Electronic Supplementary Information

Interests in new heterodinuclear transition-metal/main-group-metal complexes: DFT study of electronic structure and mechanism of fluoride sensing function

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The material enclosed in the supporting information is organized as following:

The computational strategy for optimizing the species in Table 2.

Usually, the position of a counter ion is flexible and the optimization of all possible positions is not easy. The molecular electrostatic potential (MEP) of the Pd complex suggests that the anion prefers to take a position close to the Sb center in **1, 2** and **3** (Fig. S10). This is in agreement with the computed natural charges; the Sb has the largest positive charge, 1.81*e* for **2** and 1.73*e* for **3**, and the Pd-Cl moiety has a negative charge of –0.89*e* and –0.79*e* for **2** and **3**, respectively. Four most representative sites of $[BMe_4]^-$ were examined to determine the position in **3**; see Fig. S11. The geometry optimization was carried out with the fixed geometry of the Pd moiety, where the PCM method was employed. In the most stable structure, $[BMe_4]^-$ is anchored toward the opening place of the Sb center surrounded by three phenyl rings. This structure was employed for other complexes, where the geometry optimization was performed in the similar way. Also, the full geometry optimizations were performed on $[NMe_4]BMe_4$ and $[NMe_4]F$. The relative stabilities of the optimized complexes were further refined by a single point calculation with the better basis set system BS-II.

Why is the positive charge of the Sb center smaller in 2 and 3 than in 1?

This is not surprising, as follows: In **2** and **3**, the neutral stibine group (SbR_3) coordinates with the Pd center, in which the charge transfer (CT) occurs from the lone pair of SbR_3 to the Pd center. As a result, the Sb center is more positively charged than in free SbR_3. In stibonium cation **1**, on the other hand, the Sb center is intrinsically more positively charged than those of **2** and **3**, because the positive charge tends to concentrate on the central Sb atom. Hence, the Sb center is more positively changed in **1** than in **2** and **3**.

Absorption spectra of 2 and 2F.

In **2**, all absorption peaks appear in a near ultraviolet region. Two strong absorption bands (383 and 315 nm) are mainly assigned to one-electron excitation from the HOMO to the LUMO and from the HOMO-2 to the LUMO, respectively. The HOMO and HOMO-2 mainly consist anti-bonding overlap between the Pd d_π and Cl p_π orbitals, where the Cl p_π component is larger than the Pd d_π, as shown in Fig. 4(A). The LUMO is the Pd d_σ anti-bonding MO between Pd d_σ and Sb lone pair orbitals, as expected. Thus, these transitions are assigned to ligand-field transitions (LFT) including a ligand-to-metal charge transfer (LMCT) character, where it is represented as LFT/LMCT. Additional weak absorption peaks at 360 and 353 nm mainly consist of one-electron excitations from the HOMO-1 to the LUMO and from the HOMO-3 to the LUMO. Though the HOMO-3 is similar to the HOMO-1, the mixing of d_π and p_π is different between them; see Scheme S1. The oscillator strength is considerably small. Hence, these are also assigned to LFT/LMCT, in which the LFT character is large. In the fluoride adduct **2F**, two large absorption bands disappear but one strong band appears around 330 nm, which includes one large (332 nm), two medium (302 and 348 nm), and one small (321 nm) absorption peaks. The strong absorption peak at 332 nm mainly consists of one-electron excitation from the HOMO-1 to the LUMO. As shown in Fig. 4(B), the LUMO is mainly constructed by the Pd d_σ orbital into which the Sb and Cl p orbitals mix in an anti-bonding way. The HOMO-1 is a d_π-p_π anti-bonding MO. Thus, this absorption is assigned to LFT/LMCT. Other weak absorption peaks at 302, 321 and 348 are one-electron excitations of HOMO-2 → LUMO, HOMO-3 → LUMO, and HOMO → LUMO, respectively. The HOMO mainly consists of the Pd d_σ orbital into which the Sb lone pair orbital mixes in a bonding way. The HOMO-2 is a d_π-p_π anti-bonding MO. The HOMO-3 of **2F** corresponds to that of **2**. Thus, the lowest energy absorption at 348 nm is assigned to a Pd-based LFT, while other two higher energy absorptions at 321 and 302 nm are assigned to LFT/LMCT. It should be noted that all these new absorptions are found in a near UV region. Even though some electronic photodetectors are able to observe the spectral change in this region, the visible change is much better for easy detection of the fluoride anion.

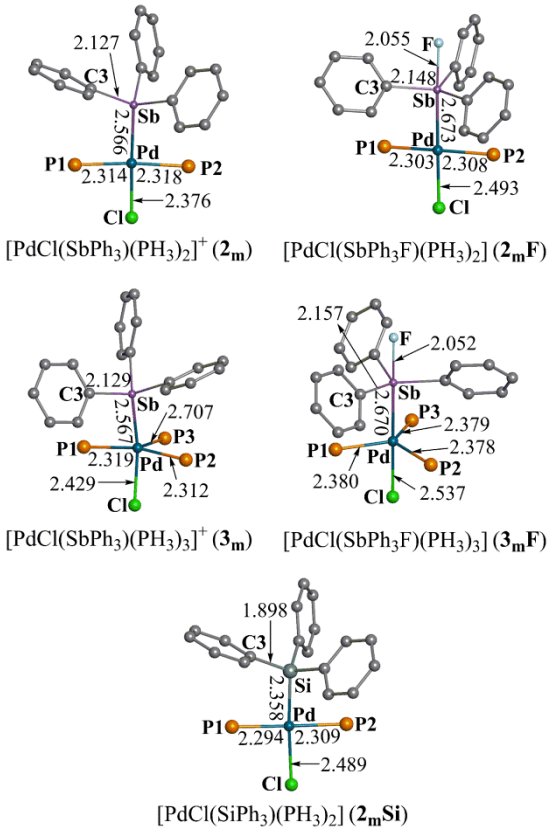


Fig. S1 Optimized structures of model systems $\mathbf{2_m}$, $\mathbf{2_mF}$, $\mathbf{3_m}$, $\mathbf{3_mF}$ and $\mathbf{2_mSi}$ calculated at the PCM(CH_2Cl_2)/PBE0/BS-II//PCM/PBE0/BS-I level. Hydrogen atoms of benzene rings and PH_3 are omitted for clarity.

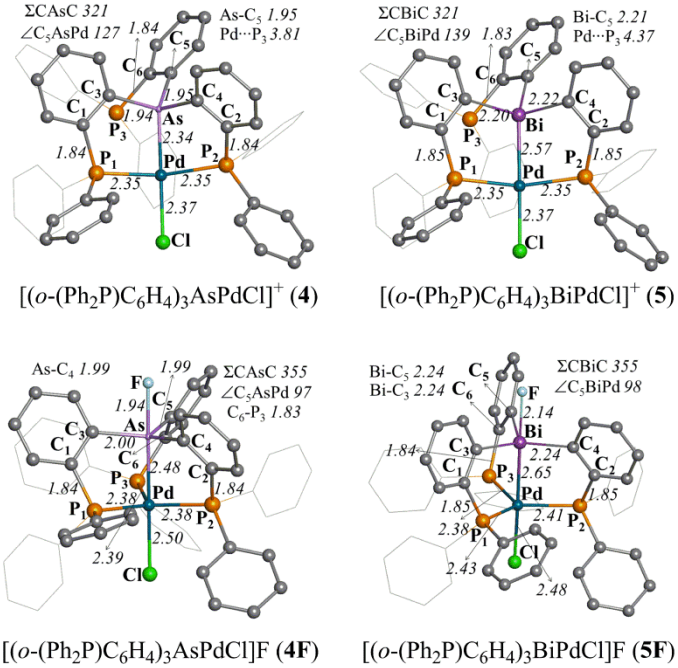


Fig. S2 Optimized structures and selected geometric parameters of **4**, **4F**, **5**, and **5F** calculated at PCM(CH_2Cl_2)/PBE0/BS-I level (bond lengths and angles in angstroms and degrees, respectively). Hydrogen atoms of benzene rings are omitted for clarity. Phenyl groups located at the back side are shown by faint black colors.

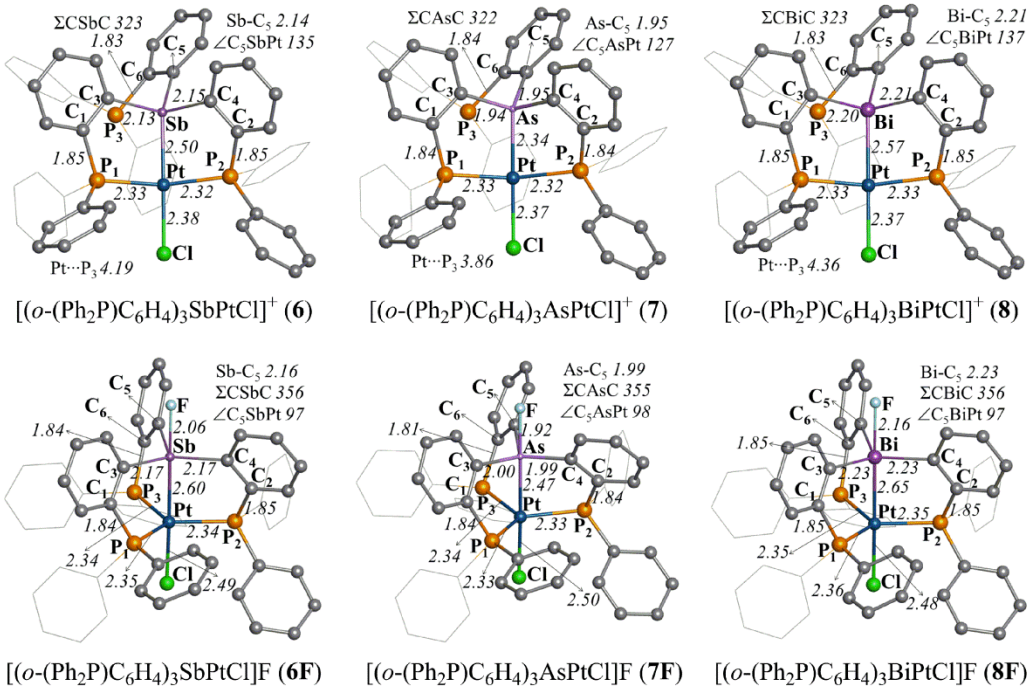


Fig. S3 Optimized structures and selected geometric parameters of **6**, **6F**, **7**, **7F**, **8**, and **8F** calculated at PCM(CH_2Cl_2)/PBE0/BS-I level (bond lengths and angles in angstroms and degrees, respectively). Hydrogen atoms of benzene rings are omitted for clarity. Phenyl groups located at the back side are shown by faint black colors.

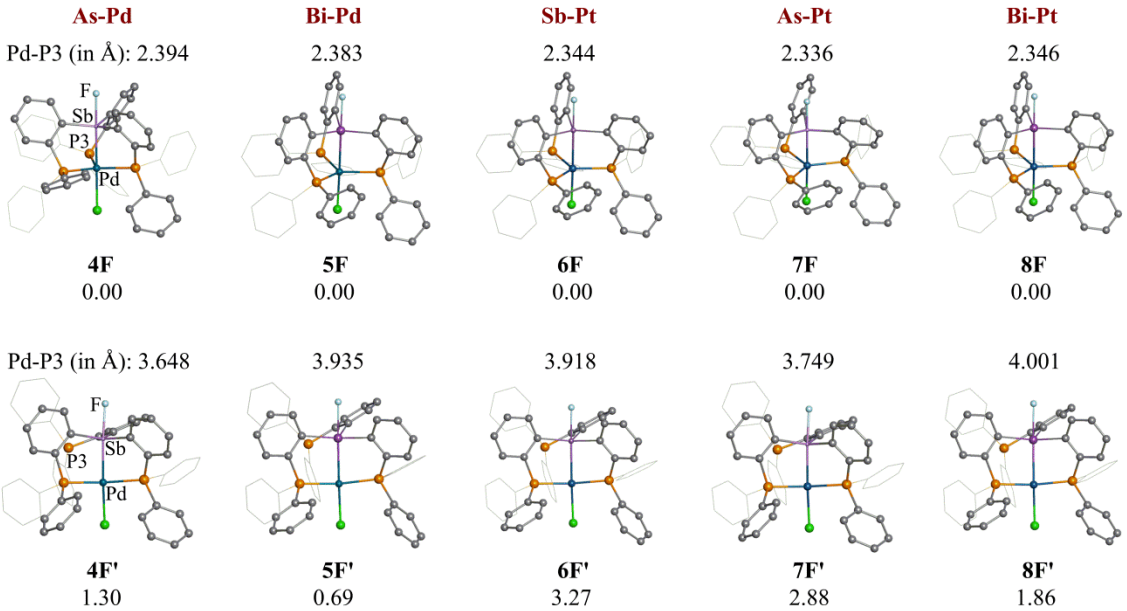


Fig. S4 Optimized structures and relative energies (in kcal mol^{-1}) of **4F**-**8F** and **4F'**-**8F'** calculated at PCM/PBE0/BS-II//PCM/PBE0/BS-I level (CH_2Cl_2 as solvent). Hydrogen atoms of benzene rings are omitted for clarity. Phenyl groups located at the back side are shown by faint black colors.

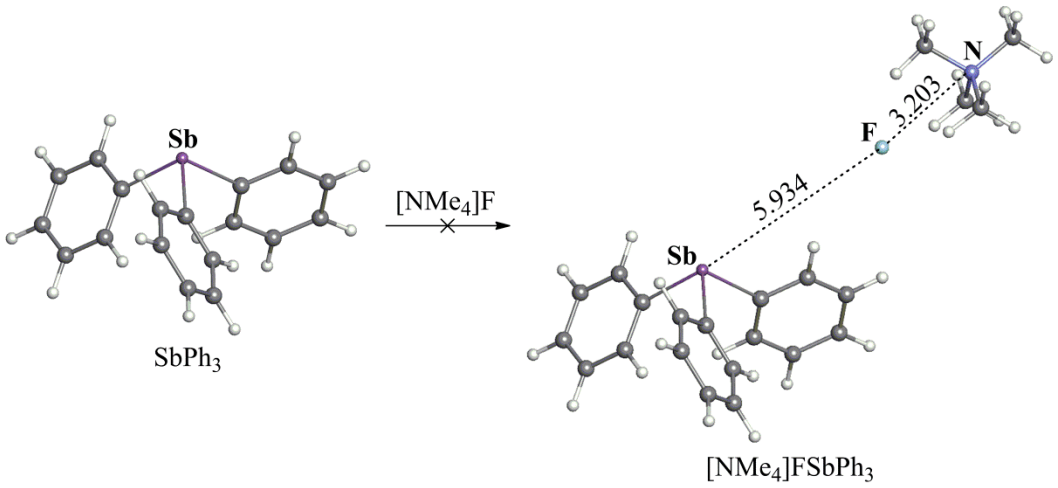


Fig. S5 Optimized structures (bond lengths in angstroms) of $SbPh_3$ and $[NMe_4]FSbPh_3$ calculated at PCM/PBE0/BS-I level (CH_2Cl_2 as solvent).

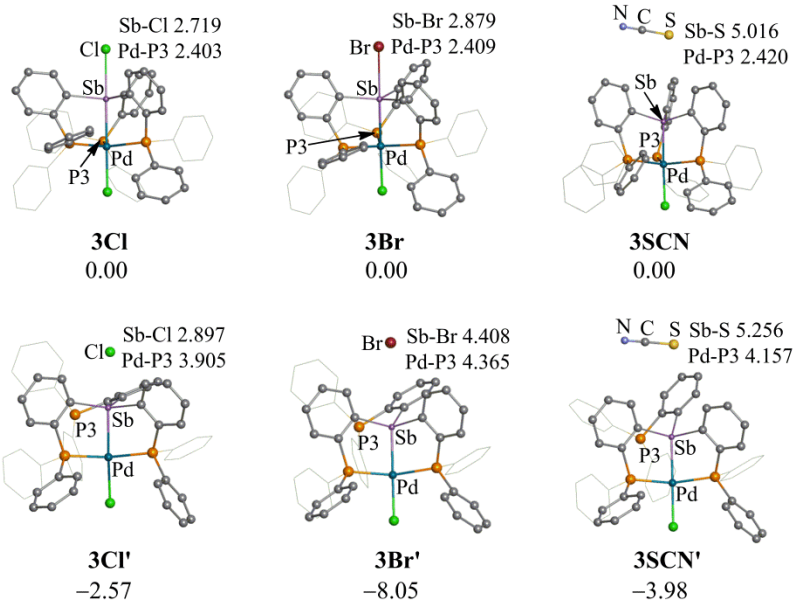


Fig. S6 Optimized structures (in Å) and relative energies (in kcal mol^{-1}) of **3Cl**, **3Cl'**, **3Br**, **3Br'**, **3SCN**, and **3SCN'** calculated at PCM/PBE0/BS-II//PCM/PBE0/BS-I level (CH_2Cl_2 as solvent). Hydrogen atoms of benzene rings are omitted for clarity. Phenyl groups located at the back side are shown by faint black colors.

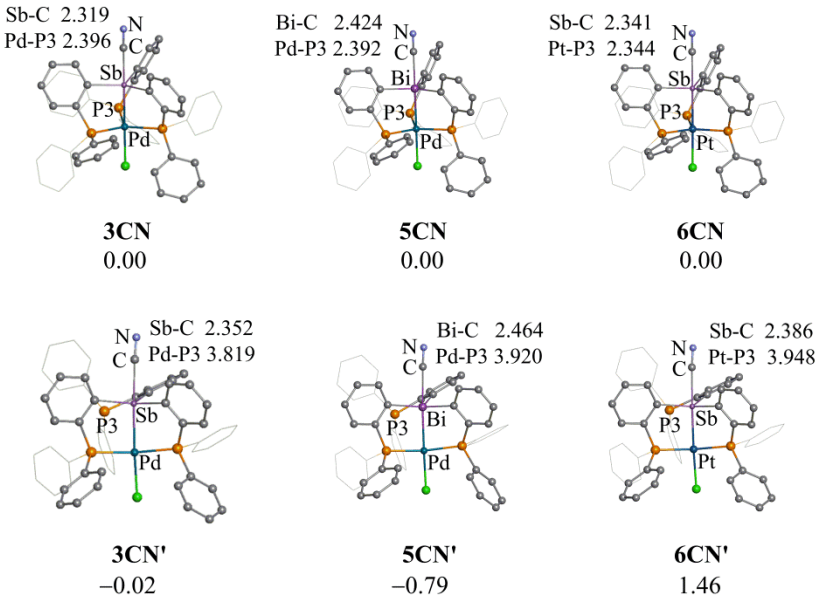


Fig. S7 Optimized structures (in Å) and relative energies (in kcal mol^{-1}) of **3CN**, **3CN'**, **5CN**, **5CN'**, **6CN**, and **6CN'** calculated at PCM/PBE0/BS-II//PCM/PBE0/BS-I level (CH_2Cl_2 as solvent). In view of the very small energy difference between **3CN** and **3CN'**, the single point calculations were performed with ωB97XD functional to verify the credibility of the results. **3CN'** is still more stable than **3CN** by 0.86 kcal mol^{-1} at PCM/ωB97XD/BS-II//PCM/PBE0/BS-I level (CH_2Cl_2 as solvent). Hydrogen atoms of benzene rings are omitted for clarity. Phenyl groups located at the back side are shown by faint black colors.

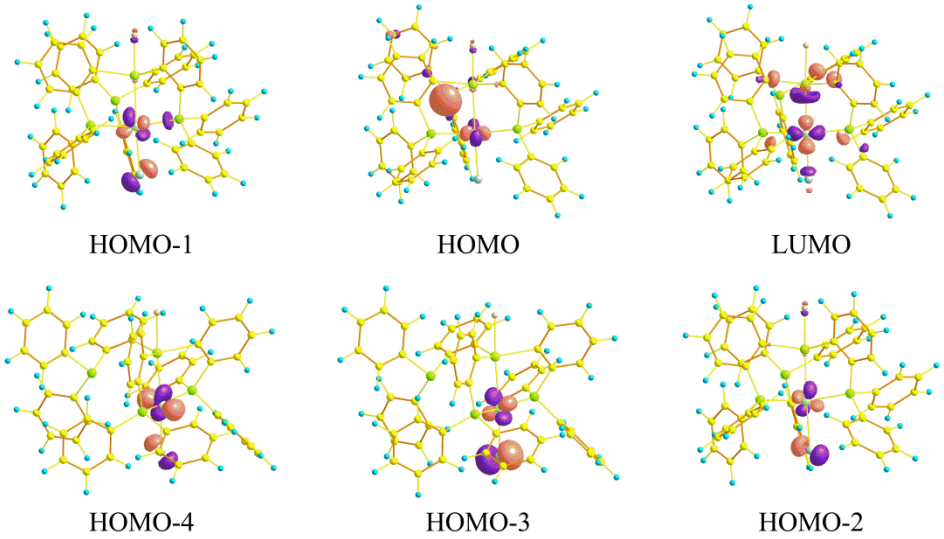


Fig. S8 Molecular orbitals for **3F'** involved in the dominant electron transitions.

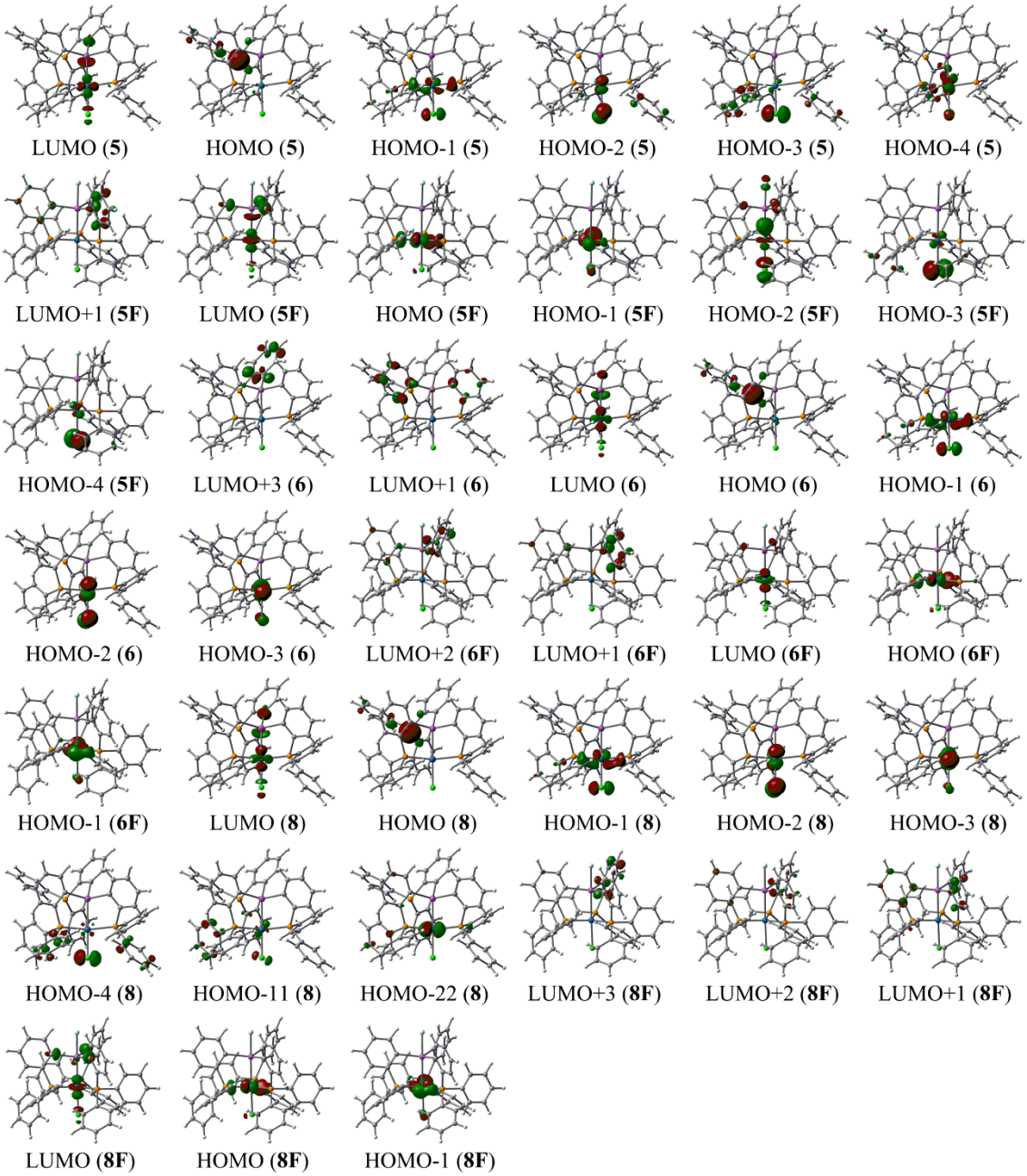


Fig. S9 Molecular orbitals for **5**, **6**, **8** and their fluoride adducts involved in the dominant electron transitions.

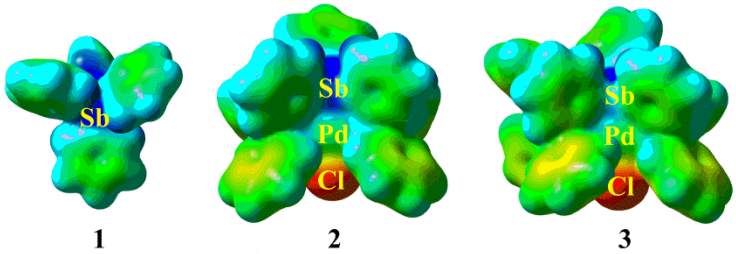


Fig. S10 Electron density maps for the PCM/PBE0/BS-I optimized structures of **1**-**3** mapped with the electrostatic potential (Isoval = 0.004) from the total SCF density. The red areas represent regions of negative electrostatic potentials, and the blue areas identify regions of positive electrostatic potentials (electrophilic sites).

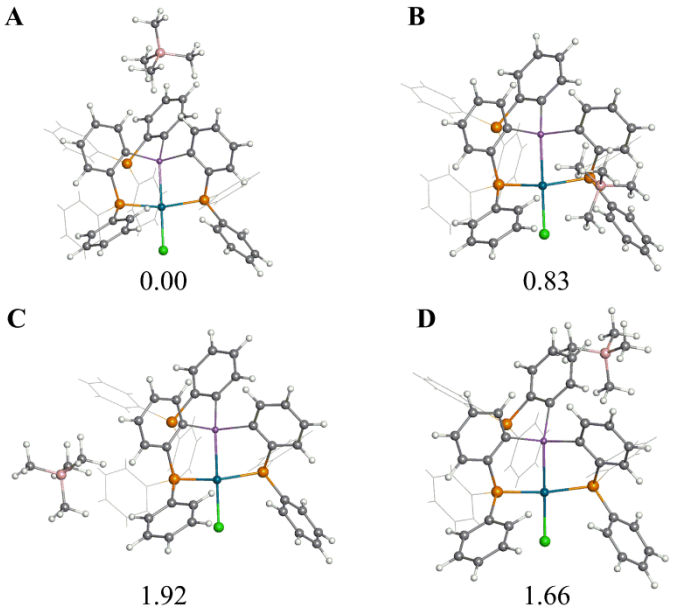
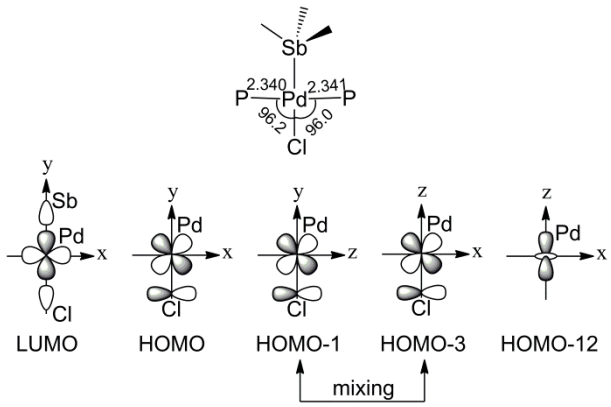


Fig. S11 Optimized structures and relative energies (in kcal mol^{-1}) for four isomers of **3**[BMe_4] calculated at PCM/PBE0/BS-II//PCM/PBE0/BS-I level (CH_2Cl_2 as solvent). Phenyl groups located at the back side are shown by faint black colors.



Scheme S1. Structure (bond lengths and angles in angstroms and degrees, respectively) and representations of five d orbitals for **2**.

Table S1 Main geometrical parameters of **3** optimized by various functionals (PBE0, mPW1PW91, B3PW91 and B3LYP) and basis set I (BS-I) in gas phase together with available experimental parameters[a] (bond lengths and angles in angstroms and degrees, respectively)

	Expt.	PBE0		mPW1PW91		B3PW91		B3LYP	
	Length	Length	Deviation	Length	Deviation	Length	Deviation	Length	Deviation
Sb-Pd	2.469	2.512	0.043	2.514	0.045	2.519	0.05	2.539	0.07
Sb-C_3	2.111	2.132	0.021	2.131	0.02	2.136	0.025	2.138	0.027
Sb-C_4	2.135	2.154	0.019	2.152	0.017	2.157	0.022	2.158	0.023
Sb-C_5	2.124	2.142	0.018	2.141	0.017	2.146	0.022	2.151	0.027
Pd-Cl	2.331	2.339	0.008	2.341	0.01	2.347	0.016	2.370	0.039
Pd-P_1	2.328	2.344	0.016	2.348	0.02	2.353	0.025	2.379	0.051
Pd-P_2	2.333	2.344	0.011	2.350	0.017	2.356	0.023	2.382	0.049
P_1-C_1	1.835	1.851	0.016	1.852	0.017	1.856	0.021	1.864	0.029
P_2-C_2	1.837	1.849	0.012	1.850	0.013	1.854	0.017	1.863	0.026
P_3-C_6	1.829	1.832	0.003	1.833	0.004	1.837	0.008	1.848	0.019
Pd···P	4.149	4.232	0.083	4.279	0.13	4.316	0.167	4.433	0.284
Sb-Pd-Cl	174.17	177.86	3.69	178.39	4.22	178.43	4.26	178.02	3.85
P_1-Pd-P_2	159.44	160.78	1.34	160.50	1.06	160.02	0.58	160.55	1.11
ΣC-Sb-C	321.30	318.63	-2.67	318.77	-2.53	318.62	-2.68	318.59	-2.71

a Experimental data see Angew. Chem. Int. Ed. 2012, 51, 478-481.

Table S2 Main geometrical parameters of **3** optimized by various functionals (TPSSh, M06, M062X and CAM-B3LYP) and basis set I (BS-I) in gas phase together with available experimental parameters[a] (bond lengths and angles in angstroms and degrees, respectively)

	Expt.	TPSSh		M06		M062X		CAM-B3LYP	
	Length	Length	Deviation	Length	Deviation	Length	Deviation	Length	Deviation
Sb-Pd	2.469	2.523	0.054	2.522	0.053	2.475	0.006	2.513	0.044
Sb-C_3	2.111	2.140	0.029	2.127	0.016	2.113	0.002	2.123	0.012
Sb-C_4	2.135	2.162	0.027	2.145	0.01	2.132	-0.003	2.139	0.004
Sb-C_5	2.124	2.151	0.027	2.131	0.007	2.115	-0.009	2.133	0.009
Pd-Cl	2.331	2.351	0.02	2.373	0.042	2.402	0.071	2.348	0.017
Pd-P_1	2.328	2.358	0.03	2.376	0.048	2.368	0.04	2.358	0.03
Pd-P_2	2.333	2.360	0.027	2.372	0.039	2.383	0.05	2.359	0.026
P_1-C_1	1.835	1.858	0.023	1.852	0.017	1.853	0.018	1.853	0.018
P_2-C_2	1.837	1.857	0.02	1.849	0.012	1.854	0.017	1.853	0.016
P_3-C_6	1.829	1.839	0.01	1.837	0.008	1.843	0.014	1.837	0.008
Pd···P	4.149	4.309	0.16	4.070	-0.079	3.877	-0.272	4.273	0.124
Sb-Pd-Cl	174.17	178.09	3.92	177.93	3.76	177.03	2.86	178.72	4.55
P_1-Pd-P_2	159.44	160.30	0.86	158.05	-1.39	157.54	-1.9	161.18	1.74
ΣC-Sb-C	321.30	317.98	-3.32	322.25	0.95	317.40	-3.9	320.72	-0.58

a Experimental data see Angew. Chem. Int. Ed. 2012, 51, 478-481.

Table S3 Main geometrical parameters of **3** optimized by various functionals (ωB97XD, BP86 and BLYP) and basis set I (BS-I) in gas phase together with available experimental parameters[a] (bond lengths and angles in angstroms and degrees, respectively)

	Expt.	ωB97XD		BP86		BLYP	
	Length	Length	Deviation	Length	Deviation	Length	Deviation
Sb-Pd	2.469	2.496	0.027	2.538	0.069	2.564	0.095
Sb-C_3	2.111	2.115	0.004	2.153	0.042	2.158	0.047
Sb-C_4	2.135	2.134	-0.001	2.175	0.04	2.180	0.045
Sb-C_5	2.124	2.122	-0.002	2.166	0.042	2.177	0.053
Pd-Cl	2.331	2.359	0.028	2.364	0.033	2.398	0.067
Pd-P_1	2.328	2.361	0.033	2.362	0.034	2.401	0.073
Pd-P_2	2.333	2.357	0.024	2.365	0.032	2.402	0.069
P_1-C_1	1.835	1.851	0.016	1.870	0.035	1.882	0.047
P_2-C_2	1.837	1.850	0.013	1.868	0.031	1.880	0.043
P_3-C_6	1.829	1.833	0.004	1.850	0.021	1.865	0.036
Pd···P	4.149	3.964	-0.185	4.354	0.205	4.506	0.357
Sb-Pd-Cl	174.17	177.74	3.57	178.41	4.24	178.33	4.16
P_1-Pd-P_2	159.44	158.92	-0.52	160.30	0.86	159.95	0.51
ΣC-Sb-C	321.30	324.09	2.79	317.76	-3.54	317.21	-4.09

a Experimental data see Angew. Chem. Int. Ed. 2012, 51, 478-481.

Table S4 Main geometrical parameters of **3** optimized by various functionals (PBE, TPSS and M06L) and basis set I (BS-I) in gas phase together with available experimental parameters[a] (bond lengths and angles in angstroms and degrees, respectively)

	Expt.	PBE		TPSS		M06L	
	Length	Length	Deviation	Length	Deviation	Length	Deviation
Sb-Pd	2.469	2.534	0.065	2.532	0.063	2.507	0.038
Sb-C_3	2.111	2.152	0.041	2.148	0.037	2.141	0.03
Sb-C_4	2.135	2.174	0.039	2.171	0.036	2.156	0.021
Sb-C_5	2.124	2.166	0.042	2.161	0.037	2.149	0.025
Pd-Cl	2.331	2.363	0.032	2.359	0.028	2.394	0.063
Pd-P_1	2.328	2.359	0.031	2.363	0.035	2.375	0.047
Pd-P_2	2.333	2.359	0.026	2.366	0.033	2.354	0.021
P_1-C_1	1.835	1.866	0.031	1.864	0.029	1.846	0.011
P_2-C_2	1.837	1.864	0.027	1.863	0.026	1.847	0.01
P_3-C_6	1.829	1.843	0.014	1.845	0.016	1.833	0.004
Pd···P	4.149	4.298	0.149	4.335	0.186	3.890	-0.259
Sb-Pd-Cl	174.17	178.77	4.6	178.10	3.93	177.64	3.47
P_1-Pd-P_2	159.44	160.36	0.92	160.09	0.65	160.83	1.39
ΣC-Sb-C	321.30	317.30	-4.0	317.39	-3.91	325.02	3.72

a Experimental data see Angew. Chem. Int. Ed. 2012, 51, 478-481.

Table S5 Main geometrical parameters of **1** and **1F** optimized at PBE0/BS-I level together with available experimental parameters[a] (bond lengths and angles in angstroms and degrees, respectively)

	1	**1F**		
	Calc.	Expt.	Calc.	Dev.
Sb-F	-	2.0530(8)	2.030	-0.02308
Sb-C_1	2.105	2.120(1)	2.138	0.0179
Sb-C_2	2.105	2.134(1)	2.139	0.0049
Sb-C_3	2.105	2.135(1)	2.151	0.0159
Sb-C_4	2.105	2.183(1)	2.202	0.0189
ΣC-Sb-C	328.44	356.81(3)	357.77	0.957

a Experimental data see Russ. J. Coord. Chem. 2005, 31, 108–114.

Table S6 Main geometrical parameters of **2** and **2F** optimized at PBE0/BS-I level together with available experimental parameters[a] (bond lengths and angles in angstroms and degrees, respectively)

	2			**2F**		
	Expt.	Calc.	Dev.	Expt.	Calc.	Dev.
Sb-Pd	2.481	2.505	0.024	2.585	2.617	0.032
Sb-F	-	-	-	2.051	2.037	-0.014
Sb-C_3	2.116	2.132	0.016	2.154	2.182	0.028
Sb-C_4	2.129	2.132	0.003	2.162	2.182	0.020
Sb-C_5	2.116	2.119	0.003	2.144	2.148	0.004
Pd-Cl	2.338	2.333	-0.005	2.406	2.423	0.017
Pd-P_1	2.310	2.338	0.028	2.305	2.302	-0.003
Pd-P_2	2.322	2.339	0.017	2.290	2.302	0.012
P_1-C_1	1.831	1.850	0.019	1.831	1.835	0.004
P_2-C_2	1.845	1.849	0.004	1.835	1.835	0.000
∠F-Sb-Pd	-	-	-	177.93	175.12	-2.81
∠Sb-Pd-Cl	176.69	179.46	2.77	173.43	173.27	-0.14
∠P_1-Pd-P_2	164.53	165.47	0.94	167.23	169.28	2.05
ΣP-Pd-P	-	-	-	-	-	-
ΣC-Sb-C	322.13	326.66	4.53	355.84	355.94	0.10

a Experimental data see Angew. Chem. Int. Ed. 2012, 51, 478-481.

Table S7 Main geometrical parameters of **3** and **3F** optimized at PBE0/BS-I level together with available experimental parameters[a] (bond lengths and angles in angstroms and degrees, respectively)

	3			**3F**		
	Expt.	Calc.	Dev.	Expt.	Calc.	Dev.
Sb-Pd	2.469	2.512	0.043	2.572	2.596	0.024
Sb-F	-	-	-	2.032	2.041	0.009
Sb-C_3	2.111	2.132	0.021	2.149	2.176	0.027
Sb-C_4	2.135	2.154	0.019	2.159	2.183	0.024
Sb-C_5	2.124	2.142	0.018	2.138	2.180	0.042
Pd-Cl	2.331	2.339	0.008	2.436	2.458	0.022
Pd-P_1	2.328	2.344	0.016	2.332	2.419	0.087
Pd-P_2	2.333	2.344	0.011	2.365	2.373	0.008
Pd···P_3/Pd-P_3	4.149	4.232	0.083	2.348	2.360	0.012
P_1-C_1	1.835	1.851	0.016	1.821	1.841	0.020
P_2-C_2	1.837	1.849	0.012	1.840	1.843	0.003
P_3-C_6	1.829	1.832	0.003	1.831	1.838	0.007
∠F-Sb-Pd	-	-	-	177.59	178.49	0.90
∠Sb-Pd-Cl	174.17	177.86	3.69	176.13	175.52	-0.61
∠P_1-Pd-P_2	159.44	160.78	1.34	-	-	-
ΣP-Pd-P	-	-	-	357.58	358.86	1.28
ΣC-Sb-C	321.30	318.63	-2.67	356.02	354.75	-1.27

a Experimental data see Angew. Chem. Int. Ed. 2012, 51, 478-481.

Table S8 Wiberg bond index (WBI) of **1**-**3** and their fluoride adducts

	1	**1F**	**2**	**2F**	**3**	**3F**
Sb-F		0.31		0.30		0.30
Sb-C_1	0.81	0.73				
Sb-C_2	0.81	0.75				
Sb-C_3	0.81	0.73	0.77	0.68	0.75	0.69
Sb-C_4	0.81	0.63	0.77	0.68	0.72	0.68
Sb-C_5			0.79	0.72	0.76	0.69
Sb-Pd			0.66	0.56	0.61	0.57
Pd-P_1			0.58	0.56	0.53	0.60
Pd-P_2			0.58	0.56	0.54	0.60
Pd-P_3						0.61
Pd-Cl			0.64	0.49	0.60	0.56

Table S9 Natural population of model systems $\mathbf{2_{mSi}}$, $\mathbf{2_m}$, $\mathbf{2_mF}$, $\mathbf{3_m}$, and $\mathbf{3_mF}$[a]

		$\mathbf{2_{mSi}}$	$\mathbf{2_m}$	$\mathbf{2_mF}$	$\mathbf{3_m}$	$\mathbf{3_mF}$
Pd	s	8.501	8.540	8.551	8.522	8.483
	p	18.572	18.665	18.605	19.065	19.142
	d	19.421	19.344	19.424	19.334	19.420
	total	46.495	46.549	46.581	46.922	47.045
Si/Sb	s	4.857	9.205	9.143	9.186	9.117
	p	7.576	19.977	19.705	19.934	19.613
	d		20.008	20.010	20.007	20.010
	total	12.458	49.190	48.857	49.127	48.740
Ph1[b]		41.472	41.324	41.377	41.333	41.373
P1 (PH_3)		14.716 (17.534)	14.705 (17.456)	14.748 (17.567)	14.662 (17.426)	14.774 (17.620)
P2 (PH_3)		14.730 (17.542)	14.718 (17.463)	14.749 (17.568)	14.645 (17.412)	14.772 (17.618)
P3 (PH_3)					14.915 (17.746)	14.772 (17.618)
Cl		17.557	17.372	17.541	17.367	17.489
F				9.755		9.752

a The PCM(CH_2Cl_2)/PBE0/BS-I geometries. *b* Average value of Ph1, Ph2 and Ph3.

Table S10 Absorption peaks (λ_{abs}) [in eV (nm)], the oscillator strength (*f*), and assignments for **5**, **5F**, **6**, **6F**, **6CN**, **8**, and **8F** at the PCM(CH_2Cl_2)/TD-PBE0/BS-II level

systems	λ_{abs}	major contributions	*f*	assignments
5	2.89 (429)	H-1 → L[a] (82%)	0.1004	LFT/LMCT
	2.97 (418)	H → L (69%) H-4 → L (14%)	0.1259	LMCT
	3.16 (393)	H-2 → L (58%) H-4 → L (20%)	0.0010	LFT/LMCT
	3.23 (384)	H-4 → L (40%) H → L (28%) H-2 → L (10%)	0.0147	LFT/LMCT
	3.59 (346)	H-3 → L (63%)	0.0866	LMCT
5F	2.27 (546)	H → L (97%)	0.0582	LFT/LMCT
	2.45 (507)	H-1 → L (97%)	0.0603	LFT/LMCT
	3.51 (354)	H-3 → L (81%)	0.0016	LMCT/LFT
	3.55 (350)	H-4 → L (71%)	0.0123	LMCT/LFT
	3.60 (345)	H-2 → L (52%) H → L+1 (31%)	0.1131	LMCT/LFT
6	3.53 (351)	H → L (38%) H-1 → L (32%) H-3 → L (18%)	0.0802	LMCT/LFT
	3.56 (348)	H-1 → L (55%) H → L (19%) H-3 → L (14%)	0.1304	LFT/LMCT
	3.72 (334)	H-2 → L (74%)	0.0123	LFT/LMCT
	3.81 (325)	H-3 → L (48%) H → L (36%)	0.0488	LFT/LMCT
	4.14 (300)	H → L+3 (75%) H → L+1 (10%)	0.0282	LLCT
6F	2.93 (423)	H → L (93%)	0.0972	LFT/LMCT
	3.10 (400)	H-1 → L (93%)	0.0720	LFT/LMCT
	3.49 (355)	H → L+1 (84%) H → L+2 (13%)	0.0144	MLCT
	3.53 (351)	H → L + 2 (84%) H → L+1 (13%)	0.0075	MLCT
	3.67 (338)	H-1 → L+1 (92%)	0.0031	MLCT
6CN	2.93 (423)	H → L (94%)	0.0972	LFT/LMCT
	3.02 (411)	H-1 → L (95%)	0.0720	LFT/LMCT
	3.43 (362)	H → L+1 (95%)	0.0144	MLCT
	3.49 (356)	H → L + 2 (93%)	0.0075	MLCT
	3.55 (349)	H-1 → L+1 (95%)	0.0031	MLCT
8	3.36 (369)	H-1 → L (60%) H-3 → L (15%) H → L (14%)	0.0446	LFT/LMCT
	3.39 (366)	H-3 → L (31%) H-1 → L (28%) H → L (28%)	0.1057	LFT/LMCT
	3.50 (354)	H-2 → L (84%)	0.0081	LFT/LMCT
	3.61 (344)	H → L (54%) H-3 → L (38%)	0.0473	LMCT/LFT
	4.08 (304)	H-4 → L (40%) H-11 → L (16%) H-22 → L (13%)	0.0128	LMCT
8F	2.57 (482)	H → L (97%)	0.0510	LFT/LMCT
	2.77 (447)	H-1 → L (97%)	0.0454	LFT/LMCT
	3.55 (349)	H → L+1 (94%)	0.0316	MLCT
	3.61 (344)	H → L+2 (94%)	0.0101	MLCT
	3.74 (331)	H → L+3 (48%) H-1 → L+1 (41%)	0.0027	MLCT

a H and L represent HOMO and LUMO, respectively.

XYZ coordinates of the optimized structure of **1**

45

C	-0.0086442444	0.045911354	-2.1036349613
C	1.2025510244	0.0324193263	-2.802253865
H	2.1529354422	0.0286501685	-2.2739324171
C	1.1869063889	0.0358149954	-4.1938191328
H	2.1238283289	0.0286740015	-4.742791905
C	-0.0260701215	0.0528356726	-4.8789005061
H	-0.0324881911	0.0566979756	-5.9649326513
C	-1.2308950636	0.0711316211	-4.1796864635
H	-2.1743255596	0.0909596673	-4.7172049675
C	-1.2295001511	0.0695116563	-2.7876285998
H	-2.1742475981	0.0991479439	-2.2495736754
C	-1.5606219771	1.2386593872	0.6793747135
C	-1.8283566158	2.4403295773	0.0135748843
H	-1.2649563256	2.73030386	-0.8704258372
C	-2.8438878757	3.2683596782	0.4835952851
H	-3.0582871587	4.2015324319	-0.0288522543
C	-3.5847764799	2.8974975625	1.6035963235
H	-4.3776218576	3.5458794236	1.9648656502
C	-3.3190844882	1.6973677775	2.2592816026
H	-3.9036714828	1.4087337653	3.1277260221
C	-2.3055923253	0.861063149	1.8008437532
H	-2.1099823516	-0.0785506581	2.3119326621
C	-0.2751230836	-1.9681864013	0.6903152541
C	-0.8693548354	-2.9178955482	-0.1464589368
H	-1.1659744357	-2.6620797798	-1.1608167322
C	-1.0715283674	-4.211270311	0.3258587686
H	-1.5295074236	-4.9547078349	-0.3197453604
C	-0.6836837903	-4.5511574369	1.6200397786
H	-0.8426556138	-5.5623156638	1.9830939141
C	-0.0876181693	-3.6037545995	2.4494905218
H	0.2192815776	-3.8741475828	3.4555132358
C	0.1218694463	-2.3068692358	1.9890652893
H	0.6015178423	-1.5776934336	2.6380688215
C	1.849888071	0.6882818147	0.7363493422
C	2.9371037161	-0.1909699096	0.798009447
H	2.8339699139	-1.233152432	0.5044709028
C	4.1654197978	0.275085507	1.2583086297
H	5.0130167786	-0.4018550491	1.3103825203
C	4.3037466805	1.6032713765	1.655262187
H	5.2635245003	1.9614121858	2.0159300272
C	3.2171110621	2.4732713465	1.5983088228
H	3.3274736918	3.5059944387	1.915406625
C	1.9839582721	2.0207258006	1.1386977523
H	1.1378147997	2.7028780042	1.1059651323
Sb	0.001138252	0.0013144073	0.0008403962

XYZ coordinates of the optimized structure of **1F**

46

C	-1.8435576069	1.077421645	0.2671688376
C	-2.7530349018	0.6570775118	1.2423515855
H	-2.5250486984	-0.2009752521	1.8664963493
C	-3.9494194019	1.347052705	1.4231032211
H	-4.6570167463	1.0097089566	2.1757316661
C	-4.2343783903	2.4702116241	0.6488429444
H	-5.1645441307	3.0118545461	0.7980606669
C	-3.3258086902	2.8987412711	-0.3155441657
H	-3.541331857	3.7766373609	-0.9185750404
C	-2.1368268502	2.1987109876	-0.513990808
H	-1.4471638869	2.5316848454	-1.2855567104
C	0.0199284499	0.2198093789	-2.1941766285
C	-1.176352488	0.1612122849	-2.921200958
H	-2.1303477602	0.111267567	-2.4007340102
C	-1.1706288975	0.1684650671	-4.3151960187
H	-2.110328468	0.126561131	-4.8601541221
C	0.0369949826	0.2284218435	-5.0073546254
H	0.0434366404	0.2354048102	-6.0941474395
C	1.2361429247	0.2751016333	-4.3002485464
H	2.1826230889	0.3166744311	-4.8333794815
C	1.2254012291	0.2675449973	-2.9057797311
H	2.1732917823	0.300530335	-2.373412461
C	1.8284128582	1.101000852	0.3077854393
C	2.0960574345	2.2662511205	-0.416009653
H	1.3942422357	2.6283018745	-1.1633419025
C	3.2747510561	2.9753637378	-0.1900269621
H	3.4707802439	3.886791229	-0.748295909
C	4.1979845495	2.5133749342	0.7446012206
H	5.1201367811	3.0624280745	0.914882951
C	3.9379028393	1.3474462982	1.4623094788
H	4.656740373	0.9843273099	2.1919278842
C	2.7521162667	0.6470106372	1.2539452469
H	2.5442496811	-0.2461337016	1.8348709563
C	0.0223152941	-2.1070315569	0.0069218524
C	-0.056681936	-2.8170643064	1.2107886433
H	-0.1225627248	-2.2759963694	2.1472823824
C	-0.0475019513	-4.2100897847	1.200574073
H	-0.1109295388	-4.7538293929	2.1394741491
C	0.043505373	-4.9038741425	-0.0040120133
H	0.0514831537	-5.9905962317	-0.0079633197
C	0.1246637226	-4.201038509	-1.2032700408
H	0.1970199261	-4.7356186799	-2.1466287924
C	0.1124373015	-2.8074906655	-1.2004770263
H	0.1739717934	-2.2743165612	-2.1440459687
Sb	0.0028470712	0.0374925945	-0.0099024116
F	-0.0158821277	-0.1158614412	2.0462731982

XYZ coordinates of the optimized structure of **[1]**BMe_4

62

C	0.0368755755	0.0444892302	-2.0881722194
C	1.2461775206	-0.0774469899	-2.7797456549
H	2.1896936581	-0.1677683972	-2.2479524451
C	1.2388502618	-0.0694722854	-4.1715260135
H	2.1751966976	-0.1577563999	-4.7142148983
C	0.0364795649	0.0612572303	-4.8634906279
H	0.0371632128	0.0728517941	-5.949512375
C	-1.1653696177	0.1867363986	-4.170455081
H	-2.1002266819	0.2968906226	-4.7117459423
C	-1.1723298713	0.1804763374	-2.7780192766
H	-2.1132007449	0.2922919194	-2.2456462866
C	-1.5280153683	1.2515691704	0.6944062822
C	-1.7775691146	2.4689622605	0.0525674453
H	-1.189761589	2.7928543858	-0.8025183783
C	-2.8053085501	3.2854731041	0.5183607856
H	-2.9987945389	4.2325607558	0.0236138313
C	-3.5758176232	2.8875716218	1.6083569021
H	-4.3771571279	3.527649271	1.9661352641
C	-3.3262639314	1.6706141521	2.240381923
H	-3.9312370548	1.3597106544	3.0870216635
C	-2.3009768446	0.8456723757	1.7868996362
H	-2.1178593302	-0.1049337542	2.281047333
C	-0.2663756053	-1.9560553998	0.6971914712
C	-0.7849156654	-2.9118529548	-0.1817322649
H	-1.0151575828	-2.655142359	-1.2125538931
C	-1.0021901257	-4.2105373378	0.2704511616
H	-1.4025605973	-4.9565215331	-0.4096390964
C	-0.7038410397	-4.5509022697	1.5882313764
H	-0.8738792483	-5.5656887057	1.9361528031
C	-0.184094027	-3.5972214503	2.4609830304
H	0.0520369711	-3.8650104504	3.4865774101
C	0.0390986896	-2.2952700413	2.0201957233
H	0.4554558741	-1.5620488901	2.7064117271
C	1.906649709	0.6547688553	0.7569845272
C	2.9109850751	-0.2919904327	0.9849892122
H	2.734782282	-1.3503467285	0.8111687863
C	4.1542915576	0.1302970831	1.4490365275
H	4.9372747222	-0.6006418694	1.6281419466
C	4.3896977825	1.4833086606	1.6824827296
H	5.3611130827	1.8083611873	2.0437663303
C	3.3851311011	2.4218987043	1.4554187585
H	3.5694469777	3.4767360877	1.6356336401
C	2.1373945694	2.0135018752	0.9931746461
H	1.3646886606	2.7577894573	0.8196236209
Sb	0.0387281197	0.0163559758	0.017150362
B	0.8059661376	5.3894049807	-2.5513032266
C	-0.6437223742	4.8703424299	-3.1466943058

C	1.1333515079	6.8962322286	-3.1380277076
C	0.734269712	5.4511556721	-0.9027580779
C	1.9963162168	4.3432610722	-3.0129038264
H	2.0926954736	7.3005599839	-2.7698413101
H	0.3654044015	7.640051322	-2.8619274059
H	1.1966448694	6.9211155353	-4.2399342374
H	-0.8990527175	3.8427313894	-2.8283290878
H	-0.6710385288	4.8522334524	-4.250366341
H	-1.490626561	5.5062837816	-2.832947011
H	2.9919712166	4.6280019086	-2.6290081471
H	2.1029443692	4.2721551443	-4.1098647702
H	1.8219856803	3.3103593896	-2.6614284269
H	1.6830823316	5.7793243259	-0.4429775426
H	0.5013020302	4.4704141524	-0.4499125834
H	-0.0408385105	6.1438825071	-0.5296934929

XYZ coordinates of the optimized structure of **2**

80

Pd	-0.0079825606	-0.0008888095	-0.0076489502
P	-2.3189895997	0.2992239914	0.2187736551
Cl	0.0012058721	-0.0696400373	-2.3872483556
Sb	-0.0076925226	0.0094246172	2.4946502687
P	2.3156940387	0.1037192612	0.2512302872
C	-1.8313721509	1.0317670328	2.9131602735
C	-2.7207563416	1.1071360884	1.8265143921
C	-3.9400537665	1.7745494498	1.9915163255
H	-4.6309182222	1.8581890441	1.1569121014
C	-4.2712602956	2.336829427	3.2211648819
H	-5.2184573351	2.8551952174	3.3361142674
C	-3.396387226	2.2332779877	4.2996885513
H	-3.6579958209	2.6710914638	5.2583919175
C	-2.1766894085	1.5772340088	4.1504545039
H	-1.504444912	1.5065182472	5.0004916833
C	-3.232594422	-1.2755795559	0.1881139576
C	-2.8790043546	-2.1991868943	-0.8061005654
H	-2.0917514964	-1.9559342108	-1.5167332196
C	-3.5375855794	-3.4216770979	-0.882251166
H	-3.2643908833	-4.1321494547	-1.6570921177
C	-4.5372654822	-3.7365177651	0.0374476578
H	-5.0449165813	-4.6951390736	-0.0198661438
C	-4.8831400811	-2.8247687564	1.031571456
H	-5.6603821881	-3.0686182261	1.7500854332
C	-4.235854724	-1.5932579981	1.1095497525
H	-4.5145576195	-0.8876925339	1.8869322751
C	-3.0680942319	1.3809038464	-1.035499209
C	-2.4227927093	2.5863269405	-1.3401022957
H	-1.4814525962	2.8390120596	-0.8572680652
C	-2.9800233425	3.4553714337	-2.2703709011
H	-2.4766846474	4.3886475731	-2.5054868279

C	-4.1744571094	3.1221638668	-2.9096526553
H	-4.604305509	3.7996965281	-3.6418354179
C	-4.8118253825	1.9200507494	-2.6162241343
H	-5.739461388	1.6566766536	-3.1160846442
C	-4.2623854488	1.0463226026	-1.6796143551
H	-4.7624610087	0.108490166	-1.4551298691
C	1.8264159803	1.0239985624	2.8850646822
C	2.7321530838	1.0024159185	1.8078653522
C	3.9642516364	1.6513087823	1.9437845582
H	4.6677232774	1.6609167325	1.1156528417
C	4.2904721653	2.2964599099	3.1341440158
H	5.2474362213	2.8014504895	3.2252981815
C	3.3964367841	2.2969423811	4.20105877
H	3.6514549983	2.804123118	5.1267406205
C	2.164027047	1.6574737639	4.0813989511
H	1.4742181944	1.6740862632	4.9199911202
C	3.0960933944	-1.5361670447	0.3738593616
C	2.5629532598	-2.5667333443	-0.412511927
H	1.7056506184	-2.3731158873	-1.0535967054
C	3.1333893144	-3.8349841265	-0.3743514006
H	2.7190157547	-4.6297687992	-0.9877414687
C	4.2260466342	-4.0850616755	0.4540208249
H	4.6655438981	-5.0778618016	0.4872925165
C	4.7523562071	-3.0650375432	1.2434830015
H	5.6015484594	-3.2592294459	1.8923047641
C	4.1923274992	-1.7906106639	1.2054535803
H	4.6080460173	-1.0019504984	1.8261126391
C	3.1897774157	1.0213535005	-1.0518999652
C	4.3288295046	0.5087524442	-1.6780757387
H	4.7135673841	-0.4687605691	-1.402207506
C	4.9730904791	1.256387656	-2.6624542919
H	5.8578171873	0.8548066922	-3.1479035669
C	4.4844749861	2.5091080139	-3.0215629711
H	4.9879325973	3.0882121082	-3.7903914414
C	3.3438489225	3.0195819159	-2.4009608463
H	2.9551882235	3.99256659	-2.6871347769
C	2.6925871096	2.2771729619	-1.4236572372
H	1.7919676054	2.6674422128	-0.9559360513
C	0.0022977163	-1.7012735779	3.7429052302
C	1.1998640041	-2.1370787355	4.3171958275
H	2.1263277063	-1.5920456904	4.1555174567
C	1.2022993865	-3.2777015494	5.1165998731
H	2.1304813297	-3.6161445767	5.5678685614
C	0.0189889689	-3.979205774	5.3364592901
H	0.0252337723	-4.8688797839	5.9595865569
C	-1.173278575	-3.5434119782	4.7608316803
H	-2.0955368182	-4.0903689626	4.9339230914
C	-1.1871976616	-2.40409017	3.961058072
H	-2.1230566529	-2.0726306619	3.5174007258

XYZ coordinates of the optimized structure of **2F**

81

Pd	0.0027272952	-0.1013265744	-0.0173530374
P	-2.2978776242	-0.0038144556	0.1856641616
Cl	0.0028984401	-0.3161642743	-2.4767064275
Sb	0.0010678332	-0.2068552484	2.5992497522
P	2.2964434096	0.1031620555	0.1885420303
C	-1.9372069458	0.7377260127	2.8653267087
C	-2.8133651625	0.7542483149	1.7728627367
C	-4.0764877367	1.3450995646	1.9048568701
H	-4.7593340081	1.3620116258	1.0593238989
C	-4.455898636	1.9254099683	3.1111671466
H	-5.4323412156	2.392909666	3.201267396
C	-3.5826557204	1.9068911214	4.1957519028
H	-3.8737176751	2.3648660785	5.1371965051
C	-2.3316664081	1.3044435692	4.0789212001
H	-1.6565929318	1.2736656603	4.9258941645
C	-3.1109316246	1.0339674693	-1.0782637887
C	-2.5070075653	2.2504040436	-1.4192663295
H	-1.5572199821	2.5276151156	-0.9680044827
C	-3.1104176244	3.0964651938	-2.3429105862
H	-2.6345940515	4.0376679141	-2.60363086
C	-4.3147146637	2.7296584293	-2.9433832877
H	-4.7814377905	3.3877661827	-3.6710113958
C	-4.913898258	1.5166632534	-2.6157012548
H	-5.8495431948	1.2250248806	-3.084646109
C	-4.3162266645	0.6688014747	-1.6843616145
H	-4.7878094885	-0.2777110638	-1.4351400424
C	-3.1316423099	-1.6257425937	0.0953302989
C	-2.7962772811	-2.4634593817	-0.9782114902
H	-2.0698587644	-2.1286603509	-1.71625792
C	-3.3861569318	-3.7174377342	-1.0924340254
H	-3.125603825	-4.3601212572	-1.928885729
C	-4.299822467	-4.1522140083	-0.1323032134
H	-4.7538914056	-5.1354002668	-0.2197911374
C	-4.624891208	-3.3281122484	0.9415373871
H	-5.3318125753	-3.6651152852	1.6945722863
C	-4.0452262674	-2.0655571634	1.0574432733
H	-4.3044053499	-1.4292949675	1.8987784638
C	1.8974919411	0.8185200787	2.8709282804
C	2.7736908871	0.8770634955	1.7800285137
C	4.0102252557	1.5208252815	1.9164773573
H	4.6928740839	1.5701507124	1.0720612376
C	4.3628882301	2.1117501356	3.1256538408
H	5.318351245	2.6201336668	3.2191939878
C	3.4898096234	2.0511258522	4.2088925674
H	3.7598770158	2.5168094857	5.152814662
C	2.2659236647	1.3962585041	4.0876140698

H	1.5918531028	1.3325633849	4.9335442003
C	3.0621831453	1.18361841	-1.0693126222
C	2.4051698235	2.3745736628	-1.401950491
H	1.4448998439	2.6074609281	-0.9475431407
C	2.9701493412	3.2528019517	-2.3198770689
H	2.4531362351	4.1739364173	-2.5737622407
C	4.1892112392	2.9437606245	-2.9230203311
H	4.6260937849	3.6268271944	-3.6461500998
C	4.8416051091	1.7563597778	-2.6034374297
H	5.7892585028	1.5097376731	-3.0741028148
C	4.2824981631	0.8766391022	-1.6777449024
H	4.796137136	-0.0494047578	-1.4349758927
C	3.2067227484	-1.476473831	0.0938585586
C	2.9387883186	-2.3106283907	-1.0012923259
H	2.2198352988	-1.9960665643	-1.7553545138
C	3.5855646317	-3.5360053088	-1.1169517166
H	3.3771095279	-4.1756934714	-1.9701398286
C	4.4901208728	-3.9462207809	-0.1375072461
H	4.9891042647	-4.9072452807	-0.2265772387
C	4.7487759024	-3.1260339714	0.9571210434
H	5.4485447479	-3.4439446807	1.7249817883
C	4.1114286033	-1.8917296674	1.0750606206
H	4.318722403	-1.258533994	1.9329206758
C	0.0459920492	-2.3502693669	2.803492164
C	0.1069393666	-3.123223288	1.6405071964
H	0.1295065502	-2.6395289215	0.6645864881
C	0.1393609581	-4.5145306709	1.7215828985
H	0.1885659463	-5.1068564393	0.8117239144
C	0.1085050694	-5.1387402209	2.9664071962
H	0.1330038096	-6.2233060369	3.0318270086
C	0.0461876195	-4.3709269051	4.1279812062
H	0.0217664646	-4.8563024004	5.1002879661
C	0.0158923349	-2.9796778647	4.0518999614
H	-0.0297584542	-2.3808550168	4.9543189557
F	-0.0032001319	-0.1827759216	4.65093627

XYZ coordinates of the optimized structure of **[2]**BMe_4

97

Pd	-0.0079825606	-0.0008888095	-0.0076489502
P	-2.3189895997	0.2992239914	0.2187736551
Cl	0.0012058721	-0.0696400373	-2.3872483556
Sb	-0.0076925226	0.0094246172	2.4946502687
P	2.3156940387	0.1037192612	0.2512302872
C	-1.8313721509	1.0317670328	2.9131602735
C	-2.7207563416	1.1071360884	1.8265143921
C	-3.9400537665	1.7745494498	1.9915163255
H	-4.6309182222	1.8581890441	1.1569121014
C	-4.2712602956	2.336829427	3.2211648819
H	-5.2184573351	2.8551952174	3.3361142674

C	-3.396387226	2.2332779877	4.2996885513
H	-3.6579958209	2.6710914638	5.2583919175
C	-2.1766894085	1.5772340088	4.1504545039
H	-1.504444912	1.5065182472	5.0004916833
C	-3.232594422	-1.2755795559	0.1881139576
C	-2.8790043546	-2.1991868943	-0.8061005654
H	-2.0917514964	-1.9559342108	-1.5167332196
C	-3.5375855794	-3.4216770979	-0.882251166
H	-3.2643908833	-4.1321494547	-1.6570921177
C	-4.5372654822	-3.7365177651	0.0374476578
H	-5.0449165813	-4.6951390736	-0.0198661438
C	-4.8831400811	-2.8247687564	1.031571456
H	-5.6603821881	-3.0686182261	1.7500854332
C	-4.235854724	-1.5932579981	1.1095497525
H	-4.5145576195	-0.8876925339	1.8869322751
C	-3.0680942319	1.3809038464	-1.035499209
C	-2.4227927093	2.5863269405	-1.3401022957
H	-1.4814525962	2.8390120596	-0.8572680652
C	-2.9800233425	3.4553714337	-2.2703709011
H	-2.4766846474	4.3886475731	-2.5054868279
C	-4.1744571094	3.1221638668	-2.9096526553
H	-4.604305509	3.7996965281	-3.6418354179
C	-4.8118253825	1.9200507494	-2.6162241343
H	-5.739461388	1.6566766536	-3.1160846442
C	-4.2623854488	1.0463226026	-1.6796143551
H	-4.7624610087	0.108490166	-1.4551298691
C	1.8264159803	1.0239985624	2.8850646822
C	2.7321530838	1.0024159185	1.8078653522
C	3.9642516364	1.6513087823	1.9437845582
H	4.6677232774	1.6609167325	1.1156528417
C	4.2904721653	2.2964599099	3.1341440158
H	5.2474362213	2.8014504895	3.2252981815
C	3.3964367841	2.2969423811	4.20105877
H	3.6514549983	2.804123118	5.1267406205
C	2.164027047	1.6574737639	4.0813989511
H	1.4742181944	1.6740862632	4.9199911202
C	3.0960933944	-1.5361670447	0.3738593616
C	2.5629532598	-2.5667333443	-0.412511927
H	1.7056506184	-2.3731158873	-1.0535967054
C	3.1333893144	-3.8349841265	-0.3743514006
H	2.7190157547	-4.6297687992	-0.9877414687
C	4.2260466342	-4.0850616755	0.4540208249
H	4.6655438981	-5.0778618016	0.4872925165
C	4.7523562071	-3.0650375432	1.2434830015
H	5.6015484594	-3.2592294459	1.8923047641
C	4.1923274992	-1.7906106639	1.2054535803
H	4.6080460173	-1.0019504984	1.8261126391
C	3.1897774157	1.0213535005	-1.0518999652
C	4.3288295046	0.5087524442	-1.6780757387

H	4.7135673841	-0.4687605691	-1.402207506
C	4.9730904791	1.256387656	-2.6624542919
H	5.8578171873	0.8548066922	-3.1479035669
C	4.4844749861	2.5091080139	-3.0215629711
H	4.9879325973	3.0882121082	-3.7903914414
C	3.3438489225	3.0195819159	-2.4009608463
H	2.9551882235	3.99256659	-2.6871347769
C	2.6925871096	2.2771729619	-1.4236572372
H	1.7919676054	2.6674422128	-0.9559360513
C	0.0022977163	-1.7012735779	3.7429052302
C	1.1998640041	-2.1370787355	4.3171958275
H	2.1263277063	-1.5920456904	4.1555174567
C	1.2022993865	-3.2777015494	5.1165998731
H	2.1304813297	-3.6161445767	5.5678685614
C	0.0189889689	-3.979205774	5.3364592901
H	0.0252337723	-4.8688797839	5.9595865569
C	-1.173278575	-3.5434119782	4.7608316803
H	-2.0955368182	-4.0903689626	4.9339230914
C	-1.1871976616	-2.40409017	3.961058072
H	-2.1230566529	-2.0726306619	3.5174007258
B	0.9769926205	1.0515742152	8.4226142443
C	0.5715377728	2.13632439	9.5963738573
C	0.9178268842	-0.4817479383	9.0274319511
C	-0.0923399805	1.1778273215	7.165364428
C	2.4982252808	1.381754717	7.8730301806
H	1.1682729291	-1.2494657231	8.2739101175
H	-0.0813437842	-0.7514721278	9.4125101718
H	1.6168123141	-0.6395266631	9.8675226047
H	0.5877635306	3.1813215946	9.2397038595
H	1.2567765742	2.1011794226	10.4611592143
H	-0.440521042	1.9709084408	10.00519298
H	2.8330628126	0.69137416	7.0788393928
H	3.2633043117	1.324024204	8.6671595526
H	2.5809110737	2.3991452629	7.4491497598
H	0.1098356087	0.4290635936	6.3774844109
H	-0.0581232476	2.1721127864	6.6825438555
H	-1.142192883	1.020894614	7.4693408811

XYZ coordinates of the optimized structure of **3**

102

Pd	-0.0235812149	-0.048445498	0.0276795572
P	-2.3121740763	0.326796656	0.3776788565
Cl	-0.0796104434	-0.0206128126	-2.3541230525
Sb	0.0599295842	-0.0032836613	2.5392614238
P	2.3068187729	0.2399902448	0.1389975949
P	1.4374371117	-2.8679820599	2.800237429
C	-1.4599109536	1.496944694	2.795365719
C	-2.4230935333	1.5344086486	1.7683333256
C	-3.460199365	2.4706557232	1.8315825065

H	-4.2024689799	2.5163601971	1.0395251594
C	-3.5386783807	3.3587731848	2.9021520683
H	-4.3439932303	4.0865090215	2.937548181
C	-2.5885164859	3.3173728385	3.9178013045
H	-2.6449654943	4.0162481093	4.747263786
C	-1.5536513776	2.3837711161	3.8685862617
H	-0.8163145534	2.3698937659	4.6665238894
C	-3.1991418138	1.1066614522	-1.004675211
C	-2.726937655	2.3292058628	-1.5011622402
H	-1.8550235276	2.8016968196	-1.0554971108
C	-3.3698200553	2.939948053	-2.5707581525
H	-3.0020653494	3.8893156573	-2.9489986822
C	-4.4756699099	2.329400742	-3.1632885486
H	-4.9728837523	2.8060067592	-4.0032770234
C	-4.9377239456	1.1081709827	-2.68219691
H	-5.7955956651	0.6274925897	-3.1434182218
C	-4.3028370489	0.4939163121	-1.6040398138
H	-4.6702222471	-0.4583248811	-1.2333608214
C	-3.3007371477	-1.1161870989	0.8856806217
C	-2.8596831127	-2.3920642893	0.5155956674
H	-1.9302540533	-2.5084563177	-0.0370564049
C	-3.6084239225	-3.5147483583	0.8608870184
H	-3.2573045938	-4.5013439444	0.5741867431
C	-4.790421072	-3.3691717809	1.5829109443
H	-5.3705345266	-4.2458874084	1.8566623972
C	-5.2282782405	-2.1006102511	1.9613537394
H	-6.1472840494	-1.9866684095	2.5290358603
C	-4.4886129633	-0.9745272025	1.6144839401
H	-4.8348583469	0.0104959019	1.915738721
C	2.0086677149	0.7745421079	2.9140541726
C	2.8658496921	0.8100159238	1.8034309754
C	4.1653321267	1.3060006221	1.9635093603
H	4.836430759	1.3606718775	1.110230597
C	4.6053986215	1.7352100207	3.2122296994
H	5.6162504854	2.1159281623	3.3233916819
C	3.7542642425	1.6783742734	4.313400642
H	4.0982295366	2.0149201859	5.2870154839
C	2.4548615755	1.197093421	4.1674618137
H	1.8013552888	1.1565455292	5.0345920097
C	2.8647029124	1.5795717735	-0.9654167235
C	2.0961130838	2.7490443044	-1.0219249441
H	1.1686140133	2.8178216098	-0.4579274062
C	2.5112510549	3.8187301627	-1.8065732952
H	1.9105936982	4.7229092584	-1.8467877814
C	3.6888380712	3.7253531419	-2.5482483716
H	4.0079621319	4.5591486128	-3.1670639935
C	4.4517350737	2.5622054089	-2.4997250307
H	5.3678366389	2.4846609884	-3.0782388567
C	4.0450225174	1.4892043292	-1.7086525036

H	4.6455873477	0.5846671467	-1.6778639639
C	3.3049774152	-1.2211642148	-0.286930871
C	3.1125270961	-1.7876498823	-1.5564851603
H	2.3994237143	-1.343114602	-2.2468730661
C	3.8268443632	-2.9226379351	-1.9252364148
H	3.6787276243	-3.3527892595	-2.9116166668
C	4.7230312446	-3.5091651783	-1.0310430816
H	5.275888014	-4.3982385609	-1.3206002163
C	4.9057210048	-2.9563906195	0.233566175
H	5.5957912311	-3.4128037057	0.9374272154
C	4.200159781	-1.8138515002	0.6085084508
H	4.3484657789	-1.395629481	1.5989442981
C	-0.4101673929	-1.3493287207	4.1361704811
C	0.3210863538	-2.5436116401	4.2137328179
C	0.1490211306	-3.3706278441	5.3279720273
H	0.7343908939	-4.2820312732	5.4212776211
C	-0.7689244902	-3.0278589333	6.3182828671
H	-0.899725991	-3.6771322288	7.1792140957
C	-1.5232489285	-1.8615582122	6.2061515344
H	-2.2415663676	-1.6010689147	6.9780062774
C	-1.3463461031	-1.0133142437	5.1142949956
H	-1.9236063732	-0.0955245563	5.0447190076
C	2.9055641568	-3.6469336851	3.5683009281
C	3.2100315084	-5.0056610221	3.4388764727
H	2.544496953	-5.661954638	2.8851761384
C	4.3678462743	-5.5226729738	4.0180011301
H	4.5942738649	-6.5801760261	3.9126147251
C	5.2281303911	-4.6912450894	4.7301233418
H	6.1298047408	-5.0972438985	5.1800235838
C	4.9323375556	-3.3345363131	4.8606043218
H	5.6028386766	-2.6799960358	5.4106758836
C	3.7831180021	-2.8125566084	4.27665983
H	3.567465097	-1.7496982304	4.3708235782
C	0.63208937	-4.2097737567	1.8501941242
C	0.983679225	-4.3155448693	0.4969679377
H	1.6971413374	-3.6175691502	0.0651527026
C	0.4279486512	-5.3124810836	-0.3003760417
H	0.7125687	-5.3861288764	-1.3463294591
C	-0.4944830427	-6.2058464888	0.2412973022
H	-0.9315917344	-6.9815402035	-0.3813104599
C	-0.8572969264	-6.1001967667	1.5826960073
H	-1.5775522028	-6.7931690418	2.0090324326
C	-0.2981284346	-5.1081023168	2.3851772469
H	-0.5953637961	-5.034377952	3.4271098647

XYZ coordinates of the optimized structure of **3F**

103

Pd	0.0637530415	0.0141647828	-0.0751970863
P	2.0726192828	1.3354683136	0.0434485535

Cl	0.0711474242	-0.246288258	-2.5530264333
Sb	0.0529164535	0.1540792966	2.5207370698
P	-2.044971674	1.1488199889	0.0085958176
P	0.2348079969	-2.3341747548	0.2897557236
C	2.158837334	0.635937019	2.7679269377
C	2.8912573837	1.1258671427	1.6801057599
C	4.2194923237	1.5277351749	1.8773125288
H	4.7850349103	1.9494737996	1.050738871
C	4.8270264049	1.3863481473	3.1195188578
H	5.8621818666	1.6887604564	3.2516839069
C	4.1042619725	0.8630789279	4.1887851432
H	4.5742765102	0.745204275	5.1613574807
C	2.7693181081	0.5069826012	4.0200155945
H	2.1926250609	0.1372885295	4.859131988
C	3.3368635984	0.8949244143	-1.2043819137
C	3.1584323893	1.3626389713	-2.5150587215
H	2.3128642916	2.0009491748	-2.7536788589
C	4.0571846793	1.0167365149	-3.5183574195
H	3.9074786484	1.3945144257	-4.5260084332
C	5.1406290157	0.1868816026	-3.2332131574
H	5.8446500693	-0.0805561366	-4.0164347213
C	5.3110390237	-0.3020420244	-1.9412937302
H	6.1470364166	-0.9567159927	-1.710083877
C	4.4123681984	0.0431148489	-0.9330955249
H	4.555375872	-0.3581891841	0.0650615122
C	2.0277107418	3.1796233933	-0.052816089
C	0.9363290426	3.8400391915	0.5221426714
H	0.1143951357	3.2639568785	0.9377919558
C	0.887348328	5.2306583204	0.5665976935
H	0.0311210357	5.7234953679	1.019078542
C	1.9256184868	5.9823750756	0.0222282967
H	1.8856992087	7.0678793254	0.0469255371
C	3.0151386811	5.3355283983	-0.5573073141
H	3.8298992662	5.9144880518	-0.9839315733
C	3.071230037	3.9439656602	-0.5897937615
H	3.9295093342	3.4564532644	-1.0426142064
C	-1.4029406878	1.7590538227	2.6853323183
C	-2.2054496102	2.0938516745	1.5857273297
C	-3.1198099664	3.1480439105	1.7080819677
H	-3.7489242123	3.420136668	0.866272452
C	-3.2214777023	3.8684564888	2.893584292
H	-3.926662726	4.6919439428	2.9647479023
C	-2.4192257346	3.5329456225	3.980428456
H	-2.4896208527	4.0949896865	4.9076912148
C	-1.5200924848	2.4745462821	3.8812384511
H	-0.9032675242	2.1999461476	4.7283917224
C	-2.3778804954	2.3943647316	-1.2990513072
C	-1.2894168028	2.938565368	-1.9876460552
H	-0.2912614374	2.5688013885	-1.7776408943

C	-1.4834998606	3.9250326259	-2.9517292379
H	-0.6274706259	4.3365967187	-3.4795444478
C	-2.769401759	4.3684896597	-3.2484892663
H	-2.9219041005	5.1329972547	-4.0055137644
C	-3.86309144	3.8196949411	-2.5810000921
H	-4.8703233042	4.1539563256	-2.8145733116
C	-3.6705625603	2.8374162625	-1.6136451983
H	-4.5339787388	2.4070009229	-1.113471535
C	-3.5724109739	0.12925019	-0.010457735
C	-4.0788686086	-0.3321324174	-1.2344570151
H	-3.6074907936	-0.0297521101	-2.166287902
C	-5.1872958173	-1.1738209201	-1.2675187046
H	-5.5748591101	-1.5121086397	-2.2248341909
C	-5.7964842215	-1.5798459538	-0.0812830802
H	-6.6609551107	-2.2372632258	-0.1084319012
C	-5.2921842843	-1.1362418844	1.1388497045
H	-5.761649183	-1.4452531146	2.0688243153
C	-4.1885902038	-0.2859171439	1.1761014789
H	-3.8142211151	0.0597670785	2.1360135489
C	-0.6481907655	-1.8609284041	2.9014365895
C	-0.5443136985	-2.8128080271	1.8823727192
C	-1.0206543633	-4.1109485211	2.1035081733
H	-0.9369624802	-4.8579909428	1.3187147348
C	-1.6109888502	-4.4464554865	3.3180342014
H	-1.9906621485	-5.4525319937	3.4733483637
C	-1.7125774966	-3.4939198651	4.3288637282
H	-2.1771635311	-3.751106285	5.2769371529
C	-1.220762971	-2.2059715531	4.1284898157
H	-1.2828890561	-1.466391207	4.9179400095
C	-0.5916641547	-3.4498486368	-0.9082679349
C	-1.8731456158	-3.0971092681	-1.3441134198
H	-2.3147036662	-2.161194134	-1.0149679417
C	-2.5812439135	-3.9321285095	-2.2012696007
H	-3.576740637	-3.644300631	-2.5285992524
C	-2.010429127	-5.1235482065	-2.6470369507
H	-2.5593642885	-5.7717322673	-3.3247612969
C	-0.732079301	-5.4775142681	-2.2243131356
H	-0.2800649735	-6.4043460474	-2.5672308071
C	-0.0248808209	-4.6479725309	-1.3549246327
H	0.9691630154	-4.9386690314	-1.0286620905
C	1.9250183913	-3.0376856173	0.4090998027
C	2.7621720653	-2.9172628605	-0.708581379
H	2.4042179844	-2.4046232701	-1.5988717474
C	4.0474456861	-3.4489049224	-0.6836734207
H	4.6814851133	-3.3578102728	-1.560978636
C	4.5248019951	-4.0782471488	0.4654487886
H	5.5314924983	-4.4866893165	0.4853109867
C	3.7085377789	-4.1761344055	1.5889872973
H	4.0751816657	-4.659101381	2.4907745956

C 2.4112214968 -3.6654149607 1.5609814076
H 1.7793001155 -3.7632920307 2.4388873682
F 0.0440902012 0.2638647147 4.564769376

XYZ coordinates of the optimized structure of **3'**
102
Pd -0.0380486218 -0.0059139058 -0.1997610615
P 2.1039010006 1.3151951789 0.0802883197
Cl -0.1425492971 -0.1704304092 -2.5908477711
Sb -0.0261687063 0.0746492483 2.2529468522
P -2.0891354963 1.2742206366 0.0222093271
P 0.2091386399 -2.3827472454 0.1934669351
C 1.85437988 0.861890586 2.8735467795
C 2.6427037996 1.4060186967 1.8480127488
C 3.8280332597 2.0677158479 2.1971678132
H 4.4334816532 2.5343127896 1.4245852914
C 4.2366971349 2.1365399762 3.5247227935
H 5.1615142353 2.6472300059 3.7762980953
C 3.4643720142 1.5550777276 4.5283982935
H 3.7873551848 1.6034774912 5.5640740339
C 2.2653403024 0.9261530762 4.2080233337
H 1.6624599291 0.496239414 5.0032673593
C 3.5149506935 0.605561305 -0.8418355433
C 3.3766628591 0.5051723929 -2.2349403795
H 2.4454786698 0.7998140738 -2.7115381461
C 4.4198288976 0.0093195489 -3.0105429478
H 4.3038687401 -0.0494896792 -4.0892027141
C 5.6004592073 -0.4181530826 -2.4064614003
H 6.4143931573 -0.8059381909 -3.0126973033
C 5.7257018356 -0.3630089184 -1.0212399114
H 6.6339272124 -0.7153279359 -0.5402618693
C 4.6909838805 0.1461057821 -0.2394593924
H 4.8088368892 0.1758090961 0.8387070912
C 2.1150972405 3.1057455262 -0.3439718756
C 1.3485535419 3.9643268123 0.4582814955
H 0.7909055963 3.5718604508 1.3057371861
C 1.2950657838 5.3261429499 0.186129183
H 0.7024710901 5.9779832744 0.821832889
C 1.994049102 5.8504726064 -0.9009602341
H 1.9492260225 6.9141667872 -1.1165725648
C 2.7495411695 5.0042740461 -1.7064486499
H 3.3021422658 5.4038696788 -2.5522512519
C 2.8146552819 3.6382979835 -1.4304736952
H 3.4214007519 2.9969864366 -2.0617509206
C -1.5741845794 1.4363340118 2.8042300223
C -2.3218189885 1.9519851209 1.7321100953
C -3.2842228608 2.9317452442 2.0014205661
H -3.8667613636 3.3586667437 1.1914619934
C -3.5015887504 3.3742789924 3.3026204441

H	-4.2482092024	4.1402125732	3.4904087585
C	-2.7708925581	2.837313047	4.3592939002
H	-2.9449847867	3.1788134524	5.3752873567
C	-1.8030050822	1.8680193457	4.1128341761
H	-1.2331074762	1.4669347655	4.9452982697
C	-2.340555023	2.6725097676	-1.1263252024
C	-1.2285487403	3.2176456546	-1.7738846741
H	-0.2481973141	2.7820431946	-1.6143279976
C	-1.3787676615	4.3001505534	-2.6375165397
H	-0.5057586636	4.7148743583	-3.1331037342
C	-2.6414268491	4.8379399848	-2.8692471439
H	-2.7592152527	5.6792063498	-3.5465874517
C	-3.7589693427	4.2859431544	-2.2441089015
H	-4.7483922038	4.6923035618	-2.4339552968
C	-3.6133874773	3.2049219025	-1.3809046408
H	-4.4959666451	2.7650117177	-0.9245947621
C	-3.5962768008	0.2602606468	-0.2101020492
C	-4.02975454	-0.0221248403	-1.5133214011
H	-3.5055074027	0.4010693151	-2.365776984
C	-5.1342583566	-0.843360808	-1.7216026344
H	-5.467661782	-1.044883155	-2.7358061489
C	-5.8077299999	-1.4033839896	-0.6369706239
H	-6.6702465062	-2.0427556662	-0.8019615621
C	-5.371780095	-1.1388520058	0.6592401235
H	-5.8924998306	-1.5700670816	1.509589038
C	-4.2718378522	-0.3112596928	0.8747072865
H	-3.9496914956	-0.1076172017	1.8923182413
C	-0.3374080536	-1.916491714	2.932283695
C	-0.2623830971	-2.8793595444	1.9137529117
C	-0.5182774044	-4.2167967468	2.2362784283
H	-0.4792774402	-4.9781841749	1.4621250867
C	-0.8316885586	-4.5785115194	3.543526074
H	-1.0346385747	-5.619377234	3.7774922025
C	-0.886279445	-3.6148240463	4.5479301084
H	-1.1310549865	-3.9005983184	5.5665914896
C	-0.6391371231	-2.278026369	4.2461860936
H	-0.6937515588	-1.5328635332	5.0347107367
C	-0.7902974458	-3.4820965038	-0.868474594
C	-2.069640516	-3.0629518013	-1.2464057837
H	-2.4213758753	-2.0754221592	-0.9626263828
C	-2.8843567464	-3.9004579522	-2.001890157
H	-3.8754893689	-3.563304923	-2.2912564062
C	-2.4242240279	-5.155340168	-2.3959985483
H	-3.0585033096	-5.8047466596	-2.9929011149
C	-1.1459409463	-5.5726608078	-2.0324148879
H	-0.7799805077	-6.5475603264	-2.3420184974
C	-0.3284063311	-4.7413951956	-1.2705797253
H	0.669309314	-5.0730386861	-0.9977816263
C	1.9141945713	-3.0136334617	0.0085823269

C	2.5022726738	-2.921678435	-1.2610833134
H	1.9480766455	-2.4789621348	-2.0852772942
C	3.790648607	-3.3994579876	-1.4684263807
H	4.2359523174	-3.3283305517	-2.4560369844
C	4.5133225726	-3.9510792287	-0.4106507023
H	5.5214420443	-4.3210599867	-0.575264712
C	3.943810088	-4.0200566856	0.8570345995
H	4.5035889235	-4.4436328587	1.6862812639
C	2.6460903298	-3.5559896066	1.0695483964
H	2.2087237119	-3.6292144696	2.0608036094

XYZ coordinates of the optimized structure of **3F'**

103

Pd	0.0153963099	0.0211436968	-0.0014690496
P	2.2945726749	0.4282113807	0.059917876
Cl	-0.1240265198	-0.1556392182	-2.4622068633
Sb	0.0910526234	-0.0945957121	2.6031210904
P	-2.2604061312	0.3536495838	0.3100446774
P	1.5697534392	-3.0569731574	1.5715809368
C	2.1696519642	0.4933166933	2.8790352583
C	2.9708279448	0.6737564536	1.7476899351
C	4.2956704922	1.1040884461	1.9005008445
H	4.9184757471	1.2637860075	1.0237174394
C	4.8216006845	1.3334768324	3.1666616134
H	5.8501370827	1.6667718868	3.2722824374
C	4.0246538567	1.1378101811	4.2917889591
H	4.4294383922	1.3147340714	5.2845763001
C	2.7029582643	0.7218063583	4.1510509027
H	2.0759393365	0.5731881911	5.0212572357
C	3.4462520837	-0.7168713652	-0.7764426881
C	3.3425231584	-0.8664034656	-2.1669757629
H	2.5962959717	-0.3002567903	-2.7168042193
C	4.1792374828	-1.7498120846	-2.8415549194
H	4.0916896489	-1.8528730452	-3.9196017857
C	5.1223573122	-2.4985750265	-2.1397377869
H	5.7776733653	-3.18503933	-2.6687013201
C	5.2195298859	-2.3653352384	-0.7571551184
H	5.9511235556	-2.9464626546	-0.2020993432
C	4.3828870698	-1.4834217844	-0.0748847562
H	4.4655664093	-1.3961431102	1.0041341306
C	2.6102146626	2.0638312169	-0.7129991013
C	1.7079810324	3.0978438646	-0.4291704808
H	0.8372118026	2.8964161769	0.1915225289
C	1.9193285557	4.3769543816	-0.9332006174
H	1.2137298835	5.1705809944	-0.7029911139
C	3.0288327022	4.6359415992	-1.7368649124
H	3.1903582713	5.6327616476	-2.1376321179
C	3.9276509177	3.613024687	-2.0257355909
H	4.7942334487	3.8082547961	-2.6514800047

C	3.7244546441	2.3327087654	-1.5134713638
H	4.4340109654	1.5444806832	-1.7471039686
C	-1.5866816612	1.2610527106	2.8707457781
C	-2.5157706835	1.3600353515	1.8251041559
C	-3.6164267428	2.2160703834	1.9531820273
H	-4.3366873671	2.3010962124	1.1433675349
C	-3.7809519667	2.9781591549	3.1068373409
H	-4.6289502435	3.6520134661	3.1912925336
C	-2.8585627709	2.8765870269	4.1447619843
H	-2.981744382	3.4748052618	5.0435671061
C	-1.7722192105	2.0096617106	4.0340777078
H	-1.0637580899	1.9125125483	4.8489678818
C	-3.0369506173	1.3552470591	-1.0080740553
C	-2.398048304	2.5382936298	-1.4009804472
H	-1.4535947646	2.8223499661	-0.9436256693
C	-2.9567821448	3.3434649351	-2.3861523367
H	-2.4533227375	4.2592066291	-2.6833268111
C	-4.1515020512	2.9682358276	-3.0013934534
H	-4.5838014722	3.5944076007	-3.7769142703
C	-4.7832954618	1.7871266014	-2.6252649712
H	-5.7105866479	1.4863112359	-3.104962357
C	-4.2305241147	0.9812191126	-1.630043597
H	-4.7316762791	0.0614566838	-1.3433611654
C	-3.3306909071	-1.1160901313	0.4807319931
C	-2.9354220056	-2.2886507009	-0.1738017559
H	-2.0014801314	-2.3056414641	-0.7310838467
C	-3.7330143985	-3.4280912568	-0.1096436658
H	-3.4183724256	-4.3344150748	-0.6193277305
C	-4.9246869122	-3.4059775565	0.612065439
H	-5.5445938086	-4.2967332627	0.6649377004
C	-5.3181249667	-2.2436435748	1.2727344315
H	-6.2436732512	-2.2254602078	1.8415896213
C	-4.5249751919	-1.1010091478	1.2095558708
H	-4.8351084802	-0.2013905225	1.7342958662
C	-0.6501992163	-2.093857113	2.9520185963
C	-0.0386382166	-3.2446136982	2.4412702134
C	-0.6465971208	-4.4895005531	2.6529781985
H	-0.1809281175	-5.3886129045	2.2579035124
C	-1.8409350072	-4.5860839372	3.3571227952
H	-2.3050568696	-5.5573263277	3.5059482166
C	-2.4361320425	-3.4374854537	3.8770317497
H	-3.3667755719	-3.5076403967	4.4336334614
C	-1.8405051782	-2.195647228	3.6802647656
H	-2.3061744007	-1.3059680919	4.0957735958
C	1.4356617849	-4.262073903	0.1912081537
C	1.0031035648	-3.7586347761	-1.0430885389
H	0.8084979671	-2.6939286624	-1.157904587
C	0.8248834221	-4.6097367021	-2.1316337448
H	0.4868183226	-4.2028254781	-3.0810256607

C	1.0926854474	-5.9709873913	-2.0054876408
H	0.9612842887	-6.6342302945	-2.8562528686
C	1.5384835996	-6.4787349096	-0.786515192
H	1.753629073	-7.539158219	-0.6834142113
C	1.7079454396	-5.6315355433	0.306052707
H	2.0629041902	-6.0388261563	1.2492187514
C	2.740335061	-3.8520959562	2.7453381456
C	3.9835002941	-4.3091084026	2.2814505207
H	4.2034939287	-4.2921614225	1.2170821891
C	4.9376627425	-4.7987565946	3.1683743302
H	5.8896809876	-5.1592283341	2.7872473192
C	4.6755692192	-4.8269128556	4.5368744489
H	5.4214391491	-5.2076109831	5.2292062683
C	3.4511051258	-4.3626587205	5.0100064654
H	3.2359975424	-4.3789029787	6.0752536459
C	2.4906112585	-3.8789096042	4.1238171248
H	1.5398992851	-3.523014147	4.5113519996
F	0.0844912482	-0.0557290823	4.6699171479

XYZ coordinates of the optimized structure of **3Cl**

103

Pd	0.0712130536	0.0815902983	-0.139905718
P	2.0721800068	1.3915355192	-0.0034998002
Cl	0.0383771447	-0.0728410973	-2.6036768718
Sb	0.0894082952	0.1640702872	2.4393250125
P	-2.0859943193	1.1005772883	0.0625187258
P	0.2712099773	-2.2849908456	0.2235073701
C	2.2494263031	0.4358667668	2.6547302194
C	2.9366645141	1.022666279	1.5815096696
C	4.2957407078	1.328590245	1.7353827756
H	4.829704889	1.8239120341	0.9294179471
C	4.9799463143	0.9833838384	2.8945891998
H	6.0373994577	1.2141671047	2.9875065822
C	4.3062734092	0.3326078026	3.9233371144
H	4.8352344235	0.0338975117	4.8239989605
C	2.9418171259	0.0789510766	3.8135238399
H	2.4158889975	-0.3855081045	4.6381345342
C	3.2815455334	1.0002352311	-1.3208814815
C	3.0966642484	1.5942655187	-2.5776836288
H	2.2888075874	2.3039265697	-2.730755491
C	3.943228936	1.2854704146	-3.6371999203
H	3.7904772492	1.7618074706	-4.6016630988
C	4.9768394777	0.3663955725	-3.4642472597
H	5.6389890026	0.1268775693	-4.2916825443
C	5.1525971435	-0.2459361663	-2.2263246377
H	5.9528735814	-0.9669481617	-2.0818554403
C	4.308752226	0.0644559826	-1.161398725
H	4.4576234358	-0.4285129891	-0.2063733054
C	2.0662006049	3.235875682	-0.0057941584

C	0.9381287047	3.9040694661	0.4793196098
H	0.0657618244	3.3354464123	0.7853118567
C	0.920160959	5.2937906098	0.5748119932
H	0.0340906141	5.7939172799	0.9560655608
C	2.0288644045	6.0338252881	0.1744649589
H	2.0150005558	7.1181881421	0.2412081106
C	3.1566827486	5.3783628528	-0.3175850532
H	4.0249398348	5.9496136883	-0.6348414661
C	3.178808614	3.9894338306	-0.4046986263
H	4.0627268866	3.4950529424	-0.7972424058
C	-1.2296579703	1.8848867989	2.6423741836
C	-2.1275664907	2.1327985585	1.5921260119
C	-3.0022690424	3.2220708724	1.6921591733
H	-3.7098966815	3.4191358944	0.8923809118
C	-2.9540521824	4.0772791728	2.7880822427
H	-3.6284528502	4.9274189742	2.8391691655
C	-2.0316165519	3.8477287865	3.803856099
H	-1.9691744728	4.5234685403	4.6521966837
C	-1.1828167859	2.7451510759	3.7403695005
H	-0.4858687357	2.5567577275	4.5479835357
C	-2.5624454234	2.2812244785	-1.2581016479
C	-1.5448027376	2.9350284222	-1.9611009944
H	-0.5093914327	2.6784728482	-1.7608658944
C	-1.8558350158	3.8886277784	-2.9269427375
H	-1.0555908352	4.3879438541	-3.4663933776
C	-3.1859910997	4.1871747395	-3.2124356384
H	-3.428178827	4.9248327568	-3.9726184592
C	-4.2063007071	3.5301770271	-2.5276741342
H	-5.246240769	3.7544918403	-2.7488892609
C	-3.8984328123	2.5830102762	-1.5543664038
H	-4.7034300257	2.0752883839	-1.0301442879
C	-3.5601275627	0.0226347189	0.2195533178
C	-4.0676657691	-0.6056141852	-0.9273961745
H	-3.6402877889	-0.3836681058	-1.9027968185
C	-5.1282232331	-1.5004929742	-0.830483185
H	-5.516124141	-1.9727031264	-1.7289874439
C	-5.6899828996	-1.7899026428	0.4125093162
H	-6.5166813686	-2.4907481112	0.4874963089
C	-5.1895829551	-1.1732789533	1.5559825449
H	-5.6243031798	-1.3894435194	2.5280462713
C	-4.1324602012	-0.269546813	1.4622928999
H	-3.7604180942	0.2109481635	2.362862041
C	-0.8807939053	-1.7649065248	2.7275536516
C	-0.7364685811	-2.7080325741	1.7006350778
C	-1.3833960681	-3.943836003	1.8129003698
H	-1.2633975156	-4.68643017	1.0291882947
C	-2.1960622783	-4.22025776	2.9082433467
H	-2.7077001675	-5.1764597189	2.972612512
C	-2.3549948482	-3.2689380777	3.9105221195

H	-3.0004944143	-3.4704592182	4.7608973485
C	-1.6865049427	-2.0487223648	3.8303520762
H	-1.7977196269	-1.3209686184	4.6251011655
C	-0.3688207927	-3.4192902449	-1.0641919093
C	-1.5143129526	-3.0320745553	-1.7671599041
H	-1.9494601124	-2.0566093387	-1.5794239982
C	-2.0842173252	-3.8835398186	-2.7082914075
H	-2.975174129	-3.5713160634	-3.2464836412
C	-1.5046028288	-5.1234966669	-2.9708287584
H	-1.9434326857	-5.7841296862	-3.7136037566
C	-0.3576977271	-5.51169964	-2.2825519242
H	0.0992975039	-6.477108135	-2.4822687389
C	0.2078356044	-4.6667499258	-1.3294661971
H	1.0983329598	-4.9830884333	-0.7943636014
C	1.9197106117	-2.9896783965	0.613819443
C	2.9122922647	-2.924210953	-0.3737737943
H	2.6917534582	-2.4681250618	-1.3361830099
C	4.1805118426	-3.4417221768	-0.1315325527
H	4.9372891016	-3.3945584869	-0.9099870376
C	4.4818885954	-4.0103111332	1.1059368053
H	5.474766831	-4.4086623946	1.2954659955
C	3.5060579126	-4.0642108703	2.0968327093
H	3.7327198687	-4.5042757204	3.0641169442
C	2.2281512207	-3.5621559714	1.8523323668
H	1.4725870061	-3.6234018619	2.6303831576
Cl	0.09755029	0.2144440961	5.1576286891

XYZ coordinates of the optimized structure of **3Cl'**

103

Pd	-0.0569237076	-0.0110732875	-0.0234098969
P	2.2302832977	0.3655174319	-0.0282223237
Cl	-0.3129127586	-0.215209646	-2.4480028535
Sb	0.1183915532	-0.2152554149	2.526411114
P	-2.303920458	0.3980083082	0.4002940933
P	1.6439332258	-3.1034754397	1.6488674059
C	2.1430655532	0.5391748362	2.8093353911
C	2.8962864287	0.7350932247	1.6432247294
C	4.1778299409	1.292865045	1.74351245
H	4.76261096	1.4628524015	0.8429572026
C	4.7056859612	1.645297827	2.9801151039
H	5.6998297589	2.0787629626	3.039948291
C	3.950445111	1.4474838724	4.1314238115
H	4.3492576439	1.7258487215	5.1029029006
C	2.6742247377	0.8952775278	4.0484896159
H	2.0910020407	0.7322969183	4.9474500299
C	3.3834129699	-0.827023548	-0.7884780803
C	3.1920537898	-1.1475625885	-2.1400664531
H	2.366483209	-0.7020885229	-2.6894584158
C	4.0475737585	-2.0430128007	-2.7735113728

H	3.8934092898	-2.2812294676	-3.822203774
C	5.093389399	-2.6341437216	-2.066543833
H	5.762274383	-3.331112336	-2.5636944133
C	5.2766671773	-2.3312468247	-0.7197300646
H	6.0895261673	-2.7893196224	-0.1625229213
C	4.4241892181	-1.43378648	-0.0784541405
H	4.5755808239	-1.2099863793	0.9730876258
C	2.5391040497	1.9399271288	-0.91807036
C	1.656282057	3.0027921433	-0.6867222374
H	0.7992782256	2.8590583514	-0.0324340132
C	1.8671289794	4.2371249362	-1.2913191558
H	1.1766817678	5.0545937766	-1.102880147
C	2.9556137346	4.4205155008	-2.1433080896
H	3.1162039916	5.382525607	-2.6218568298
C	3.8331859013	3.3668776626	-2.382110718
H	4.6821827405	3.5029515303	-3.0462969774
C	3.6306501248	2.1307817519	-1.7704250496
H	4.3223556647	1.3167691885	-1.9659462147
C	-1.5060489081	1.135650735	2.9975785863
C	-2.4880235451	1.2801361626	2.0022446213
C	-3.581721469	2.1244207271	2.2326957349
H	-4.3419956302	2.2497765552	1.4662795215
C	-3.6838908969	2.8356212335	3.4245002506
H	-4.5296324532	3.4978872625	3.5859784247
C	-2.6965011693	2.7063400056	4.3967697239
H	-2.7633888467	3.2723003472	5.3216960244
C	-1.6169588917	1.8493480195	4.190313576
H	-0.8653918937	1.7268734419	4.9625167703
C	-3.0122850291	1.5603538413	-0.8183631689
C	-2.5518825353	2.8833598574	-0.8425368429
H	-1.8212024882	3.221011905	-0.1117779776
C	-3.0349942591	3.7753600273	-1.7930882357
H	-2.6775555644	4.8012698567	-1.7991700532
C	-3.9733721086	3.3536658864	-2.7350593528
H	-4.3483207679	4.0511331222	-3.4787827186
C	-4.4275399449	2.0382096057	-2.7200736207
H	-5.1572160539	1.7033524284	-3.4519147492
C	-3.9494043904	1.1412733387	-1.7662902622
H	-4.3062177516	0.1155221494	-1.7653620716
C	-3.4353158448	-1.0321115661	0.4211318038
C	-3.0686659137	-2.1602103974	-0.3219469829
H	-2.1247011639	-2.165304204	-0.8621016125
C	-3.9116734566	-3.2675050188	-0.3703934529
H	-3.6213211946	-4.1399876699	-0.9487844466
C	-5.1168566603	-3.257495984	0.3278605406
H	-5.7712206573	-4.1241839095	0.2947103514
C	-5.4822043421	-2.1380992584	1.0743097803
H	-6.4192870859	-2.1305127558	1.6240164748
C	-4.6465886608	-1.0261619796	1.121519596

H	-4.9360338848	-0.1619694384	1.7127826668
C	-0.6871848097	-2.1928221594	2.8454073049
C	-0.0183341541	-3.3299964661	2.3868661861
C	-0.6389831375	-4.5802737771	2.5189546002
H	-0.1286488965	-5.4713159078	2.161913979
C	-1.9000497969	-4.6862463818	3.0923298209
H	-2.3735102786	-5.6598275652	3.1842262502
C	-2.5544319693	-3.5431090583	3.5524251778
H	-3.5406565153	-3.6211303116	4.0014940591
C	-1.9494392806	-2.2961136279	3.4351935431
H	-2.459167191	-1.4132584302	3.8106197764
C	1.6120916667	-4.3033622532	0.2590757258
C	1.0774527895	-3.8470318608	-0.9535144819
H	0.7523731	-2.8124383338	-1.0491532819
C	0.9614375302	-4.7070385753	-2.0424142392
H	0.5428570225	-4.3387010089	-2.975345916
C	1.3930141401	-6.028052359	-1.9389453575
H	1.3097720533	-6.6973626351	-2.7909734087
C	1.9369143805	-6.4865842934	-0.741123776
H	2.2758410276	-7.5156375336	-0.6545179077
C	2.0438013957	-5.6316458132	0.3539899653
H	2.4677733197	-6.0011348287	1.2838156934
C	2.7603776867	-3.864857542	2.8907175869
C	4.0814153602	-4.1666137468	2.5258630837
H	4.4015329607	-4.0390324757	1.4946470907
C	4.987536762	-4.640177936	3.4697798308
H	6.0033036927	-4.8798616395	3.1663584517
C	4.5961020059	-4.803802188	4.797530892
H	5.3050243818	-5.1699407534	5.5350320121
C	3.292261992	-4.4920247002	5.1728793089
H	2.9777435901	-4.6118754095	6.2061778148
C	2.3790782042	-4.0259967629	4.2285409375
H	1.3664849568	-3.7848980429	4.5388195646
Cl	0.1855117146	-0.6045867272	5.396051612

XYZ coordinates of the optimized structure of **3Br**

103

Pd	0.0643464723	0.0950620844	-0.1487606478
P	2.0737834684	1.3890723999	-0.0212971384
Cl	0.0013706086	-0.0237935758	-2.6135062357
Sb	0.096355507	0.160494612	2.4303811901
P	-2.0914971425	1.1043079643	0.0755541208
P	0.2690159945	-2.2789115405	0.2068571
C	2.2658434191	0.4100853177	2.6274853878
C	2.9478605364	1.0000845425	1.5528369279
C	4.3111946149	1.2919625011	1.6968715624
H	4.841704231	1.7902435365	0.8904479487
C	5.0038362926	0.928322777	2.8453750693
H	6.0642221379	1.148499944	2.9302146735

C	4.3339815282	0.272651689	3.8733373366
H	4.8681986553	-0.0425141918	4.7652839372
C	2.9663935844	0.03306718	3.7738141923
H	2.4434797249	-0.4282402473	4.6020400515
C	3.2705757704	1.0010949865	-1.3512659326
C	3.0822479617	1.6087681559	-2.6010014779
H	2.2808703823	2.3283992493	-2.7411596528
C	3.9172556592	1.3006902951	-3.6699360905
H	3.7622823307	1.7877483664	-4.6286766328
C	4.9416548301	0.3683988102	-3.5139692765
H	5.5943178745	0.129131395	-4.3489783177
C	5.12043762	-0.2574425966	-2.2831753574
H	5.9134633426	-0.9889929599	-2.1518529734
C	4.2888079745	0.0527812549	-1.208716053
H	4.4400765829	-0.4499699268	-0.2591966878
C	2.0770956225	3.2331241162	-0.0086737705
C	0.9545592352	3.9034240935	0.486324334
H	0.0804789497	3.3370744405	0.7916624297
C	0.9444315978	5.2924768262	0.5926110108
H	0.0626367265	5.7942738027	0.9815070237
C	2.0554116476	6.029704596	0.193457023
H	2.0475952445	7.1135739343	0.2686538632
C	3.1777620626	5.3721470861	-0.3082654318
H	4.0477323564	5.9412502817	-0.624678748
C	3.1920815168	3.9838834368	-0.4062544002
H	4.0716913702	3.4879069177	-0.806396101
C	-1.2107848107	1.8915660829	2.6442729967
C	-2.117885486	2.1397837803	1.6023016274
C	-2.9863135823	3.2335999037	1.7073924423
H	-3.7016711866	3.4302873211	0.9143031677
C	-2.9213557117	4.0932397704	2.799139017
H	-3.5905851853	4.9472138385	2.8540889811
C	-1.9888769188	3.8629337753	3.8055729879
H	-1.9122801108	4.5421519713	4.6499983941
C	-1.1473276721	2.7551818228	3.7377025032
H	-0.4486122345	2.561580182	4.5426886163
C	-2.5893379254	2.2820328723	-1.2395676359
C	-1.5845050694	2.9604091059	-1.9378661475
H	-0.5440788306	2.7234737239	-1.7392481696
C	-1.9143199151	3.9135636161	-2.8977163444
H	-1.124102105	4.4320922137	-3.4338263064
C	-3.2502269189	4.1871592245	-3.18209241
H	-3.5067723036	4.9244043665	-3.937952027
C	-4.2573170459	3.5059805013	-2.5016516001
H	-5.3014890478	3.7110463503	-2.7216081433
C	-3.9308493533	2.5592772873	-1.5337369658
H	-4.7254881097	2.0334069912	-1.011666091
C	-3.5568824276	0.0178916402	0.2481966063
C	-4.0463864255	-0.639995557	-0.8899854921

H	-3.6083214208	-0.4373774638	-1.8648375548
C	-5.1028730123	-1.5384513008	-0.7853509479
H	-5.477035733	-2.0339878083	-1.677078126
C	-5.6783630322	-1.8016378897	0.4574213668
H	-6.5021030197	-2.5052688435	0.5387856895
C	-5.1951590366	-1.1561473324	1.5920834429
H	-5.6401023918	-1.3528688571	2.563653184
C	-4.1416223217	-0.2488649294	1.4905437162
H	-3.781315913	0.2527666876	2.3842984777
C	-0.9123102654	-1.7559826044	2.6933276767
C	-0.772792817	-2.6945934883	1.6616443966
C	-1.4495909836	-3.9157216541	1.7547390834
H	-1.3326787989	-4.6561554762	0.9685628211
C	-2.2873007665	-4.1801377628	2.8344098917
H	-2.8218810906	-5.1246263547	2.883514552
C	-2.4412772199	-3.2318872385	3.8401552112
H	-3.1065293847	-3.4224691228	4.6777649519
C	-1.7430001807	-2.0274810711	3.779453091
H	-1.8455161627	-1.3051472983	4.5803454691
C	-0.3284713919	-3.426461294	-1.0895056184
C	-1.445919125	-3.0449823623	-1.8395352999
H	-1.8842552696	-2.0658931704	-1.6807465276
C	-1.9823224058	-3.9064675513	-2.7914941429
H	-2.8508925113	-3.5983397827	-3.3672752899
C	-1.3971767684	-5.1509266523	-3.0168154395
H	-1.8097189853	-5.8194090337	-3.7675873186
C	-0.2781526336	-5.5338941074	-2.2810778948
H	0.182767513	-6.5030375572	-2.4515428388
C	0.25391209	-4.6788438609	-1.3180364282
H	1.122955615	-4.9906687317	-0.7462805199
C	1.9092756943	-2.972609388	0.6491421116
C	2.9246892348	-2.9243370834	-0.315890387
H	2.7248012621	-2.491072412	-1.2931824618
C	4.1894373408	-3.4291112719	-0.0322880895
H	4.9642647449	-3.3951016873	-0.7935735727
C	4.4639765828	-3.9688805312	1.2242711421
H	5.4540520523	-4.3573239555	1.446215358
C	3.4647396768	-4.0070069945	2.1922031033
H	3.6700716499	-4.425115064	3.1738792566
C	2.1905426914	-3.5173091167	1.9064607192
H	1.4174954699	-3.564925811	2.6681593199
Br	0.1134731094	0.1838948887	5.3093801623

XYZ coordinates of the optimized structure of **3Br'**

103

Pd	-0.1064611024	0.3132865253	-0.3780674326
P	2.215925932	0.5032033323	-0.1866583672
Cl	-0.1784231302	0.9245387612	-2.6938408042
Sb	-0.047686365	-0.3921719751	2.0407439806

P	-2.3854957118	0.6110929952	0.0631370468
P	1.5716917936	-3.1746712928	1.6400393212
C	1.9053993807	0.2537169977	2.6284912243
C	2.755810131	0.6126343077	1.5696299923
C	4.0400445083	1.0860180187	1.8629464313
H	4.7025698064	1.3923111752	1.0572870234
C	4.4737255272	1.1758279427	3.1830410089
H	5.4730515389	1.5443467903	3.3957653271
C	3.6290717476	0.7951073572	4.2213833137
H	3.9640890339	0.8597673064	5.2528603603
C	2.341833345	0.333675179	3.9495654521
H	1.6899788501	0.0264978158	4.766888618
C	3.2299368389	-0.7792350229	-0.9891669973
C	2.9881467939	-1.0362196467	-2.3464559525
H	2.2124961924	-0.4838346995	-2.8723999392
C	3.7399768843	-1.9954290162	-3.0167226705
H	3.5522300079	-2.1852908763	-4.0697347616
C	4.7270245518	-2.7109854774	-2.339938044
H	5.3129621775	-3.4598519778	-2.865306296
C	4.9593884251	-2.4666515903	-0.9888876719
H	5.726366518	-3.0226109185	-0.4568606572
C	4.2132238516	-1.5047438072	-0.3097807522
H	4.4000104155	-1.3259841247	0.7448489744
C	2.7755004703	2.0946893564	-0.8858365179
C	2.0464442834	3.2457227141	-0.5594368208
H	1.1548203154	3.1674684154	0.058807325
C	2.4554403403	4.4881177949	-1.0294270602
H	1.8858547223	5.3763269419	-0.7710877126
C	3.5878857803	4.5910990311	-1.837586373
H	3.9029177877	5.5618319331	-2.2098445845
C	4.3108412792	3.4493594866	-2.1696609716
H	5.1923512659	3.5247018474	-2.8000654575
C	3.9099161488	2.2014772835	-1.6944657902
H	4.4800516402	1.3158144159	-1.9591283941
C	-1.598983316	0.9175707737	2.7415385738
C	-2.5290051651	1.3105095876	1.7602062471
C	-3.5759431292	2.1693911503	2.1100392486
H	-4.2950586547	2.4875503047	1.3600139639
C	-3.6944515551	2.626654568	3.4211776423
H	-4.5048047388	3.3013109046	3.6820842315
C	-2.7881749331	2.212601258	4.3931150852
H	-2.8895153962	2.5597621587	5.4175288784
C	-1.7426884817	1.3514523909	4.0592253684
H	-1.0654230162	0.993519425	4.8329669211
C	-3.247350722	1.7903329734	-1.0207730083
C	-2.7518036205	3.0977541636	-1.1140242061
H	-1.8788004195	3.3941129008	-0.537804301
C	-3.3721412581	4.0190723317	-1.9488283001
H	-2.9856090071	5.0320339836	-2.0142628708

C	-4.4803052967	3.6402657851	-2.7072520024
H	-4.9602575784	4.3606482359	-3.3635796778
C	-4.9668721893	2.3390148195	-2.6268835301
H	-5.8270138873	2.0391579916	-3.2186145382
C	-4.3537727324	1.4119267012	-1.7855814542
H	-4.739398124	0.3984054588	-1.7269913525
C	-3.3695345748	-0.9221128658	0.0683942157
C	-2.9037166335	-2.0051317069	-0.6864631532
H	-1.9762113462	-1.9127332436	-1.247054142
C	-3.6228594312	-3.1969592292	-0.714782415
H	-3.2551821221	-4.0346308242	-1.3003535089
C	-4.803157993	-3.3145765885	0.0156878392
H	-5.3600460452	-4.2471554731	0.0000941164
C	-5.2680346982	-2.2401750383	0.7728034626
H	-6.1855093326	-2.3334382908	1.3467619977
C	-4.5557220876	-1.045066791	0.8016748326
H	-4.9186357678	-0.2151977064	1.4021646826
C	-0.7347903303	-2.25992233	2.8247648268
C	0.0184398571	-3.4134449014	2.5824677406
C	-0.452845478	-4.6416109622	3.0567090908
H	0.1195308281	-5.5475743848	2.8776801497
C	-1.6584277226	-4.709416642	3.7477617545
H	-2.0207102034	-5.6683417442	4.1075188816
C	-2.401432377	-3.5526872165	3.9798549322
H	-3.3400873457	-3.6067436924	4.5236459134
C	-1.9401171903	-2.3206089205	3.525785478
H	-2.5141404184	-1.4218769174	3.7292794274
C	1.5443469448	-4.5221892441	0.4007569083
C	1.1108627263	-4.1824320913	-0.887174092
H	0.8644960169	-3.1477672903	-1.1160646235
C	1.0023735938	-5.1565057687	-1.876821108
H	0.6653484374	-4.879827951	-2.8720998414
C	1.3380330052	-6.4778518209	-1.5919509801
H	1.2600026693	-7.2380508452	-2.3643590744
C	1.782581504	-6.8232746256	-0.3165860795
H	2.0496780761	-7.8525350515	-0.0926985176
C	1.8853229229	-5.8528645858	0.6763177225
H	2.2423867345	-6.1314557107	1.6642641044
C	2.8666698927	-3.6365437022	2.8494514814
C	4.0966330349	-4.1512623461	2.4153679815
H	4.2499642226	-4.3812809867	1.3641872629
C	5.124554909	-4.3865930853	3.3244377173
H	6.0674403909	-4.7978855017	2.9736922147
C	4.9444622306	-4.0997611689	4.6758072264
H	5.7463280475	-4.2854939045	5.3850918333
C	3.7319098206	-3.5707457986	5.1118486312
H	3.5828238215	-3.3368936349	6.1626690325
C	2.6985132787	-3.3338915533	4.2087641534
H	1.7672870212	-2.9068837221	4.5766684239

Br 0.0442323568 -0.9927553075 6.4071372109

XYZ coordinates of the optimized structure of **3CN**

104

Pd 0.0705255994 0.0732151131 -0.1168278028
P 2.0794635495 1.366923268 0.0024115412
Cl 0.0396787714 -0.0981924663 -2.5981527208
Sb 0.0846655004 0.1665331788 2.4871587823
P -2.0711928307 1.1229786432 0.0552150713
P 0.2547762923 -2.2907738967 0.2302110413
C 2.2364511954 0.5167761845 2.68970873
C 2.937958959 1.0555431789 1.6032110243
C 4.2883032268 1.3924624455 1.7664091845
H 4.8326510075 1.8501165671 0.9450613069
C 4.9489966288 1.1345420107 2.9619468111
H 6.0002486011 1.3885740794 3.0644481356
C 4.2587217225 0.5504141836 4.0196097659
H 4.7679718231 0.3305494506 4.9537169319
C 2.9029909527 0.2617893061 3.8900608591
H 2.3695993856 -0.1559518389 4.7370350815
C 3.3042035768 0.9528519909 -1.2934201971
C 3.1311107902 1.511589138 -2.5681372679
H 2.3198077225 2.2103435055 -2.7500573822
C 3.9931672126 1.1807829647 -3.6083452948
H 3.8490905989 1.6295775844 -4.5872714544
C 5.0313099128 0.2746915772 -3.3977254961
H 5.7055615865 0.0180344325 -4.2101551634
C 5.1956085242 -0.3030629346 -2.1418483734
H 5.9985606119 -1.0145909702 -1.9682025577
C 4.3358288941 0.0290442609 -1.0963531652
H 4.474702008 -0.4387688616 -0.1271718718
C 2.0671385031 3.2122761359 -0.0314308244
C 0.9531261485 3.878889163 0.488217824
H 0.0959019464 3.3077211412 0.8316128858
C 0.9285277625 5.269176589 0.5692893002
H 0.0536602492 5.7676226243 0.9777937198
C 2.0158248283 6.0124966971 0.1185424032
H 1.9962422923 7.0974770023 0.172860325
C 3.129187435 5.3589342813 -0.4071456377
H 3.9811339516 5.9322882986 -0.7626709867
C 3.1588995858 3.9688229441 -0.4780357686
H 4.0329984207 3.4757909573 -0.8935261975
C -1.290876302 1.8486058769 2.6686338627
C -2.1519621877 2.131910809 1.5987300515
C -3.0386502156 3.2100481624 1.7085148751
H -3.7168689641 3.4366269325 0.8913031923
C -3.0456748571 4.0140545801 2.8441153658
H -3.7289389747 4.8565344851 2.9041728137
C -2.1733598001 3.7397701106 3.8925771683

H	-2.1611932265	4.3707301814	4.7768412734
C	-1.3089313584	2.6506541642	3.8109619036
H	-0.6479163405	2.4354342093	4.6439787191
C	-2.5180485301	2.3199482879	-1.2621499274
C	-1.4837886676	2.9492078785	-1.9629721217
H	-0.4557280392	2.6656156536	-1.7615974433
C	-1.7689787186	3.9118060422	-2.9280647178
H	-0.9554166551	4.3911272199	-3.4657576255
C	-3.0905424736	4.2446280985	-3.2147898811
H	-3.3129849567	4.9894718029	-3.9740497935
C	-4.1281837647	3.6120244347	-2.5328634636
H	-5.1618203573	3.8623836191	-2.755806104
C	-3.845594701	2.6552821288	-1.5613822692
H	-4.6642480864	2.1646619098	-1.0419345307
C	-3.5597403054	0.055997801	0.1708093623
C	-4.0705694086	-0.5307761176	-0.9963558343
H	-3.6363617845	-0.284828339	-1.9628734404
C	-5.140662657	-1.4175051539	-0.9308146903
H	-5.5300201696	-1.8572873883	-1.8450716761
C	-5.7100649893	-1.7399236354	0.3002700761
H	-6.544827364	-2.4333862893	0.3505896803
C	-5.2061804608	-1.1654952878	1.4642625436
H	-5.6464574569	-1.4073971943	2.4277700676
C	-4.138640208	-0.2714304188	1.4021537004
H	-3.7642936838	0.1758221511	2.3188332081
C	-0.8182127382	-1.7979438309	2.7684735501
C	-0.6996463819	-2.7363478683	1.7361797514
C	-1.3130964142	-3.9863311134	1.8748592974
H	-1.213729045	-4.7260899279	1.0855044677
C	-2.0634756755	-4.2834338329	3.0090362601
H	-2.5501822071	-5.2508710678	3.0954361869
C	-2.1887742811	-3.3415009519	4.0252477058
H	-2.7814425597	-3.5626304592	4.908557874
C	-1.5535393249	-2.1061281235	3.9131574273
H	-1.6424355646	-1.3879255229	4.7218433026
C	-0.4266027355	-3.4177709899	-1.0439622736
C	-1.5835578233	-3.0168001233	-1.7195091876
H	-2.0001662239	-2.0347916878	-1.5237239455
C	-2.1883962222	-3.8619104462	-2.6445031833
H	-3.088227652	-3.5380327124	-3.1607009645
C	-1.6327840009	-5.1102626806	-2.9186127429
H	-2.0989212992	-5.7662929563	-3.6487736306
C	-0.4745518004	-5.5127833229	-2.2579515069
H	-0.0358572851	-6.4847706197	-2.4667723858
C	0.1258282103	-4.6737170884	-1.3210864822
H	1.0251516526	-5.0013747292	-0.8078603961
C	1.9149502556	-3.0033059004	0.5583891805
C	2.8666123413	-2.9549195489	-0.4698509407
H	2.6098545728	-2.5080211699	-1.4276447776

C	4.1404660301	-3.478510598	-0.2746241043
H	4.864070389	-3.4442348832	-1.0845348067
C	4.4904707627	-4.0343980279	0.9556702679
H	5.487819654	-4.4375685617	1.1080206587
C	3.5569531178	-4.0690213677	1.9874309202
H	3.8212555942	-4.4989002305	2.9497928839
C	2.2727433455	-3.5622351902	1.7899862564
H	1.5500547648	-3.61078786	2.5994704318
C	0.0929041335	0.2178616239	4.805538665
N	0.0785573305	0.2280718405	5.9722187087

XYZ coordinates of the optimized structure of **3CN'**

104

Pd	-0.0219600531	-0.0129841286	0.0117273288
P	2.2576403984	0.3811993578	0.0262192618
Cl	-0.2397709685	-0.2753511575	-2.4367020241
Sb	0.1053633069	-0.1507786968	2.6103542172
P	-2.2800255876	0.3791411132	0.3660824395
P	1.6191035068	-3.0755535391	1.5974338083
C	2.1746283638	0.5253259165	2.8523280913
C	2.9429256292	0.7061621803	1.6976565717
C	4.2468988616	1.2066258933	1.8091439397
H	4.8429635016	1.3653853789	0.9137767211
C	4.7853425018	1.5116999769	3.0540408509
H	5.7970972766	1.9004297457	3.1256118381
C	4.0192292502	1.3226797715	4.2002030765
H	4.4277405549	1.5619091032	5.1780605823
C	2.7190761925	0.8326704164	4.0994440579
H	2.1326690954	0.6921161135	5.0014095617
C	3.4131573955	-0.785956076	-0.7730006294
C	3.243878362	-1.0433282872	-2.1410716189
H	2.4391875205	-0.5570418078	-2.685973921
C	4.0890379924	-1.9333235033	-2.7960307479
H	3.9505533603	-2.121395782	-3.8571047778
C	5.1035617039	-2.5831539413	-2.0953216911
H	5.7642423049	-3.276046017	-2.6089759591
C	5.2648184361	-2.3443722412	-0.7329526625
H	6.0517360024	-2.8493502284	-0.178980586
C	4.4220768727	-1.4530915409	-0.0705098308
H	4.5551789716	-1.2831566808	0.9934738339
C	2.5584294715	1.9863610209	-0.813824306
C	1.6895450854	3.0435363407	-0.5121075739
H	0.8585785687	2.877379714	0.1703988244
C	1.8858807456	4.3004720577	-1.0736511001
H	1.2073231061	5.1129366996	-0.8283512771
C	2.9465583131	4.5136378272	-1.9535363712
H	3.0962492031	5.493245089	-2.3988099216
C	3.8116104086	3.467400716	-2.2604485936
H	4.6402183905	3.6270243035	-2.9449254473

C	3.6236033359	2.2087338356	-1.6910697042
H	4.3067374123	1.4018270469	-1.938902725
C	-1.5630453673	1.2063206818	2.9512327849
C	-2.5075824153	1.3311796444	1.9213653001
C	-3.5997227579	2.1914860181	2.0870663792
H	-4.3337244898	2.2965379234	1.2921742757
C	-3.7390733828	2.9347999663	3.2562150483
H	-4.5818868338	3.6109987952	3.3680123477
C	-2.7961967797	2.8138732265	4.2725584543
H	-2.8942469895	3.4003274916	5.1818600969
C	-1.7188464301	1.9413032576	4.1257536301
H	-1.0005071797	1.8370298038	4.9334956628
C	-3.016565506	1.4636265831	-0.9086021109
C	-2.3699476755	2.6699233762	-1.206830527
H	-1.4474891272	2.9324649417	-0.6952508753
C	-2.8957882074	3.5294586706	-2.1637557902
H	-2.3873054082	4.4632675088	-2.386964723
C	-4.0653751874	3.1875165755	-2.8433868384
H	-4.4722243771	3.8569800212	-3.5961264906
C	-4.7053005972	1.9851808327	-2.5596173582
H	-5.6135397395	1.7110436144	-3.0891004383
C	-4.1853755051	1.1236788858	-1.5938858604
H	-4.6918717364	0.1872591218	-1.3797122715
C	-3.3938626105	-1.0637304023	0.4639368358
C	-3.0484816456	-2.1976873281	-0.281410507
H	-2.1319581966	-2.1978513444	-0.8673727249
C	-3.8760941444	-3.3170077514	-0.2728322725
H	-3.6015032868	-4.1936077309	-0.8527973804
C	-5.0464933854	-3.3142356896	0.4833668305
H	-5.6890362855	-4.1903483786	0.4933825951
C	-5.3905341088	-2.1900980374	1.2317191518
H	-6.3000097269	-2.1871304195	1.8261904296
C	-4.5684080606	-1.0664019558	1.2237777248
H	-4.8403909302	-0.1972780968	1.8164614363
C	-0.6773053253	-2.16009493	2.8702090988
C	-0.0290353327	-3.2953642049	2.3749347336
C	-0.6407165884	-4.5474192896	2.5269336141
H	-0.1455792435	-5.4358538248	2.1432241791
C	-1.8734085653	-4.6618556297	3.158403455
H	-2.3400230401	-5.6375317415	3.263057606
C	-2.5047731988	-3.5257960262	3.6638803596
H	-3.4668834559	-3.6100803117	4.1615682758
C	-1.9056081917	-2.2776324963	3.5272609236
H	-2.4014602498	-1.4003570538	3.9364111766
C	1.567176761	-4.2857042676	0.2167627187
C	1.0826207561	-3.8151014182	-1.0113108543
H	0.802835736	-2.7688306654	-1.1212473537
C	0.9585151511	-4.6763146544	-2.0988284391
H	0.5793169527	-4.2958840148	-3.0436836313

C	1.3312423923	-6.0134276894	-1.9781658666
H	1.2416836666	-6.6838293031	-2.8287463603
C	1.8253820263	-6.4871985133	-0.7645205642
H	2.1192156596	-7.5288632703	-0.6645478436
C	1.9409435625	-5.6307253658	0.3282572938
H	2.329051523	-6.0120085352	1.2690571184
C	2.7475968246	-3.8381970642	2.8306558969
C	4.0409779593	-4.21568178	2.4375481439
H	4.3282027206	-4.1545096653	1.3908066412
C	4.9601150382	-4.6820205509	3.3724199753
H	5.9528644035	-4.9811579617	3.0462461902
C	4.6115594835	-4.7634505858	4.7194550354
H	5.3304976409	-5.1249295487	5.4495288829
C	3.3366866015	-4.375947792	5.1229983864
H	3.0550263353	-4.4323175348	6.1711410134
C	2.4105158307	-3.9171613165	4.1881126781
H	1.4204162626	-3.6190104048	4.5218980784
C	0.1256701183	-0.3080907554	4.9571076456
N	0.0770743142	-0.5154267125	6.1055325878

XYZ coordinates of the optimized structure of **3SCN**

105

Pd	-0.0618921166	-0.0193670155	-0.2251399043
P	2.0932286791	1.2749854753	0.0724367166
Cl	-0.1425834099	-0.180906536	-2.6241738623
Sb	-0.0714920362	0.0616906289	2.232829967
P	-2.1010404241	1.2829402502	-0.0195528475
P	0.1497068482	-2.3970703385	0.1699594793
C	1.8012478581	0.8478083944	2.859630884
C	2.6129090856	1.373109072	1.8427540999
C	3.7939973553	2.0323246957	2.2103399822
H	4.4207685795	2.4839554348	1.445671936
C	4.1690054185	2.1212879729	3.5477078389
H	5.0905252126	2.6320175254	3.8121489385
C	3.366787186	1.5666890738	4.5432784958
H	3.6407721171	1.6301927335	5.5925778021
C	2.1734632198	0.936915143	4.2022727203
H	1.5449657898	0.5359356449	4.9929947251
C	3.5085213735	0.5542618275	-0.8357051964
C	3.3863771332	0.4475152392	-2.2298509041
H	2.4620547591	0.7443730116	-2.7184112394
C	4.4355887548	-0.0584411597	-2.9907300841
H	4.3319877114	-0.1220340842	-4.0704695378
C	5.6063845776	-0.4901906071	-2.3706750282
H	6.4251682488	-0.8857780884	-2.9653615708
C	5.7152230339	-0.4293796816	-0.9842779253
H	6.6152390292	-0.785209405	-0.490530637
C	4.6743613103	0.0898871872	-0.2174005509
H	4.7784014883	0.1244094965	0.862070165

C	2.115507012	3.0633672933	-0.3638836792
C	1.3583441035	3.9317568042	0.436883815
H	0.8061909568	3.5484885664	1.2919987383
C	1.3091735416	5.2917807203	0.1550685724
H	0.7242013484	5.9506181169	0.7906294892
C	2.0040880725	5.8054295885	-0.9396925529
H	1.9634057941	6.8679505506	-1.1620942391
C	2.7510708443	4.9498960225	-1.7432864722
H	3.3014554682	5.3409747349	-2.5946128495
C	2.8109095235	3.5854651768	-1.4580923425
H	3.4115691386	2.9370726909	-2.0880117656
C	-1.6009805858	1.4491343352	2.7601910613
C	-2.3350590971	1.9732463149	1.6830403919
C	-3.2776256933	2.9736836037	1.9455435468
H	-3.8510525925	3.4083896384	1.1331053303
C	-3.4842773056	3.4278557669	3.2450152398
H	-4.2150416921	4.2102572706	3.4283223429
C	-2.7627860722	2.8836584316	4.3043814052
H	-2.9272620433	3.2355628332	5.3186095853
C	-1.8143241693	1.892176463	4.0669794052
H	-1.2518368015	1.4809686022	4.9039112954
C	-2.3330335456	2.678176385	-1.1773412986
C	-1.2124922496	3.2082999564	-1.8225662941
H	-0.2378407184	2.7623288966	-1.6563694999
C	-1.3468527148	4.2889687551	-2.6912779445
H	-0.467064394	4.69207303	-3.1845358397
C	-2.6022535598	4.8404129526	-2.930242955
H	-2.7076441324	5.6806051697	-3.6110356077
C	-3.7283565086	4.3039925417	-2.3069329511
H	-4.7122534344	4.7215849709	-2.5014285857
C	-3.5983205925	3.2248072381	-1.4388291124
H	-4.4873142898	2.7977049086	-0.9827426619
C	-3.6175331354	0.2834473655	-0.2591432094
C	-4.048743868	0.0020188729	-1.5633087765
H	-3.5174951786	0.4192841157	-2.4144148461
C	-5.1592171582	-0.8104704132	-1.7745202744
H	-5.4904534242	-1.0111273346	-2.7896919042
C	-5.8413783104	-1.363026438	-0.6914370317
H	-6.7083349114	-1.9959306791	-0.8584300841
C	-5.4080433764	-1.0994597506	0.6058651462
H	-5.9349008753	-1.5250316144	1.4552910977
C	-4.3021187938	-0.2804612241	0.8239575796
H	-3.9816195722	-0.0777933173	1.8423171415
C	-0.4059675494	-1.9284338104	2.9029138533
C	-0.3439881022	-2.8902831924	1.8825843976
C	-0.6164520627	-4.2246730452	2.2033622791
H	-0.5856415639	-4.9860414833	1.4287276623
C	-0.9326933303	-4.5824108425	3.5113155669
H	-1.1487009369	-5.6208876528	3.7450610564

C	-0.9682343448	-3.6190492548	4.5168710109
H	-1.208025582	-3.9022843454	5.537586532
C	-0.7044300289	-2.2839951671	4.2187937989
H	-0.729914651	-1.5396404213	5.0128835156
C	-0.8453983943	-3.4882662863	-0.9057131406
C	-2.1182012944	-3.0594434401	-1.2948525129
H	-2.4664576114	-2.0711112834	-1.0094484882
C	-2.9315843121	-3.8884856687	-2.0610497025
H	-3.9177721362	-3.5434182976	-2.3581038076
C	-2.4766517917	-5.1453046817	-2.4551209413
H	-3.1096861438	-5.7883076602	-3.0603166499
C	-1.2053181203	-5.5730382417	-2.0795575003
H	-0.8435880317	-6.5500410113	-2.3877412657
C	-0.3896473297	-4.7500930328	-1.306592592
H	0.6021265502	-5.0905508017	-1.0231846842
C	1.8523909841	-3.0419184978	0.0054900002
C	2.4536504126	-2.9728441847	-1.2594722278
H	1.9080961673	-2.5446084584	-2.0969611585
C	3.7439040731	-3.4543504871	-1.4455843043
H	4.1992924311	-3.4003047438	-2.429766669
C	4.4559902015	-3.9868772315	-0.3709638181
H	5.4659886581	-4.3590320681	-0.5185946122
C	3.8737544203	-4.0326256969	0.8919692181
H	4.4253420016	-4.4396463021	1.7348749756
C	2.5740807797	-3.564694874	1.0831476597
H	2.1277648422	-3.6176909459	2.0716729528
S	-0.4255623883	0.1868853394	7.2346374575
C	1.1519113487	0.6119043332	7.5403542839
N	2.2716014482	0.9134930647	7.7447437375

XYZ coordinates of the optimized structure of **3SCN'**

105

Pd	0.0018254303	0.1794561876	-0.3222043652
P	2.2822255375	0.6004224159	0.0708220583
Cl	0.1082573546	0.71596195	-2.6504507168
Sb	-0.1029485649	-0.363023465	2.1283731209
P	-2.3248148384	0.3300640686	-0.097140448
P	1.5086558122	-3.1153641962	1.7153812422
C	1.7357964301	0.428068984	2.8514781311
C	2.6695975519	0.7777836501	1.8639133009
C	3.9040381298	1.3082839238	2.2572668398
H	4.6338862316	1.6026282593	1.5072475321
C	4.2010649178	1.4695294189	3.6079827871
H	5.162479231	1.8830936259	3.898603048
C	3.2708023896	1.1115689639	4.5811953969
H	3.4787882383	1.2447824288	5.6395802281
C	2.0351863772	0.5869669965	4.2046165457
H	1.315721578	0.3199490852	4.9750262808
C	3.4698507134	-0.5954652525	-0.616108458

C	3.4628265934	-0.7992453191	-2.0046055633
H	2.7763842217	-0.2356712609	-2.6320324058
C	4.325562736	-1.729791738	-2.5742078182
H	4.3200354793	-1.8782112015	-3.6503062995
C	5.188398528	-2.4724926096	-1.767670692
H	5.8581305391	-3.2012675341	-2.2153486062
C	5.1882405662	-2.2812473231	-0.3885993098
H	5.8519446041	-2.8616329815	0.2459525588
C	4.3320344993	-1.345225834	0.1897666257
H	4.337524853	-1.2084455605	1.2664647962
C	2.7463670467	2.2279953932	-0.6110584197
C	1.8526504909	3.2900651203	-0.4250318695
H	0.897574343	3.1148208551	0.0652981972
C	2.1803893527	4.5650924599	-0.8712484047
H	1.4829515074	5.3844550613	-0.7221458901
C	3.3969244731	4.787534126	-1.5161766423
H	3.6493150912	5.7828030423	-1.8709151947
C	4.28531746	3.7333877907	-1.7083483269
H	5.233142693	3.9022130103	-2.2115585207
C	3.9658097903	2.4546010756	-1.2550865627
H	4.6655033624	1.6384549166	-1.4099754031
C	-1.7787751826	0.8888246816	2.6081757362
C	-2.6592728239	1.1213947852	1.5339704306
C	-3.7872881056	1.9242454935	1.732595838
H	-4.4687607932	2.1213021271	0.9094667399
C	-4.0333387455	2.4872576491	2.9832356482
H	-4.9077971191	3.1155427114	3.1255507376
C	-3.1634366387	2.2492437923	4.0431001692
H	-3.3524733814	2.6933926322	5.0161447322
C	-2.0378891731	1.445286761	3.8613150727
H	-1.3712959456	1.2681964743	4.7041709206
C	-3.1467890099	1.3964836292	-1.3208434123
C	-2.7642474201	2.7418595276	-1.4069815133
H	-2.0069043511	3.1399157112	-0.7363094656
C	-3.3521462108	3.5733633721	-2.3522476984
H	-3.0549887989	4.6164607872	-2.4104271535
C	-4.3130317917	3.0671377142	-3.2281105864
H	-4.7674904687	3.7178675917	-3.9697702107
C	-4.6854331744	1.7283769134	-3.1540783793
H	-5.4307128151	1.3293864613	-3.83614942
C	-4.1051449307	0.8906564652	-2.2030315224
H	-4.40151524	-0.1527704154	-2.1510353351
C	-3.2340442581	-1.2480423745	-0.0927088567
C	-2.6679871522	-2.3430121072	-0.7557892916
H	-1.6939287912	-2.2466022646	-1.2300760771
C	-3.3491545231	-3.5570110779	-0.8026742202
H	-2.9015382854	-4.4028402624	-1.3156244952
C	-4.5881886894	-3.6851426291	-0.1796452519
H	-5.1156204894	-4.6343668019	-0.2106153185

C	-5.1501833733	-2.5997775157	0.4913172631
H	-6.1131129169	-2.7010154426	0.9836443198
C	-4.4784519868	-1.3821734848	0.5356512732
H	-4.9201123029	-0.5421626908	1.0649289624
C	-0.5724790851	-2.1445257857	3.2185484619
C	0.2465283951	-3.2675165737	3.0316140146
C	0.0501301296	-4.3896863186	3.8424629361
H	0.701646331	-5.2536512744	3.7368255627
C	-0.972313946	-4.4000856844	4.7883155661
H	-1.1180042959	-5.2755823608	5.4145567824
C	-1.80762637	-3.2946929022	4.9333513698
H	-2.6033740348	-3.3053724082	5.6722757761
C	-1.6109065682	-2.1589133125	4.1500227166
H	-2.2497775712	-1.2916502077	4.2896600378
C	0.9038022142	-4.1775185337	0.3499748956
C	1.3774909971	-3.8769898512	-0.9350306142
H	2.0634497545	-3.045705132	-1.0796882574
C	0.9778076742	-4.6372328243	-2.0310283802
H	1.356265151	-4.3953559634	-3.0204144057
C	0.0904750405	-5.6979102217	-1.8582188171
H	-0.2250794014	-6.289142378	-2.713450238
C	-0.3937980834	-5.996199171	-0.5858949869
H	-1.0876970889	-6.8207101744	-0.4457910054
C	0.0093473544	-5.2413867919	0.5135380641
H	-0.3822871257	-5.4809931515	1.4977272413
C	2.9548289064	-4.0083976634	2.3980484668
C	3.3967988508	-5.24354627	1.9135258944
H	2.855501494	-5.7388099641	1.1122434198
C	4.5322587822	-5.8438473563	2.4556283733
H	4.8658564486	-6.8045696657	2.0726373596
C	5.2330107919	-5.2198556447	3.4842314569
H	6.1168991037	-5.6907428123	3.9054549673
C	4.799637779	-3.9865983883	3.9704546075
H	5.3435544895	-3.492817684	4.7709512894
C	3.6733077227	-3.3793476422	3.4258271223
H	3.3499106581	-2.4111080689	3.8034125148
S	-0.4726527353	0.3783218391	7.3186738146
C	1.095045109	0.840794782	7.6149026192
N	2.2096397615	1.1655606493	7.8146239477

XYZ coordinates of the optimized structure of **[3]**BMe_4

119

Pd	-0.0235812149	-0.048445498	0.0276795572
P	-2.3121740763	0.326796656	0.3776788565
Cl	-0.0796104434	-0.0206128126	-2.3541230525
Sb	0.0599316705	-0.0032812368	2.5392596026
P	2.3068187729	0.2399902448	0.1389975949
P	1.4374371117	-2.8679820599	2.800237429
C	-1.4599324875	1.4969487078	2.7953605222

C	-2.4230961082	1.5344055891	1.7683356288
C	-3.460199365	2.4706557232	1.8315825065
H	-4.2024689799	2.5163601971	1.0395251594
C	-3.5386757774	3.3587761924	2.9021497554
H	-4.3439932303	4.0865090215	2.937548181
C	-2.5885124395	3.3173775177	3.9177976257
H	-2.6449697526	4.0162431857	4.7472676446
C	-1.5536177674	2.3837455079	3.8685798548
H	-0.8163285326	2.369913232	4.6665371442
C	-3.1991418138	1.1066614522	-1.004675211
C	-2.726937655	2.3292058628	-1.5011622402
H	-1.8550235276	2.8016968196	-1.0554971108
C	-3.3698200553	2.939948053	-2.5707581525
H	-3.0020653494	3.8893156573	-2.9489986822
C	-4.4756699099	2.329400742	-3.1632885486
H	-4.9728837523	2.8060067592	-4.0032770234
C	-4.9377239456	1.1081709827	-2.68219691
H	-5.7955956651	0.6274925897	-3.1434182218
C	-4.3028370489	0.4939163121	-1.6040398138
H	-4.6702222471	-0.4583248811	-1.2333608214
C	-3.3007371477	-1.1161870989	0.8856806217
C	-2.8596831127	-2.3920642893	0.5155956674
H	-1.9302540533	-2.5084563177	-0.0370564049
C	-3.6084239225	-3.5147483583	0.8608870184
H	-3.2573045938	-4.5013439444	0.5741867431
C	-4.790421072	-3.3691717809	1.5829109443
H	-5.3705345266	-4.2458874084	1.8566623972
C	-5.2282782405	-2.1006102511	1.9613537394
H	-6.1472840494	-1.9866684095	2.5290358603
C	-4.4886129633	-0.9745272025	1.6144839401
H	-4.8348583469	0.0104959019	1.915738721
C	2.0086677149	0.7745421079	2.9140541726
C	2.8658496921	0.8100159238	1.8034309754
C	4.1653321267	1.3060006221	1.9635093603
H	4.836430759	1.3606718775	1.110230597
C	4.6053986215	1.7352100207	3.2122296994
H	5.6162504854	2.1159281623	3.3233916819
C	3.7542642425	1.6783742734	4.313400642
H	4.0982295366	2.0149201859	5.2870154839
C	2.4548615755	1.197093421	4.1674618137
H	1.8013552888	1.1565455292	5.0345920097
C	2.8647029124	1.5795717735	-0.9654167235
C	2.0961130838	2.7490443044	-1.0219249441
H	1.1686140133	2.8178216098	-0.4579274062
C	2.5112510549	3.8187301627	-1.8065732952
H	1.9105936982	4.7229092584	-1.8467877814
C	3.6888380712	3.7253531419	-2.5482483716
H	4.0079621319	4.5591486128	-3.1670639935
C	4.4517350737	2.5622054089	-2.4997250307

H	5.3678366389	2.4846609884	-3.0782388567
C	4.0450225174	1.4892043292	-1.7086525036
H	4.6455873477	0.5846671467	-1.6778639639
C	3.3049774152	-1.2211642148	-0.286930871
C	3.1125270961	-1.7876498823	-1.5564851603
H	2.3994237143	-1.343114602	-2.2468730661
C	3.8268443632	-2.9226379351	-1.9252364148
H	3.6787276243	-3.3527892595	-2.9116166668
C	4.7230312446	-3.5091651783	-1.0310430816
H	5.275888014	-4.3982385609	-1.3206002163
C	4.9057210048	-2.9563906195	0.233566175
H	5.5957912311	-3.4128037057	0.9374272154
C	4.200159781	-1.8138515002	0.6085084508
H	4.3484657789	-1.395629481	1.5989442981
C	-0.4101673929	-1.3493287207	4.1361704811
C	0.3210863538	-2.5436116401	4.2137328179
C	0.1490211306	-3.3706278441	5.3279720273
H	0.7343908939	-4.2820312732	5.4212776211
C	-0.7689244902	-3.0278589333	6.3182828671
H	-0.899725991	-3.6771322288	7.1792140957
C	-1.5232489285	-1.8615582122	6.2061515344
H	-2.2415663676	-1.6010689147	6.9780062774
C	-1.3463461031	-1.0133142437	5.1142949956
H	-1.9236063732	-0.0955245563	5.0447190076
C	2.9055641568	-3.6469336851	3.5683009281
C	3.2100315084	-5.0056610221	3.4388764727
H	2.544496953	-5.661954638	2.8851761384
C	4.3678462743	-5.5226729738	4.0180011301
H	4.5942738649	-6.5801760261	3.9126147251
C	5.2281303911	-4.6912450894	4.7301233418
H	6.1298047408	-5.0972438985	5.1800235838
C	4.9323375556	-3.3345363131	4.8606043218
H	5.6028386766	-2.6799960358	5.4106758836
C	3.7831180021	-2.8125566084	4.27665983
H	3.567465097	-1.7496982304	4.3708235782
C	0.63208937	-4.2097737567	1.8501941242
C	0.983679225	-4.3155448693	0.4969679377
H	1.6971413374	-3.6175691502	0.0651527026
C	0.4279486512	-5.3124810836	-0.3003760417
H	0.7125687	-5.3861288764	-1.3463294591
C	-0.4944830427	-6.2058464888	0.2412973022
H	-0.9315917344	-6.9815402035	-0.3813104599
C	-0.8572969264	-6.1001967667	1.5826960073
H	-1.5775522028	-6.7931690418	2.0090324326
C	-0.2981284346	-5.1081023168	2.3851772469
H	-0.5953637961	-5.034377952	3.4271098647
B	0.2950614664	2.5762973116	8.1207074338
C	0.9451226533	3.6035733886	7.0030060148
C	-1.3415350023	2.4929423846	7.9182838781

C	0.9456139957	1.0708346941	7.9273195473
C	0.6292674603	3.1346195173	9.6375827275
H	-1.8300924793	1.8379406547	8.6610314768
H	-1.6342760807	2.0941176168	6.9300487649
H	-1.8380149722	3.4754316375	8.0081108545
H	2.0410356483	3.7024763758	7.1003537457
H	0.5416568706	4.6290570468	7.0725756723
H	0.7684340326	3.2838357951	5.959676051
H	0.2283346898	2.4793840941	10.430839599
H	0.2031827246	4.1353494699	9.8288608381
H	1.7116794837	3.2243895195	9.8371414122
H	0.5840122018	0.3455005042	8.6772129651
H	2.0476730715	1.0617830452	8.0024490363
H	0.6998791768	0.6258907985	6.9457754257

XYZ coordinates of the optimized structure of **4**

102

Pd	-0.0100769693	0.0217909676	-0.0198259934
P	-2.3142798977	0.362305891	0.2902595284
Cl	0.0021427093	0.1601582293	-2.3899242493
As	-0.0105172826	-0.0111343055	2.3244005817
P	2.2903092705	0.4349015795	0.1667132332
P	1.3616551596	-2.8899805003	2.0270759615
C	-1.3214880157	1.3865059506	2.6955986262
C	-2.3425138221	1.5053107377	1.7334594337
C	-3.3269462997	2.4820836723	1.8959917734
H	-4.1108174374	2.5932586536	1.1517811377
C	-3.2917765169	3.3332235645	2.9995544969
H	-4.0549610332	4.0973420829	3.1126621112
C	-2.2779520245	3.2144961173	3.9452575926
H	-2.2438030362	3.8878743722	4.7964194037
C	-1.2933514237	2.2375832338	3.7986322551
H	-0.499690937	2.1637745185	4.5361844647
C	-3.2030573079	1.2306619192	-1.0358430267
C	-2.6629483827	2.4218563329	-1.5390937425
H	-1.7272193936	2.8087196715	-1.144036077
C	-3.3188828284	3.1076242029	-2.5540267596
H	-2.8971893132	4.0316649523	-2.9386078498
C	-4.5058369458	2.6028019629	-3.08578997
H	-5.0126754917	3.1372521951	-3.8841752781
C	-5.0364502692	1.4120526988	-2.598827169
H	-5.9576629734	1.0134071783	-3.0136888643
C	-4.389250977	0.7235563342	-1.5743058113
H	-4.8101242499	-0.204088174	-1.198163326
C	-3.3340538842	-1.0691812762	0.7588192471
C	-2.9904887357	-2.3277296151	0.2520269756
H	-2.1130493809	-2.4424303887	-0.3799760691
C	-3.7712048341	-3.4380258954	0.5647112223
H	-3.4980507176	-4.4117169465	0.1697836871

C	-4.8844337853	-3.2991661351	1.3901400079
H	-5.4877178926	-4.1679077384	1.6380401505
C	-5.2231432309	-2.0484858798	1.904449419
H	-6.0882639208	-1.9398113796	2.5522060091
C	-4.4529566983	-0.9332153047	1.5902726465
H	-4.7215635365	0.0380906603	1.9967775191
C	1.7490517639	0.5391898269	2.9256558897
C	2.7166659459	0.7341447563	1.9311224242
C	3.992904584	1.1703011919	2.3000319362
H	4.7501551739	1.3459812825	1.5404254859
C	4.3010371974	1.3773505692	3.6419273426
H	5.2958721273	1.7131914745	3.9185016693
C	3.3427395733	1.1472545889	4.6268601216
H	3.5887259139	1.2991802807	5.6734764937
C	2.0633906826	0.7252489699	4.2726715199
H	1.3256444401	0.5341477814	5.0476104511
C	2.7400909587	2.0029985689	-0.6488220116
C	1.8465895843	3.0760131949	-0.5380206959
H	0.8979776633	2.9398719218	-0.023401284
C	2.167529447	4.311800452	-1.0879576545
H	1.4701762446	5.1398104228	-0.9982545907
C	3.3769428159	4.4830463382	-1.760887104
H	3.6234386682	5.4466082848	-2.1976430909
C	4.2662853872	3.418287682	-1.876050544
H	5.2085322962	3.5476076101	-2.4007923002
C	3.954005456	2.1794966272	-1.3195382164
H	4.6536273516	1.3546040241	-1.4165815752
C	3.4409569527	-0.8226791623	-0.4640875054
C	3.4318033397	-1.0818673456	-1.8431760546
H	2.7719542097	-0.5191783237	-2.4983629118
C	4.259000121	-2.0682054118	-2.3696657985
H	4.2518445688	-2.2593183348	-3.4388973885
C	5.0897509747	-2.8090266472	-1.5296022376
H	5.7334156196	-3.5797731622	-1.9438773911
C	5.0920269914	-2.5618615997	-0.1591828158
H	5.7322116674	-3.1399789472	0.5009592529
C	4.2692899939	-1.5730498232	0.3767769765
H	4.2741232363	-1.3960371217	1.4474648412
C	-0.5443641104	-1.486914695	3.4813289665
C	0.1338626688	-2.7143006965	3.3855160435
C	-0.1619747029	-3.7130552121	4.3179126714
H	0.3846567789	-4.6519286085	4.2904953948
C	-1.1420447299	-3.5142982487	5.2874585339
H	-1.3627900534	-4.3035318884	6.0003850245
C	-1.8401718018	-2.3112282399	5.3402709574
H	-2.6085411792	-2.1557338871	6.0917463592
C	-1.5406680465	-1.2914181746	4.4400622594
H	-2.0717668412	-0.3464017163	4.5034643426
C	2.6435493707	-3.9561721216	2.7888460861

C	3.0262033751	-5.1917700924	2.2566562055
H	2.5019266358	-5.5996734363	1.397163485
C	4.0777570834	-5.9087430333	2.8264471356
H	4.361832764	-6.8690444046	2.4044735903
C	4.7570865328	-5.4023477109	3.9306148659
H	5.5745789433	-5.9641712125	4.3737467035
C	4.3863373857	-4.1678977368	4.4637616203
H	4.9140435557	-3.7640260472	5.3235800965
C	3.3442873592	-3.4457549566	3.8929012303
H	3.0721095721	-2.4779298482	4.3100718415
C	0.5210025424	-3.9693685614	0.8043076199
C	0.6775641414	-3.6288426991	-0.5454764881
H	1.2655190395	-2.7554278324	-0.8171251687
C	0.0795997007	-4.3966299163	-1.5439347019
H	0.2069347929	-4.1184634369	-2.5864407702
C	-0.6809894343	-5.511844946	-1.2018271902
H	-1.1481285661	-6.1115928811	-1.9780992695
C	-0.8430236628	-5.8583096205	0.1398501767
H	-1.4352750489	-6.7283921193	0.4102963876
C	-0.2475784382	-5.0918672937	1.1374586908
H	-0.3888642715	-5.3703628353	2.1776307677

XYZ coordinates of the optimized structure of **4F**

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Pd	0.0626461593	0.1054509394	-0.169758082
P	2.035667303	1.4201565824	-0.0355965945
Cl	0.0409352829	0.0208412176	-2.672071316
As	0.0686501755	0.1676314147	2.3082903157
P	-2.1107157464	1.0505041704	0.0240023696
P	0.3291822377	-2.2527981199	0.1479590087
C	2.0377038727	0.3652667184	2.5598931701
C	2.8153082915	0.9716697288	1.5643261762
C	4.1703106189	1.2239338485	1.8130440875
H	4.7695926814	1.7306109189	1.0619040386
C	4.7667239111	0.8078198696	2.9971729097
H	5.823803417	0.9933188302	3.1657659293
C	4.0042295417	0.1467954492	3.9559149558
H	4.4632874076	-0.2000593866	4.8775076392
C	2.6427872756	-0.0532844174	3.750546697
H	2.0435012275	-0.5231301126	4.51873045
C	3.2856810733	1.0342639023	-1.3159671009
C	3.1747899916	1.6728432595	-2.5593426485
H	2.4028008279	2.4200464022	-2.7199841817
C	4.0470844649	1.3589302293	-3.596345684
H	3.9509913627	1.8688832496	-4.5509429617
C	5.03457855	0.3921704752	-3.4137732113
H	5.7169205527	0.1484317979	-4.2234435484
C	5.1371978334	-0.2629866652	-2.1895690865
H	5.8996122205	-1.0226871142	-2.0381915514

C	4.266333174	0.0513085109	-1.1478815703
H	4.3559884142	-0.4767523737	-0.2041959845
C	2.0743481677	3.2635850027	0.0078777769
C	0.9261541785	3.9514441766	0.4113099581
H	0.0207540792	3.3977289882	0.6383753054
C	0.9331586369	5.339916984	0.5278699861
H	0.0310929335	5.8564331008	0.8444382325
C	2.0879470025	6.058295911	0.2323555081
H	2.0939880197	7.1416048288	0.3163184268
C	3.2370659322	5.3829941099	-0.1771959852
H	4.1412755902	5.9377731644	-0.4130135014
C	3.2330290339	3.9956885413	-0.2870445429
H	4.1334268675	3.4853017872	-0.6172719618
C	-1.0775044743	1.7739703142	2.5211029004
C	-2.0456541507	2.0685231945	1.5520500066
C	-2.8749474458	3.1820110038	1.7294317552
H	-3.6355731776	3.4096358675	0.9880074544
C	-2.7089349429	4.0221088605	2.8259646988
H	-3.3446055228	4.8959339693	2.9384911213
C	-1.720330069	3.7448009775	3.7659283556
H	-1.5713329669	4.4058082085	4.6151692054
C	-0.9214538527	2.6127218404	3.6281782943
H	-0.1756623995	2.3794251994	4.3773059336
C	-2.6450417257	2.251227986	-1.2563832447
C	-1.6582284638	2.9409438966	-1.9696670099
H	-0.6132911483	2.6970897221	-1.8049800821
C	-2.0126391731	3.9118057005	-2.9027674505
H	-1.2365168281	4.4381596173	-3.4518053806
C	-3.3553213005	4.1931341414	-3.1448660824
H	-3.6310666056	4.944353114	-3.880008321
C	-4.3445846499	3.5017336566	-2.4487815984
H	-5.394008047	3.7132874686	-2.6354365345
C	-3.9933318135	2.5366741657	-1.5078156123
H	-4.7737754466	2.003192937	-0.9722043482
C	-3.5899344525	-0.0093184767	0.2410134372
C	-4.0902563776	-0.6985780922	-0.8738246771
H	-3.6456583882	-0.54106854	-1.8539932979
C	-5.1656925564	-1.570033509	-0.7407160294
H	-5.5469180985	-2.0909998858	-1.6148005707
C	-5.7513190458	-1.7741828889	0.5086462979
H	-6.590002613	-2.4569654391	0.6125107358
C	-5.2588236551	-1.0968087246	1.6203678657
H	-5.7118089255	-1.2474878681	2.5965553627
C	-4.1850427229	-0.2171987469	1.4894501379
H	-3.815851222	0.3100780153	2.364450557
C	-0.8360637145	-1.5793588474	2.5841014536
C	-0.6853813644	-2.5969464237	1.6344639944
C	-1.3312332325	-3.8219619143	1.8300904279
H	-1.2052323789	-4.6181631333	1.1017692475

C	-2.1534179964	-4.0184880301	2.9354240756
H	-2.667554436	-4.9668046906	3.0647506216
C	-2.3174243093	-2.996785967	3.8658739076
H	-2.9665601342	-3.1381152759	4.7256481852
C	-1.6465866044	-1.7870645124	3.7036963773
H	-1.7538715803	-1.002546571	4.4416825083
C	-0.3215824748	-3.4305864528	-1.0969638366
C	-1.4106985831	-3.02735433	-1.8765660892
H	-1.7896509184	-2.0163780464	-1.7738204908
C	-1.9867378154	-3.9047743717	-2.7906543297
H	-2.8312603683	-3.5780500168	-3.3914980714
C	-1.4709588499	-5.1895525369	-2.9468855889
H	-1.9144561534	-5.871407946	-3.6674491245
C	-0.3797348066	-5.5957869928	-2.1819225196
H	0.0280674056	-6.5961722182	-2.2995413373
C	0.1925540306	-4.7231757575	-1.2588284455
H	1.0412612254	-5.0517292973	-0.6658409626
C	1.9653329306	-2.9724520534	0.5637540936
C	2.9456849831	-3.005531038	-0.4380551656
H	2.7215916189	-2.6196450558	-1.4297842832
C	4.2059320633	-3.5313064521	-0.173223383
H	4.9526047187	-3.5600502393	-0.9623355586
C	4.5121207744	-4.0125099153	1.0997175793
H	5.4984138127	-4.4187190395	1.3064767452
C	3.5489389833	-3.9694651425	2.1035237537
H	3.7792061424	-4.3416965283	3.0981653239
C	2.2795229126	-3.4568958723	1.8377581016
H	1.5334597276	-3.4418169193	2.6271351056
F	0.0568740897	0.201627983	4.2467603759

XYZ coordinates of the optimized structure of **4F'**

103

Pd	-0.0593973052	-0.2366332647	0.0428009477
P	2.1837335572	0.2570012668	0.0121570591
Cl	-0.3148033758	-0.5955103081	-2.3987273002
As	0.0801207165	-0.2709783946	2.4990628009
P	-2.2943510702	0.2781455277	0.3771220269
P	1.738460965	-3.0639362749	1.486029582
C	1.9522763601	0.3500169159	2.8065447991
C	2.7849664712	0.5808297147	1.7052056699
C	4.0588259077	1.1288762872	1.8969597488
H	4.6923305544	1.3322557813	1.0370420379
C	4.5167021691	1.4258109752	3.1752331446
H	5.5066198332	1.8515661262	3.3119165424
C	3.6963427635	1.17651114	4.2710690205
H	4.0426449711	1.402679352	5.2757198397
C	2.4222888605	0.6437870382	4.0914742161
H	1.7856810315	0.4497628949	4.9434261333
C	3.4181735007	-0.8118532406	-0.8061107117

C	3.2375545721	-1.0944902562	-2.1676224358
H	2.3789509012	-0.6867983507	-2.694727023
C	4.1412971445	-1.9120682179	-2.8401109421
H	3.9925769993	-2.1195683039	-3.8961637501
C	5.2242289084	-2.4676394603	-2.1620104313
H	5.9285032888	-3.1061723047	-2.688031
C	5.3967504192	-2.2067800997	-0.8045782373
H	6.234794016	-2.6422926937	-0.2668175886
C	4.4983111444	-1.3850038455	-0.1266572103
H	4.6400807182	-1.1997079353	0.9334729737
C	2.3928158097	1.9082194439	-0.7693829068
C	1.5866411482	2.9480892597	-0.2835280531
H	0.8722323616	2.7500856425	0.5134092956
C	1.697671793	4.2314318476	-0.8066700069
H	1.0709258776	5.028504661	-0.4160269149
C	2.6074646831	4.4914232373	-1.8317878365
H	2.6903743083	5.4924029886	-2.245907064
C	3.4093712945	3.464471934	-2.3196181886
H	4.1230456546	3.6599632473	-3.1152859643
C	3.3085938404	2.1782441489	-1.7891319472
H	3.9465120403	1.389657272	-2.1759378229
C	-1.320298851	1.0776613052	2.8616090092
C	-2.3498242062	1.2553005786	1.9261896741
C	-3.3476843561	2.206350906	2.1673702116
H	-4.1433990887	2.3520855621	1.441245065
C	-3.3059866349	2.9936700469	3.314269007
H	-4.0741304336	3.7428737143	3.4835751227
C	-2.2734257922	2.8255135677	4.2330605999
H	-2.2292104701	3.4461589572	5.1236413521
C	-1.2936305924	1.858982764	4.018259579
H	-0.5073960463	1.7083586517	4.7481129001
C	-2.9703815893	1.4230010211	-0.8790986752
C	-2.1229346574	2.4022590911	-1.4117238588
H	-1.077907397	2.4336799907	-1.1147494117
C	-2.6077501369	3.3203088637	-2.3367522638
H	-1.9409361183	4.0742338263	-2.7461108042
C	-3.9382651894	3.2609654325	-2.7505516274
H	-4.3133943321	3.973200454	-3.4802982105
C	-4.7819206826	2.281562744	-2.2344783203
H	-5.8175685311	2.225818645	-2.5583291404
C	-4.3022333664	1.364336757	-1.3004582456
H	-4.9674987317	0.601877921	-0.9052365474
C	-3.5438026328	-1.0447376085	0.5136991816
C	-3.3850193668	-2.1562121869	-0.3234156797
H	-2.5314390549	-2.2054545466	-0.9965236776
C	-4.3150228583	-3.1907725948	-0.2916177751
H	-4.186958523	-4.0502183226	-0.9438021553
C	-5.4008017234	-3.128009917	0.5803544175
H	-6.1229796812	-3.9393845319	0.6081319234

C	-5.5581273511	-2.0270385193	1.4196236296
H	-6.4016512141	-1.9771464947	2.1027821057
C	-4.6336204989	-0.9858076351	1.3877591426
H	-4.7588207748	-0.1341679829	2.0511646732
C	-0.6274539919	-2.1136296562	2.6432875367
C	0.0425328731	-3.246690737	2.1663100923
C	-0.5885844867	-4.4951970839	2.2629245931
H	-0.0741562245	-5.3790521979	1.8944819897
C	-1.8579001283	-4.6159523731	2.8149535637
H	-2.3347806339	-5.5906077846	2.872139308
C	-2.5084655963	-3.4843073763	3.3033702038
H	-3.4986263159	-3.5667202067	3.7425668432
C	-1.8925310197	-2.2406156811	3.2271855316
H	-2.3981110277	-1.367444316	3.6283592726
C	1.7610114461	-4.3646779969	0.1881155805
C	1.2308318889	-4.0073469948	-1.0598979642
H	0.859740861	-2.9968761771	-1.2251327771
C	1.1750774353	-4.9365944274	-2.095119501
H	0.7575593072	-4.645567766	-3.0555593135
C	1.6641314049	-6.2279154909	-1.9050278436
H	1.6281031734	-6.9503317431	-2.7161062009
C	2.204038212	-6.5873635166	-0.6723824463
H	2.5871744665	-7.5926482769	-0.5167886447
C	2.2495125825	-5.6636282242	0.3704835787
H	2.6693556255	-5.9573562708	1.3287895011
C	2.7847145366	-3.7524739824	2.8313557041
C	4.1373035831	-4.0161340811	2.5615285861
H	4.5197852663	-3.9008112553	1.5498965644
C	4.996229454	-4.4348096015	3.5726312574
H	6.0369718778	-4.6458895299	3.3407758744
C	4.5265021845	-4.5776489589	4.8775109153
H	5.198524409	-4.8995157174	5.6683617032
C	3.192015724	-4.3008612339	5.160424864
H	2.8165043985	-4.4048268304	6.17507383
C	2.3259336781	-3.8928629461	4.1469464185
H	1.2872784374	-3.6822629136	4.3854472866
F	0.0510816482	-0.4970838639	4.4630663882

XYZ coordinates of the optimized structure of **[4]**BMe_4

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Pd	-0.0100769693	0.0217909676	-0.0198259934
P	-2.3142798977	0.362305891	0.2902595284
Cl	0.0021427093	0.1601582293	-2.3899242493
As	-0.0105172826	-0.0111343055	2.3244005817
P	2.2903092705	0.4349015795	0.1667132332
P	1.3616551596	-2.8899805003	2.0270759615
C	-1.3214860791	1.3865082875	2.6955967743
C	-2.3425138221	1.5053107377	1.7334594337
C	-3.3269462997	2.4820836723	1.8959917734

H	-4.1108174374	2.5932586536	1.1517811377
C	-3.2917765169	3.3332235645	2.9995544969
H	-4.0549610332	4.0973420829	3.1126621112
C	-2.2779329041	3.21451814	3.9452392032
H	-2.2438030362	3.8878743722	4.7964194037
C	-1.2934327219	2.2374782855	3.798709317
H	-0.4996082663	2.1638847369	4.5361080751
C	-3.2030573079	1.2306619192	-1.0358430267
C	-2.6629483827	2.4218563329	-1.5390937425
H	-1.7272193936	2.8087196715	-1.144036077
C	-3.3188828284	3.1076242029	-2.5540267596
H	-2.8971893132	4.0316649523	-2.9386078498
C	-4.5058369458	2.6028019629	-3.08578997
H	-5.0126754917	3.1372521951	-3.8841752781
C	-5.0364502692	1.4120526988	-2.598827169
H	-5.9576629734	1.0134071783	-3.0136888643
C	-4.389250977	0.7235563342	-1.5743058113
H	-4.8101242499	-0.204088174	-1.198163326
C	-3.3340538842	-1.0691812762	0.7588192471
C	-2.9904887357	-2.3277296151	0.2520269756
H	-2.1130493809	-2.4424303887	-0.3799760691
C	-3.7712048341	-3.4380258954	0.5647112223
H	-3.4980507176	-4.4117169465	0.1697836871
C	-4.8844337853	-3.2991661351	1.3901400079
H	-5.4877178926	-4.1679077384	1.6380401505
C	-5.2231432309	-2.0484858798	1.904449419
H	-6.0882639208	-1.9398113796	2.5522060091
C	-4.4529566983	-0.9332153047	1.5902726465
H	-4.7215635365	0.0380906603	1.9967775191
C	1.749057778	0.5391713322	2.9256570444
C	2.7166659459	0.7341447563	1.9311224242
C	3.992904584	1.1703011919	2.3000319362
H	4.7501551739	1.3459812825	1.5404254859
C	4.3010371974	1.3773505692	3.6419273426
H	5.2958721273	1.7131914745	3.9185016693
C	3.3427484811	1.1472263135	4.6268616138
H	3.5887259139	1.2991802807	5.6734764937
C	2.063372558	0.72542234	4.2726971145
H	1.3256252132	0.5339915515	5.0476017786
C	2.7400909587	2.0029985689	-0.6488220116
C	1.8465895843	3.0760131949	-0.5380206959
H	0.8979776633	2.9398719218	-0.023401284
C	2.167529447	4.311800452	-1.0879576545
H	1.4701762446	5.1398104228	-0.9982545907
C	3.3769428159	4.4830463382	-1.760887104
H	3.6234386682	5.4466082848	-2.1976430909
C	4.2662853872	3.418287682	-1.876050544
H	5.2085322962	3.5476076101	-2.4007923002
C	3.954005456	2.1794966272	-1.3195382164

H	4.6536273516	1.3546040241	-1.4165815752
C	3.4409569527	-0.8226791623	-0.4640875054
C	3.4318033397	-1.0818673456	-1.8431760546
H	2.7719542097	-0.5191783237	-2.4983629118
C	4.259000121	-2.0682054118	-2.3696657985
H	4.2518445688	-2.2593183348	-3.4388973885
C	5.0897509747	-2.8090266472	-1.5296022376
H	5.7334156196	-3.5797731622	-1.9438773911
C	5.0920269914	-2.5618615997	-0.1591828158
H	5.7322116674	-3.1399789472	0.5009592529
C	4.2692899939	-1.5730498232	0.3767769765
H	4.2741232363	-1.3960371217	1.4474648412
C	-0.5443641104	-1.486914695	3.4813289665
C	0.1338626688	-2.7143006965	3.3855160435
C	-0.1619747029	-3.7130552121	4.3179126714
H	0.3846567789	-4.6519286085	4.2904953948
C	-1.1420447299	-3.5142982487	5.2874585339
H	-1.3627900534	-4.3035318884	6.0003850245
C	-1.8401718018	-2.3112282399	5.3402709574
H	-2.6085411792	-2.1557338871	6.0917463592
C	-1.5406680465	-1.2914181746	4.4400622594
H	-2.0717668412	-0.3464017163	4.5034643426
C	2.6435493707	-3.9561721216	2.7888460861
C	3.0262033751	-5.1917700924	2.2566562055
H	2.5019266358	-5.5996734363	1.397163485
C	4.0777570834	-5.9087430333	2.8264471356
H	4.361832764	-6.8690444046	2.4044735903
C	4.7570865328	-5.4023477109	3.9306148659
H	5.5745789433	-5.9641712125	4.3737467035
C	4.3863373857	-4.1678977368	4.4637616203
H	4.9140435557	-3.7640260472	5.3235800965
C	3.3442873592	-3.4457549566	3.8929012303
H	3.0721095721	-2.4779298482	4.3100718415
C	0.5210025424	-3.9693685614	0.8043076199
C	0.6775641414	-3.6288426991	-0.5454764881
H	1.2655190395	-2.7554278324	-0.8171251687
C	0.0795997007	-4.3966299163	-1.5439347019
H	0.2069347929	-4.1184634369	-2.5864407702
C	-0.6809894343	-5.511844946	-1.2018271902
H	-1.1481285661	-6.1115928811	-1.9780992695
C	-0.8430236628	-5.8583096205	0.1398501767
H	-1.4352750489	-6.7283921193	0.4102963876
C	-0.2475784382	-5.0918672937	1.1374586908
H	-0.3888642715	-5.3703628353	2.1776307677
B	-0.0322845231	1.9870147103	8.2869089101
C	0.9195322431	2.9655048883	7.3579284205
C	-1.6196032047	2.2377772898	7.9117090732
C	0.3506437339	0.4061363933	8.0042029386
C	0.2164294124	2.3366884955	9.8797349681

H	-2.3035518353	1.6104778603	8.5099557134
H	-1.851775337	2.0131001696	6.8550430333
H	-1.9407001579	3.2810740369	8.0785359066
H	1.9976487981	2.8338751433	7.5603702515
H	0.712151093	4.0391825864	7.5110747935
H	0.7971170371	2.7903560197	6.2732866871
H	-0.4036035315	1.7200878211	10.5536715491
H	-0.0176401526	3.3868276288	10.1290752572
H	1.2616436635	2.1758618488	10.1970337914
H	-0.2237904876	-0.2919648882	8.6382474154
H	1.4151334008	0.1774222271	8.1905774456
H	0.1463237352	0.0938137492	6.9632136503

XYZ coordinates of the optimized structure of **5**

102

Pd	0.0103160496	-0.021125122	0.0188424923
P	-2.2860699829	0.3357295331	0.3685253304
Cl	-0.0407840491	0.0653968175	-2.349721486
Bi	0.0848542886	-0.0555784221	2.5858708546
P	2.3452772672	0.2400963742	0.1458758845
P	1.5259148108	-2.9556041642	2.8822245951
C	-1.5277445536	1.4461137836	2.8606254279
C	-2.4527040242	1.4890920526	1.802557231
C	-3.5125994416	2.4022744281	1.8594998659
H	-4.2313842555	2.4542654486	1.0463541207
C	-3.6466733421	3.2538726729	2.9539716987
H	-4.4700433164	3.9613729526	2.9843982893
C	-2.730615559	3.2022242231	4.0002531667
H	-2.8311908468	3.874192974	4.8477634878
C	-1.6730492352	2.2930978952	3.9576878968
H	-0.9576893917	2.2676379671	4.7759540314
C	-3.1804311738	1.145417383	-0.991385126
C	-2.6732323874	2.3475552675	-1.502678298
H	-1.7615119023	2.7747525937	-1.0926961004
C	-3.331480733	2.9932781942	-2.5419290751
H	-2.9354755821	3.9259129744	-2.9330509043
C	-4.4886885346	2.4378409746	-3.0889439257
H	-4.9977350686	2.9411028941	-3.9059993116
C	-4.9870446339	1.2371432631	-2.5925002261
H	-5.8853227573	0.7997435531	-3.0185321382
C	-4.3366917457	0.5883862406	-1.5440597135
H	-4.7324834836	-0.3472381616	-1.1603743498
C	-3.2325933255	-1.1571619878	0.8061769739
C	-2.8054514534	-2.3844603177	0.2841765153
H	-1.9205468609	-2.4290422061	-0.3470141416
C	-3.5112448573	-3.5483888703	0.5762376786
H	-3.1710215946	-4.4975666448	0.173432023
C	-4.6362997341	-3.4939940558	1.3964636754
H	-5.1822540616	-4.4038150485	1.6293899282

C	-5.0594202844	-2.275544146	1.9247347349
H	-5.9335987314	-2.2331340672	2.568062826
C	-4.3619253075	-1.1070384217	1.6323299223
H	-4.6947313619	-0.1611443969	2.0510635205
C	2.0850412478	0.7944612421	2.9362613719
C	2.9125614153	0.8245730348	1.8065143026
C	4.2105917217	1.3382210322	1.9368878426
H	4.8647272723	1.3914761707	1.0704239151
C	4.6696603866	1.7870462559	3.1714648519
H	5.6784138995	2.179690373	3.2576066321
C	3.840281157	1.7377640433	4.2896185614
H	4.1982000516	2.0943186394	5.2511601671
C	2.543751869	1.2393054541	4.1749819686
H	1.9011847785	1.2078599721	5.0507572259
C	2.9224412737	1.5630348823	-0.9686534801
C	2.1852456937	2.7532916609	-1.0116587976
H	1.2713342815	2.8485830381	-0.4295075019
C	2.6136797021	3.8100656302	-1.8063032384
H	2.037681075	4.730558378	-1.8357216541
C	3.7730340054	3.6832890274	-2.5716798404
H	4.1025396051	4.5073941141	-3.1979849718
C	4.5043099674	2.4997002362	-2.5365124931
H	5.4062544351	2.3962845198	-3.1329365896
C	4.0842718172	1.439184429	-1.7353510097
H	4.6607155552	0.5188704648	-1.7142438277
C	3.325464273	-1.2376414953	-0.2639580561
C	3.1142624363	-1.8248033141	-1.5209462137
H	2.3963231051	-1.3874005329	-2.2110464301
C	3.8193840604	-2.9688139865	-1.8797042921
H	3.6574152524	-3.4146704417	-2.8568860231
C	4.724299518	-3.5440296131	-0.986896182
H	5.2699200261	-4.4401482515	-1.2683006161
C	4.9246800596	-2.9712407924	0.2662021464
H	5.6214136083	-3.4190275088	0.9690301068
C	4.2288501893	-1.8193821601	0.6303898058
H	4.3910062255	-1.3840185116	1.6112193581
C	-0.3387274838	-1.4569023645	4.2446253542
C	0.4123511702	-2.6364224709	4.3027431267
C	0.2583868055	-3.4699239898	5.4166251852
H	0.8546598615	-4.3754396389	5.4982474237
C	-0.6536252442	-3.1432812402	6.417512592
H	-0.7672191791	-3.7981515529	7.2766302681
C	-1.4244985045	-1.9867513853	6.3184376671
H	-2.1385364784	-1.7384780543	7.0983950035
C	-1.2704171242	-1.1319804774	5.2271299288
H	-1.8623504288	-0.2228365855	5.1638501052
C	2.9842801407	-3.7608433581	3.6433572953
C	3.2170919183	-5.1391769934	3.5939435502
H	2.5025583343	-5.7939854518	3.1028381065

C	4.3661184812	-5.6772715857	4.1709790036
H	4.5373619711	-6.749417446	4.1272931601
C	5.2889329635	-4.8474253806	4.802434173
H	6.1839345689	-5.2699077109	5.2505354239
C	5.0650965395	-3.4719313626	4.8532852135
H	5.7850398231	-2.8192356435	5.3393022405
C	3.9245965915	-2.9299088578	4.2699396915
H	3.7643459632	-1.8536253689	4.2998017501
C	0.7023100097	-4.2885990621	1.9324775022
C	1.0833763304	-4.4218642463	0.5894508899
H	1.8287358773	-3.7514212673	0.1677384991
C	0.5169860481	-5.4105354143	-0.2102771778
H	0.826351631	-5.5064750451	-1.2474322412
C	-0.448068837	-6.2669338694	0.3171392173
H	-0.893835287	-7.0359770572	-0.3076613312
C	-0.8420733593	-6.1321858533	1.6468056011
H	-1.5960308771	-6.7954351584	2.0619803659
C	-0.2703734618	-5.1497208551	2.4527186713
H	-0.5898647917	-5.0549330672	3.4864913862

XYZ coordinates of the optimized structure of **5F**

103

Pd	0.0438880432	-0.0095044997	-0.0654745074
P	2.0771583224	1.3047353735	0.1033400642
Cl	0.0533456641	-0.2582004258	-2.5325608105
Bi	0.012529522	0.0983440165	2.5782839715
P	-2.0358741224	1.1994788619	0.0275724887
P	0.2062970335	-2.3635377298	0.2666594952
C	2.1264794653	0.762419405	2.8827500685
C	2.8371337346	1.250483508	1.7854704318
C	4.1174303054	1.7845271599	2.0003870443
H	4.6716859265	2.2083915553	1.1668273209
C	4.6869842488	1.7760921742	3.2680042009
H	5.6835603691	2.1836625758	3.4133596154
C	3.9766702788	1.2540643012	4.3472356418
H	4.4188497933	1.2446868634	5.339856546
C	2.6878238463	0.761711741	4.1606571808
H	2.1077903907	0.3911107743	4.9978263342
C	3.408853339	0.7740671152	-1.0355397474
C	3.2560560256	1.0512966617	-2.4028508712
H	2.3785341605	1.5859851839	-2.7534790759
C	4.2174434064	0.6386907993	-3.3196032662
H	4.0871664499	0.870328514	-4.3731619711
C	5.3384278701	-0.0699663462	-2.8896894416
H	6.0909262275	-0.388534394	-3.6059114446
C	5.4824028197	-0.3752743596	-1.539435481
H	6.3435118269	-0.9416029055	-1.1953182177
C	4.5219581372	0.0370563013	-0.6176497573
H	4.6462680215	-0.2232927661	0.4287210097

C	2.0177913908	3.1364383645	-0.1252394334
C	0.9925598193	3.8294664004	0.5312717011
H	0.2379825118	3.2807933837	1.089839176
C	0.9221133347	5.2175250774	0.4757954811
H	0.1204750505	5.7358835519	0.9948325268
C	1.8684548781	5.935511269	-0.253244986
H	1.8098564686	7.0191001844	-0.30647255
C	2.8882898514	5.2563837441	-0.9142799894
H	3.6322167999	5.807891135	-1.4830202392
C	2.9694131624	3.8659666579	-0.8458361604
H	3.7776959705	3.3543365544	-1.3593781275
C	-1.5152601013	1.7275138437	2.7574782669
C	-2.2334960177	2.1156698837	1.6222645725
C	-3.1264609587	3.1911260466	1.7350940869
H	-3.6934914826	3.5176962948	0.8690669663
C	-3.2888385252	3.8589983866	2.9444065487
H	-3.9774282453	4.6971307741	3.0064917546
C	-2.5734413136	3.4529157729	4.0675892443
H	-2.6975180907	3.9722509051	5.0140235624
C	-1.6887500373	2.3807677598	3.9779636146
H	-1.128431995	2.047603184	4.8438728977
C	-2.3300882755	2.4639141075	-1.2704054497
C	-1.2264449347	2.974247506	-1.960565706
H	-0.2400301945	2.5733298568	-1.7537692308
C	-1.3913920204	3.96777873	-2.9230092709
H	-0.5236316131	4.3533082165	-3.4512458973
C	-2.663051446	4.4523254952	-3.2160965553
H	-2.7927997899	5.2230641888	-3.9710493236
C	-3.7726271704	3.9360165202	-2.5485994461
H	-4.7693628428	4.3012324857	-2.7807579182
C	-3.6093782491	2.9460277679	-1.5840207028
H	-4.4855208695	2.5390062348	-1.0863699662
C	-3.5784423655	0.2009833581	-0.0343530895
C	-4.0842472983	-0.2155498489	-1.2743944807
H	-3.6034196103	0.1074975184	-2.194112849
C	-5.2055632878	-1.0384068751	-1.3395541262
H	-5.5925310743	-1.3403700057	-2.3091896737
C	-5.8281228909	-1.4716032164	-0.170136993
H	-6.7025244059	-2.1141826998	-0.2224255863
C	-5.324153942	-1.0736526618	1.0658231214
H	-5.8038351639	-1.403567599	1.9833120986
C	-4.2083939562	-0.241614263	1.1352909407
H	-3.8361423803	0.0689436341	2.1079530703
C	-0.5546964434	-2.0314567222	2.9591600217
C	-0.4482622001	-2.9255441287	1.8943994022
C	-0.8287122854	-4.2602335839	2.0967844921
H	-0.7507154929	-4.9735917292	1.2806860145
C	-1.3138996146	-4.6761681929	3.3323469395
H	-1.6161306232	-5.7105417222	3.4707181986

C	-1.4103547141	-3.7703358309	4.3861985987
H	-1.7925963978	-4.0930142259	5.3509535157
C	-1.0206888059	-2.4445106713	4.2064453743
H	-1.0776012586	-1.7309755357	5.0200831898
C	-0.694165058	-3.4447334332	-0.9099164369
C	-1.9787906577	-3.0537936406	-1.3000653673
H	-2.3801418691	-2.1057602552	-0.9546859847
C	-2.7386197339	-3.8634730153	-2.1376083636
H	-3.7351343368	-3.5445800763	-2.4309385924
C	-2.217674678	-5.0680669711	-2.6074743417
H	-2.8072117928	-5.6963909567	-3.2696167708
C	-0.9361773203	-5.4605754451	-2.2300416516
H	-0.5222968147	-6.3975556568	-2.5929201905
C	-0.1767947218	-4.6559626937	-1.3821081426
H	0.8202719079	-4.9751875447	-1.0936557989
C	1.9067685669	-3.0487298498	0.2322907551
C	2.6250458828	-2.9491920154	-0.9675999881
H	2.170592787	-2.465429282	-1.8297474684
C	3.9137541086	-3.4638531743	-1.0578022929
H	4.4564234694	-3.3877692459	-1.9955484712
C	4.5128985114	-4.0559680123	0.0536897364
H	5.5219000659	-4.4529835723	-0.0175320346
C	3.816220418	-4.1306346425	1.2565705194
H	4.2785595363	-4.5844062714	2.1291018473
C	2.5154614205	-3.635564368	1.3466168099
H	1.9766649025	-3.7157962283	2.286334557
F	-0.0433465531	0.1801216112	4.719773222

XYZ coordinates of the optimized structure of **5F'**

103

Pd	0.0230701428	0.1530593438	-0.0376750822
P	2.318616836	0.5020643857	0.0449869411
Cl	-0.1216088125	0.0301002231	-2.4907301039
Bi	0.0965734042	-0.0388716506	2.6148444467
P	-2.2606988383	0.4120808868	0.292721662
P	1.5367597539	-3.0639436012	1.648602787
C	2.2475816558	0.5630334321	2.8834637534
C	3.011070492	0.7470506384	1.7319840536
C	4.3415387529	1.1746027012	1.8624896709
H	4.9473754981	1.3407704699	0.9750466025
C	4.8937036535	1.3911808153	3.1195574915
H	5.925017971	1.7216199141	3.204989347
C	4.1226459778	1.1876080842	4.261835217
H	4.5505881662	1.3566250625	5.2463674187
C	2.7964244896	0.7757842094	4.1474816465
H	2.1785842843	0.622678822	5.0242344
C	3.4304290824	-0.6989159993	-0.7677628321
C	3.3073445567	-0.8832458152	-2.152657443
H	2.5667477359	-0.3158178647	-2.709227127

C	4.1168299793	-1.8027408124	-2.8117796212
H	4.0152525447	-1.9326928156	-3.8856846275
C	5.0506328355	-2.5535520701	-2.0995355198
H	5.6848040512	-3.2684062149	-2.6165382852
C	5.1653114333	-2.3863181273	-0.7220469816
H	5.8887085475	-2.9694808436	-0.158653818
C	4.3564722123	-1.4676367588	-0.0548565047
H	4.4526868329	-1.3537683751	1.0204662319
C	2.6915704742	2.108911499	-0.7577611832
C	1.8120685001	3.1730187427	-0.5182793086
H	0.9211333771	3.0096820559	0.0845963095
C	2.0682266199	4.4322357411	-1.0505893289
H	1.3794811471	5.2498872145	-0.8565745677
C	3.2000463428	4.640263978	-1.8376979683
H	3.3963805863	5.6217278994	-2.260232895
C	4.0754053484	3.5862528378	-2.084283798
H	4.9579438837	3.7417429426	-2.6987109719
C	3.8268564577	2.3254674002	-1.5446363207
H	4.5164193508	1.511045589	-1.7467036356
C	-1.7026549571	1.2739545697	2.9098937329
C	-2.5963922536	1.3542136913	1.8365839811
C	-3.7493842138	2.1421999759	1.9625791323
H	-4.4499279521	2.2193301387	1.1349618388
C	-3.9933754831	2.844473225	3.1395785264
H	-4.8829451209	3.4626844368	3.2220621177
C	-3.0999983262	2.7545465714	4.2040446427
H	-3.2875282979	3.3073053246	5.120823977
C	-1.9599005091	1.958329552	4.0958295016
H	-1.2663750007	1.8642549511	4.924101449
C	-3.0605723373	1.4144971519	-1.0073847684
C	-2.6081237652	2.7252603878	-1.2091257659
H	-1.8146498834	3.1298612046	-0.5851499201
C	-3.1686798357	3.5137047937	-2.2067051821
H	-2.8143696324	4.5302569775	-2.3529566516
C	-4.1770755959	2.9980618254	-3.021723329
H	-4.6113638974	3.6137954128	-3.8043993849
C	-4.6223644098	1.6935172557	-2.8323682285
H	-5.4048308091	1.285640764	-3.4661830059
C	-4.0673495314	0.9009446983	-1.8280784074
H	-4.4199955312	-0.1166778846	-1.6884223838
C	-3.2457140546	-1.1214640787	0.4034797813
C	-2.7299995931	-2.2746922175	-0.1986673781
H	-1.7635903915	-2.2375390632	-0.6955925682
C	-3.4475470417	-3.4673067714	-0.1568280303
H	-3.0371749835	-4.3578391981	-0.6246356169
C	-4.6797124254	-3.5165893847	0.4909473169
H	-5.2371098049	-4.4484519244	0.5289277511
C	-5.1956805621	-2.3718775535	1.0966810453
H	-6.153996246	-2.4093005925	1.6072783582

C	-4.4830018231	-1.1769684846	1.0551479236
H	-4.8875466153	-0.2925043423	1.53974994
C	-0.6521927859	-2.0874724996	3.0697685621
C	-0.0424529315	-3.2433132173	2.5756427186
C	-0.6455577681	-4.4834616739	2.8316608222
H	-0.1860128762	-5.392925629	2.4536261802
C	-1.8297213359	-4.5615360077	3.5551316314
H	-2.2898700508	-5.5290529798	3.7366663994
C	-2.4224462933	-3.4002808627	4.0501508461
H	-3.3456106393	-3.4576368044	4.6206498267
C	-1.8309542048	-2.1623249189	3.8147006221
H	-2.2903858684	-1.2608415457	4.2116510505
C	1.3294812027	-4.2335981772	0.2465740661
C	0.9071974545	-3.686621402	-0.9724893773
H	0.7697572036	-2.6108677206	-1.0664005909
C	0.6686458817	-4.5070569391	-2.0731694953
H	0.3394510931	-4.0659574127	-3.0103068349
C	0.8658792969	-5.8823918495	-1.974095764
H	0.6869580337	-6.5225716043	-2.833781671
C	1.3038124723	-6.4343998802	-0.7714391935
H	1.4662586193	-7.5060439573	-0.690659849
C	1.5336527738	-5.6171059335	0.3325073368
H	1.8844367115	-6.0591100639	1.2615352592
C	2.7378910236	-3.904266443	2.7564917179
C	3.9340363919	-4.4147620646	2.2299764852
H	4.097101364	-4.4128054738	1.155389131
C	4.9136087254	-4.9381207921	3.06887636
H	5.8283503914	-5.3396479876	2.6404482982
C	4.7238902951	-4.9485011677	4.4493895401
H	5.4894009066	-5.3562523158	5.1038317635
C	3.5463291625	-4.4318404458	4.9838443052
H	3.3879460303	-4.4340424207	6.059076135
C	2.5608792493	-3.9131485478	4.1465321632
H	1.6473090731	-3.5160831653	4.5809203791
F	0.1284669551	0.0851665508	4.7732807264

XYZ coordinates of the optimized structure of **5CN**

104

Pd	0.0627963765	0.0280328248	-0.0933305116
P	2.0831830372	1.3352898166	0.042647704
Cl	0.0625463206	-0.2016328025	-2.5556410524
Bi	0.0621788731	0.1507855049	2.555552835
P	-2.0532389642	1.1574505553	0.0369868152
P	0.2241771938	-2.3298500466	0.2757575236
C	2.2592346579	0.6227300585	2.7810369559
C	2.9394354052	1.1159418967	1.6650822442
C	4.2771310457	1.5102250277	1.8191048049
H	4.8136435897	1.9360724939	0.9755709693
C	4.9312681959	1.3558246185	3.0357691336

H	5.9713598853	1.6548832367	3.1303797995
C	4.2503776801	0.8230015202	4.1267157136
H	4.7560919624	0.6907738054	5.0792001442
C	2.9076400577	0.472986305	4.0048344464
H	2.3727020111	0.0952723396	4.8702412752
C	3.329504103	0.8977988562	-1.2244768068
C	3.1440709042	1.3884443425	-2.5256537582
H	2.3068009437	2.0442292019	-2.7451638584
C	4.0262669409	1.0439146765	-3.5441105011
H	3.8717210504	1.4399880211	-4.5439516293
C	5.0988150761	0.1921761888	-3.2842375513
H	5.7897532723	-0.0742890637	-4.0793135061
C	5.2756484457	-0.3193329328	-2.0018667485
H	6.1041135612	-0.9899558532	-1.7901096355
C	4.3942611186	0.0249523227	-0.9783450775
H	4.5428169306	-0.3932296741	0.011955621
C	2.0413229232	3.1794944567	-0.0445875047
C	0.9483824942	3.8394935048	0.5273111916
H	0.1230282852	3.2634036049	0.9357718167
C	0.9014657644	5.2301121105	0.5773622927
H	0.0437770969	5.7224337163	1.02755891
C	1.9439269708	5.9819047078	0.0415668847
H	1.9060692895	7.0673445312	0.0706815028
C	3.0351846068	5.3354504096	-0.535516358
H	3.8528291716	5.9147504212	-0.9560179004
C	3.0888889071	3.944175862	-0.5737250324
H	3.9478807829	3.4573126919	-1.0259369888
C	-1.4198913678	1.8418091578	2.7169623836
C	-2.202624005	2.1420684635	1.5968704449
C	-3.1006365169	3.2156804634	1.6801135488
H	-3.7212833006	3.4680779402	0.8258456195
C	-3.1971401628	3.9787617075	2.8391723814
H	-3.8900318852	4.8146624112	2.8767628023
C	-2.4058419346	3.6715576434	3.9415164801
H	-2.468559522	4.2680101341	4.8474465226
C	-1.5232189261	2.5948492297	3.8841665931
H	-0.9185613852	2.3516196713	4.7520748375
C	-2.4185361138	2.3748668743	-1.2874004702
C	-1.3431325398	2.9448595351	-1.9761423798
H	-0.3344519023	2.611777567	-1.7547148994
C	-1.5627252517	3.9114757908	-2.9545245062
H	-0.7169503676	4.3439113657	-3.4821426702
C	-2.8605309136	4.3079516679	-3.2663315889
H	-3.0325258281	5.0562258884	-4.0352661685
C	-3.9402535519	3.7335011524	-2.5979706591
H	-4.9561283715	4.0320503911	-2.8421072825
C	-3.7226410237	2.7720519667	-1.6149561189
H	-4.5744789914	2.3234356084	-1.111063152
C	-3.5719031674	0.1250785289	0.0700106148

C	-4.0760689702	-0.3924005589	-1.1323749716
H	-3.6097115232	-0.1239126813	-2.0774095047
C	-5.1772300763	-1.2435852117	-1.1281464263
H	-5.5623304213	-1.6268206699	-2.0693342891
C	-5.7829582419	-1.6017732002	0.0751568564
H	-6.6420642778	-2.2667097798	0.0773624865
C	-5.2829639017	-1.1000172557	1.274160574
H	-5.7507205083	-1.3704144498	2.21691015
C	-4.1858156649	-0.24037732	1.2737844035
H	-3.8164365429	0.1521490859	2.2174242509
C	-0.7256210826	-1.9294608142	2.8970731283
C	-0.6126388393	-2.8323345974	1.8383582557
C	-1.1347499884	-4.1231979975	1.9975202666
H	-1.0460529751	-4.8434269567	1.1888703254
C	-1.7740883111	-4.4875458157	3.1786459492
H	-2.1864748094	-5.4873893614	3.2810469916
C	-1.8834593109	-3.5736060598	4.2224655045
H	-2.3887685622	-3.8502650162	5.1437121425
C	-1.3463765543	-2.293937978	4.0882237547
H	-1.41956758	-1.5906695032	4.911848417
C	-0.5414018187	-3.4390692107	-0.9663645818
C	-1.7641597889	-3.0494153371	-1.5215218575
H	-2.1903916672	-2.0879310628	-1.2541683381
C	-2.4282665675	-3.8803768893	-2.4175855695
H	-3.3794699726	-3.5654975039	-2.8383735898
C	-1.8682227977	-5.10324673	-2.7837022663
H	-2.3816050803	-5.7482501003	-3.491635611
C	-0.6455160208	-5.4936440316	-2.2434935627
H	-0.202540742	-6.4452210824	-2.5247311673
C	0.0156735416	-4.668587117	-1.3351720104
H	0.9660378399	-4.9866930131	-0.916819674
C	1.9099414917	-3.0312946036	0.46107871
C	2.782748068	-2.9273314294	-0.6307945204
H	2.4537377737	-2.4308420076	-1.5413432312
C	4.0672145752	-3.45589142	-0.5554171257
H	4.7293354674	-3.3784786892	-1.4131396368
C	4.5076293835	-4.0668124447	0.6183074678
H	5.513579268	-4.4732127067	0.6771307386
C	3.6549673126	-4.1498375249	1.715511561
H	3.9918649841	-4.619565407	2.6356604251
C	2.3586952759	-3.6415368234	1.6372675844
H	1.6982660437	-3.728736322	2.4951578136
C	0.0564243801	0.2514190928	4.9772665843
N	0.0445184554	0.2812308046	6.1449364723

XYZ coordinates of the optimized structure of **5CN'**

104

Pd	0.0129563358	0.1330297674	-0.0201830118
P	2.3058949185	0.4851770901	0.0399868884

Cl	-0.1487828216	0.0032203245	-2.4679642608
Bi	0.1052616778	-0.0655725265	2.6297517094
P	-2.2674556461	0.4062305536	0.3243558798
P	1.5499420902	-3.069999608	1.6354188712
C	2.2652895979	0.5660160912	2.886962351
C	3.007850067	0.7492812677	1.7211474801
C	4.3335073605	1.1973318686	1.8277818242
H	4.9229776875	1.3607210056	0.9289914437
C	4.9026334195	1.4396301964	3.0725013146
H	5.9298644917	1.7866610184	3.1375589515
C	4.1511860429	1.2415714206	4.2274516289
H	4.5869863439	1.4317146897	5.204429792
C	2.8301814137	0.8068447308	4.1353831351
H	2.2450219735	0.6611201278	5.038292359
C	3.4197958063	-0.7173349883	-0.7672906392
C	3.2878009368	-0.9165972445	-2.1492901161
H	2.5373620738	-0.362042712	-2.7057292707
C	4.1022336152	-1.8336960554	-2.8056686664
H	3.9938450353	-1.9752270522	-3.8774104178
C	5.0492217345	-2.5676430143	-2.093382527
H	5.687060272	-3.2807220524	-2.6082626368
C	5.1726323433	-2.3858311794	-0.7184967191
H	5.9069795399	-2.9554614744	-0.155408451
C	4.359556648	-1.468916248	-0.0540214606
H	4.463640668	-1.3432199573	1.0192734608
C	2.6694389887	2.0864011807	-0.7781579063
C	1.7921898388	3.1522426869	-0.5380720159
H	0.9082794145	2.9942619832	0.0763664171
C	2.0417547337	4.4068915616	-1.08393632
H	1.3548721155	5.2258894601	-0.8891153486
C	3.1645006256	4.6085829661	-1.8855566782
H	3.355585584	5.5864326807	-2.3186904792
C	4.037515725	3.5528645059	-2.1328378463
H	4.9130271761	3.7032987701	-2.7584309731
C	3.7957227065	2.2966709968	-1.5796045033
H	4.4836548867	1.4811025285	-1.7824130652
C	-1.6838366742	1.2730688842	2.942297593
C	-2.5809144934	1.3542589088	1.8707562956
C	-3.7205363004	2.1613353227	1.9943864753
H	-4.4253956897	2.2369393413	1.1704091433
C	-3.9462513933	2.8867667196	3.1610519657
H	-4.8258766043	3.519409002	3.2394441747
C	-3.045052587	2.8033200564	4.2182365245
H	-3.2121199968	3.3769493385	5.1258574938
C	-1.9198061306	1.9853859156	4.1138898833
H	-1.2296337828	1.9059694316	4.9489161823
C	-3.0581038391	1.4214762674	-0.971103872
C	-2.5966341175	2.7300627335	-1.165830305
H	-1.804126563	3.1277418988	-0.5363079239

C	-3.1474145257	3.5254883068	-2.1632847787
H	-2.7864456676	4.5404765899	-2.3038782703
C	-4.1547258135	3.0187960789	-2.9852002047
H	-4.5813988308	3.6399498177	-3.7677605989
C	-4.6086879566	1.7162416906	-2.8029008701
H	-5.3902515109	1.3153051515	-3.4421908937
C	-4.0636288049	0.9166598473	-1.7987721538
H	-4.4229578835	-0.0993499921	-1.665015763
C	-3.276538038	-1.1107883391	0.4355605458
C	-2.7794904757	-2.2729677355	-0.1648210258
H	-1.8079762358	-2.2549051564	-0.6529613939
C	-3.5238030324	-3.4494804649	-0.1337604195
H	-3.1291773984	-4.3475733313	-0.6005346983
C	-4.7629218091	-3.4735660172	0.5019690536
H	-5.3411142915	-4.3929760181	0.5309475903
C	-5.2595334537	-2.3199790139	1.1071518394
H	-6.2231866644	-2.3380664174	1.6086009702
C	-4.5207464307	-1.1409030363	1.0757720138
H	-4.9112221649	-0.24910585	1.5583740772
C	-0.6703131014	-2.1267810447	3.0262920198
C	-0.0473695789	-3.2702555826	2.5238030302
C	-0.6538822892	-4.5158576648	2.7444471371
H	-0.183250606	-5.4174145173	2.3609648771
C	-1.8532348392	-4.6077902151	3.4403011291
H	-2.3155997494	-5.5787386196	3.5954509391
C	-2.4580561203	-3.4564311803	3.9439591729
H	-3.3936519035	-3.5244854955	4.4923613251
C	-1.8628949682	-2.2139624848	3.7452529053
H	-2.3320093682	-1.3222546762	4.1547288973
C	1.380182904	-4.238203478	0.227832328
C	0.9393484185	-3.6987606176	-0.9881325903
H	0.7681875343	-2.6274472611	-1.077498107
C	0.7248599868	-4.5214653623	-2.0918513875
H	0.3809798593	-4.08676804	-3.0266877842
C	0.9644185087	-5.8905866332	-1.9989971251
H	0.8043329095	-6.5321587463	-2.861337097
C	1.419126568	-6.4343334678	-0.7989453757
H	1.6129101047	-7.5010570985	-0.7224845127
C	1.6247257621	-5.6152879768	0.3086191132
H	1.9861395525	-6.0507345714	1.2366239694
C	2.7355487013	-3.8961100604	2.7700226348
C	3.9549560796	-4.3800896672	2.2726438398
H	4.1475731078	-4.3664769805	1.2030275922
C	4.9205935049	-4.8920451558	3.1344152413
H	5.8539837606	-5.2734249953	2.728456153
C	4.6934232582	-4.9161990429	4.5090719148
H	5.4482278614	-5.3146746225	5.1813841454
C	3.4926608775	-4.4248094703	5.014861429
H	3.305270749	-4.4371480822	6.0852889934

C	2.5207658166	-3.918287297	4.154578682
H	1.5892916421	-3.5402839206	4.567475273
C	0.1156853787	-0.0759365811	5.093273006
N	0.0656846656	-0.2064837639	6.254166535

XYZ coordinates of the optimized structure of **[5]**BMe_4

119

Pd	0.0103160496	-0.021125122	0.0188424923
P	-2.2860699829	0.3357295331	0.3685253304
Cl	-0.0407840491	0.0653968175	-2.349721486
Bi	0.0848542886	-0.0555784221	2.5858708546
P	2.3452772672	0.2400963742	0.1458758845
P	1.5259148108	-2.9556041642	2.8822245951
C	-1.5277450815	1.4461131218	2.8606258689
C	-2.4527040242	1.4890920526	1.802557231
C	-3.5125994416	2.4022744281	1.8594998659
H	-4.2313842555	2.4542654486	1.0463541207
C	-3.6466733421	3.2538726729	2.9539716987
H	-4.4700433164	3.9613729526	2.9843982893
C	-2.7306118849	3.2022286407	4.0002500916
H	-2.8311908468	3.874192974	4.8477634878
C	-1.673092308	2.2931242545	3.9577263924
H	-0.9576317306	2.2675879104	4.77591052
C	-3.1804311738	1.145417383	-0.991385126
C	-2.6732323874	2.3475552675	-1.502678298
H	-1.7615119023	2.7747525937	-1.0926961004
C	-3.331480733	2.9932781942	-2.5419290751
H	-2.9354755821	3.9259129744	-2.9330509043
C	-4.4886885346	2.4378409746	-3.0889439257
H	-4.9977350686	2.9411028941	-3.9059993116
C	-4.9870446339	1.2371432631	-2.5925002261
H	-5.8853227573	0.7997435531	-3.0185321382
C	-4.3366917457	0.5883862406	-1.5440597135
H	-4.7324834836	-0.3472381616	-1.1603743498
C	-3.2325933255	-1.1571619878	0.8061769739
C	-2.8054514534	-2.3844603177	0.2841765153
H	-1.9205468609	-2.4290422061	-0.3470141416
C	-3.5112448573	-3.5483888703	0.5762376786
H	-3.1710215946	-4.4975666448	0.173432023
C	-4.6362997341	-3.4939940558	1.3964636754
H	-5.1822540616	-4.4038150485	1.6293899282
C	-5.0594202844	-2.275544146	1.9247347349
H	-5.9335987314	-2.2331340672	2.568062826
C	-4.3619253075	-1.1070384217	1.6323299223
H	-4.6947313619	-0.1611443969	2.0510635205
C	2.0850417836	0.7944597442	2.9362617114
C	2.9125614153	0.8245730348	1.8065143026
C	4.2105917217	1.3382210322	1.9368878426
H	4.8647272723	1.3914761707	1.0704239151

C	4.6696603866	1.7870462559	3.1714648519
H	5.6784138995	2.179690373	3.2576066321
C	3.8402798111	1.7377677405	4.2896177062
H	4.1982000516	2.0943186394	5.2511601671
C	2.5437824402	1.2393086531	4.175004521
H	1.9011322653	1.207869887	5.0507403437
C	2.9224412737	1.5630348823	-0.9686534801
C	2.1852456937	2.7532916609	-1.0116587976
H	1.2713342815	2.8485830381	-0.4295075019
C	2.6136797021	3.8100656302	-1.8063032384
H	2.037681075	4.730558378	-1.8357216541
C	3.7730340054	3.6832890274	-2.5716798404
H	4.1025396051	4.5073941141	-3.1979849718
C	4.5043099674	2.4997002362	-2.5365124931
H	5.4062544351	2.3962845198	-3.1329365896
C	4.0842718172	1.439184429	-1.7353510097
H	4.6607155552	0.5188704648	-1.7142438277
C	3.325464273	-1.2376414953	-0.2639580561
C	3.1142624363	-1.8248033141	-1.5209462137
H	2.3963231051	-1.3874005329	-2.2110464301
C	3.8193840604	-2.9688139865	-1.8797042921
H	3.6574152524	-3.4146704417	-2.8568860231
C	4.724299518	-3.5440296131	-0.986896182
H	5.2699200261	-4.4401482515	-1.2683006161
C	4.9246800596	-2.9712407924	0.2662021464
H	5.6214136083	-3.4190275088	0.9690301068
C	4.2288501893	-1.8193821601	0.6303898058
H	4.3910062255	-1.3840185116	1.6112193581
C	-0.3387275424	-1.4569024056	4.2446253122
C	0.4123511702	-2.6364224709	4.3027431267
C	0.2583868055	-3.4699239898	5.4166251852
H	0.8546598615	-4.3754396389	5.4982474237
C	-0.6536252442	-3.1432812402	6.417512592
H	-0.7672191791	-3.7981515529	7.2766302681
C	-1.4244958476	-1.9867495281	6.3184394968
H	-2.1385364784	-1.7384780543	7.0983950035
C	-1.2704273563	-1.131987031	5.2271314814
H	-1.8623377774	-0.2228272197	5.1638492604
C	2.9842801407	-3.7608433581	3.6433572953
C	3.2170919183	-5.1391769934	3.5939435502
H	2.5025583343	-5.7939854518	3.1028381065
C	4.3661184812	-5.6772715857	4.1709790036
H	4.5373619711	-6.749417446	4.1272931601
C	5.2889329635	-4.8474253806	4.802434173
H	6.1839345689	-5.2699077109	5.2505354239
C	5.0650965395	-3.4719313626	4.8532852135
H	5.7850398231	-2.8192356435	5.3393022405
C	3.9245965915	-2.9299088578	4.2699396915
H	3.7643459632	-1.8536253689	4.2998017501

C	0.7023100097	-4.2885990621	1.9324775022
C	1.0833763304	-4.4218642463	0.5894508899
H	1.8287358773	-3.7514212673	0.1677384991
C	0.5169860481	-5.4105354143	-0.2102771778
H	0.826351631	-5.5064750451	-1.2474322412
C	-0.448068837	-6.2669338694	0.3171392173
H	-0.893835287	-7.0359770572	-0.3076613312
C	-0.8420733593	-6.1321858533	1.6468056011
H	-1.5960308771	-6.7954351584	2.0619803659
C	-0.2703734618	-5.1497208551	2.4527186713
H	-0.5898647917	-5.0549330672	3.4864913862
B	0.561654941	2.5869997472	8.1127834635
C	1.0578822691	3.6222512848	6.9266348729
C	-1.0875614724	2.5617534137	8.1728836607
C	1.123729646	1.067673541	7.7925489999
C	1.1571575909	3.0932411811	9.5651491398
H	-1.4771241805	1.8850798141	8.9538862456
H	-1.5503652593	2.2265773908	7.2265568191
H	-1.5226491867	3.553713977	8.3876568958
H	2.1577617307	3.6787737081	6.8390129494
H	0.7142422949	4.6586969406	7.0905731786
H	0.6927124711	3.342425991	5.9215726691
H	0.8570448175	2.4370325519	10.4009445306
H	0.8167464447	4.1075459606	9.8382250039
H	2.2605892105	3.1268009734	9.5867749839
H	0.8571067033	0.3350459418	8.5741971231
H	2.2239157221	1.0265826047	7.7023576591
H	0.7216058479	0.6505429299	6.8512886567

XYZ coordinates of the optimized structure of **6**

102

Pt	-0.0205728298	-0.0673186245	0.0840168976
P	-2.291676476	0.3031334853	0.3957020909
Cl	-0.0899038695	-0.089057798	-2.2983578643
Sb	0.075869535	0.0308184515	2.5847149752
P	2.288249308	0.2337237577	0.1325424589
P	1.4870656515	-2.8497786552	2.8259370002
C	-1.4758344766	1.4914413815	2.8322310922
C	-2.4302482753	1.5019938025	1.7955870151
C	-3.4871117682	2.4161204306	1.8459150756
H	-4.2239996863	2.4406175012	1.0478111811
C	-3.593287708	3.3097645157	2.9097602589
H	-4.414395946	4.0200877918	2.9336644206
C	-2.6487997481	3.2979965216	3.9311769567
H	-2.7255856017	4.0024085115	4.7542858068
C	-1.5937566565	2.386564012	3.8957939156
H	-0.859840287	2.3958475754	4.6973207934
C	-3.171956799	1.0987018343	-0.9836825481
C	-2.6232989303	2.2610513416	-1.5416262645

H	-1.687755651	2.6609307461	-1.1588918721
C	-3.2696454752	2.8999894358	-2.5924787702
H	-2.8407783615	3.8014312929	-3.0203919681
C	-4.4578227211	2.3770929561	-3.1039222922
H	-4.9579178931	2.874628056	-3.9299978411
C	-4.9988558765	1.2161675403	-2.5601947109
H	-5.9213328333	0.8036641014	-2.9584466419
C	-4.3600688462	0.5751568285	-1.4997912304
H	-4.7899485444	-0.3287346682	-1.0786717942
C	-3.2831910452	-1.1447601339	0.8816780785
C	-2.8815247999	-2.4041773348	0.4212464198
H	-1.9787458696	-2.4989342325	-0.1776385523
C	-3.6336057465	-3.5325794882	0.7369652204
H	-3.3139017126	-4.5068197305	0.3800575462
C	-4.7795289586	-3.4100757471	1.5197899889
H	-5.3621381793	-4.2920732523	1.7704127828
C	-5.1767723188	-2.1589745089	1.9886987249
H	-6.0668400149	-2.0633946779	2.6038954229
C	-4.4333475812	-1.0261434269	1.6714994033
H	-4.7472556036	-0.0544473199	2.0430703424
C	2.0213931593	0.8244152937	2.9098739082
C	2.8584422173	0.8399620187	1.7829355843
C	4.1573141205	1.3455847786	1.9126461051
H	4.8153030467	1.3857867473	1.0485139159
C	4.6155648041	1.8050210147	3.1441672645
H	5.6261649619	2.1929760579	3.2295804142
C	3.782788932	1.770867572	4.260011959
H	4.1404374801	2.1323058078	5.2196538933
C	2.483975353	1.2801908714	4.1449911134
H	1.8408599668	1.2578184483	5.0206333937
C	2.8200467509	1.560359548	-1.0009407334
C	2.0136677686	2.7000973599	-1.106801714
H	1.0720633577	2.7456501905	-0.5649897896
C	2.4082959805	3.7611526183	-1.9136027021
H	1.7764949626	4.6409652422	-1.9947126496
C	3.605304357	3.689074627	-2.6255826845
H	3.9092256832	4.5157900431	-3.261376155
C	4.4071752819	2.5555279482	-2.5269241713
H	5.3380406037	2.4942717723	-3.0833958411
C	4.0197226318	1.4911852583	-1.7150083093
H	4.6496135948	0.6088035614	-1.6472954576
C	3.3164524169	-1.2134897494	-0.278214756
C	3.140740177	-1.7919264376	-1.5445453834
H	2.4300851346	-1.3603803894	-2.2453223282
C	3.8684998732	-2.9229614058	-1.8987186151
H	3.7307974759	-3.3634647313	-2.8819962045
C	4.7644290673	-3.4924762951	-0.9935418383
H	5.3277975149	-4.3787160315	-1.2712903685
C	4.933224284	-2.9262836751	0.2669493624

H	5.6232612323	-3.3690769315	0.9795111739
C	4.2127390017	-1.7882758724	0.6270670518
H	4.349257542	-1.3601690682	1.614905043
C	-0.3622328058	-1.3353843899	4.1738533453
C	0.3746228882	-2.5268435239	4.2447392132
C	0.208724341	-3.357736907	5.3568582032
H	0.7970983014	-4.2679168188	5.4433144201
C	-0.7050447124	-3.0216708401	6.3534355312
H	-0.8288952017	-3.6742596962	7.2129238725
C	-1.4639384544	-1.8580519862	6.2486483498
H	-2.1797038621	-1.6020857916	7.0243718811
C	-1.2949213773	-1.0066009842	5.1580041207
H	-1.8772685764	-0.0916188548	5.0933520511
C	2.9287612681	-3.688957157	3.5829556159
C	3.1526651686	-5.0667544094	3.4954750095
H	2.4389130121	-5.7018251294	2.9781963466
C	4.291785082	-5.6301215269	4.0682843561
H	4.4556426509	-6.7017967479	3.9947054666
C	5.2139458622	-4.8262419274	4.7331614217
H	6.1010892891	-5.2683269093	5.1779595894
C	4.9994528844	-3.4511037418	4.821543813
H	5.718970303	-2.8181431406	5.3336184509
C	3.8690081834	-2.8838699734	4.2427794451
H	3.7171843591	-1.8075716147	4.3018073613
C	0.6383219132	-4.1555204498	1.8605855108
C	0.9493368947	-4.2255394344	0.4954053416
H	1.6567978119	-3.5217027645	0.0637306489
C	0.3611390286	-5.1938699106	-0.3138983486
H	0.613230436	-5.2380872165	-1.3697974811
C	-0.5521251128	-6.0956389506	0.2288009677
H	-1.0137946551	-6.84980037	-0.402607302
C	-0.8755215413	-6.025452719	1.5826675884
H	-1.5897963218	-6.7241928567	2.0096782697
C	-0.2850786843	-5.0609409042	2.3960136416
H	-0.5524851764	-5.0135771331	3.4476593663

XYZ coordinates of the optimized structure of **6F**

103

Pt	0.0303073992	0.0410623654	-0.0174642711
P	2.0372053939	1.2660764623	0.0696528823
Cl	0.0435458133	-0.2128856033	-2.4979041062
Sb	0.0006251445	0.1904507539	2.5739045881
P	-2.0236941597	1.1667960989	-0.0106054403
P	0.2154706871	-2.2755307322	0.2901463171
C	2.097119911	0.6810740284	2.8270921832
C	2.8474617147	1.0840895073	1.7157191613
C	4.1893790831	1.4471380932	1.8913369061
H	4.7718440915	1.7957254754	1.0428833936
C	4.7899953147	1.3599759184	3.1419301377

H	5.8359203367	1.6304133573	3.2580124461
C	4.0466432555	0.9339205351	4.2397807442
H	4.5102912973	0.8627616473	5.2199635254
C	2.7013422815	0.6117716133	4.0867545958
H	2.1096701606	0.3102783923	4.9426230893
C	3.3025932405	0.7962940907	-1.1645464284
C	3.1851633916	1.2987407484	-2.4690561263
H	2.3860310335	1.9918247359	-2.7151386182
C	4.0889710908	0.9204803113	-3.4562585862
H	3.9881529028	1.3253955255	-4.4594780415
C	5.1157398432	0.0254055993	-3.1601774499
H	5.8242071999	-0.2667498839	-3.9304993165
C	5.2219063185	-0.4995500146	-1.8756739816
H	6.0089592663	-1.2099034317	-1.6381246078
C	4.3171866907	-0.1245352402	-0.8844730628
H	4.4056634761	-0.5583055498	0.1070237346
C	2.0246514603	3.1131566008	-0.0325906685
C	0.943285154	3.7960349927	0.5337297519
H	0.1024560103	3.2348031896	0.9321061432
C	0.9280637321	5.1869630954	0.5893090374
H	0.0785298891	5.6972830845	1.0350056679
C	1.9913719587	5.9172386702	0.0642904006
H	1.977754394	7.0032019521	0.0969641293
C	3.0724397517	5.2479566471	-0.5050837384
H	3.907086335	5.8096012198	-0.9161610928
C	3.0949738151	3.8557430787	-0.5467618999
H	3.9490029434	3.3515955437	-0.9890262783
C	-1.498483832	1.7517968449	2.7098611599
C	-2.2526821032	2.0875842961	1.5761235244
C	-3.1941823234	3.1205481393	1.6687323869
H	-3.7857042936	3.395927792	0.8015848318
C	-3.3730156833	3.8182676408	2.8586515596
H	-4.098912888	4.6253636473	2.9054928885
C	-2.6214239303	3.480789998	3.9801537531
H	-2.7531130067	4.0238457373	4.9120735949
C	-1.6939329452	2.4452544432	3.9083933021
H	-1.112970282	2.1687351425	4.7797318678
C	-2.3114830245	2.428477223	-1.316720767
C	-1.205026574	2.9704768928	-1.9771166223
H	-0.2149788114	2.5933264071	-1.745707388
C	-1.3696627461	3.9668218789	-2.9365281929
H	-0.4984791029	4.3757106752	-3.4410061085
C	-2.6445022682	4.4255046946	-3.2561648052
H	-2.77410601	5.1986948433	-4.0086280715
C	-3.7564440191	3.8806784207	-2.6165061178
H	-4.7557252357	4.2258643258	-2.8675119019
C	-3.5929111425	2.8869380891	-1.6557214796
H	-4.4720113519	2.4587787236	-1.1820022258
C	-3.5552044833	0.1520546333	-0.0972174572

C	-4.0701388067	-0.2385860963	-1.3416407329
H	-3.6091678081	0.1199042563	-2.2583053516
C	-5.1756335784	-1.082149824	-1.415306071
H	-5.5694521806	-1.3652252872	-2.3879087613
C	-5.774071583	-1.5592068352	-0.2509304252
H	-6.6361323656	-2.2177298683	-0.3098991054
C	-5.2612784115	-1.1861151672	0.9893018238
H	-5.7217083581	-1.5515881197	1.9031720489
C	-4.1610860173	-0.3351533367	1.067365788
H	-3.7789906908	-0.047283756	2.0432677656
C	-0.5985763882	-1.8512407735	2.9511813413
C	-0.4832504681	-2.7862255609	1.9162227495
C	-0.8818808194	-4.1095731697	2.1412761209
H	-0.7932355158	-4.8449744321	1.3466973959
C	-1.4078068765	-4.4893921285	3.3719729489
H	-1.7277784132	-5.5160885493	3.5271832653
C	-1.5230563533	-3.5546787788	4.3974333435
H	-1.9369894388	-3.8461116071	5.3589906689
C	-1.108498001	-2.2411557646	4.1927915724
H	-1.1790878929	-1.5123719713	4.9914624024
C	-0.6394185328	-3.3928734561	-0.8872828701
C	-1.859474701	-2.9669916533	-1.4192013245
H	-2.2241654498	-1.9728147949	-1.1829700332
C	-2.597178341	-3.8023499943	-2.2522246571
H	-3.5446134084	-3.4553787957	-2.6556002204
C	-2.1166416622	-5.0697940924	-2.5745162048
H	-2.6876250498	-5.71939197	-3.2324668772
C	-0.8986040391	-5.5003010774	-2.0537890841
H	-0.5170314941	-6.4875657668	-2.2999654412
C	-0.1631912464	-4.6691402845	-1.2113438992
H	0.7836902284	-5.0192687141	-0.8111143881
C	1.9185671587	-2.9642428069	0.3430140496
C	2.6309497312	-3.104448947	-0.8558743988
H	2.1664383581	-2.8293998782	-1.7995489288
C	3.9296414175	-3.6026894625	-0.8484872775
H	4.4637851173	-3.7181906589	-1.7874236015
C	4.5472473973	-3.9378978704	0.3555979308
H	5.5631707475	-4.32342835	0.3594391876
C	3.856559216	-3.7738350425	1.5534077329
H	4.3306468714	-4.0286076738	2.4974857432
C	2.5465923197	-3.2969875513	1.5486384001
H	2.0138965831	-3.1916783081	2.4896528356
F	-0.0319028189	0.3192505521	4.6270816867

XYZ coordinates of the optimized structure of **6F'**

103

Pt	-0.0016826962	0.1509511432	0.0324732765
P	2.2723879653	0.4862980976	0.0370930226
Cl	-0.1587867439	0.1584790367	-2.423663381

Sb	0.0863626803	-0.0762487925	2.6158588314
P	-2.2639887883	0.4073329195	0.3213945523
P	1.5917961976	-3.0504792324	1.6333548595
C	2.1588287287	0.5418029876	2.8678754613
C	2.9412248635	0.7500448764	1.7258900404
C	4.2594255103	1.205114838	1.8628848645
H	4.8651337224	1.3867905743	0.9785219889
C	4.8023369961	1.4321512586	3.1222634167
H	5.8255203948	1.7853973229	3.2141591693
C	4.0277099866	1.2084432181	4.2572036944
H	4.444133089	1.3839607645	5.2454752715
C	2.7124530282	0.7678516418	4.1317280544
H	2.1015889241	0.5989338152	5.009627831
C	3.3872432561	-0.7272585793	-0.7578655351
C	3.2461791692	-0.9490019261	-2.1351647027
H	2.4880798378	-0.4076984536	-2.6944912955
C	4.0658124139	-1.8661435147	-2.7850914321
H	3.9481468612	-2.0274801409	-3.8530528331
C	5.0313751745	-2.5736657784	-2.0711504857
H	5.6743244407	-3.2858088858	-2.5810249543
C	5.1677489388	-2.3656722321	-0.7011956379
H	5.9181171826	-2.9131996232	-0.1371921132
C	4.3468596878	-1.4508947498	-0.0431837013
H	4.4589241621	-1.3055255515	1.0267772045
C	2.6646195885	2.0719184679	-0.799586177
C	1.7784939814	3.1418943679	-0.6229485011
H	0.8684017874	2.9914301686	-0.0466641601
C	2.0521154733	4.3833799447	-1.1870497759
H	1.3551227486	5.2048343821	-1.0461499156
C	3.2108290239	4.568185606	-1.9397249735
H	3.4212034814	5.5358145318	-2.3868751975
C	4.0947128511	3.5082025281	-2.1221533241
H	4.9976722222	3.6451061214	-2.7108061003
C	3.8265424881	2.2644773404	-1.5532577839
H	4.5213565001	1.4441605937	-1.7081027927
C	-1.6330812343	1.2115280517	2.933591796
C	-2.5595059052	1.3238844219	1.885080277
C	-3.697907273	2.1233907523	2.0441884493
H	-4.4139867406	2.2201136011	1.2321110969
C	-3.9062351521	2.8182885915	3.2324814426
H	-4.7849055464	3.4478145582	3.3417900846
C	-2.9864742847	2.7080492742	4.2716193914
H	-3.1429695117	3.2548056694	5.1976815204
C	-1.8612964985	1.8976989359	4.1275253244
H	-1.1532967072	1.7917258221	4.9416218432
C	-3.0717480371	1.4424978778	-0.9497073175
C	-2.587989052	2.7415725239	-1.1534403376
H	-1.7567966939	3.111131215	-0.5578796015
C	-3.1604275187	3.5581954783	-2.1208047419

H	-2.7795691767	4.5644996123	-2.2709449562
C	-4.2142805025	3.0832673811	-2.9023839437
H	-4.6582888401	3.7211641154	-3.6615736705
C	-4.6916066977	1.7905840492	-2.7111618827
H	-5.5087660098	1.4137760885	-3.3199637415
C	-4.1237388833	0.9697599317	-1.7370869679
H	-4.5029345537	-0.0377652094	-1.594760808
C	-3.265611482	-1.1171195007	0.4093264013
C	-2.7654391664	-2.2678748125	-0.2099935623
H	-1.7938910065	-2.2379540413	-0.6970485117
C	-3.5054371795	-3.4472754749	-0.1972980236
H	-3.107633993	-4.3363683119	-0.678471875
C	-4.7450947054	-3.4854149169	0.4368877029
H	-5.3202914614	-4.4071028942	0.4511820428
C	-5.246314718	-2.3426635085	1.0584892974
H	-6.2108121648	-2.3714143694	1.5578593812
C	-4.5106599021	-1.1612242291	1.0467831322
H	-4.904341317	-0.278147895	1.5427904933
C	-0.6468576975	-2.0768965776	2.9759893914
C	-0.0204869553	-3.2330718559	2.4965862098
C	-0.6243953599	-4.4787956414	2.7172500201
H	-0.1447593244	-5.3807939167	2.3457506006
C	-1.8318777087	-4.5727208188	3.3985072639
H	-2.2927665993	-5.5444530285	3.5542354389
C	-2.4449738397	-3.4187974397	3.8848976974
H	-3.3868595975	-3.4851574667	4.4228956334
C	-1.8513747324	-2.1770819398	3.6815796848
H	-2.331494744	-1.2843724047	4.0736511951
C	1.4290160682	-4.2270527462	0.2300995853
C	0.9700016301	-3.6961081326	-0.983056866
H	0.7787703881	-2.6276750999	-1.0667947476
C	0.763627948	-4.5215793584	-2.085775133
H	0.4061586528	-4.0935183274	-3.0186024862
C	1.0295239449	-5.8860976033	-1.9957469897
H	0.8764715676	-6.5300295361	-2.8576784107
C	1.5011328003	-6.4217495632	-0.7987119663
H	1.7145036141	-7.4849247207	-0.7238144025
C	1.6982270413	-5.5994705128	0.308237793
H	2.0718061394	-6.0288763568	1.2342088187
C	2.753845222	-3.8857703434	2.7864154176
C	3.9881499967	-4.3546742135	2.3107228564
H	4.2039575865	-4.3255211523	1.245754565
C	4.9390093063	-4.8702185098	3.1864801302
H	5.8839956759	-5.2392851216	2.796126816
C	4.6828332482	-4.912802366	4.555717514
H	5.4263115499	-5.3133736281	5.2393807553
C	3.4675640133	-4.4367026101	5.0408659198
H	3.2574974319	-4.4634074883	6.1069218249
C	2.5102793889	-3.9272890807	4.1657606884

H 1.56688967 -3.5615836441 4.5620362324
F 0.1238804599 -0.0576006695 4.6969124486

XYZ coordinates of the optimized structure of **6CN**
104
Pt 0.0695799871 0.0614119724 -0.0379109262
P 2.0503815929 1.3153586733 0.0304449952
Cl 0.0772264635 -0.1709691772 -2.5172283322
Sb 0.0675457374 0.192341833 2.5611061588
P -2.019551467 1.1217794388 0.0261112455
P 0.2326887206 -2.25542481 0.2804130375
C 2.2084893936 0.581243545 2.7581083407
C 2.908735659 1.0618158079 1.6430143142
C 4.2592741419 1.4065800431 1.7833043871
H 4.8013720158 1.8210609175 0.9380675796
C 4.9242611559 1.2112757853 2.9883462364
H 5.9763694974 1.468495261 3.0728354732
C 4.2366555004 0.6869790684 4.0782582714
H 4.7485125795 0.5179455689 5.0215034342
C 2.8802661541 0.3935036576 3.9676999475
H 2.3485829928 0.0223995385 4.8372434347
C 3.2841456931 0.9032991664 -1.2572988914
C 3.117174972 1.4536081907 -2.536409891
H 2.306122771 2.1501970344 -2.7271990559
C 3.9869119443 1.1198916172 -3.5693283167
H 3.8466638587 1.5612163783 -4.552208613
C 5.0290820995 0.2219931696 -3.3452466241
H 5.7100878658 -0.0363324314 -4.1515184935
C 5.1884874112 -0.3461899418 -2.0846587763
H 5.993810054 -1.0523494988 -1.9010148686
C 4.3188458717 -0.0140954866 -1.0477013293
H 4.4525143049 -0.4763537795 -0.075041269
C 2.0228023412 3.1634467448 -0.0232597689
C 0.9166843178 3.830250217 0.5116631945
H 0.0660369844 3.2571662169 0.867993761
C 0.8910524244 5.2204291068 0.5898864539
H 0.0216660675 5.7183575808 1.0105919458
C 1.9698481143 5.9646722266 0.120174811
H 1.9491098596 7.0498029949 0.1712559597
C 3.0761806576 5.3110648733 -0.4192838232
H 3.9221133628 5.884325324 -0.7890774182
C 3.1074739722 3.9205969243 -0.485416911
H 3.9779908447 3.4288088546 -0.9094151086
C -1.3718079529 1.8224143565 2.6996755766
C -2.1852556757 2.0969875462 1.5893577744
C -3.113479803 3.1421368491 1.6712765761
H -3.7553327872 3.3638962316 0.8245743735
C -3.2112390032 3.9241121232 2.8177831931
H -3.9269766601 4.7406145203 2.8539866894

C	-2.3866992156	3.6611151236	3.9062648426
H	-2.4441017286	4.2744232078	4.8011306375
C	-1.4803460861	2.6054424676	3.8501077353
H	-0.855235373	2.3994126837	4.7124673233
C	-2.4003088463	2.3413267326	-1.2943932953
C	-1.3342941752	2.9355040486	-1.976827368
H	-0.321150884	2.617458811	-1.7549688212
C	-1.5678522776	3.9096508992	-2.9444699682
H	-0.7282136366	4.3605007939	-3.4663294165
C	-2.8709302299	4.2923713389	-3.2508598919
H	-3.0539076945	5.0473077275	-4.0106973303
C	-3.9415859519	3.696491453	-2.5870203538
H	-4.9617899576	3.9847052733	-2.8253436412
C	-3.7096784603	2.7265019303	-1.6158460436
H	-4.5558702236	2.2627407533	-1.1165276071
C	-3.5233140938	0.064991588	0.0529974879
C	-4.0759839705	-0.4005168178	-1.1488780874
H	-3.6642185044	-0.0728936113	-2.1002332156
C	-5.1566673345	-1.2781294543	-1.1364598296
H	-5.579882505	-1.6202262657	-2.077131922
C	-5.6927030483	-1.7148437683	0.0733275126
H	-6.535257381	-2.4006143147	0.0816953113
C	-5.1431468472	-1.2661277295	1.2718451427
H	-5.5548334488	-1.5994804797	2.2205679371
C	-4.0678755511	-0.3802952419	1.2634937455
H	-3.6578238245	-0.0333713901	2.2082406212
C	-0.733152462	-1.8039821675	2.8831104307
C	-0.6179668801	-2.732664986	1.8408622805
C	-1.1544524896	-4.0149017051	2.003483379
H	-1.0581934851	-4.7454140081	1.2052491083
C	-1.8269815948	-4.3576850222	3.1727709012
H	-2.2537725482	-5.3512040446	3.2780065994
C	-1.9533769355	-3.4263019819	4.1982716819
H	-2.4868145974	-3.6822670092	5.1095039232
C	-1.394747283	-2.1573808943	4.0595151472
H	-1.4829264519	-1.4465003709	4.8745774225
C	-0.5235116193	-3.3747182398	-0.9595230246
C	-1.7329206928	-2.9825328158	-1.5406716099
H	-2.1500737056	-2.0114103892	-1.2966188024
C	-2.3949312912	-3.8238128026	-2.4287332666
H	-3.3358930356	-3.5055782616	-2.8695166623
C	-1.8467771256	-5.0618560072	-2.7591763676
H	-2.3584847619	-5.715757044	-3.4601798231
C	-0.638358691	-5.4569414729	-2.1908854975
H	-0.2049940343	-6.4210003737	-2.4430434642
C	0.0207952844	-4.6205995317	-1.2916528362
H	0.9593381232	-4.9437835461	-0.8514704451
C	1.9130774842	-2.9677057893	0.4876807287
C	2.779006444	-2.9433190601	-0.6142915769

H	2.4496550756	-2.5023102442	-1.5525479273
C	4.0575239498	-3.481811855	-0.5153204652
H	4.7132848691	-3.467974684	-1.3814982774
C	4.5001159682	-4.0234908805	0.6913705635
H	5.5016615755	-4.4377057399	0.7683227169
C	3.6546736312	-4.0280876285	1.7968089583
H	3.9926577315	-4.4441036567	2.7420729555
C	2.3634876988	-3.5110326645	1.695303577
H	1.708062608	-3.5386253363	2.5610130556
C	0.0726212842	0.3012417576	4.8998206453
N	0.064905373	0.3361331791	6.0665550938

XYZ coordinates of the optimized structure of **6CN'**

104

Pt	-0.0364438854	0.1044336373	0.007506543
P	2.2371464856	0.4290847067	-0.0125743204
Cl	-0.2219529108	0.0993811186	-2.4455169912
Sb	0.0865017722	-0.1568677453	2.5836809974
P	-2.2871563199	0.429214959	0.3331539084
P	1.6337000777	-3.0831154119	1.631673021
C	2.1544659816	0.5130901936	2.8251469863
C	2.9160944627	0.7195027617	1.668209333
C	4.2235084072	1.2098556977	1.780310451
H	4.8130254851	1.3870107199	0.8841527802
C	4.7759114315	1.4812136774	3.0269371063
H	5.7906510318	1.8621035819	3.0981589704
C	4.0186031147	1.2691084406	4.1744644399
H	4.4364255686	1.4830758411	5.1542758586
C	2.7148603678	0.7888334778	4.072175695
H	2.13406762	0.6307173068	4.975025882
C	3.3546448739	-0.7815713144	-0.8057181128
C	3.183445166	-1.0356737591	-2.173898754
H	2.4000660836	-0.522063795	-2.7247295421
C	4.0060979817	-1.9492694685	-2.8250167346
H	3.8656459002	-2.1359305064	-3.8860408669
C	5.0026816987	-2.6222016276	-2.1204771104
H	5.646945655	-3.3326587217	-2.6309597113
C	5.1685696302	-2.3824470503	-0.7589076432
H	5.943673192	-2.9032048751	-0.2030139358
C	4.3465666513	-1.4695436746	-0.0999653897
H	4.4824678365	-1.298427132	0.9634838342
C	2.6088117483	2.0140879726	-0.8598398119
C	1.7505890976	3.0951035304	-0.6210640894
H	0.8800782007	2.9545341306	0.01589791
C	2.0046445218	4.3362464505	-1.194124616
H	1.3305045421	5.1665994454	-1.0030728068
C	3.1157051552	4.5099832243	-2.0183785215
H	3.3108558373	5.4775270589	-2.4724596166
C	3.9719992698	3.4398448625	-2.2609984003

H	4.8386146136	3.5686368502	-2.9035884849
C	3.7239717611	2.1958944741	-1.6826267081
H	4.3982646668	1.3685409941	-1.8829977077
C	-1.5965161625	1.1672633869	2.9601758129
C	-2.5287667014	1.323360969	1.9212801158
C	-3.631323897	2.1665091527	2.1009343242
H	-4.3539791624	2.2939686989	1.2990666421
C	-3.7970378831	2.86423058	3.2946683032
H	-4.6487211794	3.5271983893	3.417913103
C	-2.8675991381	2.7158593434	4.3191532675
H	-2.9850989669	3.2673468144	5.2478702601
C	-1.7785678255	1.8607463335	4.1555051689
H	-1.0691406516	1.7349268009	4.9680417863
C	-3.0769104863	1.5219841264	-0.9012522603
C	-2.4275497845	2.7160830743	-1.2396740718
H	-1.4644437086	2.9535321258	-0.7954706365
C	-3.000751992	3.5897168488	-2.1557111284
H	-2.4886831157	4.5125438841	-2.4133860469
C	-4.2216153535	3.2745421727	-2.7529794556
H	-4.6654459325	3.954980364	-3.4743772261
C	-4.8653766787	2.0844615449	-2.4291485629
H	-5.8132018625	1.8308355002	-2.8956724678
C	-4.2972512843	1.2085096119	-1.5044496756
H	-4.8076183924	0.282199854	-1.2579373723
C	-3.3457315389	-1.0558231206	0.4056890381
C	-2.9496610115	-2.1725913752	-0.3394214056
H	-2.0229087314	-2.1388138622	-0.9076093624
C	-3.7367960333	-3.320466251	-0.3484072032
H	-3.4217953512	-4.1844650395	-0.9266688199
C	-4.9191497459	-3.3617339858	0.3879224755
H	-5.5305303356	-4.2598914401	0.3838338397
C	-5.314740073	-2.2539886439	1.1351147011
H	-6.233462381	-2.2855595723	1.7142319528
C	-4.5315652532	-1.1029659464	1.1463960312
H	-4.842111082	-0.2467702871	1.7391826685
C	-0.6827228774	-2.166883795	2.8633091637
C	-0.017684233	-3.3062243487	2.3999629416
C	-0.6164665791	-4.5622888776	2.5703952609
H	-0.1063338263	-5.4524145834	2.2107945588
C	-1.8556710868	-4.6781879246	3.1882226336
H	-2.3131342142	-5.6566096007	3.3070618383
C	-2.5052101695	-3.5385550917	3.6618476958
H	-3.4726010327	-3.6232505436	4.149291008
C	-1.9172006705	-2.287170743	3.508727083
H	-2.4267994083	-1.4077387944	3.8955901533
C	1.5905917586	-4.3021218862	0.2583409942
C	1.0957420914	-3.8401903123	-0.9687897051
H	0.8069632388	-2.7959388768	-1.0745613104
C	0.9745488805	-4.7040819943	-2.0539163454

H	0.5879589222	-4.3306910342	-2.9984979155
C	1.3614338578	-6.03705861	-1.9316622589
H	1.2748984158	-6.7102476271	-2.7803389187
C	1.8654406518	-6.5030604033	-0.7191479205
H	2.1695187338	-7.5416875591	-0.6181336746
C	1.9773324809	-5.6431181045	0.3712764663
H	2.3726814223	-6.018457953	1.311397854
C	2.7598734613	-3.8296781041	2.876146809
C	4.0505185582	-4.226257548	2.4931025416
H	4.3380189224	-4.1955442772	1.4450955421
C	4.9668194058	-4.6741382539	3.4399231608
H	5.9573295917	-4.9887249254	3.1215547531
C	4.6182567808	-4.7176068756	4.7886035146
H	5.3349437369	-5.0646303886	5.5278590953
C	3.3462458303	-4.3103147141	5.1820112598
H	3.0648082305	-4.3362877602	6.2314145124
C	2.4230991759	-3.8699359478	4.2356338707
H	1.4359105108	-3.5537075164	4.561563498
C	0.1302522035	-0.3363282598	4.9629063609
N	0.0895274066	-0.5651259315	6.10831499

XYZ coordinates of the optimized structure of **[6]**BMe_4

119

Pt	-0.0205728298	-0.0673186245	0.0840168976
P	-2.291676476	0.3031334853	0.3957020909
Cl	-0.0899038695	-0.089057798	-2.2983578643
Sb	0.075869535	0.0308184515	2.5847149752
P	2.288249308	0.2337237577	0.1325424589
P	1.4870656515	-2.8497786552	2.8259370002
C	-1.4758332473	1.4914429018	2.8322299489
C	-2.4302482753	1.5019938025	1.7955870151
C	-3.4871117682	2.4161204306	1.8459150756
H	-4.2239996863	2.4406175012	1.0478111811
C	-3.593287708	3.3097645157	2.9097602589
H	-4.414395946	4.0200877918	2.9336644206
C	-2.6488009626	3.297995072	3.9311780855
H	-2.7255856017	4.0024085115	4.7542858068
C	-1.5937409522	2.3865479899	3.8957797215
H	-0.859851255	2.3958674632	4.6973399468
C	-3.171956799	1.0987018343	-0.9836825481
C	-2.6232989303	2.2610513416	-1.5416262645
H	-1.687755651	2.6609307461	-1.1588918721
C	-3.2696454752	2.8999894358	-2.5924787702
H	-2.8407783615	3.8014312929	-3.0203919681
C	-4.4578227211	2.3770929561	-3.1039222922
H	-4.9579178931	2.874628056	-3.9299978411
C	-4.9988558765	1.2161675403	-2.5601947109
H	-5.9213328333	0.8036641014	-2.9584466419
C	-4.3600688462	0.5751568285	-1.4997912304

H	-4.7899485444	-0.3287346682	-1.0786717942
C	-3.2831910452	-1.1447601339	0.8816780785
C	-2.8815247999	-2.4041773348	0.4212464198
H	-1.9787458696	-2.4989342325	-0.1776385523
C	-3.6336057465	-3.5325794882	0.7369652204
H	-3.3139017126	-4.5068197305	0.3800575462
C	-4.7795289586	-3.4100757471	1.5197899889
H	-5.3621381793	-4.2920732523	1.7704127828
C	-5.1767723188	-2.1589745089	1.9886987249
H	-6.0668400149	-2.0633946779	2.6038954229
C	-4.4333475812	-1.0261434269	1.6714994033
H	-4.7472556036	-0.0544473199	2.0430703424
C	2.0213932131	0.8244151424	2.9098739439
C	2.8584422173	0.8399620187	1.7829355843
C	4.1573141205	1.3455847786	1.9126461051
H	4.8153030467	1.3857867473	1.0485139159
C	4.6155648041	1.8050210147	3.1441672645
H	5.6261649619	2.1929760579	3.2295804142
C	3.7827893284	1.7708664611	4.2600122218
H	4.1404374801	2.1323058078	5.2196538933
C	2.4839718968	1.2801884105	4.1449885121
H	1.8408681323	1.257819838	5.0206289781
C	2.8200467509	1.560359548	-1.0009407334
C	2.0136677686	2.7000973599	-1.106801714
H	1.0720633577	2.7456501905	-0.5649897896
C	2.4082959805	3.7611526183	-1.9136027021
H	1.7764949626	4.6409652422	-1.9947126496
C	3.605304357	3.689074627	-2.6255826845
H	3.9092256832	4.5157900431	-3.261376155
C	4.4071752819	2.5555279482	-2.5269241713
H	5.3380406037	2.4942717723	-3.0833958411
C	4.0197226318	1.4911852583	-1.7150083093
H	4.6496135948	0.6088035614	-1.6472954576
C	3.3164524169	-1.2134897494	-0.278214756
C	3.140740177	-1.7919264376	-1.5445453834
H	2.4300851346	-1.3603803894	-2.2453223282
C	3.8684998732	-2.9229614058	-1.8987186151
H	3.7307974759	-3.3634647313	-2.8819962045
C	4.7644290673	-3.4924762951	-0.9935418383
H	5.3277975149	-4.3787160315	-1.2712903685
C	4.933224284	-2.9262836751	0.2669493624
H	5.6232612323	-3.3690769315	0.9795111739
C	4.2127390017	-1.7882758724	0.6270670518
H	4.349257542	-1.3601690682	1.614905043
C	-0.3622309257	-1.3353830979	4.1738546954
C	0.3746228882	-2.5268435239	4.2447392132
C	0.208724341	-3.357736907	5.3568582032
H	0.7970983014	-4.2679168188	5.4433144201
C	-0.7050447124	-3.0216708401	6.3534355312

H	-0.8288952017	-3.6742596962	7.2129238725
C	-1.4639385918	-1.8580520803	6.248648255
H	-2.1797038621	-1.6020857916	7.0243718811
C	-1.2949152341	-1.0065976918	5.1579953821
H	-1.877286373	-0.0916249483	5.0933613079
C	2.9287612681	-3.688957157	3.5829556159
C	3.1526651686	-5.0667544094	3.4954750095
H	2.4389130121	-5.7018251294	2.9781963466
C	4.291785082	-5.6301215269	4.0682843561
H	4.4556426509	-6.7017967479	3.9947054666
C	5.2139458622	-4.8262419274	4.7331614217
H	6.1010892891	-5.2683269093	5.1779595894
C	4.9994528844	-3.4511037418	4.821543813
H	5.718970303	-2.8181431406	5.3336184509
C	3.8690081834	-2.8838699734	4.2427794451
H	3.7171843591	-1.8075716147	4.3018073613
C	0.6383219132	-4.1555204498	1.8605855108
C	0.9493368947	-4.2255394344	0.4954053416
H	1.6567978119	-3.5217027645	0.0637306489
C	0.3611390286	-5.1938699106	-0.3138983486
H	0.613230436	-5.2380872165	-1.3697974811
C	-0.5521251128	-6.0956389506	0.2288009677
H	-1.0137946551	-6.84980037	-0.402607302
C	-0.8755215413	-6.025452719	1.5826675884
H	-1.5897963218	-6.7241928567	2.0096782697
C	-0.2850786843	-5.0609409042	2.3960136416
H	-0.5524851764	-5.0135771331	3.4476593663
B	0.3019141192	2.6880598107	8.1056981804
C	0.9362963459	3.7107553976	6.9748954996
C	-1.3364947255	2.596621542	7.9214828055
C	0.958679103	1.1852136816	7.9149058373
C	0.6471823076	3.2568384191	9.6162660582
H	-1.8147057929	1.9499178955	8.6780741369
H	-1.6396918904	2.1844236881	6.9421278845
H	-1.8348047628	3.5787985864	8.004295316
H	2.033202429	3.8118202496	7.0581726365
H	0.5321930893	4.7360261111	7.0441088623
H	0.7469665409	3.3851876391	5.9355485386
H	0.2560781625	2.6039306609	10.4164075905
H	0.2176367632	4.2564624942	9.8057183109
H	1.7307856173	3.3528469932	9.8061804571
H	0.6023077331	0.4596972634	8.6671006091
H	2.0608996671	1.1822680091	7.9883493377
H	0.7146963747	0.7364365694	6.9346250146

XYZ coordinates of the optimized structure of **7**

102

Pt	-0.0060906875	-0.2139838656	0.187203274
P	-2.2733940686	0.1798434498	0.4956853016

Cl	-0.1331155147	-0.5277430821	-2.159070601
As	0.104036332	0.1369625262	2.493158879
P	2.2915772398	0.1489153386	0.1611944608
P	1.5452204506	-2.7760578467	2.6211416293
C	-1.2357805188	1.5321302378	2.7248030549
C	-2.2972760864	1.481214767	1.8011293881
C	-3.3184549878	2.4304767661	1.8818539982
H	-4.1359939449	2.4135442335	1.166233747
C	-3.279175136	3.4196357839	2.8632252052
H	-4.0727069576	4.1592353398	2.9117324162
C	-2.2220855915	3.4705862651	3.7668598232
H	-2.1850615174	4.2517214402	4.5201663709
C	-1.2008214216	2.5235336588	3.7030992284
H	-0.3761714005	2.5761284512	4.4078297287
C	-3.1678249922	0.9065607587	-0.9107492747
C	-2.5976265787	2.0042145318	-1.5691379044
H	-1.6354554175	2.3949438475	-1.2482585739
C	-3.2567478745	2.5886565979	-2.6434884439
H	-2.8110769748	3.4395072971	-3.1504475993
C	-4.4794200161	2.0751700893	-3.0771836119
H	-4.9895039775	2.5297762587	-3.9216579867
C	-5.0422717303	0.9778207339	-2.4329518233
H	-5.9915440995	0.572191369	-2.7706376591
C	-4.3904369221	0.3913591687	-1.3493255298
H	-4.8362252725	-0.4637484802	-0.850152939
C	-3.2877048362	-1.1986096606	1.1091609676
C	-2.9442469952	-2.4973404796	0.7160163326
H	-2.0625572364	-2.6647814405	0.1015564112
C	-3.7294691569	-3.5741032604	1.1195040132
H	-3.4577133627	-4.5790461123	0.8118787868
C	-4.8462944394	-3.3613976988	1.9243564878
H	-5.4539197974	-4.2038434453	2.2424437056
C	-5.18206761	-2.0706008014	2.3295028471
H	-6.0484768024	-1.9045706776	2.9631677804
C	-4.4078092535	-0.9884480686	1.9228577384
H	-4.6745097989	0.0148744748	2.2436034667
C	1.8890042152	0.7827252392	2.8815288976
C	2.8034654886	0.7654889752	1.8186053646
C	4.1000444233	1.2425576682	2.0320725333
H	4.8170314302	1.2568664558	1.2153438768
C	4.4815980569	1.7000227151	3.2906527644
H	5.4922108734	2.0656786926	3.4450913893
C	3.5752385834	1.6843326755	4.3484642379
H	3.8768048244	2.0342693777	5.3311107156
C	2.2762020631	1.2239157063	4.1471589691
H	1.5782754179	1.2012525604	4.9797882238
C	2.7270093558	1.5317208751	-0.9490265037
C	1.8445480307	2.616119506	-1.0308808441
H	0.9050712865	2.5882670561	-0.4839319968

C	2.1636621564	3.7194355541	-1.8142613213
H	1.4721642121	4.5548416093	-1.875986736
C	3.3624895489	3.7468475106	-2.525565853
H	3.6080771593	4.6061064136	-3.1431264132
C	4.2423388145	2.6707564597	-2.4481414317
H	5.1760551536	2.6873341457	-3.0029442378
C	3.9303351009	1.5645219465	-1.660397949
H	4.6215555748	0.728326235	-1.610438775
C	3.4129724389	-1.2119938435	-0.2891758241
C	3.30834956	-1.7319292771	-1.5881686129
H	2.5965046399	-1.3057227066	-2.2902214862
C	4.1074534489	-2.8028596771	-1.9748087918
H	4.0222033804	-3.1989450927	-2.9825481123
C	5.0086580197	-3.3669040227	-1.0723330619
H	5.6298171801	-4.2045994999	-1.3762209104
C	5.1099748597	-2.8568104951	0.2193112666
H	5.8060862538	-3.2948362782	0.9288464311
C	4.3142325686	-1.7829693968	0.6141420082
H	4.3954801481	-1.4030291229	1.6272547648
C	-0.3291848722	-1.1524075913	3.895066086
C	0.3731642504	-2.367892681	3.9781277783
C	0.1494643397	-3.1927212236	5.08498179
H	0.7159185576	-4.1149394605	5.1869898069
C	-0.7844563173	-2.8454568209	6.0583593754
H	-0.9480266265	-3.502136951	6.9080363252
C	-1.5094201219	-1.6640581494	5.9384328496
H	-2.2440327454	-1.3920729599	6.6905038303
C	-1.279636939	-0.8120530051	4.8604950742
H	-1.832085116	0.1196992803	4.7903960854
C	2.8765882733	-3.6702562091	3.5143028529
C	3.0868338691	-5.0496891711	3.4201235283
H	2.413709859	-5.6624921194	2.827084092
C	4.1585580501	-5.645365067	4.0843727339
H	4.310255682	-6.7183944603	4.0033307472
C	5.0274952902	-4.8730240485	4.8499481559
H	5.8611904954	-5.3400830953	5.3668408954
C	4.8279994582	-3.4959701857	4.945898319
H	5.5061541053	-2.8860081193	5.5365826048
C	3.7669566139	-2.8972607127	4.2752845021
H	3.6290423551	-1.8193527783	4.3431362626
C	0.6815539912	-4.0878525267	1.6699998225
C	1.029667746	-4.2032416038	0.3166811383
H	1.7626863323	-3.5249474262	-0.1129749901
C	0.4454011486	-5.1809409278	-0.4847927273
H	0.7263563215	-5.2573021427	-1.5315422605
C	-0.5005540336	-6.0502594064	0.0539297544
H	-0.9597987399	-6.8114557228	-0.5707320119
C	-0.8591154653	-5.9382380875	1.3961144691
H	-1.5975895918	-6.6128434828	1.8212980919

C	-0.2742512838	-4.9623953841	2.2000672289
H	-0.572562865	-4.8826605047	3.241250178

XYZ coordinates of the optimized structure of **7F**

103

Pt	0.0766641256	0.0861066513	-0.0897616355
P	2.0317611923	1.3530453838	-0.0000996898
Cl	0.107563566	-0.0983302335	-2.579659052
As	0.0601522877	0.1902142592	2.3771706979
P	-2.0341485813	1.0757050168	-0.0053256345
P	0.2710165214	-2.2229716762	0.2089326476
C	2.0244032756	0.4189203506	2.6436653372
C	2.8053950826	0.9735031601	1.6199432693
C	4.1599516236	1.2394148752	1.8538857928
H	4.7580801537	1.7104105178	1.078966646
C	4.7578499043	0.8806626368	3.0559890214
H	5.8153537498	1.0731180165	3.2139758304
C	3.9952677144	0.2681818111	4.0460055126
H	4.4547968714	-0.0339079746	4.9830582894
C	2.6329343495	0.0610511707	3.8521892304
H	2.0325349441	-0.3684831554	4.6423728385
C	3.2883892289	0.9569230685	-1.2698415946
C	3.1733098309	1.5659526067	-2.5275409995
H	2.3942838356	2.3014814445	-2.7066285755
C	4.0525759671	1.2391902442	-3.5547369987
H	3.9530054451	1.7255431411	-4.5212341012
C	5.0521319199	0.2904979925	-3.3463371156
H	5.7401930157	0.0371173071	-4.1481996249
C	5.1592230434	-0.335241481	-2.1074375484
H	5.9306113989	-1.0814681742	-1.9365817154
C	4.2801856567	-0.0099796629	-1.0764309437
H	4.3720778299	-0.5160806587	-0.120954247
C	2.0531945291	3.199952345	0.0044966045
C	0.9151926779	3.888669045	0.4327561525
H	0.0186117906	3.3330735731	0.6878694543
C	0.9208815115	5.27787651	0.5366180587
H	0.025984298	5.7943772264	0.8730252497
C	2.0646591229	5.9971749094	0.2022669052
H	2.0695157972	7.0812924365	0.275388184
C	3.2040111782	5.3209529854	-0.2314314938
H	4.1000072645	5.8756284654	-0.4970143644
C	3.2017393874	3.9323751332	-0.326466545
H	4.0958957316	3.4219783897	-0.6727408707
C	-1.1432651808	1.7604472737	2.5697633255
C	-2.0648644669	2.051611616	1.5535183294
C	-2.9393733915	3.1331433473	1.7085453276
H	-3.6637844886	3.356533336	0.931092763
C	-2.8655503054	3.9518904691	2.8305117832
H	-3.5365496605	4.8010752123	2.925290356

C	-1.9213548146	3.6847842037	3.8171008051
H	-1.8414296343	4.3295030066	4.6879516075
C	-1.0786892344	2.5829611911	3.6986563812
H	-0.3682779142	2.3551538465	4.4820541138
C	-2.4862435544	2.3002454407	-1.2964833009
C	-1.4575673257	2.9309872586	-2.0041137898
H	-0.4299249343	2.6327945875	-1.8233071759
C	-1.7482944061	3.9160264211	-2.9447960611
H	-0.9386848724	4.3957668776	-3.4879477535
C	-3.070180559	4.2732858943	-3.1979525768
H	-3.2971000634	5.0367932183	-3.9371128796
C	-4.1027633776	3.642344882	-2.5068393174
H	-5.1369120586	3.9127154649	-2.7023028298
C	-3.8144567834	2.6614091196	-1.5618069142
H	-4.6300810256	2.1725803686	-1.0361225137
C	-3.5298399842	0.0179835775	0.1071293718
C	-4.1040891765	-0.5023945584	-1.0620256218
H	-3.7181772327	-0.2081058788	-2.0353181491
C	-5.1749503259	-1.3879693371	-0.9892368606
H	-5.6144546567	-1.7750434505	-1.9046543168
C	-5.6812814284	-1.7760802136	0.2500716313
H	-6.5160699085	-2.4691744618	0.3057923902
C	-5.1128398443	-1.2696974842	1.4160307467
H	-5.5020076921	-1.5650661749	2.3866545483
C	-4.0464412559	-0.3754819653	1.3470509091
H	-3.6184812966	0.0159893753	2.2655369144
C	-0.7865423067	-1.5760164449	2.7058254079
C	-0.6523496858	-2.5884386904	1.7478803988
C	-1.2529673883	-3.8325559263	1.9662502058
H	-1.1376208648	-4.6228443779	1.2297292949
C	-2.0224096078	-4.0544449394	3.1039371591
H	-2.5040042647	-5.0170571114	3.251739579
C	-2.1770183317	-3.0380397613	4.0418400987
H	-2.7863446107	-3.1984203978	4.9270932906
C	-1.5459611457	-1.8105255953	3.8559179194
H	-1.6417188424	-1.0303163885	4.5995773107
C	-0.4668741619	-3.3683032091	-1.0168495833
C	-1.6226217098	-2.9553562297	-1.6867210613
H	-2.0049307876	-1.9549012991	-1.5159068433
C	-2.2699961119	-3.8126264485	-2.5708287746
H	-3.1685445014	-3.4783775277	-3.0825283895
C	-1.7601727069	-5.0877205281	-2.8075695929
H	-2.2600077225	-5.7543608829	-3.5051529017
C	-0.6045326104	-5.5040606382	-2.1508498549
H	-0.2014660322	-6.4971089153	-2.3303269654
C	0.0395178087	-4.6512730357	-1.2565947997
H	0.9373721952	-4.9893456476	-0.7476531553
C	1.9264586458	-2.9595845918	0.5013487801
C	2.8307257313	-3.0043424845	-0.5689597996

H	2.5403959422	-2.6131516278	-1.54121462
C	4.0990284067	-3.5481677934	-0.3959031188
H	4.785568151	-3.587248345	-1.2372981697
C	4.4912605871	-4.0310517889	0.8525765762
H	5.484541195	-4.4503600969	0.9873978858
C	3.6060116838	-3.9714396396	1.9248173376
H	3.9045109922	-4.34294005	2.9014190687
C	2.3265295398	-3.444977014	1.7505351439
H	1.6400470155	-3.4182852463	2.5919401918
F	0.0487191115	0.266962553	4.3376577645

XYZ coordinates of the optimized structure of **7F'**

103

Pt	-0.0612959576	-0.111016737	0.0446052622
P	2.1862190059	0.2932509952	-0.007386746
Cl	-0.2864660516	-0.2904076349	-2.4055881945
As	0.0686994779	-0.2443116197	2.4778693732
P	-2.2888041794	0.3198189959	0.3595128107
P	1.7355560209	-3.0528698282	1.5173481959
C	1.9331094817	0.3921470155	2.7921266443
C	2.7676426044	0.6240341746	1.6904267389
C	4.0392793205	1.1777717497	1.8795877352
H	4.671533563	1.3808297392	1.0185962852
C	4.4965301821	1.4825462142	3.1561841383
H	5.4847498541	1.912894584	3.2906964576
C	3.6758024002	1.2361555447	4.2520917602
H	4.0196987468	1.4703906505	5.2557847021
C	2.4045568485	0.6962221949	4.0738931665
H	1.7662011941	0.501664997	4.9244004713
C	3.3914371779	-0.8346032147	-0.7920118111
C	3.1891755792	-1.1739607885	-2.1369269158
H	2.3276572015	-0.7798671443	-2.6697416662
C	4.0786569045	-2.0252366509	-2.7864145813
H	3.9123360192	-2.2791670513	-3.8295753758
C	5.1707973385	-2.5535586674	-2.1017150553
H	5.8646787151	-3.2173717906	-2.6099556283
C	5.3665661294	-2.232524966	-0.7603388928
H	6.2124233252	-2.6460046453	-0.2174849212
C	4.4811137154	-1.3792652673	-0.1049699851
H	4.6387258325	-1.1498550891	0.9441644109
C	2.4584350295	1.9168417974	-0.8249964703
C	1.6975984293	3.001507501	-0.3646354894
H	0.977655695	2.8526405744	0.4375516835
C	1.8593355825	4.2634491528	-0.9242883175
H	1.2651631375	5.0958154256	-0.5572142512
C	2.7776432879	4.457661771	-1.9563500718
H	2.9000768905	5.4425634119	-2.3983574817
C	3.5363091983	3.3864683002	-2.4165603106
H	4.2554786561	3.5307451177	-3.2181579866

C	3.3831852825	2.1201908297	-1.8514206727
H	3.9857160755	1.2950052917	-2.2180444015
C	-1.3577634209	1.0616077094	2.8821162925
C	-2.3785461954	1.2466505386	1.9366549337
C	-3.4021083536	2.1666018712	2.1881388916
H	-4.1879634466	2.317975514	1.4524665844
C	-3.3981834522	2.9175499721	3.3599702214
H	-4.1868821023	3.6425431424	3.5398319069
C	-2.3757052972	2.7452092988	4.2889638884
H	-2.3605105285	3.3386862294	5.1988896417
C	-1.3689090252	1.8099222362	4.0600545293
H	-0.5894672564	1.6536035952	4.7956367208
C	-2.9999253608	1.4753395938	-0.8662034256
C	-2.2168222088	2.5546829949	-1.2951468297
H	-1.1960347082	2.6593666887	-0.9364130866
C	-2.7329122264	3.4787405815	-2.1961261046
H	-2.1161100751	4.3099754181	-2.5262491864
C	-4.030204742	3.3292450392	-2.686620684
H	-4.4293669248	4.0482332397	-3.3966986356
C	-4.8085940698	2.252985471	-2.2720056422
H	-5.8173203442	2.1274986041	-2.6555909913
C	-4.2976449896	1.327136843	-1.3629672156
H	-4.9123900081	0.4896214798	-1.0462915595
C	-3.4761349129	-1.061573405	0.4554499629
C	-3.2265141348	-2.1811366737	-0.3469408306
H	-2.3352196722	-2.2083778408	-0.9698285039
C	-4.1139212223	-3.2532857315	-0.342803278
H	-3.9142529133	-4.1200596246	-0.9664659666
C	-5.2483289322	-3.2174583947	0.4659768754
H	-5.9375958067	-4.057374014	0.4723967883
C	-5.496529483	-2.1076024293	1.2711729132
H	-6.3776645219	-2.0797288766	1.9062966816
C	-4.6142659936	-1.0304447125	1.2676539983
H	-4.8095191897	-0.1727384107	1.905747022
C	-0.6262592109	-2.086510474	2.6690267053
C	0.0463917233	-3.226656974	2.2140922474
C	-0.5757699207	-4.4774629372	2.3398546928
H	-0.056540732	-5.3654265927	1.9879927112
C	-1.8420927831	-4.5948138244	2.8979606342
H	-2.3129510407	-5.5708477371	2.9779889204
C	-2.4982356677	-3.455837092	3.3619510896
H	-3.4868226082	-3.5344777696	3.8056795044
C	-1.8894744083	-2.2109163028	3.2580391593
H	-2.3988544078	-1.3327374614	3.6428239843
C	1.7249481183	-4.3446731999	0.2085115965
C	1.1512252746	-3.9813562529	-1.0185262974
H	0.7670052389	-2.9721628738	-1.1589523468
C	1.0682786208	-4.9000244891	-2.0607295504
H	0.6174639016	-4.6034068538	-3.0042331563

C	1.573859135	-6.1889836339	-1.8996719494
H	1.516994043	-6.9038477606	-2.7162251487
C	2.1564678379	-6.5553642145	-0.6888650843
H	2.551991596	-7.5590583866	-0.5554262014
C	2.2288174973	-5.6413823897	0.3611413623
H	2.6820759026	-5.9413730652	1.3020290447
C	2.7911977321	-3.7628163686	2.8440243419
C	4.1358399872	-4.0475855346	2.5562365493
H	4.5066360978	-3.9370888891	1.5397756576
C	5.001567461	-4.4806393148	3.5555000054
H	6.0355790638	-4.7082377284	3.3094731556
C	4.5474467559	-4.6165254734	4.8665689394
H	5.2248561444	-4.9495304093	5.6481831791
C	3.221598813	-4.3178363716	5.1676126748
H	2.8584183914	-4.4153464301	6.1873990092
C	2.3485614724	-3.8957670944	4.1660936185
H	1.3170134797	-3.6675391885	4.4185341736
F	0.0675002956	-0.4879077942	4.4838462562

XYZ coordinates of the optimized structure of **[7]**BMe_4

119

Pt	-0.0060906875	-0.2139838656	0.187203274
P	-2.2733940686	0.1798434498	0.4956853016
Cl	-0.1331155147	-0.5277430821	-2.159070601
As	0.104036332	0.1369625262	2.493158879
P	2.2915772398	0.1489153386	0.1611944608
P	1.5452204506	-2.7760578467	2.6211416293
C	-1.2357788757	1.5321322225	2.7248009848
C	-2.2972760864	1.481214767	1.8011293881
C	-3.3184549878	2.4304767661	1.8818539982
H	-4.1359939449	2.4135442335	1.166233747
C	-3.279175136	3.4196357839	2.8632252052
H	-4.0727069576	4.1592353398	2.9117324162
C	-2.2220873627	3.4705842051	3.7668620489
H	-2.1850615174	4.2517214402	4.5201663709
C	-1.2007923372	2.5235579971	3.7030633885
H	-0.3762126739	2.5760954112	4.4078794648
C	-3.1678249922	0.9065607587	-0.9107492747
C	-2.5976265787	2.0042145318	-1.5691379044
H	-1.6354554175	2.3949438475	-1.2482585739
C	-3.2567478745	2.5886565979	-2.6434884439
H	-2.8110769748	3.4395072971	-3.1504475993
C	-4.4794200161	2.0751700893	-3.0771836119
H	-4.9895039775	2.5297762587	-3.9216579867
C	-5.0422717303	0.9778207339	-2.4329518233
H	-5.9915440995	0.572191369	-2.7706376591
C	-4.3904369221	0.3913591687	-1.3493255298
H	-4.8362252725	-0.4637484802	-0.850152939
C	-3.2877048362	-1.1986096606	1.1091609676

C	-2.9442469952	-2.4973404796	0.7160163326
H	-2.0625572364	-2.6647814405	0.1015564112
C	-3.7294691569	-3.5741032604	1.1195040132
H	-3.4577133627	-4.5790461123	0.8118787868
C	-4.8462944394	-3.3613976988	1.9243564878
H	-5.4539197974	-4.2038434453	2.2424437056
C	-5.18206761	-2.0706008014	2.3295028471
H	-6.0484768024	-1.9045706776	2.9631677804
C	-4.4078092535	-0.9884480686	1.9228577384
H	-4.6745097989	0.0148744748	2.2436034667
C	1.8890054294	0.7827215415	2.8815298151
C	2.8034654886	0.7654889752	1.8186053646
C	4.1000444233	1.2425576682	2.0320725333
H	4.8170314302	1.2568664558	1.2153438768
C	4.4815980569	1.7000227151	3.2906527644
H	5.4922108734	2.0656786926	3.4450913893
C	3.5752375548	1.6843359161	4.3484634635
H	3.8768048244	2.0342693777	5.3311107156
C	2.2761916673	1.2238762944	4.1471491876
H	1.5782979453	1.2013012064	4.9797838104
C	2.7270093558	1.5317208751	-0.9490265037
C	1.8445480307	2.616119506	-1.0308808441
H	0.9050712865	2.5882670561	-0.4839319968
C	2.1636621564	3.7194355541	-1.8142613213
H	1.4721642121	4.5548416093	-1.875986736
C	3.3624895489	3.7468475106	-2.525565853
H	3.6080771593	4.6061064136	-3.1431264132
C	4.2423388145	2.6707564597	-2.4481414317
H	5.1760551536	2.6873341457	-3.0029442378
C	3.9303351009	1.5645219465	-1.660397949
H	4.6215555748	0.728326235	-1.610438775
C	3.4129724389	-1.2119938435	-0.2891758241
C	3.30834956	-1.7319292771	-1.5881686129
H	2.5965046399	-1.3057227066	-2.2902214862
C	4.1074534489	-2.8028596771	-1.9748087918
H	4.0222033804	-3.1989450927	-2.9825481123
C	5.0086580197	-3.3669040227	-1.0723330619
H	5.6298171801	-4.2045994999	-1.3762209104
C	5.1099748597	-2.8568104951	0.2193112666
H	5.8060862538	-3.2948362782	0.9288464311
C	4.3142325686	-1.7829693968	0.6141420082
H	4.3954801481	-1.4030291229	1.6272547648
C	-0.3291848722	-1.1524075913	3.895066086
C	0.3731642504	-2.367892681	3.9781277783
C	0.1494643397	-3.1927212236	5.08498179
H	0.7159185576	-4.1149394605	5.1869898069
C	-0.7844563173	-2.8454568209	6.0583593754
H	-0.9480266265	-3.502136951	6.9080363252
C	-1.5094201219	-1.6640581494	5.9384328496

H	-2.2440327454	-1.3920729599	6.6905038303
C	-1.279636939	-0.8120530051	4.8604950742
H	-1.832085116	0.1196992803	4.7903960854
C	2.8765882733	-3.6702562091	3.5143028529
C	3.0868338691	-5.0496891711	3.4201235283
H	2.413709859	-5.6624921194	2.827084092
C	4.1585580501	-5.645365067	4.0843727339
H	4.310255682	-6.7183944603	4.0033307472
C	5.0274952902	-4.8730240485	4.8499481559
H	5.8611904954	-5.3400830953	5.3668408954
C	4.8279994582	-3.4959701857	4.945898319
H	5.5061541053	-2.8860081193	5.5365826048
C	3.7669566139	-2.8972607127	4.2752845021
H	3.6290423551	-1.8193527783	4.3431362626
C	0.6815539912	-4.0878525267	1.6699998225
C	1.029667746	-4.2032416038	0.3166811383
H	1.7626863323	-3.5249474262	-0.1129749901
C	0.4454011486	-5.1809409278	-0.4847927273
H	0.7263563215	-5.2573021427	-1.5315422605
C	-0.5005540336	-6.0502594064	0.0539297544
H	-0.9597987399	-6.8114557228	-0.5707320119
C	-0.8591154653	-5.9382380875	1.3961144691
H	-1.5975895918	-6.6128434828	1.8212980919
C	-0.2742512838	-4.9623953841	2.2000672289
H	-0.572562865	-4.8826605047	3.241250178
B	0.2826026635	2.7979792296	8.1336055545
C	1.0256621643	3.8014585631	7.053075638
C	-1.3393282837	2.7500617806	7.8289319898
C	0.9069814926	1.2765221606	7.9882352372
C	0.5399727491	3.3562019518	9.6653324044
H	-1.8855480191	2.091593793	8.5273955478
H	-1.5742866604	2.3742657662	6.8163536528
H	-1.8239825814	3.7397176773	7.9050519744
H	2.1137420284	3.8818607658	7.2247697432
H	0.6375453378	4.8348780797	7.0814143975
H	0.9156397324	3.4699686557	6.0040039238
H	0.0720370759	2.7190845942	10.436117694
H	0.1356341279	4.3711414182	9.8263301246
H	1.6108925176	3.4131495549	9.9284322685
H	0.4952733247	0.5703604788	8.7305832583
H	2.0040650333	1.2424185643	8.1120376829
H	0.6949480825	0.8234462038	7.0026703178

XYZ coordinates of the optimized structure of **8**

102

Pt	0.0145453354	-0.0270944721	0.05717902
P	-2.2624503367	0.3259943611	0.3766751699
Cl	-0.0522001638	0.0499931076	-2.3092889559
Bi	0.0942791181	-0.0430920499	2.621195847

P	2.3260597298	0.2404924221	0.1385006622
P	1.5510442344	-2.9538709195	2.902770981
C	-1.5273001653	1.4413551598	2.8830968784
C	-2.4405817629	1.4789941076	1.8139652108
C	-3.503248987	2.3886649946	1.8605857402
H	-4.2140787223	2.4381586168	1.0403268303
C	-3.6501754917	3.2434070342	2.9514123977
H	-4.4759740198	3.9484344595	2.9715894866
C	-2.7423569127	3.2002354709	4.0049135418
H	-2.852125762	3.8753068306	4.8487884417
C	-1.681653085	2.2943643661	3.9736260953
H	-0.9698125977	2.2739529381	4.7952611188
C	-3.1553529712	1.140763782	-0.9830535376
C	-2.6320829118	2.3303190246	-1.5069578431
H	-1.7084932161	2.7421945428	-1.1087470519
C	-3.2892709434	2.9823093988	-2.5430475854
H	-2.8801033221	3.9049761682	-2.944170665
C	-4.4630303491	2.4461375153	-3.0735707835
H	-4.9716676384	2.9542701188	-3.8878983891
C	-4.9788688956	1.2586871034	-2.5636254592
H	-5.8902050172	0.8360607652	-2.9766541289
C	-4.3291983512	0.6041750827	-1.5182396625
H	-4.73974733	-0.3203240861	-1.1234615831
C	-3.2218955765	-1.1592068704	0.8140247544
C	-2.7809506808	-2.3947530243	0.3252999043
H	-1.8735132905	-2.4461967272	-0.2720657846
C	-3.4993541594	-3.5528213697	0.6100169466
H	-3.1483153023	-4.5083955009	0.2324262814
C	-4.6523394806	-3.4833190178	1.3891711899
H	-5.2090819399	-4.3881596358	1.6160258657
C	-5.0900656243	-2.2560839994	1.8845300453
H	-5.9861451469	-2.2021460035	2.4960726712
C	-4.3792388568	-1.094044776	1.599437957
H	-4.7241099246	-0.1410757219	1.9916355587
C	2.0940734361	0.8065722886	2.9386433977
C	2.9021448701	0.8368696468	1.7942689702
C	4.1988876949	1.3576049916	1.9042254906
H	4.8399967389	1.4118268137	1.0282189222
C	4.6751420076	1.8145294035	3.1294348403
H	5.6829205628	2.2131456467	3.1974500655
C	3.8639158939	1.7667181874	4.2606104101
H	4.2348049779	2.1296841181	5.2147938194
C	2.5684781172	1.2612104017	4.1675440959
H	1.9383110736	1.2307681597	5.0525106947
C	2.8948718832	1.5578925956	-0.9877239741
C	2.1358186464	2.7325137589	-1.0588178304
H	1.212460655	2.8128183441	-0.4900631729
C	2.5546319878	3.7854369995	-1.8637374378
H	1.960195267	4.6929626066	-1.9172900694

C	3.7281028817	3.6704825453	-2.6089333758
H	4.0507439562	4.4913226421	-3.2431141571
C	4.4823498354	2.5025231777	-2.5446216171
H	5.3949146675	2.4083315518	-3.1262348474
C	4.070796588	1.4457002379	-1.7343518361
H	4.66413484	0.5368666646	-1.6920372716
C	3.3259258173	-1.2292759677	-0.2637338797
C	3.1248585247	-1.8215308254	-1.5197247603
H	2.4087021528	-1.3907049117	-2.2155971612
C	3.8376657496	-2.9627210278	-1.8721780166
H	3.6813660541	-3.4131942071	-2.8481346912
C	4.7425837684	-3.5293942333	-0.9741043243
H	5.2942333465	-4.4235187579	-1.2500570578
C	4.9349028701	-2.9506333031	0.2773918437
H	5.6318077784	-3.3916121787	0.9843519421
C	4.2302487724	-1.8019208772	0.6350092757
H	4.3850470302	-1.3632202523	1.6155438461
C	-0.3350838667	-1.4707354069	4.2542673655
C	0.4216355254	-2.6464074604	4.3142223843
C	0.256330751	-3.4865225414	5.4214129139
H	0.8558568139	-4.3896724688	5.5058685825
C	-0.669602713	-3.169969694	6.4128537886
H	-0.7904054479	-3.8302282066	7.2668621923
C	-1.4447039219	-2.0167270369	6.310878283
H	-2.1699060056	-1.7762290409	7.0828987404
C	-1.2798161308	-1.154647908	5.2269400034
H	-1.8741389496	-0.2472132109	5.1613717987
C	2.992298751	-3.7836433348	3.6712463742
C	3.2052391706	-5.1652688115	3.6228888555
H	2.4840053954	-5.8093073079	3.1273525679
C	4.3428839892	-5.7205273303	4.2061706767
H	4.4986830387	-6.7950576119	4.1628407689
C	5.2743315006	-4.9045846298	4.8430707501
H	6.1604470095	-5.3404036982	5.2960637314
C	5.0709703548	-3.5259127457	4.8924121588
H	5.7981379755	-2.8840165945	5.3820758302
C	3.9420121696	-2.9670140872	4.302473866
H	3.7981354625	-1.8883368649	4.3301500987
C	0.7205658128	-4.2689542308	1.9323617291
C	1.0743493155	-4.3605623042	0.5786977419
H	1.8036236271	-3.6704254562	0.1612386493
C	0.5015433648	-5.3324729967	-0.2369341797
H	0.7877567071	-5.393536698	-1.2832837215
C	-0.4410432667	-6.2155052425	0.2864129998
H	-0.8914647684	-6.9720004259	-0.3503204684
C	-0.8079059097	-6.1231279048	1.6276172443
H	-1.5449722615	-6.8070226737	2.0396934038
C	-0.2314784303	-5.1558499521	2.4480837202
H	-0.5318002107	-5.0923509554	3.4899739093

XYZ coordinates of the optimized structure of **8F**

103

Pt	0.0286308951	0.0230203831	-0.0152696579
P	2.0417543357	1.2568809066	0.0934022029
Cl	0.0152337632	-0.2184795028	-2.4867708712
Bi	0.0059738609	0.1385347558	2.6281288548
P	-2.0108992551	1.1904010454	0.0324402182
P	0.1997795971	-2.2980490297	0.2761025089
C	2.1208072485	0.7842696853	2.894163603
C	2.8283902684	1.205960159	1.7671142766
C	4.1298379565	1.7013587869	1.9412247932
H	4.6856278924	2.0736521049	1.0847194823
C	4.7204721998	1.7214808104	3.1991345344
H	5.733664334	2.0973060333	3.3116255881
C	4.0105600739	1.2704945401	4.310049608
H	4.468853315	1.2858633242	5.2952619214
C	2.703098918	0.8161557825	4.1619813688
H	2.1235877673	0.4958459841	5.0202269998
C	3.3529016645	0.7277571497	-1.0696052453
C	3.2064586201	1.0527953895	-2.4269375556
H	2.3477462876	1.6287520067	-2.7580774729
C	4.1533780439	0.64048114	-3.3587882961
H	4.0280719856	0.9082259939	-4.4043654884
C	5.2550318555	-0.1113513116	-2.9535206966
H	5.9971589919	-0.4284285213	-3.6811379487
C	5.3929326435	-0.4617080281	-1.6138517918
H	6.2383957247	-1.0620995791	-1.2894518006
C	4.4450432544	-0.0532055526	-0.6778278393
H	4.5622542021	-0.3515696199	0.3593501856
C	2.0055213726	3.0947477113	-0.1161113834
C	0.9887593432	3.7968433235	0.542856312
H	0.2157006449	3.2516425594	1.0790949842
C	0.9493519171	5.1869401368	0.5157595799
H	0.153246386	5.7120586258	1.0365484072
C	1.9193336357	5.8989127784	-0.1876876466
H	1.8846641538	6.9843960848	-0.2194956248
C	2.9320134765	5.211111213	-0.8502862198
H	3.694305048	5.7573541449	-1.3994779173
C	2.9824409852	3.8182806905	-0.8084840343
H	3.7868349981	3.3007247212	-1.3220344063
C	-1.5586976419	1.7194687127	2.7893724912
C	-2.2562376703	2.0907142544	1.6348845481
C	-3.1843539734	3.1376483087	1.728578337
H	-3.7364215027	3.4544802264	0.8497944891
C	-3.4024841352	3.7932152557	2.9359878184
H	-4.1182376463	4.6093925817	2.9811962949
C	-2.7081388521	3.4033945672	4.0777191337
H	-2.8766684213	3.9124824398	5.0228392608

C	-1.7875750143	2.3608703658	4.0066911078
H	-1.2399548681	2.0393548501	4.8851302993
C	-2.2947535035	2.4655915767	-1.260692629
C	-1.1882857349	2.9916797362	-1.933377918
H	-0.2015928437	2.5988920538	-1.7153334759
C	-1.3489252458	3.9931078005	-2.8882731598
H	-0.477325187	4.3902158982	-3.4013172431
C	-2.6201004648	4.4724661921	-3.1911058055
H	-2.7467497064	5.2500743494	-3.9395125118
C	-3.7328958508	3.9421964232	-2.5405002712
H	-4.7297060519	4.3026954795	-2.7794578975
C	-3.5733614847	2.9432378891	-1.5846815251
H	-4.4535255036	2.5253734381	-1.1038101385
C	-3.5499870203	0.1853384559	-0.066137296
C	-4.0721674898	-0.178588935	-1.3155858097
H	-3.6107026234	0.191743399	-2.2270593449
C	-5.1847091826	-1.0119763443	-1.40106739
H	-5.5839423268	-1.2733679447	-2.3775233491
C	-5.7822440554	-1.5072147278	-0.2438616768
H	-6.6493995067	-2.1580945299	-0.3120561458
C	-5.2617491786	-1.161733524	1.0011414751
H	-5.7211115053	-1.5413325191	1.9097579277
C	-4.1554797591	-0.3199395477	1.0911290687
H	-3.7694030725	-0.0530478149	2.071416993
C	-0.5274648721	-1.9899513913	2.9934877761
C	-0.4370488872	-2.868509737	1.9126579173
C	-0.8060259724	-4.2074618117	2.1045473537
H	-0.7425184222	-4.9100108935	1.2782909297
C	-1.2640198956	-4.6445486219	3.3433936543
H	-1.5581199901	-5.682627843	3.4713869971
C	-1.3437614858	-3.7558915268	4.4127715355
H	-1.702889469	-4.0956195066	5.3805457412
C	-0.9664928799	-2.425505044	4.2427962643
H	-1.0107543715	-1.722611085	5.0667369303
C	-0.6936173384	-3.3876616663	-0.8995105764
C	-1.9487475384	-2.9702203145	-1.3503550489
H	-2.325634234	-1.9971942799	-1.0522024163
C	-2.7060608067	-3.7852532402	-2.1856587468
H	-3.6798434947	-3.4444564915	-2.5266789667
C	-2.2114428544	-5.0233692867	-2.5908497475
H	-2.7983526986	-5.656557244	-3.2507638198
C	-0.9587356354	-5.4443842353	-2.1514897089
H	-0.5653447069	-6.408145559	-2.4634129654
C	-0.2025036097	-4.6335005229	-1.3073768698
H	0.7720410439	-4.9752334201	-0.971672079
C	1.9015844786	-2.988420548	0.2425816134
C	2.5883825908	-2.9946254085	-0.9795133242
H	2.1095762367	-2.5957410575	-1.870998898
C	3.8767027456	-3.5116838093	-1.0581510816

H	4.3930061108	-3.5199000523	-2.0138157698
C	4.5088838985	-4.0000229766	0.0850040471
H	5.5172963804	-4.3999748356	0.0220239776
C	3.845026057	-3.9671059276	1.3078854483
H	4.3323253026	-4.3394837422	2.2050415584
C	2.5440532459	-3.4710320546	1.3875113393
H	2.0306549296	-3.4703409885	2.3447955049
F	-0.0343052391	0.2356099295	4.7827122404

XYZ coordinates of the optimized structure of **8F'**

103

Pt	0.0207681593	0.2102398229	-0.0205919478
P	2.3013343421	0.5295964945	0.0346931235
Cl	-0.0863886015	0.2394872574	-2.4622105227
Bi	0.0785602516	-0.0465389572	2.6164180511
P	-2.2492370753	0.4379070769	0.2581941457
P	1.5566901416	-3.0710075438	1.6770442175
C	2.2189853612	0.5675107409	2.8827065577
C	2.978924986	0.7696117957	1.7297837274
C	4.3068282106	1.2041024363	1.8598504123
H	4.9082733556	1.3845013718	0.9723157283
C	4.8644120286	1.4095345379	3.1163979427
H	5.8941486853	1.745230638	3.2003615469
C	4.0998364934	1.1883265894	4.2594717127
H	4.5310355165	1.3489230383	5.2440253571
C	2.7756580913	0.7704851034	4.1451166376
H	2.1611249813	0.6049998241	5.0220586791
C	3.4050525953	-0.6941126761	-0.7599182065
C	3.2927018508	-0.8874128086	-2.1443166107
H	2.5671221734	-0.3129621518	-2.7132803499
C	4.0998156679	-1.8185533718	-2.7898858955
H	4.0053613173	-1.9567661201	-3.8633697229
C	5.0236828072	-2.5689813605	-2.064591807
H	5.6570363281	-3.2921143873	-2.5709720997
C	5.1309753452	-2.3893535658	-0.6881389821
H	5.848546489	-2.9702484307	-0.1150746596
C	4.3225781909	-1.4605936372	-0.0344204709
H	4.4123156587	-1.3371343029	1.0403493891
C	2.7133124422	2.1197828771	-0.7819037454
C	1.8342372515	3.1944398141	-0.5976923964
H	0.9206584361	3.045600789	-0.0262763477
C	2.1204239964	4.4398834749	-1.1466373399
H	1.4296942382	5.2654640344	-0.999328125
C	3.2843622422	4.6236143853	-1.8915245436
H	3.5048069091	5.5945534172	-2.326434328
C	4.1608123203	3.5588004243	-2.0815792835
H	5.0677845922	3.6952518101	-2.6640905916
C	3.8802819595	2.31097561	-1.5278385145
H	4.5692956846	1.4868322224	-1.6884452733

C	-1.7272282461	1.2475282924	2.9084256345
C	-2.5978082459	1.355206298	1.8163625427
C	-3.7474638123	2.1486442721	1.9301211246
H	-4.4283747816	2.2451435271	1.0882867708
C	-4.0157362286	2.8297887875	3.1145919603
H	-4.9034030231	3.4519248348	3.1876544874
C	-3.1474975809	2.7148084552	4.1967509754
H	-3.3532111336	3.2508650924	5.11957583
C	-2.0088517355	1.9151435553	4.0983258608
H	-1.3324234291	1.8040230259	4.9386762134
C	-3.0849644625	1.4347077645	-1.025491099
C	-2.5336788434	2.678452097	-1.3600349623
H	-1.6190580229	3.0135977146	-0.8772932673
C	-3.1437950598	3.4800498763	-2.317081638
H	-2.7090883347	4.442950505	-2.5701585635
C	-4.3029479578	3.0432223871	-2.9592225435
H	-4.7758199121	3.6683079746	-3.7116110348
C	-4.8480470026	1.8038537424	-2.6393213945
H	-5.7473815351	1.4561833512	-3.1400155519
C	-4.2431045225	0.9995527457	-1.6737317357
H	-4.6770656315	0.0346317034	-1.4290519077
C	-3.2044417248	-1.1149294878	0.3687292285
C	-2.6906724592	-2.2485352535	-0.2713406245
H	-1.7399783868	-2.1873117905	-0.794964869
C	-3.3897792663	-3.4516936129	-0.2318384408
H	-2.9805479516	-4.3270493808	-0.7284649274
C	-4.6033122864	-3.5309507578	0.4481550371
H	-5.1463522634	-4.4713830854	0.4830322711
C	-5.1184695999	-2.4056227556	1.088997179
H	-6.0622918746	-2.4659636514	1.6237623491
C	-4.4221867299	-1.2006993693	1.0527993166
H	-4.8245139204	-0.3311328863	1.5656471248
C	-0.6496145493	-2.0992105585	3.0784921937
C	-0.0288935308	-3.2532751137	2.5926846029
C	-0.6238555505	-4.497242515	2.8493230787
H	-0.1552176163	-5.4039906879	2.4757897109
C	-1.8095479375	-4.5831437362	3.5690400434
H	-2.2627208863	-5.553727455	3.7519522803
C	-2.4114152348	-3.4249941316	4.059875156
H	-3.335244748	-3.4876706818	4.6288166682
C	-1.8294802658	-2.1831777515	3.8210751818
H	-2.2972854315	-1.2841286256	4.2135070028
C	1.3504550581	-4.227470543	0.2631409458
C	0.9295968914	-3.6663068192	-0.949853155
H	0.7923316229	-2.5891100341	-1.0262917031
C	0.6933500333	-4.4725736047	-2.0610679342
H	0.3662367991	-4.0208085902	-2.9938412118
C	0.8912846409	-5.848879707	-1.9786949675
H	0.7145592969	-6.4784863029	-2.8466434231

C	1.3271578477	-6.4154733722	-0.7820914877
H	1.4898229775	-7.4880115872	-0.7143390719
C	1.5547598164	-5.6118216885	0.3323077536
H	1.9042119934	-6.0652105481	1.2563201132
C	2.7465170399	-3.9297215263	2.7832612642
C	3.9415646731	-4.4448428158	2.2585436543
H	4.1084844446	-4.4380030328	1.1845521236
C	4.9147477922	-4.979462072	3.0978075016
H	5.8284852104	-5.384281437	2.6702856259
C	4.7198969047	-4.996894966	4.4775169219
H	5.4803626371	-5.4133734244	5.1323621976
C	3.5436038838	-4.4757984483	5.0105548204
H	3.3812517094	-4.4832047376	6.0851883262
C	2.5646473555	-3.9458364111	4.1727083208
H	1.6521659968	-3.5451184868	4.606038567
F	0.110063667	0.0779111678	4.7926220885

XYZ coordinates of the optimized structure of **[8]**BMe_4

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Pt	0.0145453354	-0.0270944721	0.05717902
P	-2.2624503367	0.3259943611	0.3766751699
Cl	-0.0522001638	0.0499931076	-2.3092889559
Bi	0.0942791181	-0.0430920499	2.621195847
P	2.3260597298	0.2404924221	0.1385006622
P	1.5510442344	-2.9538709195	2.902770981
C	-1.5272885609	1.4413696573	2.8830871828
C	-2.4405817629	1.4789941076	1.8139652108
C	-3.503248987	2.3886649946	1.8605857402
H	-4.2140787223	2.4381586168	1.0403268303
C	-3.6501754917	3.2434070342	2.9514123977
H	-4.4759740198	3.9484344595	2.9715894866
C	-2.742355518	3.2002371441	4.0049123748
H	-2.852125762	3.8753068306	4.8487884417
C	-1.6816301215	2.2943035837	3.9736047
H	-0.9698745879	2.2740159567	4.7953023764
C	-3.1553529712	1.140763782	-0.9830535376
C	-2.6320829118	2.3303190246	-1.5069578431
H	-1.7084932161	2.7421945428	-1.1087470519
C	-3.2892709434	2.9823093988	-2.5430475854
H	-2.8801033221	3.9049761682	-2.944170665
C	-4.4630303491	2.4461375153	-3.0735707835
H	-4.9716676384	2.9542701188	-3.8878983891
C	-4.9788688956	1.2586871034	-2.5636254592
H	-5.8902050172	0.8360607652	-2.9766541289
C	-4.3291983512	0.6041750827	-1.5182396625
H	-4.73974733	-0.3203240861	-1.1234615831
C	-3.2218955765	-1.1592068704	0.8140247544
C	-2.7809506808	-2.3947530243	0.3252999043
H	-1.8735132905	-2.4461967272	-0.2720657846

C	-3.4993541594	-3.5528213697	0.6100169466
H	-3.1483153023	-4.5083955009	0.2324262814
C	-4.6523394806	-3.4833190178	1.3891711899
H	-5.2090819399	-4.3881596358	1.6160258657
C	-5.0900656243	-2.2560839994	1.8845300453
H	-5.9861451469	-2.2021460035	2.4960726712
C	-4.3792388568	-1.094044776	1.599437957
H	-4.7241099246	-0.1410757219	1.9916355587
C	2.0940680143	0.8065870189	2.9386400424
C	2.9021448701	0.8368696468	1.7942689702
C	4.1988876949	1.3576049916	1.9042254906
H	4.8399967389	1.4118268137	1.0282189222
C	4.6751420076	1.8145294035	3.1294348403
H	5.6829205628	2.2131456467	3.1974500655
C	3.8639139149	1.7667234839	4.2606091827
H	4.2348049779	2.1296841181	5.2147938194
C	2.5684667118	1.2611701801	4.1675345957
H	1.9383559073	1.2307699475	5.052515778
C	2.8948718832	1.5578925956	-0.9877239741
C	2.1358186464	2.7325137589	-1.0588178304
H	1.212460655	2.8128183441	-0.4900631729
C	2.5546319878	3.7854369995	-1.8637374378
H	1.960195267	4.6929626066	-1.9172900694
C	3.7281028817	3.6704825453	-2.6089333758
H	4.0507439562	4.4913226421	-3.2431141571
C	4.4823498354	2.5025231777	-2.5446216171
H	5.3949146675	2.4083315518	-3.1262348474
C	4.070796588	1.4457002379	-1.7343518361
H	4.66413484	0.5368666646	-1.6920372716
C	3.3259258173	-1.2292759677	-0.2637338797
C	3.1248585247	-1.8215308254	-1.5197247603
H	2.4087021528	-1.3907049117	-2.2155971612
C	3.8376657496	-2.9627210278	-1.8721780166
H	3.6813660541	-3.4131942071	-2.8481346912
C	4.7425837684	-3.5293942333	-0.9741043243
H	5.2942333465	-4.4235187579	-1.2500570578
C	4.9349028701	-2.9506333031	0.2773918437
H	5.6318077784	-3.3916121787	0.9843519421
C	4.2302487724	-1.8019208772	0.6350092757
H	4.3850470302	-1.3632202523	1.6155438461
C	-0.3350838667	-1.4707354069	4.2542673655
C	0.4216355254	-2.6464074604	4.3142223843
C	0.256330751	-3.4865225414	5.4214129139
H	0.8558568139	-4.3896724688	5.5058685825
C	-0.669602713	-3.169969694	6.4128537886
H	-0.7904054479	-3.8302282066	7.2668621923
C	-1.4447039219	-2.0167270369	6.310878283
H	-2.1699060056	-1.7762290409	7.0828987404
C	-1.2798161308	-1.154647908	5.2269400034

H	-1.8741389496	-0.2472132109	5.1613717987
C	2.992298751	-3.7836433348	3.6712463742
C	3.2052391706	-5.1652688115	3.6228888555
H	2.4840053954	-5.8093073079	3.1273525679
C	4.3428839892	-5.7205273303	4.2061706767
H	4.4986830387	-6.7950576119	4.1628407689
C	5.2743315006	-4.9045846298	4.8430707501
H	6.1604470095	-5.3404036982	5.2960637314
C	5.0709703548	-3.5259127457	4.8924121588
H	5.7981379755	-2.8840165945	5.3820758302
C	3.9420121696	-2.9670140872	4.302473866
H	3.7981354625	-1.8883368649	4.3301500987
C	0.7205658128	-4.2689542308	1.9323617291
C	1.0743493155	-4.3605623042	0.5786977419
H	1.8036236271	-3.6704254562	0.1612386493
C	0.5015433648	-5.3324729967	-0.2369341797
H	0.7877567071	-5.393536698	-1.2832837215
C	-0.4410432667	-6.2155052425	0.2864129998
H	-0.8914647684	-6.9720004259	-0.3503204684
C	-0.8079059097	-6.1231279048	1.6276172443
H	-1.5449722615	-6.8070226737	2.0396934038
C	-0.2314784303	-5.1558499521	2.4480837202
H	-0.5318002107	-5.0923509554	3.4899739093
B	0.5706889468	2.5666754055	8.1065978084
C	1.0686557409	3.6045057175	6.9233807759
C	-1.0784962534	2.5463915094	8.1698755005
C	1.1274893043	1.0462390787	7.7817163944
C	1.1699077123	3.0668744385	9.5595922278
H	-1.4683466641	1.8688948679	8.9500019871
H	-1.5447824468	2.215187509	7.2239610882
H	-1.5098893098	3.5391594874	8.3882758344
H	2.1686512668	3.6590725884	6.8357742657
H	0.727438161	4.6410985184	7.0913280858
H	0.7030810536	3.329842903	5.9170960896
H	0.8687624153	2.4092375564	10.3938826576
H	0.8331113421	4.0815092572	9.8360761685
H	2.2734637904	3.0967861311	9.5798343911
H	0.8592063742	0.3129300991	8.5621704959
H	2.2274458685	1.0016351737	7.6904929165
H	0.7230547396	0.6321569571	6.8399502483

XYZ coordinates of the optimized structure of $[NMe_4]F$

18

F	0.0071840419	0.0627748138	3.2025571011
C	0.0022431822	-1.397033002	0.5395368546
N	0.0007875159	-0.0026411584	0.0014678014
C	-1.2105042123	0.7031577015	0.5207518706
C	1.2145203079	0.7034678246	0.5145403496
C	-0.002886567	-0.0192370513	-1.4845641939

H	0.8954915155	-1.9090188308	0.1770816775
H	-0.8926279588	-1.9091702927	0.1813126668
H	0.0047662795	-1.3063552155	1.6314385674
H	-1.2056284561	1.7267569523	0.1416794843
H	-2.0987697265	0.1779549839	0.1648959775
H	-1.13516409	0.6767720456	1.6142709186
H	1.2073682449	1.7270717867	0.1354917621
H	2.1011137999	0.1785941768	0.154065479
H	1.1449494058	0.677127098	1.6084027624
H	-0.897151249	-0.5392588113	-1.8317391038
H	-0.0039038393	1.0086970919	-1.8505309864
H	0.8897908058	-0.5390491129	-1.8361269886

XYZ coordinates of the optimized structure of $[NMe_4]Cl$

18

Cl	0.0088735313	0.0564050562	3.8816497745
C	0.002158792	-1.4010076641	0.499272007
N	0.0007077076	-0.0022867265	-0.0272675625
C	-1.2147750394	0.7065024924	0.4771655109
C	1.2185552382	0.7068331061	0.4709322891
C	-0.0029636777	-0.0207606008	-1.5167905605
H	0.8953627895	-1.9106366511	0.1350536958
H	-0.8929728856	-1.9106417104	0.1398114722
H	0.0050342291	-1.3486101102	1.5908608126
H	-1.2069943638	1.7284804019	0.095421353
H	-2.1006641381	0.1798750889	0.1192456367
H	-1.1764084374	0.7012953201	1.5695263449
H	1.2087553267	1.7286366075	0.0887337471
H	2.1027410482	0.1802035559	0.1088235328
H	1.1856128302	0.7020622034	1.5634715353
H	-0.897133906	-0.5415396023	-1.86206281
H	-0.0041539091	1.0067978493	-1.8829197857
H	0.8898438644	-0.5409976164	-1.8663949932

XYZ coordinates of the optimized structure of $[NMe_4]Br$

18

Br	0.01015663	0.0584795797	3.961450742
C	0.0020361553	-1.4003187714	0.4948887464
N	0.0006249303	-0.0024402881	-0.0350773542
C	-1.2144999338	0.7059405881	0.4719165232
C	1.2180154386	0.706299278	0.4659201977
C	-0.0028863626	-0.0209034119	-1.5240975436
H	0.8956952449	-1.9110782066	0.1333618719
H	-0.8935399646	-1.9110378178	0.1380623411
H	0.0048978622	-1.3405230128	1.5866184147
H	-1.2065519862	1.7294058345	0.0941882612
H	-2.1013281674	0.1802969196	0.1148779165
H	-1.1715184993	0.695737198	1.5644327695
H	1.2082140191	1.7295334316	0.0875783272

H 2.1032234634 0.1805552065 0.1050256378
H 1.1801208186 0.6966600926 1.5586277217
H -0.89705722 -0.54164706 -1.869502094
H -0.0040361354 1.0067387439 -1.8901097703
H 0.890012707 -0.541087304 -1.8736307087

XYZ coordinates of the optimized structure of $[NMe_4]CN$
19
N 0.0096100709 0.0459274323 4.766688592
C 0.0084078973 0.040936513 3.5907150566
C 0.0019398783 -1.3934415405 0.499300333
N 0.0005825243 -0.0005794387 -0.0437888068
C -1.2115304028 0.7083676731 0.4693921015
C 1.2148531164 0.7087251408 0.4637542846
C -0.0027492164 -0.0245332728 -1.5307142738
H 0.8955023593 -1.9073230084 0.1412447905
H -0.8933650562 -1.9073041948 0.1455800338
H 0.0045686414 -1.3081603455 1.5906791756
H -1.2054279174 1.7313073567 0.0895185237
H -2.1003242915 0.1827689138 0.116506749
H -1.1495289747 0.6913707563 1.5620948767
H 1.2069292719 1.7314720035 0.0833663976
H 2.1021475905 0.1831057384 0.1071441748
H 1.1577233278 0.6921933211 1.5567286514
H -0.8969124859 -0.5467966669 -1.8744219025
H -0.0038468585 1.0016433285 -1.9013191255
H 0.8901835676 -0.546293896 -1.8783805309

XYZ coordinates of the optimized structure of $[NMe_4]SCN$
20
N 0.2138857396 0.27499614 3.4972065738
C 0.5637189084 0.622105621 4.5690383619
S 1.0509148795 1.1057367876 6.0710547218
C 0.051985305 -1.4447907584 0.6897395004
N -0.106291248 -0.1113618856 0.0328916872
C -1.3229397617 0.5597535296 0.5844705346
C 1.0925653073 0.7264422655 0.3407479311
C -0.2429821017 -0.2828702595 -1.4397783352
H 0.9448273756 -1.9265450771 0.2883963421
H -0.8295079012 -2.0484700227 0.468533892
H 0.1493622618 -1.2742913323 1.7641049084
H -1.4289068601 1.5360054354 0.1088096886
H -2.1932323957 -0.060048831 0.363044186
H -1.1829900688 0.6638847629 1.6626430161
H 0.9710852052 1.6991312525 -0.1380415596
H 1.9788840807 0.2251368416 -0.0510371056
H 1.1535596601 0.8310866438 1.4262628261
H -1.1206540995 -0.897725497 -1.643533136
H -0.3590542936 0.6988926308 -1.9009171366

H 0.6529409466 -0.7727459202 -1.8238062746

XYZ coordinates of the optimized structure of $[NMe_4]BMe_4$

34

B 0.008821885 -0.0016337119 -2.5312913819
C 0.0230167927 1.5636337892 -2.0062255813
C -1.3626427352 -0.7488162003 -1.9977045302
C 0.0331195352 -0.0281973037 -4.1805865419
C 1.3398199438 -0.7924151539 -1.9578559147
H 0.9257913903 2.1163785453 -2.3193281309
H -0.0151136069 1.6563014814 -0.9043900673
H -0.8362992162 2.1472319292 -2.379693044
H -1.4357001504 -1.7980361642 -2.3322569141
H -2.283219088 -0.2518532711 -2.3498396785
H -1.4475774666 -0.7828340937 -0.89525781
H 0.0201013736 -1.0530066417 -4.5909039103
H 0.9300065054 0.4565673304 -4.6040468827
H -0.8323357106 0.4888383652 -4.6303730602
H 1.3664772202 -1.8571621982 -2.2478916886
H 1.4194720194 -0.783332999 -0.8548751958
H 2.2843226239 -0.3538597309 -2.3236195352
N -0.0081810361 0.0009904819 2.470565042
C 1.1601514862 0.7861918579 1.9693086555
C 0.0638532138 -1.3916832315 1.9336068616
C 0.0172719639 -0.0363701653 3.9621475572
C -1.2738096941 0.6472839255 2.0091150658
H 1.0936849947 1.8024097343 2.3600011805
H 1.1319696378 0.7993150954 0.8786316851
H 2.077628752 0.309866734 2.3167556401
H -0.7922882631 -1.9561513799 2.3045655857
H 0.0440377293 -1.349407313 0.843547198
H 0.9924488359 -1.8509297263 2.2747930162
H -0.8424181161 -0.6072010441 4.3150087442
H -0.0309056465 0.9851105132 4.3410898123
H 0.9424992007 -0.5134669982 4.2873672529
H -1.2789975878 0.6701026891 0.918334649
H -2.1196812368 0.0656954508 2.3779176889
H -1.3141955497 1.6616094038 2.4077042326

XYZ coordinates of the optimized structure of PPh_3

34

P 2.1904612189 0.1854721251 0.2717550849
C 1.9490206 0.8954595348 2.9436226488
C 2.7668946927 1.0148178599 1.8113354731
C 3.9505221062 1.7564572551 1.9108062828
H 4.5941700258 1.8666777307 1.0419313551
C 4.3106671616 2.3555071037 3.1164865924
H 5.2316351022 2.9294230957 3.1785785346
C 3.4964272521 2.2183805659 4.2388712632

H	3.7787514604	2.6870954914	5.1777317172
C	2.3144832431	1.4848371972	4.1509546253
H	1.6706891629	1.3801828888	5.0202182246
C	3.0102403091	-1.4600908971	0.3751280441
C	2.4849887729	-2.4842670016	-0.4251890819
H	1.6242011016	-2.2828684542	-1.0598002074
C	3.0495953619	-3.7568822062	-0.4139746178
H	2.6323220266	-4.5388591192	-1.0428152998
C	4.1382936162	-4.0291595468	0.4127236681
H	4.5743302448	-5.0243566748	0.4300909998
C	4.6603503808	-3.0229441854	1.2229643369
H	5.5069827286	-3.2307236589	1.8721747044
C	4.102465948	-1.745956679	1.2034717546
H	4.5193610067	-0.9671342602	1.8366993532
C	3.1735215918	1.0383907536	-1.0308431411
C	4.4444851498	0.6298439322	-1.4533549648
H	4.910812358	-0.2411531445	-1.0003006977
C	5.1175358561	1.3317999807	-2.4516648069
H	6.1029465581	1.0021909656	-2.7706394407
C	4.5326691523	2.4526175556	-3.0374836334
H	5.0588162458	2.9978630335	-3.8164085386
C	3.2668578305	2.8671286382	-2.6266249819
H	2.8013235018	3.7358540943	-3.0844889948
C	2.589582135	2.1593815529	-1.6372671367
H	1.5942858011	2.4777079254	-1.3334224915
H	1.0165102965	0.3385065479	2.8769333718

XYZ coordinates of the optimized structure of $SbPh_3$

34

Sb	1.7788298757	0.1767843974	0.2084126433
C	1.8934528457	0.9818755822	3.1835737394
C	2.6112475077	1.092537034	1.986175636
C	3.8201417166	1.7973052114	1.9885527663
C	4.3045773123	2.3697125279	3.1643295945
C	3.5856402306	2.2459250409	4.3514243164
C	2.3784546478	1.5503614397	4.3601765535
C	2.8948352976	-1.6757383461	0.3272433016
C	2.4763783627	-2.7501044353	-0.4677012366
C	3.1528663212	-3.9682631682	-0.4325999457
C	4.2530845674	-4.129802956	0.4067818546
C	4.6738167308	-3.0705102993	1.2082475076
C	3.9984219753	-1.8510937135	1.1695551857
C	3.0729837421	1.1674079786	-1.2181663848
C	4.3408020138	0.6871055893	-1.5643735305
C	5.1260894788	1.3666598028	-2.4951758334
C	4.6529407236	2.5334671216	-3.0918963691
C	3.3902087609	3.0186794635	-2.7581642021
C	2.6045964419	2.3363822951	-1.8308901732
H	0.9443290208	0.449020549	3.2067216914

H	4.3900942088	1.9033499342	1.0684790437
H	5.2455288639	2.9142930048	3.151930126
H	3.9633661793	2.6937314249	5.2668789242
H	1.8110867569	1.453421472	5.2823875821
H	1.6133660495	-2.6439776961	-1.1228567992
H	2.81756337	-4.7921141752	-1.0575932503
H	4.7791743479	-5.0803016876	0.4389943536
H	5.5299204298	-3.1929103553	1.8671912434
H	4.3355633325	-1.0334789506	1.8023883709
H	4.7213782619	-0.2234884551	-1.1075931053
H	6.1094792792	0.9824753837	-2.7549132058
H	5.2652764509	3.0614230412	-3.8182277008
H	3.0139036299	3.9264977116	-3.2229778626
H	1.6168032665	2.7245672323	-1.5881148346

XYZ coordinates of the optimized structure of $AsPh_3$

34

As	2.0215581135	0.181142034	0.2461387811
C	1.9477609152	0.8984607366	3.0429218043
C	2.706665197	1.0459194351	1.8756850524
C	3.8790952178	1.8064826751	1.921842532
C	4.2881421068	2.4001713864	3.1150062599
C	3.5317714672	2.2392538537	4.273915809
C	2.3602815832	1.4855271553	4.2367745748
C	2.9654284813	-1.54197106	0.3596671953
C	2.5070923397	-2.5750349634	-0.4667371921
C	3.1160015314	-3.8274951215	-0.4414692835
C	4.1836674118	-4.0655681341	0.4218079083
C	4.6401596355	-3.0467398963	1.255303829
C	4.0355456481	-1.7909839276	1.2245761831
C	3.1344207674	1.084078749	-1.102607659
C	4.3837430969	0.6183384025	-1.5236750686
C	5.1019989081	1.3090185901	-2.4987016819
C	4.581270658	2.4723362777	-3.0613005388
C	3.3357447493	2.9426658116	-2.6496658297
C	2.6147187587	2.2482919474	-1.6812284699
H	1.0247537153	0.3221591475	3.0214338172
H	4.4759494138	1.9380817605	1.0231198408
H	5.2011767641	2.9897079977	3.1380770901
H	3.8517792922	2.7039712225	5.20270692
H	1.7628125166	1.360098638	5.136015392
H	1.66575509	-2.402992605	-1.1353859162
H	2.7517023622	-4.6192905541	-1.0908397038
H	4.6556501683	-5.044115353	0.4481765244
H	5.4707975703	-3.2282718942	1.9326594626
H	4.3990555905	-1.002851998	1.8787483619
H	4.7989211768	-0.2878937327	-1.0905935226
H	6.0718595533	0.9363027349	-2.8183416547
H	5.1423528029	3.0086171345	-3.8219583659

H 2.9213589236 3.8468856943 -3.0878487422
H 1.6372104729 2.6168968556 -1.3760237093

XYZ coordinates of the optimized structure of $BiPh_3$
34
Bi 1.6842312092 0.1809339332 0.1911630705
C 1.8878756459 0.9898720743 3.2295684011
C 2.5852423704 1.1082795339 2.0217819563
C 3.794812628 1.8101167881 2.0087837381
C 4.3004220788 2.3740264629 3.1805581137
C 3.6004635396 2.2449228258 4.3784323094
C 2.3921733871 1.551571751 4.4022254984
C 2.8728683125 -1.7149743057 0.315969112
C 2.4588210171 -2.8036646443 -0.4601667003
C 3.1513558813 -4.0135213681 -0.4185152229
C 4.2657772559 -4.1497371494 0.4064748308
C 4.6838872565 -3.0742387994 1.1876125513
C 3.9902050522 -1.8645818809 1.1437901916
C 3.0605994189 1.1976394749 -1.2561487837
C 4.3345246529 0.7144338822 -1.5716129116
C 5.1409391904 1.3871050586 -2.4901741071
C 4.6812388101 2.5492912911 -3.1063229753
C 3.4118736001 3.0371509863 -2.8032321273
C 2.6068974691 2.3624414358 -1.8858164896
H 0.9395669952 0.4555544141 3.2683717567
H 4.3503881418 1.9212686621 1.0801777499
H 5.2426423608 2.9164338804 3.1565568517
H 3.9941801322 2.6858112419 5.2905987134
H 1.8401258354 1.4492980192 5.3333746232
H 1.5874189238 -2.7189543664 -1.1080339146
H 2.8187607524 -4.8498412751 -1.0285959391
H 4.8055057382 -5.0925142365 0.4425302848
H 5.5516063446 -3.176636722 1.8350121164
H 4.3252354614 -1.0348461636 1.7624080018
H 4.7050902555 -0.1936414535 -1.1010292917
H 6.1298399225 1.0009314838 -2.7257503204
H 5.3094099608 3.0718753972 -3.8230753299
H 3.0462895234 3.9420589733 -3.2825562771
H 1.615932876 2.7573337951 -1.6661594807

XYZ coordinates of the optimized structure of $\mathbf{2_m}$
44
Pd -0.21252309 0.1752672249 0.5648306663
P -2.4867014282 -0.2714328868 0.6202119347
Cl -0.5200024378 0.3918307391 -1.781626174
Sb 0.0295843469 -0.0178074154 3.1124059788
P 2.0296404852 0.6967188528 0.3248437037
C -1.5914121497 0.948141107 4.0938881048
C -2.12734624 0.4196727596 5.2719855653

C	-3.188767889	1.0695552863	5.8979570165
H	-3.6068020431	0.6576024039	6.8119168004
C	-3.7136131205	2.2398505292	5.353339313
H	-4.5418664666	2.7420552948	5.8447903154
C	-3.1820549091	2.7648888051	4.1774520362
H	-3.5919197646	3.6755625887	3.7502511094
C	-2.1234062423	2.1189943206	3.541791998
H	-1.722926656	2.5344264752	2.6189252365
C	1.7686241545	0.8683079796	3.9586026112
C	2.9513231366	0.1279610508	4.0701858891
C	4.0950016529	0.7283035257	4.5934121516
H	5.0102207195	0.1509458246	4.687324419
C	4.0615590301	2.0610253623	4.9982618875
H	4.9546567588	2.5257611463	5.4059254371
C	2.8836974562	2.7977001265	4.8872381888
H	2.8553486235	3.8343601856	5.2101910309
C	1.735335155	2.2057734967	4.367364904
H	0.8187589687	2.7866528169	4.2974169263
C	0.0777655277	-2.0136234788	3.8242401205
C	0.5360476783	-2.2853739758	5.1186211718
H	0.8970849832	-1.4880123793	5.7633653037
C	0.5407986007	-3.597790376	5.5856099489
H	0.8951649323	-3.8088853562	6.5903799767
C	0.0982518618	-4.6338761286	4.7658865983
H	0.1068598921	-5.6559065274	5.1334740993
C	-0.3493527485	-4.3641786412	3.4743195053
H	-0.6874418218	-5.1728148363	2.8328818832
C	-0.3598321487	-3.0548448589	2.9994585657
H	-0.7031201781	-2.8540314171	1.9870930969
H	-1.7306958217	-0.4954958051	5.7040775837
H	2.98720112	-0.9166398052	3.7692055619
H	-3.2542776749	0.8049434698	0.1479530426
H	-2.8682289969	-1.3053423987	-0.2492216643
H	-3.1864826519	-0.6140820924	1.7914164366
H	2.4659440546	0.708888991	-1.0094473651
H	2.4144163743	1.9725504285	0.7719790373
H	3.0049198866	-0.1040068225	0.9429748763

XYZ coordinates of the optimized structure of **2_mF**

45

Pd	-0.0434124393	-0.3427745094	-0.0351771656
P	-2.3069324005	-0.7950883125	-0.0457014796
Cl	-0.1455501809	-0.2596630293	-2.5245293592
Sb	-0.0166771767	-0.3067227087	2.6377310522
P	2.2521179613	-0.2279685804	-0.1827401947
C	-1.8034359733	0.8759922819	2.8774480477
C	-2.0874964362	1.8762589541	1.9430051481
C	-3.2283658311	2.6657214269	2.0856330525
H	-3.4330725856	3.453103292	1.3651196946

C	-4.1027336044	2.4396171932	3.1464464314
H	-4.9979534974	3.0462897373	3.2518424336
C	-3.8254896959	1.4373268849	4.0740741426
H	-4.5052430214	1.2594849885	4.9031939734
C	-2.6719345102	0.6640965297	3.9510837532
H	-2.443359799	-0.0926030552	4.6938636998
C	1.7527092837	0.8697457956	2.9554690691
C	1.9372124061	2.044562668	2.2221264303
C	3.0757582221	2.8242547267	2.424535826
H	3.2048913094	3.7463736969	1.8641964949
C	4.0440613178	2.4177894878	3.3401757045
H	4.9361057668	3.0194643112	3.4908935264
C	3.8653484694	1.2411748792	4.0656295907
H	4.6184446735	0.9228035707	4.7815105939
C	2.7164527243	0.4722735258	3.885031566
H	2.5710100875	-0.4273330802	4.4755560382
C	0.048365243	-2.4580915104	2.8523408698
C	0.1859765003	-3.2407430277	1.7026988949
H	0.2533480533	-2.7648600102	0.7245208432
C	0.2373999024	-4.6307112912	1.7965664057
H	0.3478391384	-5.2285392252	0.895762315
C	0.1463423321	-5.2462206878	3.042516632
H	0.1839096469	-6.3295732694	3.1186071695
C	0.0073394454	-4.4697117672	4.1911444225
H	-0.0640874996	-4.9467938249	5.1650940982
C	-0.0395857586	-3.0795038784	4.1028108733
H	-0.1417351987	-2.475450889	4.9960689372
F	-0.0567847889	-0.339651556	4.6918252431
H	1.1974850587	2.3637144081	1.4896606911
H	-1.4240833538	2.049128272	1.0963963472
H	-3.0763764407	-1.1149469689	1.0904412012
H	-3.1275205813	0.1944026798	-0.6176838758
H	-2.6287229736	-1.8864644848	-0.8744934308
H	2.7544954425	-1.0797415028	-1.1847043239
H	2.7966981196	0.9963609017	-0.6128258293
H	3.1399436429	-0.5281250429	0.868028446

XYZ coordinates of the optimized structure of **3$_m$**

48

Pd	0.3017592932	-0.119406266	0.3323718344
P	-1.5136962486	1.2674846576	-0.0199675207
Cl	0.935834619	0.4269901755	-1.9480714772
Sb	0.0512536801	0.0333062893	2.8821425904
P	2.448133419	-0.9808088478	0.5002620333
P	-0.9203237653	-2.3454438531	-0.6043549546
C	-1.5352890875	1.2454375484	3.6211590529
C	-2.8304685678	0.7225846587	3.7142375641
C	-3.8733598973	1.5324955849	4.1586121333
H	-4.8764700172	1.1232723601	4.237573693

C	-3.628386659	2.8606533533	4.503106799
H	-4.4435512778	3.4896671194	4.8490542175
C	-2.3396764382	3.3817215576	4.4090027689
H	-2.1468394976	4.4148598326	4.6835190749
C	-1.290450711	2.577983809	3.9672166538
H	-0.2873524163	2.9933208723	3.9064821136
C	1.7890728	0.8848876844	3.7688062356
C	2.1880765911	0.5233409614	5.0592566847
C	3.3213135675	1.1086622462	5.6190959981
H	3.6330382504	0.8262708416	6.6206066263
C	4.0532435889	2.0504168227	4.8979502668
H	4.9366589439	2.5029924735	5.3390863573
C	3.6577231217	2.4094115347	3.6113843242
H	4.228901078	3.1410246265	3.0470191876
C	2.527611876	1.8250755406	3.0419352511
H	2.2293328332	2.1032151223	2.0326027766
C	-0.2690577147	-1.815703846	3.8805406844
C	0.0573364749	-3.0226873675	3.2545095855
C	-0.1276078515	-4.2273529096	3.929100974
H	0.1267684569	-5.1634977142	3.4403997092
C	-0.6403976107	-4.2292803183	5.2246264498
H	-0.7854161155	-5.169630502	5.7485397287
C	-0.9726014722	-3.0284070234	5.8475798325
H	-1.3771393241	-3.0292706526	6.8556096891
C	-0.7914744453	-1.8193886138	5.1790770681
H	-1.0669849543	-0.8908385975	5.6728936713
H	-3.0323728216	-0.3145851894	3.4565720276
H	1.6288065943	-0.2139332569	5.6298057048
H	0.449327196	-3.033303896	2.240262538
H	-0.0620950669	-3.2449198707	-1.2788956573
H	-1.7488134048	-3.3312522319	-0.0137887281
H	-1.7586993459	-2.0736043167	-1.7098676089
H	-1.1851638804	2.6250652724	-0.1723136701
H	-2.181888463	1.0050504628	-1.2269566683
H	-2.5836386448	1.3465207205	0.8897014633
H	3.4393453714	-0.037992021	0.1843532499
H	2.9854011264	-1.5464284553	1.6720070409
H	2.7156967475	-1.9948604785	-0.4342013895

XYZ coordinates of the optimized structure of **3_mF**

49

Pd	0.0714567629	0.0651304186	-0.0444432547
P	0.0762318966	2.425823108	-0.3270697527
Cl	0.1151661272	-0.0571058222	-2.5784038068
Sb	0.0180377068	0.1976633797	2.6215047713
P	-1.969638083	-1.147518135	-0.1916923268
P	2.1343390401	-1.1202276815	-0.1127157466
C	2.1144109831	0.5987498739	2.9332840444
C	2.8501176615	1.3769609578	2.0372880249

C	4.2063147297	1.6124471732	2.2602241593
H	4.765892902	2.2332300296	1.5656984561
C	4.8394663463	1.0468415898	3.364655175
H	5.8987714793	1.2204339731	3.5326468244
C	4.1107651161	0.2590445052	4.2530462431
H	4.6001273603	-0.185815599	5.115341449
C	2.7486315126	0.0434825206	4.048927564
H	2.1814095189	-0.5437806548	4.762744547
C	-1.3684467434	1.8410863596	2.7959107101
C	-2.421427608	2.0078649467	1.8940619348
C	-3.2952735968	3.0864723971	2.0259783917
H	-4.1215112202	3.197862985	1.328972116
C	-3.1027867885	4.0191794218	3.0426296068
H	-3.7764517794	4.8661859926	3.1387774931
C	-2.0448387879	3.8626760734	3.9354386299
H	-1.8890300876	4.588373969	4.7291700161
C	-1.1852007854	2.7707575189	3.8241637233
H	-0.3837251607	2.6382871541	4.542784739
C	-0.7082307649	-1.7994693929	2.9925938662
C	-0.3316989572	-2.8767650859	2.1879293322
C	-0.8255725182	-4.1545001972	2.4487048952
H	-0.5131767015	-4.9893082305	1.8271112201
C	-1.7209849652	-4.3552693378	3.4968409591
H	-2.1149466223	-5.348607948	3.6932244914
C	-2.1092408551	-3.2795314416	4.2923983253
H	-2.808920691	-3.4302521999	5.110116908
C	-1.5966249536	-2.0055135327	4.0524958785
H	-1.8780913604	-1.1792829825	4.6962283003
F	-0.0272480932	0.2994399216	4.6705105761
H	-2.5635317778	1.3071544968	1.0758034108
H	0.3395456456	-2.7289296177	1.3462957524
H	2.3766489138	1.7967603773	1.1539396417
H	-2.8869588622	-1.4544915937	0.8401515661
H	-2.89760161	-0.6446056928	-1.1301393168
H	-1.8556569135	-2.4498227383	-0.7238311873
H	3.2028167938	-0.4330320049	-0.7278447379
H	2.8688286727	-1.6673899792	0.9649840371
H	2.14315112	-2.2596547264	-0.9473923937
H	1.0520965972	2.9197810643	-1.2207299379
H	-1.0577115203	2.9562317099	-0.978880739
H	0.1995599706	3.4269802767	0.6642696101

XYZ coordinates of the optimized structure of **2_mSi**

44

Pd	-0.2272197172	0.1445672323	0.871930643
P	-2.438000804	-0.468895986	1.1311989844
Cl	-0.6586323572	0.3609548116	-1.5699027167
Si	0.033691403	-0.0122413974	3.2104838592
P	1.9779657598	0.7387735098	0.6550830002

C	-1.4361313304	0.8844883857	4.012500639
C	-2.1053308735	0.366499301	5.1318061037
C	-3.1751731498	1.0466524011	5.7119809242
H	-3.6799941953	0.6225266343	6.5763031968
C	-3.5988506592	2.2646504915	5.1849831741
H	-4.4330613754	2.7948586937	5.6367247556
C	-2.9512838329	2.7970998977	4.0714802857
H	-3.2782838827	3.7447643888	3.6511178894
C	-1.8873576523	2.109487494	3.4909520629
H	-1.4054487753	2.528826994	2.60818496
C	1.6085896627	0.7956191664	3.895472431
C	2.7967862996	0.0593248504	4.0401619138
C	3.966126646	0.6555581572	4.5094041483
H	4.8698638808	0.0616283087	4.6197594567
C	3.9738785372	2.0085999097	4.8417149821
H	4.8837245221	2.4755960548	5.2094821339
C	2.8064265394	2.7585678663	4.7074141291
H	2.8025657897	3.8125578191	4.9734200593
C	1.640033517	2.1569219982	4.24135335
H	0.7361488576	2.756416435	4.1571992025
C	0.0699299745	-1.8288702464	3.7424504517
C	0.3749387388	-2.1694813071	5.0721270497
H	0.6201916507	-1.3883508259	5.7892653442
C	0.3833848829	-3.4964875652	5.495190206
H	0.6189533501	-3.7334070617	6.5295590513
C	0.0970253366	-4.5186470397	4.591923962
H	0.1068288297	-5.5547794682	4.9197980139
C	-0.1915769615	-4.2070266636	3.2655635428
H	-0.4028544815	-4.9994929314	2.5521969547
C	-0.2032735717	-2.8762975809	2.8498327664
H	-0.4130657229	-2.648461165	1.8058459356
H	-1.7939680113	-0.5851645014	5.5562820406
H	2.807418711	-1.0009856919	3.7954248618
H	-3.3516769419	0.5687432347	0.8696774757
H	-2.8913573284	-1.4322212235	0.2100652517
H	-2.9894468117	-0.9789434224	2.3215606938
H	2.4093191269	0.9113438932	-0.6747280686
H	2.4146089564	1.948535206	1.2252529489
H	2.9830183837	-0.1202134678	1.1356567792