0	3.259556	.000775	2.561824
22	6	0	2.449761	.000193	1.267601

23	6	0	2.457953	.000175	-.101870
24	6	0	1.179807	.000000	-.733234
25	1	0	-.949125	.000044	-.523606
26	1	0	-.930884	.000095	1.978451
27	1	0	1.063203	-.004422	5.275915
28	1	0	3.033627	1.020083	8.334885
29	1	0	5.326018	1.454741	11.619976
30	1	0	9.090785	-.978577	9.278554
31	1	0	7.453312	-.272586	5.943452
32	1	0	5.438248	.009392	2.558823
33	1	0	3.366132	.000909	-.691517
34	1	0	1.130650	.000490	-1.816073
35	27	0	4.486323	-1.394289	8.065451
36	6	0	3.553849	-2.677835	9.627465
37	6	0	2.837628	-2.759365	8.395118
38	6	0	3.735928	-3.267558	7.380560
39	6	0	5.015092	-3.445314	7.981563
40	6	0	4.909191	-3.039974	9.370229
41	1	0	3.162937	-2.319439	10.567373
42	1	0	1.795032	-2.524077	8.247577
43	1	0	3.482973	-3.448830	6.347675
44	1	0	5.908339	-3.800088	7.492357
45	1	0	5.717083	-3.033717	10.085292
46	1	0	7.473324	.934109	12.796530
47	1	0	9.295406	-.243631	11.658277

E_{TOT} = -1260.41270836

Structure *f*:

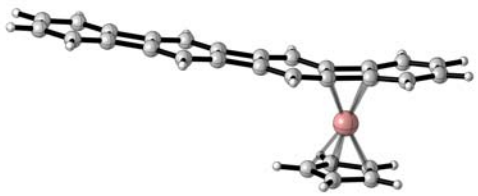


1	6	0	.000000	.000000	.000000
2	6	0	.000000	.000000	1.427333
3	6	0	1.230785	.000000	2.025690
4	6	0	2.036291	.001912	3.323882
5	6	0	1.987259	.004556	4.711091
6	6	0	3.260286	.007104	5.292236
7	6	0	4.035259	.021231	6.585459
8	6	0	3.972780	.048537	7.945450
9	6	0	5.265764	-.031450	8.580293
10	6	0	6.044184	.518373	9.778807
11	6	0	6.004673	.907738	11.095935
12	6	0	7.240592	1.321600	11.666816
13	6	0	8.422432	1.327100	10.932483
14	6	0	8.460752	.920430	9.569510
15	6	0	7.265356	.523934	9.020060
16	6	0	6.538260	-.025766	7.790487
17	6	0	6.541459	.052508	6.349828
18	6	0	5.293967	.021228	5.803555
19	6	0	4.478135	.007028	4.535745
20	6	0	4.521452	.004507	3.136990
21	6	0	3.256244	.001974	2.566026
22	6	0	2.449374	.000000	1.268685
23	6	0	2.458333	.000132	-.099812
24	6	0	1.178777	.000246	-.732272
25	1	0	-.949420	.000183	-.523077
26	1	0	-.931037	.000773	1.980165
27	1	0	1.067946	.005084	5.281702
28	1	0	3.052309	.116249	8.513583
29	1	0	5.092535	.922708	11.680762
30	1	0	9.388798	.945622	9.010624
31	1	0	7.457948	.122295	5.775517

32	1	0	5.440429	.005179	2.565830
33	1	0	3.366481	.001141	-.689489
34	1	0	1.130504	.000610	-1.815174
35	27	0	6.130533	-1.869276	8.534679
36	6	0	5.618481	-3.441560	9.949485
37	6	0	5.470499	-3.910703	8.623718
38	6	0	6.772717	-3.849467	7.959503
39	6	0	7.708885	-3.325146	8.875438
40	6	0	6.979903	-2.973044	10.079314
41	1	0	4.843278	-3.355398	10.693772
42	1	0	4.559152	-4.265719	8.166856
43	1	0	6.968452	-4.153227	6.942805
44	1	0	8.752889	-3.127453	8.691671
45	1	0	7.401639	-2.500809	10.953223
46	1	0	7.256745	1.652098	12.699385
47	1	0	9.338685	1.662187	11.405651

E_{TOT} = -1260.38299488

Structure **g**:



1	6	0	.000000	.000000	.000000
2	6	0	.000000	.000000	1.472975
3	6	0	1.493687	.000000	1.485388
4	6	0	1.493706	.000000	-.012385
5	6	0	2.684644	-.244791	-.784650
6	6	0	3.782936	-.433265	-.009916
7	6	0	3.782895	-.433261	1.483070
8	6	0	2.684568	-.244723	2.257736
9	6	0	5.263363	-.698609	1.452941

10	6	0	5.263448	-.698429	.020310
11	1	0	2.683302	-.280904	3.340504
12	1	0	2.683457	-.280977	-1.867419
13	27	0	.847579	1.763191	.736495
14	6	0	-.011451	3.585448	1.455698
15	6	0	1.339411	3.492400	1.904948
16	6	0	2.180622	3.387782	.739810
17	6	0	1.346337	3.491372	-.430474
18	6	0	-.007154	3.585041	.010509
19	1	0	-.889544	3.636852	2.080308
20	1	0	1.672228	3.462697	2.930452
21	1	0	3.253665	3.274397	.743011
22	1	0	1.685371	3.460672	-1.453912
23	1	0	-.881484	3.636230	-.619369
24	6	0	-1.210428	-.050141	-.723700
25	6	0	-1.210409	-.050140	2.196701
26	6	0	-2.378567	-.074302	.022087
27	6	0	-2.378559	-.074329	1.450933
28	1	0	-1.232403	-.101344	-1.806272
29	1	0	-3.333629	-.117524	-.489652
30	1	0	-3.333615	-.117557	1.962681
31	1	0	-1.232361	-.101319	3.279273
32	6	0	6.411979	-.906909	-.755433
33	6	0	6.411788	-.907316	2.228776
34	6	0	7.543294	-1.115140	.017165
35	6	0	7.543209	-1.115289	1.456268
36	1	0	6.411865	-.906133	-1.837405
37	1	0	6.411568	-.906638	3.310749
38	6	0	9.044470	-1.395466	1.453775
39	6	0	9.044496	-1.395659	.019783
40	6	0	10.182530	-1.610929	-.710110

41	6	0	10.182495	-1.610436	2.183770
42	6	0	11.373042	-1.835414	.042664
43	6	0	11.373024	-1.835184	1.431101
44	1	0	10.203358	-1.615956	-1.792693
45	1	0	10.203268	-1.615247	3.266356
46	1	0	12.302144	-2.010706	1.961126
47	1	0	12.302188	-2.011051	-.487277

E_{TOT} = -1260.42618253