Supporting material

Dispersion Energy Enforced Dimerization of a Cyclic Disilylated Plumbylene

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Crystallographic Material

Table S1.Crystallographic Data for Compounds **2**, **3**, and **4**.

	2	**3**	**4**
Empirical formula	$PbPSi_8C_{22}H_{63}$	$PbBSi_8F_{15}C_{34}H_{48}$	$Pb_2Si_{16}C_{32}H_{96}$
M_w	790.60	1184.44	1344.91
Temperature [K]	100(2)	100(2)	110(2)
Size [mm]	0.36x0.20x0.20	0.36x0.26x0.12	0.38x0.33x0.20
Crystal system	monoclinic	triclinic	monoclinic
Space group	P2(1)/c	P-1	P2(1)/n
a [Å]	9.701(2)	11.896(2)	15.913(3)
b [Å]	21.430(4)	12.182(3)	18.062(4)
c [Å]	19.585(4)	20.051(4)	23.793(5)
α [°]	90	81.96(3)	90
β [°]	104.19(3)	74.89(3)	98.49(3)
γ [°]	90	61.25(3)	90
V [$Å^3$]	3947(2)	2459(2)	6764(2)
Z	4	2	4
ρ_{calc} [gcm^{-3}]	1.330	1.600	1.321
Absorption coefficient [mm-1]	4.569	3.707	5.274
F(000)	1616	1172	2704
θ range	1.43<θ<26.37	1.05<θ<26.37	1.45<θ<25.00
Reflections collected/unique	30193/7996	19515/9890	20045/11463
Completeness to θ [%]	99.0	98.3	96.3
Data/restraints/parameters	7996/0/308	9890/0/548	11463/0/483
Goodness of fit on F^2	1.07	1.04	0.95
Final R indices [I>2σ(I)]	R1=0.058, *w*R2=0.160	R1=0.049, *w*R2=0.113	R1=0.069, *w*R2=0.161
R indices (all data)	R1=0.064, *w*R2=0.162	R1=0.056, *w*R2=0.116	R1=0.109, *w*R2=0.177
Largest diff. Peak/hole [e^-/ $Å^3$]	5.00/-4.56	4.36/-1.77	2.21/-1.96

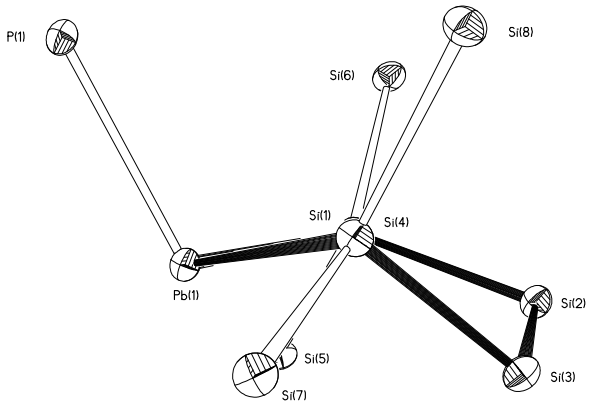


Figure S1. Part of the molecular structure of **2**: Plane: Si(1)-Pb(1)-Si(4) orthogonal distance P1-plane = 259 pm β P(1)Pb(1)-plane: 71.2º α Si(4)-Pb(1)-Si(1) = 95.67(8)°

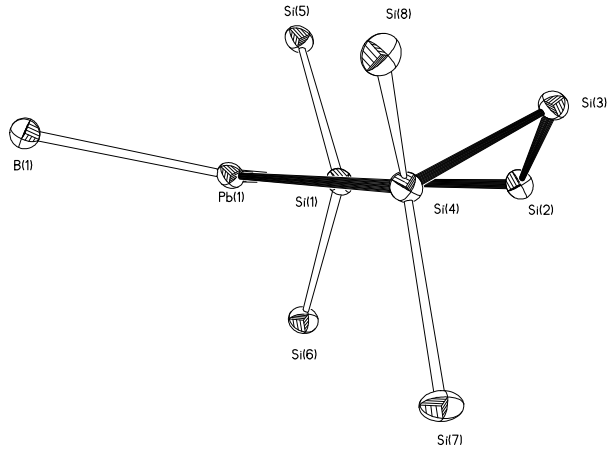


Figure S2. Part of the molecular structure of **3**: Plane: Si(1)-Pb(1)-Si(4) orthogonal distance B(1)-plane = 34 pm, β B-Pb-plane: 7.9º, α Si(1)-Pb(1)-Si(4) = 102.80(6)°

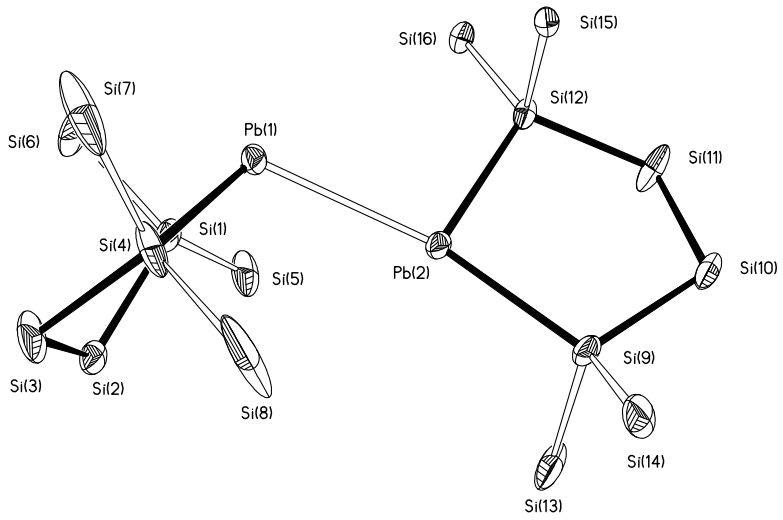


Figure S3. Part of molecular structure of **4**: Plane: Si(1)-Pb(1)-Si(4) orthogonal distance Pb(2)-plane = 280 pm, β Pb(2)-Pb(1)-plane = 66º, α Si(4)-Pb(1)-Si(1) = 94.38(12)°

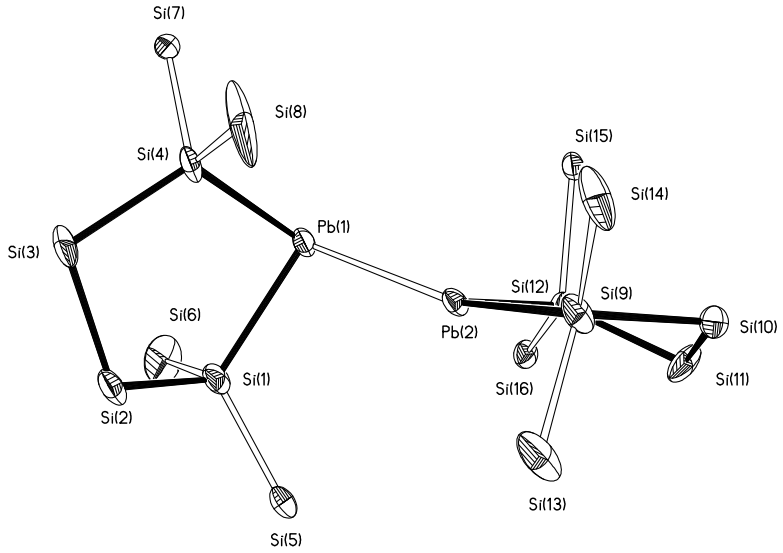


Figure S4. Part of the molecular structure of **4**: Plane: Si(1)-Pb(2)-Si(4) orthogonal distance Pb(1)-plane = 80 pm, β Pb(1)-Pb(2)-plane = 15.1º, α Si(12)-Pb(2)-Si(9) = 96.49(10)°

Computational Details.

All geometry optimizations and natural bond orbital[1] (NBO) analyses were carried out using Gaussian09 package.[2] Unless otherwise noted all quantum chemical calculations were performed at the M06-2X level of theory[3] using the standard 6-31G(d) Pople basis set[4-6] for all second and third row elements and quasirelativistic Stuttgart Dresden pseudo potential SDD[7] for lead (6-31G(d) for H, B, C, F, Si, P, SDD for Pb). This basis set is denoted as basis set A. Every stationary point was identified by a subsequent frequency calculation. To verify the calculated structural data small molecules (PbH_2, Pb_2H_4) were computed at the CCSD[8] level of theory using a cc-pVTZ basis set for hydrogen[9] and a cc-pVTZ-PP basis set for lead.[10] The calculated energies for all calculated compounds are summarized in Table S4 and the xyz coordinates for all optimized molecular structures are given in Table S5. The NBO5.0 program as implemented in the Gaussian suite of programs was applied for the NBO analysis. The analysis was based on molecular structures obtained at the M06-2X/A optimized structures and densities obtained using the M06-2X functional in combination with Ahlrichs and Wigands def2-TZVP[11] basis sets and the corresponding effective core potentials (ECP) to realize a high accuracy with respect to the bonding situation of the heavy element lead. Orbital figures were calculated by ChemCraft 1.6[12] package and graphically arranged by GaussView.[13]

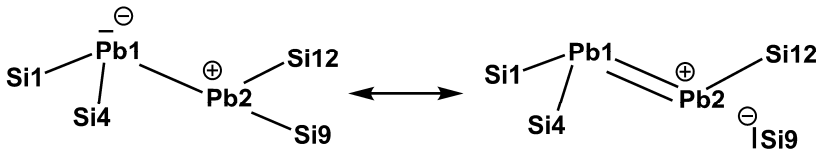
Binding energies, BE, were computed using the total energy of the complex and subtracting the total energies of its constituent molecules. The contribution of the dispersion forces to the overall binding energy was estimated by comparing the calculated binding energies BE obtained for the M06-2X optimized structures with that calculated with the B3LYP functional using the same molecular structure. The basis set superposition error (BSSE) was estimated using the counterpoise method from Boys and Bernardi.[14] The computed binding energies are given in Table S2.

Vertical singlet-triplet energy differences, $\Delta E(ST)$, for plumbylenes PbH_2, **5** and **6** were calculated at the M06-2X/A level and are summarized in Table S3.

The ^{29}Si nuclear magnetic shielding tensors of compounds **4**, **5** and **6** were computed by single point calculations at the B3LYP level using the GIAO-method[15] and molecular structures obtained at the M06-2X/A level of theory. For hydrogen, carbon and silicon atoms the 6-311+G(2d,p) basis set was used,[4-6] for lead atoms the def2-TZVP[11] basis and the corresponding ECP were used. Isotropic ^{29}Si NMR chemical shifts, $\delta^{29}Si$, were calculated using isotropic ^{29}Si

NMR shielding value of tetramethylsilane σ^{29}Si(TMS) computed at the same level of theory. These results are summarized in Table S4.

Figures S5-S8 show the calculated LMOs of dimer **4** which are according to the NBO analysis involved in negative hyperconjugation (see Schemes 2 and S1) and show pictorially the contribution of negative hyperconjugation to the Pb(1) Pb(2) bond.



Scheme S1. Canonical structures which describe the negative hyperconjugation in dimer **4**.

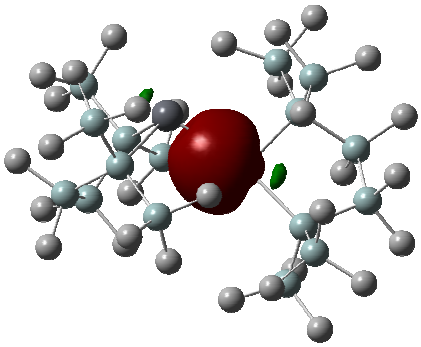


Figure S5. LMO describing the Pb(1)Pb(2) σ-bond.

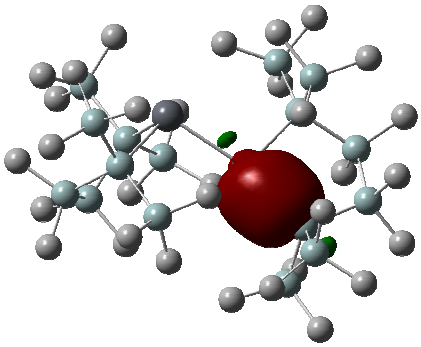


Figure S6. LMO describing the Pb(2)Si(9) σ-bond.

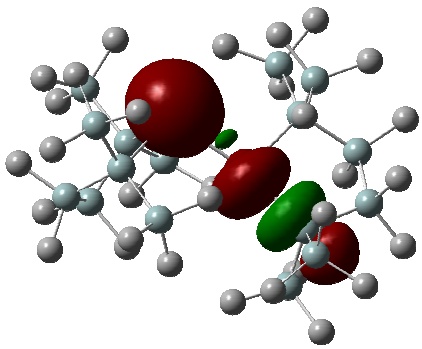


Figure S7. Illustration of the interaction of the lone pair at Pb(1) and σ* -orbital of the Pb(2)Si(9) bond.

The dissociation of plumbylene dimer **4** into two plumbylene monomers **6** is enforced by entropy and solvation effects. The results of the computations at the M06-2X/A level suggests that in benzene solution dimer **4** and plumbylene **6** form complexes with the solvent, namely [**4**$(C_6H_6)_2$] and [**6**(C_6H_6)]. While the calculated total energies E^{tot} strongly favor the formation of the dimer solvate [**4**$(C_6H_6)_2$] (see Figure S8a), inspection of the relative Gibbs free enthalpies for these solvates reveals that at T=298K the free plumbylene **6** is the dominant species (see Figure S8b). Inclusion of solvation effects using a PCM model[16] into the calculation indicates that solvation further favors the formation of the plumbylene **6** in benzene solution (Figure S8c).

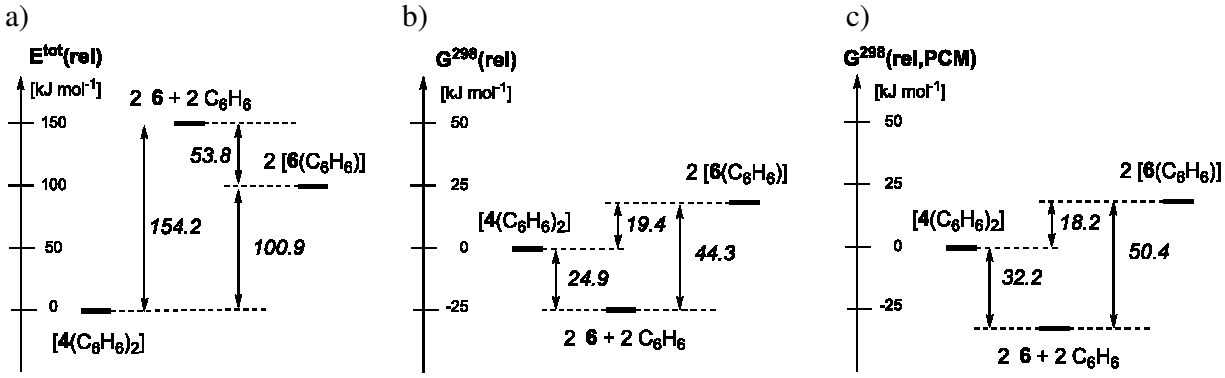


Figure S8. Calculated relative total energies E^{tot}(rel) (a), relative Gibbs free enthalpies G^{298}(rel) (b) and G^{298}(rel) corrected for solvent effects (c), of plumbylene **6** and solvates [**6**(C_6H_6)] and [**4**$(C_6H_6)_2$]. (At M06-2X/A (a,b) and at PCM/M06-2X/A (c)).

Table S2. Calculated bond energies (BE) and Gibbs free energies at 298.15K (G^{298}) for donor-acceptor complexes of plumbylenes and related compounds (at M06-2X/SDD(Pb) 6-31G(d)(P, Si, F, C, B, H)).

entry	compound	method	BE [kJmol^{-1}]	G^{298} [kJmol^{-1}]
1	**4**	M06-2X//M06-2X	-110.8[b]	-22.3
2		B3LYP//M06-2X	+1.0[c]	+89.5[a]
3		B3LYP//B3LYP	-26.5[d]	+51.0
4	**7**	M06-2X//M06-2X	-76.4	+0.1
5		B3LYP//M06-2X	-0.5	+77.1[a]
6		B3LYP//B3LYP	-28.2	+48.4
7	**Pb_2H_6**	M06-2X//M06-2X	-237.1	-179.9
8		B3LYP//M06-2X	-202.2	-144.9[a]
9	**Pb_2H_4**	M06-2X//M06-2X	-62.4	-15.6
10		B3LYP//M06-2X	-54.4	-7.6[a]
11	**3**	M06-2X//M06-2X	-65.1	+14.2
12		B3LYP//M06-2X	+48.6	+127.8
13	**2**	M06-2X//M06-2X	+76.0	+0.9
14		B3LYP//M06-2X	-1.8	+75.1

a) Correction terms for translation, rotation, and vibration energies taken from frequency analyses of optimized molecular structures at M06-2X level of theory G^{corr} ($G = G^{corr}$(M06-2X)+ E^{tot}(B3LYP).[17] b) Basis Set Superposition Error[14] E_{BSSE} = 18.7 kJmol^{-1}, c) E_{BSSE} = 14.4 kJmol^{-1}, d) E_{BSSE} = 21.4 kJmol^{-1}.

Table S3. Calculated vertical singlet-triplet energy differences ΔE(ST) of plumbylenes (at M06-2X/A//M06-2X/A).

Entry	Compound	ΔE(ST) [a.u]	ΔE(ST) [kJmol^{-1}]	α(SiPbSi) [°]
1	**6**	-0.055367	-145.4	90.5
2	**:PbH$_2$**	-0.082049	-215.4	90.9
3	**5**	-0.049106	-128.9	108.2

Table S4. Calculated isotropic shieldings, σ^{iso} ^{29}Si and ^{29}Si NMR chemical shifts, δ^{29}Si for silylsubstituted plumbylenes (GIAO B3LYP/H,C,Si: 6-311+G(2d,p), Pb: def2-TZVP//M06-2X/A).

Entry	Compound	Core	σ^{iso} ^{29}Si	δ ^{29}Si
1	**SiMe$_4$**	Si	328.61	0
2	**4**	Si(1)	409.72	-81
		Si(4)	429.87	-101
		α–Si(Pb(1)) [a]	419.80	-91
		Si(9)	353.35	-25
		Si(12)	373.41	-45
		α–Si(Pb(2)) [b]	363.38	-35
3	**6**	Si(1)[a]	365.57	-37
		Si(2)	361.90	-33
		α–Si(Pb) [c]	363.74	-35
4	**5**	Si(1)	380.16	-52
		Si(2)	390.34	-62
		α–Si(Pb) [c]	385.25	-57

a) mean value from Si(1) and Si(4). b) mean value from Si(9) and Si(12). c) mean value from Si(1) and Si(2).

Table S5. Computed absolute energies, E^{tot}, free Gibbs enthalpies at 298.15K, G^{298}, zero point energies (ZPE) and number (NImag) and size of imaginary frequencies of plumbylenes and related compounds. The correction terms G^{corr} for translation, rotation and vibration energies are given in parentheses. The following basis sets were used : For B3LYP and M06-2X calculations Basis A; for CCSD calculation H cc-pVTZ, Pb cc-pVTZ-PP.

Cpd. (point group)	method	E^{tot} [a.u.]	G^{298} [a.u.]	ZPE [kJmol^{-1}]	NImag [cm^{-1}]
2 (C_1)	M06-2X	-3536.41124	-3535.68864 (0.72261)	2142.669	0
	B3LYP//M06-2X	-3537.24848	-3536.52587[a]		
3 (C_1)	M06-2X	-5165.05982	-5164.40523 (0.65460)	2023.212	0
	B3LYP//M06-2X	-2208.22775	-2208.12988[a]		
4 (C_1)	M06-2X	-5915.10082	-5914.01402 (1.08681)	3212.363	0
	B3LYP//M06-2X	-5916.43210	-5915.34529[a]		
	B3LYP	-5916.45467	-5915.38263	3190.573	0
	scrf M06-2X//M06-2X	-5915.10323	-5914.01643[b]		
[4(C_6H_6)$_2$] (C_1)	M06-2X	-6379.39029	-6378.11590 (1.27439)	3748.733	0
	scrf M06-2X//M06-2X	-6379.39392	-6378.11952[b]		
7 (C_1)	M06-2X	-5915.08773	-5914.00549 (1.08224)	3209.628	0
	B3LYP//M06-2X	-5916.43226	-5915.35002[a]		
	B3LYP	-5916.45532	-5915.38362	3192.179	0
6 ^{1}A (C_1)	M06-2X	-2957.52931	-2957.00277 (0.52654)	1601.354	0
	B3LYP//M06-2X	-2958.21623	-2957.68969		
	B3LPY	-2958.22228	-2957.70102	1592.202	0
	scrf M06-2X//M06-2X	-2957.53119	-2957.00465[b]		
6 ^{3}A (C_1)	M06-2X//M06-2X	-2957.47394			

[6(C_6H_6)] (C_1)	M06-2X	-3189.67594	-3189.05426 (0.62168)	1873.191	0
	scrf M06-2X//M06-2X	-3189.67797	-3189.05629[b]		
Pb_2H_4 (C_{2h})	M06-2X	-9.14487	-9.15481 (-0.00994)	58.779	0
	B3LYP//M06-2X	-9.21481	-9.22475[a]		
	CCSD	-386.40648	-386.41598 (-0.00950)	59.630	0
Pb_2H_6 (D_{3d})	M06-2X	-10.31616	-10.30913 (0.00703)	100.808	0
	B3LYP//M06-2X	-10.39596	-10.38893		
	CCSD	-387.58826	-387.58208 (0.00618)	101.449	0
:PbH_2 ^{1}A (C_{2v})	M06-2X	-4.56055	-4.57444 (-0.01389)	24.129	0
	B3LYP//M06-2X	-4.59704	-4.61093[a]		
:PbH_2 ^{3}B (C_{2v})	M06-2X//M06-2X	-4.47850			
5 ^{1}A (C_1)	M06-2X	-3037.31234	-3036.71567 (0.59667)	300.729	0
5 ^{3}A (C_1)	M06-2X//M06-2X	-3037.26324			
PEt_3 (C_3)	M06-2X	-578.85300	-578.68621 (0.16679)	529.527	0
	B3LYP//M06-2X	-579.03156	-578.86477[a]		
B(C_6F_5)$_3$ (C_3)	M06-2X	-2207.50572	-2207.40785 (0.09787)	413.918	0
	B3LYP//M06-2X	-2208.22775	-2208.12988[a]		
$SiMe_4$ (T_d)	M06-2X	-449.04694	-448.92740	392.925	0
C_6H_6 (D_{6h})	M06-2X	-232.1364659	-232.059929 (0.076537)	266.859	0
	scrf M06-2X//M06-2X	-232.1377824	-232.061245[b]		

a) $G(B3LYP//M06\text{-}2X) = G^{corr}(M06\text{-}2X) + E^{tot}(B3LYP)$[17]

b) $G(scrf\ M06\text{-}2X//M06\text{-}2X) = G^{corr}(M06\text{-}2X) + E^{tot}(scrf\ M06\text{-}2X//M06\text{-}2X)$

Table S6. Cartesian coordinates for all optimized molecular structures
Compound 2. M06-2X / H, C, Si, P: 6-31G(d); Pb: SDD C_1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	2.098844	-0.416232	0.166777
2	14	0	1.306208	-2.409606	1.119829
3	14	0	-0.852065	-1.981242	1.918654
4	14	0	-1.910516	-0.842877	0.138764
5	14	0	3.309339	0.726833	1.825842
6	14	0	3.720899	-1.073766	-1.397543
7	14	0	-2.773245	-2.405379	-1.421755
8	14	0	-3.811017	0.176800	1.077374
9	6	0	1.066413	-3.710944	-0.254840
10	1	0	2.008587	-3.957799	-0.756355
11	1	0	0.366374	-3.348190	-1.017304
12	1	0	0.653458	-4.637860	0.161599
13	6	0	2.479562	-3.171749	2.413109
14	1	0	2.059399	-4.100628	2.815377
15	1	0	2.659715	-2.491977	3.252366
16	1	0	3.449127	-3.408305	1.959278
17	6	0	-0.808376	-0.874063	3.468928
18	1	0	-1.809234	-0.782581	3.906343
19	1	0	-0.436612	0.130680	3.242393
20	1	0	-0.150683	-1.308630	4.230893
21	6	0	-1.684784	-3.603569	2.473544
22	1	0	-1.229918	-3.940522	3.412711
23	1	0	-1.562482	-4.399641	1.734358
24	1	0	-2.757965	-3.469014	2.647374
25	6	0	3.743960	2.511636	1.337550
26	1	0	4.122213	2.563142	0.310574
27	1	0	4.522790	2.901679	2.003567
28	1	0	2.882508	3.183540	1.415280
29	6	0	2.456977	0.786879	3.520606
30	1	0	3.144427	1.221052	4.256760
31	1	0	2.189234	-0.217336	3.866068
32	1	0	1.542428	1.387719	3.524416
33	6	0	4.962493	-0.158908	2.113060
34	1	0	5.605490	-0.111833	1.227729
35	1	0	4.812899	-1.214096	2.365192
36	1	0	5.500095	0.316125	2.942783
37	6	0	4.813020	0.400282	-1.888040
38	1	0	5.415995	0.758507	-1.045985
39	1	0	4.198187	1.237157	-2.239312
40	1	0	5.499696	0.125014	-2.697100
41	6	0	4.851290	-2.469025	-0.785403
42	1	0	4.275653	-3.368699	-0.541781
43	1	0	5.411407	-2.180656	0.109187
44	1	0	5.574238	-2.737754	-1.565262
45	6	0	2.877100	-1.693293	-2.979951
46	1	0	3.621187	-2.078106	-3.687379
47	1	0	2.327859	-0.887452	-3.479660
48	1	0	2.167516	-2.501454	-2.769748
49	6	0	-1.733873	-2.425458	-3.012526
50	1	0	-2.096379	-3.214006	-3.682970
51	1	0	-0.669178	-2.612073	-2.831277
52	1	0	-1.816574	-1.472111	-3.546518
53	6	0	-2.852471	-4.186764	-0.781845
54	1	0	-3.441954	-4.264480	0.137672
55	1	0	-1.852908	-4.584486	-0.576500
56	1	0	-3.318118	-4.827866	-1.540312
57	6	0	-4.526457	-1.938064	-1.974883
58	1	0	-4.554267	-0.930641	-2.403282
59	1	0	-5.242164	-1.972182	-1.146467
60	1	0	-4.870141	-2.641147	-2.743055
61	6	0	-4.808187	-1.177523	1.955590
62	1	0	-5.767756	-0.791024	2.319212
63	1	0	-4.248436	-1.554644	2.819615
64	1	0	-5.010907	-2.028522	1.295841
65	6	0	-4.935270	1.032156	-0.197783

66	1	0	-5.634052	0.322556	-0.649698
67	1	0	-4.367285	1.496709	-1.011444
68	1	0	-5.526312	1.815948	0.291533
69	6	0	-3.470294	1.486340	2.418160
70	1	0	-3.114340	2.436181	2.006395
71	1	0	-2.746452	1.153239	3.168196
72	1	0	-4.415076	1.693432	2.936405
73	82	0	-0.005008	0.466302	-1.460184
74	15	0	-0.384272	2.893549	-0.152748
75	6	0	-2.054112	3.577101	-0.578929
76	1	0	-2.776065	3.002221	0.011818
77	1	0	-2.236526	3.292431	-1.622496
78	6	0	-0.234180	2.843859	1.683662
79	1	0	0.814356	2.573904	1.853966
80	1	0	-0.820899	1.975485	2.004896
81	6	0	-0.610504	4.083643	2.492785
82	1	0	-0.331906	3.940286	3.541547
83	1	0	-0.097993	4.981168	2.131828
84	1	0	-1.688119	4.267770	2.463152
85	6	0	-2.267848	5.081484	-0.402904
86	1	0	-1.613805	5.659348	-1.062717
87	1	0	-3.300428	5.342340	-0.653301
88	1	0	-2.079913	5.408022	0.622114
89	6	0	0.788352	4.213664	-0.693880
90	1	0	0.546138	5.155919	-0.188335
91	1	0	1.784452	3.908293	-0.356259
92	6	0	0.782788	4.391156	-2.213601
93	1	0	1.478858	5.180149	-2.511151
94	1	0	1.083685	3.466221	-2.715343
95	1	0	-0.210237	4.662988	-2.586712

Compound 3. M06-2X / H, C, Si, F, B: 6-31G(d); Pb: SDD C_1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	2.212028	1.956909	0.168510
2	14	0	4.283748	0.904548	-0.178607
3	14	0	4.115542	-1.313292	0.567061
4	14	0	2.103326	-2.238219	-0.236627
5	14	0	1.814869	2.885471	2.303307
6	14	0	1.942202	3.676787	-1.415612
7	14	0	1.974175	-2.616387	-2.558193
8	14	0	1.529372	-4.035176	1.183412
9	6	0	4.615684	0.872248	-2.051554
10	1	0	4.728347	1.880624	-2.463365
11	1	0	3.792088	0.384231	-2.586473
12	1	0	5.534080	0.314509	-2.269596
13	6	0	5.706530	1.821828	0.686487
14	1	0	6.664762	1.325427	0.496346
15	1	0	5.554639	1.858136	1.770698
16	1	0	5.781567	2.852215	0.321517
17	6	0	3.980469	-1.255981	2.463283
18	1	0	3.946479	-2.253937	2.910925
19	1	0	3.069147	-0.727115	2.762711
20	1	0	4.833659	-0.722480	2.898556
21	6	0	5.651671	-2.313850	0.065645
22	1	0	6.554959	-1.868837	0.498029
23	1	0	5.771455	-2.335730	-1.022328
24	1	0	5.581311	-3.347591	0.419955
25	6	0	-0.021803	3.273198	2.538043
26	1	0	-0.379715	4.022401	1.825159
27	1	0	-0.177804	3.676243	3.546090
28	1	0	-0.657161	2.385505	2.439001
29	6	0	2.364769	1.781201	3.732917
30	1	0	2.264523	2.339334	4.671667
31	1	0	3.410767	1.472689	3.638102
32	1	0	1.745997	0.882198	3.816287
33	6	0	2.806813	4.494218	2.390940
34	1	0	2.474644	5.210338	1.632182
35	1	0	3.874883	4.307477	2.234195

36	1	0	2.685987	4.965027	3.373489
37	6	0	0.548309	4.825043	-0.851572
38	1	0	0.924729	5.578154	-0.150850
39	1	0	-0.233697	4.258692	-0.339440
40	1	0	0.086886	5.348899	-1.697401
41	6	0	3.553836	4.670302	-1.475853
42	1	0	4.400503	4.054621	-1.797135
43	1	0	3.798950	5.090114	-0.494231
44	1	0	3.458587	5.502375	-2.183474
45	6	0	1.593006	2.988785	-3.138274
46	1	0	1.465351	3.810098	-3.853004
47	1	0	0.683143	2.383233	-3.166776
48	1	0	2.427994	2.368999	-3.483425
49	6	0	1.041530	-1.164858	-3.355200
50	1	0	1.061708	-1.246180	-4.448448
51	1	0	1.470551	-0.184953	-3.103179
52	1	0	-0.016564	-1.164576	-3.057396
53	6	0	3.688629	-2.774523	-3.336112
54	1	0	4.240241	-3.605515	-2.883471
55	1	0	4.283552	-1.864599	-3.205458
56	1	0	3.604616	-2.970488	-4.411356
57	6	0	0.993026	-4.188573	-2.916062
58	1	0	0.048852	-4.226101	-2.362486
59	1	0	1.569483	-5.079788	-2.647011
60	1	0	0.762507	-4.250109	-3.986183
61	6	0	3.152211	-4.903416	1.635953
62	1	0	2.946194	-5.744286	2.308859
63	1	0	3.875057	-4.248473	2.130046
64	1	0	3.627325	-5.307466	0.734760
65	6	0	0.441700	-5.365801	0.412012
66	1	0	0.938921	-5.846121	-0.435921
67	1	0	-0.522198	-4.983865	0.074216
68	1	0	0.255006	-6.138817	1.167813
69	6	0	0.682755	-3.353928	2.729161
70	1	0	-0.314611	-2.982621	2.469126
71	1	0	1.244866	-2.533700	3.186598
72	1	0	0.561901	-4.144408	3.478661
73	82	0	0.485697	-0.087026	-0.100452
74	6	0	-2.285568	-0.255543	1.585565
75	6	0	-3.623196	-0.449421	1.932660
76	6	0	-1.397357	-0.425059	2.635715
77	6	0	-4.043234	-0.803812	3.205539
78	6	0	-1.759028	-0.786232	3.926262
79	6	0	-3.100350	-0.979494	4.212609
80	6	0	-2.529498	-1.018857	-0.974875
81	6	0	-3.391819	-0.776478	-2.046099
82	6	0	-2.195895	-2.364302	-0.806079
83	6	0	-3.846909	-1.769519	-2.907214
84	6	0	-2.628019	-3.384027	-1.639202
85	6	0	-3.460819	-3.084568	-2.707733
86	6	0	-2.204873	1.636692	-0.403631
87	6	0	-2.825155	2.617920	0.365407
88	6	0	-1.810173	2.061530	-1.674085
89	6	0	-3.059943	3.911378	-0.096874
90	6	0	-2.022056	3.330563	-2.175949
91	6	0	-2.664000	4.267598	-1.375372
92	9	0	-4.568535	-0.262740	1.005905
93	9	0	-5.333714	-0.969910	3.477992
94	9	0	-3.484546	-1.323120	5.436202
95	9	0	-0.831188	-0.946433	4.866928
96	9	0	-0.052599	-0.248455	2.453368
97	9	0	-1.386771	-2.727008	0.209833
98	9	0	-2.246805	-4.646958	-1.433057
99	9	0	-3.886121	-4.047091	-3.518038
100	9	0	-4.662132	-1.464037	-3.913310
101	9	0	-3.848010	0.453231	-2.303990
102	9	0	-1.173095	1.182070	-2.477523
103	9	0	-1.578851	3.680145	-3.383514
104	9	0	-2.839019	5.508778	-1.816730
105	9	0	-3.656523	4.807144	0.686079
106	9	0	-3.239839	2.359848	1.611693
107	5	0	-1.960590	0.109722	0.035938

Compound 4. M06-2X / H, C, Si: 6-31G(d); Pb: SDD C_1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	82	0	1.715241	0.407122	-1.196570
2	82	0	-1.100831	-0.076484	0.003705
3	14	0	2.682694	1.708580	1.086738
4	14	0	3.654311	0.060030	2.456284
5	14	0	4.618990	-1.609718	1.119133
6	14	0	3.121980	-1.924239	-0.661795
7	14	0	1.254259	2.924215	2.503570
8	14	0	4.276145	3.288208	0.397804
9	14	0	4.312094	-2.405647	-2.626854
10	14	0	1.747930	-3.773869	-0.269039
11	14	0	-3.242545	-1.600739	0.865384
12	14	0	-5.216814	-0.447473	0.274795
13	14	0	-4.722856	1.828332	0.027547
14	14	0	-2.647614	1.896825	-1.060021
15	14	0	-3.112074	-1.682810	3.222528
16	14	0	-3.525669	-3.817550	0.104941
17	14	0	-2.732479	1.007492	-3.245984
18	14	0	-1.824679	4.085561	-1.215355
19	6	0	4.930020	0.742111	3.696225
20	1	0	4.506238	1.525641	4.332477
21	1	0	5.789205	1.166261	3.164413
22	1	0	5.301443	-0.059779	4.345142
23	6	0	2.216906	-0.765373	3.397309
24	1	0	2.555170	-1.627769	3.983716
25	1	0	1.476733	-1.126801	2.672446
26	1	0	1.710621	-0.071420	4.078229
27	6	0	6.331186	-1.068024	0.488055
28	1	0	6.945042	-0.678064	1.308767
29	1	0	6.258470	-0.292054	-0.277702
30	1	0	6.861252	-1.922605	0.053786
31	6	0	4.931836	-3.185952	2.144520
32	1	0	5.602111	-2.968014	2.984179
33	1	0	5.413803	-3.947374	1.520414
34	1	0	4.012207	-3.617237	2.550511
35	6	0	-0.450916	2.098498	2.696612
36	1	0	-1.009382	2.540908	3.531465
37	1	0	-0.342309	1.023620	2.900725
38	1	0	-1.056864	2.241706	1.790386
39	6	0	0.969945	4.712644	1.946790
40	1	0	0.260689	5.203517	2.624853
41	1	0	0.566091	4.783031	0.933205
42	1	0	1.905128	5.282364	1.975549
43	6	0	2.017124	3.041579	4.236754
44	1	0	3.010867	3.500058	4.188702
45	1	0	2.124891	2.063171	4.715627
46	1	0	1.387962	3.666280	4.881952
47	6	0	5.769532	2.451136	-0.406930
48	1	0	5.470106	1.790092	-1.228829
49	1	0	6.320654	1.851748	0.325403
50	1	0	6.457223	3.202152	-0.813020
51	6	0	4.926726	4.286818	1.873782
52	1	0	5.704897	4.984997	1.542655
53	1	0	5.365627	3.628895	2.631968
54	1	0	4.137950	4.873139	2.356610
55	6	0	3.537210	4.489052	-0.865278
56	1	0	2.713109	5.070707	-0.439629
57	1	0	3.148186	3.953813	-1.738940
58	1	0	4.304466	5.191497	-1.211836
59	6	0	3.121521	-3.053705	-3.952774
60	1	0	2.670338	-4.005612	-3.650360
61	1	0	3.648114	-3.219280	-4.899886
62	1	0	2.309600	-2.341285	-4.138906
63	6	0	5.136682	-0.840068	-3.308097
64	1	0	5.878373	-0.444552	-2.606128
65	1	0	4.399110	-0.051466	-3.499743
66	1	0	5.650705	-1.051672	-4.253016

67	6	0	5.661312	-3.711433	-2.367751
68	1	0	6.409556	-3.372028	-1.644235
69	1	0	6.177972	-3.916573	-3.313081
70	1	0	5.243629	-4.653703	-1.999072
71	6	0	1.061755	-3.743144	1.497466
72	1	0	0.274937	-2.982335	1.579584
73	1	0	1.831976	-3.499166	2.235215
74	1	0	0.623317	-4.708033	1.777577
75	6	0	2.689895	-5.396934	-0.529654
76	1	0	2.061345	-6.255646	-0.265309
77	1	0	3.594666	-5.434693	0.086408
78	1	0	2.991811	-5.512727	-1.576647
79	6	0	0.263056	-3.763672	-1.455451
80	1	0	-0.238105	-4.739114	-1.475745
81	1	0	0.555371	-3.511370	-2.480211
82	1	0	-0.476088	-3.020965	-1.125345
83	6	0	-5.899070	-1.053558	-1.398978
84	1	0	-6.193847	-2.107566	-1.361341
85	1	0	-5.169779	-0.938524	-2.207230
86	1	0	-6.788049	-0.469382	-1.666126
87	6	0	-6.591738	-0.737620	1.560783
88	1	0	-7.485838	-0.163733	1.290484
89	1	0	-6.286071	-0.430642	2.566107
90	1	0	-6.871576	-1.796514	1.600362
91	6	0	-4.594626	2.676481	1.726504
92	1	0	-4.582144	3.765274	1.613699
93	1	0	-3.685648	2.384885	2.262297
94	1	0	-5.454766	2.415217	2.354004
95	6	0	-6.112403	2.703217	-0.934332
96	1	0	-7.059289	2.632703	-0.386487
97	1	0	-6.259859	2.267638	-1.927002
98	1	0	-5.879372	3.766184	-1.063159
99	6	0	-1.402927	-2.229626	3.813404
100	1	0	-1.136342	-3.223190	3.438677
101	1	0	-1.385089	-2.265141	4.909349
102	1	0	-0.618669	-1.534277	3.493173
103	6	0	-3.456724	0.018286	3.972009
104	1	0	-3.435501	-0.047571	5.066456
105	1	0	-4.433102	0.415722	3.677379
106	1	0	-2.695457	0.744451	3.667222
107	6	0	-4.379079	-2.906384	3.918711
108	1	0	-4.143944	-3.935208	3.625835
109	1	0	-5.397202	-2.681014	3.585412
110	1	0	-4.363896	-2.860417	5.014340
111	6	0	-2.296963	-4.990875	0.925751
112	1	0	-2.358595	-4.932568	2.018420
113	1	0	-1.271453	-4.752857	0.633759
114	1	0	-2.505877	-6.026092	0.630762
115	6	0	-5.270862	-4.346377	0.627444
116	1	0	-6.042309	-3.741415	0.140047
117	1	0	-5.417850	-4.270662	1.708634
118	1	0	-5.436261	-5.391062	0.336275
119	6	0	-3.441116	-4.026270	-1.772473
120	1	0	-3.602924	-5.083878	-2.015243
121	1	0	-2.476680	-3.727572	-2.192871
122	1	0	-4.225637	-3.447575	-2.272076
123	6	0	-2.448085	-0.870890	-3.187410
124	1	0	-2.695664	-1.342515	-4.146198
125	1	0	-3.042601	-1.367866	-2.413130
126	1	0	-1.387618	-1.089339	-2.992295
127	6	0	-4.374794	1.388178	-4.103443
128	1	0	-4.564208	2.467343	-4.110201
129	1	0	-5.218411	0.902558	-3.602858
130	1	0	-4.352262	1.040173	-5.142865
131	6	0	-1.330214	1.717012	-4.298547
132	1	0	-0.352884	1.487728	-3.857835
133	1	0	-1.403143	2.803128	-4.413147
134	1	0	-1.358831	1.271459	-5.300209
135	6	0	-2.760744	4.992757	-2.592016
136	1	0	-2.433306	6.037578	-2.651517
137	1	0	-3.838655	4.989253	-2.395640
138	1	0	-2.599281	4.535278	-3.573246
139	6	0	0.021386	4.098597	-1.619220

140	1	0	0.204552	3.657890	-2.605411
141	1	0	0.601724	3.520954	-0.889739
142	1	0	0.414478	5.122876	-1.626879
143	6	0	-2.179528	5.030846	0.387778
144	1	0	-1.906577	4.468149	1.286393
145	1	0	-3.249781	5.259370	0.446712
146	1	0	-1.633544	5.981525	0.406753

Compound 4. B3LYP / H, C, Si 6-31G(d); Pb: SDD C_1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	82	0	-1.692135	-0.365895	-0.918314
2	82	0	1.381489	0.015078	0.102460
3	14	0	-3.065758	-1.676595	1.180219
4	14	0	-4.347631	0.001871	2.288314
5	14	0	-5.071813	1.644350	0.729076
6	14	0	-3.284958	1.956998	-0.826129
7	14	0	-1.775499	-2.842898	2.815632
8	14	0	-4.488577	-3.326343	0.193834
9	14	0	-4.120865	2.121269	-3.058412
10	14	0	-2.131847	3.972675	-0.326251
11	14	0	3.511032	1.642328	0.957044
12	14	0	5.537844	0.593334	0.249301
13	14	0	5.128342	-1.707486	-0.155561
14	14	0	2.962799	-1.894742	-1.134649
15	14	0	3.294561	1.569797	3.340862
16	14	0	3.608201	3.948228	0.331530
17	14	0	2.910936	-1.142464	-3.419226
18	14	0	2.182339	-4.147038	-1.042112
19	6	0	-5.844349	-0.709334	3.251640
20	1	0	-5.524978	-1.429732	4.013926
21	1	0	-6.551836	-1.216343	2.585605
22	1	0	-6.388977	0.095487	3.762250
23	6	0	-3.228898	0.893006	3.562733
24	1	0	-3.783944	1.690745	4.072115
25	1	0	-2.358774	1.351119	3.079510
26	1	0	-2.862121	0.203092	4.331514
27	6	0	-6.700826	1.109657	-0.121977
28	1	0	-7.456618	0.845406	0.628800
29	1	0	-6.572380	0.248841	-0.783895
30	1	0	-7.107354	1.934110	-0.719972
31	6	0	-5.527414	3.238258	1.692442
32	1	0	-6.330073	3.030931	2.412132
33	1	0	-5.890405	4.017057	1.010557
34	1	0	-4.680045	3.649484	2.250027
35	6	0	-0.147731	-1.939269	3.233100
36	1	0	0.357334	-2.418472	4.082054
37	1	0	-0.318836	-0.888028	3.491467
38	1	0	0.540988	-1.974395	2.378062
39	6	0	-1.306591	-4.603205	2.258040
40	1	0	-0.661574	-5.075841	3.010709
41	1	0	-0.763796	-4.606037	1.307064
42	1	0	-2.191415	-5.238287	2.137836
43	6	0	-2.744042	-3.026821	4.449264
44	1	0	-3.700216	-3.540688	4.297975
45	1	0	-2.957484	-2.058767	4.915365
46	1	0	-2.158099	-3.617606	5.166009
47	6	0	-5.860985	-2.573407	-0.887033
48	1	0	-5.456222	-1.935321	-1.680643
49	1	0	-6.562058	-1.973096	-0.297479
50	1	0	-6.436623	-3.375319	-1.368149
51	6	0	-5.350266	-4.359459	1.545286
52	1	0	-6.003728	-5.112637	1.084871
53	1	0	-5.971366	-3.734564	2.196963
54	1	0	-4.631078	-4.889232	2.180063
55	6	0	-3.507974	-4.524260	-0.915403
56	1	0	-2.720762	-5.046664	-0.362232
57	1	0	-3.032539	-4.007225	-1.756961
58	1	0	-4.184108	-5.282958	-1.331946

59	6	0	-2.745094	2.625339	-4.278621
60	1	0	-2.386005	3.643321	-4.089699
61	1	0	-3.128921	2.597360	-5.307208
62	1	0	-1.881227	1.952171	-4.228883
63	6	0	-4.796988	0.443163	-3.661341
64	1	0	-5.631847	0.091631	-3.045228
65	1	0	-4.022203	-0.333949	-3.651357
66	1	0	-5.161064	0.528593	-4.693816
67	6	0	-5.522509	3.401195	-3.235841
68	1	0	-6.389054	3.145878	-2.615926
69	1	0	-5.862940	3.447628	-4.279151
70	1	0	-5.194028	4.406412	-2.948336
71	6	0	-1.591127	4.017893	1.500034
72	1	0	-0.935211	3.176029	1.750507
73	1	0	-2.449623	3.978784	2.179270
74	1	0	-1.043380	4.944587	1.715561
75	6	0	-3.198629	5.521196	-0.641990
76	1	0	-2.646306	6.426790	-0.356681
77	1	0	-4.126941	5.500445	-0.060438
78	1	0	-3.470092	5.620118	-1.699366
79	6	0	-0.566854	4.138455	-1.399511
80	1	0	-0.019766	5.055165	-1.145278
81	1	0	-0.805668	4.178641	-2.467763
82	1	0	0.111292	3.290936	-1.245253
83	6	0	6.182209	1.364103	-1.380343
84	1	0	6.419686	2.427506	-1.264058
85	1	0	5.455626	1.271730	-2.194668
86	1	0	7.101119	0.854020	-1.696078
87	6	0	6.939992	0.797913	1.538904
88	1	0	7.860641	0.319510	1.180468
89	1	0	6.684141	0.344465	2.502937
90	1	0	7.164363	1.856667	1.715635
91	6	0	5.205448	-2.665848	1.498994
92	1	0	5.205002	-3.747596	1.323409
93	1	0	4.368948	-2.434819	2.165677
94	1	0	6.133906	-2.422172	2.030761
95	6	0	6.528297	-2.442862	-1.235143
96	1	0	7.486637	-2.373827	-0.704209
97	1	0	6.638094	-1.927052	-2.193657
98	1	0	6.344904	-3.503417	-1.446426
99	6	0	1.545605	2.104452	3.866923
100	1	0	1.281010	3.096709	3.486195
101	1	0	1.475917	2.137416	4.962219
102	1	0	0.784627	1.400007	3.510722
103	6	0	3.586533	-0.174630	4.045270
104	1	0	3.502716	-0.148284	5.139944
105	1	0	4.581125	-0.562928	3.800660
106	1	0	2.845466	-0.896020	3.680443
107	6	0	4.543761	2.740775	4.175080
108	1	0	4.368981	3.787391	3.901616
109	1	0	5.577628	2.493345	3.910036
110	1	0	4.451600	2.665149	5.266833
111	6	0	2.308777	4.994345	1.242988
112	1	0	2.486302	5.006242	2.324689
113	1	0	1.291435	4.629181	1.074680
114	1	0	2.353965	6.033504	0.890576
115	6	0	5.316965	4.654441	0.798964
116	1	0	6.134921	4.147262	0.275614
117	1	0	5.514039	4.582621	1.874047
118	1	0	5.359756	5.717341	0.525016
119	6	0	3.388841	4.190601	-1.541496
120	1	0	3.453467	5.258598	-1.788913
121	1	0	2.417817	3.828166	-1.894093
122	1	0	4.169669	3.672865	-2.109665
123	6	0	2.497118	0.714194	-3.533514
124	1	0	2.538703	1.044017	-4.580157
125	1	0	3.190217	1.342508	-2.964008
126	1	0	1.480618	0.921647	-3.174080
127	6	0	4.569917	-1.427479	-4.307188
128	1	0	4.878117	-2.478380	-4.268962
129	1	0	5.376012	-0.826399	-3.872734
130	1	0	4.477328	-1.143788	-5.364125
131	6	0	1.567845	-2.054862	-4.409226

132	1	0	0.574448	-1.924970	-3.965301
133	1	0	1.766164	-3.129670	-4.487473
134	1	0	1.531136	-1.650605	-5.429663
135	6	0	3.271683	-5.248367	-2.153243
136	1	0	2.931532	-6.291229	-2.100591
137	1	0	4.322731	-5.227268	-1.841935
138	1	0	3.230287	-4.941024	-3.204697
139	6	0	0.384446	-4.300947	-1.636569
140	1	0	0.278979	-4.022767	-2.689904
141	1	0	-0.293014	-3.662236	-1.059013
142	1	0	0.039136	-5.337747	-1.528786
143	6	0	2.280094	-4.846560	0.724713
144	1	0	1.769883	-4.207919	1.453703
145	1	0	3.315786	-4.967884	1.057721
146	1	0	1.802402	-5.834471	0.760892

Compound [4(C_6H_6)$_2$]. M06-2X / H, C, Si: 6-31G(d); Pb: SDD C_1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	82	0	-1.695097	0.175051	-0.502139
2	82	0	1.220190	-0.562085	0.150904
3	14	0	-2.571091	-2.483276	-0.433185
4	14	0	-3.305062	-2.908116	1.760544
5	14	0	-4.209153	-0.968135	2.724985
6	14	0	-2.909240	0.802816	1.906903
7	14	0	-1.189529	-4.294203	-1.015573
8	14	0	-4.386922	-2.554510	-1.912780
9	14	0	-4.241648	2.688451	1.491072
10	14	0	-1.322512	1.487233	3.479535
11	14	0	3.511401	-0.426225	1.691207
12	14	0	5.346485	-0.466339	0.203453
13	14	0	4.686699	-1.437709	-1.822919
14	14	0	2.537465	-0.607887	-2.239831
15	14	0	3.580267	-2.411469	2.968942
16	14	0	3.907476	1.396476	3.140854
17	14	0	2.503578	1.735269	-2.540367
18	14	0	1.536544	-1.589004	-4.116976
19	6	0	-4.546487	-4.346438	1.904826
20	1	0	-4.154907	-5.277700	1.483733
21	1	0	-5.477768	-4.103178	1.380977
22	1	0	-4.794436	-4.527676	2.957346
23	6	0	-1.741211	-3.308076	2.774953
24	1	0	-1.965023	-3.441273	3.839952
25	1	0	-1.035327	-2.472879	2.683641
26	1	0	-1.237058	-4.214040	2.419499
27	6	0	-6.051128	-0.731590	2.297515
28	1	0	-6.588754	-1.686960	2.304919
29	1	0	-6.194615	-0.269668	1.316794
30	1	0	-6.516971	-0.083702	3.048138
31	6	0	-4.152484	-1.135698	4.624390
32	1	0	-4.744137	-2.000161	4.948363
33	1	0	-4.582550	-0.241972	5.090972
34	1	0	-3.136112	-1.260456	5.009520
35	6	0	0.600232	-4.029254	-0.425983
36	1	0	1.187582	-4.953774	-0.493737
37	1	0	0.616349	-3.698582	0.622559
38	1	0	1.100845	-3.276969	-1.050933
39	6	0	-1.156860	-4.647681	-2.876975
40	1	0	-0.456398	-5.464002	-3.092636
41	1	0	-0.851943	-3.780297	-3.468400
42	1	0	-2.147183	-4.960482	-3.226041
43	6	0	-1.831703	-5.883300	-0.204150
44	1	0	-2.858813	-6.090007	-0.525365
45	1	0	-1.828242	-5.828157	0.888979
46	1	0	-1.208907	-6.735683	-0.500974
47	6	0	-5.748413	-1.395550	-1.297018
48	1	0	-5.350849	-0.392508	-1.097996
49	1	0	-6.186104	-1.772622	-0.366602
50	1	0	-6.553124	-1.299744	-2.035030

51	6	0	-5.108175	-4.302970	-2.038136
52	1	0	-6.002027	-4.307791	-2.672983
53	1	0	-5.392582	-4.680042	-1.049963
54	1	0	-4.389324	-5.008265	-2.468873
55	6	0	-3.866620	-1.988002	-3.643542
56	1	0	-3.101183	-2.647311	-4.066480
57	1	0	-3.451869	-0.973079	-3.617661
58	1	0	-4.727475	-1.986337	-4.322480
59	6	0	-3.105818	4.198283	1.328326
60	1	0	-2.612278	4.442641	2.275891
61	1	0	-3.668322	5.078667	0.994817
62	1	0	-2.331601	3.989141	0.581887
63	6	0	-5.213525	2.524059	-0.124416
64	1	0	-5.952080	1.716446	-0.066797
65	1	0	-4.550520	2.323072	-0.975478
66	1	0	-5.750950	3.454283	-0.344683
67	6	0	-5.477167	3.025870	2.887608
68	1	0	-6.249759	2.251097	2.921820
69	1	0	-5.976513	3.989334	2.730003
70	1	0	-4.985868	3.054822	3.865498
71	6	0	-0.385894	-0.003423	4.186821
72	1	0	0.389415	-0.329278	3.480589
73	1	0	-1.045705	-0.857349	4.369139
74	1	0	0.110531	0.244110	5.132041
75	6	0	-2.113564	2.434319	4.918199
76	1	0	-1.351821	2.725424	5.651774
77	1	0	-2.857902	1.815559	5.430987
78	1	0	-2.614109	3.346194	4.574166
79	6	0	-0.041907	2.627760	2.653242
80	1	0	0.532841	3.194454	3.396613
81	1	0	-0.512102	3.342672	1.969551
82	1	0	0.671778	2.033169	2.067446
83	6	0	5.945518	1.294341	-0.216676
84	1	0	6.344971	1.813253	0.661206
85	1	0	5.143731	1.911064	-0.634998
86	1	0	6.748551	1.239041	-0.961947
87	6	0	6.828487	-1.376776	0.978692
88	1	0	7.674483	-1.390691	0.281670
89	1	0	6.583371	-2.412965	1.232380
90	1	0	7.155937	-0.873317	1.895157
91	6	0	4.638806	-3.335605	-1.704712
92	1	0	4.541803	-3.776295	-2.702147
93	1	0	3.796559	-3.687416	-1.100523
94	1	0	5.562008	-3.721285	-1.256726
95	6	0	5.937147	-0.986501	-3.184464
96	1	0	6.940263	-1.339627	-2.918269
97	1	0	5.988375	0.094500	-3.345960
98	1	0	5.658217	-1.456363	-4.134360
99	6	0	1.975915	-2.714022	3.919207
100	1	0	1.760119	-1.913588	4.634044
101	1	0	2.054620	-3.654734	4.477715
102	1	0	1.113385	-2.799597	3.248622
103	6	0	3.843543	-3.897835	1.829906
104	1	0	3.900862	-4.819192	2.421689
105	1	0	4.763272	-3.816808	1.241790
106	1	0	3.008333	-4.004717	1.128290
107	6	0	4.987343	-2.353258	4.234210
108	1	0	4.811606	-1.576142	4.986092
109	1	0	5.958378	-2.162175	3.766433
110	1	0	5.048350	-3.314730	4.758211
111	6	0	2.843418	1.325368	4.699529
112	1	0	2.863969	0.331871	5.161620
113	1	0	1.802141	1.570707	4.475825
114	1	0	3.214803	2.049299	5.434640
115	6	0	5.720195	1.254202	3.683678
116	1	0	6.410255	1.348324	2.838939
117	1	0	5.924167	0.299677	4.178426
118	1	0	5.951666	2.057966	4.393513
119	6	0	3.700928	3.104661	2.350604
120	1	0	3.924926	3.866830	3.108377
121	1	0	2.686140	3.282473	1.981499
122	1	0	4.390586	3.252107	1.512436
123	6	0	2.360774	2.572432	-0.845902

124	1	0	2.638026	3.631302	-0.907251
125	1	0	2.998069	2.111431	-0.083443
126	1	0	1.320010	2.546348	-0.488314
127	6	0	4.013153	2.408631	-3.459599
128	1	0	4.116964	1.943040	-4.445638
129	1	0	4.943067	2.240083	-2.907111
130	1	0	3.899125	3.490397	-3.602775
131	6	0	0.944848	2.226774	-3.493513
132	1	0	0.063317	1.795109	-3.003731
133	1	0	0.950813	1.896658	-4.537458
134	1	0	0.834579	3.318498	-3.480017
135	6	0	2.310903	-0.823255	-5.667469
136	1	0	1.891750	-1.275068	-6.574252
137	1	0	3.394599	-0.983790	-5.680615
138	1	0	2.132887	0.255946	-5.717313
139	6	0	-0.323813	-1.247523	-4.140625
140	1	0	-0.508617	-0.173905	-4.259066
141	1	0	-0.810626	-1.564688	-3.210473
142	1	0	-0.812822	-1.767785	-4.973409
143	6	0	1.892679	-3.447267	-4.186297
144	1	0	1.678985	-3.960956	-3.243669
145	1	0	2.949481	-3.609895	-4.425787
146	1	0	1.294897	-3.925145	-4.971720
147	6	0	-2.277267	3.622533	-2.389490
148	6	0	-3.002611	4.776931	-2.099883
149	6	0	-2.810971	2.663836	-3.251398
150	6	0	-4.265487	4.966447	-2.658470
151	1	0	-2.586027	5.529414	-1.435140
152	6	0	-4.074688	2.852284	-3.807496
153	1	0	-2.239705	1.770431	-3.490632
154	6	0	-4.802989	4.002312	-3.507911
155	1	0	-4.831114	5.864003	-2.427430
156	1	0	-4.490504	2.103033	-4.474398
157	1	0	-5.789204	4.146777	-3.938305
158	1	0	-1.294674	3.469229	-1.946256
159	6	0	0.663693	5.713116	-1.647937
160	6	0	1.948197	6.121467	-2.006055
161	6	0	0.359023	5.473338	-0.309117
162	6	0	2.924263	6.293785	-1.025257
163	1	0	2.185723	6.311244	-3.048785
164	6	0	1.335887	5.640253	0.671190
165	1	0	-0.641965	5.160397	-0.023256
166	6	0	2.618260	6.052070	0.313349
167	1	0	3.923485	6.613715	-1.304935
168	1	0	1.097667	5.444861	1.712938
169	1	0	3.379672	6.177450	1.077362
170	1	0	-0.100658	5.588472	-2.410658

Compound 5. M06-2X / H, C, Si: 6-31G(d); Pb: SDD C_1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	82	0	0.078814	0.151377	-1.776181
2	14	0	-1.895267	-0.031210	0.123746
3	14	0	-1.049025	-0.041030	2.309019
4	14	0	1.139328	-0.884897	2.194853
5	14	0	2.011602	-0.054326	0.175752
6	14	0	-2.973282	-2.074301	-0.333936
7	14	0	-3.565439	1.605129	-0.090974
8	14	0	2.499355	2.248391	0.351079
9	14	0	3.869668	-1.310883	-0.505053
10	6	0	-0.920801	1.746989	2.956958
11	1	0	-1.906945	2.217355	3.042042
12	1	0	-0.311301	2.367003	2.289945
13	1	0	-0.455413	1.766587	3.949797
14	6	0	-2.153244	-1.016216	3.515319
15	1	0	-1.721503	-1.022527	4.522737
16	1	0	-2.274748	-2.056844	3.195301
17	1	0	-3.150096	-0.564681	3.578039
18	6	0	1.169332	-2.785799	2.145316

19	1	0	2.202832	-3.147465	2.203917
20	1	0	0.726566	-3.176059	1.224808
21	1	0	0.618891	-3.208810	2.993714
22	6	0	2.129801	-0.377834	3.740608
23	1	0	1.724602	-0.884394	4.624552
24	1	0	2.088567	0.699841	3.920038
25	1	0	3.183186	-0.663032	3.642273
26	6	0	-3.279096	-2.260794	-2.195412
27	1	0	-3.817657	-1.404437	-2.613150
28	1	0	-3.869019	-3.162713	-2.397050
29	1	0	-2.333444	-2.356040	-2.742090
30	6	0	-1.909684	-3.547992	0.198043
31	1	0	-2.435054	-4.489844	0.000523
32	1	0	-1.664630	-3.516267	1.264894
33	1	0	-0.966046	-3.569478	-0.359901
34	6	0	-4.637168	-2.180295	0.562433
35	1	0	-5.337443	-1.426796	0.186015
36	1	0	-4.519999	-2.021899	1.639881
37	1	0	-5.091667	-3.166462	0.410600
38	6	0	-4.593310	1.294449	-1.649967
39	1	0	-5.128202	0.340501	-1.587852
40	1	0	-3.961941	1.267048	-2.544821
41	1	0	-5.337827	2.087281	-1.785988
42	6	0	-4.721767	1.569584	1.410236
43	1	0	-4.175795	1.790703	2.333819
44	1	0	-5.197081	0.590940	1.531467
45	1	0	-5.513799	2.320305	1.302795
46	6	0	-2.824019	3.343467	-0.207970
47	1	0	-3.618283	4.090874	-0.319560
48	1	0	-2.151625	3.436483	-1.068155
49	1	0	-2.252387	3.594476	0.692202
50	6	0	1.014999	3.229827	-0.322494
51	1	0	1.128206	4.305464	-0.142517
52	1	0	0.072181	2.915638	0.140694
53	1	0	0.922081	3.101538	-1.411278
54	6	0	2.835558	2.824337	2.119943
55	1	0	3.651412	2.252522	2.574654
56	1	0	1.951643	2.713260	2.756266
57	1	0	3.119496	3.883637	2.120494
58	6	0	3.995992	2.716390	-0.708010
59	1	0	3.867360	2.399364	-1.748254
60	1	0	4.913119	2.255230	-0.326192
61	1	0	4.137588	3.803666	-0.698816
62	6	0	5.107529	-1.480257	0.917620
63	1	0	5.983982	-2.064577	0.614496
64	1	0	4.645698	-1.985501	1.773405
65	1	0	5.454760	-0.498499	1.258028
66	6	0	4.745986	-0.561470	-2.006513
67	1	0	5.281593	0.357618	-1.753370
68	1	0	4.035109	-0.328334	-2.807023
69	1	0	5.474722	-1.276935	-2.405376
70	6	0	3.290431	-3.042659	-1.010454
71	1	0	2.612832	-2.991294	-1.870284
72	1	0	2.764662	-3.551600	-0.196783
73	1	0	4.147708	-3.662303	-1.298835

Compound 5. B3LYP / H, C, Si: 6-31G(d); Pb: SDD C_1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	82	0	0.045486	-0.038750	-1.713533
2	14	0	-1.993098	-0.013273	0.161477
3	14	0	-1.084773	0.287094	2.342093
4	14	0	1.132421	-0.578575	2.326191
5	14	0	2.056495	-0.030070	0.196218
6	14	0	-3.123469	-2.103499	-0.086486
7	14	0	-3.561542	1.705829	-0.364392
8	14	0	2.829873	2.238207	0.079527
9	14	0	3.767204	-1.555233	-0.451212
10	6	0	-0.978183	2.153053	2.759494

11	1	0	-1.970793	2.617966	2.781497
12	1	0	-0.369880	2.699457	2.029706
13	1	0	-0.522202	2.298056	3.747002
14	6	0	-2.145742	-0.523785	3.715694
15	1	0	-1.704042	-0.351166	4.705517
16	1	0	-2.236983	-1.606915	3.576466
17	1	0	-3.158512	-0.102355	3.726488
18	6	0	1.085356	-2.477373	2.566947
19	1	0	2.098926	-2.885448	2.663074
20	1	0	0.589900	-2.997943	1.741997
21	1	0	0.544008	-2.723982	3.489282
22	6	0	2.128904	0.083605	3.822768
23	1	0	1.677144	-0.266833	4.759931
24	1	0	2.167198	1.176250	3.857107
25	1	0	3.161800	-0.285160	3.797233
26	6	0	-3.455501	-2.466823	-1.927602
27	1	0	-4.050891	-1.680367	-2.403739
28	1	0	-4.005141	-3.411627	-2.033151
29	1	0	-2.523541	-2.562814	-2.498188
30	6	0	-2.099229	-3.558051	0.593074
31	1	0	-2.654304	-4.497293	0.468291
32	1	0	-1.878477	-3.443587	1.660019
33	1	0	-1.143602	-3.668971	0.066900
34	6	0	-4.797733	-2.115843	0.823640
35	1	0	-5.484560	-1.358519	0.428414
36	1	0	-4.677721	-1.928769	1.896962
37	1	0	-5.282593	-3.094652	0.708359
38	6	0	-4.534116	1.301403	-1.951602
39	1	0	-5.180436	0.425646	-1.821696
40	1	0	-3.869101	1.102370	-2.800069
41	1	0	-5.177785	2.148135	-2.224663
42	6	0	-4.823481	1.954897	1.041932
43	1	0	-4.337626	2.261836	1.975481
44	1	0	-5.388014	1.038561	1.248206
45	1	0	-5.545051	2.737695	0.772007
46	6	0	-2.676508	3.369658	-0.645990
47	1	0	-3.408535	4.159952	-0.859050
48	1	0	-1.985100	3.324399	-1.496093
49	1	0	-2.102644	3.679297	0.234727
50	6	0	1.513161	3.339427	-0.757149
51	1	0	1.839671	4.387780	-0.771307
52	1	0	0.549246	3.305813	-0.235706
53	1	0	1.345197	3.044498	-1.802081
54	6	0	3.193440	2.999593	1.785370
55	1	0	3.938469	2.420971	2.342518
56	1	0	2.290773	3.063926	2.402768
57	1	0	3.583930	4.018583	1.660904
58	6	0	4.413754	2.401332	-0.963438
59	1	0	4.268582	2.042416	-1.988219
60	1	0	5.252599	1.845415	-0.529122
61	1	0	4.710058	3.457305	-1.019810
62	6	0	5.185395	-1.594890	0.820501
63	1	0	5.963579	-2.305902	0.512677
64	1	0	4.829171	-1.901134	1.811340
65	1	0	5.657463	-0.611240	0.928747
66	6	0	4.501275	-1.127656	-2.155635
67	1	0	5.070434	-0.192893	-2.140090
68	1	0	3.721275	-1.031656	-2.920283
69	1	0	5.182546	-1.926937	-2.476581
70	6	0	3.057232	-3.318534	-0.596064
71	1	0	2.273454	-3.375551	-1.361758
72	1	0	2.629523	-3.675102	0.346668
73	1	0	3.851021	-4.018803	-0.888462

Compound [6(C_6H_6)]. M06-2X / H, C, Si: 6-31G(d); Pb: SDD C_1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	2.022458	-0.355247	0.077809
2	14	0	1.324480	-2.563761	0.476396
3	14	0	-0.833755	-2.477848	1.384668
4	14	0	-1.901769	-0.790137	0.142767
5	14	0	3.167791	0.356493	1.999347
6	14	0	3.616189	-0.427079	-1.640120
7	14	0	-2.738728	-1.601559	-1.909040
8	14	0	-3.660327	0.095841	1.407233
9	6	0	1.113035	-3.476005	-1.185089
10	1	0	2.048598	-3.521359	-1.753321
11	1	0	0.363733	-2.979086	-1.812914
12	1	0	0.773921	-4.504850	-1.015223
13	6	0	2.549547	-3.576317	1.524372
14	1	0	2.177388	-4.597035	1.669045
15	1	0	2.702731	-3.130739	2.512988
16	1	0	3.524669	-3.639390	1.028230
17	6	0	-0.851845	-2.031404	3.233008
18	1	0	-1.862160	-2.163072	3.637657
19	1	0	-0.546190	-0.997704	3.414367
20	1	0	-0.179858	-2.690029	3.795568
21	6	0	-1.652008	-4.194097	1.270859
22	1	0	-1.164564	-4.879648	1.974227
23	1	0	-1.575129	-4.626453	0.269817
24	1	0	-2.714401	-4.141643	1.534169
25	6	0	3.557526	2.212766	2.015188
26	1	0	3.918664	2.567725	1.044117
27	1	0	4.334887	2.421580	2.759602
28	1	0	2.675850	2.800172	2.292319
29	6	0	2.181983	-0.009335	3.572859
30	1	0	2.760811	0.270057	4.461040
31	1	0	1.925224	-1.070541	3.656457
32	1	0	1.244609	0.558670	3.591915
33	6	0	4.829255	-0.547752	2.109362
34	1	0	5.494719	-0.239707	1.295057
35	1	0	4.707238	-1.634000	2.050830
36	1	0	5.328854	-0.310606	3.056387
37	6	0	4.614545	1.183687	-1.675674
38	1	0	5.213875	1.298011	-0.765277
39	1	0	3.951353	2.053067	-1.751302
40	1	0	5.298466	1.205159	-2.531907
41	6	0	4.823143	-1.876094	-1.454522
42	1	0	4.296339	-2.836390	-1.470868
43	1	0	5.377294	-1.818176	-0.512334
44	1	0	5.549847	-1.879867	-2.275631
45	6	0	2.738386	-0.613980	-3.310857
46	1	0	3.462197	-0.662669	-4.132726
47	1	0	2.070578	0.233585	-3.507094
48	1	0	2.136977	-1.529658	-3.340872
49	6	0	-1.569024	-1.129197	-3.334930
50	1	0	-1.861806	-1.647379	-4.255906
51	1	0	-0.521436	-1.389854	-3.137941
52	1	0	-1.618006	-0.053027	-3.542005
53	6	0	-2.961310	-3.479014	-1.960439
54	1	0	-3.580938	-3.835619	-1.131371
55	1	0	-1.996073	-3.993450	-1.904701
56	1	0	-3.443874	-3.772272	-2.900468
57	6	0	-4.402362	-0.793551	-2.316259
58	1	0	-4.307954	0.297076	-2.354811
59	1	0	-5.166772	-1.039202	-1.571244
60	1	0	-4.762155	-1.136170	-3.293635
61	6	0	-4.954073	-1.229164	1.806369
62	1	0	-5.772262	-0.815939	2.407907
63	1	0	-4.500477	-2.049801	2.373675
64	1	0	-5.386284	-1.654670	0.894407
65	6	0	-4.525043	1.516349	0.492262
66	1	0	-5.223988	1.125585	-0.253744
67	1	0	-3.807092	2.156571	-0.031437

68	1	0	-5.095306	2.139365	1.191863
69	6	0	-3.006513	0.745845	3.072728
70	1	0	-1.990925	1.150262	3.001403
71	1	0	-2.977480	-0.061923	3.810659
72	1	0	-3.660551	1.532494	3.467873
73	82	0	-0.143875	1.087273	-0.921320
74	6	0	-0.102942	3.341969	1.300194
75	6	0	0.788366	4.047908	0.484371
76	6	0	0.302685	4.914210	-0.492925
77	6	0	-1.070848	5.074719	-0.663501
78	6	0	-1.961854	4.370720	0.143536
79	6	0	-1.481371	3.505928	1.126329
80	1	0	0.274314	2.682707	2.079847
81	1	0	1.858386	3.920294	0.612282
82	1	0	0.996734	5.459336	-1.124349
83	1	0	-1.447313	5.747304	-1.427652
84	1	0	-3.032302	4.495288	0.012444
85	1	0	-2.179623	2.968287	1.760570

Pb_2H_4. M06-2X / H: 6-31G(d); Pb: SDD C_{2h}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	82	0	1.454492	0.063808	0.000000
2	1	0	2.189302	-0.849316	-1.362482
3	1	0	2.189302	-0.849316	1.362482
4	82	0	-1.454492	-0.063808	0.000000
5	1	0	-2.189302	0.849316	1.362482
6	1	0	-2.189302	0.849316	-1.362482

Pb_2H_4. CCSD / H: cc-pVTZ; Pb: cc-pVTZ-PP C_{2h}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	82	0	1.424677	0.072330	0.000000
2	1	0	2.162295	-0.842545	-1.356006
3	1	0	2.162295	-0.842545	1.356006
4	82	0	-1.424677	-0.072330	0.000000
5	1	0	-2.162295	0.842545	1.356006
6	1	0	-2.162295	0.842545	-1.356006

Pb_2H_6. M06-2X / H: 6-31G(d); Pb: SDD D_{3d}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	82	0	0.000000	0.000000	-1.444173
2	1	0	0.000000	1.636490	-2.058676
3	1	0	-1.417242	-0.818245	-2.058676
4	1	0	1.417242	-0.818245	-2.058676
5	82	0	0.000000	0.000000	1.444173
6	1	0	-1.417242	0.818245	2.058676
7	1	0	0.000000	-1.636490	2.058676
8	1	0	1.417242	0.818245	2.058676

Pb_2H_6. CCSD / H: cc-pVTZ; Pb: cc-pVTZ-PP D_{3d}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	82	0	0.000000	0.000000	-1.409829
2	1	0	0.000000	1.632155	-2.035527
3	1	0	-1.413488	-0.816078	-2.035527
4	1	0	1.413488	-0.816078	-2.035527
5	82	0	0.000000	0.000000	1.409829
6	1	0	-1.413488	0.816078	2.035527
7	1	0	0.000000	-1.632155	2.035527
8	1	0	1.413488	0.816078	2.035527

PEt_3. M06-2X / 6-31G(d) C_3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.000000	0.000000	-0.694170
2	6	0	1.623581	0.208616	0.201070
3	1	0	2.072591	1.144804	-0.149131
4	1	0	1.442683	0.319637	1.279101
5	6	0	2.587931	-0.948434	-0.064297
6	1	0	3.568022	-0.752629	0.381136
7	1	0	2.214836	-1.885248	0.360622
8	1	0	2.731556	-1.101792	-1.138849
9	6	0	-0.992457	1.301754	0.201070
10	1	0	-2.027725	1.222514	-0.149131
11	1	0	-0.998155	1.089582	1.279101
12	6	0	-0.472598	2.715431	-0.064297
13	1	0	-1.132215	3.466313	0.381136
14	1	0	0.525255	2.860729	0.360622
15	1	0	-0.411599	2.916493	-1.138849
16	6	0	-0.631123	-1.510370	0.201070
17	1	0	-0.044866	-2.367318	-0.149131
18	1	0	-0.444528	-1.409218	1.279101
19	6	0	-2.115334	-1.766997	-0.064297
20	1	0	-2.435807	-2.713683	0.381136
21	1	0	-2.740091	-0.975480	0.360622
22	1	0	-2.319958	-1.814701	-1.138849

C_6H_6 M06-2X / 6-31G(d) D_{6h}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.392659	0.000000
2	6	0	1.206078	0.696329	0.000000
3	6	0	1.206078	-0.696329	0.000000
4	6	0	0.000000	-1.392659	0.000000
5	6	0	-1.206078	-0.696329	0.000000
6	6	0	-1.206078	0.696329	0.000000
7	1	0	0.000000	2.478596	0.000000
8	1	0	2.146527	1.239298	0.000000
9	1	0	2.146527	-1.239298	0.000000
10	1	0	0.000000	-2.478596	0.000000
11	1	0	-2.146527	-1.239298	0.000000
12	1	0	-2.146527	1.239298	0.000000

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