Influence of the ligand framework

To investigate the effects of cyclopentadienyl substitution and bridging, intermediates and products of the displacement reaction are calculated for different ligand frameworks: Figure S1 and Table S8 show the relative energies for reactions of $H_2Si(C_5H_4)_2ZrMe^+MeB(CF_3)_3^-$, **9a**, $(C_5H_5)_2ZrMe^+MeB(CF_3)_3^-$, **13a**, and *rac*-$H_2Si(C_9H_6)_2ZrMe^+MeB(CF_3)_3^-$, **14a**, with dimethyl ether to form the corresponding five-coordinated intermediates, **9b-14b**, and the outer-sphere ion pairs, **9c-14c**. Reaction energies for the formation of the outer-sphere complexes in toluene solution are in the range of –41 to –34 kJ/mol. Formation of the outer-sphere complex was most favored for the indenyl complex **14c**, in deviation from the experimental results (Table 4). However, differences between the $MeB(CF_3)_3^-$ anion used in these calculations and the $MeB(C_6F_5)_3^-$ used in NMR experiments would be expected to be most pronounced in the case of the outer-sphere complexes.

Table S8. Relative energies [a] calculated for the five-coordinated intermediates, 9b-14b, and the outer-sphere reaction products, 9c-14c, for the reaction of 9a, 13a and 14a with dimethyl ether.

Contact ion pair	9-14b		9-14c	
	$E_{toluene}$	$E_{gas\ phase}$	$E_{toluene}$	$E_{gas\ phase}$
9a	–27	–21	–38	–32
13a	–25	–17	–34	–28
14a	–22	–13	–41	–37

[a] in kJ/mol, relative to non-interacting **9-14a** + Me_2O.

Better agreement with the experimental data is obtained for the energies associated with the formation of the five-coordinated intermediates: **9a** shows the highest tendency to form **9b**, followed by the unbridged complex **13b**, which is more endothermic by 2 kJ/mol (Table S8). Formation of the five-coordinated indenyl complex **14b**, finally, is accompanied with a reaction enthalpy which is higher by 5 kJ/mol than the one calculated for **9a**. These energy values are in the same order as the corresponding activation energies experimentally obtained for anion substitution by DBE in complexes **1a** and **5a** with differences of 7 and 15 kJ/mol, respectively, in comparison to the barrier found for **3a** (Table 4). The strong effects of the substitution pattern on the reaction rate are reproduced in the energy ordering of the five-coordinated intermediates, which thus seem to resemble the transition state of the anion substitution reaction.

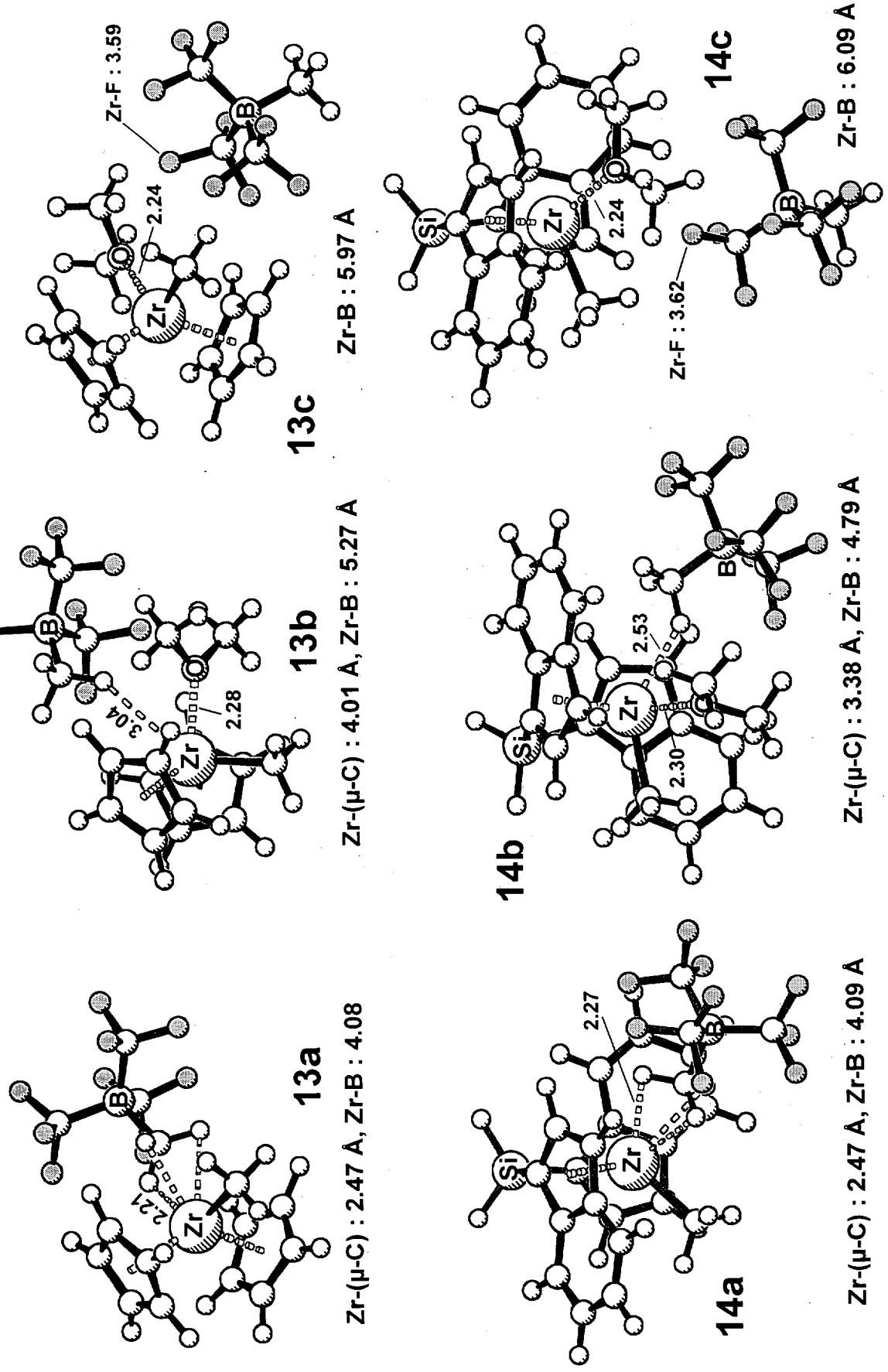

Zr-F : 3.59
2.24
Zr
O
B
13c
Zr-B : 5.97 Å
2.28
2.04
13b
Zr-(μ-C) : 4.01 Å, Zr-B : 5.27 Å
2.24
13a
Zr-(μ-C) : 2.47 Å, Zr-B : 4.08
Si
2.24
14c
Zr-F : 3.62
Zr-B : 6.09 Å
2.53
2.30
14b
Zr-(μ-C) : 3.38 Å, Zr-B : 4.79 Å
2.27
14a
Zr-(μ-C) : 2.47 Å, Zr-B : 4.09 Å

Figure S1

Determination of the rate constant *k* from 2D-NMR experiments

For a two-site exchange with unequal population of the exchanging sites k_{obs} can be determined according to Perrin and Dwyer:[45]

$$k_{obs} = k_{AB} + k_{BA} \tag{1}$$

$$k_{obs} = \frac{1}{\tau_M} \ln \frac{r+1}{r-1}, \qquad r = 4X_A X_B \frac{I_{AA} + I_{BB}}{I_{AB} + I_{BA}} - (X_A - X_B)^2 \tag{2}$$

(I = integral of cross and diagonal signals, X_A=[A]/([A]+[B]). Since the system is in equilibrium :

$$k_{AB}[\mathrm{A}] = k_{BA}[\mathrm{B}]$$
$$\Leftrightarrow \quad k_{BA} = \frac{[\mathrm{A}]}{[\mathrm{B}]} k_{AB} = \frac{X_A}{X_B} k_{AB} \tag{3}$$

With (1) und (3):

$$k_{obs} = (1 + \frac{X_A}{X_B}) k_{AB}$$
$$\Leftrightarrow \quad k_{AB} = X_B k_{obs} \tag{4}$$

Comparison of the rate laws for the magnetisation transfer (5) and the substitution process (6) yields (7) with k_{obs} determined from the experimental data according to (2):

$$v_{mag.-transfer} = k_{AB}[\mathrm{Zr^+A^-}] = k_{BA}[\mathrm{Zr(Lb)^+A^-}] \tag{5}$$

$$v_{substitution} = k[\mathrm{Zr^+A^-}] \cdot [\mathrm{Lb}] \tag{6}$$

$$k = \frac{1}{[\mathrm{Lb}]} k_{AB} = \frac{X_B}{[\mathrm{Lb}]} k_{obs} \tag{7}$$

Determination of relative molecular weights

Molecular weights (M_w / 1000) for ethene and propene polymerizations with catalysts 1/MAO-7/MAO.

	Ref. 61a	Ref. 61b	Ref. 61c	Ref. 61c	Ref. 61c	Ref. 61c	Ref. 61d	Ref. 61e	
1/MAO		25							
3/MAO	5								
4/MAO	42								
5/MAO		91	195	36	30	25	62	87.4	95
6/MAO	146	140	249	195	82		135	297	300
7/MAO		172	532	330	100	55	137	516	605

Values in the same coloumn are obtained under identical conditions.

Since M_w depends strongly on polymerization conditions (and of course on the monomer used) estimates for relativ molecular weights are determined as follows :

1. data from ref. 61b-61e is scaled according to:

$$M_w^r(\text{ref. i, cat. j}) = \frac{1}{2}\left(\frac{M_w(\text{ref. i, }\mathbf{5})}{\overline{M_w}(\mathbf{5})} + \frac{M_w(\text{ref. i, }\mathbf{7})}{\overline{M_w}(\mathbf{7})}\right) M_w(\text{ref. i, cat. j})$$

Average molecular weights $\overline{M_w}$ are determined from all results of ref. 61b-61e for the respective catalyst.

	Ref. 61a	Ref. 61b	Ref. 61c	Ref. 61c	Ref. 61c	Ref. 61c	Ref. 61d	Ref. 61e	
1/MAO		32.9							
3/MAO									
4/MAO									
5/MAO		119.8	94.9	55.5	84.7	108.4	108.1	64.7	62.9
6/MAO		184.2	121.2	300.7	231.6		235.3	220.0	198.5
7/MAO		226.3	258.9	508.9	282.4	238.4	238.8	382.2	400.3

2. data from ref. 61a is scaled according to :

$$M_w^r(\text{cat. j}) = \frac{M_w(\text{ref. i, }\mathbf{6})}{\overline{M_w}(\mathbf{6})} M_w(\text{cat. j})$$

3. all data is scaled relativ to **3**/MAO

	Ref. 61a	Ref. 61b	Ref. 61c	Ref. 61c	Ref. 61c	Ref. 61c	Ref. 61d	Ref. 61e	
1/MAO		4.5							
3/MAO	1								
4/MAO	8.4								
5/MAO		16.4	13.0	7.6	11.6	14.9	14.8	8.9	8.6
6/MAO	29.2	25.2	16.6221	41.2	31.7		32.2	30.2	27.2
7/MAO		31.0	35.5	69.7	38.7	32.7	32.7	52.4	54.9

Molecular Mechanics calculations

Substantial steric differences exists between the Lewis bases studied here and olefins such as ethene and propene. To clarify to which extend experimentally observed trends in coordination constants can be extended to anion displacement by olefins, we estimated the steric contribution to the reaction energy of the anion substitution by molecular mechanics methods. For this we used coordination geometries constrained to values obtained by the DFT-calculations and a modified AMBER94 force-field (Schneider, N.; Schaper, F.; Schmidt, K.; Kirsten, R.; Geyer, A.; Brintzinger, H. H. *Organometallics* **2000**, *19* , 3597). The atom type CA (aromatic carbon) was assigned to the carbon atoms of the olefin ligand, B4 to the boron and F to fluorine atoms. Parameters for the silicon bridge were taken from : Doman, T. N.; Hollis, T. K.; Bosnich, B. *J. Am. Chem. Soc.* **1995**, *117* , 1352. The following parameters were added to the force-field :

Bond distance	K [kcal/Å]	r_{eq} [Å]
B4 - CT	310	1.66
B4 - CA	310	1.62
CA - F	317	1.355

Bond angle	K [kcal/deg]	α_{eq} [deg]
CA - B4 - CA	50	109.5
CA - B4 - CT	50	109.5
B4 – CT - HC	50	109.5
CA – CA – B4	70	120
CA – CA – F	70	120
CT – CA – HA	35	120
HA – CA – HA	35	120

Since reduced coordination constants for DBE in comparison to diethyl ether are probably caused by a hindered rotation of the n-butyl chains, dibutyl ether was modeled by a diethyl ether molecule with increased vdW-parameters on the β-carbon atoms. The coordination geometry in the equatorial plane was restrained to the values obtained from the DFT-calculations: The positions of the zirconium atom, the carbon atom of the methyl group attached to zirconium and the coordinated atoms of the Lewis base (μ-C for the contact ion pair, oxygen for the ether adducts and the carbon atoms of ethene or propene) were frozen in the geometry optimization. As a model for the MAO^- anion we used the methyl adduct of hexameric MAO ($Me-(AlOMe)_6^-$), the geometry of which was restrained to that calculated by Vanka et al.[13c] For oxygen-coordination, d_{Zr-Me}, d_{Zr-O} and $\alpha_{Me-Zr-O}$ were fixed to the values calculated by these authors for $(C_5H_3Me_2)_2ZrMe^+Me(AlOMe)_6^-$. In the methyl-bridged MAO-contact ion pair, the Zr-bound and the bridging methyl group were fixed at the positions calculated for the methyl bridged $MeB(C_6F_5)_3^-$ contact ion pair **8a**, while the Zr-(μ-Me)-Al angle was restrained to 180°.

The energy difference $\Delta E_R = E(Zr\text{-}Lb^+) + E(A^-) - E(Lb) - E(Zr^+A^-)$ reflects the steric strain associated with the displacement of $MeB(C_6F_5)_3^-$ by the Lewis base (Figure S3). For all ligands studied (ethene, propene, Me_2O and $^nBu_2O$) more unfavorable reaction energies are calculated for the sterically more demanding complexes. The values calculated for the displacement of $MeB(C_6F_5)_3^-$ by DBE compare surprisingly well to reaction energies experimentally obtained for this reaction, although the energy differences obtained in the molecular mechanics calculations are generally higher. We can thus conclude that anion displacement is increasingly disfavored with

increasing steric bulk at the ligand framework and that olefins as well as DBE are sterically more demanding than a methylborate anion.

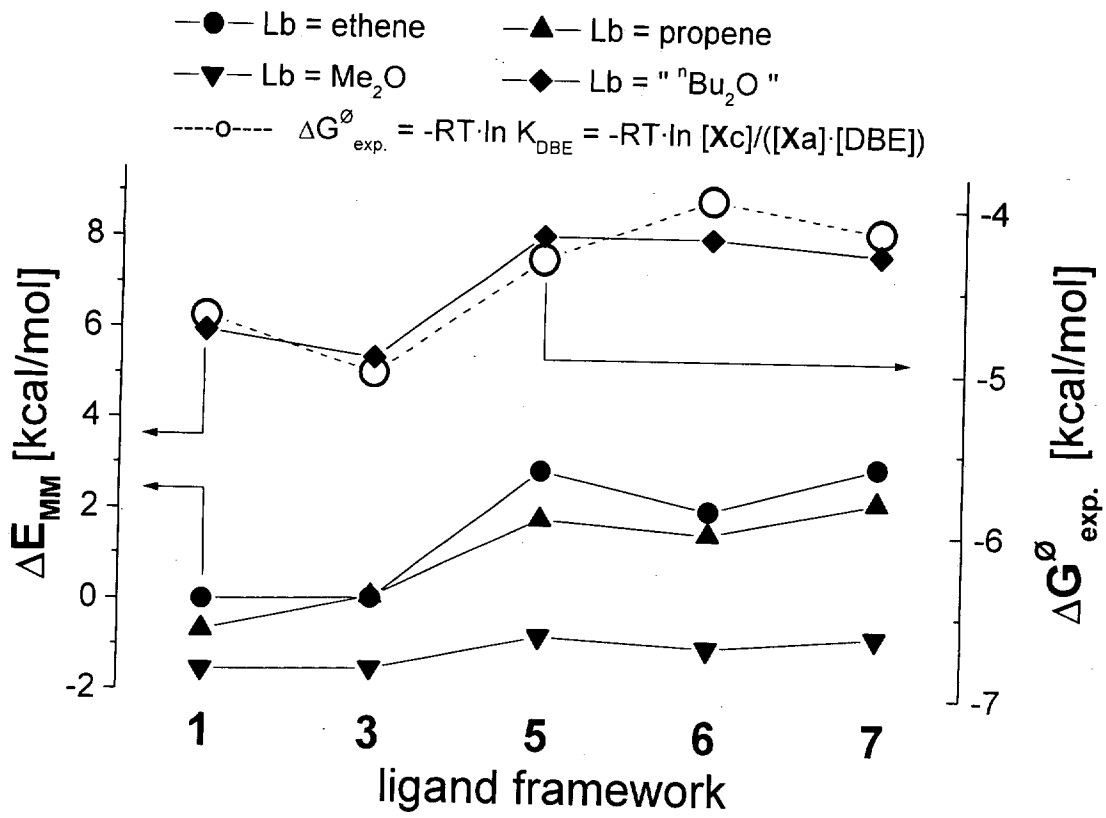


Figure S3

Energy differences ΔE obtained for the substitution of $MeB(C_6F_5)_3^-$ by $MeMAO^-$ indicate steric interactions of the ligand framework with methyl coordinated $MeMAO^-$ comparable to that with the methylborate anion, while oxygen coordination of $MeMAO^-$ becomes sterically unfavorable with increasing ligand substitution (Figure S4). These calculations indicate, despite the approximations made, that methyl-coordinated $MeMAO^-$ contact ion pairs (or $AlMe_3$ adducts) are comparable in their steric demands to contact ion pairs with the $MeB(C_6F_5)_3^-$ anion and that the trends in steric contributions to the reaction energies calculated for the displacement of $MeB(C_6F_5)_3^-$ by DBE, ethene or propene are the same as for displacement of methyl coordinated $MeMAO^-$.

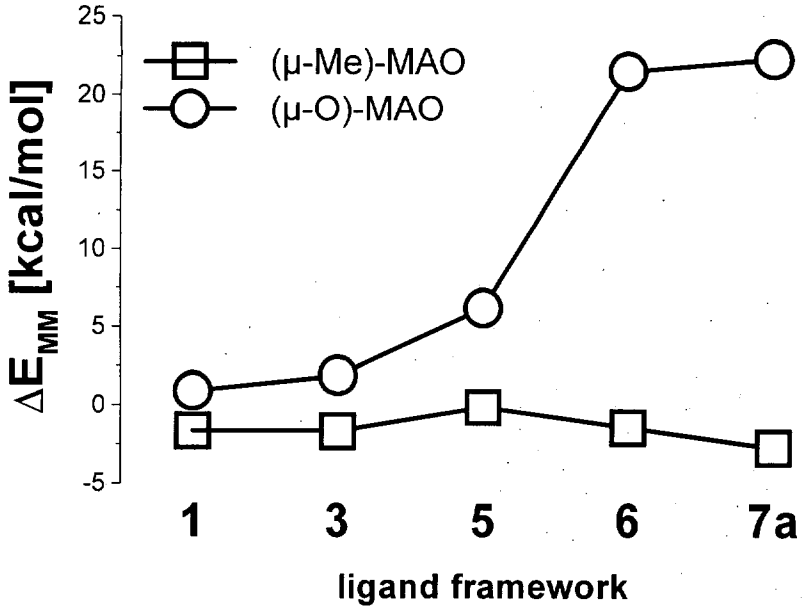
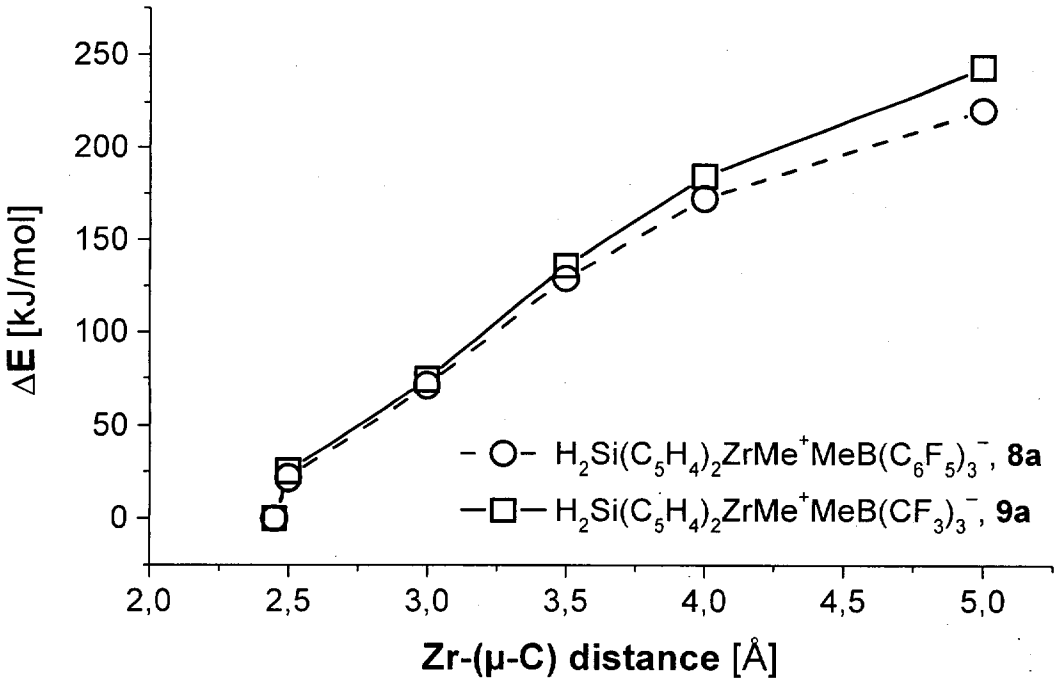


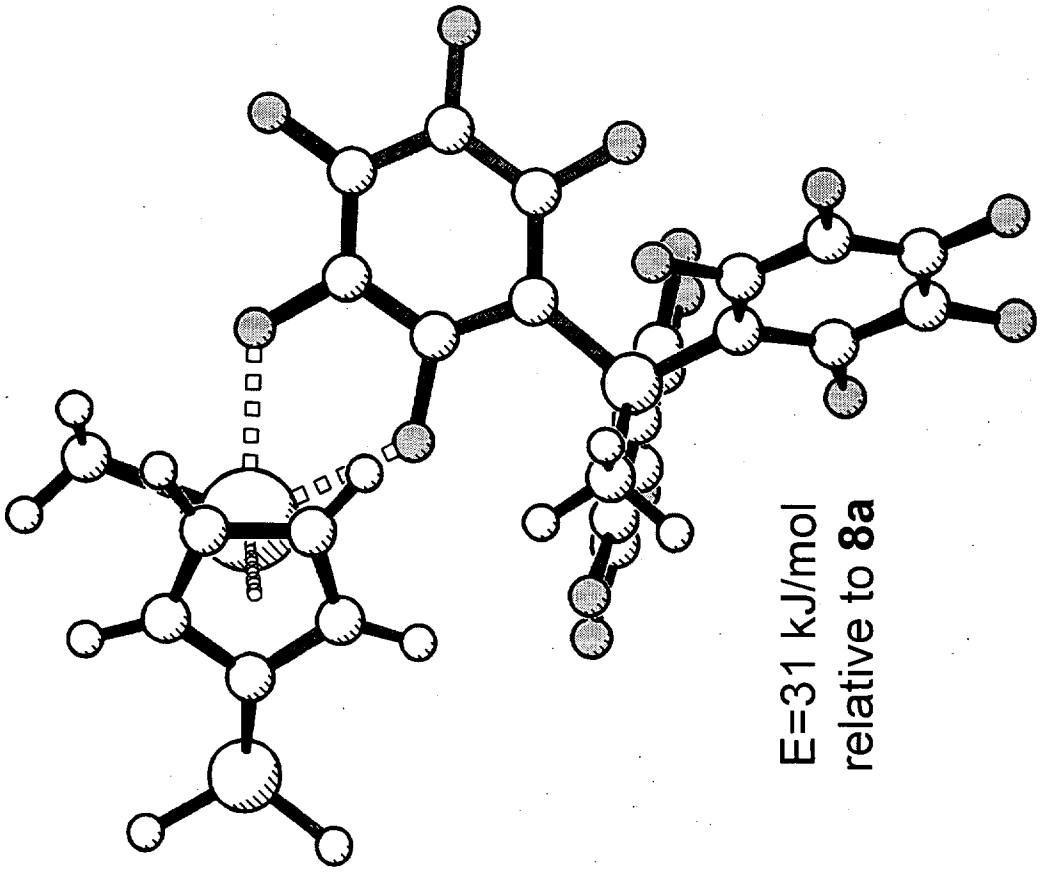
Figure S4

Energy profiles for anion dissociation

Energies were obtained as single-point energies in the gas phase (relative to the corresponding contatct ion pair). Geometries were identical to those of the contact ion pairs **8a** and **9a**, with exception of the elongated Zr-(μ-Me) distance.



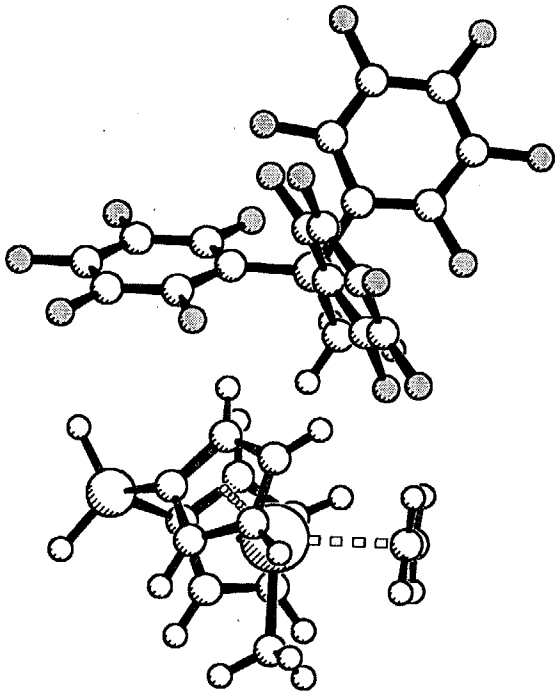
Isomers for complex 8a



E=31 kJ/mol
relative to **8a**

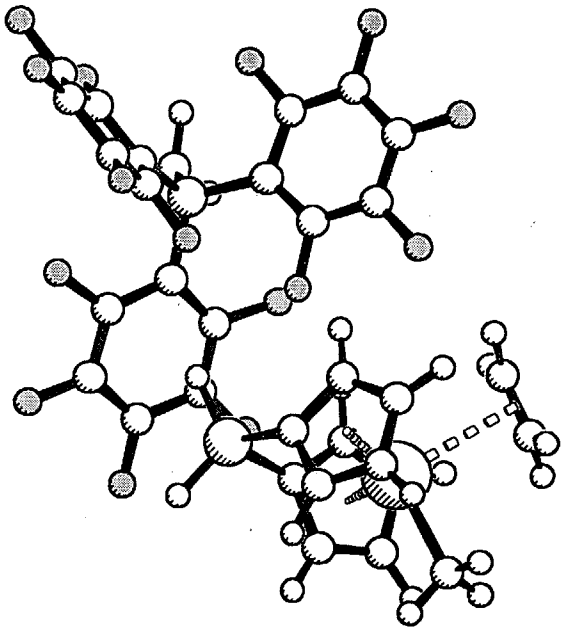
Isomers for complex 8c

Energies relative to **8c**



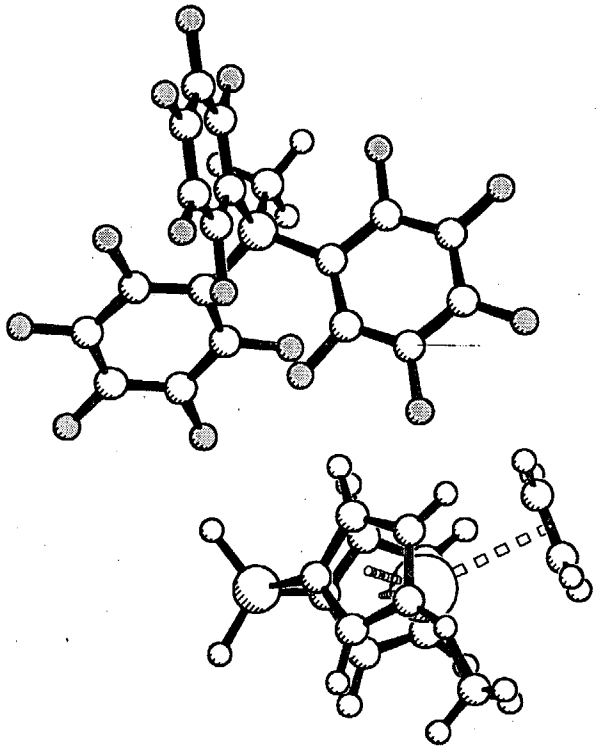
8c-2

E=6 kJ/mol



8c-3

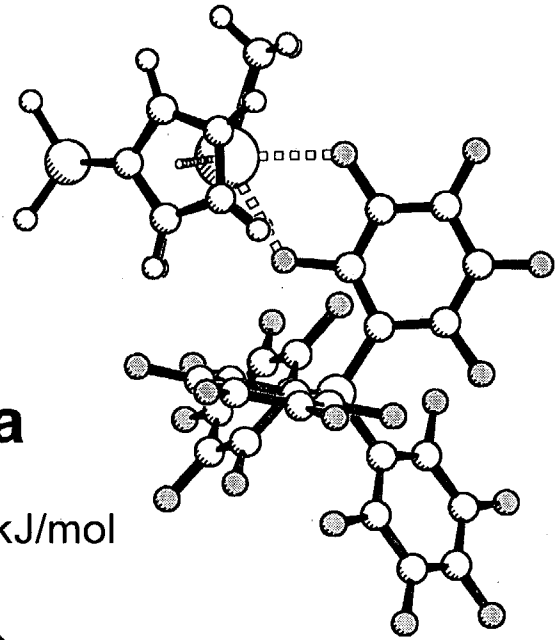
E=33 kJ/mol



8c-4

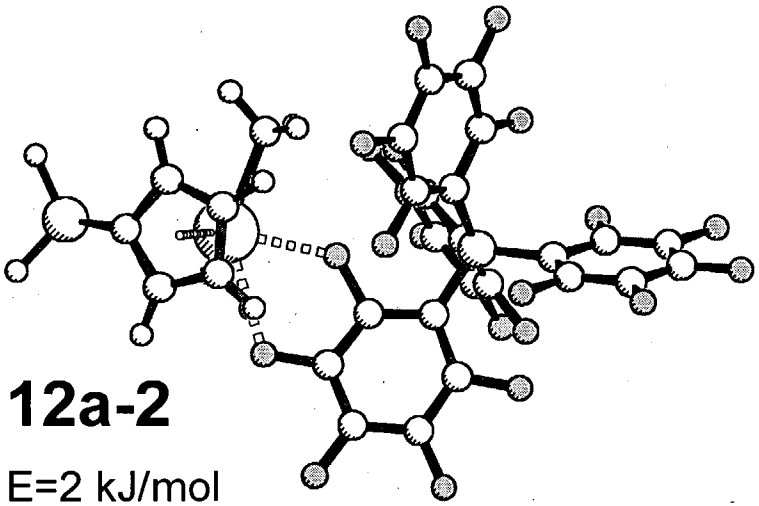
E=47 kJ/mol

Isomers for complex 12a



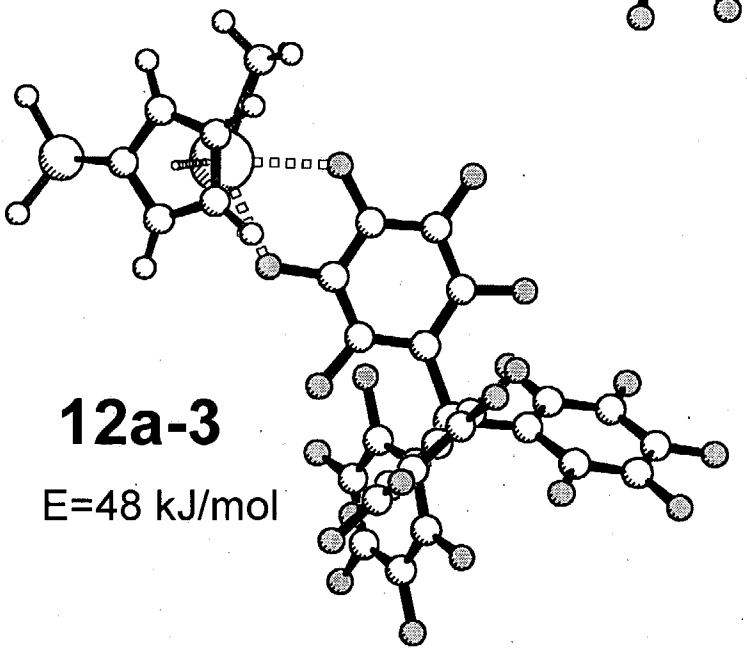
12a

E=0 kJ/mol



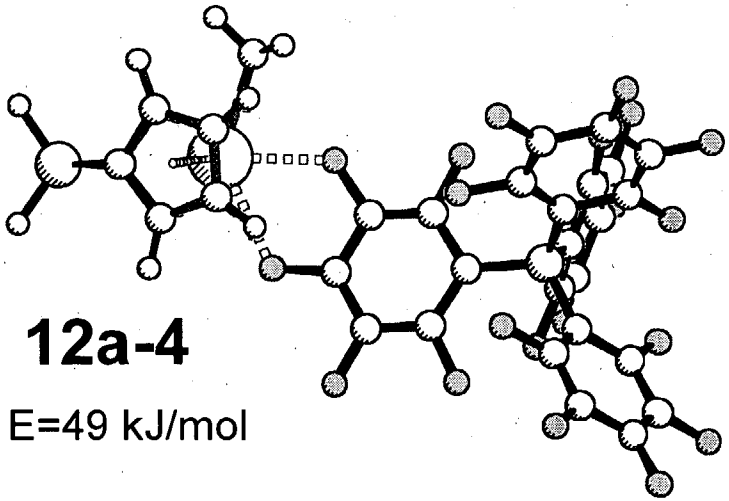
12a-2

E=2 kJ/mol



12a-3

E=48 kJ/mol



12a-4

E=49 kJ/mol

Calculated energies (in Hartree) and reactions energies (in kJ/mol) as well as zero point energies (kJ/mol) and entropies (J/(mol·K)) obtained from calculated second derivatives in the gas phase.

	SVP		TZVP		S	ZPE
	gas phase	toluene	gas phase	toluene	SVP, gas phase	
Me_2O	-154,913428	-154,915327	-155,088053	-155,090422	182,2	270,3
Ethene	-78,528697	-78,529646	-78,616465	-78,617689	116,4	232,7
Propene	-117,820312	-117,821329	-117,948768	-117,950082	182	269,8
8a	-3009,97636	-3009,98442	-3013,02694	-3013,03663	903	1209,1
9a	-1840,29334	-1840,30272	-1842,0637	-1842,07442	658,3	847
12a	-3697,39361	-3697,40314	-3701,21106	-3701,22233		
13a	-1550,85269	-1550,86285	-1552,534	-1552,5456	667,1	823,4
14a	-2147,36301	-2147,37251	-2149,43688	-2149,44783	874,3	948,5
8b	-3088,49008	-3088,49962	-3091,62828	-3091,63944		
9b	-1995,21617	-1995,2304	-1997,15964	-1997,17525	855,9	893,2
10b	-1918,81046	-1918,82343	-1920,66912	-1920,6836	782,9	899,9
11b	-1958,10214	-1958,11556	-1960,00101	-1960,01583	846,6	933,3
12b	-3775,91098	-3775,92671	-3779,82064	-3779,83799		
13b	-1705,77416	-1705,78985	-1707,62833	-1707,64553	867,3	859,8
14b	-2302,28122	-2302,29683	-2304,52968	-2304,54664	1063	1036
8c	-3088,48879	-3088,50081	-3091,62131	-3091,6346		
9c	-1995,22425	-1995,23844	-1997,16412	-1997,17934	845,8	957,8
10c	-1918,81278	-1918,82728	-1920,66942	-1920,68503		
11c	-1958,10811	-1958,12269	-1960,00459	-1960,02026	843,4	949,5
12c	-3775,91241	-3775,92609	-3779,82054	-3779,83576		
13c	-1705,78173	-1705,79688	-1707,63256	-1707,64884	854,7	935,5
14c	-2302,29518	-2302,30914	-2304,539	-2304,55403	1061	1075,8
10e	-1918,80874	-1918,81997	-1920,66719	-1920,67993	783,9	890,6
1-III	-3565,10799	-3565,11823	-3569,0017	-3569,013	[a]	
1-III	-3565,11227	-3565,12126	-3569,00205	-3569,01269	[b]	
C_2H_4-1-III	-3643,62226	-3643,64084	-3647,60648	-3647,62682	[a]	

five-coordinated intermediates $H_2Si(C_5H_4)ZrMe(OMe_2)^+MeB(CF_3)_3^-$, Zr-O fixed to 2.6 Å

-1995,21116	(attack in the middle position)
-1995,19549	(attack from methyl side)
-1995,20404	(attack from anion side)

12a-contact ion pair conformations

12a	-3697,3936
12a-2	-3697,39298
12a-3	-3697,37556
12a-4	-3697,37507

[a] reoptimized geometry from ref. 13d, [b] contact ion pair with alternative anion orientation.

Reaction energies relative to the contact ion pair + free Lewis base.

	SVP		TZVP		ZPE	S
	gas phase	toluene	gas phase	toluene	SVP, gas phase	
8b	39,3	37,9	39,7	39		
9b	-24,7	-32,4	-20,7	-27,3	15,4	-224,1
10b	30,4	23,4	29	22,3	8,2	-179,8
11b	30,2	22,3	30,1	22,8	6,3	-183,4
12b	29,7	15,9	18,1	5,3		
13b	-21,1	-30,6	-16,5	-25	18	-233,8
14b	-12,6	-23,6	-12,5	-22	6,5	-182,7
8c	42,7	34,8	58	51,7		
9c	-45,9	-53,5	-32,4	-38	5,3	-159,46
10c	24,3	13,3	28,2	18,6		
11c	14,5	3,6	20,7	11,1	3,1	-167,29
12c	26	17,6	18,3	11,2		
13c	-41	-49,1	-27,6	-33,6	5,4	-158,18
14c	-49,2	-55,9	-36,9	-41,4	4,5	-142,98
10e	34,9	32,5	34,1	32	9,2	-189,2
C_2H_4-1-III	37,9	18,5	30,7	10,2	[a]	
C_2H_4-1-III	49,1	26,4	31,6	9,4	[b]	

[a] reoptimized geometry from ref. 13d, [b] contact ion pair with alternative anion orientation.

Atomic coordinates in bohr

Complex **8a** :

E = -3009.9763529752 hartree

0.0000	0.0000	4.2755	zr
4.6057	0.0000	4.7800	c
0.0000	0.0000	0.0000	c
-3.1422	-2.5987	6.7190	c
-3.0936	2.6751	6.7127	c
-3.4182	3.3281	4.0902	c
-1.2311	4.6567	3.2404	c
0.5017	4.7850	5.2891	c
-0.6228	3.5474	7.4167	c
-4.8844	0.0568	8.3487	si
-0.6809	-3.5110	7.4108	c
0.4143	-4.7747	5.2829	c
-1.3259	-4.6116	3.2425	c
-3.4863	-3.2445	4.0981	c
7.6440	0.1543	5.7921	b
3.5368	-0.0409	6.6206	h
4.2488	1.7479	3.6741	h
4.3220	-1.7416	3.6494	h
1.0359	1.6873	-0.6976	h
-1.8933	0.0068	-0.9039	h
1.0222	-1.6980	-0.6910	h
-1.0635	-5.4131	1.3504	h
-5.1587	-2.8050	2.9500	h
-7.6392	0.0804	7.6947	h
-4.4487	0.0597	11.1434	h
0.2664	3.3265	9.2808	h
0.2069	-3.3078	9.2780	h
2.2610	-5.7153	5.2337	h
2.3561	5.7134	5.2725	h
-0.9500	5.4527	1.3485	h
-5.0948	2.9210	2.9365	h
8.2453	-2.3727	7.5572	c
9.4852	-2.3408	9.9150	c
10.0038	-4.5274	11.3381	c
9.2967	-6.9061	10.4023	c
8.0791	-7.0510	8.0508	c
7.6333	-4.8119	6.6979	c
9.6309	0.0546	3.3880	c
8.9824	-0.0836	0.8188	c
10.7544	-0.3264	-1.1487	c
13.3363	-0.4336	-0.5604	c
14.0962	-0.2748	1.9788	c
12.2491	-0.0425	3.8678	c
7.6948	2.8283	7.4283	c
6.1585	3.0956	9.5834	c
5.9848	5.2848	11.0637	c
7.4281	7.4057	10.3835	c
8.9735	7.2701	8.2332	c
9.0534	5.0262	6.7971	c
9.7779	-9.0025	11.7305	f
7.3593	-9.2963	7.1160	f
6.5213	-5.1360	4.3903	f
10.2728	-0.1589	10.9578	f
11.1781	-4.3572	13.5740	f
4.6924	1.1178	10.3660	f
4.4459	5.3716	13.0794	f
6.5256	0.0160	0.0657	f
9.9972	-0.4524	-3.5651	f
15.0593	-0.6694	-2.3959	f
16.5582	-0.3394	2.5648	f
13.1012	0.1449	6.2627	f
10.5352	5.1127	4.7297	f
10.3426	9.2848	7.5483	f
7.3234	9.5232	11.7586	f

Complex **8a**-fluorcoordination :

E = -3009.9645817603 hartree

-1.1781	0.2601	6.8275	zr
-0.5058	3.9011	-1.9025	c
-3.4549	-2.0638	9.6722	c
-1.1259	4.7437	8.3081	c
2.9196	1.4440	8.8406	c
2.1048	-0.8019	10.1388	c
2.2315	-2.8886	8.4337	c
3.0621	-1.9636	6.0548	c
3.4615	0.7011	6.2784	c
2.1127	4.7842	9.8175	si
-1.5091	4.7912	5.6155	c
-3.9782	3.8340	5.0747	c
-5.1277	3.1398	7.4004	c
-3.3751	3.6597	9.3853	c
0.0331	1.1285	-3.2204	b
-2.4519	4.5409	-2.3514	h
0.8006	5.3414	-2.6875	h
-0.2784	3.9582	0.1754	h
-2.8801	-4.0768	9.5176	h
-3.2540	-1.5149	11.6842	h
-5.4944	-1.9332	9.1939	h
-7.0252	2.3383	7.6324	h
-3.7176	3.3296	11.4033	h
1.9580	5.0444	12.6307	h
3.8205	6.7068	8.6440	h
4.1170	1.9338	4.7413	h
-0.1570	5.4719	4.1959	h
-4.8257	3.6842	3.1856	h
3.3699	-3.0891	4.3392	h
1.7667	-4.8574	8.8862	h
1.5246	-0.9106	12.1262	h
-1.9403	-1.0529	-1.9892	c
-3.4498	-2.8366	-3.2953	c
-5.0596	-4.6063	-2.1087	c
-5.2079	-4.7429	0.5439	c
-3.6955	-3.0490	1.8872	c
-2.1518	-1.3447	0.6145	c
2.8588	-0.1061	-2.5961	c
4.6572	0.8673	-0.9035	c
6.9785	-0.3147	-0.3563	c
7.5880	-2.6085	-1.5352	c
5.8593	-3.6745	-3.2456	c

3.5628	-2.4255	-3.7015	c
-0.4664	1.6218	-6.2652	c
-2.9137	2.1823	-7.1465	c
-3.4933	2.8479	-9.6470	c
-1.5270	3.0222	-11.4200	c
0.9581	2.5323	-10.6412	c
1.4327	1.8700	-8.1075	c
-6.7144	-6.3987	1.7048	f
-3.6589	-3.0046	4.5115	f
-0.6858	0.1029	2.3070	f
-3.4326	-2.9578	-5.8168	f
-6.4515	-6.1924	-3.4929	f
-4.9073	2.0835	-5.5312	f
-5.8830	3.3331	-10.3507	f
4.2512	3.0636	0.3755	f
8.5918	0.7192	1.3157	f
9.7878	-3.7625	-1.0445	f
6.4088	-5.8659	-4.3943	f
1.9765	-3.5671	-5.3426	f
3.8930	1.5014	-7.5199	f
2.8617	2.7260	-12.3073	f
-2.0210	3.6553	-13.8226	f

Complex **9a** :

E = -1840.2933388314 hartree

1.0026	-0.0069	-3.1850	zr
0.9440	-0.0238	1.4445	c
5.2630	-0.0166	-3.6359	c
-1.1827	2.6635	-6.4024	c
-1.1932	-2.6194	-6.4443	c
1.3410	-3.5984	-6.3284	c
1.6951	-4.8212	-3.9497	c
-0.5837	-4.5938	-2.5438	c
-2.3483	-3.2097	-4.0492	c
-2.3061	0.0413	-8.5520	si
-2.3346	3.2234	-3.9984	c
-0.5632	4.5745	-2.4722	c
1.7172	4.8119	-3.8750	c
1.3566	3.6283	-6.2722	c
-0.9843	4.6439	4.0703	f
-2.0711	2.3371	4.6504	c
-4.0278	2.1108	2.9180	f
-3.1726	2.6222	6.9340	f
1.8212	0.4182	8.7659	f
2.3884	0.3914	6.2618	c
3.6330	2.6226	5.7723	f
4.1770	-1.4604	5.9365	f
0.2078	-4.7371	4.5317	f
-1.4300	-2.7413	4.8773	c
-3.3330	-3.1740	3.1182	f
-2.5007	-3.0715	7.1718	f
-0.0580	-0.0052	4.4163	b
2.0331	1.7387	1.1140	h
-0.9429	-0.0596	0.4572	h
2.0660	-1.7699	1.1376	h
6.0355	-1.7287	-2.6962	h
6.0087	-0.0006	-5.5959	h
6.0461	1.6721	-2.6637	h
3.4474	5.7545	-3.2312	h
2.7799	3.5003	-7.7760	h
-0.9422	0.0588	-11.0314	h
-5.1170	0.0495	-8.8799	h
-4.2860	-2.7322	-3.4782	h
-4.2729	2.7444	-3.4309	h
-0.9093	5.2751	-0.5492	h
-0.9395	-5.3260	-0.6354	h
3.4199	-5.7841	-3.3217	h
2.7652	-3.4543	-7.8297	h

Complex **13a** :

E = hartree

-3.8354	0.0256	-0.5057	zr
0.8193	0.3093	-0.7688	c
-4.4386	-0.0527	-4.7600	c
-7.2948	2.8379	1.1122	c
-7.0192	-3.2584	0.6988	c
-5.6463	-4.3447	-1.3563	c
-3.1162	-4.7560	-0.5315	c
-2.9279	-3.9733	2.0486	c
-5.3360	-3.0514	2.8118	c
-5.2195	3.1189	2.8301	c
-3.2279	4.3801	1.5249	c
-4.0528	4.8449	-0.9993	c
-6.5700	3.9128	-1.2529	c
4.5732	4.7500	0.3120	f
4.5916	2.5374	1.6550	c
2.8157	2.9244	3.5659	f
6.8598	2.4129	2.8327	f
7.9789	0.0885	-2.4764	f
5.4264	0.0323	-2.7390	c
4.8051	2.0445	-4.2607	f
4.8817	-2.0766	-4.1588	f
3.1840	-4.6161	0.2881	f
4.2337	-2.5614	1.5183	c
2.9718	-2.4975	3.8214	f
6.6439	-3.2048	2.0521	f
3.8662	0.0697	-0.0696	b
0.4897	2.1391	-1.7261	h
-0.0323	0.2408	1.1833	h
0.3333	-1.3511	-1.9612	h
-3.3825	-1.6707	-5.5823	h
-6.4302	-0.2309	-5.3970	h
-3.6753	1.7153	-5.5958	h
-2.9470	5.7759	-2.4862	h
-7.7453	4.0287	-2.9540	h
-5.8290	-2.3578	4.7011	h
-5.1896	2.5498	4.8224	h
-1.3672	4.8553	2.3128	h
-1.2076	-4.0544	3.2054	h
-1.5685	-5.5658	-1.6486	h
-6.4122	-4.8054	-3.2236	h
-9.1486	2.0314	1.5662	h
-9.0369	-2.7847	0.6928	h

Complex **14a** :

E = -2147.3630120755 hartree

0.6482	2.6396	-0.2774	zr
0.6479	-2.0217	0.0288	c

4.3913	3.0960	1.7147	c
-0.6386	5.0167	-4.1136	c
-3.1100	5.3441	0.5563	c
-1.2243	6.3532	2.2870	c
-0.7425	4.4750	4.2423	c
-2.2357	2.2836	3.6564	c
-3.7217	2.8641	1.4857	c
-3.6140	6.4538	-2.7901	si
-0.2835	2.4590	-5.0390	c
2.4142	1.8723	-4.9661	c
3.6939	4.0402	-3.9491	c
1.8553	5.9340	-3.4887	c
-0.0396	-4.9566	0.9264	b
-1.2639	-1.2029	-0.3824	h
1.6143	-1.1552	1.6988	h
1.8726	-2.1068	-1.6616	h
4.3326	2.2248	3.6206	h
4.9537	5.1028	1.9541	h
5.8917	2.1287	0.6086	h
5.7379	4.2361	-3.6802	h
2.2785	7.8194	-2.7301	h
-3.6350	9.2778	-3.0285	h
-5.9523	5.3168	-3.9086	h
-5.0900	1.5602	0.6205	h
-2.3364	0.5293	4.7529	h
-1.2440	-4.8330	3.7767	c
-2.1092	-6.1257	-1.0643	c
2.6089	-6.5589	0.8947	c
3.3028	-0.5107	-5.8718	c
1.5590	-2.2559	-6.7606	c
-2.0212	0.5835	-5.9208	c
-1.0881	-1.7169	-6.7692	c
2.2090	-4.1101	-7.4340	h
-2.4063	-3.1732	-7.4420	h
5.3356	-0.9461	-5.8549	h
-4.0611	0.9816	-5.9719	h
0.0359	8.7430	2.4028	c
1.6380	9.2354	4.4209	c
0.9070	5.0517	6.2940	c
2.0627	7.4031	6.3623	c
2.5757	11.0867	4.5580	h
3.3209	7.8870	7.9454	h
-0.3394	10.2011	0.9675	h
1.2259	3.6531	7.7983	h
-1.1099	-6.6700	-3.3987	f
-3.2578	-8.2740	-0.2651	f
-4.0431	-4.4239	-1.5586	f
0.2026	-3.3660	5.3975	f
-3.5953	-3.6808	3.8170	f
-1.5398	-7.0859	4.9421	f
3.8572	-6.3506	-1.3835	f
4.3015	-5.6888	2.6627	f
2.3396	-9.0751	1.3267	f

Complex **12a** :

E = -3697.3936027012 hartree

-1.1475	7.1797	0.1146	zr
-4.2770	10.0787	-0.5627	c
1.5095	8.7839	3.6586	c
2.8797	9.0971	-1.3925	c
0.9261	10.3021	-2.8514	c
-0.1614	8.4799	-4.5169	c
1.0505	6.1240	-4.0768	c
2.9017	6.4811	-2.1416	c
4.1591	10.2271	1.7462	si
1.1726	6.1053	4.0199	c
-1.4038	5.6425	4.7016	c
-2.6953	7.9937	4.7074	c
-0.9295	9.9212	4.0366	c
0.0395	-3.0955	-0.2413	b
-4.9309	9.9280	-2.5500	h
-3.7989	12.0889	-0.2160	h
-5.8894	9.6034	0.6966	h
-4.6995	8.2802	5.1540	h
-1.3592	11.9432	3.8827	h
4.1477	13.0515	1.9271	h
6.6844	9.1128	2.3526	h
4.1588	5.0086	-1.3978	h
2.6430	4.6514	3.8463	h
-2.2325	3.7934	5.1405	h
0.6589	4.3404	-5.0627	h
-1.6731	8.8379	-5.8901	h
0.3852	12.3001	-2.7411	h
-2.6015	-1.6457	-1.2178	c
-4.6857	-2.7876	-2.4433	c
-6.8294	-1.4542	-3.3189	c
-6.9924	1.1807	-3.0305	c
-4.9363	2.3620	-1.8727	c
-2.8591	0.9709	-1.0743	c
2.0834	-2.1923	-2.4481	c
4.0181	-0.3976	-2.1678	c
5.6378	0.3588	-4.1369	c
5.3118	-0.6528	-6.5639	c
3.3789	-2.4277	-6.9631	c
1.8072	-3.1079	-4.9351	c
-0.2927	-6.1985	0.0123	c
-2.2766	-7.1654	1.4988	c
-2.6456	-9.7380	2.0186	c
-0.9175	-11.5024	1.0468	c
1.1144	-10.6439	-0.4223	c
1.3989	-8.0393	-0.8917	c
-8.9988	2.4855	-3.8191	f
-4.9086	4.9538	-1.4762	f
-0.9731	2.4973	-0.0110	f
-4.7618	-5.2775	-2.8514	f
-8.7205	-2.6852	-4.4449	f
-3.9926	-5.5549	2.5079	f
-4.6017	-10.5151	3.4315	f
4.4317	0.7869	0.0777	f
7.4366	2.1082	-3.7224	f
6.8176	0.0559	-8.4679	f
3.0318	-3.4149	-9.2678	f
-0.0553	-4.7621	-5.4699	f
3.4362	-7.4016	-2.2822	f
2.7836	-12.3074	-1.3530	f
-1.2105	-13.9724	1.5118	f
0.8609	-2.3162	2.6947	c
-0.7048	-1.2417	4.5491	c
-0.0069	-0.9339	7.0969	c
2.3873	-1.7277	7.9040	c
4.0290	-2.8371	6.1358	c
3.2335	-3.1119	3.6177	c
-3.0626	-0.3770	3.9805	f

-1.6123	0.1542	8.7409	f	
4.8888	-4.2309	2.0388	f	
6.3206	-3.6235	6.8704	f	
3.0959	-1.4413	10.3151	f	11

Compe x **12a**-2 :

E = -3697.3929790559 hartr

-0.0112	0.3871	-6.6965	zr
3.4471	2.5032	-5.3569	c
1.2605	-1.7520	-10.6849	c
-1.5306	2.7156	-10.4966	c
-0.2923	4.5953	-8.9731	c
-1.7311	4.9958	-6.7268	c
-3.8470	3.3451	-6.7973	c
-3.7255	1.9185	-9.0913	c
0.0450	0.6960	-12.9904	si
-0.3731	-3.4670	-9.3381	c
0.9306	-4.3581	-7.1452	c
3.3477	-3.1901	-7.0758	c
3.5468	-1.5693	-9.2223	c
0.0328	-0.1514	3.2780	b
2.7599	3.9864	-4.0387	h
4.6754	3.4412	-6.7719	h
4.6315	1.1638	-4.2673	h
4.7887	-3.4619	-5.6076	h
5.1961	-0.4055	-9.6902	h
2.1552	2.0712	-14.2774	h
-1.8059	-0.3924	-14.8335	h
-5.1150	0.5075	-9.7082	h
-2.2736	-4.0524	-9.9289	h
0.2003	-5.7199	-5.7605	h
-5.3181	3.2123	-5.3408	h
-1.2844	6.3181	-5.1933	h
1.4574	5.5916	-9.4654	h
-2.5463	-1.1134	1.7015	c
-4.7920	-2.1184	2.7474	c
-6.8092	-3.0993	1.2964	c
-6.6707	-3.1393	-1.3556	c
-4.4584	-2.1993	-2.4549	c
-2.5418	-1.2598	-0.9238	c
1.9641	-2.5567	2.6660	c
4.0045	-2.5286	0.9705	c
5.4171	-4.6811	0.3100	c
4.8084	-7.0289	1.3732	c
2.7846	-7.1716	3.0865	c
1.4122	-4.9709	3.6528	c
-0.4969	0.3330	6.3184	c
-2.4356	2.0028	7.0472	c
-2.9692	2.6658	9.5580	c
-1.4561	1.6664	11.4969	c
0.5357	0.0323	10.8742	c
0.9819	-0.5900	8.3252	c
-8.5538	-4.0509	-2.7662	f
-4.1270	-2.1529	-5.0289	f
-0.4382	-0.3942	-2.3310	f
-5.1446	-2.2219	5.2453	f
-8.8735	-4.0012	2.4314	f
-3.9446	3.0377	5.2556	f
-4.8802	4.2344	10.1211	f
4.7248	-0.3733	-0.2135	f
7.2922	-4.5051	-1.4077	f
6.1253	-9.0995	0.7600	f
2.1566	-9.3994	4.1142	f
-0.5636	-5.2650	5.2367	f
2.9565	-2.1466	7.9120	f
2.0081	-0.9158	12.7066	f
-1.9139	2.2674	13.9118	f
1.0901	2.6484	2.3032	c
-0.1928	4.4268	0.8078	c
0.7360	6.8559	0.2583	c
3.0728	7.6255	1.2364	c
4.4287	5.9372	2.7720	c
3.4170	3.5321	3.2631	c
-2.4721	3.8952	-0.2657	f
-0.5930	8.4291	-1.2494	f
4.8213	2.0135	4.7456	f
6.6647	6.6331	3.7334	f
3.9892	9.9277	0.7292	f

Compe x **12a**-3 :

E = -3697.3755546226 hartr

0.0000	0.0000	4.7093	zr
4.1050	0.0000	6.0187	c
0.0000	0.0000	0.0000	c
-0.9308	4.2605	2.9212	c
1.0992	4.6575	4.6855	c
0.1753	4.2459	7.1873	c
-2.4079	3.5380	7.0114	c
-3.0916	3.5097	4.3958	c
-0.5483	3.4900	-0.5490	si
-1.9566	-1.7135	0.8033	c
-0.8017	-3.8932	1.9098	c
1.8595	-3.5390	1.8533	c
2.3609	-1.1432	0.7188	c
-9.0161	-7.9651	11.6337	b
4.1792	0.7420	7.9813	h
5.4506	1.1319	4.8798	h
4.8136	-1.9746	6.0413	h
3.2806	-4.8728	2.5600	h
4.2440	-0.3354	0.4038	h
1.7210	4.7543	-1.6643	h
-2.9106	3.9836	-2.0223	h
-4.9740	3.0522	3.6522	h
-3.9983	-1.4368	0.5526	h
-1.8005	-5.5579	2.6466	h
-3.6682	3.1106	8.6042	h
1.2687	4.4435	8.9373	h
3.0307	5.2336	4.2008	h
-6.2258	-6.7031	10.8231	c
-3.8894	-7.0559	12.0513	c
-1.6182	-5.7956	11.3810	c
-1.7456	-4.0668	9.4012	c
-4.0227	-3.6289	8.1680	c
-6.2188	-4.8982	8.8582	c
-10.4674	-5.4117	12.7583	c
-12.4484	-4.0743	11.5946	c
-13.4894	-1.8379	12.5963	c
-12.5075	-0.8177	14.8362	c
-10.5057	-2.0629	16.0547	c
-9.5284	-4.2812	14.9787	c

-8.8187	-10.3119	13.6972	c
-7.3324	-12.4398	13.1117	c
-7.2154	-14.6372	14.5917	c
-8.6840	-14.7796	16.7979	c
-10.2130	-12.7219	17.4649	c
-10.2685	-10.5606	15.9132	c
0.3209	-2.6948	8.5443	f
-3.9461	-1.8586	6.2154	f
-8.3183	-4.3301	7.5627	f
-3.6438	-8.6501	13.9946	f
0.5495	-6.2293	12.5962	f
-5.8897	-12.4248	10.9969	f
-5.7442	-16.5935	13.9215	f
-13.4683	-4.8527	9.3939	f
-15.3850	-0.6487	11.4003	f
-13.4623	1.3217	15.7991	f
-9.5365	-1.1082	18.1969	f
-7.5666	-5.3591	16.2122	f
-11.8472	-8.7191	16.6901	f
-11.6337	-12.8336	19.5621	f
-8.6236	-16.8564	18.2450	f
-10.4419	-9.3141	9.1851	c
-9.3269	-9.9800	6.8695	c
-10.5955	-11.2896	4.9351	c
-13.1077	-12.0431	5.3011	c
-14.3074	-11.4616	7.5961	c
-12.9556	-10.1489	9.4640	c
-6.8889	-9.3745	6.3346	f
-9.4109	-11.8346	2.7530	f
-14.2091	-9.6713	11.6314	f
-16.7100	-12.1725	7.9812	f
-14.3493	-13.2914	3.4807	f

Complex **12a**-4 :

E = -3697.3750721584 hartree

0.0000	0.0000	4.7168	zr
4.0945	0.0000	6.0326	c
0.0000	0.0000	0.0000	c
-0.9595	4.2524	2.9355	c
1.0717	4.6600	4.6983	c
0.1544	4.2393	7.2000	c
-2.4233	3.5085	7.0278	c
-3.1125	3.4864	4.4124	c
-0.5832	3.4865	-0.5363	si
-1.9307	-1.7375	0.8135	c
-0.7402	-3.8997	1.9215	c
1.9146	-3.5113	1.8521	c
2.3772	-1.1092	0.7146	c
-4.0117	-5.9263	16.5247	b
4.1705	0.7843	7.9772	h
5.4712	1.0724	4.8736	h
4.7588	-1.9901	6.1072	h
3.3568	-4.8230	2.5575	h
4.2480	-0.2747	0.3954	h
1.6681	4.7702	-1.6656	h
-2.9576	3.9582	-1.9984	h
-4.9919	3.0188	3.6682	h
-3.9758	-1.4891	0.5627	h
-1.7067	-5.5791	2.6653	h
-3.6707	3.0724	8.6287	h
1.2466	4.4357	8.9510	h
2.9994	5.2478	4.2121	h
-4.2851	-4.6283	13.6453	c
-6.5424	-4.3181	12.2662	c
-6.6643	-3.4141	9.7466	c
-4.3877	-2.8313	8.5639	c
-2.1160	-3.1345	9.8515	c
-2.0443	-4.0284	12.3251	c
-2.6786	-8.6705	15.7673	c
-0.1744	-9.4095	16.2736	c
0.8761	-11.7050	15.4269	c
-0.5823	-13.3530	13.9512	c
-3.0820	-12.6878	13.3605	c
-4.0433	-10.3844	14.2543	c
-6.7479	-6.1921	18.0240	c
-8.1745	-3.9948	18.4884	c
-10.4012	-3.9293	19.9243	c
-11.2936	-6.1821	21.0071	c
-9.9454	-8.4283	20.6121	c
-7.7105	-8.3906	19.1664	c
-4.2275	-1.9292	6.1159	f
0.0622	-2.4578	8.5057	f
0.2325	-4.3006	13.3892	f
-8.7960	-4.8795	13.2590	f
-8.8651	-3.1408	8.5389	f
-7.4137	-1.7635	17.4862	f
-11.6691	-1.7586	20.2777	f
1.4114	-7.9233	17.6018	f
3.2772	-12.3052	15.9835	f
0.3935	-15.5332	13.1085	f
-4.5016	-14.2306	11.9305	f
-6.4489	-9.8398	13.5805	f
-6.5209	-10.6322	18.9535	f
-10.7828	-10.5934	21.6332	f
-13.4110	-6.1839	22.3961	f
-2.3283	-4.1584	18.4930	c
-1.6650	-1.6081	18.1767	c
-0.4297	-0.1569	20.0314	c
0.1580	-1.2548	22.3693	c
-0.4920	-3.7914	22.8024	c
-1.7176	-5.1557	20.8863	c
-2.1986	-0.3496	16.0027	f
0.1638	2.2733	19.5836	f
-2.3148	-7.5717	21.4352	f
0.0435	-4.8697	25.0333	f
1.3286	0.0924	24.1668	f

Complex **8b** :

E = -3088.4900792975 hartree

0.0000	0.0000	4.4021	zr
5.3067	0.0000	2.9159	c
4.6898	2.4777	2.6875	c
0.0000	0.0000	0.0000	c
-4.3385	1.6783	5.1259	c
-3.1610	-3.4307	5.1334	c
-1.8023	-4.2029	2.9158	c
0.7313	-4.8154	3.6149	c
0.9776	-4.4373	6.2642	c
-1.3822	-3.5388	7.2021	c
-6.1122	-1.4206	5.1992	si

-2.7994	2.5461	7.2074	c				
-1.0770	4.4033	6.2873	c				
-1.4489	4.6421	3.6344	c				
-3.4521	2.9816	2.9179	c				
1.3874	-1.3980	-0.7261	h				
-1.8411	-0.4919	-0.8720	h				
0.5164	1.8883	-0.7535	h				
-0.4262	5.9299	2.3727	h				
-4.2141	2.7764	1.0037	h				
-7.6801	-1.7905	2.8724	h				
-7.6180	-1.7621	7.5690	h				
-1.7859	-3.1080	9.1897	h				
5.1826	-1.2940	1.2923	h				
6.1423	-0.7484	4.6668	h				
-2.9718	1.9513	9.1852	h				
0.2956	5.4580	7.4296	h				
4.9807	3.8400	4.2345	h				
4.0314	3.2468	0.8722	h				
2.6651	-4.7762	7.4157	h				
2.2043	-5.5229	2.3389	h				
-2.5882	-4.3419	1.0063	h				
4.5375	2.0738	11.5767	b				
4.8438	0.0284	13.9346	c				
4.1055	-2.5188	13.9408	c				
4.2412	-4.1057	16.0709	c				
5.1560	-3.1317	18.3578	c				
5c9426	-0.59759	4172	5.7588	0.9009			
2.5273	4.2406	12.6703	c				
3.1076	6.7656	13.2946	c				
1.3349	8.4922	14.2763	c				
-1.1613	7.7134	14.7149	c				
-1.8338	5.2062	14.1727	c				
0.0121	3.5600	13.2118	c				
5.2869	-4.5997	20.4146	f				
6.8455	0.3512	20.6289	f				
6.5603	3.3127	16.4959	f				
3.1722	-3.6503	11.8201	f				
3.4891	-6.5261	15.9350	f				
5.4582	7.6925	12.9977	f				
2.0136	10.8720	14.8137	f				
-2.8689	9.3335	15.6389	f				
-4.2105	4.4025	14.5620	f				
-0.8052	1.1446	12.8047	f				
7.2634	3.2590	10.5811	c				
9.6913	2.4137	11.2688	c				
11.9475	3.4143	10.2642	c				
11.8423	5.3154	8.4208	c				
9.4686	6.1965	7.6269	c				
7.2935	5.1523	8.7172	c				
10.0121	0.5351	12.9590	f				
14.1948	2.5360	11.0334	f				
5.0605	6.1066	7.8169	f				
9.2930	7.9805	5.8288	f				
13.9663	6.2646	7.4272	f				
3.3040	0.6889	8.9789	c				
4.6033	-0.8069	8.3233	h				
3.1256	2.2143	7.5449	h				
1.4541	-0.1408	9.4513	h				

Complex **9b** :

E = -1995.2161662063 hartree

0.7701	0.1667	-4.2494	zr
4.0858	0.8802	-1.5874	o
-0.8815	-1.5230	2.3230	c
3.5536	1.5092	-7.2679	c
-3.4351	1.7126	-5.8139	c
-1.7410	-3.2069	-6.4501	c
0.7468	-3.3554	-7.5265	c
2.4569	-4.2588	-5.6445	c
1.0665	-4.6444	-3.3759	c
-1.4982	-3.9619	-3.8433	c
-4.4448	-1.1916	-7.6217	si
-3.4755	1.8534	-3.0924	c
-1.8068	3.8147	-2.2907	c
-0.6634	4.8597	-4.4874	c
-1.6353	3.5648	-6.6474	c
0.3301	3.9820	3.3132	f
-1.0975	2.6781	5.1586	c
-3.5442	3.2422	4.5209	f
-0.6141	3.9360	7.3375	f
3.2600	-3.2555	5.5895	f
2.3995	-0.8635	6.1493	c
2.8206	-0.5301	8.6528	f
4.1786	0.7147	4.9573	f
-1.8870	-4.3246	7.3834	f
-2.5644	-1.8229	7.0421	c
-4.9216	-1.8510	6.0767	f
-2.7189	-0.8216	9.4088	f
-0.5021	-0.3619	5.1703	b
0.3749	-0.5624	0.9252	h
-2.8621	-1.2890	1.6883	h
-0.4395	-3.5696	2.2755	h
5.2417	0.2617	-7.1801	h
2.9218	1.5569	-9.2641	h
4.1553	3.4586	-6.7643	h
0.6995	6.4226	-4.5399	h
-1.1218	3.9568	-8.6166	h
-4.3203	-0.7904	-10.4209	h
-6.9664	-2.1768	-6.7985	h
-3.0251	-4.0707	-2.4440	h
-4.6472	0.7102	-1.8201	h
-1.4708	4.3674	-0.3179	h
1.7983	-5.3552	-1.5706	h
4.4814	-4.6135	-5.9249	h
1.2491	-2.8968	-9.4837	h
4.6966	3.3582	-0.5552	c
5.8130	-1.0096	-0.5914	c
5.3778	-2.8246	-1.5073	h
5.5629	-1.1484	1.4800	h
7.7735	-0.4377	-1.0645	h
3.4710	4.7548	-1.4903	h
6.7034	3.7826	-0.9837	h
4.3354	3.3452	1.5029	h

Complex **13b** :

E = -1705.7728016481 hartree

0.0000	0.0000	4.3162	zr
4.3007	0.0000	4.0881	o
3.7987	-0.2361	10.8843	c

0.0000	0.0000	0.0000	c
-3.5767	2.7434	5.9271	c
-3.6240	-3.0389	4.9261	c
-2.1000	-4.1549	3.0078	c
0.2609	-4.8333	4.1169	c
0.1784	-4.1737	6.7347	c
-2.2108	-3.0487	7.2368	c
-1.4162	3.2688	7.4559	c
0.4052	4.5279	5.9069	c
-0.6098	4.7289	3.4255	c
-3.0648	3.6027	3.4228	c
5.5686	5.1391	8.8508	f
5.0606	4.6402	11.4190	c
2.5103	5.1593	11.6310	f
6.2553	6.5131	12.6834	f
9.4414	-1.2838	12.0106	f
8.6814	1.0987	11.3563	c
10.4878	2.6970	12.2275	f
8.9945	1.1482	8.7035	f
5.7009	-1.0660	16.0549	f
5.5230	1.4157	15.3051	c
3.2108	2.2223	16.1880	f
7.2826	2.6916	16.6958	f
5.7772	1.7364	12.2298	b
3.5098	0.2376	8.8537	h
1.9255	-0.1859	11.8248	h
4.5028	-2.2092	10.9925	h
1.0425	-1.6865	-0.6923	h
-1.8714	0.0056	-0.9459	h
1.0178	1.7102	-0.6727	h
0.2994	5.6224	1.7913	h
-4.3485	3.4878	1.8006	h
-2.8535	-2.3627	9.0831	h
-1.1803	2.8950	9.4805	h
2.2368	5.2206	6.5930	h
1.6791	-4.4336	8.1432	h
1.8309	-5.7534	3.1234	h
-2.6546	-4.4640	1.0382	h
5.7470	2.2340	3.3763	c
6.0371	-2.0491	4.6948	c
4.9331	-3.6424	5.4390	h
7.3861	-1.3820	6.1457	h
7.0316	-2.6200	2.9398	h
4.4169	3.6510	2.6346	h
7.1012	1.6998	1.8701	h
6.7456	2.9571	5.0663	h
-5.3438	1.8801	6.5776	h
-5.5713	-2.3748	4.6831	h

Complex **14b** :

E = -2302.2812238156 hartree

-0.0250	0.0184	4.2404	zr
4.2385	0.0319	3.9742	o
4.6806	1.8079	10.6759	c
-0.0009	-0.0609	-0.0288	c
-3.8481	2.5949	5.0758	c
-3.7372	-2.6873	5.2102	c
-2.4610	-3.8957	3.1382	c
-0.0918	-4.8789	3.9559	c
0.0789	-4.5142	6.6492	c
-2.1458	-3.1024	7.4249	c
-6.1857	-0.0909	5.0588	si
-2.0951	3.0426	7.1298	c
-0.0178	4.5107	6.2797	c
-0.4801	5.1571	3.6854	c
-2.8543	3.9902	2.9257	c
5.8454	6.0138	6.7984	f
6.2910	6.4579	9.3891	c
4.0645	7.5636	10.1776	f
8.0465	8.3225	9.4230	f
10.1342	0.2997	10.7872	f
9.6294	2.6696	9.8678	c
11.7494	4.0543	10.2764	f
9.5916	2.3038	7.2220	f
8.0221	2.4602	15.3638	f
7.3094	4.5352	13.9684	c
5.0868	5.3456	15.0531	f
9.0467	6.3677	14.5119	f
6.9793	3.8683	10.9533	b
4.2209	1.3848	8.6695	h
2.9319	2.5081	11.5966	h
5.1811	-0.0050	11.6001	h
1.2608	-1.6416	-0.6027	h
-1.8340	-0.3160	-1.0045	h
0.8108	1.7457	-0.7287	h
-7.6401	-0.2101	2.6330	h
-7.9336	-0.0998	7.2894	h
-2.3067	2.3664	9.0777	h
1.5545	5.1969	7.4411	h
1.2504	-5.9350	2.7805	h
-3.1775	-4.0012	1.1976	h
5.5718	2.0023	2.5869	c
6.0039	-1.8774	4.8587	c
5.0005	-3.0872	6.2204	h
7.5957	-0.9227	5.8197	h
6.6723	-2.9954	3.2153	h
4.1530	3.3528	1.8773	h
6.5698	1.1172	0.9703	h
6.8976	2.9559	3.8892	h
1.8462	-5.3553	8.5074	c
-2.5156	-2.5272	10.0392	c
-0.7438	-3.3427	11.7914	c
1.4229	-4.7581	11.0276	c
-1.0214	-2.9308	13.8093	h
2.7611	-5.4131	12.4770	h
-3.8382	4.4705	0.4616	c
-2.4886	6.0284	-1.1584	c
-0.1466	7.1615	-0.4126	c
0.8648	6.7512	1.9716	c
2.6132	7.6868	2.5971	h
-4.2278	-1.5238	10.6620	h
3.4647	-6.5420	7.9633	h
-5.6572	3.6510	-0.1231	h
-3.2468	6.4429	-3.0502	h
0.8323	8.4221	-1.7459	h

Complex **10b** :

E = -1918.8104553393 hartree

0.0000	0.0000	4.3727	zr
5.2200	0.0000	3.2121	c

4.5510	2.4785	3.2409	c
3.8052	1.3023	9.4051	c
0.0000	0.0000	0.0000	c
-4.3617	1.4824	5.3181	c
-2.9158	-3.5497	5.3424	c
-1.6461	-4.2951	3.0562	c
0.9483	-4.7633	3.6196	c
1.3271	-4.3068	6.2460	c
-1.0211	-3.5206	7.3087	c
-5.9693	-1.7014	5.5310	si
-2.7537	2.4419	7.3042	c
-1.1594	4.3485	6.2666	c
-1.6922	4.5500	3.6358	c
-3.6528	2.7937	3.0468	c
2.8482	-3.8256	11.7474	f
4.3553	-2.1219	13.0939	c
6.7719	-2.7377	12.3882	f
4.1229	-2.8252	15.5494	f
-0.0990	3.7747	12.5872	f
0.7754	1.4771	13.4751	c
0.4543	1.5385	16.0084	f
-1.0411	-0.2426	12.5942	f
5.0625	5.2515	13.3859	f
5.6808	2.7520	13.7754	c
8c0607	2.4 559	3983	5.9592
3.6289	0.8226	12.4697	b
2.2162	0.2707	8.4347	h
5.6153	0.5747	8.6517	h
3.6643	3.3416	8.9714	h
1.4134	-1.3661	-0.7358	h
-1.8308	-0.5144	-0.8805	h
0.4870	1.9086	-0.7283	h
-0.8006	5.8643	2.3031	h
-4.5014	2.5249	1.1761	h
-7.6112	-2.1930	3.2782	h
-7.3500	-2.0803	7.9676	h
-1.2922	-3.0289	9.3062	h
5.1799	-1.1121	1.4552	h
6.0045	-0.9174	4.9075	h
-2.7683	1.8653	9.2961	h
0.2106	5.4676	7.3468	h
4.7805	3.6218	4.9638	h
3.9513	3.4552	1.5047	h
3.0798	-4.5303	7.3300	h
2.3799	-5.4206	2.2719	h
-2.5308	-4.5081	1.1957	h

Complex **12b** :
E = -3775.9109749178 hartree

0.0000	0.0000	4.3279	zr
5.1909	0.0000	3.5518	c
4.5849	2.4975	3.5776	c
0.0000	0.0000	0.0000	c
-4.1266	1.6368	5.9475	c
-2.8399	-3.4125	5.9291	c
-2.1905	-4.1455	3.3872	c
0.4198	-4.7940	3.3077	c
1.4477	-4.4051	5.7671	c
-0.5442	-3.5390	7.3759	c
-5.6677	-1.4470	6.9295	si
-2.1686	2.8622	7.3721	c
-0.8391	4.5626	5.7454	c
-1.9387	4.3893	3.2920	c
-3.9200	2.5720	3.3963	c
1.3429	-1.4248	-0.7578	h
-1.8634	-0.4374	-0.8565	h
0.5586	1.8828	-0.7439	h
-1.3757	5.4773	1.6203	h
-5.1273	2.0200	1.8029	h
-7.9429	-2.0028	5.3445	h
-6.1088	-1.6306	9.6993	h
-0.3547	-3.0620	9.3854	h
5.1095	-1.1269	1.8038	h
5.9906	-0.9048	5.2451	h
-1.8167	2.5806	9.3945	h
0.6704	5.8619	6.3220	h
4.9023	3.6397	5.2867	h
3.9859	3.4889	1.8477	h
3.3938	-4.8057	6.3590	h
1.4495	-5.4871	1.6473	h
-3.4993	-4.2392	1.7814	h
-1.0335	2.9339	17.0164	b
-3.3561	4.0072	15.1656	c
-5.2773	2.5637	14.0249	c
2.4827	-7.1863	13.5783	12.3567
-6.9889	6.1397	11.6963	c
-5.0904	7.6618	12.7512	c
-3.3345	6.5647	14.4131	c
1.4466	3.2531	15.0795	c
3.3641	5.0934	15.2248	c
5.2534	5.4222	13.3665	c
5.2411	3.8957	11.2056	c
3.3633	2.0437	10.9869	c
1.5452	1.7702	12.8817	c
-1.4433	-0.0155	18.0052	c
-3.6368	-0.6124	19.3924	c
-4.1147	-2.9813	20.4880	c
-2.2956	-4.8995	20.2557	c
-0.0648	-4.4023	18.9183	c
0.3231	-1.9933	17.8597	c
-8.6742	7.1139	10.0747	f
-4.9542	10.1186	12.1363	f
-1.5382	8.1344	15.3147	f
-5.4918	0.0502	14.4332	f
-8.8761	2.0850	11.3160	f
-5.4469	1.1572	19.7083	f
-6.2647	-3.4264	21.7581	f
3.5090	6.7116	17.1652	f
7.0263	7.2052	13.6312	f
6.9704	4.1996	9.3581	f
3.2985	0.5521	8.8550	f
-0.2416	-0.0335	12.4656	f
2.5641	-1.6981	16.6577	f
1.6954	-6.2170	18.6716	f
-2.6916	-7.1789	21.2884	f
-0.7095	4.5163	19.6964	c
-2.4700	6.1940	20.7661	c
-2.1486	7.3316	23.1503	c
-0.0070	6.7564	24.5995	c
1.7942	5.0649	23.6330	c
1.3929	3.9933	21.2421	c
-4.6209	6.8177	19.5442	f
-3.8846	8.9427	24.0588	f

3.1963	2.3797	20.4130	f
3.8540	4.4880	24.9970	f
0.3210	7.8121	26.8781	f

Complex **8c** :
E = -3088.4887899096 hartree

0.0000	0.0000	4.6916	zr
3.9782	0.0000	6.2780	c
0.0000	0.0000	0.0000	c
-1.1199	-4.2014	2.9063	c
-3.2827	-3.3344	4.3060	c
-2.6782	-3.3536	6.9392	c
-0.1355	-4.2007	7.2002	c
0.8364	-4.6938	4.7340	c
-0.6725	-3.4729	-0.5718	si
2.4244	1.0130	0.7140	c
2.0593	3.4245	1.8560	c
-0.5826	3.9240	1.9138	c
-1.8620	1.8169	0.7997	c
-11.8322	2.0509	0.9601	b
3.9331	-0.7581	8.2383	h
4.6963	1.9749	6.3402	h
-1.4740	5.6645	2.6024	h
-3.9186	1.6335	0.5640	h
-2.9875	-3.9430	-2.1047	h
1.6288	-4.7656	-1.5958	h
2.7504	-5.3713	4.3102	h
4.2590	0.0981	0.3976	h
3.5545	4.6848	2.5445	h
0.8936	-4.4530	8.9821	h
-3.9949	-2.8700	8.4660	h
-5.0971	-2.7607	3.4805	h
-11.8982	-0.4240	-0.9879	c
-13.9698	-1.1541	-2.4877	c
-13.9858	-3.3450	-4.0039	c
-11.8485	-4.9102	-4.0863	c
-9.7309	-4.2638	-2.6270	c
-9.8214	-2.0678	-1.1510	c
-11.8505	0.6829	3.8259	c
-9.7857	0.3041	5.4452	c
-9.9423	-0.7726	7.8645	c
-12.2600	-1.6725	8.7668	c
-14.3787	-1.4611	7.1877	c
-14.1225	-0.3431	4.7857	c
-11.8289	-6.9935	-5.5274	f
-7.6466	-5.7315	-2.6818	f
-7.6658	-1.5481	0.1911	f
-16.0986	0.2328	-2.5665	f
-16.0224	-3.9427	-5.3905	f
-7.3875	0.9796	4.7412	f
-7.8475	-0.9518	9.3568	f
-12.4460	-2.7153	11.0662	f
-16.6165	-2.3490	7.9732	f
-16.2458	-0.3317	3.3863	f
-9.3317	3.8697	0.3708	c
-8.3406	4.1800	-2.0849	c
-6.3784	5.8683	-2.7148	c
-5.2909	7.3597	-0.8148	c
-6.2489	7.1675	1.6464	c
-8.2572	5.5122	2.1657	c
-9.2767	2.8517	-4.0502	f
-5.5202	6.0364	-5.0950	f
-9.1189	5.5780	4.5780	f
-5.1210	8.4860	3.5395	f
-3.3322	8.8965	-1.3160	f
-1.0103	3.0950	8.5618	c
-0.4594	1.6443	9.9581	h
-3.4499	3.3567	7.8197	c
-4.0678	4.9034	6.5686	h
-4.9371	2.0547	8.4700	h
0.4477	4.4850	8.0196	h
5.4156	-1.1212	5.2416	h
-14.1970	4.0571	0.6838	c
-14.2063	4.9370	-1.2201	h
-13.9665	5.6208	2.0672	h
-16.0849	3.2209	0.9862	h

Complex **9c** :

E = -1995.2242505908 hartree

0.0000	0.0000	4.2691	zr
4.0071	0.0000	5.6084	o
0.0000	0.0000	0.0000	c
-3.4122	2.8539	5.9284	c
-3.6944	-2.3999	5.9729	c
-3.3244	-3.3831	3.4656	c
-1.0031	-4.7425	3.3945	c
0.1247	-4.6070	5.8316	c
-1.5053	-3.1521	7.4176	c
-5.8034	0.3494	6.7992	si
-1.1767	3.3487	7.4071	c
0.6168	4.6395	5.8545	c
-0.4276	4.8721	3.3966	c
-2.8881	3.7576	3.4246	c
1.2556	-1.6197	-0.4733	h
-1.8068	-0.2853	-1.0213	h
0.8592	1.7653	-0.7415	h
-8.1009	0.4621	5.1519	h
-6.4647	0.4343	9.5516	h
-0.9433	2.9149	9.4238	h
2.4745	5.3368	6.4579	h
-0.1744	-5.7285	1.7727	h
-4.6258	-3.1401	1.8691	h
6.0100	0.8561	3.9324	c
4.8679	-0.4807	8.1546	c
3.2083	-1.0492	9.2835	h
5.6923	1.2762	8.9522	h
6.2817	-2.0206	8.1154	h
5.1844	1.0729	2.0274	h
7.5076	-0.5986	3.8363	h
6.7393	2.6949	4.6299	h
1.9330	-5.4919	6.3379	h
-1.2034	-2.7418	9.4307	h
-4.1708	3.6468	1.7993	h
0.4816	5.7684	1.7637	h
8.7900	-9.9279	0.7871	c
12.7361	-5.5053	1.8192	f
10.4748	-5.1451	0.6144	c
10.9670	-5.4477	-1.9017	f
9.9765	-2.5699	0.8817	f
5.8775	-7.6987	5.7994	f
8.1353	-6.8654	4.7639	c

8.4063	-4.4202	5.7599	f
9.9557	-8.2305	5.9442	f
3.5702	-7.7951	0.9026	f
5.5114	-6.1109	0.4924	c
5.5109	-5.6803	-2.0401	f
4.5713	-3.8305	1.5299	f
8.2335	-7.0230	1.6606	b
10.7064	-10.5369	1.3761	h
8.6812	-10.1385	-1.2955	h
7.4200	-11.2767	1.6250	h

Complex **13c** :

E = -1705.7817316058 hartree

0.0000	0.0000	4.2772	zr
4.0832	0.0000	5.4242	o
0.0000	0.0000	0.0000	c
-3.4715	3.1434	5.0933	c
-3.4066	-2.6733	6.2501	c
-3.3021	-3.4439	3.6658	c
-0.9311	-4.6555	3.2544	c
0.4457	-4.6228	5.5667	c
-1.0782	-3.3857	7.4240	c
-1.8810	3.1906	7.2912	c
0.4716	4.2772	6.5730	c
0.3698	4.8478	3.9416	c
-2.0836	4.1835	3.0363	c
1.3057	-1.5738	-0.4898	h
-1.8144	-0.3760	-0.9825	h
0.7770	1.7853	-0.7805	h
-5.0169	-1.7735	7.1932	h
-5.4427	2.5098	5.0258	h
-2.4147	2.5843	9.2004	h
2.0926	4.5928	7.8270	h
-0.2393	-5.4920	1.4920	h
-4.7981	-3.1832	2.2546	h
5.9961	0.8536	3.6443	c
5.0907	-0.5133	7.9087	c
3.4945	-1.0462	9.1408	h
6.0057	1.2204	8.6578	h
6.4681	-2.0810	7.7775	h
5.0709	1.0745	1.7869	h
7.4826	-0.6052	3.4676	h
6.7691	2.6881	4.3053	h
2.3384	-5.4352	5.8197	h
-0.6108	-3.1191	9.4278	h
-2.7823	4.4434	1.1056	h
1.8919	5.6923	2.8145	h
8.8527	-9.9477	0.3833	c
12.7749	-5.4832	1.2926	f
10.4759	-5.1427	0.1530	c
10.9003	-5.4368	-2.3767	f
9.9614	-2.5747	0.4401	f
6.0598	-7.7316	5.4744	f
8.2760	-6.8756	4.3654	c
8.5432	-4.4224	5.3421	f
10.1453	-8.2119	5.5009	f
3.5882	-7.8208	0.6878	f
5.5257	-6.1649	0.1610	c
5.4478	-5.8184	-2.3839	f
4.6342	-3.8506	1.1537	f
8.2856	-7.0464	1.2611	b
10.7862	-10.5382	0.9337	h
8.7029	-10.1627	-1.6964	h
7.5124	-11.3076	1.2509	h

Complex **14c** :

E = -2302.2951827579 hartree

0.0000	0.0000	4.2295	zr
4.1215	0.0000	5.1623	o
0.0000	0.0000	0.0000	c
-3.3377	2.8791	5.8565	c
-3.6841	-2.3902	5.8863	c
-3.1768	-3.4505	3.4275	c
-0.8498	-4.7815	3.4512	c
0.1015	-4.7435	5.9993	c
-1.6368	-3.2449	7.5173	c
-5.7926	0.3929	6.5574	si
-1.1324	3.2691	7.4192	c
0.7612	4.5745	6.0320	c
-0.2323	5.1243	3.5694	c
-2.7745	4.0627	3.4460	c
1.4618	-1.4655	-0.4034	h
-1.7455	-0.5857	-0.9948	h
0.6076	1.8430	-0.7944	h
-7.9713	0.5113	4.7538	h
-6.6881	0.4957	9.2441	h
-0.9504	2.6586	9.3952	h
2.6051	5.1826	6.7592	h
0.0369	-5.7867	1.8735	h
-4.3848	-3.2080	1.7590	h
5.9024	0.9249	3.2803	c
5.2558	-0.2365	7.6339	c
3.7775	-0.8804	8.9569	h
5.9970	1.6337	8.2345	h
6.7961	-1.6466	7.5334	h
4.9235	0.9627	1.4401	h
7.5078	-0.4041	3.1460	h
6.5215	2.8533	3.8265	h
2.2131	-5.9722	7.1473	c
-1.2022	-2.9926	10.1734	c
0.8294	-4.2673	11.2466	c
2.5209	-5.7472	9.7427	c
1.1316	-4.1630	13.3023	h
4.1091	-6.7249	10.6618	h
-4.2463	4.4014	1.2075	c
-3.2243	5.7532	-0.7921	c
-0.7311	6.7922	-0.6629	c
0.7631	6.4936	1.4713	c
2.6647	7.3293	1.5674	h
-2.5271	-1.9160	11.3624	h
3.5309	-7.0880	5.9949	h
-6.1793	3.6428	1.1004	h
-4.3531	6.0545	-2.5119	h
-0.0022	7.8663	-2.2873	h
9.4902	-9.5531	-0.1550	c
12.8426	-4.6453	-0.1322	f
10.3169	-4.5797	-0.6776	c
10.1497	-4.8025	-3.2469	f
9.5974	-2.0918	-0.1887	f
7.7459	-8.0383	5.3671	f

9.2805	-6.5266	3.8871	c
8.9560	-4.1063	4.9229	f
11.6773	-7.1789	4.5296	f
4.1076	-8.1169	1.3730	f
5.6639	-6.2990	0.3235	c
5.0075	-6.2160	-2.1598	f
4.6904	-4.0314	1.3244	f
8.6896	-6.7461	0.8449	b
11.5524	-9.8671	0.0456	h
9.0138	-9.8132	-2.1795	h
8.5187	-11.0707	0.9175	h

Complex **10c** :

E = -1918.8127755523 hartree

-10.6014	0.1678	0.9224	c
-8.1938	2.1885	5.9719	f
-7.2570	0.1126	4.7461	c
-8.4397	-1.9231	5.8104	f
-4.7597	-0.0745	5.5668	f
-6.0266	3.0278	-1.9331	f
-6.4114	2.9504	0.6360	c
-4.0027	3.5877	1.6259	f
-7.8486	5.0000	1.1827	f
-6.2986	-2.1831	-2.2529	f
-6.1866	-2.1439	0.3411	c
-7.0733	-4.4254	1.1052	f
-3.5479	-2.2931	0.8230	f
-7.6065	0.2722	1.6647	b
-11.6743	1.6889	1.8834	h
-11.4606	-1.6587	1.4853	h
-10.9085	0.3933	-1.1402	h
3.2951	-0.7983	-0.5487	zr
1.8283	-4.6268	-1.5658	c
7.8280	-0.6150	-1.8041	c
3.9260	1.5705	-4.5349	c
1.8809	-0.1539	-5.0592	c
-0.2758	0.5935	-3.6316	c
0.3909	2.7678	-2.1897	c
2.9706	3.3551	-2.7089	c
7.4026	0.9302	-4.9985	si
7.6195	0.7686	0.5381	c
7.1269	-0.9809	2.5289	c
6.9559	-3.4401	1.4578	c
7.3719	-3.2254	-1.1962	c
2.5536	-6.0481	-0.2039	h
-0.2034	-4.2199	-1.1369	h
6.5829	-5.1989	2.4911	h
7.3658	-4.8004	-2.5441	h
7.8871	-0.8821	-7.1152	h
8.9301	3.3009	-5.2487	h
4.0223	4.9609	-1.9189	h
7.8998	2.8115	0.7709	h
6.9618	-0.5123	4.5437	h
-0.9224	3.8087	-0.9691	h
-2.1424	-0.3115	-3.6140	h
1.0101	-1.2817	4.1878	c
2.6250	-2.2767	5.0473	h
1.0162	1.2520	3.7781	c
-0.7352	2.1931	3.1604	h
2.6659	2.4407	4.2556	h
-0.7324	-2.3629	3.8181	h
1.8832	-5.4771	-3.4762	h
1.9578	-1.7473	-6.3823	h

Complex **11c** :

E = -1958.1081072503 hartree

-4.4888	2.2884	2.8109	c
-2.6734	3.9564	8.2214	f
-1.6194	1.9563	6.9702	c
-2.9447	-0.1258	7.7384	f
0.7611	1.6641	8.0647	f
0.2545	5.3021	0.6340	f
-0.2675	5.0321	3.1735	c
2.0926	5.4775	4.3331	f
-1.6684	7.0838	3.8049	f
0.0000	0.0000	0.0000	f
0.0000	0.0000	2.6000	c
-0.7816	-2.3458	3.2865	f
2.6184	0.0000	3.1943	f
-1.5986	2.3209	3.8893	b
-5.6596	3.7474	3.7554	h
-5.4134	0.4370	3.1446	h
-4.5641	2.6640	0.7493	h
9.4255	1.6169	1.7809	zr
7.9761	-2.2898	0.9458	c
13.8857	1.7954	0.2645	c
9.8276	3.8930	-2.3085	c
7.7806	2.1377	-2.6773	c
5.6931	2.8957	-1.1528	c
6.4144	5.0990	0.2108	c
8.9563	5.7034	-0.4636	c
13.2715	3.2464	-2.9457	si
13.7979	3.2574	2.5643	c
13.4476	1.5753	4.6411	c
13.2452	-0.9234	3.6676	c
13.5015	-0.7967	0.9891	c
8.7117	-3.6178	2.3960	h
5.9059	-2.0336	1.2319	h
12.9620	-2.6502	4.7794	h
13.4362	-2.4177	-0.3010	h
13.6438	1.3740	-5.0329	h
14.7890	5.6035	-3.3472	h
10.0329	7.3354	0.2343	h
14.0698	5.3095	2.7097	h
13.4114	2.1201	6.6426	h
5.1736	6.1347	1.5104	h
3.8426	1.9693	-1.0282	h
7.7451	0.6289	7.3295	c
9.6669	0.4906	8.1392	h
7.1516	2.7222	5.9362	c
5.1913	3.0889	5.3199	h
8.5172	4.3184	5.8663	h
5.9847	-1.4677	7.9762	c
8.2454	-3.1881	-0.9262	h
7.8026	0.5086	-3.9588	h
4.1120	-1.2456	7.0882	h
6.8207	-3.3274	7.4791	h
5.7448	-1.4974	10.0653	h

Complex **12c** :

E = -3775.9124125885 hartree

0.0000	0.0000	4.6963	zr
3.9210	0.0000	6.4085	c
0.0000	0.0000	0.0000	c
-1.2322	-4.1701	2.8925	c
-3.3454	-3.2831	4.3512	c
-2.6779	-3.3397	6.9705	c
-0.1445	-4.2279	7.1624	c
0.7609	-4.7053	4.6687	c
-0.8257	-3.4362	-0.5904	si
2.4650	0.9062	0.7207	c
2.2027	3.3319	1.8636	c
-0.4160	3.9416	1.9209	c
-1.7815	1.8902	0.8020	c
-11.7561	2.3965	0.2926	b
3.8212	-0.7586	8.3665	h
4.6277	1.9779	6.4923	h
-1.2342	5.7194	2.6046	h
-3.8434	1.7877	0.5674	h
-3.1975	-3.7918	-2.0664	h
1.3944	-4.8225	-1.6677	h
2.6551	-5.4039	4.1916	h
4.2601	-0.0843	0.4034	h
3.7507	4.5284	2.5481	h
0.9206	-4.5190	8.9169	h
-3.9505	-2.8689	8.5371	h
-5.1689	-2.6663	3.5772	h
-11.9833	-0.0715	-1.6416	c
-14.1377	-0.7955	-3.0245	c
-14.2567	-3.0089	-4.5030	c
-12.1656	-4.6336	-4.6184	c
-9.9835	-4.0150	-3.2421	c
-9.9656	-1.7949	-1.7990	c
-11.8971	0.9588	3.0978	c
-9.8866	0.4621	4.7451	c
-10.1286	-0.8300	7.0504	c
-12.4752	-1.8016	7.7879	c
-14.5483	-1.4386	6.1702	c
-14.2087	-0.1101	3.8946	c
-13.9644	4.6042	-0.0499	c
-14.4485	5.6370	-2.4565	c
-16.1454	7.6243	-2.9176	c
-17.4264	8.7291	-0.8736	c
-16.9841	7.8088	1.5712	c
-15.2672	5.8081	1.9330	c
-12.2472	-6.7467	-6.0115	f
-7.9500	-5.5487	-3.3190	f
-7.7845	-1.3416	-0.4864	f
-16.2563	0.6082	-3.0049	f
-16.3616	-3.5853	-5.7901	f
-13.2332	4.7116	-4.5017	f
-16.5278	8.4929	-5.2698	f
-7.4731	1.2242	4.1982	f
-8.0852	-1.1402	8.5866	f
-12.7307	-3.0474	9.9761	f
-16.8155	-2.3632	6.8101	f
-16.2789	0.1387	2.4435	f
-14.9319	5.1029	4.3660	f
-18.1787	8.8573	3.5498	f
-19.0461	10.6387	-1.2545	f
-9.1333	4.0761	-0.2094	c
-7.8043	4.1732	-2.5187	c
-5.7373	5.7950	-2.9760	c
-4.8719	7.3842	-1.0430	c
-6.1225	7.3469	1.2926	c
-8.2285	5.7718	1.6326	c
-8.4272	2.6771	-4.4769	f
-4.5550	5.7811	-5.2173	f
-9.3638	5.9323	3.9158	f
-5.1992	8.7354	3.2377	f
-2.8245	8.8478	-1.3739	f
-1.2151	3.1038	8.4948	c
-0.7310	1.6385	9.9007	h
-3.6041	3.3375	7.5959	c
-4.1641	4.8991	6.3364	h
-5.1119	2.0023	8.1215	h
0.2522	4.5235	8.0681	h
5.3946	-1.1134	5.4146	h

Complex **8c-2** :

E = -3088.4864006265 hartree

0.0000	0.0000	4.6780	zr
4.1381	0.0000	5.8320	c
0.0000	0.0000	0.0000	c
-0.8418	-4.2483	2.8978	c
-3.1157	-3.4774	4.1972	c
-2.6359	-3.4865	6.8485	c
-0.0616	-4.1919	7.2316	c
1.0429	-4.6552	4.8200	c
-0.2338	-3.5307	-0.5617	si
2.2334	1.3960	0.6927	c
1.4842	3.7160	1.8326	c
-1.2125	3.7922	1.8821	c
-2.1302	1.5084	0.7916	c
-10.3165	3.0999	0.4973	b
4.3611	-0.9111	7.7109	h
4.7481	2.0084	5.9803	h
-2.4051	5.3513	2.5477	h
-4.1289	1.0098	0.5408	h
-2.3507	-4.2643	-2.2670	h
2.2694	-4.5810	-1.3631	h
3.0009	-5.2492	4.4883	h
4.1888	0.7933	0.3626	h
2.7638	5.2010	2.5099	h
0.8902	-4.3884	9.0630	h
-4.0321	-3.0605	8.3204	h
-4.9294	-3.0226	3.2966	h
-9.9434	1.2315	3.0248	c
-11.5183	-0.9020	3.3264	c
-11.5310	-2.4826	5.4621	c
-9.8873	-1.9405	7.4739	c
-8.2885	0.1569	7.2695	c
-8.3174	1.6468	5.0713	c
-13.2718	4.1503	0.8611	c
-13.8016	5.9340	2.7686	c
-16.1952	7.0034	3.1974	c
-18.2446	6.2258	1.7074	c
-17.8475	4.3980	-0.1694	c
-15.4141	3.3825	-0.5209	c
-9.8091	-3.4136	9.5380	f

-6.6431	0.6645	9.1838	f
-6.5589	3.5495	5.0383	f
-13.1304	-1.5478	1.4720	f
-13.0622	-4.4948	5.5953	f
-11.9597	6.7226	4.3686	f
-16.5434	8.7250	5.0323	f
-15.2498	1.5782	-2.3155	f
-19.7994	3.6158	-1.5908	f
-20.5493	7.2146	2.0740	f
-9.8277	1.5243	-2.1779	c
-8.3807	-0.6831	-2.4160	c
-7.8602	-1.9179	-4.7094	c
-8.7643	-0.8800	-6.9704	c
-10.1647	1.3720	-6.8693	c
-10.6146	2.5262	-4.5202	c
-7.2983	-1.8031	-0.3338	f
-6.4615	-4.0500	-4.7585	f
-11.9012	4.7258	-4.6024	f
-11.0264	2.4059	-9.0171	f
-8.2942	-2.0102	-9.1895	f
-0.8383	1.8804	9.4562	c
-2.5237	0.8669	10.1252	h
-1.0793	3.9156	7.9022	c
0.5552	5.1059	7.4023	h
-2.9648	4.5339	7.2679	h
1.0075	1.3219	10.2456	h
5.5038	-0.9360	4.5480	h
-8.3459	5.5127	0.3173	c
-8.3259	6.7329	2.0130	h
-8.8897	6.7149	-1.3125	h
-6.3750	4.8913	-0.0572	h

Complex **8c**-3 :

E = -3088.4760675583 hartree

0.0000	0.0000	4.7058	zr
3.6858	0.0000	6.8867	c
0.0000	0.0000	0.0000	c
-1.6814	-4.0111	2.8984	c
-3.6157	-3.0269	4.5226	c
-2.7613	-3.1840	7.0883	c
-0.2898	-4.2485	7.0834	c
0.3946	-4.7149	4.5177	c
-1.3691	-3.2648	-0.6048	si
2.5783	0.4338	0.7714	c
2.7599	2.8719	1.9068	c
0.2944	3.9495	1.9210	c
-1.4039	2.1879	0.7637	c
-10.6340	-0.3353	-4.3832	b
3.3719	-0.6665	8.8557	h
4.4974	1.9370	6.9732	h
-0.1973	5.8489	2.5975	h
-3.4409	2.4579	0.4652	h
-3.8308	-3.2861	-1.9576	h
0.6087	-4.9279	-1.7603	h
2.1985	-5.5232	3.8849	h
4.1638	-0.8747	0.4835	h
4.4934	3.7642	2.6072	h
0.8714	-4.6619	8.7483	h
-3.8613	-2.6712	8.7718	h
-5.4375	-2.2643	3.8851	h
-11.9255	-3.2064	-4.4347	c
-14.0442	-3.9317	-5.8647	c
-15.1962	-6.3306	-5.6778	c
-14.2123	-8.1368	-4.0066	c
-12.0764	-7.5209	-2.5606	c
-11.0129	-5.1026	-2.8109	c
-11.2510	0.5833	-1.4094	c
-9.5771	0.6098	0.6471	c
-10.2543	1.2580	3.1262	c
-12.7510	1.9103	3.7014	c
-14.5263	1.8933	1.7334	c
-13.7554	1.2068	-0.7206	c
-15.2867	-10.4225	-3.7961	f
-11.0909	-9.2296	-0.9586	f
-8.9453	-4.6483	-1.3572	f
-15.1169	-2.3447	-7.5393	f
-17.2304	-6.9022	-7.0795	f
-7.0921	-0.0575	0.3836	f
-8.4960	1.1866	5.0103	f
-13.4143	2.5308	6.0680	f
-16.9429	2.4790	2.2198	f
-15.6347	1.1175	-2.4347	f
-7.5826	-0.4170	-5.1373	c
-6.5055	-2.2785	-6.7083	c
-4.0063	-2.2000	-7.6280	c
-2.4406	-0.1609	-6.9830	c
-3.4371	1.7807	-5.4742	c
-5.9419	1.6095	-4.6137	c
-7.8659	-4.2916	-7.4835	f
-3.1115	-4.0522	-9.1159	f
-6.7323	3.5886	-3.1775	f
-1.9760	3.7727	-4.8468	f
-0.0463	-0.0442	-7.8227	f
-1.4139	3.3465	8.3360	c
-1.0508	2.0998	9.9667	h
-3.6764	3.3429	7.1303	c
-4.1030	4.6801	5.5924	h
-5.2293	2.0739	7.6774	h
0.0721	4.7317	7.8660	h
5.1849	-1.2301	6.0797	h
-11.7923	1.6996	-6.4355	c
-11.3997	1.0862	-8.4025	h
-10.8634	3.5662	-6.1884	h
-13.8531	1.9970	-6.2830	h

Complex **8c**-4 :

E = -3088.4708271334 hartree

6.2895	0.7997	4.7792	zr
9.8056	1.3316	7.1957	c
7.2406	0.5155	0.1795	c
5.8480	-3.5955	3.1357	c
3.4071	-2.8588	4.0763	c
3.5350	-2.6711	6.7678	c
6.0509	-3.2613	7.5251	c
7.4832	-3.7885	5.3036	c
6.8914	-3.0242	-0.2446	si
9.3845	1.7656	1.3024	c
8.6194	4.2066	2.1516	c
5.9916	4.4800	1.6226	c
5.1334	2.2134	0.4280	c

-5.8809	0.4752	-4.5902	b
9.4563	0.7070	9.1707	h
10.3928	3.3490	7.2355	h
4.8469	6.1760	1.9735	h
3.1967	1.8347	-0.2133	h
4.8979	-3.7071	-2.1194	h
9.3864	-4.2499	-0.7687	h
9.4929	-4.2966	5.2644	h
11.3043	0.9918	1.4405	h
9.8507	5.6288	3.0265	h
6.7636	-3.3242	9.4702	h
1.9480	-2.2436	8.0351	h
1.7291	-2.4870	2.9157	h
-7.7109	-2.0223	-4.0267	c
-10.2960	-2.2269	-4.6085	c
-11.7824	-4.3531	-3.9834	c
-10.6796	-6.4038	-2.7218	c
-8.1017	-6.2988	-2.1067	c
-6.7098	-4.1334	-2.7582	c
-5.1783	1.4877	-1.6704	c
-2.8890	1.1234	-0.3766	c
-2.4634	1.9652	2.0951	c
-4.3459	3.2183	3.4587	c
-6.6928	3.5847	2.2900	c
-7.0536	2.6851	-0.1922	c
-12.0607	-8.4394	-2.1130	f
-7.0010	-8.2456	-0.9032	f
-4.2336	-4.1717	-2.1091	f
-11.5317	-0.3742	-5.8388	f
-14.2435	-4.4287	-4.5932	f
-0.8942	-0.1081	-1.4279	f
-0.1862	1.5156	3.2411	f
-3.8868	4.0234	5.8331	f
-8.5661	4.7422	3.5438	f
-9.4053	3.0147	-1.1040	f
-3.3833	-0.2683	-6.3352	c
-3.3352	-2.3024	-8.0547	c
-1.3511	-2.7569	-9.7674	c
0.7114	-1.0965	-9.8408	c
0.7552	0.9794	-8.1860	c
-1.2805	1.3573	-6.5280	c
-5.2732	-3.9593	-8.1814	f
-1.4285	-4.7401	-11.3491	f
-1.1333	3.4523	-5.0561	f
2.7302	2.5814	-8.2293	f
2.6138	-1.4773	-11.4738	f
4.7076	4.0653	8.5968	c
5.1002	2.7964	10.2011	h
2.5295	3.8989	7.2492	c
2.0503	5.2682	5.7588	h
1.0605	2.4898	7.6726	h
6.0825	5.5936	8.2607	h
11.4770	0.2508	6.5254	h
-7.2244	2.7669	-6.2395	c
-7.7301	2.0923	-8.1596	h
-5.8701	4.3509	-6.4827	h
-8.9613	3.5353	-5.3722	h

Complex ref.13d : I-3 :

E = -3565.1109741285 hartree

0.0000	0.0000	3.1464	b
3.1048	0.0000	3.7668	c
4.5719	2.0153	4.7272	c
7.2141	1.8967	5.1102	c
8.5745	-0.2937	4.4737	c
7.1802	-2.3023	3.4746	c
4.5890	-2.0786	3.1237	c
0.0000	0.0000	0.0000	c
-0.6861	-2.0059	-1.5975	c
-0.5726	-1.8892	-4.2521	c
0.3458	0.2947	-5.4370	c
1.1100	2.3423	-3.9291	c
0.9498	2.1311	-1.2878	c
-1.4968	2.4412	4.4109	c
-1.3237	2.8388	7.0366	c
-2.6043	4.7556	8.3462	c
-4.2154	6.3768	6.9972	c
-4.4943	6.0403	4.3836	c
-3.1672	4.0865	3.1578	c
11.0696	-0.4487	4.8068	f
8.3197	-4.5526	2.7935	f
3.5180	-4.2497	2.0689	f
3.5190	4.2252	5.3532	f
8.4517	3.8832	6.0552	f
0.1925	1.3311	8.4430	f
-2.3187	5.0450	10.8491	f
-1.4797	-4.2641	-0.6665	f
-1.2467	-3.9052	-5.6528	f
0.4903	0.4273	-7.9587	f
2.0018	4.4491	-5.0146	f
1.7476	4.1531	0.0431	f
-3.6087	3.8825	0.6551	f
-6.0393	7.5630	3.0723	f
-5.4618	8.2252	8.1937	f
-1.5002	-2.4547	4.4172	c
-0.5946	-4.1034	6.2902	c
-2.0556	-6.0122	7.4297	c
-4.5915	-6.3122	6.7256	c
-5.6133	-4.6913	4.8875	c
-4.0690	-2.8238	3.8054	c
1.8353	-3.9784	7.1260	f
-1.0270	-7.5556	9.1661	f
-5.1746	-1.3308	2.0617	f
-8.0360	-4.9414	4.1922	f
-6.0156	-8.1165	7.7844	f
1.8398	-9.4468	2.3305	c
3.9356	-7.0071	-3.5258	c
5.5245	-9.1547	-3.9734	c
8.1131	-8.3633	-3.8845	c
8.1290	-5.7043	-3.3170	c
5.5578	-4.8974	-3.1181	c
3.6221	-9.3669	4.3705	c
5.4212	-11.3182	3.9573	c
4.7948	-12.6042	1.6564	c
2.5105	-11.4775	0.6843	c
6.0862	-14.9252	0.6467	c
0.9070	-12.4790	-1.4328	c
4.9338	-2.9576	-2.7234	h
3.5561	-8.0524	5.9743	h
7.0180	-11.7917	5.1888	h
10.4221	-4.0381	-3.1784	c
10.3624	-9.9321	-4.6031	c
4.8865	-11.0574	-4.4869	h

5.9383	-7.9895	0.5324	zr
9.9545	-9.3316	1.4028	c
11.3801	-8.0677	0.5272	h
10.3797	-11.2884	0.7820	h
10.2522	-9.2649	3.4800	h
0.2002	-8.1985	2.0993	h
1.8661	-6.9497	-3.5720	h
5.0797	-16.6555	1.2811	h
8.0569	-15.0669	1.3315	h
6.1231	-14.9774	-1.4463	h
-0.1378	-10.9621	-2.4240	h
-0.5293	-13.7947	-0.6480	h
2.0080	-13.5645	-2.8415	h
11.1738	-3.6740	-5.1042	h
11.9745	-4.9103	-2.0750	h
9.9775	-2.1807	-2.3260	h
10.8594	-9.5792	-6.6127	h
9.9772	-11.9788	-4.4066	h
12.0544	-9.4771	-3.4605	h

Complex ref.13d : C_2H_4-I-3 :

E = -3643.5767619695 hartree

0.0450	-0.0158	0.0004	zr
4.7658	0.0664	-0.3438	c
4.0556	2.6514	-0.1688	c
2.8862	3.0255	2.2409	c
3.0013	0.6786	3.5925	c
4.1653	-1.1428	1.9999	c
-2.5820	-0.7755	-3.8637	c
-0.4984	0.8181	-4.5077	c
-0.8297	3.1600	-3.1839	c
-3.1248	3.0141	-1.7535	c
-4.1998	0.5726	-2.1759	c
4.7745	4.6408	-1.9753	c
6.7225	5.2567	-1.5496	h
-6.6959	-0.2755	-1.2612	c
-4.2631	5.1125	-0.3389	c
-4.9251	6.5512	-1.6927	h
-2.4460	0.2960	3.3025	c
4.5621	-3.0713	2.4987	h
5.7746	-0.7523	-1.9491	h
2.3632	0.3914	5.4849	h
-2.9534	-2.6331	-4.5861	h
0.9916	0.4077	-5.8185	h
0.9130	13.7125	-1.8511	b
2.7173	12.3624	0.1946	c
1.7734	16.6116	-1.6956	c
1.2589	12.5792	-4.6519	c
2.2654	12.8727	2.7324	c
3.6858	11.8769	4.7055	c
5.7403	10.3374	4.1376	c
6.3356	9.8710	1.6236	c
4.8362	10.8998	-0.2735	c
0.4204	18.5965	-0.6533	c
1.3268	21.0648	-0.5908	c
3.7123	21.5825	-1.5567	c
5.1808	19.6290	-2.5412	c
4.1701	17.2103	-2.5634	c
1.0248	9.9942	-4.9505	c
1.4265	8.6844	-7.1742	c
1.9667	10.0499	-9.3497	c
2.0764	12.6756	-9.1981	c
1.7264	13.8724	-6.8843	c
-2.0391	13.2698	-1.3005	c
-3.1114	11.5218	0.3254	c
-5.6998	11.1875	0.6144	c
-7.3502	12.6560	-0.8074	c
-6.3660	14.4163	-2.4888	c
-3.7642	14.6499	-2.7173	c
1.9457	5.4418	3.2721	c
1.5650	6.8371	1.7819	h
3.3960	6.2518	4.5363	h
0.2100	5.1518	4.3819	h
3.5786	6.3191	-1.8059	h
4.7122	3.9713	-3.9372	h
0.3283	4.7934	-3.3408	h
-6.9402	-2.3310	-1.4978	h
-8.1761	0.6909	-2.3711	h
-6.9918	0.2164	0.7483	h
1.8609	16.3924	-6.9757	f
2.5595	13.9918	-11.2733	f
2.3381	8.8492	-11.5142	f
1.3016	6.1482	-7.3011	f
0.4537	8.5801	-2.8792	f
5.6440	15.3735	-3.5107	f
7.4825	20.1153	-3.4562	f
4.6177	23.9243	-1.5493	f
-0.0448	22.9271	0.3790	f
-1.8908	18.2641	0.3415	f
0.3262	14.3533	3.4013	f
3.0957	12.3084	7.1021	f
7.0860	9.2540	5.9766	f
8.3042	8.3893	1.0746	f
5.5663	10.2970	-2.6353	f
-5.9179	4.4837	0.7939	h
-2.9036	6.0506	0.9256	h
-1.6891	9.9652	1.7777	f
-6.6228	9.4581	2.2091	f
-9.8338	12.2800	-0.5557	f
-7.9363	15.8340	-3.8595	f
-2.9139	16.4074	-4.4434	f
-0.1555	-4.9611	-0.3206	c
1.7103	-4.5206	-2.1436	c
-2.2260	-4.9809	-0.8393	h
0.4010	-5.5076	1.6329	h
1.2238	-4.1296	-4.1153	h
3.6975	-4.7400	-1.6517	h
-2.4921	-1.8008	3.0172	h
-1.7825	0.7107	5.2323	h
-4.4144	1.0081	3.0705	h

Complex ref.13d : I-3
(reoptimized,not included in the paper) :

E = -3565,107992 hartree

0.0000	0.0000	3.1413	b
3.0874	0.0000	3.7346	c
0.0000	0.0000	0.0000	c
-1.5313	-2.4898	4.3670	c
4.5153	2.1545	3.0762	c
7.1651	2.2770	3.1524	c

8.5389	0.1264	3.8787	c
7.2196	-2.0805	4.5100	c
4.5606	-2.0895	4.4485	c
-0.5854	2.0576	-1.5790	c
-0.3417	1.9868	-4.2292	c
0.5655	-0.2041	-5.4108	c
1.2042	-2.3036	-3.9187	c
0.9246	-2.1375	-1.2882	c
-1.3654	-3.1240	6.9248	c
-2.7172	-5.0450	8.1016	c
-4.4190	-6.5468	6.7571	c
-4.6976	-6.0028	4.1767	c
-3.3073	-4.0107	3.0658	c
-1.5764	2.4141	4.3923	c
-0.6922	4.0938	6.2507	c
-2.1079	6.1444	7.1823	c
-4.5938	6.5154	6.3444	c
-5.6017	4.8467	4.5445	c
-4.1016	2.8433	3.6611	c
0.7220	-3.0709	13.2967	zr
4.5888	-6.1457	12.6162	c
2.3429	-7.6649	12.5977	c
1.1500	-7.4096	15.0198	c
2.6850	-5.7903	16.5519	c
4.7702	-4.9835	15.0546	c
6.5244	-6.0154	10.5510	c
1.5437	-9.3968	10.4913	c
-1.0995	1.2111	14.9373	c
-0.3706	-0.3523	17.0264	c
-2.0141	-2.4989	17.1188	c
-3.6711	-2.3383	15.0186	c
-3.1143	-0.0657	13.6365	c
-0.1666	3.8356	14.4220	c
1.1116	0.1131	18.4008	h
3.7445	-0.1757	12.3846	c
-0.5695	-8.4015	15.6233	h
2.3704	-5.3212	18.5435	h
6.3113	-3.7437	15.6709	h
5.6754	-5.8538	8.6492	h
7.6872	-7.7639	10.5511	h
7.8324	-4.4072	10.8135	h
1.8632	-8.5517	8.6020	h
-0.4669	-9.9462	10.6431	h
2.6801	-11.1607	10.5559	h
-2.0238	-3.9831	18.5634	h
-5.1604	-3.6998	14.5395	h
-4.5997	0.9393	11.4328	c
1.7626	4.1375	15.1683	h
-1.4276	5.2183	15.3753	h
-0.1616	4.3201	12.3896	h
-7.9749	5.1599	3.7169	f
4.7173	0.6884	14.0296	h
2.8568	1.3718	11.2849	h
-3.7936	-3.6545	0.6131	f
-6.2999	-7.3703	2.7876	f
-5.6959	-8.4113	7.8845	f
-2.3535	-5.4349	10.6628	f
0.2480	-1.8678	8.5916	f
1.5792	-4.2240	0.0441	f
2.0776	-4.4215	-5.0070	f
0.8135	-0.2972	-7.9278	f
-0.9531	4.0094	-5.6284	f
-1.4288	4.2686	-0.6333	f
3.3260	4.2605	2.2743	f
8.3930	4.4001	2.5225	f
11.0677	0.1754	3.9509	f
8.5142	-4.1670	5.1807	f
3.4694	-4.3254	5.1190	f
-5.7300	-0.5602	10.5123	h
-5.9440	2.4155	12.0807	h
-3.3874	1.8269	9.9776	h
1.6320	3.8276	7.2918	f
-1.1296	7.6853	8.9548	f
-5.9812	8.4327	7.2416	f
5.2125	-1.0470	11.1681	h
-5.1996	1.3009	1.9529	f

Complex ref.13d : I-3 (reoptimized,different anion orientation) :

E = -3565,110974 hartree

0.0000	0.0000	3.1464	b
3.1048	0.0000	3.7668	c
4.5719	2.0153	4.7272	c
7.2141	1.8967	5.1102	c
8.5745	-0.2937	4.4737	c
7.1802	-2.3023	3.4746	c
4.5890	-2.0786	3.1237	c
0.0000	0.0000	0.0000	c
-0.6861	-2.0059	-1.5975	c
-0.5726	-1.8892	-4.2521	c
0.3458	0.2947	-5.4370	c
1.1100	2.3423	-3.9291	c
0.9498	2.1311	-1.2878	c
-1.4968	2.4412	4.4109	c
-1.3237	2.8388	7.0366	c
-2.6043	4.7556	8.3462	c
-4.2154	6.3768	6.9972	c
-4.4943	6.0403	4.3836	c
-3.1672	4.0865	3.1578	c
11.0696	-0.4487	4.8068	f
8.3197	-4.5526	2.7935	f
3.5180	-4.2497	2.0689	f
3.5190	4.2252	5.3532	f
8.4517	3.8832	6.0552	f
0.1925	1.3311	8.4430	f
-2.3187	5.0450	10.8491	f
-1.4797	-4.2641	-0.6665	f
-1.2467	-3.9052	-5.6528	f
0.4903	0.4273	-7.9587	f
2.0018	4.4491	-5.0146	f
1.7476	4.1531	0.0431	f
-3.6087	3.8825	0.6551	f
-6.0393	7.5630	3.0723	f
-5.4618	8.2252	8.1937	f
-1.5002	-2.4547	4.4172	c
-0.5946	-4.1034	6.2902	c
-2.0556	-6.0122	7.4297	c
-4.5915	-6.3122	6.7256	c
-5.6133	-4.6913	4.8875	c
-4.0690	-2.8238	3.8054	c
1.8353	-3.9784	7.1260	f
-1.0270	-7.5556	9.1661	f
-5.1746	-1.3308	2.0617	f

-8.0360	-4.9414	4.1922	f
-6.0156	-8.1165	7.7844	f
1.8398	-9.4468	2.3305	c
3.9356	-7.0071	-3.5258	c
5.5245	-9.1547	-3.9734	c
8.1131	-8.3633	-3.8845	c
8.1290	-5.7043	-3.3170	c
5.5578	-4.8974	-3.1181	c
3.6221	-9.3669	4.3705	c
5.4212	-11.3182	3.9573	c
4.7948	-12.6042	1.6564	c
2.5105	-11.4775	0.6843	c
6.0862	-14.9252	0.6467	c
0.9070	-12.4790	-1.4328	c
4.9338	-2.9576	-2.7234	h
3.5561	-8.0524	5.9743	h
7.0180	-11.7917	5.1888	h
10.4221	-4.0381	-3.1784	c
10.3624	-9.9321	-4.6031	c
4.8865	-11.0574	-4.4869	h
5.9383	-7.9895	0.5324	zr
9.9545	-9.3316	1.4028	c
11.3801	-8.0677	0.5272	h
10.3797	-11.2884	0.7820	h
10.2522	-9.2649	3.4800	h
0.2002	-8.1985	2.0993	h
1.8661	-6.9497	-3.5720	h
5.0797	-16.6555	1.2811	h
8.0569	-15.0669	1.3315	h
6.1231	-14.9774	-1.4463	h
-0.1378	-10.9621	-2.4240	h
-0.5293	-13.7947	-0.6480	h
2.0080	-13.5645	-2.8415	h
11.1738	-3.6740	-5.1042	h
11.9745	-4.9103	-2.0750	h
9.9775	-2.1807	-2.3260	h
10.8594	-9.5792	-6.6127	h
9.9772	-11.9788	-4.4066	h
12.0544	-9.4771	-3.4605	h

Complex ref.13d : I-3
(reoptimized, different anion-orientation and Cp-torsion) :

E = -3565.1122731029 hartree

0.0000	0.0000	3.1438	b
3.0464	0.0000	3.8439	c
0.0000	0.0000	0.0000	c
-1.5503	-2.4558	4.4183	c
4.5282	2.1077	3.1738	c
7.1496	2.2628	3.5502	c
8.4263	0.1899	4.6078	c
7.0502	-1.9757	5.2689	c
4.4250	-2.0371	4.8464	c
-0.6524	2.0434	-1.5768	c
-0.3967	1.9997	-4.2297	c
0.5629	-0.1617	-5.4250	c
1.2993	-2.2250	-3.9300	c
1.0074	-2.0876	-1.2999	c
-3.2207	-4.1225	3.2554	c
-4.7469	-5.8681	4.5086	c
-4.6634	-6.1234	7.1300	c
-2.9861	-4.5196	8.4314	c
-1.5292	-2.7524	7.0797	c
-1.6493	2.3775	4.3719	c
-0.8266	4.1233	6.2026	c
-2.4046	5.9972	7.2507	c
-4.9536	6.1352	6.5348	c
-5.8787	4.4106	4.7446	c
-4.2207	2.6061	3.7475	c
-6.7198	-6.9473	-1.6702	zr
-4.8936	-11.5647	-1.7172	c
-2.8077	-9.8605	-1.3968	c
-2.6596	-8.3079	-3.6221	c
-4.6214	-9.0575	-5.3074	c
-6.0383	-11.0148	-4.1072	c
-5.5594	-13.7150	0.0091	c
-0.9334	-9.9060	0.7375	c
-10.8574	-4.8152	-3.2949	c
-9.1061	-5.1933	-5.3203	c
-6.9559	-3.5892	-4.9175	c
-7.3614	-2.2674	-2.6168	c
-9.7265	-3.0488	-1.5573	c
-13.5299	-5.7507	-3.2038	c
-9.4582	-6.3766	-6.9867	h
-10.0039	-9.2633	-0.1211	c
-1.2032	-6.8807	-3.9926	h
-4.9494	-8.3012	-7.2068	h
-7.6682	-12.0134	-4.9107	h
-5.4741	-13.1780	2.0316	h
-4.1938	-15.2876	-0.2586	h
-7.4679	-14.4703	-0.3879	h
-1.8268	-10.3410	2.5806	h
0.1078	-8.1037	0.9027	h
0.4904	-11.4109	0.3939	h
-5.3343	-3.3500	-6.1846	h
-6.0682	-0.8953	-1.7570	h
-10.9360	-1.9993	0.7939	c
-13.7961	-7.4722	-4.3610	h
-14.8085	-4.2731	-3.9738	h
-14.1722	-6.1652	-1.2574	h
-8.3188	4.4751	4.0385	f
-11.2226	-10.1880	-1.5536	h
-11.2325	-8.0122	1.0330	h
-0.0515	-1.2563	8.4878	f
-2.8234	-4.6745	10.9452	f
-6.1023	-7.8001	8.3470	f
-6.3737	-7.3182	3.0715	f
-3.5928	-4.2095	0.6376	f
1.7582	-4.1576	0.0162	f
2.2155	-4.3339	-5.0330	f
0.7893	-0.2543	-7.9449	f
-1.0727	4.0054	-5.6193	f
-1.5679	4.2165	-0.6285	f
3.4150	4.1442	2.1119	f
8.4442	4.3404	2.8961	f
10.9277	0.2835	4.9812	f
8.2450	-3.9789	6.2662	f
3.2758	-4.2394	5.4678	f
-9.6167	-0.7534	1.8287	h
-12.6184	-0.8476	0.2961	h
-11.6005	-3.5021	2.0960	h
1.5540	4.0945	7.0906	f
-1.4967	7.6247	8.9640	f

-6.4828	7.8842	7.5350	f
-9.2791	-10.7662	1.1443	h
-5.2574	0.9758	2.0343	f

Complex ref.13d : C_2H_4-I-3
(reoptimized) :

E = -3643,622261 hartree

0.0000	0.0000	4.7991	zr
3.1300	2.2953	2.0184	c
2.6452	0.0000	0.6858	c
0.0000	0.0000	0.0000	c
-1.0608	2.3637	0.8259	c
0.8513	3.7715	2.0715	c
1.7380	-2.8202	8.2721	c
2.7407	-3.6096	5.9021	c
0.6891	-4.6112	4.4516	c
-1.5724	-4.4937	5.9447	c
-0.9218	-3.3566	8.3243	c
4.5905	-1.8957	-0.1277	c
4.9585	-1.6739	-2.1813	h
-2.6417	-3.1025	10.5678	c
-4.0828	-5.6152	5.2490	c
-4.3097	-7.4748	6.1972	h
-4.1635	0.9048	5.2849	c
0.6309	5.6783	2.8560	h
4.9905	2.8774	2.7317	h
-3.0084	2.9795	0.4859	h
2.8266	-2.0383	9.8588	h
4.7255	-3.5609	5.3110	h
1.2433	-10.8351	-5.1784	b
0.9632	-7.8849	-6.2423	c
1.5205	-12.4435	-7.8555	c
3.6782	-11.2252	-3.2167	c
-1.1989	-7.2299	-7.6565	c
-1.5826	-4.8667	-8.8034	c
0.2906	-3.0016	-8.5693	c
2.5021	-3.5715	-7.2300	c
2.7994	-5.9694	-6.1191	c
-0.2931	-14.0593	-8.9317	c
0.0094	-15.2299	-11.3039	c
2.1804	-14.7415	-12.7440	c
4.0306	-13.1063	-11.7766	c
3.6499	-12.0044	-9.3943	c
3.8298	-9.7370	-1.0262	c
5.6779	-9.9692	0.8504	c
7.5310	-11.8487	0.5990	c
7.4652	-13.4220	-1.5315	c
5.5560	-13.1038	-3.3633	c
-1.1578	-11.7509	-3.3587	c
-2.9674	-10.1863	-2.2093	c
-4.8135	-11.0588	-0.5074	c
-4.8746	-13.6159	0.1725	c
-3.0944	-15.2652	-0.8997	c
-1.2908	-14.2988	-2.5892	c
-1.3275	-1.9158	-1.6148	c
-0.5695	-3.8483	-1.3952	h
-1.0821	-1.4115	-3.6390	h
-3.3844	-1.9668	-1.2405	h
3.9805	-3.8763	0.1303	h
6.4037	-1.6169	0.8768	h
0.8573	-5.5319	2.6029	h
-1.8326	-1.8613	12.0481	h
-2.9479	-4.9805	11.4544	h
-4.5333	-2.3665	10.0505	h
5.6424	-14.7501	-5.2960	f
9.2140	-15.2346	-1.8012	f
9.3257	-12.1317	2.3649	f
5.6961	-8.4102	2.8768	f
2.0835	-7.8648	-0.6386	f
5.4983	-10.4396	-8.5784	f
6.1146	-12.5998	-13.1325	f
2.4849	-15.8233	-15.0137	f
-1.7755	-16.7852	-12.2139	f
-2.4827	-14.5869	-7.7372	f
-3.0685	-8.9320	-7.9607	f
-3.7079	-4.3611	-10.0924	f
-0.0350	-0.7076	-9.6015	f
4.3041	-1.7868	-6.9483	f
5.0132	-6.3005	-4.8825	f
-5.6907	-4.4223	5.8575	h
-4.2480	-5.9684	3.1962	h
-3.0383	-7.6559	-2.6417	f
-6.4783	-9.4259	0.5346	f
-6.6019	-14.4756	1.8170	f
-3.1111	-17.7201	-0.2678	f
0.3993	-15.9775	-3.4909	f
0.0570	3.3398	8.8921	c
2.4336	3.6368	7.9739	c
-0.4293	1.8080	10.2133	h
-1.4424	4.7205	8.4746	h
3.9786	2.3343	8.4873	h
2.9569	5.2870	6.8247	h
-4.5935	2.9421	5.0095	h
-5.2533	-0.1182	3.8008	h
-4.9652	0.3088	7.1295	h

able S1. ^{1}H-NMR data for reaction products of 1a with different Lewis bases

ewis base	C_5H_5	Zr^+-CH_3	$(C_6F_5)_3BCH_3^-$	Lewis base
one [a]	5.39 (s, 10H)	0.28 (s, 3H)	0.1 (bs, 3H)	
$C_5H_5)_2ZrMe_2$ [a]	5.62 (20H)	–0.12 (6H)	1.3 (3H)	–1.19 (3H, μ-CH_3)
$C_6H_5)_3PCH_2$	5.45 (10H)	n. r.	1.19	n.r., 5.53 (m), -0.14 (d, J=13 Hz, C$\underline{H}_2$)
Me_3	5.38 (10H)	0.05 (3H)	1.07	1.25 (9H)
$NMe_3)_2$ [b]	5.42 (10H)	0.09 (3H)	1.07	1.27 (18H)
$e_2N(SiMe_3)$	5.39 (10H)	0.12 (3H)	n.r.	2.65 (s, 6H, N-Me), –0.48 (s, 9H, Si-Me)
$Me_2(C_6H_5)$	5.20 (10H)	0.22 (3H)	1.38	6.7-7.0, 6.2 (d, 2H), 1.79 (s, 6H)
$Me_2(C_6H_5)$ [c]	5.29 (5H), 5.04 (5H)	-	n.r.	2.6 (d, 1H), 2.18 (s, 3H), 1.6 (d, 1H)
6-Lutidine [d]	5.55 (A), 5.54 (B)	-	1.29 (A), 1.01 (B)	2.20 (s, 2H, A), 2.17 (s, 2H, B), 1.28 (s, 3H, A), 1.21 (s, 3H, B)
yridazine [e]	5.52 (bs, A), 5.47 (s, B)	0.33 (6H, A+B)	1.27 (A), 0.75 (B)	n.r.
$C_4H_9)_2O$	5.53 (10H)	0.26 (3H)	1.35	2.74 (t, 6 Hz, 4H), 1.36 (m, 4H), 0.77 (m, 4H), 0.67 (t, 6H, 7 Hz)
$C_2H_5)_2O$	5.47 (10H)	0.19 (3H)	1.34	2.57 (q, 4H), 0.36 (t, 6H)
$CH_2)_5O$	5.51	0.18	1.39	2.61 (α-CH_2), 0.88 (γ-CH_2), 0.75 (β-CH_2)
$CH_2)_5O)_2$ [b]	5.48 (10H)	–0.05 (3H)	1.36	2.49 (t, 8H, α-C$\underline{H}_2$), n.r.
$CH_2)_3(CH)_2O$	5.49 (bs)	0.26 (bs)	1.33	n. r.
$CH_2)_2(CH)_2O$	n. r.	n. r.	n. r.	n. r.
$CH_2)_4S$	n. r.	n. r.	n. r.	n. r.

nless otherwise stated, signals of the C_5H_5-ring and of the Zr-methyl group appear as singlets, signals of the $B(CH_3)$-protons appear as broad nglets. [a] taken from ref. 40b, [b] bis-adduct, [c] product of the CH-activation reaction, $(C_5H_5)_2Zr(CH_2)NMe(C_6H_5)^+MeB(C_6F_5)^-$, [d] CH-activation eaction (c.f. ref. 18g) results in a 1:2 mixture of two products, probably the N-coordinated (A) and borate coordinated (B) isomer, [e] mixture of vo species

ble S2. ^{1}H-NMR data for reaction products of 2a with different Lewis bases

wis base	C_5H_4	B-CH_3^-	$C_2(CH_3)_4$	Zr^+-CH_3	Lewis base
ne [a]	6.08 (β, methyl-side), 5.88 (β, borate-side), 5.58 (α, borate-side), 5.03 (α, methyl-side)	0.23	0.73 (borate-side), 0.58(methyl-side)	0.38	
$e_4C_2(C_5H_4)_2ZrMe_2$ [b]	n.r.	1.3	n.r.	0.15	–0.71 (μ-CH_3)
$e_2N(CH_2C_6H_5)$	5.98, 5.93, 5.36, 5.33	1.41	0.97, 0.61	0.36	7.0-7.2, 6.67 (m, 2H), 2.93 (s, 2H), 1.56 (s, 6H)
$e_2N(C_6H_5)$	5.88, 5.63, 5.17, 5.10	1.3	0.90, 0.63	0.39	6.7-7.2, 6.32 (m, 2H), 1.94 (s, 6H)
$e_2N(C_6H_5)$ oluene-d^8, 273 K)	5.67 (α, amine-side), 5.65 (β, methyl-side), 5.08 (β, amine-side), 5.05 (α, methyl-side)	1.4	0.88 (amine-side), 0.57 (methyl-side)	0.31	6.97 (meta-C_6H_5), 6.86 (para-C_6H_5), 6.30 (ortho-C_6H_5), 1.88 (NMe_2)
$le_2N(C_6H_5)$ H-activation [c]	6.13, 6.03, 5.60, 5.47, 5.37, 5.22, 4.93, 4.61 (each 1H)	0.65	0.96, 0.86, 0.71, 0.64 (each 3H)		6.7-7.0, 2.67 (1H, d, J=8.5 Hz, Zr-CH_2), 2.17 (NCH_3), 1.77 (1H, d, J=8.5, Zr-CH_2)
-Me-1-pyrroline	6.10, 5.73, 5.49, 5.29	1.35.	0.94, 0.69	0.24	3.5 (b), 2.52, 1.84 (t), 1.11
$^2(OMe)_3$	5.83, 5.66, 5.31, n.r.	1.38	0.96, 0.70	0.08	2.67 (d, J=10 Hz)

Unless otherwise stated, signals of the C_5H_4-ring appear as multipletts, signals of the C_2Me_4-bridge and of the Zr-methyl group as singlets with ntensities of 2H, 6H and 3H, respectively. Signals of the $B(CH_3)$-protons appear as broad singlets. [a] assignment by comparison with NOESY-ata in toluene, [b] taken from ref. 40b, [c] product of the CH-activation reaction : $Me_4C_2(C_5H_4)_2Zr(CH_2)NMe(C_6H_5)^+MeB(C_6F_5)^-$.

able S3. ^{1}H-NMR data for reaction products of 3a with different Lewis bases

ewis base	C_5H_4	$B\text{-}CH_3^-$	$Si\text{-}CH_3$, $Zr^+\text{-}CH_3$	Lewis base
one [a]	6.31 (β, methyl-side), 6.23 (β, borate-side), 5.28 (α, borate-side), 4.85 (α, methyl-side)	0.44	0.31 (Zr-Me), –0.06 (Si-Me, borate-side), –0.24 (Si-Me, methyl-side)	
$Me_2Si(C_5H_4)_2ZrMe_2$ [b]	n.r.	1.3	n.r.	–0.50 (μ-CH_3)
$Me_2N(SiMe_3)$	6.15, 5.92, 5.34, 5.13	n.r.	0.21, 0.17, –0.18	1.56 (s, 6H), –0.37 (s, 9H)
$Me_2N(CH_2C_6H_5)$	6.13, 5.62, 5.50, 5.22	1.4	0.44, 0.25, –0.23	n.r., 2.88 (s, 2H), 1.56 (s, 6H)
$Me_2N(C_6H_5)$ oluene, 273 K) [d]	5.85 (β, methyl-side), 5.40 (β, amine-side), 5.37 (α, amine-side), 4.94 (α, methyl-side)	1.4	0.19 (Zr-Me), 0.17 (Si-Me, amine-side), –0.24 (Si-Me, methyl-side)	6.94 (m-C_6H_5), 6.86 (p-C_6H_5), 6.26 (o-C_6H_5), 1.88 (NMe_2)
BU	6.26, 6.04, 5.45, 5.29	n.r.	0.21, 0.19, -0.04	2.9 (br, 2H), 2.5 (br, 6H), 2.35 (br, 2H), 1.9 (br, 2H), n.r.
$_2H_5)O(C_2H_5)$	6.43, 5.94, 5.58, 4.86	1.3	0.29, 0.18, –0.13	2.84 (α-CH_2), 0.93 (γ-CH_2), 0.83 (β-CH_2)
$_4H_9)O(C_4H_9)$ [d]	6.43 (β, methyl-side), 6.02 (β, ether-side), 5.63 (α, erher-side), 4.94 (α, methyl-side)	1.4	0.28 (Si-Me, borate-side), 0.26 (Si-Me, methyl-side), –0.21 (Zr-Me)	2.92 (t, OCH_2-), 0.99 (m, $OCCH_2$-), 0.83 (m, $OCCCH_2$-), 0.71 (t, $OCCCCH_3$)
HF	6.40, 5.86, 5.41, 4.95	1.33	0.29, 0.19, -0.13	2.82, 1.10
$CH_2C_6H_5)_3$	n.r., 6.26, 5.05, 4.48	1.44	0.15, –0.04, –0.10	6.6-7.2, 2.67 (d, 6H, J = 7 Hz)
$Me_2(C_6H_5)$	6.41, 6.21, 5.08, 4.90	1.41	0.13, –0.02, –0.04	n.r., 7.04, 6.63, 0.95 (d, J = 5 Hz)
$Me_2(C_6H_5))_2$ [c]	6.2 (4H), 4.98 (4H)	1.41	0.0 (6H), –0.17 (3H)	6.7-7.1, 1.01 (12H)

nless otherwise stated, signals of the C_5H_4-ring appear as multipletts, signals of the $SiMe_2$-bridge and of the Zr-methyl group as singlets with ensities of 2H, 3H and 3H, respectively. Signals of the $B(CH_3)$-protons appear as broad singlets. [a] assignment by comparison with NOESY-data toluene, [b] taken from ref. 40b, [c] bis-adduct, [d] assignement by NOESY-data

able S4. ^{1}H-NMR data for reaction products of 4a with different Lewis bases

ewis base	C_9H_7	B-CH_3^-	Zr^+-CH_3	Lewis base
one	n.r., 6.87, 6.76, 5.61, 5.46, 5.30	–0.20	–0.58	
$_9H_7)_2ZrMe_2$	6.5-7.0, 5.79 (4H), 5.67 (4H), 5.57 (4H)	1.53	–1.06 (6H)	–2.53 (μ-CH_3, 3H)
$e_2NCH_2(C_6H_5)$	n.r., 5.80, 5.71, 5.53	1.33	–1.34	n.r., 3.02 (s, 2H), 1.57 (s, 6H)
BU	n.r., 5.82, 5.4-5.5 (4H)	n.r.	n.r.	2.95 (bm), n.r.
6-Lutidine [a]	A: 6.1-6.9, 6.02 (t), 5.89, 5.67 B: 6.1-6.9, n.r., 5.49, 5.38	A: 1.45 B: 1.05	-	A: 6.1-6.9, 1.38 (3H), 0.46 (2H) B: 6.1-6.9, 1.21 (3H), 0.43 (2H)
yridazine	n.r., 5.65, 5.51, 5,19	1.35	0.12	n.r.
HF	6.87, 6.74, 5.69 (t), 5.57 (m), 5.47	1.44	–0.62	2.41 (4H), 0.98 (4H)
$_4H_9)O(C_4H_9)$	6.6-7.0, 5.85, 5.65, 5.42	1.46	–0.99	2.75 (OCH_2-), 0.92 ($OCCH_2$-), 0.80 (CH_2Me), 0.68 (-CH_3)
$(CH_2C_6H_5)_3$	7.2-6.6, 6.18, 5.84, 5.10 (t)	1.51	–1.80	6.5-7.2, 2.77 (d, J=6 Hz)
$le_2P(C_6H_5)$	6.4-7.1, 5.79, 5.74, 5.32	1.45	–1.80	7.1-6.4, 0.82 (d, 8 Hz)

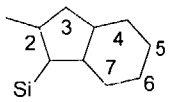
nless otherwise stated, signals of the C_9H_7-ligand appear as multipletts, signals of the Zr-methyl group as singlets with intensities of 2H and H, respectively. Signals of the B(CH_3)-protons appear as broad singlets. [a] CH-activation reaction (c.f. ref. 18g) results in a mixture of two roducts, probably the N-coordinated (A) and borate coordinated (B) isomer.

Table S5. ^{1}H-NMR data for reaction products of 5a with different Lewis bases

Lewis base	C_9H_6	B^--CH_3	Zr^+-CH_3, Si-CH_3	Lewis base
none [a]	7.50 (1H), 7.03 (2H), 6.89 (1H), 6.69 (1H), 6.63 (1H), 6.57 (1H, β-C_5H_2, methyl-side), 6.29 (2H), 6.22 (1H, β-C_5H_2, borate-side), 5.66 (1H, α-C_5H_2, borate-side), 4.97 (1H, α-C_5H_2, methyl-side)	-0.44	0.34 (Si, borate-side), 0.20 (Si-methyl-side), –0.51 (Zr-Me)	
$Me_2Si(C_9H_7)_2ZrMe_2$ [b]	n.r.	1.4/1.1	–0.96/–0.99 (Zr-CH_3), n.r.	–3.10/–3.22 (μ-CH_3)
$(C_4H_9)O(C_4H_9)$ [c]	n.r., 6.04 (1H, β-C_5H_2, ether-side), 5.83 (1H, α-C_5H_2, ether-side), 5.09 (1H, α-C_5H_2, methyl-side),	n.r.	0.58, 0.23, –0.72	2.69 (O-CH_2), 2.40 (O-CH_2), n.r.

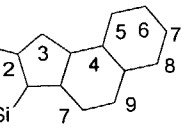
Signals of the B(CH_3)-protons appear as broad singlets. [a] taken from ref. 31, [b] 2 isomers, data taken from ref. 40b, [c] assignment by comparison with NOESY-data at 328 K.

Table S6. ^{1}H-NMR data of reactions of 6a with different Lewis bases

ewis base	$C_9H_5(CH_3)$	B-CH_3^-	Zr^+-CH_3, Si-CH_3	Lewis base
	6.8-7.5,6.55 (m, 1H), 6.37 (s, 1H), 6.34 (m, 1H), 6.2 (m, 1H), 6.12 (s, 1H), 1.71 (s, 3H), 1.44 (s, 3H)	–0.26	0.48, 0.43, –0.28	
$e_2Si(C_9H_6Me)_2ZrMe_2$ [a]	A: 6.1-7.4, 5.75 (2H), 1.79 (6H), 1.63 (6H) B: 6.1-7.4, 5.80 (2H), 1.83 (6H), 1.63 (6H)	A: 1.47 B: n.r.	A: 0.78 (6H), 0.62 (6H), –0.76 (6H) B: 0.78 (6H), 0.62 (6H), –0.76 (6H)	A: –2.86 (3H, μ-CH_3) B: –2.53 (3H, μ-CH_3)
Me_3	6.6-7.6, 5.53 (1H), 1.76 (s, 3H), 1.43 (s, 3H)	n.r.	0.62, 0.41, –0.71	1.24 (9H)
$e_2N(CH_2)(C_6H_5)$ [a] 	methyl-side: 7.19 (C_{4a}), 7.02 (C_{7a}), 6.76 (C_{6a}), n.r., 6.35 (C_{3b}), 1.49 (C_{2b}-Me), amine-side: 7.36 (C_{7b}), 6.96 (C_{4b}), 6.65 (C_{6b}), n.r., 5.85 (C_{3a}), 1.85 (C_{2a}-Me)	1.39	0.65 (Si-Me, amine-side), 0.47 (Si-Me, methyl-side), –0.55 (Zr-Me)	n.r., 7.18 (meta-C_6H_5), 6.70 (ortho-C_6H_5), n.r.
-Me-1-pyrroline	6.5-7.4, 6.23 (1H), 6.05 (1H), 1.74 (s, 3H), 1.49 (s, 3H)	1.37	0.63, 0.51, –0.76	2.8 (bm), n.r.
$_4H_9)O(C_4H_9)$	6.4-7.5, 6.69 (1H), 5.88 (1H), 1.82 (s, 3H), n.r.	n.r.	0.70, 0.49, –0.46	2.70 (2H, O-CH_2), 2.48 (2H, O-CH_2), n.r.
$CH_2)_5O$	6.6-7.4, 6.42 (1H), 5.78 (1H), 1.80 (s, 3H), 1.47 (3s, H)	1.42	0.68, 0.47, -0.65	2.7 (m, 4H), 1.0 (m, 6H)
$CH)_2(CH_2)_3O$	6.0-7.6, 5.79 (1H), 1.74 (s, 3H), 1.41 (s, 3H)	n.r.	0.65, 0.44, -0.59	n.r., 4.45 (m), n.r.

ignals of the B(CH_3)-protons appear as broad singlets. [a] assignement by ROESY spectra, 600MHz, benzene, 300 K.

Table S7. ^{1}H-NMR data of reactions of 7a with different Lewis bases

ewis base	$C_{13}H_9(CH_3)$	BCH_3^-	Zr^+-CH_3, Si-CH_3	Lewis base
one [a]	methyl-side: 7.86 (C_{4a}), 7.61 (C_{5a}), 7.49 (C_{7a}), 7.29 (C_{6a}), 7.04 (C_{8a}), 6.97 (C_{9a}), 6.97 (C_{3b}), 1.65 (C_{2b}-Me), borate-side: 6.74 (C_{9b}), 6.95 (C_{8b}), 7.16 (C_{7b}), 7.08 (C_{6b}), 7.12 (C_{5b}), 7.68 (C_{4b}), 6.73 (C_{3a}), 1.87 (C_{2a}-Me)	–0.34	0.564 ($SiCH_3$), 0.558 ($SiCH_3$), –0.41 (Zr-CH_3)	-
$e_2N(CH_2)(C_6H_5)$ [b] 	methyl-side: 7.03 (C_{9a}), 6.98 (C_{8a}), 7.59 (C_{7a}), 7.15 (C_{6a}), 7.43 (C_{5a}), 7.77 (C_{4a}), 6.82 (C_{3b}), 1.70 (C_{2b}-Me), amine-side: 7.36 (C_{9b}), 7.07 (C_{8b}), 7.49 (C_{7b}), n.r. (C_{6b}, C_{5a}), 7.30 (C_{4b}), 6.59 (C_{3a}), 2.14 (C_{2a}-Me)	1.36	0.75 (Si-Me, amine-side), 0.59 (Si-Me, methyl-side), –0.58 (Zr-Me)	n.r. (p-C_6H_5), 6.93 (m-C_6H_5), 5.73 (o-C_6H_5), 1.44 (3H, NCH_3), 1.33 (2H, NCH_3), 2.85 (d, 1H, NCH_2), n.r. (d, 1H, NCH_2)
$C_4H_9)O(C_4H_9)$	n.r., 6.59 (1H), 2.03 (3H), 1.65 (3H)	n.r.	0.78, n.r., –0.62	2.51 (1H, dt), 2.04 (1H, dt), n.r.

ignals of the $B(CH_3)$-protons appear as broad singlets. [a] taken from ref. 29, [b] assignement by ROESY spectra, 600MHz, benzene, 300 K.