

Supporting Information

Theoretical study on the unusual square-planar structure of bis(imino)pyridine-ligated Group 13 complexes

*Weiyi Li, * Yajing Lyu, Huifang Zhang, Maoqin Zhu and Hanping Tang*

School of Science, Xihua University, Chengdu, Sichuan, 610039, P. R. China.

E-mail: weiyili@mail.xhu.edu.cn; Fax: +86-028-87727663; Tel: +86-028-87727663

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S1: Computational details

Optimization and frequency calculation in gas phase: M06-2X/6-31G*, the key words (Opt = tight and Int = ultrafine) are used to get more accurate results.

Single-point energy calculation in benzene solvent: M06-2X/6-311++G(d, p), LANL2DZ using SMD solvent model.

S2: Assessment on the computational protocol

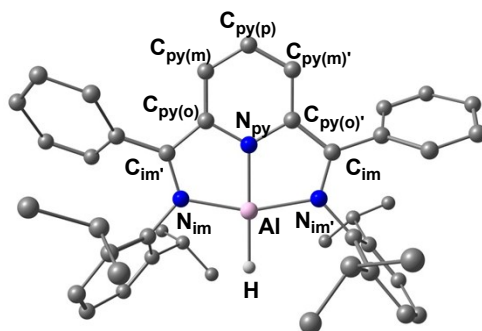
To assess the present computational method, the optimization and frequency calculations for the C_2 -symmetric Bis(imino)pyridine complex of Al^{III} , denoted as ${}^1(PhI_2P)AlH-SP$ (complex **1**), were carried out with different functionals (*e.g.* B3LYP, BP86 and M06-2X) and basis sets (6-31G* and cc-PVDZ), respectively. The calculations show that the closed-shell single state ($S=0$) structure is the ground state of complex **1**, which lies approximately 7.0~10.0 kcal mol⁻¹ (depending on the computational method) below the analogue biradical triplet state ($S=1$) structure. This computed result is in good agreement with the experimental observation that the complex **1** was found to be diamagnetic.^{6a,b} As a result, the key geometrical parameters and IR frequency of the Al–H stretching vibration for the ground state of the complex **1** are listed in Table S1 to make a further comparison of the computational and experimentally determined results.

As shown in Fig. S1 and Table S1, the geometric optimization of complex **1** with the three different DFT functionals and two basis sets could generally well reproduce the SP geometry for the Al^{III} center in four-coordinate complex **1**, as indicated by the comparable τ_4 values (0.14 vs 0.13). However, the structural parameters and of IR frequencies of the Al–H stretching vibration obtained from the B3LYP and BP86 functional with correlation-consistent cc-PVDZ basis set deviated somewhat from those of the solid-state complex. Especially for the Al– N_{im} and Al– N_{py} bond lengths, the largest discrepancies between the computational and experimental data exceed the accepted error of the calculations (0.05 Å). On the contrary, the geometries and IR frequency of the Al–H stretching vibration of complex calculated at the M06-2X/6-31G* level of theory are closed to the corresponding experimental data, in which the differences in bond lengths and bond angles are less than 0.03 Å and 2.0 degree. In addition, geometric optimization of complex **1** was also performed with the SMD solvation model in THF solvent. However, the calculation accuracy is not significantly

improved (Table S2), suggesting that solvent effect may have small impact on the geometric structure of the present complex. Considering the above results and the computational cost, we believe that the geometric optimization in gas phase at the M06-2X/6-31G* level of theory is reliable for the present system.

Table S1 Structural parameters and the Al-H stretching vibration frequency of complex **1** calculated in the gas phase.

	B3LYP	BP86	M06-2X	B3LYP	BP86	M06-2X	exp. Data ^{6a,b}
	cc-PVDZ			6-31G*			
Al-N _{im}	2.015	2.017	1.989	1.996	1.999	1.972	1.942
Al-N _{py}	1.860	1.881	1.855	1.849	1.869	1.845	1.833
Al-H	1.583	1.599	1.583	1.583	1.597	1.584	1.570
N _{im} -C _{im}	1.359	1.370	1.348	1.359	1.370	1.347	1.363
N _{py} -C _{py(p)}	1.392	1.396	1.385	1.389	1.394	1.384	1.386
C _{im} -C _{py(o)}	1.430	1.441	1.426	1.427	1.439	1.423	1.427
C _{py(o)} -C _{py(m)}	1.396	1.404	1.392	1.394	1.403	1.390	1.395
C _{py(m)} -C _{py(p)}	1.403	1.410	1.401	1.400	1.408	1.399	1.403
N _{im} -Al-N _{py}	80.1	80.0	79.9	80.4	80.2	80.2	81.0
N _{im} -Al-N _{im} '	160.2	159.9	159.8	160.8	160.6	160.4	161.9
N _{im} -Al-H	99.9	100.0	100.1	99.6	99.0	99.8	99.0
N _{py} -Al-H	180.0	180.0	180.0	180.0	180.0	180.0	180.0
τ_4	0.14	0.14	0.14	0.14	0.14	0.14	0.13
Al-H stretching vibration	1898	1841	1920	1935	1842	1939	1966



Complex 1

Fig. S1 Optimized-structure of the complex **1**. All H atoms except hydride atom are omitted for clarity.

Table S2 Structural parameters and the Al–H stretching vibration frequency of complex 1 calculated in THF solvent with SMD model.

	B3LYP	BP86	M06–2X	B3LYP	BP86	M06–2X	exp. Data ^{6a,b}
	cc–PVDZ			6–31G*			
Al–N _{im}	2.017	2.019	1.990	2.000	1.999	1.970	1.942
Al–N _{py}	1.858	1.879	1.854	1.847	1.868	1.843	1.833
Al–H	1.584	1.599	1.584	1.584	1.598	1.586	1.570
N _{im} –C _{im}	1.360	1.371	1.348	1.360	1.371	1.348	1.363
N _{py} –C _{py(p)}	1.392	1.396	1.386	1.390	1.395	1.385	1.386
C _{im} –C _{py(o)}	1.429	1.440	1.426	1.427	1.439	1.423	1.427
C _{py(o)} –C _{py(m)}	1.396	1.404	1.392	1.394	1.403	1.390	1.395
C _{py(m)} –C _{py(p)}	1.403	1.410	1.401	1.400	1.408	1.399	1.403
N _{im} –Al–N _{py}	80.20	80.05	79.94	80.50	80.372	80.27	80.96
N _{im} –Al–N _{im} '	160.40	160.09	159.87	160.99	160.74	160.54	161.93
N _{im} –Al–H	99.80	99.95	100.06	99.50	99.63	99.73	99.00
N _{py} –Al–H	180.00	180.00	180.00	180.00	180.00	180.00	180.00
τ_4	0.14	0.14	0.14	0.13	0.14	0.14	0.13
Al–H stretching vibration	1891	1835	1911	1925	1863	1970	1966

Table S3 Comparison of the key bond lengths (in Å), bond angles and dihedral angles (in degree) in the free (PhI₂P)²⁻ ligand and ¹(PhI₂P)AlX complexes (X = H, , NH₂, NHPH and NHDipp).

${}^1(\text{PhI}_2\text{P})\text{AlX}$	Free (PhI_2P) $^{2-}$	X = H		X = NH $_2$		X = NHPH		X = NHDipp	
		SP	TET	SP	TET	SP	TET	SP	TET
$\text{N}_{\text{im}}-\text{C}_{\text{im}}$	1.338	1.347	1.328	1.353	1.331	1.350	1.344	1.340	1.375
$\text{C}_{\text{im}}-\text{C}_{\text{py(o)}}$	1.479	1.422	1.454	1.422	1.452	1.423	1.438	1.430	1.415
$\text{N}_{\text{py}}-\text{C}_{\text{py(o)}}$	1.346	1.383	1.378	1.386	1.377	1.384	1.384	1.386	1.393
$\text{C}_{\text{py(o)}}-\text{C}_{\text{py(m)}}$	1.413	1.390	1.374	1.390	1.375	1.390	1.379	1.383	1.397
$\text{C}_{\text{py(m)}}-\text{C}_{\text{py(p)}}$	1.387	1.399	1.429	1.400	1.429	1.400	1.417	1.407	1.397
$\text{N}_{\text{im}}-\text{C}_{\text{im}}-\text{C}_{\text{py(o)}}$	116.1	112.7	114.7	112.9	114.6	113.4	114.0	113.6	113.6
$\text{N}_{\text{im}'}-\text{C}_{\text{im}'}-\text{C}_{\text{py(o)'}}$	116.1	112.7	115.5	112.9	116.1	112.4	114.7	113.4	114.2
$\text{C}_{\text{im}}-\text{C}_{\text{py(o)}}-\text{N}_{\text{py}}$	117.3	111.8	113.3	112.1	113.1	112.0	113.4	112.5	113.5
$\text{C}_{\text{im}'}-\text{C}_{\text{py(o)'}}-\text{N}_{\text{py}}$	117.3	111.8	114.6	112.1	114.6	112.1	113.8	113.1	113.3
$\text{C}_{\text{py(o)}}-\text{N}_{\text{py}}-\text{C}_{\text{py(o)'}}$	119.7	121.5	116.7	121.5	116.9	120.9	118.8	119.4	119.3
$\text{N}_{\text{im}}-\text{C}_{\text{im}}-\text{C}_{\text{py(o)}}-\text{N}_{\text{py}}$	32.4	2.8	9.3	6.2	10.0	2.4	10.1	0.0	9.1
$\text{N}_{\text{im}'}-\text{C}_{\text{im}'}-\text{C}_{\text{py(o)'}}-\text{N}_{\text{py}}$	32.4	2.8	2.7	6.1	4.4	4.1	6.8	5.2	8.4
$\text{N}_{\text{py}}-\text{C}_{\text{py(o)}}-\text{C}_{\text{py(m)}}-\text{C}_{\text{py(p)}}$	1.4	3.0	2.6	1.3	2.5	0.1	10.0	0.4	12.5
$\text{N}_{\text{py}}-\text{C}_{\text{py(o)'}}-\text{C}_{\text{py(m)'}}-\text{C}_{\text{py(p)'}}$	1.4	3.0	22.2	1.2	23.1	5.7	6.5	10.3	4.5

S3: Nature bond orbital analysis

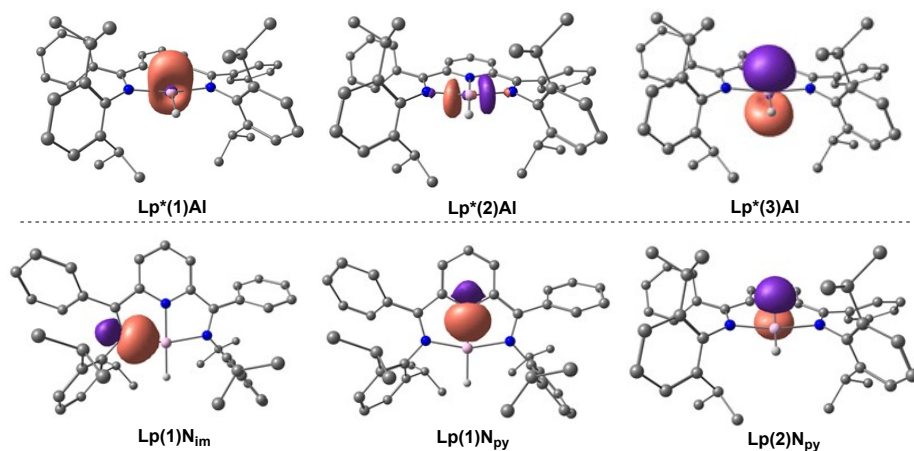


Fig.S2 The nature bond orbitals of $\text{Lp}^*(n)\text{Al}$, $\text{Lp}(n)\text{N}_{\text{im}}$ and $\text{Lp}(n)\text{N}_{\text{py}}$ in the SP structure of the ${}^1(\text{PhI}_2\text{P})\text{AlH}$ complex.

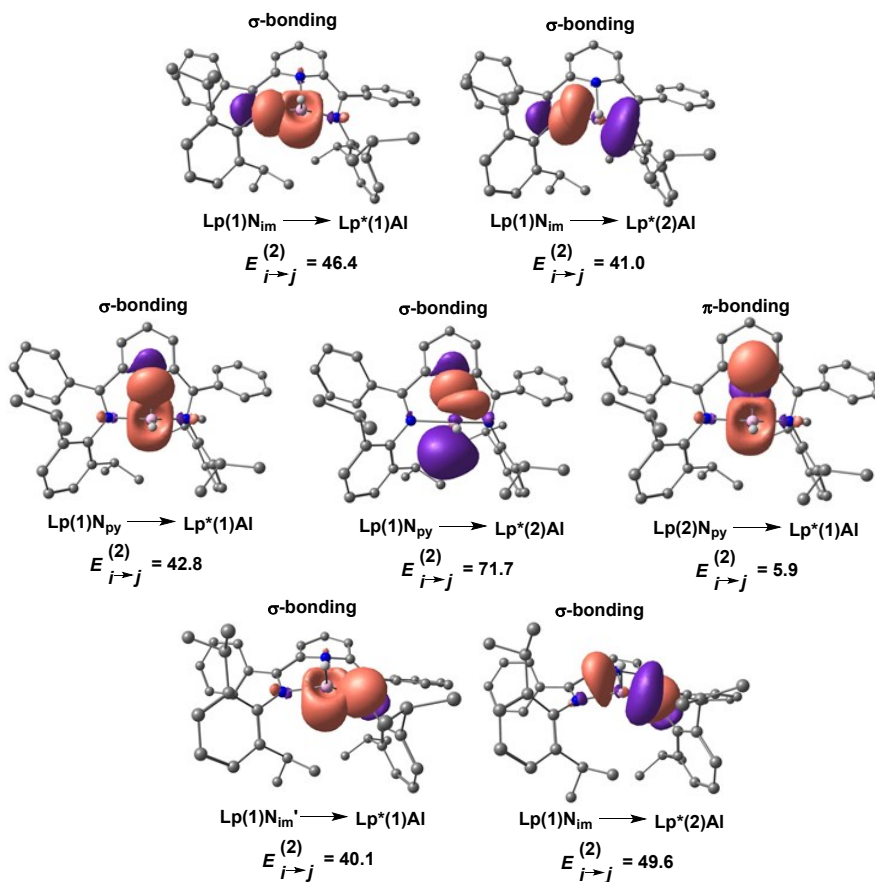


Fig. S3 NBO analysis showing σ - and π -interactions between the coordinating nitrogen atoms and the Al ion in the TET structure of the $(\text{PhI}_2\text{P})\text{AlH}$ complex. The isodensity contour value is 0.05 a.u. All the second order perturbation energies are given in kcal mol^{-1} .

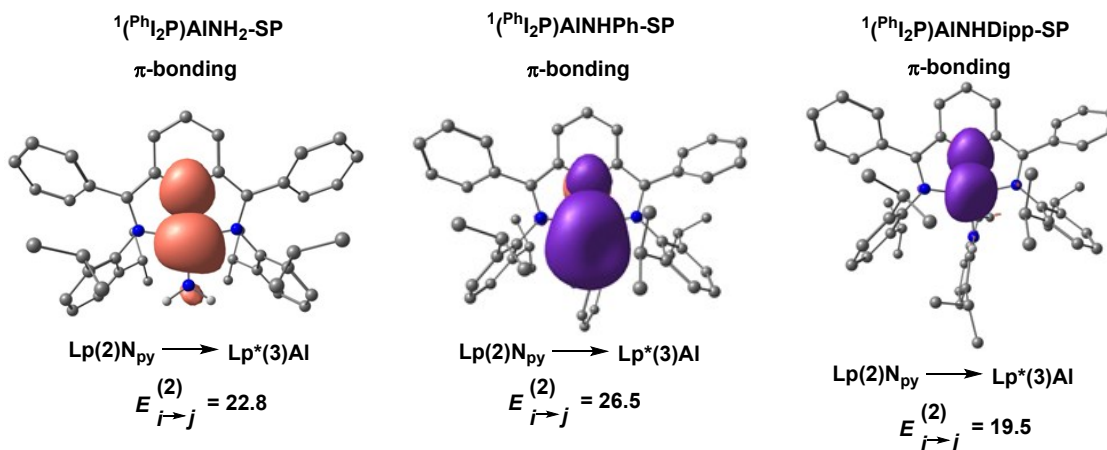


Fig. S4 NBO analysis showing π -interactions between the N_{py} nitrogen atoms and the Al^{III} ion in the SP structures of the ${}^1(\text{PhI}_2\text{P})\text{AlNH}_2$, ${}^1(\text{PhI}_2\text{P})\text{AlNHPh}$ and ${}^1(\text{PhI}_2\text{P})\text{AlNHdipp}$ complexes. The isodensity contour value is 0.05 a.u. All the second order perturbation energies are given in kcal mol^{-1} .

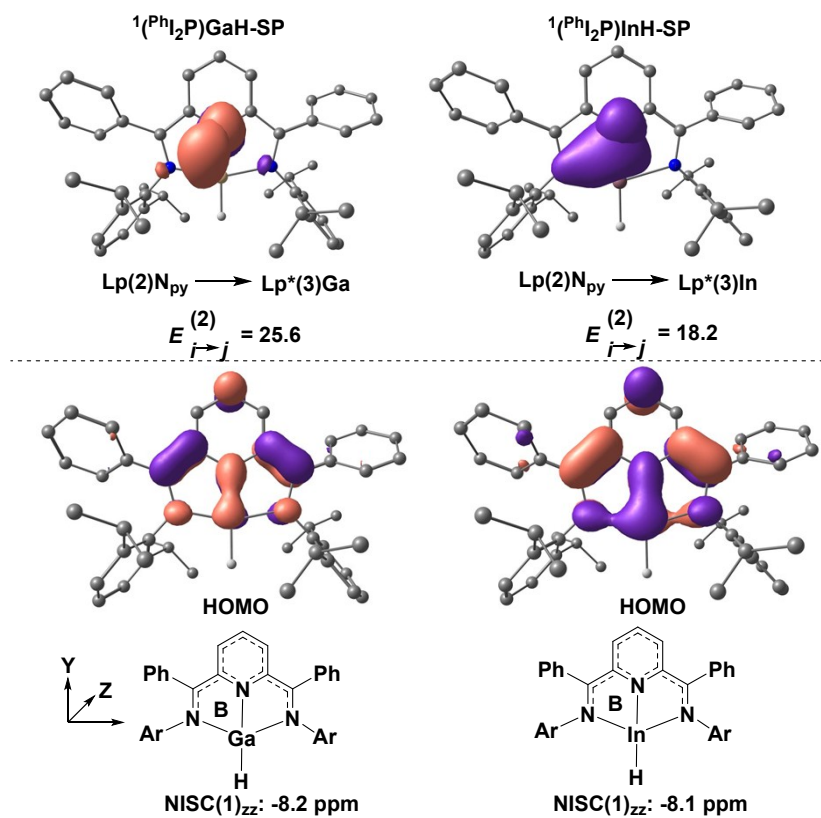


Fig. S5 NBO and FMO analyses of the SP structure of the ${}^1(\text{PhI}_2\text{P})\text{GaH}$ and ${}^1(\text{PhI}_2\text{P})\text{InH}$ complexes. The isodensity contour value is 0.05 a.u. All the second order perturbation energies are given in kcal mol^{-1} .

S4: Summary of energy and spin-contamination of the optimized structures

Table S4 Electronic energy and spin-contamination $\langle S^2 \rangle$ values of optimized structures

Species	E_{ZPE} (a.u.) ^a	E_{sln} (a.u.) ^b	$\langle S^2 \rangle$
$^1(\text{PhI}_2\text{P})^{2-}$	0.79634	-1830.97906	0.00
$^3(\text{PhI}_2\text{P})^{2-}$	0.79595	-1830.98461	2.02
BS ^c - $^1(\text{PhI}_2\text{P})^{2-}$	0.79598	-1830.90792	1.02
$^1(\text{PhI}_2\text{P})\text{AlH-SP}$	0.81309	-2073.95826	0.00
$^1(\text{PhI}_2\text{P})\text{AlH-TET}$	0.81320	-2073.94459	0.00
$^3(\text{PhI}_2\text{P})\text{AlH-SP}$	0.81249	-2073.94654	2.00
BS- $^1(\text{PhI}_2\text{P})\text{AlH-SP}$	0.81305	-2073.95865	0.29
$^1(\text{PhI}_2\text{P})\text{AlNH}_2\text{-SP}$	0.83286	-2129.36712	0.00
$^1(\text{PhI}_2\text{P})\text{AlNH}_2\text{-TET}$	0.83205	-2129.34756	0.00
$^1(\text{PhI}_2\text{P})\text{AlNHPh-SP}$	0.91603	-2360.37297	0.00
$^1(\text{PhI}_2\text{P})\text{AlNHPh-TET}$	0.91477	-2360.38042	0.00
$^1(\text{PhI}_2\text{P})\text{AlNHDIpp-SP}$	1.08933	-2596.19190	0.00
$^1(\text{PhI}_2\text{P})\text{AlNHDIpp-TET}$	1.08705	-2596.21205	0.00
$^1(\text{PhI}_2\text{P})\text{BH-SP}$	0.81843	-1856.31606	0.00
$^1(\text{PhI}_2\text{P})\text{BH-T}$	0.82050	-1856.37651	0.00
$^1(\text{PhI}_2\text{P})\text{GaH-SP}$	0.81183	-1833.55976	0.00
$^1(\text{PhI}_2\text{P})\text{GaH-TET}$	0.81232	-1833.54535	0.00
$^3(\text{PhI}_2\text{P})\text{GaH-SP}$	0.81145	-1833.54740	2.02
BS- $^1(\text{PhI}_2\text{P})\text{GaH}$	0.81167	-1833.55989	0.06
$^1(\text{PhI}_2\text{P})\text{InH-SP}$	0.80953	-1833.36215	0.00
$^1(\text{PhI}_2\text{P})\text{InH-TET}$	0.81009	-1833.34397	0.00
$^3(\text{PhI}_2\text{P})\text{InH-SP}$	0.80935	-1833.35402	2.02
BS- $^1(\text{PhI}_2\text{P})\text{InH}$	0.80961	-1833.36284	0.25
$^1(\text{PhI}_2\text{P})\text{TIH-SP}$	0.80764	-1882.88800	0.00
$^1(\text{PhI}_2\text{P})\text{TIH-T}$	0.81002	-1882.93506	0.00

a: E_{ZPE} is the Zero-point correction calculated in gas phase at the M06-2X/6-31G* level

b: E_{sln} is the single point energy after PCM correction calculated at the M06-2X/(SMD,THF)/6-311++G(d,p) level

c: BS represents for the open-shell singlet state

S5: Cartesian coordinates of the optimized structures.

$1^{(\text{PhI}_2\text{P})^{2-}}$:							
				1	4.788097000	-2.391286000	3.373399000
7	2.162870000	-0.030080000	0.523485000	6	5.229038000	-2.778563000	1.308626000
7	-0.152235000	1.219609000	-0.262261000	1	6.009027000	-3.502382000	1.529778000
7	-2.433907000	-0.157832000	-0.922118000	6	4.899792000	-2.477805000	-0.005277000
6	2.234280000	1.138526000	-0.001542000	1	5.423826000	-2.978530000	-0.817757000
6	0.966441000	1.919498000	-0.184868000	6	3.908480000	-1.544792000	-0.320814000
6	1.074646000	3.317244000	-0.157821000	6	2.728915000	-0.555023000	3.184881000
1	2.027439000	3.821848000	-0.056006000	1	2.643910000	0.508367000	2.924105000
6	-0.149539000	4.026846000	-0.229869000	6	3.388054000	-0.647686000	4.561234000
1	-0.150027000	5.116064000	-0.258351000	1	4.422241000	-0.284378000	4.546443000
6	-1.330112000	3.342631000	-0.310585000	1	3.396545000	-1.681067000	4.928747000
1	-2.254190000	3.895091000	-0.443782000	1	2.822553000	-0.050151000	5.283770000
6	-1.369161000	1.897513000	-0.296519000	6	1.300707000	-1.121399000	3.235552000
6	-2.550220000	1.141357000	-0.436440000	1	0.791363000	-0.965818000	2.281463000
6	3.517668000	1.764058000	-0.451808000	1	0.720336000	-0.624546000	4.021427000
6	4.690576000	1.682051000	0.309289000	1	1.331845000	-2.194794000	3.458232000
1	4.668042000	1.168914000	1.266180000	6	3.568904000	-1.281671000	-1.777849000
6	5.875867000	2.251135000	-0.143603000	1	2.785436000	-0.520175000	-1.815760000
1	6.773292000	2.181592000	0.465226000	6	4.785526000	-0.759113000	-2.551965000
6	5.913386000	2.908131000	-1.375939000	1	5.227161000	0.113395000	-2.060404000
1	6.841624000	3.346349000	-1.733777000	1	4.496169000	-0.471768000	-3.569572000
6	4.755025000	2.994011000	-2.142905000	1	5.558531000	-1.534573000	-2.631441000
1	4.775765000	3.499875000	-3.104763000	6	3.000287000	-2.542168000	-2.440262000
6	3.564996000	2.429846000	-1.687823000	1	2.101945000	-2.882295000	-1.918521000
1	2.658342000	2.493882000	-2.280090000	1	3.737528000	-3.355187000	-2.433756000
6	-3.872711000	1.746073000	-0.314050000	1	2.728214000	-2.338184000	-3.482055000
6	-4.976229000	1.193940000	-1.018705000	6	-3.101677000	-1.224343000	-0.485760000
1	-4.786973000	0.342279000	-1.663893000	6	-3.814508000	-1.428622000	0.762722000
6	-6.255588000	1.715019000	-0.905381000	6	-4.539903000	-2.599979000	0.969728000
1	-7.063079000	1.261931000	-1.479202000	1	-5.070799000	-2.709672000	1.918507000
6	-6.528171000	2.799712000	-0.064175000	6	-4.591186000	-3.646307000	0.053518000
1	-7.536239000	3.195643000	0.032756000	1	-5.173509000	-4.543537000	0.249070000
6	-5.470301000	3.332466000	0.676794000	6	-3.820685000	-3.515868000	-1.111149000
1	-5.655096000	4.146409000	1.377381000	1	-3.805185000	-4.340675000	-1.823720000
6	-4.186989000	2.815038000	0.567684000	6	-3.083876000	-2.378992000	-1.381368000
1	-3.406118000	3.204339000	1.214977000	6	-3.678077000	-0.475591000	1.945453000
6	3.229333000	-0.898467000	0.733507000	1	-3.072985000	0.376369000	1.632099000
6	3.531629000	-1.226260000	2.081634000	6	-2.919957000	-1.148223000	3.100392000
6	4.537671000	-2.149745000	2.343909000	1	-1.944751000	-1.506345000	2.756849000
				1	-3.477236000	-2.010360000	3.489849000

1	-3.929911000	-0.091075000	-3.080822000	1	1.946052000	4.002767000	-0.559880000
1	-3.696557000	-1.312564000	-1.812305000	6	-0.187436000	4.003713000	-0.894388000
6	1.840578000	-2.675259000	-1.001948000	1	-0.242159000	5.065050000	-1.132784000
6	3.005267000	-2.079293000	-1.577984000	6	-1.338162000	3.228605000	-0.889382000
6	3.601348000	-2.676179000	-2.688394000	1	-2.302597000	3.651660000	-1.150004000
1	4.487489000	-2.205569000	-3.115056000	6	-1.234770000	1.860247000	-0.560650000
6	3.096231000	-3.828740000	-3.279924000	6	-2.427013000	0.980344000	-0.586621000
1	3.587923000	-4.275680000	-4.140334000	6	3.597860000	1.854616000	-0.488818000
6	1.926182000	-4.382966000	-2.757660000	6	4.830541000	1.687100000	0.203147000
1	1.508360000	-5.272519000	-3.224915000	1	4.820139000	1.225453000	1.185062000
6	1.290139000	-3.828488000	-1.655577000	6	6.034161000	2.105311000	-0.340365000
6	3.547595000	-0.740893000	-1.096349000	1	6.948800000	1.961251000	0.232409000
1	2.961208000	-0.424610000	-0.231590000	6	6.093522000	2.704695000	-1.603416000
6	3.358337000	0.334106000	-2.175543000	1	7.042099000	3.020467000	-2.029280000
1	2.303148000	0.420980000	-2.449654000	6	4.894482000	2.875069000	-2.307195000
1	3.929911000	0.091075000	-3.080822000	1	4.908451000	3.320206000	-3.300826000
1	3.696557000	1.312564000	-1.812305000	6	3.685642000	2.463112000	-1.772070000
6	5.018400000	-0.824151000	-0.669982000	1	2.777724000	2.575114000	-2.357738000
1	5.168827000	-1.596460000	0.090146000	6	-3.735791000	1.527661000	-0.267027000
1	5.353342000	0.135433000	-0.256698000	6	-4.928289000	0.959714000	-0.797498000
1	5.660981000	-1.057427000	-1.529968000	1	-4.848129000	0.125890000	-1.487216000
6	0.000000000	-4.399900000	-1.094657000	6	-6.180224000	1.449585000	-0.463106000
1	0.104739000	-4.397797000	-0.001988000	1	-7.061758000	0.985011000	-0.901814000
6	-0.297580000	-5.829243000	-1.548889000	6	-6.329423000	2.522358000	0.422871000
1	-1.176707000	-6.216303000	-1.020504000	1	-7.314686000	2.894551000	0.690438000
1	0.546058000	-6.501750000	-1.355226000	6	-5.170878000	3.094625000	0.963389000
1	-0.519923000	-5.868823000	-2.622724000	1	-5.253224000	3.917967000	1.671162000
6	-1.183015000	-3.477962000	-1.427079000	6	-3.914602000	2.614825000	0.633358000
1	-0.991536000	-2.479263000	-1.026685000	1	-3.036944000	3.055557000	1.097471000
1	-2.113839000	-3.863074000	-0.989824000	6	3.157074000	-0.593927000	1.183970000
1	-1.317673000	-3.413402000	-2.514391000	6	3.471138000	-0.933843000	2.542041000
				6	4.368784000	-1.955217000	2.821839000
				1	4.614620000	-2.182387000	3.857273000
				6	4.970418000	-2.696449000	1.803500000
				1	5.676210000	-3.490083000	2.035437000
				6	4.624213000	-2.411629000	0.487236000
				1	5.050132000	-3.013883000	-0.315554000
				6	3.731213000	-1.395654000	0.149155000
				6	2.783889000	-0.138661000	3.637976000
				1	2.807211000	0.913045000	3.324536000
BS ⁻¹ (^{Ph} I ₂ P) ²⁻ :							
7	2.252669000	0.408931000	0.991460000				
7	-0.047668000	1.288677000	-0.284432000				
7	-2.220031000	-0.273388000	-1.007406000				
6	2.343593000	1.373375000	0.067529000				
6	1.071369000	2.036412000	-0.304756000				
6	1.033398000	3.417110000	-0.593651000				

6	-0.732391000	-6.324855000	-2.633384000	1	-0.161873000	-5.365962000	4.073077000
1	-0.903702000	-7.340229000	-2.976890000	6	1.056456000	-4.031139000	2.907573000
6	-1.497508000	-5.276254000	-3.136335000	1	1.952182000	-4.225392000	3.492278000
1	-2.276802000	-5.469932000	-3.866976000	6	1.122850000	-3.135289000	1.838706000
6	-1.283660000	-3.977426000	-2.685538000	6	-2.550869000	-3.253941000	0.668906000
1	-1.913890000	-3.168512000	-3.043017000	1	-2.319646000	-2.655010000	-0.216188000
6	0.046605000	2.895246000	1.090743000	6	-3.498524000	-2.425353000	1.545632000
6	-1.122850000	3.135289000	1.838706000	1	-3.023358000	-1.488304000	1.855470000
6	-1.056456000	4.031139000	2.907573000	1	-3.772319000	-2.977296000	2.451793000
1	-1.952182000	4.225392000	3.492278000	1	-4.418823000	-2.185778000	1.001991000
6	0.129079000	4.673628000	3.237424000	6	-3.221959000	-4.546316000	0.190686000
1	0.161873000	5.365962000	4.073077000	1	-2.520110000	-5.170528000	-0.371642000
6	1.274421000	4.419457000	2.494362000	1	-4.073846000	-4.314222000	-0.457339000
1	2.205637000	4.913297000	2.759567000	1	-3.600539000	-5.133497000	1.034637000
6	1.258218000	3.533058000	1.416753000	6	2.452695000	-2.468789000	1.519280000
6	-2.452695000	2.468789000	1.519280000	1	2.318519000	-1.851625000	0.624370000
1	-2.318519000	1.851625000	0.624370000	6	3.546394000	-3.498625000	1.207376000
6	-3.546394000	3.498625000	1.207376000	1	4.481485000	-2.990549000	0.949964000
1	-3.270237000	4.143072000	0.367092000	1	3.270237000	-4.143072000	0.367092000
1	-3.743764000	4.140812000	2.072420000	1	3.743764000	-4.140812000	2.072420000
1	-4.481485000	2.990549000	0.949964000	6	2.897762000	-1.554032000	2.667079000
6	-2.897762000	1.554032000	2.667079000	1	2.132335000	-0.806150000	2.892803000
1	-2.132335000	0.806150000	2.892803000	1	3.828217000	-1.037593000	2.406538000
1	-3.828217000	1.037593000	2.406538000	1	3.080951000	-2.135503000	3.577743000
1	-3.080951000	2.135503000	3.577743000	1	0.000000000	0.000000000	1.946987000
6	2.550869000	3.253941000	0.668906000	¹ (^{Ph} I ₂ P)AIH-TET:			
1	2.319646000	2.655010000	-0.216188000	13	0.048238000	-0.215260000	-1.014969000
6	3.221959000	4.546316000	0.190686000	7	1.813488000	-0.024581000	-0.111971000
1	2.520110000	5.170528000	-0.371642000	7	0.138691000	1.630157000	-1.120270000
1	4.073846000	4.314222000	-0.457339000	7	-1.773349000	-0.010051000	-0.576520000
1	3.600539000	5.133497000	1.034637000	6	2.208841000	1.241174000	-0.044398000
6	3.498524000	2.425353000	1.545632000	6	1.227187000	2.209597000	-0.505829000
1	3.023358000	1.488304000	1.855470000	6	1.241146000	3.561692000	-0.259815000
1	3.772319000	2.977296000	2.451793000	1	2.075061000	4.034320000	0.245599000
1	4.418823000	2.185778000	1.001991000	6	0.076463000	4.312835000	-0.609525000
6	-0.046605000	-2.895246000	1.090743000	1	0.095310000	5.394813000	-0.539415000
6	-1.258218000	-3.533058000	1.416753000	6	-1.102921000	3.660106000	-0.878653000
6	-1.274421000	-4.419457000	2.494362000	1	-2.025330000	4.220225000	-0.999208000
1	-2.205637000	-4.913297000	2.759567000	6	-1.114173000	2.233433000	-0.897532000
6	-0.129079000	-4.673628000	3.237424000				

6	-2.144175000	1.344842000	-0.636757000	1	-0.920354000	-2.626047000	1.975162000
6	3.536169000	1.670252000	0.437451000	1	0.298230000	-3.816003000	1.456058000
6	4.114278000	1.091739000	1.576105000	6	4.107226000	-0.460454000	-1.966300000
1	3.578654000	0.316049000	2.114810000	1	3.450538000	0.413410000	-1.950716000
6	5.361142000	1.513675000	2.019123000	6	5.558929000	0.033855000	-1.914611000
1	5.796425000	1.062330000	2.904933000	1	5.803720000	0.460846000	-0.937343000
6	6.051557000	2.512062000	1.331670000	1	5.726318000	0.799796000	-2.679094000
1	7.028367000	2.834390000	1.678332000	1	6.258343000	-0.786092000	-2.111793000
6	5.487766000	3.087980000	0.196475000	6	3.828156000	-1.202688000	-3.280022000
1	6.025537000	3.855341000	-0.351290000	1	2.780028000	-1.508913000	-3.338678000
6	4.239399000	2.668820000	-0.251659000	1	4.454526000	-2.097834000	-3.362768000
1	3.812183000	3.091056000	-1.155934000	1	4.048789000	-0.554918000	-4.134873000
6	-3.553175000	1.767721000	-0.514571000	6	-2.628431000	-1.016419000	-0.035080000
6	-4.573196000	1.043082000	-1.148510000	6	-3.108981000	-0.956232000	1.293084000
1	-4.311586000	0.164939000	-1.730602000	6	-3.830701000	-2.040534000	1.797723000
6	-5.899875000	1.443389000	-1.047445000	1	-4.194771000	-1.998942000	2.821367000
1	-6.673452000	0.868314000	-1.547276000	6	-4.075258000	-3.174171000	1.034803000
6	-6.237870000	2.581615000	-0.316093000	1	-4.624207000	-4.011569000	1.454466000
1	-7.274865000	2.893416000	-0.238995000	6	-3.620595000	-3.215501000	-0.275390000
6	-5.237523000	3.307354000	0.324457000	1	-3.824393000	-4.091341000	-0.886647000
1	-5.491813000	4.181760000	0.916036000	6	-2.916195000	-2.147696000	-0.834039000
6	-3.910819000	2.896051000	0.238768000	6	-2.861574000	0.219794000	2.226933000
1	-3.145130000	3.425311000	0.798096000	1	-2.348705000	1.010280000	1.674857000
6	2.694134000	-1.134611000	0.089605000	6	-1.949918000	-0.174930000	3.395155000
6	2.384188000	-2.054102000	1.111457000	1	-0.964144000	-0.483224000	3.035209000
6	3.208111000	-3.165507000	1.284013000	1	-2.376507000	-1.005584000	3.969451000
1	2.982938000	-3.878767000	2.071206000	1	-1.812672000	0.671386000	4.076908000
6	4.307084000	-3.376777000	0.461504000	6	-4.187924000	0.785711000	2.754085000
1	4.941342000	-4.245312000	0.608775000	1	-4.896952000	0.961877000	1.940207000
6	4.577592000	-2.479429000	-0.561319000	1	-4.018805000	1.734176000	3.275512000
1	5.421303000	-2.660685000	-1.221688000	1	-4.651513000	0.094145000	3.466856000
6	3.783076000	-1.350966000	-0.777945000	6	-2.499288000	-2.243091000	-2.294420000
6	1.145772000	-1.887537000	1.975315000	1	-2.038480000	-1.293364000	-2.580332000
1	0.836877000	-0.836685000	1.921237000	6	-3.711329000	-2.463420000	-3.210142000
6	1.388630000	-2.217093000	3.451273000	1	-3.398242000	-2.452798000	-4.259188000
1	2.235549000	-1.652145000	3.853095000	1	-4.468710000	-1.685552000	-3.072416000
1	1.590762000	-3.282787000	3.598542000	1	-4.187961000	-3.430064000	-3.014626000
1	0.499625000	-1.972246000	4.040929000	6	-1.471657000	-3.360295000	-2.513593000
6	0.011749000	-2.759063000	1.415979000	1	-0.585749000	-3.228477000	-1.885006000
1	-0.204584000	-2.536149000	0.361529000	1	-1.138588000	-3.375567000	-3.556496000

1	-1.908009000	-4.338415000	-2.280227000	1	-3.353257000	3.134704000	1.427780000
1	0.448072000	-0.846579000	-2.416637000	6	2.821387000	-1.094452000	0.303871000
$^3(\text{PhI}_2\text{P})\text{AlH}$:				6	2.882623000	-1.879771000	1.472179000
13	-0.000014000	-0.341319000	0.000044000	6	3.782881000	-2.946597000	1.512843000
7	1.888448000	-0.017213000	0.248418000	1	3.845034000	-3.554274000	2.412241000
7	-0.000006000	1.579717000	0.000043000	6	4.598088000	-3.243140000	0.429249000
7	-1.888456000	-0.017205000	-0.248436000	1	5.293074000	-4.075718000	0.479215000
6	2.286179000	1.285698000	0.195441000	6	4.510445000	-2.473172000	-0.723604000
6	1.196424000	2.215427000	0.097197000	1	5.135177000	-2.717018000	-1.578905000
6	1.212635000	3.628808000	0.133067000	6	3.627103000	-1.397006000	-0.810911000
1	2.141210000	4.166106000	0.272616000	6	2.026083000	-1.597154000	2.697327000
6	0.000000000	4.299243000	0.000037000	1	1.376660000	-0.743804000	2.471289000
1	0.000001000	5.385622000	0.000041000	6	2.886956000	-1.203755000	3.904738000
6	-1.212638000	3.628814000	-0.133004000	1	3.488315000	-0.313335000	3.697098000
1	-2.141208000	4.166117000	-0.272563000	1	3.569400000	-2.015347000	4.179672000
6	-1.196431000	2.215433000	-0.097140000	1	2.253333000	-0.989925000	4.771776000
6	-2.286186000	1.285708000	-0.195436000	6	1.132803000	-2.794547000	3.042185000
6	3.690080000	1.732555000	0.173740000	1	0.504957000	-3.073686000	2.191035000
6	4.667616000	1.172620000	1.010854000	1	0.485085000	-2.555146000	3.892618000
1	4.389684000	0.397037000	1.716025000	1	1.735270000	-3.666592000	3.319189000
6	5.988980000	1.599026000	0.941927000	6	3.523151000	-0.628514000	-2.117541000
1	6.727864000	1.153999000	1.601083000	1	2.910966000	0.261568000	-1.951308000
6	6.366358000	2.589015000	0.036619000	6	4.892107000	-0.155773000	-2.618115000
1	7.399738000	2.917192000	-0.015226000	1	5.427501000	0.395374000	-1.838153000
6	5.408708000	3.148192000	-0.806393000	1	4.771614000	0.502550000	-3.484979000
1	5.693263000	3.907467000	-1.528427000	1	5.515977000	-1.000353000	-2.930677000
6	4.087306000	2.721628000	-0.741899000	6	2.807338000	-1.484638000	-3.170433000
1	3.353197000	3.134729000	-1.427766000	1	1.814885000	-1.787837000	-2.817837000
6	-3.690087000	1.732561000	-0.173764000	1	3.376720000	-2.396299000	-3.383126000
6	-4.667596000	1.172638000	-1.010917000	1	2.689543000	-0.929733000	-4.107514000
1	-4.389636000	0.397072000	-1.716099000	6	-2.821400000	-1.094440000	-0.303884000
6	-5.988964000	1.599032000	-0.942018000	6	-3.627101000	-1.396999000	0.810908000
1	-6.727827000	1.154013000	-1.601203000	6	-4.510436000	-2.473171000	0.723613000
6	-6.366374000	2.588999000	-0.036698000	1	-5.135155000	-2.717022000	1.578922000
1	-7.399759000	2.917166000	0.015126000	6	-4.598086000	-3.243142000	-0.429238000
6	-5.408751000	3.148166000	0.806351000	1	-5.293064000	-4.075728000	-0.479193000
1	-5.693331000	3.907425000	1.528392000	6	-3.782896000	-2.946594000	-1.512842000
6	-4.087344000	2.721613000	0.741884000	1	-3.845052000	-3.554275000	-2.412238000
				6	-2.882648000	-1.879758000	-1.472191000
				6	-3.523131000	-0.628512000	2.117540000

1	-2.910960000	0.261578000	1.951300000	6	-0.234489000	6.065936000	-1.664575000
6	-2.807285000	-1.484633000	3.170413000	1	-0.826877000	6.879071000	-1.256793000
1	-1.814838000	-1.787821000	2.817792000	6	0.741708000	6.325928000	-2.625194000
1	-3.376654000	-2.396301000	3.383113000	1	0.915552000	7.341876000	-2.965696000
1	-2.689475000	-0.929732000	4.107493000	6	1.498936000	5.275622000	-3.136818000
6	-4.892082000	-0.155787000	2.618142000	1	2.274871000	5.468584000	-3.871246000
1	-5.427495000	0.395359000	1.838192000	6	1.281632000	3.976135000	-2.690187000
1	-4.771580000	0.502533000	3.485007000	1	1.905839000	3.166087000	-3.055794000
1	-5.515938000	-1.000374000	2.930711000	6	-0.290928000	-3.698969000	-1.734839000
6	-2.026111000	-1.597141000	-2.697340000	6	0.458932000	-4.767621000	-1.222573000
1	-1.376771000	-0.743718000	-2.471340000	1	1.218749000	-4.576599000	-0.472615000
6	-2.886985000	-1.203902000	-3.904802000	6	0.234489000	-6.065936000	-1.664575000
1	-2.253353000	-0.990045000	-4.771827000	1	0.826877000	-6.879071000	-1.256793000
1	-3.488455000	-0.313540000	-3.697231000	6	-0.741708000	-6.325928000	-2.625194000
1	-3.569327000	-2.015584000	-4.179723000	1	-0.915552000	-7.341876000	-2.965696000
6	-1.132720000	-2.794483000	-3.042093000	6	-1.498936000	-5.275622000	-3.136818000
1	-0.504864000	-3.073506000	-2.190911000	1	-2.274871000	-5.468584000	-3.871246000
1	-0.485010000	-2.555095000	-3.892535000	6	-1.281632000	-3.976135000	-2.690187000
1	-1.735113000	-3.666600000	-3.319033000	1	-1.905839000	-3.166087000	-3.055794000
1	-0.000031000	-1.927730000	0.000167000	6	0.046350000	2.885936000	1.091288000
				6	-1.121867000	3.120310000	1.842983000
				6	-1.056967000	4.016659000	2.911602000
				1	-1.952135000	4.207097000	3.498442000
				6	0.126381000	4.664722000	3.238217000
				1	0.158059000	5.357623000	4.073445000
				6	1.271231000	4.414951000	2.492786000
				1	2.201023000	4.912472000	2.756076000
				6	1.256164000	3.528357000	1.415407000
				6	-2.449805000	2.448230000	1.527385000
				1	-2.312858000	1.822905000	0.638495000
				6	-3.543416000	3.473921000	1.201953000
				1	-3.266197000	4.107300000	0.353662000
				1	-3.740390000	4.127022000	2.058906000
				1	-4.478655000	2.963097000	0.950523000
				6	-2.896756000	1.543809000	2.682554000
				1	-2.130983000	0.799027000	2.917381000
				1	-3.825788000	1.023719000	2.424273000
				1	-3.083664000	2.133097000	3.587353000
				6	2.548549000	3.252366000	0.665915000
				1	2.316943000	2.655911000	-0.220680000
BS ⁻¹ (^{Ph} I ₂ P)AIH:							
13	0.000000000	0.000000000	0.357136000				
7	0.000000000	1.936772000	0.024841000				
7	0.000000000	0.000000000	-1.497675000				
7	0.000000000	-1.936772000	0.024841000				
6	0.095349000	2.311169000	-1.269061000				
6	0.060133000	1.205140000	-2.166996000				
6	0.028721000	1.213066000	-3.559517000				
1	0.023086000	2.156255000	-4.094246000				
6	0.000000000	0.000000000	-4.253244000				
1	0.000000000	0.000000000	-5.337428000				
6	-0.028721000	-1.213066000	-3.559517000				
1	-0.023086000	-2.156255000	-4.094246000				
6	-0.060133000	-1.205140000	-2.166996000				
6	-0.095349000	-2.311169000	-1.269061000				
6	0.290928000	3.698969000	-1.734839000				
6	-0.458932000	4.767621000	-1.222573000				
1	-1.218749000	4.576599000	-0.472615000				

6	3.219143000	4.545868000	0.190292000	^{13}C (PbI ₂ P)AlNH ₂ -SP:			
1	2.516888000	5.170904000	-0.370612000	13	-0.000164000	0.249243000	0.269205000
1	4.070786000	4.315259000	-0.458566000	7	1.919618000	0.054035000	-0.078004000
1	3.598022000	5.131449000	1.035221000	7	0.000115000	-1.476101000	-0.376232000
6	3.496684000	2.421707000	1.540205000	7	-1.918833000	0.055115000	-0.077104000
1	3.021753000	1.483831000	1.848180000	6	2.306096000	-1.172973000	-0.497318000
1	3.770517000	2.971311000	2.447770000	6	1.209035000	-2.041555000	-0.748765000
1	4.416921000	2.183542000	0.995826000	6	1.212736000	-3.257635000	-1.421407000
6	-0.046350000	-2.885936000	1.091288000	1	2.153591000	-3.689145000	-1.746328000
6	-1.256164000	-3.528357000	1.415407000	6	-0.000147000	-3.881853000	-1.737092000
6	-1.271231000	-4.414951000	2.492786000	1	-0.000111000	-4.816444000	-2.285483000
1	-2.201023000	-4.912472000	2.756076000	6	-1.212453000	-3.256897000	-1.423098000
6	-0.126381000	-4.664722000	3.238217000	1	-2.153172000	-3.687821000	-1.749207000
1	-0.158059000	-5.357623000	4.073445000	6	-1.209250000	-2.040518000	-0.749960000
6	1.056967000	-4.016659000	2.911602000	6	-2.305474000	-1.171880000	-0.498771000
1	1.952135000	-4.207097000	3.498442000	7	0.001572000	1.692377000	1.328980000
6	1.121867000	-3.120310000	1.842983000	1	0.835648000	2.167569000	1.650604000
6	-2.548549000	-3.252366000	0.665915000	6	-3.706299000	-1.626174000	-0.610184000
1	-2.316943000	-2.655911000	-0.220680000	6	-4.052406000	-2.897274000	-0.120584000
6	-3.496684000	-2.421707000	1.540205000	6	-4.725368000	-0.821829000	-1.144826000
1	-3.021753000	-1.483831000	1.848180000	6	-5.361437000	-3.361371000	-0.193111000
1	-3.770517000	-2.971311000	2.447770000	1	-3.288104000	-3.506327000	0.352197000
1	-4.416921000	-2.183542000	0.995826000	6	-6.033653000	-1.286385000	-1.208698000
6	-3.219143000	-4.545868000	0.190292000	1	-4.493842000	0.171894000	-1.511495000
1	-2.516888000	-5.170904000	-0.370612000	6	-6.358766000	-2.557634000	-0.738228000
1	-4.070786000	-4.315259000	-0.458566000	1	-5.604128000	-4.345110000	0.196889000
1	-3.598022000	-5.131449000	1.035221000	1	-6.805017000	-0.648516000	-1.628923000
6	2.449805000	-2.448230000	1.527385000	1	-7.383320000	-2.912952000	-0.786599000
1	2.312858000	-1.822905000	0.638495000	6	3.706783000	-1.628637000	-0.605521000
6	3.543416000	-3.473921000	1.201953000	6	4.050464000	-2.899311000	-0.113074000
1	4.478655000	-2.963097000	0.950523000	6	4.727875000	-0.826026000	-1.138926000
1	3.266197000	-4.107300000	0.353662000	6	5.359268000	-3.364638000	-0.181543000
1	3.740390000	-4.127022000	2.058906000	1	3.284415000	-3.506997000	0.358597000
6	2.896756000	-1.543809000	2.682554000	6	6.035854000	-1.291979000	-1.199011000
1	2.130983000	-0.799027000	2.917381000	1	4.498353000	0.167384000	-1.507622000
1	3.825788000	-1.023719000	2.424273000	6	6.358633000	-2.562736000	-0.725636000
1	3.083664000	-2.133097000	3.587353000	1	5.600110000	-4.347950000	0.210658000
1	0.000000000	0.000000000	1.941539000	1	6.808810000	-0.655529000	-1.618450000
				1	7.382964000	-2.919092000	-0.770957000

1	5.766492000	1.091747000	2.934825000	1	5.737079000	0.542475000	-0.837179000
6	5.999440000	2.563547000	1.378782000	1	5.725904000	0.836968000	-2.588629000
1	6.969931000	2.898865000	1.730887000	1	6.291032000	-0.713266000	-1.956151000
6	5.426613000	3.142874000	0.249945000	6	3.959936000	-1.270599000	-3.219439000
1	5.951037000	3.926381000	-0.287867000	1	2.952831000	-1.689472000	-3.292740000
6	4.186915000	2.706093000	-0.205411000	1	4.674779000	-2.099489000	-3.262859000
1	3.754345000	3.131586000	-1.105397000	1	4.140251000	-0.626804000	-4.087003000
6	-3.574727000	1.721353000	-0.578565000	6	-2.620765000	-0.974669000	0.125573000
6	-4.544629000	0.961074000	-1.247874000	6	-3.069190000	-0.804704000	1.456601000
1	-4.229000000	0.081153000	-1.799874000	6	-3.791515000	-1.836117000	2.061409000
6	-5.882320000	1.332857000	-1.224185000	1	-4.126270000	-1.710961000	3.088134000
1	-6.616976000	0.731353000	-1.751102000	6	-4.071100000	-3.021893000	1.396308000
6	-6.281281000	2.477741000	-0.534401000	1	-4.619219000	-3.816054000	1.893898000
1	-7.327227000	2.767958000	-0.516712000	6	-3.652748000	-3.169707000	0.082000000
6	-5.331084000	3.239147000	0.139532000	1	-3.886620000	-4.085802000	-0.455060000
1	-5.634038000	4.120310000	0.697257000	6	-2.949775000	-2.158339000	-0.574858000
6	-3.992222000	2.857189000	0.129202000	6	-2.773280000	0.427319000	2.300781000
1	-3.266606000	3.416892000	0.712174000	1	-2.287118000	1.179858000	1.676361000
6	2.678841000	-1.117946000	0.124138000	6	-1.804879000	0.095552000	3.442627000
6	2.380062000	-2.006575000	1.176472000	1	-0.843289000	-0.249090000	3.052663000
6	3.218517000	-3.098724000	1.393983000	1	-2.210987000	-0.691742000	4.088631000
1	2.999506000	-3.785578000	2.205854000	1	-1.622929000	0.980759000	4.061699000
6	4.328035000	-3.320879000	0.588386000	6	-4.065864000	1.034203000	2.865302000
1	4.975237000	-4.173069000	0.770824000	1	-4.821523000	1.159614000	2.085302000
6	4.595340000	-2.451136000	-0.458195000	1	-3.863309000	2.014462000	3.310659000
1	5.452908000	-2.635448000	-1.099768000	1	-4.487959000	0.397344000	3.650934000
6	3.784443000	-1.343354000	-0.718843000	6	-2.579744000	-2.369863000	-2.035209000
6	1.137860000	-1.817576000	2.027570000	1	-2.123328000	-1.449913000	-2.412571000
1	0.853214000	-0.760659000	1.968773000	6	-3.819556000	-2.663611000	-2.891882000
6	1.350271000	-2.158445000	3.504849000	1	-3.543647000	-2.715197000	-3.950165000
1	2.211917000	-1.625732000	3.919434000	1	-4.583953000	-1.889363000	-2.775880000
1	1.510243000	-3.231301000	3.652736000	1	-4.275225000	-3.621819000	-2.619272000
1	0.462838000	-1.881938000	4.082620000	6	-1.566858000	-3.511799000	-2.195466000
6	-0.006008000	-2.658968000	1.447144000	1	-0.650856000	-3.334459000	-1.621617000
1	-0.197737000	-2.416093000	0.392658000	1	-1.290967000	-3.636434000	-3.249127000
1	-0.944115000	-2.510650000	1.992403000	1	-1.992299000	-4.460250000	-1.848352000
1	0.257157000	-3.722402000	1.477237000	7	0.362826000	-0.885270000	-2.685499000
6	4.126893000	-0.474927000	-1.917556000	1	0.236349000	-1.816863000	-3.057934000
1	3.429622000	0.368037000	-1.956639000	1	1.120270000	-0.423685000	-3.180023000
6	5.553000000	0.083760000	-1.812666000				

¹ (²¹⁰ Pb)AINHPh-SP:							
				6	4.132583000	2.755743000	-0.229809000
13	0.031661000	0.066102000	-0.100334000	1	4.340494000	3.624114000	-0.846038000
7	1.965298000	-0.246975000	-0.255043000	6	4.799820000	2.607422000	0.983410000
7	0.010932000	-1.558305000	-0.959338000	1	5.523439000	3.352781000	1.299250000
7	-1.885016000	-0.371627000	0.109788000	6	4.531087000	1.511694000	1.789115000
6	2.326919000	-1.453326000	-0.745106000	1	5.047060000	1.402580000	2.739740000
6	1.215981000	-2.204228000	-1.204772000	6	3.602184000	0.541815000	1.399705000
6	1.204872000	-3.452740000	-1.818974000	6	2.499218000	1.971856000	-2.007168000
1	2.143759000	-3.931941000	-2.075707000	1	1.460301000	1.653190000	-1.873823000
6	-0.010614000	-4.091868000	-2.071760000	6	3.118927000	1.064655000	-3.080341000
1	-0.022871000	-5.072724000	-2.532080000	1	3.020181000	0.003410000	-2.833768000
6	-1.209282000	-3.498215000	-1.657876000	1	4.183482000	1.294569000	-3.210093000
1	-2.144376000	-4.039678000	-1.742718000	1	2.621000000	1.231046000	-4.041362000
6	-1.193649000	-2.225190000	-1.100296000	6	2.461293000	3.414895000	-2.511466000
6	-2.270752000	-1.510133000	-0.504767000	1	2.079967000	4.100192000	-1.748872000
6	3.697620000	-2.015496000	-0.699552000	1	1.798034000	3.479258000	-3.379188000
6	4.842956000	-1.291640000	-1.067005000	1	3.454211000	3.754126000	-2.830228000
1	4.750116000	-0.274078000	-1.427108000	6	3.307666000	-0.627363000	2.323452000
6	6.105454000	-1.866172000	-0.971205000	1	2.659342000	-1.331178000	1.792646000
1	6.975859000	-1.288377000	-1.266015000	6	4.581772000	-1.380130000	2.721296000
6	6.258729000	-3.168690000	-0.500081000	1	5.151527000	-1.685421000	1.838044000
1	7.247619000	-3.609977000	-0.424315000	1	4.328432000	-2.277364000	3.295929000
6	5.134916000	-3.892596000	-0.113231000	1	5.230428000	-0.758259000	3.348198000
1	5.240583000	-4.899894000	0.277718000	6	2.543857000	-0.140829000	3.560848000
6	3.870585000	-3.319376000	-0.204177000	1	1.627718000	0.388330000	3.273389000
1	3.003460000	-3.871071000	0.144932000	1	3.154542000	0.551142000	4.151652000
6	-3.638694000	-2.070792000	-0.521763000	1	2.266300000	-0.983558000	4.204227000
6	-4.413129000	-2.189215000	0.641764000	6	-2.813695000	0.394266000	0.890152000
1	-4.028011000	-1.821389000	1.587012000	6	-3.919235000	1.047949000	0.312279000
6	-5.672313000	-2.776513000	0.591862000	6	-4.796905000	1.738971000	1.154891000
1	-6.256424000	-2.863999000	1.502670000	1	-5.654904000	2.242328000	0.717631000
6	-6.185441000	-3.250413000	-0.614786000	6	-4.598278000	1.795434000	2.522281000
1	-7.170619000	-3.704934000	-0.647675000	1	-5.294203000	2.334967000	3.157183000
6	-5.432251000	-3.124073000	-1.778807000	6	-3.490649000	1.164297000	3.078072000
1	-5.830300000	-3.469850000	-2.727800000	1	-3.335885000	1.226289000	4.149117000
6	-4.173588000	-2.533595000	-1.733614000	6	-2.582126000	0.463935000	2.287242000
1	-3.601940000	-2.401130000	-2.647570000	6	-4.231984000	1.060169000	-1.176685000
6	2.945485000	0.701530000	0.169764000	1	-3.469436000	0.471627000	-1.699047000
6	3.196579000	1.816747000	-0.661709000	6	-4.199829000	2.491928000	-1.731800000
				1	-3.278003000	3.010625000	-1.468010000

1	-5.037598000	3.075125000	-1.333747000	6	-0.637847000	3.149432000	-0.100117000
1	-4.298801000	2.477082000	-2.823183000	6	-1.028406000	-0.994434000	-2.147700000
6	-5.613806000	0.453409000	-1.470568000	6	-0.603965000	4.441937000	0.451114000
1	-5.765778000	-0.507055000	-0.976129000	6	-1.053937000	-1.862357000	-3.219586000
1	-5.743629000	0.313495000	-2.549241000	1	-1.990308000	-2.301747000	-3.548579000
1	-6.403082000	1.133718000	-1.131155000	6	-3.467370000	-1.202900000	-1.482261000
6	-1.396708000	-0.241791000	2.939385000	6	3.711283000	1.500911000	0.383173000
1	-0.505131000	-0.012771000	2.339391000	6	-1.324409000	5.482968000	-0.120118000
6	-1.562073000	-1.767843000	2.962158000	1	-1.280864000	6.468506000	0.334938000
1	-0.683417000	-2.234449000	3.421396000	6	0.178689000	-2.307397000	-3.758794000
1	-1.682471000	-2.190347000	1.960597000	1	0.178004000	-3.021841000	-4.573871000
1	-2.439429000	-2.041239000	3.560232000	6	-2.427133000	-0.644926000	1.217227000
6	-1.092914000	0.257162000	4.353384000	6	3.737513000	-1.393385000	-1.206233000
1	-0.974471000	1.344767000	4.380937000	6	-3.463417000	0.243262000	1.537242000
1	-0.166889000	-0.199575000	4.714106000	6	-1.035746000	-2.753274000	1.644136000
1	-1.885948000	-0.022108000	5.055394000	1	-0.200592000	-2.168691000	1.236744000
6	-0.143914000	2.980782000	-0.163786000	6	2.876677000	0.485253000	0.901356000
6	0.262680000	4.227800000	0.349653000	6	4.396527000	-1.319984000	-2.442375000
6	-0.781803000	2.978298000	-1.417813000	1	3.897174000	-0.839939000	-3.279544000
6	0.039927000	5.403130000	-0.355689000	6	-1.394380000	2.958941000	-1.271525000
6	-0.993898000	4.158448000	-2.120846000	6	1.364977000	-1.105162000	-2.023634000
6	-0.586792000	5.384831000	-1.600838000	6	2.359769000	-0.900307000	-1.055155000
1	0.367942000	6.346064000	0.073310000	6	-2.124319000	4.002066000	-1.827384000
1	-1.488423000	4.113852000	-3.087927000	1	-2.707230000	3.818816000	-2.725856000
1	-0.753475000	6.303632000	-2.152517000	6	4.558575000	2.178791000	1.261892000
1	-1.112260000	2.029118000	-1.843971000	1	5.200819000	2.963704000	0.871162000
1	0.767425000	4.259917000	1.311589000	6	-2.103360000	5.273696000	-1.256620000
7	0.105530000	1.802595000	0.513892000	1	-2.670019000	6.087085000	-1.697038000
1	0.735040000	1.966214000	1.295700000	6	2.884844000	0.194185000	2.282053000
				6	3.685757000	1.945344000	-1.071632000
				1	3.056859000	1.258981000	-1.644926000
				6	-5.307191000	-0.858758000	-3.033368000
				1	-5.691996000	-0.401242000	-3.939319000
				6	-3.983880000	-1.133582000	3.466102000
				1	-4.594274000	-1.326730000	4.343044000
				6	-2.942603000	-1.998990000	3.140033000
				1	-2.751396000	-2.860865000	3.771537000
				6	1.943733000	-0.841665000	2.874014000
				1	1.673863000	-1.539674000	2.072690000
				6	-2.059071000	-0.891321000	-1.150541000
$^{1}(\text{PbI}_2\text{P})\text{AlNHPh-TET}$:							
13	0.145779000	0.372775000	-0.102787000				
7	1.947571000	-0.189381000	0.052349000				
7	0.169300000	-0.419889000	-1.760286000				
7	-1.623516000	-0.456308000	0.044196000				
7	0.050558000	2.094626000	0.484160000				
1	0.693807000	2.402897000	1.207981000				
6	4.423998000	-1.942739000	-0.112537000				
1	3.927804000	-1.998491000	0.852102000				

1	6.770532000	-2.232608000	-1.307820000	1	4.703854000	-2.591677000	1.923674000
6	5.897343000	-4.009837000	-0.460890000	1	3.614424000	-3.164392000	3.203311000
1	6.841672000	-4.540077000	-0.386488000	1	4.691735000	-1.799515000	3.508269000
6	4.719044000	-4.606640000	-0.024225000	6	2.240790000	-0.690945000	3.468699000
1	4.737091000	-5.602198000	0.408746000	1	1.482872000	0.025597000	3.135702000
6	3.514413000	-3.915464000	-0.106969000	1	2.944736000	-0.146989000	4.108841000
1	2.613620000	-4.362684000	0.300901000	1	1.754279000	-1.462892000	4.076409000
6	-3.820722000	-2.252484000	-0.208948000	6	-2.856562000	0.274155000	0.900772000
6	-4.558580000	-2.222215000	0.983325000	6	-3.988635000	0.915075000	0.370131000
1	-4.122825000	-1.796679000	1.880743000	6	-4.836191000	1.614559000	1.235949000
6	-5.850450000	-2.734559000	1.024694000	1	-5.717862000	2.101230000	0.828531000
1	-6.405213000	-2.704987000	1.957213000	6	-4.576963000	1.697564000	2.590417000
6	-6.433156000	-3.281350000	-0.117497000	1	-5.247046000	2.241770000	3.248599000
1	-7.443333000	-3.676743000	-0.078931000	6	-3.438431000	1.085979000	3.101700000
6	-5.715977000	-3.304999000	-1.310155000	1	-3.236660000	1.170928000	4.162464000
1	-6.165722000	-3.709976000	-2.211355000	6	-2.563644000	0.370019000	2.284758000
6	-4.424627000	-2.789480000	-1.356888000	6	-4.348877000	0.925096000	-1.103985000
1	-3.879221000	-2.776495000	-2.295655000	1	-3.623577000	0.309704000	-1.649783000
6	2.968181000	0.140032000	0.139434000	6	-4.271110000	2.365534000	-1.627246000
6	3.493642000	1.238376000	-0.580590000	1	-3.291489000	2.811266000	-1.429212000
6	4.567729000	1.947003000	-0.042941000	1	-5.024005000	2.987898000	-1.131817000
1	4.974649000	2.789505000	-0.591394000	1	-4.468341000	2.398624000	-2.703138000
6	5.121018000	1.605777000	1.184814000	6	-5.754848000	0.362889000	-1.360259000
1	5.955642000	2.171852000	1.587135000	1	-5.911417000	-0.597650000	-0.865106000
6	4.585242000	0.544651000	1.894782000	1	-5.918519000	0.230767000	-2.435105000
1	5.001902000	0.283541000	2.863937000	1	-6.519104000	1.058479000	-0.996054000
6	3.514717000	-0.201912000	1.393163000	6	-1.362427000	-0.329182000	2.913578000
6	2.933490000	1.631275000	-1.934618000	1	-0.493229000	-0.154583000	2.263391000
1	1.851815000	1.548904000	-1.849361000	6	-1.550249000	-1.850248000	3.016178000
6	3.406023000	0.680592000	-3.041833000	1	-0.657774000	-2.307406000	3.457739000
1	3.060971000	-0.345636000	-2.877231000	1	-1.721695000	-2.321759000	2.044619000
1	4.501551000	0.674452000	-3.096900000	1	-2.402465000	-2.079903000	3.666771000
1	3.028032000	1.009633000	-4.015801000	6	-1.009016000	0.223839000	4.297136000
6	3.222108000	3.079950000	-2.324743000	1	-0.865631000	1.309269000	4.278808000
1	2.925334000	3.771546000	-1.529279000	1	-0.090472000	-0.238456000	4.663023000
1	2.644190000	3.336669000	-3.218041000	1	-1.793285000	-0.007245000	5.025314000
1	4.281294000	3.237758000	-2.560014000	7	0.004988000	1.553581000	0.241984000
6	2.964116000	-1.312490000	2.270082000	1	0.296892000	1.636853000	1.208766000
1	2.228245000	-1.888256000	1.699833000	6	0.077794000	2.781012000	-0.406888000
6	4.060696000	-2.273532000	2.748422000	6	0.479981000	3.934869000	0.325332000

6	-0.260237000	2.926146000	-1.783667000	6	-1.284248000	-3.192895000	-2.370698000
6	0.651968000	5.145577000	-0.339052000	1	-2.220427000	-3.720660000	-2.512061000
6	-0.051006000	4.162893000	-2.398018000	6	-1.210798000	-2.098317000	-1.547509000
6	0.422777000	5.267356000	-1.704493000	6	-2.240481000	-1.644910000	-0.620160000
1	0.966723000	6.018763000	0.224405000	6	3.614913000	-2.153066000	-0.989291000
1	-0.282017000	4.269100000	-3.453863000	6	4.828992000	-1.451057000	-1.078267000
1	0.576696000	6.214305000	-2.211190000	1	4.828121000	-0.372587000	-1.176479000
6	0.707656000	3.838991000	1.828423000	6	6.046386000	-2.122124000	-1.036797000
1	-0.070691000	3.173454000	2.234461000	1	6.968080000	-1.552698000	-1.108387000
6	0.539922000	5.172959000	2.559775000	6	6.091243000	-3.508566000	-0.906552000
1	1.358912000	5.862079000	2.327683000	1	7.045160000	-4.025788000	-0.873666000
1	-0.403637000	5.660259000	2.297021000	6	4.899855000	-4.220374000	-0.803601000
1	0.554384000	5.006417000	3.641488000	1	4.915731000	-5.298875000	-0.677648000
6	2.085346000	3.242688000	2.158036000	6	3.681586000	-3.549502000	-0.831151000
1	2.872143000	3.917475000	1.802278000	1	2.760329000	-4.106581000	-0.691874000
1	2.208213000	3.113443000	3.239996000	6	-3.650744000	-2.049091000	-0.814613000
1	2.253929000	2.275808000	1.674074000	6	-4.496642000	-2.455004000	0.228526000
6	-0.919837000	1.806558000	-2.593458000	1	-4.125048000	-2.509569000	1.244933000
1	-1.574163000	1.253522000	-1.899368000	6	-5.819759000	-2.790181000	-0.033551000
6	-1.819821000	2.350446000	-3.717836000	1	-6.460005000	-3.106577000	0.783685000
1	-1.216389000	2.641926000	-4.584650000	6	-6.326738000	-2.716254000	-1.329802000
1	-2.510177000	1.568648000	-4.051887000	1	-7.363872000	-2.970346000	-1.524726000
1	-2.400534000	3.218977000	-3.405672000	6	-5.498616000	-2.306610000	-2.370900000
6	0.027984000	0.805632000	-3.286282000	1	-5.886130000	-2.232236000	-3.381965000
1	0.660227000	0.201524000	-2.629088000	6	-4.171981000	-1.975997000	-2.116582000
1	-0.559105000	0.102981000	-3.887727000	1	-3.533150000	-1.631643000	-2.923608000
1	0.701957000	1.352579000	-3.955437000	6	2.956490000	0.330449000	0.463627000
				6	3.404835000	1.552129000	-0.091288000
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				1	4.765390000	3.193799000	0.157333000
				6	4.964620000	1.780789000	1.756221000
				1	5.744750000	2.345383000	2.258073000
				6	4.508182000	0.588121000	2.295343000
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				1	1.764583000	1.839183000	-1.391148000
				6	3.461991000	1.411702000	-2.616290000
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¹ (^{Ph} I ₂ P)AlNHDipp-TET:							
13	0.068784000	-0.104225000	-0.110441000				
7	1.933887000	-0.407764000	-0.212113000				
7	-0.019694000	-1.453745000	-1.344148000				
7	-1.783778000	-0.848409000	0.331080000				
6	2.279341000	-1.511464000	-0.992338000				
6	1.194809000	-2.070359000	-1.660087000				
6	1.137222000	-3.154820000	-2.574607000				
1	2.062405000	-3.584076000	-2.946424000				
6	-0.076038000	-3.671774000	-2.963158000				
1	-0.114912000	-4.503771000	-3.657057000				

7	-0.265008000	-1.774570000	0.141352000	1	-1.840259000	4.705921000	-2.696393000
6	0.323157000	2.261775000	1.367199000	6	-0.918112000	3.381696000	-1.283714000
6	0.185610000	1.188690000	2.288356000	6	2.398138000	1.465937000	-1.824255000
6	0.226855000	1.181420000	3.672830000	1	2.310105000	0.991459000	-0.842155000
1	0.431926000	2.110336000	4.194262000	6	3.700212000	2.277937000	-1.840640000
6	0.000000000	0.000000000	4.381376000	1	3.693315000	3.064695000	-1.079289000
1	0.000000000	0.000000000	5.464520000	1	3.856345000	2.756122000	-2.813912000
6	-0.226855000	-1.181420000	3.672830000	1	4.558297000	1.625813000	-1.647116000
1	-0.431926000	-2.110336000	4.194262000	6	2.444020000	0.355458000	-2.881626000
6	-0.185610000	-1.188690000	2.288356000	1	1.562053000	-0.289743000	-2.812715000
6	-0.323157000	-2.261775000	1.367199000	1	3.337421000	-0.263702000	-2.747004000
6	0.461333000	3.683282000	1.743810000	1	2.483980000	0.775460000	-3.892859000
6	1.353363000	4.517371000	1.058853000	6	-2.070292000	3.532511000	-0.302300000
1	1.958298000	4.105129000	0.257032000	1	-1.819238000	3.012400000	0.624205000
6	1.460396000	5.861436000	1.397218000	6	-2.326633000	5.003357000	0.046556000
1	2.157406000	6.496333000	0.859386000	1	-1.408670000	5.496465000	0.382443000
6	0.676616000	6.393290000	2.420202000	1	-3.071289000	5.079837000	0.846150000
1	0.759492000	7.444184000	2.679265000	1	-2.712500000	5.554189000	-0.818373000
6	-0.221002000	5.574211000	3.099971000	6	-3.333475000	2.861010000	-0.854214000
1	-0.848601000	5.985448000	3.884499000	1	-3.158141000	1.792865000	-1.015643000
6	-0.332433000	4.229399000	2.761257000	1	-3.631538000	3.304537000	-1.810778000
1	-1.066641000	3.602463000	3.258811000	1	-4.166548000	2.973632000	-0.152005000
6	-0.461333000	-3.683282000	1.743810000	6	-0.193410000	-2.545019000	-1.045443000
6	-1.353363000	-4.517371000	1.058853000	6	0.918112000	-3.381696000	-1.283714000
1	-1.958298000	-4.105129000	0.257032000	6	0.987470000	-4.061129000	-2.499930000
6	-1.460396000	-5.861436000	1.397218000	1	1.840259000	-4.705921000	-2.696393000
1	-2.157406000	-6.496333000	0.859386000	6	0.000000000	-3.919942000	-3.466565000
6	-0.676616000	-6.393290000	2.420202000	1	0.073311000	-4.458701000	-4.406305000
1	-0.759492000	-7.444184000	2.679265000	6	-1.073957000	-3.075263000	-3.225587000
6	0.221002000	-5.574211000	3.099971000	1	-1.842450000	-2.956279000	-3.985134000
1	0.848601000	-5.985448000	3.884499000	6	-1.189433000	-2.367707000	-2.026667000
6	0.332433000	-4.229399000	2.761257000	6	2.070292000	-3.532511000	-0.302300000
1	1.066641000	-3.602463000	3.258811000	1	1.819238000	-3.012400000	0.624205000
6	0.193410000	2.545019000	-1.045443000	6	3.333475000	-2.861010000	-0.854214000
6	1.189433000	2.367707000	-2.026667000	1	3.158141000	-1.792865000	-1.015643000
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1	1.842450000	2.956279000	-3.985134000	1	4.166548000	-2.973632000	-0.152005000
6	0.000000000	3.919942000	-3.466565000	6	2.326633000	-5.003357000	0.046556000
1	-0.073311000	4.458701000	-4.406305000	1	1.408670000	-5.496465000	0.382443000
6	-0.987470000	4.061129000	-2.499930000	1	3.071289000	-5.079837000	0.846150000

1	2.712500000	-5.554189000	-0.818373000	6	3.536083000	1.764838000	-0.288351000
6	-2.398138000	-1.465937000	-1.824255000	6	4.745753000	1.559001000	0.382645000
1	-2.310105000	-0.991459000	-0.842155000	1	4.766666000	0.946815000	1.278978000
6	-3.700212000	-2.277937000	-1.840640000	6	5.918657000	2.132874000	-0.097122000
1	-4.558297000	-1.625813000	-1.647116000	1	6.851583000	1.971789000	0.433591000
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6	-2.444020000	-0.355458000	-2.881626000	6	4.696492000	3.117585000	-1.928469000
1	-1.562053000	0.289743000	-2.812715000	1	4.674649000	3.718871000	-2.831891000
1	-3.337421000	0.263702000	-2.747004000	6	3.520070000	2.556032000	-1.442522000
1	-2.483980000	-0.775460000	-3.892859000	1	2.580763000	2.720616000	-1.962880000
1	0.000000000	0.000000000	-1.110328000	6	-2.851317000	-1.098561000	-0.601003000
5	0.000000000	0.000000000	0.106534000	6	-3.031316000	-1.479652000	-1.942650000
				6	-3.825358000	-2.596970000	-2.207833000
				1	-3.966140000	-2.918614000	-3.236149000
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				1	-5.058611000	-4.164001000	-1.405211000
				6	-4.274150000	-2.887096000	0.135719000
				1	-4.762243000	-3.435790000	0.936902000
				6	-3.478281000	-1.784424000	0.451467000
				6	-2.394161000	-0.714573000	-3.091680000
				1	-2.019196000	0.234895000	-2.695723000
				6	-3.403299000	-0.386836000	-4.198489000
				1	-4.276584000	0.142313000	-3.804291000
				1	-3.757388000	-1.291983000	-4.702746000
				1	-2.933727000	0.248040000	-4.956557000
				6	-1.203928000	-1.492904000	-3.666388000
				1	-0.452436000	-1.688578000	-2.896844000
				1	-0.730246000	-0.930737000	-4.478567000
				1	-1.535304000	-2.457173000	-4.068590000
				6	-3.297136000	-1.382882000	1.905207000
				1	-2.720443000	-0.454087000	1.938224000
				6	-4.646114000	-1.118668000	2.584798000
				1	-5.238627000	-0.390782000	2.021240000
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				6	-2.495173000	-2.450734000	2.659722000
				1	-1.522857000	-2.618226000	2.186448000
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$^{1}(\text{PbI}_2\text{P})\text{BH-T:}$							
7	-2.002525000	0.015441000	-0.307579000				
7	-0.191750000	1.335305000	0.077208000				
7	2.156764000	-0.087976000	0.585167000				
6	-2.469743000	1.265326000	0.120347000				
6	-1.377994000	2.071783000	0.326486000				
6	-1.291090000	3.465771000	0.630016000				
1	-2.213512000	4.020055000	0.767015000				
6	-0.077685000	4.065427000	0.702481000				
1	0.006292000	5.125498000	0.914281000				
6	1.113650000	3.286312000	0.509594000				
1	2.088320000	3.745147000	0.624947000				
6	1.044684000	1.958562000	0.225127000				
6	2.273018000	1.118592000	0.186981000				
6	-3.878678000	1.591893000	0.367079000				
6	-4.900891000	1.202690000	-0.511008000				
1	-4.650670000	0.660551000	-1.417338000				
6	-6.228767000	1.503456000	-0.229073000				
1	-7.006074000	1.189062000	-0.918783000				
6	-6.563519000	2.209982000	0.924749000				
1	-7.601453000	2.443336000	1.140522000				
6	-5.557625000	2.608204000	1.801659000				
1	-5.807954000	3.146687000	2.710690000				
6	-4.230515000	2.291604000	1.531810000				
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6	3.201334000	-1.033823000	0.600977000	1	0.037931000	2.154190000	-4.065124000
6	3.762808000	-1.545135000	-0.581969000	6	0.000000000	0.000000000	-4.234073000
6	4.735395000	-2.544020000	-0.467226000	1	0.000000000	0.000000000	-5.317579000
1	5.177965000	-2.952437000	-1.372548000	6	-0.036724000	-1.209050000	-3.533412000
6	5.146439000	-3.019614000	0.767833000	1	-0.037931000	-2.154190000	-4.065124000
1	5.910845000	-3.787733000	0.831518000	6	-0.067032000	-1.204789000	-2.143631000
6	4.565134000	-2.513155000	1.928718000	6	-0.106184000	-2.331105000	-1.269724000
1	4.886068000	-2.892815000	2.893500000	6	0.314912000	3.707118000	-1.771070000
6	3.578652000	-1.534512000	1.868213000	6	-0.448349000	4.784979000	-1.301825000
6	3.327829000	-1.094735000	-1.966404000	1	-1.228031000	4.607308000	-0.569105000
1	2.592049000	-0.292075000	-1.859651000	6	-0.212342000	6.073679000	-1.765881000
6	2.637467000	-2.242624000	-2.714002000	1	-0.814766000	6.895590000	-1.392231000
1	1.785535000	-2.624616000	-2.143099000	6	0.789463000	6.312055000	-2.705806000
1	3.330806000	-3.074623000	-2.880126000	1	0.972750000	7.320216000	-3.063669000
1	2.276448000	-1.903978000	-3.691337000	6	1.559506000	5.251178000	-3.174824000
6	4.508964000	-0.547025000	-2.776678000	1	2.353765000	5.428450000	-3.893198000
1	5.042252000	0.234103000	-2.226320000	6	1.330018000	3.961250000	-2.705874000
1	4.159422000	-0.125404000	-3.725258000	1	1.961271000	3.142513000	-3.038114000
1	5.223610000	-1.343996000	-3.011138000	6	-0.314912000	-3.707118000	-1.771070000
6	2.885616000	-1.002015000	3.113137000	6	0.448349000	-4.784979000	-1.301825000
1	2.772942000	0.083360000	2.991142000	1	1.228031000	-4.607308000	-0.569105000
6	3.670299000	-1.244382000	4.402303000	6	0.212342000	-6.073679000	-1.765881000
1	3.179951000	-0.733876000	5.236601000	1	0.814766000	-6.895590000	-1.392231000
1	4.697922000	-0.873672000	4.329236000	6	-0.789463000	-6.312055000	-2.705806000
1	3.709521000	-2.310540000	4.651347000	1	-0.972750000	-7.320216000	-3.063669000
6	1.475037000	-1.601454000	3.226683000	6	-1.559506000	-5.251178000	-3.174824000
1	0.885608000	-1.376326000	2.334140000	1	-2.353765000	-5.428450000	-3.893198000
1	0.953981000	-1.195582000	4.100760000	6	-1.330018000	-3.961250000	-2.705874000
1	1.538937000	-2.689418000	3.340850000	1	-1.961271000	-3.142513000	-3.038114000
1	0.090486000	-0.917912000	-0.669403000	6	0.052059000	2.968117000	1.073549000
5	-0.576070000	0.001427000	-0.338057000	6	-1.122464000	3.235901000	1.805086000
				6	-1.049891000	4.126185000	2.877916000
				1	-1.948168000	4.338944000	3.451829000
				6	0.145834000	4.741080000	3.224619000
				1	0.183782000	5.429417000	4.063148000
				6	1.293791000	4.466275000	2.492834000
				1	2.231471000	4.941660000	2.768557000
				6	1.272293000	3.582305000	1.413112000
				6	-2.460411000	2.600298000	1.459125000
				1	-2.331749000	2.019576000	0.539756000
$^{1}(\text{PbI}_2\text{P})\text{GaH-SP:}$							
7	0.000000000	2.004672000	0.024453000	6	0.145834000	4.741080000	3.224619000
7	0.000000000	0.000000000	-1.466985000	1	0.183782000	5.429417000	4.063148000
7	0.000000000	-2.004672000	0.024453000	6	1.293791000	4.466275000	2.492834000
6	0.106184000	2.331105000	-1.269724000	1	2.231471000	4.941660000	2.768557000
6	0.067032000	1.204789000	-2.143631000	6	1.272293000	3.582305000	1.413112000
6	0.036724000	1.209050000	-3.533412000	6	-2.460411000	2.600298000	1.459125000
				1	-2.331749000	2.019576000	0.539756000

6	-3.543576000	3.653819000	1.192938000	1	4.478395000	-3.166835000	0.896918000
1	-3.253506000	4.342997000	0.393841000	1	3.253506000	-4.342997000	0.393841000
1	-3.748834000	4.248289000	2.089525000	1	3.748834000	-4.248289000	2.089525000
1	-4.478395000	3.166835000	0.896918000	6	2.916603000	-1.643860000	2.568297000
6	-2.916603000	1.643860000	2.568297000	1	2.162844000	-0.875382000	2.762215000
1	-2.162844000	0.875382000	2.762215000	1	3.855164000	-1.152046000	2.289768000
1	-3.855164000	1.152046000	2.289768000	1	3.086940000	-2.190252000	3.502968000
1	-3.086940000	2.190252000	3.502968000	1	0.000000000	0.000000000	1.983828000
6	2.565387000	3.285310000	0.673815000	31	0.000000000	0.000000000	0.411570000
1	2.333477000	2.671513000	-0.200890000				
6	3.237335000	4.569769000	0.175088000		¹ (^{Ph} I ₂ P)GaH-TET:		
1	2.537500000	5.182204000	-0.402358000	7	1.858340000	-0.024575000	-0.071739000
1	4.093432000	4.327697000	-0.463731000	7	0.133001000	1.616602000	-1.110883000
1	3.608993000	5.172777000	1.010985000	7	-1.837711000	-0.019589000	-0.583216000
6	3.512852000	2.471917000	1.564878000	6	2.221843000	1.240219000	-0.029675000
1	3.039157000	1.539583000	1.890255000	6	1.222035000	2.197393000	-0.502486000
1	3.787284000	3.039207000	2.461248000	6	1.239681000	3.548196000	-0.260916000
1	4.433133000	2.223765000	1.025180000	1	2.073691000	4.021018000	0.243043000
6	-0.052059000	-2.968117000	1.073549000	6	0.075107000	4.302378000	-0.620262000
6	-1.272293000	-3.582305000	1.413112000	1	0.101668000	5.385422000	-0.572869000
6	-1.293791000	-4.466275000	2.492834000	6	-1.101769000	3.652556000	-0.884503000
1	-2.231471000	-4.941660000	2.768557000	1	-2.019976000	4.213458000	-1.029436000
6	-0.145834000	-4.741080000	3.224619000	6	-1.120646000	2.219420000	-0.881370000
1	-0.183782000	-5.429417000	4.063148000	6	-2.161620000	1.349488000	-0.614869000
6	1.049891000	-4.126185000	2.877916000	6	3.540981000	1.702021000	0.452461000
1	1.948168000	-4.338944000	3.451829000	6	4.114940000	1.156279000	1.608416000
6	1.122464000	-3.235901000	1.805086000	1	3.581519000	0.389445000	2.161660000
6	-2.565387000	-3.285310000	0.673815000	6	5.355758000	1.599001000	2.049264000
1	-2.333477000	-2.671513000	-0.200890000	1	5.788471000	1.173914000	2.949009000
6	-3.512852000	-2.471917000	1.564878000	6	6.043021000	2.584627000	1.340588000
1	-3.039157000	-1.539583000	1.890255000	1	7.014879000	2.923315000	1.685172000
1	-3.787284000	-3.039207000	2.461248000	6	5.482615000	3.127339000	0.187334000
1	-4.433133000	-2.223765000	1.025180000	1	6.017989000	3.885107000	-0.375609000
6	-3.237335000	-4.569769000	0.175088000	6	4.239542000	2.688426000	-0.257487000
1	-2.537500000	-5.182204000	-0.402358000	1	3.812441000	3.087874000	-1.171965000
1	-4.093432000	-4.327697000	-0.463731000	6	-3.560519000	1.799423000	-0.473429000
1	-3.608993000	-5.172777000	1.010985000	6	-4.602917000	1.082944000	-1.080183000
6	2.460411000	-2.600298000	1.459125000	1	-4.365040000	0.193961000	-1.656045000
1	2.331749000	-2.019576000	0.539756000	6	-5.921796000	1.504301000	-0.959920000
6	3.543576000	-3.653819000	1.192938000				

1	2.141432000	4.165460000	0.265721000	6	-1.199699000	-2.739175000	-3.058968000
6	1.197007000	2.213455000	0.091542000	1	-0.554542000	-2.994856000	-2.213259000
6	2.300390000	1.297473000	0.188712000	1	-0.568015000	-2.489506000	-3.918493000
6	-3.696964000	1.768781000	-0.155388000	1	-1.780069000	-3.630954000	-3.320168000
6	-4.683605000	1.232783000	-0.996988000	6	-3.550732000	-0.613938000	2.123218000
1	-4.415682000	0.465238000	-1.714637000	1	-2.928772000	0.268391000	1.952493000
6	-5.999879000	1.673499000	-0.917355000	6	-4.914707000	-0.124992000	2.622325000
1	-6.746312000	1.247228000	-1.580188000	1	-5.442601000	0.431980000	1.841533000
6	-6.362089000	2.654708000	0.003705000	1	-4.788099000	0.532059000	3.489301000
1	-7.391133000	2.994387000	0.064138000	1	-5.548234000	-0.963043000	2.933207000
6	-5.394621000	3.190524000	0.851044000	6	-2.844679000	-1.473521000	3.180009000
1	-5.667579000	3.942919000	1.584472000	1	-1.854938000	-1.789069000	2.830734000
6	-4.078515000	2.749255000	0.775756000	1	-3.423852000	-2.377876000	3.397026000
1	-3.336430000	3.144661000	1.463281000	1	-2.721531000	-0.915677000	4.114573000
6	3.696970000	1.768793000	0.155400000	6	2.879434000	-1.076422000	0.307815000
6	4.683590000	1.232816000	0.997039000	6	3.666972000	-1.384518000	-0.819208000
1	4.415644000	0.465300000	1.714710000	6	4.544455000	-2.466509000	-0.745020000
6	5.999868000	1.673520000	0.917417000	1	5.154469000	-2.714123000	-1.609759000
1	6.746286000	1.247265000	1.580277000	6	4.643824000	-3.238494000	0.405807000
6	6.362102000	2.654698000	-0.003667000	1	5.332401000	-4.076801000	0.443997000
1	7.391150000	2.994367000	-0.064092000	6	3.849267000	-2.935150000	1.502982000
6	5.394654000	3.190496000	-0.851040000	1	3.921493000	-3.542977000	2.401421000
1	5.667632000	3.942868000	-1.584484000	6	2.957770000	-1.860630000	1.476892000
6	4.078543000	2.749238000	-0.775764000	6	3.550682000	-0.613961000	-2.123210000
1	3.336474000	3.144628000	-1.463315000	1	2.928738000	0.268379000	-1.952478000
6	-2.879420000	-1.076438000	-0.307782000	6	2.844591000	-1.473545000	-3.179975000
6	-2.957726000	-1.860667000	-1.476849000	1	1.854856000	-1.789080000	-2.830670000
6	-3.849249000	-2.935165000	-1.502955000	1	3.423749000	-2.377907000	-3.397000000
1	-3.921462000	-3.542999000	-2.401390000	1	2.721425000	-0.915707000	-4.114540000
6	-4.643849000	-3.238478000	-0.405802000	6	4.914651000	-0.125036000	-2.622353000
1	-5.332444000	-4.076769000	-0.444005000	1	5.442567000	0.431942000	-1.841580000
6	-4.544497000	-2.466484000	0.745020000	1	4.788031000	0.532004000	-3.489336000
1	-5.154544000	-2.714074000	1.609743000	1	5.548163000	-0.963099000	-2.933236000
6	-3.666998000	-1.384508000	0.819222000	6	2.125461000	-1.565599000	2.715448000
6	-2.125384000	-1.565668000	-2.715392000	1	1.502802000	-0.689264000	2.505011000
1	-1.502605000	-0.689430000	-2.504908000	6	3.011209000	-1.215664000	3.918302000
6	-3.011106000	-1.215533000	-3.918207000	1	2.393134000	-0.982689000	4.791557000
1	-3.646204000	-0.348664000	-3.711893000	1	3.646460000	-0.348894000	3.712042000
1	-3.662723000	-2.055129000	-4.183257000	1	3.662677000	-2.055379000	4.183341000
1	-2.393018000	-0.982626000	-4.791471000	6	1.199619000	-2.739011000	3.058928000

1	0.554427000	-2.994541000	2.213198000	1	-2.352759000	-5.428368000	-3.894548000
1	0.567970000	-2.489336000	3.918477000	6	-1.329363000	-3.961049000	-2.707152000
1	1.779878000	-3.630888000	3.320043000	1	-1.959305000	-3.142091000	-3.041372000
1	0.000038000	-1.966090000	-0.000185000	6	0.052188000	2.965896000	1.073712000
31	0.000014000	-0.386247000	-0.000041000	6	-1.121958000	3.232346000	1.806366000
				6	-1.049440000	4.122380000	2.879423000
				1	-1.947498000	4.334119000	3.454070000
				6	0.145942000	4.738347000	3.225363000
				1	0.183866000	5.426536000	4.064014000
				6	1.293634000	4.464724000	2.492692000
				1	2.231095000	4.940835000	2.767912000
				6	1.272136000	3.581006000	1.412782000
				6	-2.459688000	2.595816000	1.461276000
				1	-2.330766000	2.013705000	0.542816000
				6	-3.542827000	3.648817000	1.192939000
				1	-3.252834000	4.335938000	0.392054000
				1	-3.747541000	4.245478000	2.088198000
				1	-4.477857000	3.161327000	0.898412000
				6	-2.916068000	1.641183000	2.571920000
				1	-2.162203000	0.873223000	2.767526000
				1	-3.854407000	1.148668000	2.293888000
				1	-3.086976000	2.189066000	3.505602000
				6	2.565037000	3.284969000	0.672755000
				1	2.332939000	2.671658000	-0.202228000
				6	3.236415000	4.569869000	0.174433000
				1	2.536174000	5.182353000	-0.402465000
				1	4.092330000	4.328360000	-0.464839000
				1	3.608226000	5.172576000	1.010481000
				6	3.513094000	2.471370000	1.563012000
				1	3.039814000	1.538732000	1.888177000
				1	3.787694000	3.038239000	2.459593000
				1	4.433248000	2.223745000	1.022852000
				6	-0.052188000	-2.965896000	1.073712000
				6	-1.272136000	-3.581006000	1.412782000
				6	-1.293634000	-4.464724000	2.492692000
				1	-2.231095000	-4.940835000	2.767912000
				6	-0.145942000	-4.738347000	3.225363000
				1	-0.183866000	-5.426536000	4.064014000
				6	1.049440000	-4.122380000	2.879423000
				1	1.947498000	-4.334119000	3.454070000

BS-¹(^{Ph}I₂P)GaH-SP:

6	1.121958000	-3.232346000	1.806366000	6	-3.726730000	1.826755000	-0.047148000
6	-2.565037000	-3.284969000	0.672755000	6	-4.725425000	1.459587000	-0.958808000
1	-2.332939000	-2.671658000	-0.202228000	1	-4.485680000	0.767519000	-1.758935000
6	-3.513094000	-2.471370000	1.563012000	6	-6.010183000	1.977344000	-0.848216000
1	-3.039814000	-1.538732000	1.888177000	1	-6.770270000	1.683076000	-1.565030000
1	-3.787694000	-3.038239000	2.459593000	6	-6.322697000	2.871935000	0.174567000
1	-4.433248000	-2.223745000	1.022852000	1	-7.327753000	3.272717000	0.259988000
6	-3.236415000	-4.569869000	0.174433000	6	-5.340631000	3.242702000	1.089129000
1	-2.536174000	-5.182353000	-0.402465000	1	-5.577416000	3.927995000	1.897056000
1	-4.092330000	-4.328360000	-0.464839000	6	-4.055231000	2.718934000	0.983949000
1	-3.608226000	-5.172576000	1.010481000	1	-3.299843000	2.978044000	1.720213000
6	2.459688000	-2.595816000	1.461276000	6	3.726739000	1.826747000	0.047186000
1	2.330766000	-2.013705000	0.542816000	6	4.725437000	1.459536000	0.958826000
6	3.542827000	-3.648817000	1.192939000	1	4.485694000	0.767431000	1.758921000
1	4.477857000	-3.161327000	0.898412000	6	6.010195000	1.977297000	0.848253000
1	3.252834000	-4.335938000	0.392054000	1	6.770284000	1.682996000	1.565051000
1	3.747541000	-4.245478000	2.088198000	6	6.322707000	2.871933000	-0.174491000
6	2.916068000	-1.641183000	2.571920000	1	7.327763000	3.272717000	-0.259898000
1	2.162203000	-0.873223000	2.767526000	6	5.340638000	3.242742000	-1.089033000
1	3.854407000	-1.148668000	2.293888000	1	5.577422000	3.928070000	-1.896931000
1	3.086976000	-2.189066000	3.505602000	6	4.055238000	2.718972000	-0.983873000
1	0.000000000	0.000000000	1.982751000	1	3.299849000	2.978115000	-1.720123000
31	0.000000000	0.000000000	0.410214000	6	-3.149914000	-1.031207000	-0.248699000
				6	-3.411348000	-1.717030000	-1.452480000
				6	-4.357433000	-2.742844000	-1.444353000
				1	-4.562909000	-3.283189000	-2.364669000
				6	-5.038623000	-3.084832000	-0.283247000
				1	-5.769677000	-3.887155000	-0.294408000
				6	-4.776739000	-2.393663000	0.892423000
				1	-5.306692000	-2.664405000	1.801921000
				6	-3.837020000	-1.362458000	0.934695000
				6	-2.693537000	-1.369177000	-2.747513000
				1	-2.144736000	-0.434986000	-2.585393000
				6	-3.666639000	-1.141708000	-3.911379000
				1	-4.419185000	-0.383561000	-3.673450000
				1	-4.194856000	-2.063645000	-4.176133000
				1	-3.118969000	-0.810124000	-4.799358000
				6	-1.681950000	-2.461163000	-3.121107000
				1	-0.967451000	-2.641179000	-2.312297000
				1	-1.125600000	-2.182024000	-4.022700000
$^{1}(\text{PbI}_2\text{P})\text{InH-SP:}$							
7	-2.113585000	-0.052798000	-0.225543000	6	-5.038623000	-3.084832000	-0.283247000
7	0.000004000	1.413181000	-0.000002000	1	-5.769677000	-3.887155000	-0.294408000
7	2.113588000	-0.052805000	0.225516000	6	-4.776739000	-2.393663000	0.892423000
6	-2.360522000	1.259067000	-0.129567000	1	-5.306692000	-2.664405000	1.801921000
6	-1.203930000	2.093810000	-0.051348000	6	-3.837020000	-1.362458000	0.934695000
6	-1.204833000	3.485137000	-0.079783000	6	-2.693537000	-1.369177000	-2.747513000
1	-2.145871000	4.016309000	-0.169747000	1	-2.144736000	-0.434986000	-2.585393000
6	0.000004000	4.187698000	0.000058000	6	-3.666639000	-1.141708000	-3.911379000
1	0.000006000	5.271230000	0.000081000	1	-4.419185000	-0.383561000	-3.673450000
6	1.204844000	3.485129000	0.079873000	1	-4.194856000	-2.063645000	-4.176133000
1	2.145882000	4.016296000	0.169864000	1	-3.118969000	-0.810124000	-4.799358000
6	1.203936000	2.093808000	0.051380000	6	-1.681950000	-2.461163000	-3.121107000
6	2.360530000	1.259057000	0.129581000	1	-0.967451000	-2.641179000	-2.312297000
				1	-1.125600000	-2.182024000	-4.022700000

1	-0.521614000	6.937954000	-1.522333000	1	2.731771000	5.111412000	-0.476539000
6	1.063431000	6.243440000	-2.803796000	1	4.232081000	4.161406000	-0.491106000
1	1.305554000	7.232555000	-3.179352000	1	3.783970000	5.078585000	0.951960000
6	1.776234000	5.130518000	-3.245275000	6	3.511360000	2.402104000	1.575467000
1	2.584557000	5.248470000	-3.960328000	1	2.978170000	1.509215000	1.922835000
6	1.468852000	3.865650000	-2.757024000	1	3.810117000	2.972110000	2.462087000
1	2.047454000	3.005240000	-3.081256000	1	4.420203000	2.081311000	1.055143000
6	-0.434825000	-3.682672000	-1.824136000	6	-0.099492000	-3.083575000	1.036998000
6	0.272373000	-4.812465000	-1.387665000	6	-1.347081000	-3.647716000	1.368537000
1	1.071312000	-4.694833000	-0.663703000	6	-1.408106000	-4.566511000	2.417114000
6	-0.040000000	-6.077670000	-1.872762000	1	-2.367306000	-5.002474000	2.684090000
1	0.521614000	-6.937954000	-1.522333000	6	-0.271943000	-4.923788000	3.132075000
6	-1.063431000	-6.243440000	-2.803796000	1	-0.340991000	-5.636592000	3.947809000
1	-1.305554000	-7.232555000	-3.179352000	6	0.952174000	-4.360034000	2.796908000
6	-1.776234000	-5.130518000	-3.245275000	1	1.841606000	-4.638445000	3.356508000
1	-2.584557000	-5.248470000	-3.960328000	6	1.063048000	-3.442187000	1.751282000
6	-1.468852000	-3.865650000	-2.757024000	6	-2.626893000	-3.251342000	0.653076000
1	-2.047454000	-3.005240000	-3.081256000	1	-2.364332000	-2.634504000	-0.210675000
6	0.099492000	3.083575000	1.036998000	6	-3.511360000	-2.402104000	1.575467000
6	-1.063048000	3.442187000	1.751282000	1	-2.978170000	-1.509215000	1.922835000
6	-0.952174000	4.360034000	2.796908000	1	-3.810117000	-2.972110000	2.462087000
1	-1.841606000	4.638445000	3.356508000	1	-4.420203000	-2.081311000	1.055143000
6	0.271943000	4.923788000	3.132075000	6	-3.385497000	-4.475433000	0.128683000
1	0.340991000	5.636592000	3.947809000	1	-2.731771000	-5.111412000	-0.476539000
6	1.408106000	4.566511000	2.417114000	1	-4.232081000	-4.161406000	-0.491106000
1	2.367306000	5.002474000	2.684090000	1	-3.783970000	-5.078585000	0.951960000
6	1.347081000	3.647716000	1.368537000	6	2.427164000	-2.863885000	1.407586000
6	-2.427164000	2.863885000	1.407586000	1	2.318879000	-2.279359000	0.487514000
1	-2.318879000	2.279359000	0.487514000	6	3.466008000	-3.959197000	1.135890000
6	-3.466008000	3.959197000	1.135890000	1	4.416929000	-3.510778000	0.830462000
1	-3.139921000	4.637579000	0.341707000	1	3.139921000	-4.637579000	0.341707000
1	-3.655357000	4.558846000	2.032385000	1	3.655357000	-4.558846000	2.032385000
1	-4.416929000	3.510778000	0.830462000	6	2.926277000	-1.930726000	2.519147000
6	-2.926277000	1.930726000	2.519147000	1	2.204034000	-1.136672000	2.733592000
1	-2.204034000	1.136672000	2.733592000	1	3.880319000	-1.470088000	2.240060000
1	-3.880319000	1.470088000	2.240060000	1	3.081080000	-2.490168000	3.448636000
1	-3.081080000	2.490168000	3.448636000	1	0.000000000	0.000000000	2.323649000
6	2.626893000	3.251342000	0.653076000	49	0.000000000	0.000000000	0.600969000
1	2.364332000	2.634504000	-0.210675000				
6	3.385497000	4.475433000	0.128683000				

BS- ¹ (^{Ph} I ₂ P)InH-SP:							
				1	-1.914377000	4.738919000	3.286401000
7	0.000000000	2.119172000	0.050897000	6	0.202598000	5.023412000	3.097022000
7	0.000000000	0.000000000	-1.429027000	1	0.255418000	5.749282000	3.902389000
7	0.000000000	-2.119172000	0.050897000	6	1.351869000	4.658024000	2.408228000
6	0.129577000	2.358714000	-1.262697000	1	2.304988000	5.101940000	2.683671000
6	0.080716000	1.202124000	-2.102767000	6	1.311844000	3.722482000	1.373196000
6	0.052249000	1.207958000	-3.496949000	6	-2.460358000	2.924190000	1.361034000
1	0.063945000	2.151908000	-4.029475000	1	-2.342427000	2.352312000	0.434247000
6	0.000000000	0.000000000	-4.194712000	6	-3.517789000	4.005985000	1.106795000
1	0.000000000	0.000000000	-5.278706000	1	-3.198494000	4.715270000	0.337018000
6	-0.052249000	-1.207958000	-3.496949000	1	-3.732827000	4.575574000	2.016941000
1	-0.063945000	-2.151908000	-4.029475000	1	-4.454785000	3.545828000	0.776996000
6	-0.080716000	-1.202124000	-2.102767000	6	-2.945940000	1.967044000	2.457978000
6	-0.129577000	-2.358714000	-1.262697000	1	-2.214276000	1.177780000	2.655895000
6	0.373649000	3.706667000	-1.826025000	1	-3.894845000	1.499835000	2.172378000
6	-0.399984000	4.812024000	-1.446789000	1	-3.104636000	2.510552000	3.396377000
1	-1.217057000	4.674451000	-0.746755000	6	2.603772000	3.327605000	0.679220000
6	-0.130947000	6.075145000	-1.960656000	1	2.358234000	2.687127000	-0.172642000
1	-0.742484000	6.918556000	-1.655986000	6	3.349264000	4.552428000	0.137253000
6	0.914669000	6.260123000	-2.864092000	1	2.692600000	5.167720000	-0.485811000
1	1.123232000	7.248165000	-3.262039000	1	4.206463000	4.238794000	-0.468124000
6	1.693775000	5.171451000	-3.246674000	1	3.731200000	5.177042000	0.952311000
1	2.519657000	5.306954000	-3.938062000	6	3.492396000	2.512239000	1.627592000
6	1.431019000	3.907810000	-2.726260000	1	2.968835000	1.619600000	1.987945000
1	2.064484000	3.067268000	-2.994429000	1	3.775838000	3.107328000	2.502788000
6	-0.373649000	-3.706667000	-1.826025000	1	4.410066000	2.194347000	1.121169000
6	0.399984000	-4.812024000	-1.446789000	6	-0.072135000	-3.147596000	1.034417000
1	1.217057000	-4.674451000	-0.746755000	6	-1.311844000	-3.722482000	1.373196000
6	0.130947000	-6.075145000	-1.960656000	6	-1.351869000	-4.658024000	2.408228000
1	0.742484000	-6.918556000	-1.655986000	1	-2.304988000	-5.101940000	2.683671000
6	-0.914669000	-6.260123000	-2.864092000	6	-0.202598000	-5.023412000	3.097022000
1	-1.123232000	-7.248165000	-3.262039000	1	-0.255418000	-5.749282000	3.902389000
6	-1.693775000	-5.171451000	-3.246674000	6	1.014521000	-4.452492000	2.748245000
1	-2.519657000	-5.306954000	-3.938062000	1	1.914377000	-4.738919000	3.286401000
6	-1.431019000	-3.907810000	-2.726260000	6	1.105192000	-3.515520000	1.717912000
1	-2.064484000	-3.067268000	-2.994429000	6	-2.603772000	-3.327605000	0.679220000
6	0.072135000	3.147596000	1.034417000	1	-2.358234000	-2.687127000	-0.172642000
6	-1.105192000	3.515520000	1.717912000	6	-3.492396000	-2.512239000	1.627592000
6	-1.014521000	4.452492000	2.748245000	1	-2.968835000	-1.619600000	1.987945000
				1	-3.775838000	-3.107328000	2.502788000

1	-4.410066000	-2.194347000	1.121169000	6	1.732634000	5.146495000	-3.358120000
6	-3.349264000	-4.552428000	0.137253000	1	2.588395000	5.273957000	-4.013853000
1	-2.692600000	-5.167720000	-0.485811000	6	1.481764000	3.902457000	-2.785195000
1	-4.206463000	-4.238794000	-0.468124000	1	2.149006000	3.067368000	-2.979674000
1	-3.731200000	-5.177042000	0.952311000	6	-0.385893000	-3.715567000	-1.931577000
6	2.460358000	-2.924190000	1.361034000	6	0.443205000	-4.810285000	-1.654726000
1	2.342427000	-2.352312000	0.434247000	1	1.296227000	-4.676365000	-0.997226000
6	3.517789000	-4.005985000	1.106795000	6	0.188894000	-6.052939000	-2.222138000
1	4.454785000	-3.545828000	0.776996000	1	0.843982000	-6.889310000	-1.999295000
1	3.198494000	-4.715270000	0.337018000	6	-0.899513000	-6.225780000	-3.076313000
1	3.732827000	-4.575574000	2.016941000	1	-1.097842000	-7.197904000	-3.516521000
6	2.945940000	-1.967044000	2.457978000	6	-1.732634000	-5.146495000	-3.358120000
1	2.214276000	-1.177780000	2.655895000	1	-2.588395000	-5.273957000	-4.013853000
1	3.894845000	-1.499835000	2.172378000	6	-1.481764000	-3.902457000	-2.785195000
1	3.104636000	-2.510552000	3.396377000	1	-2.149006000	-3.067368000	-2.979674000
1	0.000000000	0.000000000	2.341644000	6	0.140965000	3.323982000	0.935096000
49	0.000000000	0.000000000	0.625669000	6	-1.007892000	3.816505000	1.589504000
				6	-0.852411000	4.790461000	2.576165000
				1	-1.730024000	5.172634000	3.090529000
$^{1}(\text{PbI}_2\text{P})\text{TIH-SP:}$				6	0.403635000	5.281386000	2.910447000
7	0.000000000	2.248286000	0.017838000	1	0.507610000	6.037660000	3.682130000
7	0.000000000	0.000000000	-1.399519000	6	1.524836000	4.798683000	2.248322000
7	0.000000000	-2.248286000	0.017838000	1	2.507387000	5.182155000	2.511139000
6	0.141286000	2.394411000	-1.299119000	6	1.419493000	3.822278000	1.256166000
6	0.087426000	1.202425000	-2.088194000	6	-2.395245000	3.302100000	1.240024000
6	0.060654000	1.201806000	-3.479896000	1	-2.320160000	2.769611000	0.285364000
1	0.079532000	2.147805000	-4.008893000	6	-3.417359000	4.432349000	1.069026000
6	0.000000000	0.000000000	-4.186609000	1	-3.067408000	5.193743000	0.364759000
1	0.000000000	0.000000000	-5.270009000	1	-3.627260000	4.931357000	2.020838000
6	-0.060654000	-1.201806000	-3.479896000	1	-4.364151000	4.029483000	0.695612000
1	-0.079532000	-2.147805000	-4.008893000	6	-2.891203000	2.307768000	2.298054000
6	-0.087426000	-1.202425000	-2.088194000	1	-2.199284000	1.467614000	2.415457000
6	-0.141286000	-2.394411000	-1.299119000	1	-3.874178000	1.906952000	2.027726000
6	0.385893000	3.715567000	-1.931577000	1	-2.976989000	2.799399000	3.273682000
6	-0.443205000	4.810285000	-1.654726000	6	2.681136000	3.296242000	0.593323000
1	-1.296227000	4.676365000	-0.997226000	1	2.391109000	2.647652000	-0.238550000
6	-0.188894000	6.052939000	-2.222138000	6	3.536164000	4.430880000	0.018464000
1	-0.843982000	6.889310000	-1.999295000	1	2.944149000	5.071093000	-0.642566000
6	0.899513000	6.225780000	-3.076313000	1	4.374256000	4.021017000	-0.555415000
1	1.097842000	7.197904000	-3.516521000	1	3.955915000	5.055676000	0.814441000

6	3.490360000	2.445310000	1.581155000	7	2.325409000	0.075390000	0.460075000
1	2.892859000	1.611037000	1.966808000	6	-2.418688000	1.281243000	0.000680000
1	3.813063000	3.046387000	2.438536000	6	-1.152972000	2.086523000	0.061448000
1	4.382854000	2.033185000	1.098361000	6	-1.198196000	3.486173000	0.044282000
6	-0.140965000	-3.323982000	0.935096000	1	-2.150677000	4.001920000	0.021076000
6	-1.419493000	-3.822278000	1.256166000	6	-0.003569000	4.190616000	0.048146000
6	-1.524836000	-4.798683000	2.248322000	1	-0.003307000	5.275733000	0.043808000
1	-2.507387000	-5.182155000	2.511139000	6	1.193186000	3.485730000	0.052318000
6	-0.403635000	-5.281386000	2.910447000	1	2.143941000	4.004555000	0.063718000
1	-0.507610000	-6.037660000	3.682130000	6	1.152094000	2.087539000	0.043461000
6	0.852411000	-4.790461000	2.576165000	6	2.423245000	1.284357000	0.069690000
1	1.730024000	-5.172634000	3.090529000	6	-3.688642000	1.940977000	0.437753000
6	1.007892000	-3.816505000	1.589504000	6	-4.859877000	1.854178000	-0.322281000
6	-2.681136000	-3.296242000	0.593323000	1	-4.858325000	1.303805000	-1.257444000
1	-2.391109000	-2.647652000	-0.238550000	6	-6.028842000	2.466227000	0.120935000
6	-3.490360000	-2.445310000	1.581155000	1	-6.929548000	2.397953000	-0.480395000
1	-2.892859000	-1.611037000	1.966808000	6	-6.046909000	3.155780000	1.331269000
1	-3.813063000	-3.046387000	2.438536000	1	-6.962535000	3.625752000	1.676001000
1	-4.382854000	-2.033185000	1.098361000	6	-4.888295000	3.235283000	2.100905000
6	-3.536164000	-4.430880000	0.018464000	1	-4.897581000	3.760960000	3.050304000
1	-2.944149000	-5.071093000	-0.642566000	6	-3.715288000	2.636733000	1.653097000
1	-4.374256000	-4.021017000	-0.555415000	1	-2.812005000	2.696989000	2.254745000
1	-3.955915000	-5.055676000	0.814441000	6	3.687393000	1.965234000	-0.349839000
6	2.395245000	-3.302100000	1.240024000	6	4.853650000	1.876374000	0.416415000
1	2.320160000	-2.769611000	0.285364000	1	4.853035000	1.302704000	1.337845000
6	3.417359000	-4.432349000	1.069026000	6	6.016960000	2.514633000	-0.004263000
1	4.364151000	-4.029483000	0.695612000	1	6.914800000	2.445809000	0.601334000
1	3.067408000	-5.193743000	0.364759000	6	6.032712000	3.230852000	-1.199095000
1	3.627260000	-4.931357000	2.020838000	1	6.943663000	3.721789000	-1.526641000
6	2.891203000	-2.307768000	2.298054000	6	4.879690000	3.307028000	-1.977517000
1	2.199284000	-1.467614000	2.415457000	1	4.889769000	3.849305000	-2.917512000
1	3.874178000	-1.906952000	2.027726000	6	3.711943000	2.681991000	-1.552529000
1	2.976989000	-2.799399000	3.273682000	1	2.813535000	2.732900000	-2.162278000
1	0.000000000	0.000000000	2.561390000	6	-3.405955000	-0.794870000	-0.620873000
81	0.000000000	0.000000000	0.800775000	6	-3.633006000	-1.217391000	-1.949645000
				6	-4.694194000	-2.087410000	-2.189779000
				1	-4.899003000	-2.411597000	-3.205003000
				6	-5.479184000	-2.568311000	-1.145531000
				1	-6.297057000	-3.252341000	-1.349367000
				6	-5.192313000	-2.194670000	0.159082000
¹ (^{Ph} I ₂ P)TIH-T:							
7	-2.310679000	0.086485000	-0.438939000				
7	-0.000647000	1.408296000	0.061736000				

1	-5.782587000	-2.602930000	0.975301000	6	5.109033000	-0.271066000	-2.603216000
6	-4.153988000	-1.306521000	0.454190000	1	5.525683000	0.544691000	-2.005602000
6	-2.748130000	-0.700039000	-3.073405000	1	4.843604000	0.123149000	-3.589927000
1	-1.730551000	-0.611756000	-2.672505000	1	5.897160000	-1.019071000	-2.748036000
6	-3.189257000	0.698675000	-3.527662000	6	2.732281000	-0.846184000	3.046539000
1	-3.112306000	1.432041000	-2.718426000	1	1.724717000	-0.723447000	2.629465000
1	-4.228266000	0.680115000	-3.879200000	6	3.183046000	0.520641000	3.580832000
1	-2.557706000	1.048096000	-4.351029000	1	2.546400000	0.836982000	4.414020000
6	-2.690968000	-1.644038000	-4.275029000	1	3.130529000	1.294977000	2.808999000
1	-2.454626000	-2.667378000	-3.968321000	1	4.216117000	0.466386000	3.944449000
1	-1.911889000	-1.308559000	-4.965704000	6	2.642816000	-1.853744000	4.193419000
1	-3.637071000	-1.659960000	-4.828680000	1	2.387124000	-2.852462000	3.827273000
6	-3.848201000	-0.987694000	1.908143000	1	1.869740000	-1.540215000	4.901483000
1	-3.045753000	-0.244339000	1.943738000	1	3.584985000	-1.920630000	4.748920000
6	-5.069979000	-0.404351000	2.628594000	1	0.586569000	-0.834301000	-1.910253000
1	-5.494891000	0.442320000	2.081827000	81	-0.007777000	-1.418783000	-0.020426000
1	-4.793419000	-0.065393000	3.632676000				
1	-5.853288000	-1.162418000	2.740405000				
6	-3.338609000	-2.238917000	2.635944000				
1	-2.440811000	-2.635511000	2.152477000				
1	-4.102134000	-3.024703000	2.639236000				
1	-3.094008000	-2.000877000	3.676714000				
6	3.411577000	-0.820490000	0.599365000				
6	4.165373000	-1.285100000	-0.494234000				
6	5.194464000	-2.194247000	-0.229729000				
1	5.790038000	-2.564874000	-1.059828000				
6	5.466187000	-2.636324000	1.056378000				
1	6.277924000	-3.335085000	1.232992000				
6	4.672963000	-2.205393000	2.115909000				
1	4.864398000	-2.583342000	3.115032000				
6	3.622726000	-1.315422000	1.906642000				
6	3.878854000	-0.897719000	-1.934907000				
1	3.056818000	-0.176208000	-1.951891000				
6	3.398059000	-2.117833000	-2.729955000				
1	2.486833000	-2.530211000	-2.289731000				
1	4.166913000	-2.898643000	-2.757447000				
1	3.167295000	-1.826765000	-3.759866000				

S6: Reference 12 details.

12. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G.

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