

Supporting Information

The Nature of Pd–Carbene and Pd–Halogen Bonds in (BisNHC)PdX₂ Type Catalysts : Insights from Density Functional Theory

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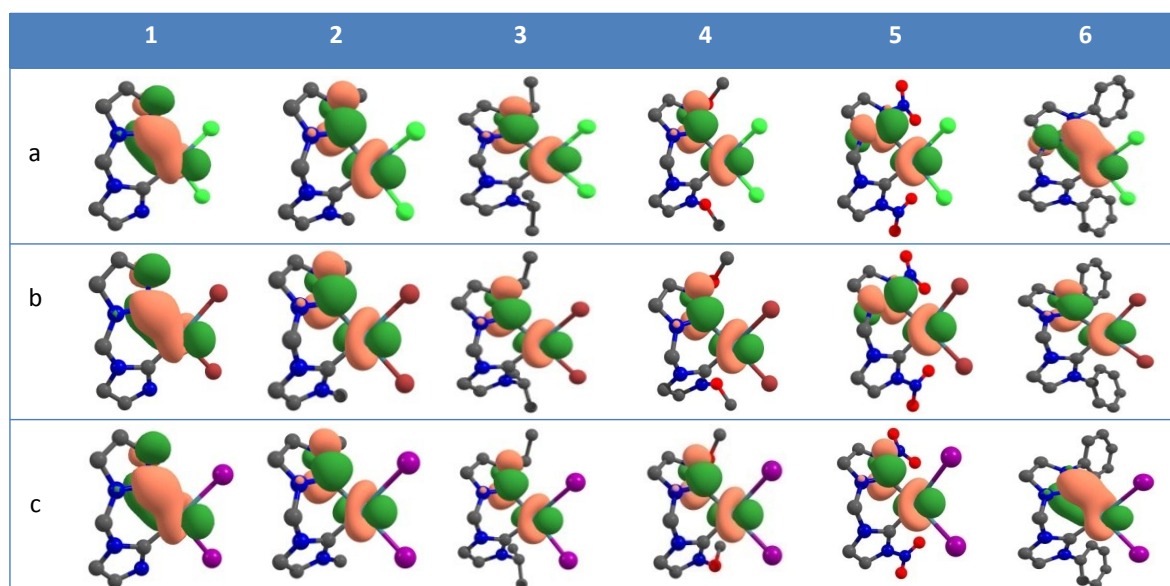
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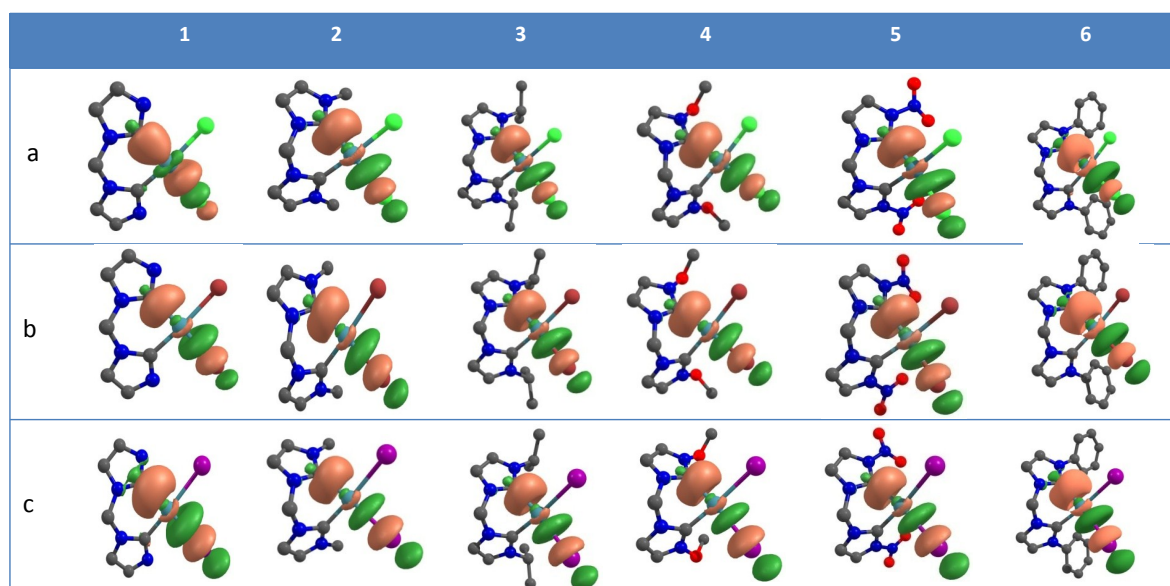
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SIF1. Backbonding interaction ($n \rightarrow \pi^*$) between Palladium and bis(NHC) ligand computed at B3LYP/LANL2DZ[#] (# LANL2DZ for Pd, Br and I atom, 6-31g(d) for all other atoms) level.



SIF2. Stabilization interaction between Pd-C_{Carbene} and Pd-X bonds ($\sigma_{\text{C-Pd}} \rightarrow \sigma^*_{\text{Pd-X}}$) at B3LYP/LANL2DZ[#] (# LANL2DZ for Pd, Br and I atom, 6-31g(d) for all other atoms) level.



SIT1. Selected optimized geometrical parameters computed with various functionals and LANL2DZ[#] (# LANL2DZ for Pd, Br and I atom, 6-31g(d) for all other atoms) basis set along with crystal data* for 2a.

Bond Parameter	B3LYP	B3LYP-D3	B3PW91	M06	PBE	BP86	Exp*
Pd-X	2.397	2.396	2.363	2.375	2.388	2.391	2.378
Pd-C	2.020	2.018	1.998	2.018	2.388	1.999	1.966
Pd-C-Pd	86.0	85.7	86.0	85.7	86.4	86.5	83.8
X-Pd-X	92.5	93.1	92.6	92.6	91.9	91.9	91.2

*T. Strassner, M. Muehlhofer, A. Zeller, E. Herdtweck and W. A. Herrmann, *J. Organomet. Chem.*, 2004, **689**, 1418-1424.

SIT2. Selected bond lengths (Å) and bond angles (°) of the optimized [L_nPdX₂] complexes. (L_n=bisNHC, X=Cl, Br and I)

Complex	Pd-C _{carbene}	Pd-X	N ₁ -C ₂	N ₃ -C ₂	X-Pd-X	C ₂ -Pd-C _{2'}	N ₁ -C ₂ -N ₃
1a	1.989	2.414	1.344	1.362	96.3	87.5	104.7
1b	2.003	2.587	1.346	1.363	95.0	87.4	104.4
1c	2.023	2.746	1.347	1.363	93.3	87.1	104.1
2a	2.019	2.397	1.353	1.365	92.5	86.0	104.6
	1.966*	2.378*			91.2*	83.8*	
2b	2.026	2.574	1.353	1.365	92.4	85.7	104.6
2c	2.037	2.738	1.353	1.365	93.1	85.0	104.5
3a	2.020	2.397	1.353	1.365	92.7	86.0	104.8
3b	2.025	2.567	1.353	1.365	93.3	85.6	104.8
3c	2.039	2.740	1.353	1.365	92.8	84.9	104.8
4a	2.017	2.388	1.349	1.367	91.8	84.9	103.1
4b	2.023	2.567	1.349	1.368	92.3	84.8	103.1
4c	2.042	2.729	1.349	1.368	92.9	84.9	102.9
5a	2.003	2.377	1.357	1.360	94.7	86.2	102.7
5b	2.012	2.558	1.359	1.360	94.6	86.1	102.6
5c	2.028	2.721	1.360	1.360	94.0	85.5	102.5
6a	2.019	2.384	1.360	1.364	93.9	86.7	104.4
6b	2.025	2.564	1.360	1.364	94.0	86.4	104.4
6c	2.040	2.728	1.361	1.364	93.7	85.9	104.3

*T. Strassner, M. Muehlhofer, A. Zeller, E. Herdtweck and W. A. Herrmann, *J. Organomet. Chem.*, 2004, **689**, 1418-1424.

SIT3. Natural Hybrid Orbital (NHO) Analysis of Pd-C_{carbene} bond in complexes 1a-6c

Complex	Occ.	polarization		hybridization	
		Pd	C	Pd	C
1a	1.82	24.2%	75.8%	s (25.5%), p (45.4%),d (29.1%)	s (39.5%), p (60.5%)
1b	1.83	24.2%	75.8%	s (25.6%), p (45.1%),d (29.3%)	s (39.8%), p (60.2%)
1c	1.84	24.0%	76.0%	s (26.4%), p (43.7%),d (29.9%)	s (40.2%), p(59.8%)
2a	1.83	23.3%	76.7%	s (25.4%), p (46.5%),d (28.1%)	s (40.1%), p(59.9%)
2b	1.84	23.4%	76.6%	s (25.4%), p (46.1%),d (28.5%)	s (40.2%), p (59.8%)
2c	1.84	23.6%	76.4%	s (25.9%), p (44.5%),d (29.6%)	s (40.4%), p (59.6%)
3a	1.83	23.4%	76.6%	s (25.3%), p (46.4%),d (28.2%)	s (40.0%), p (60.0%)
3b	1.83	23.6%	76.4%	s (25.3%), p (46.1%),d (28.6%)	s (40.0%), p (60.0%)
3c	1.84	23.5%	76.5%	s (25.8%), p (44.6%),d (29.6%)	s (40.0%), p (60.0%)
4a	1.83	22.6%	77.4%	s (25.4%), p (46.7%),d (27.8%)	s (40.7%), p (59.3%)
4b	1.84	22.7%	77.3%	s (25.5%), p (46.3%),d (28.2%)	s (40.9%), p (59.1%)
4c	1.85	22.7%	77.3%	s (25.9%), p (45.1%),d (28.9%)	s (41.3%), p (58.7%)
5a	1.83	21.8%	78.2%	s (25.1%), p (47.4%),d (27.5%)	s (41.5%), p (58.5%)
5b	1.84	21.8%	78.1%	s (25.1%), p (47.1%),d (27.8%)	s (41.7%), p (58.3%)
5c	1.85	21.7%	78.3%	s (25.8%), p (45.4%),d (28.7%)	s (41.9%), p (58.1%)
6a	1.83	22.8%	77.2%	s (25.0%), p (47.3%),d (27.7%)	s (40.8%), p (59.2%)
6b	1.84	22.9%	77.1%	s (24.9%), p (47.1%),d (28.1%)	s (41.0%), p (59.0%)
6c	1.84	22.8%	77.2%	s (25.5%), p (45.4%),d (29.1%)	s (41.0%), p (59.0%)

SIT4. Second-order perturbation (back-bonding) interaction between palladium d-orbitals and π^* antibonding orbital of NHC computed at B3LYP/LANL2DZ# (# LANL2DZ for Pd, Br and I atom, 6-31g(d) for all other atoms) level.

Complex	Donor(i)	Acceptor(j)	E(2) (kcal/mol)	E(j)-E(i) (a.u)	F(i,j) (a.u)
1a	LP (4)Pd	$\pi^*(N_1 - C_2)$	7.82	0.23	0.042
1b	LP (4)Pd	$\pi^*(N_1 - C_2)$	7.47	0.23	0.041
1c	LP (4)Pd	$\pi^*(N_1 - C_2)$	7.11	0.23	0.040
2a	LP (4)Pd	$\pi^*(N_1 - C_2)$	8.06	0.24	0.043
2b	LP (4)Pd	$\pi^*(N_1 - C_2)$	8.00	0.24	0.043
2c	LP (4)Pd	$\pi^*(N_1 - C_2)$	7.81	0.24	0.043
3a	LP (4)Pd	$\pi^*(N_1 - C_2)$	8.00	0.24	0.043
3b	LP (4)Pd	$\pi^*(N_1 - C_2)$	7.89	0.24	0.043
3c	LP (4)Pd	$\pi^*(N_1 - C_2)$	7.62	0.24	0.042
4a	LP (4)Pd	$\pi^*(N_1 - C_2)$	8.62	0.24	0.044
4b	LP (4)Pd	$\pi^*(N_1 - C_2)$	8.55	0.24	0.044
4c	LP (4)Pd	$\pi^*(N_1 - C_2)$	7.95	0.24	0.043
5a	LP (4)Pd	$\pi^*(N_1 - C_2)$	9.56	0.22	0.045
5b	LP (4)Pd	$\pi^*(N_1 - C_2)$	9.43	0.22	0.045
5c	LP (4)Pd	$\pi^*(N_1 - C_2)$	9.04	0.22	0.045
6a	LP (4)Pd	$\pi^*(N_1 - C_2)$	8.33	0.24	0.044
6b	LP (4)Pd	$\pi^*(N_1 - C_2)$	8.26	0.24	0.044
6c	LP (4)Pd	$\pi^*(N_1 - C_2)$	8.13	0.24	0.044

SIT5. Energies (eV) of the Highest Occupied Molecular orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO) of the complexes, the Highest Occupied Fragment orbital (HOMO) of PdX₂ fragment and the Lowest Unoccupied Fragment Orbital (LUMO) of [N-R(bisNHC)] fragment.

Complex	Complex		Fragment	
	HOMO	LUMO	HOMO of PdX ₂	LUMO of bis(NHC)
1a	-5.9473	-1.2180	-7.9544	0.8626
1b	-5.6417	-1.5497	-7.4075	0.8626
1c	-5.2904	-1.7100	-7.0491	0.8626
2a	-5.6382	-1.0544	-7.9544	0.8670
2b	-5.2251	-1.3505	-7.4075	0.8670
2c	-4.8989	-1.4798	-7.0491	0.8670
3a	-5.5702	-0.9780	-7.9544	0.9464
3b	-5.2137	-1.2776	-7.4075	0.9464
3c	-4.8673	-1.4332	-7.0491	0.9464
4a	-5.6121	-1.2000	-7.9544	0.6876
4b	-5.2657	-1.4830	-7.4075	0.6876
4c	-4.8488	-1.6153	-7.0491	0.6876
5a	-5.9095	-3.0754	-7.9544	-2.4958
5b	-5.6069	-3.1579	-7.4075	-2.4958
5c	-5.2880	-3.1772	-7.0491	-2.4958
6a	-5.2853	-1.0474	-7.9544	-0.3086
6b	-4.9536	-1.1780	-7.4075	-0.3086
6c	-4.6597	-1.3565	-7.0491	-0.3086

SIT6. Charge transfer values (Δq) from carbene C atom to Pd atom and halogen atom to Pd atom in the complexes.

Complex	$C_{\text{carbene}} \rightarrow \text{Pd}$			$X \rightarrow \text{Pd}$		
	a	b	c	a	b	c
1	-0.389	-0.361	-0.321	-0.230	-0.275	-0.317
2	-0.440	-0.415	-0.378	-0.228	-0.251	-0.316
3	-0.441	-0.419	-0.377	-0.221	-0.271	-0.313
4	-0.419	-0.392	-0.391	-0.242	-0.286	-0.335
5	-0.427	-0.406	-0.366	-0.246	-0.299	-0.346
6	-0.466	-0.440	-0.400	-0.230	-0.280	-0.348

SIT7. Natural Hybrid Orbital (NHO) Analysis of Pd-X bond

Complex	Occ.	polarization		hybridization	
		Pd	X	Pd	X
1a	1.91	16.9%	83.1%	s (23.2%), p (58.7%),d (23.1%)	s (16.2%), p (83.7%)
1b	1.90	19.8%	80.2%	s (23.2%), p (54.1%),d (22.7%)	s (15.1%), p (84.8%)
1c	1.89	23.4%	76.6%	s (22.5%), p (54.9%),d (22.6%)	s (13.3%), p (86.7%)
2a	1.90	18.1%	81.9%	s (23.3%), p (52.6%),d (24.1%)	s (16.1%), p (83.8%)
2b	1.89	20.8%	79.2%	s (23.4%), p (52.9%),d (23.7%)	s (15.1%), p (84.7%)
2c	1.87	24.2%	75.8%	s (22.9%), p (54.1%),d (2.9%)	s (13.7%), p (86.3%)
3a	1.90	17.9%	82.1%	s (23.4%), p (52.5%),d (24.1%)	s (16.3%), p (83.6%)
3b	1.89	20.6%	79.4%	s (23.5%), p (52.9%),d (23.6%)	s (15.5%), p (84.4%)
3c	1.88	23.9%	76.1%	s (23.5%), p (52.9%),d (23.6%)	s (14.1%), p (85.9%)
4a	1.89	18.3%	81.7%	s (23.3%), p (52.4%),d (24.3%)	s (15.4%), p (84.5%)
4b	1.88	21.1%	78.9%	s (23.4%), p (52.7%),d (23.9%)	s (14.4%), p (85.4%)
4c	1.87	24.4%	75.6%	s (23.4%), p (53.6%),d (23.0%)	s (13.8%), p (86.2%)
5a	1.88	19.6%	80.4%	s (23.6%), p (51.7%),d (24.7%)	s (14.5%), p (85.4%)
5b	1.87	22.6%	77.4%	s (23.7%), p (52.0%),d (24.3%)	s (13.5%), p (86.3%)
5c	1.85	26.2%	73.8%	s (23.0%), p (53.4%),d (23.6%)	s (12.0%), p (88.0%)
6a	1.89	18.8%	81.2%	s (23.7%), p (51.7%),d (24.6%)	s (16.1%), p (83.8%)
6b	1.88	23.8%	78.5%	s (23.5%), p (52.0%),d (24.1%)	s (15.3%), p (84.5%)
6c	1.87	24.8%	75.2%	s (23.5%), p (53.0%),d (23.5%)	s (14.1%), p (86.0%)

SIT8. $\sigma \rightarrow \sigma^*$ stabilization interaction between C-Pd and Pd-X.

Complex	Donor(i)	Acceptor(j)	E(2) (kcal/mol)	E(j)-E(i) (a.u)	F(i,j) (a.u)
1a	$\sigma_{\text{C-Pd}}$	$\sigma^*_{\text{Pd-Cl}}$	18.02	0.65	0.097
1b	$\sigma_{\text{C-Pd}}$	$\sigma^*_{\text{Pd-Br}}$	15.87	0.64	0.090
1c	$\sigma_{\text{C-Pd}}$	$\sigma^*_{\text{Pd-I}}$	15.40	0.66	0.090
2a	$\sigma_{\text{C-Pd}}$	$\sigma^*_{\text{Pd-Cl}}$	17.97	0.63	0.096
2b	$\sigma_{\text{C-Pd}}$	$\sigma^*_{\text{Pd-Br}}$	15.88	0.62	0.089
2c	$\sigma_{\text{C-Pd}}$	$\sigma^*_{\text{Pd-I}}$	15.77	0.65	0.091
3a	$\sigma_{\text{C-Pd}}$	$\sigma^*_{\text{Pd-Cl}}$	18.38	0.63	0.096
3b	$\sigma_{\text{C-Pd}}$	$\sigma^*_{\text{Pd-Br}}$	16.31	0.61	0.090
3c	$\sigma_{\text{C-Pd}}$	$\sigma^*_{\text{Pd-I}}$	16.45	0.64	0.092
4a	$\sigma_{\text{C-Pd}}$	$\sigma^*_{\text{Pd-Cl}}$	16.92	0.64	0.093
4b	$\sigma_{\text{C-Pd}}$	$\sigma^*_{\text{Pd-Br}}$	14.89	0.63	0.087
4c	$\sigma_{\text{C-Pd}}$	$\sigma^*_{\text{Pd-I}}$	14.38	0.65	0.087
5a	$\sigma_{\text{C-Pd}}$	$\sigma^*_{\text{Pd-Cl}}$	15.70	0.66	0.091
5b	$\sigma_{\text{C-Pd}}$	$\sigma^*_{\text{Pd-Br}}$	13.61	0.65	0.084
5c	$\sigma_{\text{C-Pd}}$	$\sigma^*_{\text{Pd-I}}$	13.15	0.67	0.084
6a	$\sigma_{\text{C-Pd}}$	$\sigma^*_{\text{Pd-Cl}}$	16.47	0.62	0.091
6b	$\sigma_{\text{C-Pd}}$	$\sigma^*_{\text{Pd-Br}}$	14.47	0.61	0.084
6c	$\sigma_{\text{C-Pd}}$	$\sigma^*_{\text{Pd-I}}$	14.61	0.63	0.086

SIT9. Energy decomposition analysis (kcal/mol) of the interaction between X⁻ and [N-R bis(NHC) PdX]⁺ fragments in the equilibrium [N-R bis(NHC) PdX₂] structures.

Complex	ΔE_{Pauli}	$\Delta E_{\text{elestat}}$	ΔE_{steric}	ΔE_{orb}	ΔE_{int}
1a	89.26	-161.14	-71.88	-56.89	-128.78
1b	97.92	-161.77	-63.86	-56.99	-120.85
1c	92.82	-148.96	-56.14	-57.70	-113.84
2a	95.11	-152.50	-57.39	-59.52	-116.91
2b	103.37	-154.29	-50.92	-58.34	-109.26
2c	97.18	-143.07	-45.89	-57.74	-103.63
3a	94.97	-149.59	-54.61	-59.48	-114.09
3b	103.48	-151.94	-48.46	-57.98	-106.44
3c	97.69	-141.50	-43.81	-54.51	-98.33
4a	96.39	-153.72	-57.33	-60.15	-117.49
4b	104.93	-155.58	-50.64	-58.98	-109.62
4c	99.99	-145.46	-45.47	-58.55	-104.02
5a	97.40	-159.45	-62.06	-62.06	-124.11
5b	106.06	-161.32	-55.26	-63.14	-118.40
5c	100.91	-150.02	-49.11	-64.47	-113.58
6a	94.97	-144.16	-49.19	-60.70	-109.88
6b	103.33	-146.99	-43.66	-58.97	-102.63
6c	98.04	-137.33	-39.29	-58.89	-98.18

SIT10. Bond dissociation energy (BDE) of Pd-X bond obtained using different functional with def2TZVP basis set along with B3LYP/LANL2DZ# results.

Complex	B3LYP/ LANL2DZ#	B3LYP-D3/ def2TZVP*	B3PW91/ def2TZVP*	M06/ def2TZVP *	PBE0/ def2TZVP *
1a	130.16	134.47	132.95	138.04	135.61
1b	126.94	125.69	124.06	130.55	126.71
1c	115.96	117.54	116.18	124.21	118.83
2a	118.98	123.86	121.39	128.09	124.17
2b	116.27	115.27	112.68	120.73	115.42
2c	105.97	107.84	105.79	115.05	108.52
3a	116.48	122.27	118.89	126.64	121.98
3b	113.87	113.97	110.39	119.69	113.44
3c	103.67	106.84	103.38	114.26	106.52
4a	118.14	122.77	120.62	127.84	123.41
4b	115.22	114.04	111.80	120.36	114.56
4c	104.69	106.72	104.49	114.65	107.41
5a	123.73	129.51	127.13	133.17	129.77
5b	121.81	121.63	119.20	126.65	121.83
5c	113.00	115.34	113.24	122.08	115.97
6a	108.59	116.01	112.50	119.89	115.27
6b	106.63	108.18	104.53	113.53	107.26
6c	94.59	102.21	99.00	110.02	101.95

LANL2DZ for Pd, Br and I atom, 6-31g(d) for all other atoms

* Single point energy calculation

SIT11. Bond dissociation energy (BDE) of Pd-C_{Carbene} bond obtained using different functional with def2TZVP basis set along with B3LYP/LANL2DZ[#] results.

Complex	B3LYP/ LANL2DZ [#]	B3LYP-D3/ def2TZVP*	B3PW91/ def2TZVP*	M06/ def2TZVP*	PBE0/ def2TZVP*
1a	120.22	124.82	124.06	123.46	128.42
1b	115.16	120.58	119.49	115.18	124.11
1c	102.76	108.20	106.35	99.48	111.03
2a	109.32	117.45	113.76	115.76	118.29
2b	104.82	113.37	109.38	107.70	114.17
2c	93.30	102.18	97.29	93.20	102.21
3a	108.72	120.72	114.75	118.66	119.74
3b	104.34	116.93	110.52	110.94	115.78
3c	92.64	105.64	98.24	96.36	103.69
4a	98.74	109.40	104.61	107.05	109.35
4b	94.12	105.20	100.07	99.05	105.08
4c	82.22	93.90	87.65	84.65	92.76
5a	79.86	96.27	91.43	93.77	95.66
5b	76.34	93.04	87.84	86.88	92.36
5c	66.84	83.17	77.16	73.92	81.84
6a	92.60	111.90	103.54	108.27	108.11
6b	89.10	108.94	99.91	101.44	104.79
6c	75.82	98.61	88.46	87.92	93.59

[#] LANL2DZ for Pd, Br and I atom, 6-31g(d) for all other atoms

* Single point energy calculation

SIT12. Cartesian coordinates of all the geometries and E (*in a.u.*).

1a E=-1537.7723451

7	2.674967000	0.430529000	-0.299823000
6	1.375283000	0.588873000	0.004766000
7	1.208418000	1.935989000	0.119958000
6	2.417580000	2.600502000	-0.094606000
6	3.340235000	1.639332000	-0.362959000
6	-0.000007000	2.568953000	0.625411000
7	-1.208410000	1.935999000	0.119897000
6	-2.417559000	2.600524000	-0.094712000
6	-3.340215000	1.639361000	-0.363084000
7	-2.674966000	0.430550000	-0.299898000
6	-1.375283000	0.588883000	0.004700000
1	4.389789000	1.717548000	-0.599137000
1	2.505701000	3.674627000	-0.041306000
1	-2.505668000	3.674651000	-0.041436000
1	-4.389760000	1.717586000	-0.599296000
1	-0.000033000	2.528545000	1.720845000
1	0.000005000	3.614905000	0.311107000
46	-0.000004000	-0.845647000	0.079901000
17	-1.798731000	-2.454873000	0.017577000
17	1.798724000	-2.454852000	0.017331000
1	-3.026706000	-0.526397000	-0.408882000
1	3.026698000	-0.526417000	-0.408834000

1b E=-643.7305985

7	-0.975728000	2.673868000	-0.377636000
6	-1.095683000	1.384633000	-0.011054000
7	-2.434685000	1.204909000	0.165499000
6	-3.130190000	2.390824000	-0.073119000
6	-2.197886000	3.316881000	-0.418466000
6	-3.017853000	-0.000368000	0.732109000
7	-2.434555000	-1.205327000	0.164976000
6	-3.130020000	-2.391095000	-0.074480000
6	-2.197628000	-3.316929000	-0.420146000
7	-0.975489000	-2.673919000	-0.378715000
6	-1.095507000	-1.384873000	-0.011487000
1	-2.302820000	4.354433000	-0.693955000
1	-4.202700000	2.462736000	0.021135000
1	-4.202550000	-2.463068000	0.019528000
1	-2.302482000	-4.354337000	-0.696205000
1	-2.868127000	-0.000592000	1.817345000
1	-4.088928000	-0.000384000	0.521247000
46	0.349444000	0.000013000	0.072818000
35	2.098760000	-1.905786000	0.020103000
35	2.098330000	1.906058000	0.018685000
1	-0.036734000	3.055033000	-0.527251000
1	-0.036446000	-3.055063000	-0.528083000

1c E= -640.1679056

7	-1.431406000	2.661743000	-0.485346000
6	-1.492547000	1.394053000	-0.033625000
7	-2.814573000	1.201348000	0.235641000
6	-3.555244000	2.352026000	-0.032327000
6	-2.670080000	3.275469000	-0.489193000
6	-3.325028000	-0.000034000	0.874637000
7	-2.814558000	-1.201390000	0.235608000
6	-3.555219000	-2.352064000	-0.032405000
6	-2.670047000	-3.275480000	-0.489308000
7	-1.431389000	-2.661723000	-0.485497000
6	-1.492527000	-1.394077000	-0.033649000
1	-2.816520000	4.292570000	-0.817012000
1	-4.621346000	2.405997000	0.125292000
1	-4.621319000	-2.406053000	0.125218000
1	-2.816478000	-4.292569000	-0.817171000
1	-3.035637000	-0.000047000	1.930328000
1	-4.413754000	-0.000039000	0.801576000
46	-0.029334000	-0.000001000	0.053806000
53	1.855883000	1.996699000	0.023535000
53	1.855910000	-1.996681000	0.023608000
1	-0.521488000	-3.071798000	-0.704868000
1	-0.521504000	3.071850000	-0.704649000

2a E= -1616.3809892

7	-2.539498000	0.776439000	0.707708000
6	-1.377305000	0.612351000	0.035154000
7	-1.192020000	1.792742000	-0.624586000
6	-2.227166000	2.684036000	-0.370488000
6	-3.075562000	2.036033000	0.466225000
6	-0.000001000	2.030593000	-1.425309000
7	1.192018000	1.792743000	-0.624586000
6	2.227161000	2.684040000	-0.370485000
6	3.075559000	2.036037000	0.466224000
7	2.539498000	0.776442000	0.707706000
6	1.377305000	0.612352000	0.035153000
1	-4.009084000	2.351145000	0.905818000
1	-2.277192000	3.665396000	-0.816172000
1	2.277184000	3.665401000	-0.816168000
1	4.009081000	2.351150000	0.905816000
1	-0.000001000	1.355972000	-2.284479000
1	-0.000002000	3.066224000	-1.767885000
46	0.000000000	-0.856745000	-0.117141000
6	-3.131125000	-0.196745000	1.630099000
1	-2.822240000	0.028245000	2.655679000
1	-4.219168000	-0.135595000	1.552633000
1	-2.797882000	-1.192387000	1.333618000
6	3.131130000	-0.196743000	1.630092000

1	4.219173000	-0.135615000	1.552601000
1	2.822274000	0.028262000	2.655678000
1	2.797865000	-1.192383000	1.333627000
17	1.731102000	-2.477230000	-0.457823000
17	-1.731100000	-2.477231000	-0.457823000

2b E = -722.3401532

7	-2.516405000	1.339387000	0.733207000
6	-1.377219000	1.075228000	0.052945000
7	-1.191145000	2.167056000	-0.744278000
6	-2.202560000	3.103001000	-0.567061000
6	-3.038067000	2.573244000	0.360907000
6	-0.000108000	2.295622000	-1.571959000
7	1.190947000	2.167158000	-0.744289000
6	2.202282000	3.103190000	-0.567073000
6	3.037841000	2.573501000	0.360887000
7	2.516287000	1.339597000	0.733185000
6	1.377118000	1.075346000	0.052931000
1	-3.954355000	2.955034000	0.783599000
1	-2.249495000	4.026696000	-1.122723000
1	2.249134000	4.026892000	-1.122732000
1	3.954099000	2.955367000	0.783574000
1	-0.000079000	1.508484000	-2.328861000
1	-0.000153000	3.275022000	-2.052004000
46	0.000015000	-0.410235000	0.026560000
6	-3.094547000	0.493558000	1.780374000
1	-2.696670000	0.784837000	2.757298000
1	-4.179353000	0.620693000	1.772801000
1	-2.846342000	-0.545742000	1.559994000
6	3.094509000	0.493813000	1.780344000
1	4.179304000	0.621044000	1.772768000
1	2.696610000	0.785051000	2.757272000
1	2.846396000	-0.545508000	1.559960000
35	1.863198000	-2.162891000	-0.261146000
35	-1.863000000	-2.163065000	-0.261176000

2c E=-718.7788319

7	-2.485357000	1.793484000	0.742505000
6	-1.371992000	1.441629000	0.058906000
7	-1.182374000	2.456848000	-0.833876000
6	-2.166684000	3.430210000	-0.712207000
6	-2.990418000	3.003208000	0.276830000
6	0.008892000	2.500554000	-1.671393000
7	1.199414000	2.448868000	-0.833318000
6	2.190035000	3.415702000	-0.710732000
6	3.010218000	2.983081000	0.278823000
7	2.496848000	1.776632000	0.743895000
6	1.381687000	1.432289000	0.059429000
1	-3.887505000	3.442113000	0.685331000

1	-2.206626000	4.304767000	-1.343021000
1	2.236274000	4.290044000	-1.341410000
1	3.909916000	3.415928000	0.688041000
1	0.006201000	1.643217000	-2.347416000
1	0.012107000	3.428658000	-2.244311000
46	-0.000254000	-0.064019000	0.108208000
6	-3.055553000	1.061959000	1.874158000
1	-2.811643000	1.577060000	2.808692000
1	-4.140272000	1.004698000	1.756282000
1	-2.645381000	0.052772000	1.876443000
6	3.061072000	1.041091000	1.875946000
1	4.145834000	0.979547000	1.760695000
1	2.816963000	1.555786000	2.810651000
1	2.646628000	0.033625000	1.875689000
53	-1.994484000	-1.917773000	-0.175690000
53	1.981766000	-1.930764000	-0.176692000

3a E=-1773.6448387

7	-2.545935000	0.810836000	0.354593000
6	-1.377977000	0.632471000	-0.304106000
7	-1.192205000	1.789420000	-1.004308000
6	-2.235787000	2.681126000	-0.791575000
6	-3.088061000	2.057764000	0.059516000
6	0.000152000	2.003537000	-1.810384000
7	1.192675000	1.789123000	-1.004629000
6	2.236523000	2.680578000	-0.792131000
6	3.088746000	2.057058000	0.058912000
7	2.546269000	0.810369000	0.354261000
6	1.378136000	0.632285000	-0.304173000
1	-4.025246000	2.390394000	0.475698000
1	-2.284990000	3.648463000	-1.267248000
1	2.285912000	3.647868000	-1.267879000
1	4.026067000	2.389474000	0.474966000
1	-0.000053000	1.305083000	-2.650605000
1	0.000230000	3.028957000	-2.182677000
46	-0.000026000	-0.840092000	-0.418389000
6	-3.159510000	-0.160187000	1.297017000
1	-2.502094000	-1.029455000	1.256749000
6	3.159282000	-0.160421000	1.297329000
1	2.502577000	-1.030176000	1.255923000
17	1.734669000	-2.465566000	-0.725376000
17	-1.734610000	-2.465646000	-0.725150000
6	-4.540307000	-0.586721000	0.794874000
1	-4.946595000	-1.350369000	1.465916000
1	-5.249854000	0.250095000	0.770890000
1	-4.455677000	-1.023164000	-0.203621000
6	-3.179600000	0.424280000	2.712814000
1	-3.568940000	-0.325449000	3.409161000
1	-2.171933000	0.701938000	3.039598000

1	-3.822835000	1.310248000	2.783752000
6	3.177134000	0.423798000	2.713287000
1	2.169848000	0.707456000	3.036042000
1	3.559119000	-0.328286000	3.411178000
1	3.825431000	1.305863000	2.786823000
6	4.541013000	-0.585905000	0.796954000
1	5.250195000	0.251262000	0.774428000
1	4.946791000	-1.349660000	1.468206000
1	4.458142000	-1.021917000	-0.201882000

3b E= -879.6041919

7	-2.510033000	1.298170000	0.259089000
6	-1.375296000	0.947472000	-0.388073000
7	-1.191040000	1.922953000	-1.324790000
6	-2.200846000	2.874944000	-1.266087000
6	-3.032374000	2.473318000	-0.272737000
6	-0.000008000	1.946553000	-2.161862000
7	1.191054000	1.922925000	-1.324835000
6	2.200895000	2.874882000	-1.266184000
6	3.032433000	2.473254000	-0.272843000
7	2.510066000	1.298137000	0.259026000
6	1.375322000	0.947438000	-0.388127000
1	-3.944480000	2.916203000	0.093648000
1	-2.247928000	3.720471000	-1.934931000
1	2.247982000	3.720398000	-1.935041000
1	3.944555000	2.916126000	0.093519000
1	-0.000029000	1.072648000	-2.816845000
1	-0.000008000	2.858838000	-2.759795000
46	-0.000003000	-0.530343000	-0.228234000
6	-3.088729000	0.578629000	1.422237000
1	-2.500268000	-0.337590000	1.492932000
6	3.088744000	0.578630000	1.422203000
1	2.500273000	-0.337580000	1.492927000
35	1.873003000	-2.298182000	-0.285771000
35	-1.873044000	-2.298137000	-0.285894000
6	-4.542494000	0.190885000	1.145661000
1	-4.922394000	-0.396603000	1.987571000
1	-5.192650000	1.067248000	1.031270000
1	-4.604625000	-0.427277000	0.246097000
6	-2.912589000	1.415096000	2.693404000
1	-3.269026000	0.845015000	3.557480000
1	-1.857971000	1.660247000	2.857836000
1	-3.483295000	2.351074000	2.650711000
6	2.912608000	1.415144000	2.693340000
1	1.857992000	1.660311000	2.857758000
1	3.269035000	0.845090000	3.557438000
1	3.483323000	2.351115000	2.650615000
6	4.542505000	0.190859000	1.145648000
1	5.192674000	1.067210000	1.031232000

1	4.922392000	-0.396605000	1.987581000
1	4.604636000	-0.427334000	0.246106000

3c E= -876.0425762

7	-2.485277000	1.697682000	0.196771000
6	-1.376642000	1.243259000	-0.431768000
7	-1.190390000	2.104327000	-1.474804000
6	-2.171197000	3.087868000	-1.498799000
6	-2.988979000	2.822906000	-0.449903000
6	-0.000047000	2.018546000	-2.310228000
7	1.190487000	2.104109000	-1.475018000
6	2.171514000	3.087419000	-1.499298000
6	2.989622000	2.822181000	-0.450728000
7	2.485715000	1.697217000	0.196230000
6	1.376743000	1.243083000	-0.431942000
1	-3.880508000	3.328500000	-0.115501000
1	-2.212416000	3.854779000	-2.256878000
1	2.212776000	3.854223000	-2.257483000
1	3.881452000	3.327480000	-0.116680000
1	-0.000188000	1.064729000	-2.841707000
1	-0.000036000	2.843861000	-3.023313000
46	-0.000045000	-0.235535000	-0.153282000
6	-3.047211000	1.134037000	1.449042000
1	-2.487508000	0.210130000	1.604862000
6	3.047629000	1.133766000	1.448576000
1	2.487720000	0.210029000	1.604704000
53	-1.985322000	-2.124362000	-0.132943000
53	1.984904000	-2.124669000	-0.132348000
6	-2.794473000	2.095535000	2.614941000
1	-3.329820000	3.044062000	2.484676000
1	-3.142681000	1.639391000	3.547336000
1	-1.726088000	2.312280000	2.718907000
6	-4.523910000	0.779013000	1.266108000
1	-4.889831000	0.287678000	2.173269000
1	-5.145772000	1.666421000	1.094883000
1	-4.646704000	0.084240000	0.430947000
6	4.524254000	0.778423000	1.265568000
1	5.146233000	1.665699000	1.094068000
1	4.890192000	0.287237000	2.172800000
1	4.646846000	0.083456000	0.430543000
6	2.795270000	2.095581000	2.614258000
1	3.143619000	1.639520000	3.546648000
1	3.330780000	3.043977000	2.483725000
1	1.726943000	2.312515000	2.718413000

4a E= -1766.6735257

7	-2.480916000	0.899396000	0.664387000
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6	-1.362209000	0.653321000	-0.048188000
7	-1.192126000	1.805494000	-0.764341000
6	-2.179957000	2.744210000	-0.482377000
6	-3.002914000	2.164765000	0.427032000
6	-0.000053000	1.995675000	-1.581255000
7	1.191946000	1.805552000	-0.764226000
6	2.180070000	2.744056000	-0.482645000
6	3.003072000	2.164566000	0.426700000
7	2.480894000	0.899312000	0.664273000
6	1.361957000	0.653412000	-0.048009000
1	-3.888293000	2.516663000	0.931029000
1	-2.217484000	3.712924000	-0.956363000
1	2.217690000	3.712729000	-0.956708000
1	3.888594000	2.516398000	0.930487000
1	0.000002000	1.266434000	-2.393775000
1	-0.000069000	3.008750000	-1.985880000
46	-0.000059000	-0.825199000	-0.209340000
17	1.715523000	-2.427130000	-0.648278000
17	-1.715376000	-2.427304000	-0.648667000
8	2.959473000	0.100581000	1.669761000
8	-2.959538000	0.100688000	1.669875000
6	4.058175000	-0.734830000	1.220209000
1	4.332470000	-1.297875000	2.113383000
1	3.710859000	-1.405167000	0.431501000
1	4.899713000	-0.110815000	0.895830000
6	-4.057978000	-0.735069000	1.220190000
1	-3.710101000	-1.405996000	0.432233000
1	-4.332993000	-1.297347000	2.113627000
1	-4.899211000	-0.111251000	0.894663000

4b E= -872.6324693

7	-2.455367000	1.420786000	0.641323000
6	-1.363834000	1.057672000	-0.062653000
7	-1.191238000	2.102900000	-0.927566000
6	-2.149172000	3.094933000	-0.741197000
6	-2.957116000	2.658450000	0.257112000
6	0.000041000	2.170731000	-1.765186000
7	1.191453000	2.102719000	-0.927773000
6	2.149523000	3.094645000	-0.741525000
6	2.957470000	2.658122000	0.256759000
7	2.455611000	1.420528000	0.641056000
6	1.364054000	1.057448000	-0.062909000
1	-3.821043000	3.094224000	0.732031000
1	-2.181745000	3.994881000	-1.335858000
1	2.182142000	3.994576000	-1.336210000
1	3.821453000	3.093836000	0.731630000
1	-0.000077000	1.327646000	-2.458328000
1	0.000064000	3.112273000	-2.315964000
46	-0.000016000	-0.436300000	-0.048353000

35	1.850914000	-2.188740000	-0.355396000
35	-1.851292000	-2.188323000	-0.355659000
8	2.914714000	0.765181000	1.754036000
8	-2.914534000	0.765356000	1.754227000
6	4.094090000	-0.029014000	1.467055000
1	4.336516000	-0.483847000	2.428351000
1	3.854170000	-0.796985000	0.728687000
1	4.917107000	0.617023000	1.138599000
6	-4.093797000	-0.028946000	1.467080000
1	-3.853697000	-0.796871000	0.728719000
1	-4.336308000	-0.483829000	2.428331000
1	-4.916837000	0.617015000	1.138531000

4c E= -869.0705536

7	-2.410828000	1.791196000	0.593153000
6	-1.348376000	1.367478000	-0.122591000
7	-1.189422000	2.360345000	-1.050078000
6	-2.124244000	3.378726000	-0.889805000
6	-2.905744000	3.014978000	0.157188000
6	-0.010358000	2.377425000	-1.906640000
7	1.193885000	2.375856000	-1.084466000
6	2.161979000	3.371642000	-1.007784000
6	3.006480000	3.001275000	-0.011753000
7	2.510382000	1.804338000	0.481163000
6	1.404785000	1.383021000	-0.167344000
1	-3.748362000	3.492212000	0.630613000
1	-2.163733000	4.242845000	-1.535188000
1	2.176189000	4.225431000	-1.667347000
1	3.906227000	3.442577000	0.384635000
1	-0.014182000	1.488599000	-2.540172000
1	-0.024550000	3.278069000	-2.521823000
46	0.043031000	-0.124419000	-0.034456000
53	-1.883943000	-2.038548000	-0.299923000
53	2.064741000	-1.942117000	-0.169024000
8	3.194572000	1.134037000	1.462503000
8	-2.832729000	1.208576000	1.761496000
6	2.399532000	0.943373000	2.651777000
1	3.085349000	0.455507000	3.345273000
1	2.070228000	1.910113000	3.050709000
1	1.549635000	0.289261000	2.444821000
6	-4.072641000	0.479599000	1.587394000
1	-3.936942000	-0.327603000	0.864446000
1	-4.273847000	0.072321000	2.579034000
1	-4.879051000	1.161017000	1.291109000

5a E= -1946.6413016

7	-2.586979000	0.788633000	0.492425000
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6	-1.369174000	0.663913000	-0.093418000
7	-1.200127000	1.871784000	-0.694576000
6	-2.306234000	2.707747000	-0.510618000
6	-3.196386000	2.015609000	0.236845000
6	0.000043000	2.166039000	-1.474497000
7	1.200199000	1.871753000	-0.694568000
6	2.306332000	2.707683000	-0.510611000
6	3.196452000	2.015527000	0.236873000
7	2.586998000	0.788580000	0.492476000
6	1.369210000	0.663878000	-0.093409000
1	-4.174271000	2.258621000	0.616815000
1	-2.361598000	3.702012000	-0.926621000
1	2.361729000	3.701942000	-0.926623000
1	4.174335000	2.258518000	0.616861000
1	0.000038000	1.554022000	-2.379737000
1	0.000057000	3.224968000	-1.735925000
46	0.000000000	-0.770889000	-0.376679000
17	1.748743000	-2.237862000	-1.041057000
17	-1.748816000	-2.237892000	-1.040797000
7	3.196891000	-0.211288000	1.379211000
8	4.393408000	-0.060401000	1.521158000
8	2.443367000	-1.007237000	1.868216000
7	-3.196931000	-0.211245000	1.379109000
8	-4.393441000	-0.060303000	1.521055000
8	-2.443441000	-1.007218000	1.868128000

5b E= -1052.6020095

7	-2.565101000	1.312534000	0.416502000
6	-1.372849000	0.998559000	-0.154322000
7	-1.198645000	2.003630000	-1.053286000
6	-2.274577000	2.897061000	-1.057426000
6	-3.152607000	2.452916000	-0.129498000
6	-0.000007000	2.066113000	-1.886995000
7	1.198640000	2.003628000	-1.053299000
6	2.274575000	2.897056000	-1.057452000
6	3.152610000	2.452912000	-0.129530000
7	2.565103000	1.312538000	0.416486000
6	1.372852000	0.998556000	-0.154337000
1	-4.109849000	2.817731000	0.202434000
1	-2.322014000	3.750160000	-1.716759000
1	2.322008000	3.750152000	-1.716788000
1	4.109855000	2.817727000	0.202396000
1	-0.000011000	1.222335000	-2.580846000
1	-0.000009000	3.008020000	-2.436776000
46	0.000000000	-0.471102000	-0.093155000
35	1.881261000	-2.155669000	-0.500721000
35	-1.881262000	-2.155658000	-0.500757000
7	-3.166044000	0.597041000	1.546192000
8	-4.339088000	0.863027000	1.715709000

8	-2.429473000	-0.123229000	2.163622000
7	3.166045000	0.597058000	1.546184000
8	4.339093000	0.863033000	1.715688000
8	2.429476000	-0.123210000	2.163619000

5c E= -1049.0439061

7	-2.538057000	1.735879000	0.342837000
6	-1.377445000	1.290830000	-0.210026000
7	-1.197628000	2.149486000	-1.249335000
6	-2.236791000	3.079857000	-1.350896000
6	-3.099312000	2.812229000	-0.344567000
6	0.000015000	2.069452000	-2.084379000
7	1.197627000	2.149509000	-1.249295000
6	2.236761000	3.079920000	-1.350792000
6	3.099244000	2.812309000	-0.344428000
7	2.537994000	1.735930000	0.342937000
6	1.377425000	1.290846000	-0.209989000
1	-4.031065000	3.259831000	-0.043392000
1	-2.274839000	3.828881000	-2.127045000
1	2.274821000	3.828953000	-2.126932000
1	4.030969000	3.259936000	-0.043206000
1	0.000034000	1.118251000	-2.621436000
1	0.000018000	2.902835000	-2.787701000
46	-0.000002000	-0.179682000	0.021203000
53	-1.990368000	-2.011368000	-0.274525000
53	1.990426000	-2.011297000	-0.274620000
7	3.128432000	1.209136000	1.571977000
8	4.260000000	1.604671000	1.774572000
8	2.428103000	0.478541000	2.221283000
7	-3.128532000	1.209089000	1.571865000
8	-4.260092000	1.604657000	1.774443000
8	-2.428155000	0.478643000	2.221286000

6a E= -1999.8339393

7	2.575239000	0.895403000	-0.660202000
6	1.386158000	1.155027000	-0.054344000
7	1.194508000	2.491947000	-0.243492000
6	2.249068000	3.068943000	-0.941385000
6	3.118371000	2.062965000	-1.199592000
6	0.000001000	3.161321000	0.251375000
7	-1.194505000	2.491947000	-0.243494000
6	-2.249066000	3.068944000	-0.941385000
6	-3.118368000	2.062967000	-1.199594000
7	-2.575237000	0.895405000	-0.660204000
6	-1.386156000	1.155027000	-0.054348000
1	4.052229000	2.055667000	-1.737833000
1	2.286792000	4.120045000	-1.182218000
1	-2.286789000	4.120047000	-1.182217000
1	-4.052227000	2.055670000	-1.737834000

1	0.000000000	3.139254000	1.343770000
1	0.000002000	4.194283000	-0.099481000
46	0.000000000	0.102209000	0.968313000
6	-3.210918000	-0.386211000	-0.792871000
6	-4.579956000	-0.489431000	-0.542727000
6	-2.472833000	-1.492229000	-1.212611000
6	-5.215663000	-1.718258000	-0.716765000
1	-5.133390000	0.371535000	-0.180252000
6	-3.115806000	-2.717985000	-1.373209000
1	-1.408511000	-1.392148000	-1.392390000
6	-4.486048000	-2.833716000	-1.130939000
1	-6.278502000	-1.804745000	-0.510744000
1	-2.541528000	-3.584804000	-1.686345000
1	-4.981712000	-3.791984000	-1.256326000
6	3.210919000	-0.386213000	-0.792869000
6	4.579959000	-0.489431000	-0.542739000
6	2.472830000	-1.492234000	-1.212596000
6	5.215665000	-1.718259000	-0.716776000
1	5.133396000	0.371537000	-0.180273000
6	3.115802000	-2.717990000	-1.373194000
1	1.408506000	-1.392155000	-1.392364000
6	4.486047000	-2.833719000	-1.130938000
1	6.278506000	-1.804743000	-0.510766000
1	2.541522000	-3.584812000	-1.686319000
1	4.981711000	-3.791988000	-1.256325000
17	-1.742429000	-0.887129000	2.259475000
17	1.742424000	-0.887125000	2.259484000

6b E= -1105.7947560

7	-2.555368000	1.226740000	0.731424000
6	-1.385617000	1.311898000	0.043834000
7	-1.193849000	2.649976000	-0.135241000
6	-2.231504000	3.395327000	0.412493000
6	-3.089514000	2.497598000	0.953310000
6	-0.000001000	3.157197000	-0.798245000
7	1.193857000	2.649978000	-0.135260000
6	2.231523000	3.395326000	0.412457000
6	3.089532000	2.497594000	0.953271000
7	2.555375000	1.226738000	0.731400000
6	1.385629000	1.311899000	0.043802000
1	-4.009821000	2.637156000	1.496932000
1	-2.268143000	4.472604000	0.363929000
1	2.268164000	4.472603000	0.363895000
1	4.009841000	2.637150000	1.496891000
1	-0.000008000	2.830858000	-1.840763000
1	-0.000002000	4.246853000	-0.747525000
46	-0.000001000	0.042793000	-0.710781000
6	3.176889000	0.027004000	1.218567000
6	4.550496000	-0.144464000	1.040356000

6	2.416954000	-0.926069000	1.895898000
6	5.167841000	-1.286658000	1.548635000
1	5.121732000	0.587769000	0.478009000
6	3.041921000	-2.069642000	2.389771000
1	1.350434000	-0.775648000	2.018873000
6	4.416021000	-2.250976000	2.222036000
1	6.234235000	-1.429154000	1.400533000
1	2.450935000	-2.820449000	2.905728000
1	4.897928000	-3.144621000	2.607717000
6	-3.176893000	0.027008000	1.218580000
6	-4.550492000	-0.144470000	1.040323000
6	-2.416974000	-0.926055000	1.895944000
6	-5.167847000	-1.286664000	1.548591000
1	-5.121713000	0.587755000	0.477949000
6	-3.041951000	-2.069627000	2.389806000
1	-1.350459000	-0.775625000	2.018953000
6	-4.416044000	-2.250971000	2.222026000
1	-6.234236000	-1.429168000	1.400453000
1	-2.450978000	-2.820426000	2.905790000
1	-4.897959000	-3.144615000	2.607698000
35	1.876020000	-1.256684000	-1.878758000
35	-1.876015000	-1.256660000	-1.878788000

6c E= -1102.235177

7	-2.530598000	1.724298000	-0.112145000
6	-1.389709000	1.292873000	-0.715167000
7	-1.192782000	2.177490000	-1.734699000
6	-2.195320000	3.138911000	-1.783768000
6	-3.040359000	2.848179000	-0.766464000
6	-0.000015000	2.106150000	-2.569003000
7	1.192755000	2.177495000	-1.734702000
6	2.195296000	3.138913000	-1.783785000
6	3.040348000	2.848178000	-0.766493000
7	2.530589000	1.724302000	-0.112163000
6	1.389686000	1.292885000	-0.715165000
1	-3.935253000	3.343825000	-0.426850000
1	-2.221472000	3.920516000	-2.527197000
1	2.221442000	3.920516000	-2.527216000
1	3.935251000	3.343817000	-0.426894000
1	-0.000014000	1.162040000	-3.118166000
1	-0.000018000	2.945317000	-3.265813000
46	-0.000007000	-0.184249000	-0.492759000
53	-1.990495000	-2.042842000	-0.646346000
53	1.990505000	-2.042822000	-0.646311000
6	3.145900000	1.162538000	1.056780000
6	4.532424000	1.000536000	1.082216000
6	2.364910000	0.821366000	2.160884000
6	5.140640000	0.494293000	2.230187000
1	5.124080000	1.231537000	0.201720000

6	2.981858000	0.305271000	3.299151000
1	1.289248000	0.947914000	2.117496000
6	4.368105000	0.145048000	3.339225000
1	6.217742000	0.356520000	2.248148000
1	2.374826000	0.027216000	4.155544000
1	4.843845000	-0.258218000	4.228382000
6	-3.145898000	1.162530000	1.056801000
6	-4.532426000	1.000571000	1.082266000
6	-2.364893000	0.821309000	2.160881000
6	-5.140633000	0.494323000	2.230241000
1	-5.124096000	1.231611000	0.201789000
6	-2.981832000	0.305208000	3.299150000
1	-1.289227000	0.947820000	2.117470000
6	-4.368084000	0.145029000	3.339252000
1	-6.217738000	0.356585000	2.248223000
1	-2.374788000	0.027114000	4.155522000
1	-4.843815000	-0.258241000	4.228412000