

A DFT Study on Dihydropyrazine Annulated Linear Polyacenes: Aromaticity, Stability and HOMO-LUMO Energy Modulation

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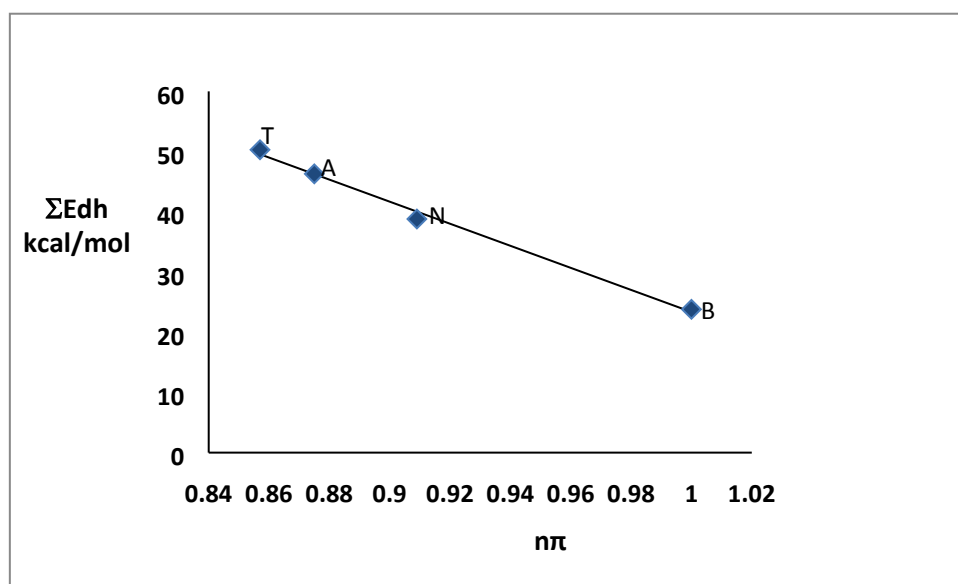
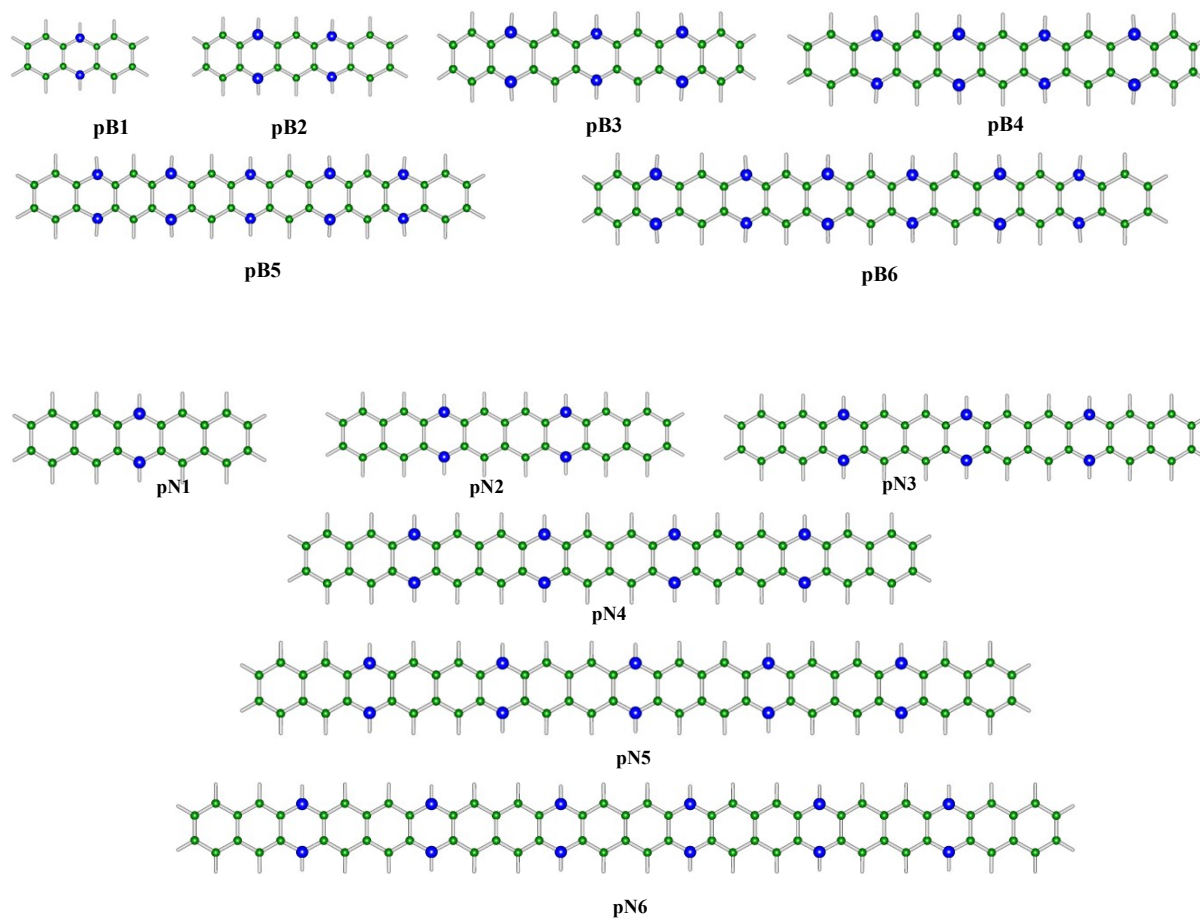


Figure S1. Correlation between n_π and E_{dh} of benzene(B), naphthalene(N), anthracene(A) and tetracene(T)



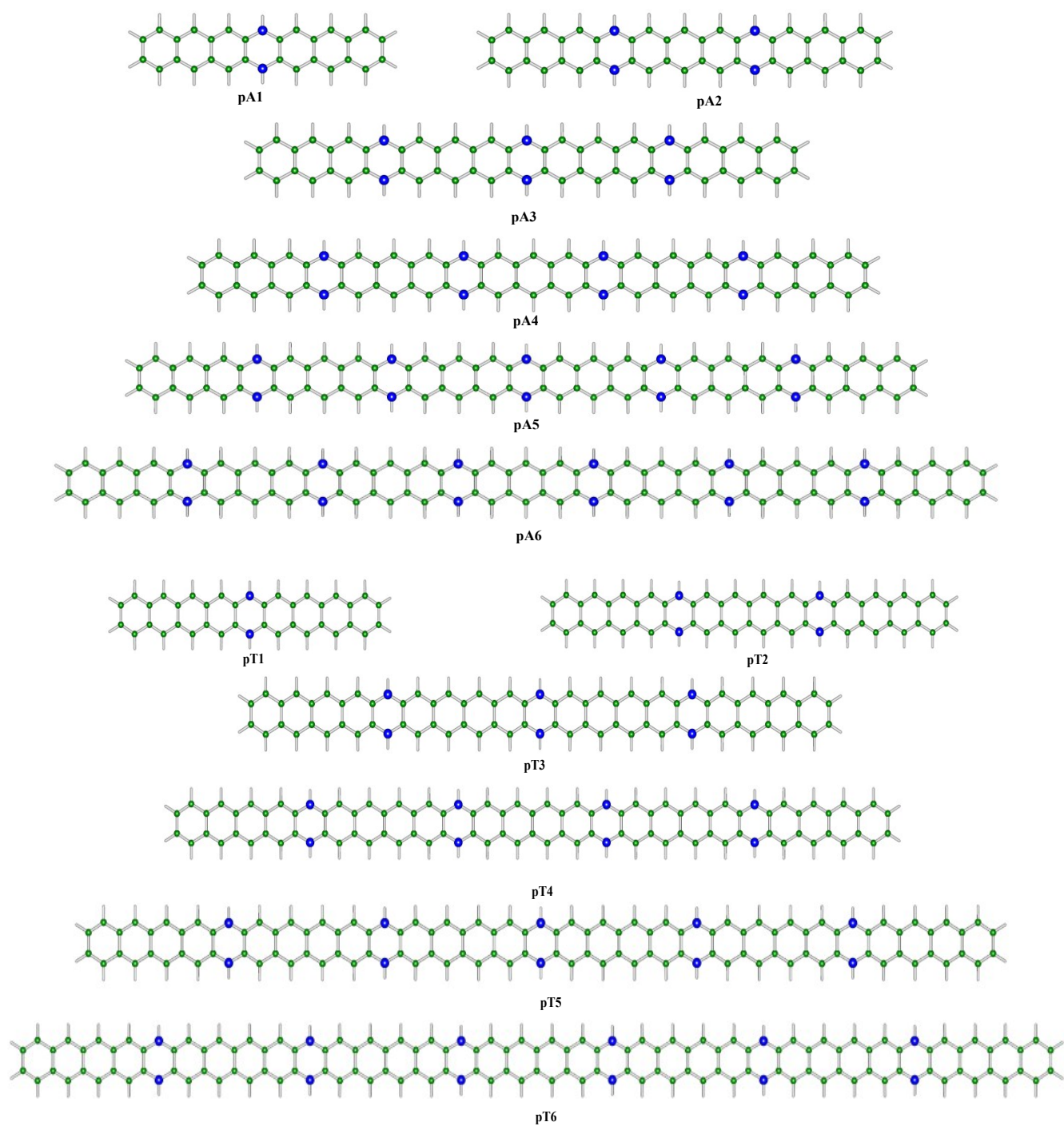
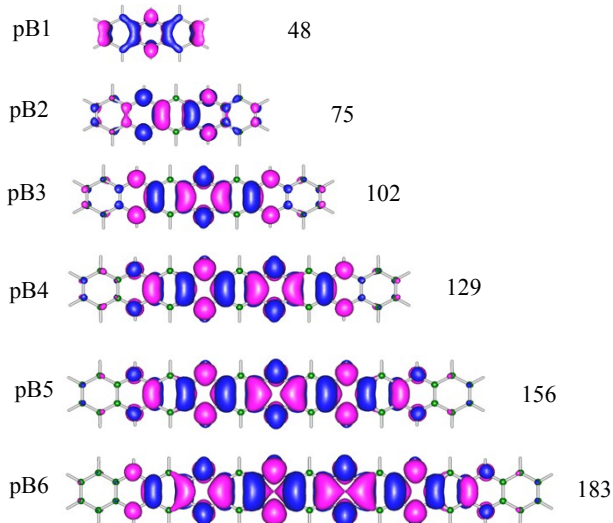
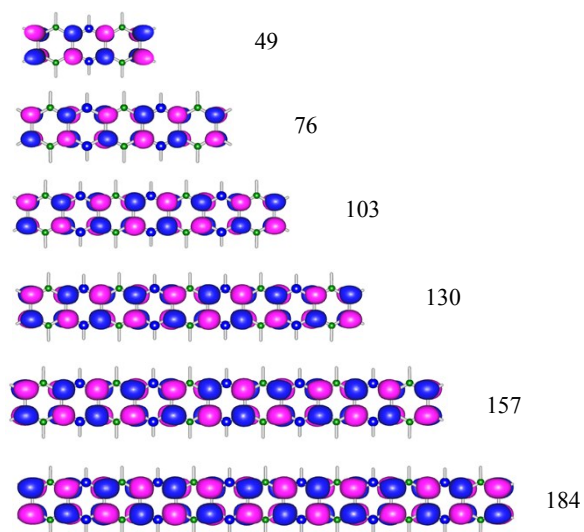


Figure S2. Optimised geometries of LPA mimics at M06L/6-311++G(d,p) level of theory.

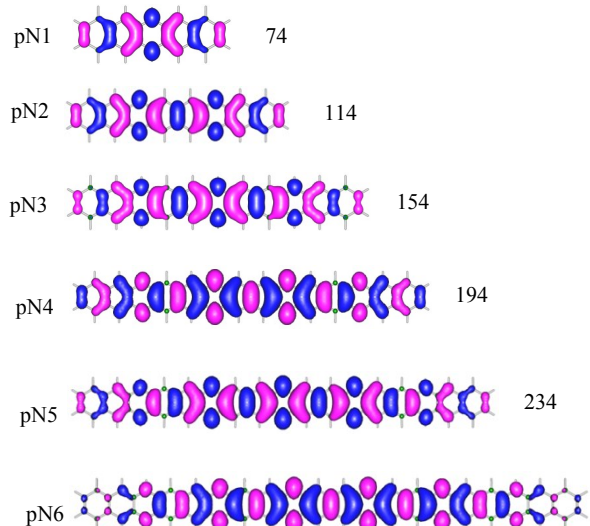
HOMO



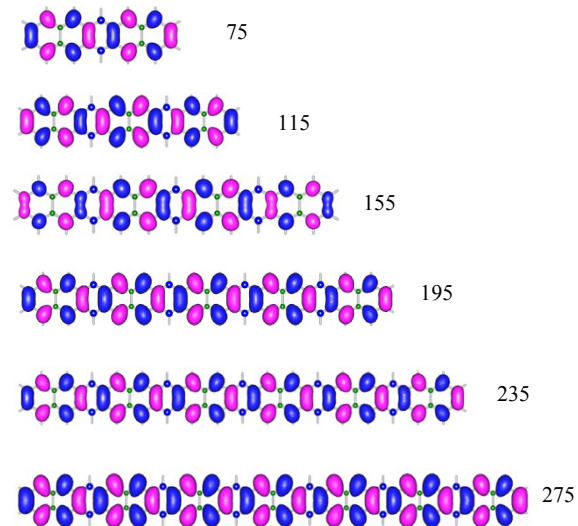
LUMO



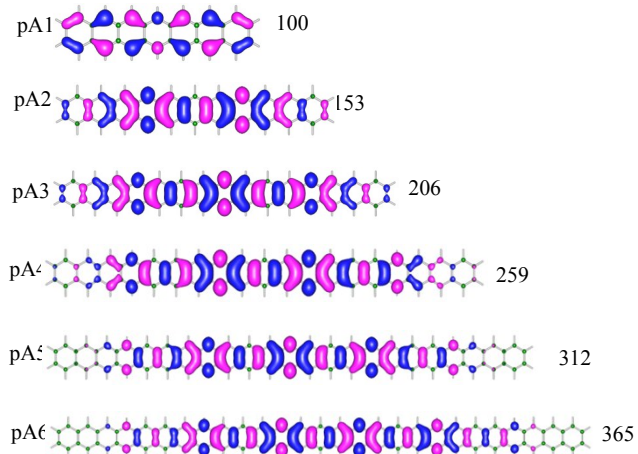
HOMO



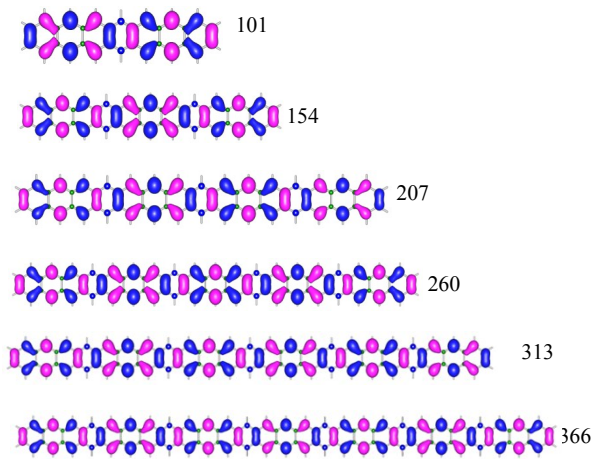
LUMO



HOMO



LUMO



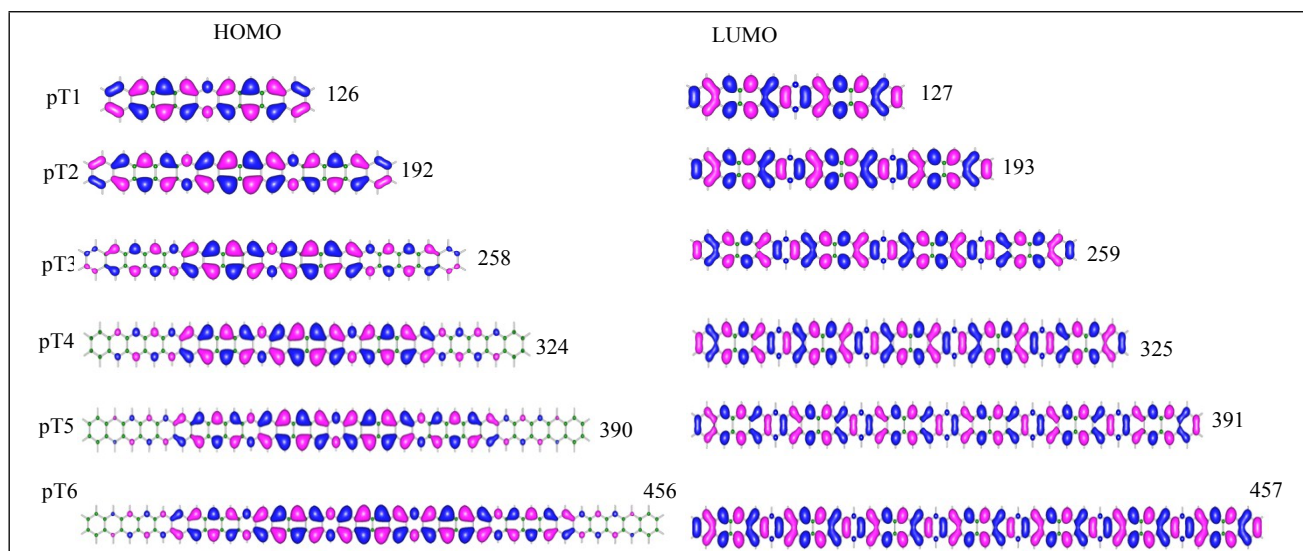
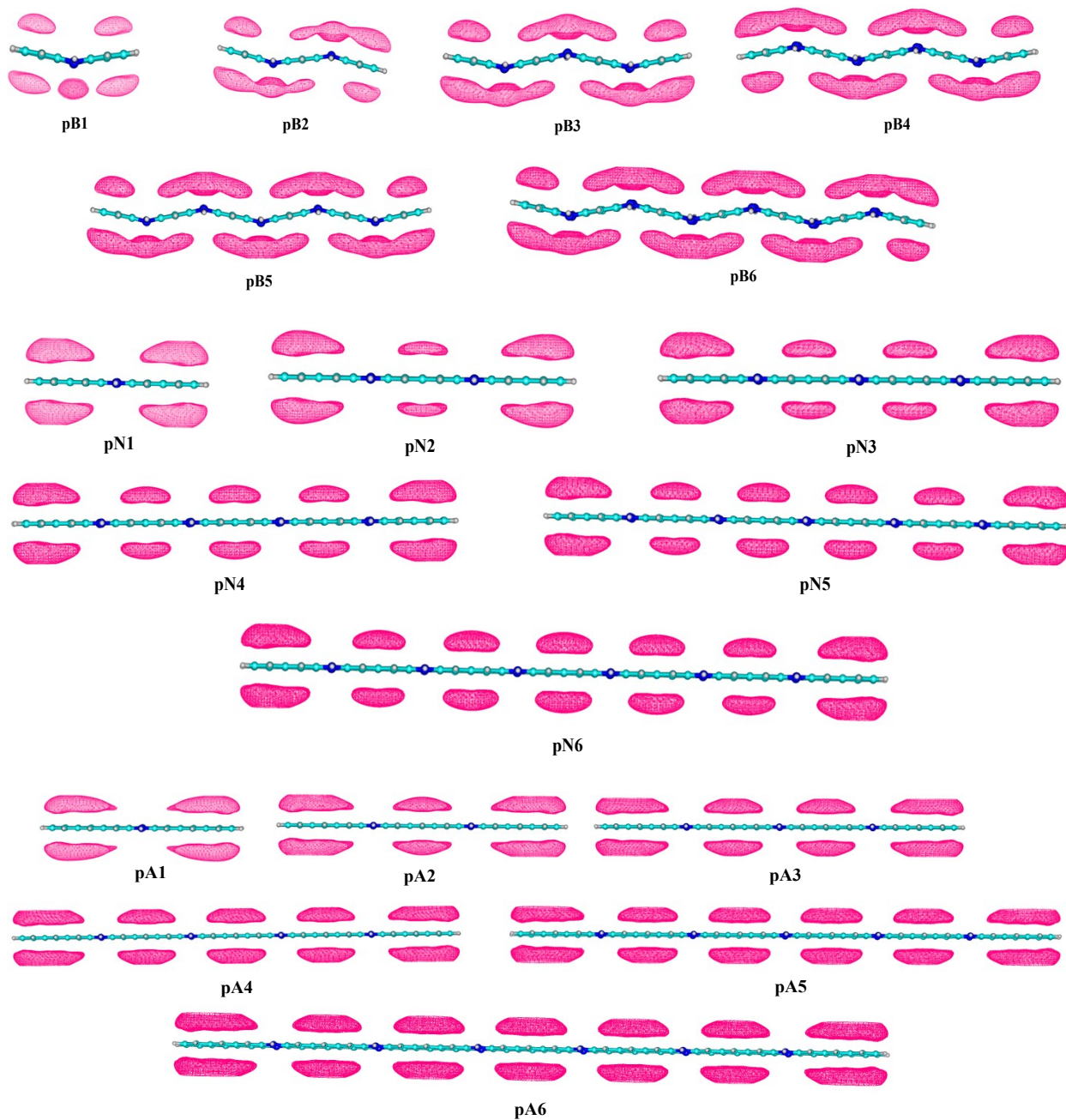


Figure S3. HOMO and LUMO of LPA mimics including their MO number.



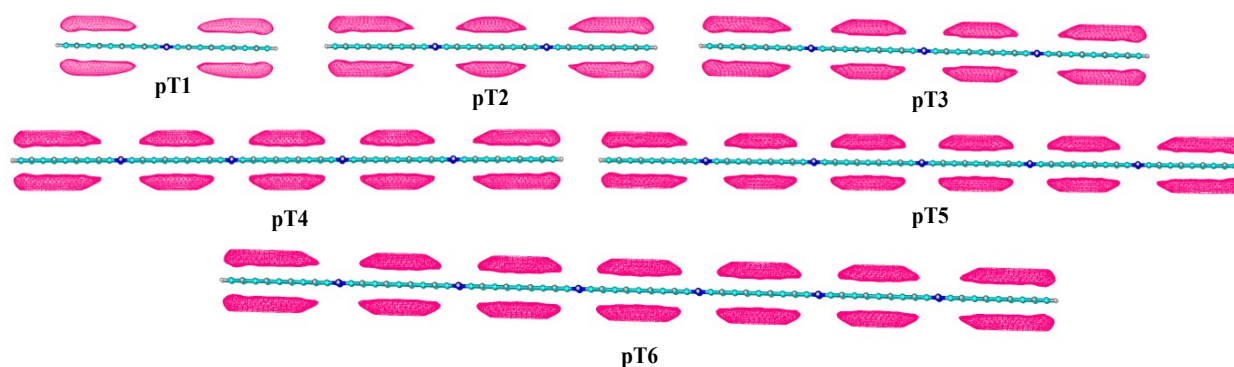


Figure S4. Plots of MESP isosurface of LPA mimics. (MESP value used for the plots are 12kcal/mol for pB and 9.0 kcal/mol for pN, pA and pT series)

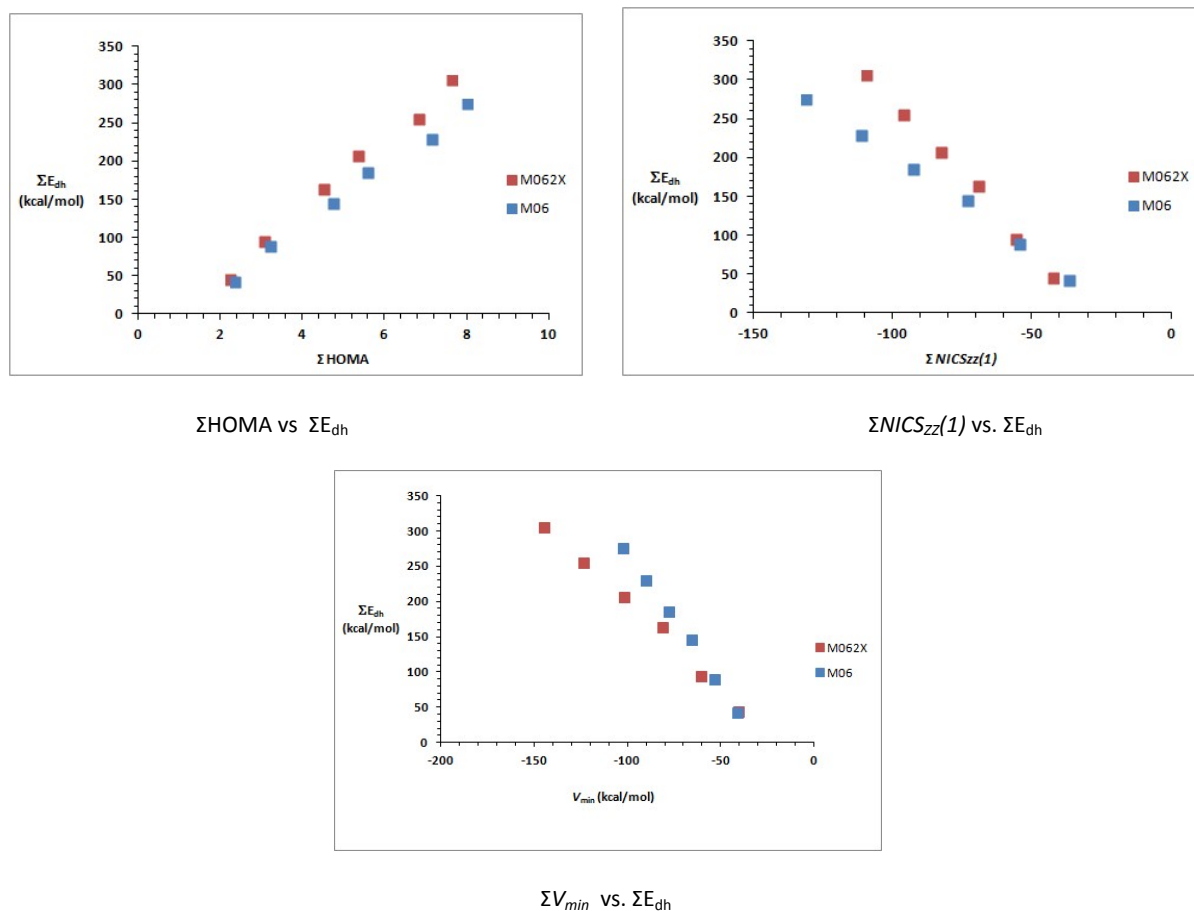


Figure S5. Correlation between dehydrogenation energy and HOMA index, $NICS_{zz}(1)$ values and V_{min} values for pN series of molecules at M06 and M062X level of theories.

Table S1 : Average CC and CN bond lengths of optimized geometries at M06L/6-311++g(d,p) level (in Angstroms)

system	C-C bond	C-N bond
pB ₁	1.393	1.401
pB ₂	1.394	1.404
pB ₃	1.394	1.405
pB ₄	1.394	1.406
pB ₅	1.394	1.406

pB ₆	1.394	1.406
pN ₁	1.402	1.387
pN ₂	1.402	1.388
pN ₃	1.403	1.388
pN ₄	1.403	1.388
pN ₅	1.403	1.388
pN ₆	1.403	1.388
pA ₁	1.405	1.384
pA ₂	1.406	1.385
pA ₃	1.406	1.385
pA ₄	1.406	1.385
pA ₅	1.406	1.385
pA ₆	1.406	1.385
pT ₁	1.407	1.383
pT ₂	1.407	1.384
pT ₃	1.407	1.384
pT ₄	1.408	1.384
pT ₅	1.408	1.384
pT ₆	1.408	1.384

Table S2 : SCF energy of optimized geometries and M06L/6-311++g(d,p) level (in A. U.). The notation pX_n_0 indicates the full LPA mimic and pX_n_i (i is an integer) indicates a state obtained by dehydrogenating i N-heterocycles, from one terminal to the interior.

system	pX _n _0	pX _n _1	pX _n _2	pX _n _3	pX _n _4	pX _n _5	pX _n _6
pB ₁	-572.87769	-571.66820					
pB ₂	-913.47950	-912.28856	-911.05324				
pB ₃	-1254.08138	-1252.89185	-1251.67924	-1250.43509			
pB ₄	-1594.68334	-1593.49379	-1592.28411	-1591.06410	-1589.81625		
pB ₅	-1935.28511	-1934.09587	-1932.88515	-1931.67023	-1930.44654	-1929.19725	
pB ₆	-2275.88688	-2274.69044	-2273.48906	-2272.27389	-2271.05426	-2269.82834	-2268.57791
pN ₁	-880.20333	-878.96990					
pN ₂	-1374.47511	-1373.25107	-1372.00296				
pN ₃	-1868.74664	-1867.52423	-1866.28635	-1865.03896			
pN ₄	-2363.01811	-2361.79625	-2360.56042	-2359.31877	-2358.08454		
pN ₅	-2857.28956	-2856.06748	-2854.80419	-2853.59334	-2852.36660	-2851.12445	
pN ₆	-3351.56099	-3350.33943	-3349.10476	-3347.86660	-3346.62607	-3345.38274	-3344.16130
pA ₁	-1187.51463	-1186.26925					
pA ₂	-1835.44522	-1834.20499	-1832.95113				

pA ₃	-2483.37564	-2482.13628	-2480.88786	-2479.65460			
pA ₄	-3131.30601	-3130.06641	-3128.81898	-3127.56903	-3126.34509		
pA ₅	-3779.23638	-3777.99738	-3776.75027	-3775.52183	-3774.28130	-3773.03151	
pA ₆	-4427.16669	-4425.92776	-4424.68310	-4423.43230	-4422.18290	-4420.93229	-4419.73128
pT ₁	-1494.81952	-1493.56785					
pT ₂	-2296.40400	-2295.15559	-2293.91866				
pT ₃	-3097.98836	-3096.74043	-3095.50544	-3094.22980			
pT ₄	-3899.57270	-3898.32489	-3897.07202	-3895.84874	-3894.60675		
pT ₅	-4701.15688	-4699.90926	-4698.65654	-4697.40300	-4696.14882	-4694.95188	
pT ₆	-5502.74117	-5501.49358	-5500.24092	-5499.01834	-5497.77107	-5496.52044	-5495.29526

[illegible]

ring16												-4.92
ring17												-8.33
NICS(0)												
	pB ₁	pB ₂	pB ₃	pB ₄	pB ₅	pB ₆	pN ₁	pN ₂	pN ₃	pN ₄	pN ₅	pN ₆
ring1	-5.54	-5.93	-5.87	-6	-6.17	-6.18	-9.03	-8.98	-9.02	-8.91	-8.9	-8.81
ring2	8.59	7.11	7.02	7.05	7	7.03	-6.77	-6.82	-6.71	-6.74	-6.73	-6.73
ring3		-2.38	-2.6	-2.54	-2.62	-2.58	5.04	4.93	4.94	4.93	4.97	4.97
ring4			5.28	5.52	5.52	5.59		-5.51	-5.4	-5.34	-5.3	-5.21
ring5				-3.02	-2.86	-2.93			-5.74	-5.78	-5.78	-5.87
ring6					5.67	5.6			4.57	4.53	4.62	4.63
ring7						-2.72				-5.7	-5.6	-5.54
ring8											-5.65	-5.71
ring9											4.68	4.67
ring10												-5.6
	pA ₁	pA ₂	pA ₃	pA ₄	pA ₅	pA ₆	pT ₁	pT ₂	pT ₃	pT ₄	pT ₅	pT ₆
ring1	-9.22	-9.03	-8.98	-8.93	-8.83	-8.83	-8.83	-8.61	-8.4	-8.24	-8.15	-7.86
ring2	-10.82	-10.7	-10.57	-10.48	-10.42	-10.38	-11.89	-11.74	-11.66	-11.56	-11.45	-11.37
ring3	-6.9	-7.02	-7.19	-7.32	-7.42	-7.56	-11.19	-11.12	-11.17	-11.26	-11.39	-11.39
ring4	3.49	3.56	3.55	3.58	3.61	3.54	-7.01	-7.03	-7.12	-7.27	-7.3	-7.49
ring5		-6.24	-6.01	-5.9	-5.76	-5.62	3.06	2.99	2.83	2.76	2.7	2.62
ring6		-9.21	-9.16	-9.15	-9.16	-9.16		-6.58	-6.41	-6.2	-6.22	-5.95
ring7			-6.41	-6.5	-6.57	-6.74		-10.25	-10.22	-10.17	-10.14	-10.23
ring8			3.68	3.67	3.7	3.72			-10.17	-10.18	-10.22	-10.21
ring9				-6.28	-6.12	-6.05			-6.62	-6.71	-6.79	-6.97
ring10				-9.11	-9.08	-9.07			3.04	3.02	2.99	3.05
ring11					-6.36	-6.5				-6.46	-6.31	-6.18
ring12					3.69	3.68				-10.14	-10.1	-10.1
ring13						-6.25					-10.13	-10.15
ring14											-6.53	-6.66
ring15											3.01	3.04
ring16												-6.36
ring17												-10.08

Table S4. Dehydrogenation energy E_{dh} (kcal/mol) of the pN series of LPA mimics at M06 and M062X level of theory

	system	pN _{n_0}	pN _{n_1}	pN _{n_2}	pN _{n_3}	pN _{n_4}	pN _{n_5}	pN _{n_6}
M06	pN ₁	-879.64296	-878.40498					
	pN ₂	-1373.61298	-1372.38297	-1371.12980				
	pN ₃	-1867.58273	-1866.35386	-1865.10956	-1863.84092			
	pN ₄	-2361.55252	-2360.32397	-2359.08050	-2357.83282	-2356.57604		
	pN ₅	-2855.52220	-2854.29375	-2853.05111	-2851.80474	-2850.55464	-2849.30513	
	pN ₆	-3349.49198	-3348.26362	-3347.02103	-3345.75914	-3344.52592	-3343.28472	-3342.03135
	system	pN _{n_0}	pN _{n_1}	pN _{n_2}	pN _{n_3}	pN _{n_4}	pN _{n_5}	pN _{n_6}
M062X	pN ₁	-879.95954	-878.71990					

pN ₂	-1374.10157	-1372.86976	-1371.61352				
pN ₃	-1868.24333	-1867.01250	-1865.76508	-1864.47734			
pN ₄	-2362.38515	-2361.15456	-2359.90814	-2358.65669	-2357.38117		
pN ₅	-2856.52689	-2855.29637	-2854.05022	-2852.79988	-2851.53140	-2850.27737	
pN ₆	-3350.66869	-3349.43816	-3348.19205	-3346.94199	-3345.69034	-3344.42870	-3343.17151

Table S5. Dehydrogenation energy E_{dh} (kcal/mol) of the pN series of LPA mimics at M06 and M062X level of theory

	N1	N2	N3	N4	N5	N6	ΣE_{dh}
M06							
pN₁	-42.4						-42.4
pN₂	-37.4	-51.9					-89.3
pN₃	-36.7	-46.4	-61.7				-144.7
pN₄	-36.5	-45.9	-48.5	-54.2			-185.1
pN₅	-36.4	-45.3	-47.7	-50.0	-49.6		-229.1
pN₆	-36.4	-45.3	-57.4	-39.4	-44.4	-52.1	-275.0
M062X							
pN₁	-44.8						-44.8
pN₂	-39.8	-55.2					-95.0
pN₃	-39.2	-49.6	-75.0				-163.8
pN₄	-39.1	-49.0	-52.2	-67.3			-207.6
pN₅	-39.0	-48.9	-51.5	-62.9	-53.8		-256.0
pN₆	-39.0	-48.8	-51.3	-52.3	-58.6	-55.8	-305.8

Table S6. HOMA index of pN series of LPA mimics at M06 and M062X level of theory

M06						
	pN ₁	pN ₂	pN ₃	pN ₄	pN ₅	pN ₆
Cring1	0.88	0.88	0.88	0.88	0.88	0.88
Cring2	0.79	0.79	0.78	0.78	0.78	0.79
Nring1	0.70	0.71	0.71	0.71	0.71	0.71
Cring3		0.84	0.84	0.84	0.84	0.84
Cring4			0.83	0.83	0.83	0.83
Nring2			0.72	0.73	0.72	0.72
Cring5				0.84	0.84	0.84
Cring6					0.84	0.84
Nring3					0.70	0.72
Cring7						0.84
Σ HOMA	2.37	3.22	4.77	5.60	7.15	8.01
M062X						
Cring1	0.86	0.86	0.86	0.86	0.86	0.86
Cring2	0.75	0.74	0.73	0.74	0.74	0.74
Nring1	0.65	0.65	0.65	0.65	0.65	0.65
Cring3		0.81	0.81	0.82	0.82	0.82

Cring4			0.80	0.80	0.80	0.80
Nring2			0.67	0.67	0.67	0.66
Cring5				0.81	0.81	0.81
Cring6					0.80	0.81
Nring3					0.67	0.67
Cring7						0.81
Σ HOMA	2.25	3.06	4.53	5.35	6.83	7.63

Table S7. *NICSzz(1)* values of pN series of LPA mimics(M06 and M062X level)

	pN ₁	pN ₂	pN ₃	pN ₄	pN ₅	pN ₆
M06						
Cring1	-24.65	-24.52	-23.92	-23.46	-23.25	-22.94
Cring2	-16.34	-15.95	-15.51	-15.13	-14.95	-14.69
Nring1	19.06	19.26	19.30	19.35	19.44	19.48
Cring3		-12.90	-12.98	-12.95	-12.94	-12.91
Cring4			-13.12	-13.07	-13.04	-13.13
Nring2			18.70	18.65	18.47	19.04
Cring5				-13.06	-12.96	-13.02
Cring6					-12.85	-12.88
Nring3					18.15	19.23
Cring7						-12.86
M062X						
Cring1	-25.04	-24.25	-23.16	-22.46	-21.78	-21.10
Cring2	-17.31	-17.58	-18.22	-18.76	-19.34	-19.87
Nring1	20.65	20.33	20.49	20.49	20.44	20.40
Cring3		-13.92	-13.39	-12.68	-12.03	-11.36
Cring4			-14.29	-14.84	-15.46	-16.10
Nring2			20.33	20.45	20.41	20.45
Cring5				-13.78	-13.06	-12.34
Cring6					-14.29	-14.93
Nring3					20.32	20.42
Cring7						-13.56

Table S8 .MESP minimum (kcal/mol) observed on the LPA units for pN series of molecules(M06 and M062X level).

System	$V_{\min}$ on the LPA unit from left to right							$\Sigma V_{\min}$
	1	2	3	4	5	6	7	
M06								
pN ₁	-18.42	-18.42						-36.85
pN ₂	-19.88	-15.16	-19.88					-54.92
pN ₃	-20.41	-16.38	-16.38	-20.41				-73.57
pN ₄	-20.78	-17.01	-17.37	-17.01	-20.78			-92.95
pN ₅	-20.81	-17.23	-17.85	-17.85	-17.23	-20.81		-111.76
pN ₆	-20.85	-17.41	-18.20	-18.39	-18.20	-17.41	-20.85	-131.31

M062X								
pN ₁	-20.34	-20.34					-40.68	
pN ₂	-21.66	-17.52	-21.66				-60.83	
pN ₃	-22.14	-18.59	-18.59	-22.14			-81.48	
pN ₄	-22.40	-19.01	-19.52	-19.01	-22.40		-102.34	
pN ₅	-22.48	-19.40	-20.12	-20.12	-19.40	-22.48	-124.01	
pN ₆	-22.45	-19.48	-20.33	-20.58	-20.33	-19.48	-22.45	-145.10

Table S9. HOMO (ϵ_1), LUMO (ϵ_2) and HOMO-LUMO energy gap ($\Delta\epsilon$) for pN series of molecules. All values in eV. N represents Naphthalene.

M06				M062X			
System	ϵ_1	ϵ_2	$\Delta\epsilon$	System	ϵ_1	ϵ_2	$\Delta\epsilon$
N	-6.42	-1.25	5.17	N	-7.37	-0.49	6.89
pN ₁	-5.29	-1.23	4.05	pN ₁	-6.10	-0.51	5.58
pN ₂	-4.81	-1.27	3.53	pN ₂	-5.57	-0.51	5.06
pN ₃	-4.58	-1.29	3.29	pN ₃	-5.33	-0.49	4.84
pN ₄	-4.46	-1.29	3.17	pN ₄	-5.20	-0.48	4.72
pN ₅	-4.38	-1.28	3.10	pN ₅	-5.12	-0.47	4.65
pN ₆	-4.33	-1.28	3.06	pN ₆	-5.07	-0.46	4.61

Table S10. NICS values for pN series of molecules at M06 and M06-2X level of theory.

M06						M062X					
pN ₁	pN ₂	pN ₃	pN ₄	pN ₅	pN ₆	pN ₁	pN ₂	pN ₃	pN ₄	pN ₅	pN ₆
NICS(0)											
-7.00	-6.83	-6.22	-5.75	-5.46	-5.07	-6.49	-5.86	-4.93	-4.30	-3.71	-3.09
-6.14	-6.45	-6.50	-6.59	-6.76	-6.85	-6.63	-7.50	-8.40	-9.16	-9.93	-10.67
6.76	6.99	7.05	7.17	7.34	7.44	8.03	7.67	7.77	7.80	7.80	7.80
	-5.23	-5.03	-4.85	-4.65	-4.43		-5.38	-4.71	-3.99	-3.32	-2.61
		-5.71	-5.93	-6.07	-6.46			-6.08	-6.80	-7.53	-8.24
		6.45	6.31	6.08	6.69			7.59	7.65	7.53	7.55
			-5.52	-5.22	-5.03				-5.44	-4.68	-3.97
				-5.54	-5.88					-6.12	-6.88
				5.61	6.72					7.41	7.47
					-5.41						-5.37
NICS(1)											
-9.34	-9.30	-9.14	-8.99	-8.91	-8.81	-9.27	-9.00	-8.69	-8.45	-8.22	-8.00
-6.96	-6.80	-6.71	-6.64	-6.56	-6.44	-7.28	-7.36	-7.63	-7.83	-7.98	-8.17
4.98	4.98	5.00	5.01	5.07	5.05	5.59	5.44	5.48	5.48	5.48	5.44
	-5.96	-5.88	-5.88	-5.94	-5.90		-6.24	-6.01	-5.78	-5.58	-5.35
		-6.16	-6.15	-6.08	-6.17			-6.43	-6.63	-6.83	-7.06
		4.83	4.78	4.69	4.94			5.51	5.50	5.48	5.50
			-6.16	-6.07	-6.06				-6.29	-5.97	-5.75
				-6.07	-6.03					-6.40	-6.64
				4.49	4.97					5.43	5.47
					-5.99						-6.16

Table S11-S118: SCF energy (E) and Cartesian coordinates of all the optimized structures at M06L/6-311++g(d,p) level. Atomic number followed by X, Y, Z coordinates in Angstrom.

Table S11: Coordinates pB₁

atom	x	y	z
6	3.597429000	0.693015000	-0.250281000
6	2.401823000	1.387852000	-0.064189000
6	1.212062000	0.703091000	0.142102000
6	1.212062000	-0.703091000	0.142102000
6	2.401823000	-1.387852000	-0.064189000
6	3.597429000	-0.693015000	-0.250281000
7	0.000000000	1.357958000	0.395701000
7	0.000000000	-1.357958000	0.395701000
6	-1.212062000	-0.703091000	0.142102000
6	-1.212062000	0.703091000	0.142102000
6	-2.401823000	1.387852000	-0.064189000
1	-2.391660000	2.474425000	-0.067469000
6	-3.597430000	0.693015000	-0.250281000
6	-3.597430000	-0.693015000	-0.250281000
6	-2.401823000	-1.387852000	-0.064189000
1	4.520061000	1.243608000	-0.397576000
1	2.391660000	2.474425000	-0.067469000
1	2.391660000	-2.474425000	-0.067469000
1	4.520061000	-1.243608000	-0.397576000
1	-2.391660000	-2.474425000	-0.067469000
1	-4.520060000	1.243608000	-0.397576000
1	-4.520060000	-1.243608000	-0.397576000
1	0.000000000	2.353523000	0.228598000
1	0.000000000	-2.353523000	0.228598000

Table S12: Coordinates of pB₂ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	5.999138000	0.693132000
6	-0.152607000	4.798662000	1.387148000
6	-0.327986000	3.602726000	0.703407000
6	-0.327986000	3.602726000	-0.703407000
6	-0.152607000	4.798662000	-1.387148000
6	0.000000000	5.999138000	-0.693132000
7	-0.553877000	2.386409000	1.362107000
7	-0.553877000	2.386409000	-1.362107000
6	-0.248529000	1.185247000	-0.698676000
6	-0.248529000	1.185247000	0.698676000
6	0.000000000	0.000000000	1.384883000
1	0.000000000	0.000000000	2.472007000
6	0.248529000	-1.185247000	0.698676000
6	0.248529000	-1.185247000	-0.698676000

6	0.000000000	0.000000000	-1.384883000
1	0.122584000	6.925322000	1.243886000
1	-0.148360000	4.788644000	2.473852000
1	-0.148360000	4.788644000	-2.473852000
1	0.122584000	6.925322000	-1.243886000
1	0.000000000	0.000000000	-2.472007000
7	0.553877000	-2.386409000	-1.362107000
7	0.553877000	-2.386409000	1.362107000
6	0.327986000	-3.602726000	-0.703407000
6	0.327986000	-3.602726000	0.703407000
6	0.152607000	-4.798662000	1.387148000
6	0.152607000	-4.798662000	-1.387148000
6	0.000000000	-5.999138000	-0.693132000
6	0.000000000	-5.999138000	0.693132000
1	0.148360000	-4.788644000	2.473852000
1	-0.122584000	-6.925322000	1.243886000
1	-0.122584000	-6.925322000	-1.243886000
1	0.148360000	-4.788644000	-2.473852000
1	-0.354061000	2.394474000	-2.351724000
1	-0.354061000	2.394474000	2.351724000
1	0.354061000	-2.394474000	-2.351724000
1	0.354061000	-2.394474000	2.351724000

Table S13: Coordinates of pB₃ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-3.590091000	-0.698617000	0.180834000
6	-2.398773000	-1.384190000	-0.036249000
6	-1.206295000	-0.698986000	-0.254009000
6	-1.206298000	0.698981000	-0.254026000
6	-2.398776000	1.384184000	-0.036263000
6	-3.590096000	0.698613000	0.180822000
7	0.000068000	-1.367259000	-0.532648000
7	0.000062000	1.367248000	-0.532667000
6	1.206388000	0.698990000	-0.253870000
6	1.206391000	-0.698989000	-0.253854000
6	2.398838000	-1.384194000	-0.035955000
1	2.399164000	-2.471434000	-0.036144000
6	3.590132000	-0.698613000	0.181278000
6	3.590120000	0.698600000	0.181276000
6	2.398836000	1.384188000	-0.035955000
1	-2.399102000	-2.471430000	-0.036420000
1	-2.399106000	2.471425000	-0.036457000
1	2.399171000	2.471428000	-0.036152000
7	4.799623000	1.361781000	0.455761000
7	4.799636000	-1.361769000	0.455680000
6	6.008090000	0.703450000	0.189810000

6	6.008089000	-0.703455000	0.189811000
6	7.197528000	-1.387182000	-0.026066000
6	7.197516000	1.387187000	-0.026065000
6	8.391991000	0.693173000	-0.220063000
6	8.391993000	-0.693157000	-0.220059000
1	7.187331000	-2.473900000	-0.030301000
1	9.313462000	-1.243918000	-0.374328000
1	9.313458000	1.243938000	-0.374334000
1	7.187311000	2.473904000	-0.030317000
7	-4.799597000	-1.361790000	0.455090000
7	-4.799595000	1.361794000	0.455056000
6	-6.008106000	-0.703462000	0.189598000
6	-6.008110000	0.703459000	0.189601000
6	-7.197618000	1.387184000	-0.025847000
6	-7.197611000	-1.387179000	-0.025895000
6	-8.392157000	0.693165000	-0.219460000
6	-8.392152000	-0.693160000	-0.219489000
1	-7.187406000	-2.473898000	-0.030149000
1	-7.187420000	2.473901000	-0.030060000
1	-9.313676000	1.243932000	-0.373405000
1	-9.313663000	-1.243928000	-0.373476000
1	-4.801789000	2.351300000	0.254239000
1	-4.801794000	-2.351287000	0.254304000
1	0.000042000	2.348846000	-0.294995000
1	0.000052000	-2.348839000	-0.294918000
1	4.801799000	2.351260000	0.254720000
1	4.801819000	-2.351287000	0.254854000

Table S14: Coordinates of pB₄ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	1.191440000	0.698918000	0.225747000
6	0.000107000	1.383457000	0.001916000
6	-1.191225000	0.698923000	-0.221927000
6	-1.191225000	-0.698923000	-0.221927000
6	0.000107000	-1.383457000	0.001916000
6	1.191440000	-0.698917000	0.225747000
6	-3.604004000	-0.699126000	-0.235195000
6	-3.604004000	0.699126000	-0.235194000
6	-4.797898000	1.384114000	-0.024570000
1	-4.798326000	2.471379000	-0.024706000
6	-5.990483000	0.698509000	0.185569000
6	-5.990483000	-0.698510000	0.185568000
6	-4.797898000	-1.384114000	-0.024573000
1	0.000106000	2.470811000	0.001902000
1	0.000106000	-2.470810000	0.001902000
1	-4.798326000	-2.471379000	-0.024710000

6	-8.408349000	-0.703547000	0.178440000
6	-8.408349000	0.703546000	0.178442000
6	-9.596191000	1.387171000	-0.046185000
6	-9.596191000	-1.387171000	-0.046189000
6	-10.789424000	-0.693146000	-0.248432000
6	-10.789424000	0.693147000	-0.248430000
1	-9.586170000	2.473912000	-0.050535000
1	-9.586169000	-2.473911000	-0.050542000
6	3.604102000	0.699092000	0.237866000
6	3.604102000	-0.699092000	0.237867000
6	4.797818000	-1.384108000	0.026091000
6	4.797818000	1.384107000	0.026089000
6	5.990179000	-0.698541000	-0.185243000
6	5.990179000	0.698540000	-0.185245000
1	4.798218000	2.471371000	0.026227000
1	4.798218000	-2.471371000	0.026231000
7	-7.201802000	1.361719000	0.452698000
7	-7.201803000	-1.361720000	0.452695000
7	-2.396402000	1.367324000	-0.507074000
7	-2.396401000	-1.367323000	-0.507076000
7	2.396689000	1.367316000	0.510837000
7	2.396689000	-1.367316000	0.510839000
7	7.201222000	1.361712000	-0.453572000
7	7.201222000	-1.361713000	-0.453569000
6	8.408114000	0.703504000	-0.180977000
6	8.408114000	-0.703504000	-0.180975000
6	9.596313000	1.387189000	0.042003000
6	9.596313000	-1.387189000	0.042006000
6	10.789761000	0.693171000	0.242475000
6	10.789761000	-0.693171000	0.242477000
1	7.202321000	-2.351302000	-0.253172000
1	7.202320000	2.351302000	-0.253177000
1	2.397861000	-2.348777000	0.272643000
1	2.397861000	2.348777000	0.272641000
1	-2.397668000	2.348847000	-0.269195000
1	-2.397668000	-2.348847000	-0.269196000
1	-7.202624000	2.351276000	0.252084000
1	-7.202624000	-2.351276000	0.252079000
1	9.586107000	-2.473923000	0.046334000
1	11.710412000	-1.243948000	0.401585000
1	11.710412000	1.243948000	0.401581000
1	9.586107000	2.473923000	0.046328000
1	-11.709750000	-1.244067000	-0.408844000
1	-11.709750000	1.244068000	-0.408840000

Table S15: Coordinates of pB₅ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-3.589535000	-0.698961000	0.212766000
6	-2.397814000	-1.383450000	-0.009179000
6	-1.206011000	-0.699027000	-0.231026000
6	-1.206028000	0.698972000	-0.230939000
6	-2.397822000	1.383337000	-0.008854000
6	-3.589526000	0.698789000	0.213006000
6	1.206011000	0.699028000	-0.231018000
6	1.206028000	-0.698971000	-0.230948000
6	2.397822000	-1.383338000	-0.008872000
1	2.397800000	-2.470712000	-0.008059000
6	3.589526000	-0.698793000	0.212996000
6	3.589535000	0.698958000	0.212773000
6	2.397814000	1.383449000	-0.009163000
1	-2.397785000	-2.470824000	-0.008605000
1	-2.397800000	2.470711000	-0.008029000
1	2.397785000	2.470823000	-0.008578000
6	6.002635000	0.699202000	0.227119000
6	6.002623000	-0.699112000	0.227476000
6	7.197142000	-1.384070000	0.019970000
6	7.197151000	1.384032000	0.019158000
6	8.390233000	0.698407000	-0.187872000
6	8.390236000	-0.698574000	-0.187413000
1	7.197592000	-2.471340000	0.020727000
1	7.197609000	2.471302000	0.019281000
6	-6.002635000	-0.699205000	0.227114000
6	-6.002623000	0.699109000	0.227486000
6	-7.197142000	1.384070000	0.019989000
6	-7.197151000	-1.384032000	0.019145000
6	-8.390236000	0.698576000	-0.187402000
6	-8.390233000	-0.698405000	-0.187877000
1	-7.197609000	-2.471303000	0.019256000
1	-7.197591000	2.471340000	0.020758000
6	10.807887000	-0.703579000	-0.171661000
6	10.807884000	0.703457000	-0.172181000
6	11.994767000	1.387235000	0.057531000
6	11.994771000	-1.387185000	0.058568000
6	13.187006000	0.693276000	0.265361000
6	13.187007000	-0.693071000	0.265888000
1	11.984519000	2.473972000	0.061524000
1	11.984525000	-2.473918000	0.063374000
1	14.106699000	-1.243787000	0.430663000
1	14.106698000	1.244119000	0.429724000
7	9.602484000	-1.361769000	-0.450885000
7	9.602467000	1.361432000	-0.451848000
7	4.794853000	-1.367605000	0.497380000
7	4.794901000	1.367849000	0.496804000

7	0.000033000	-1.367047000	-0.513299000
7	-0.000033000	1.367052000	-0.513284000
7	-4.794901000	-1.367856000	0.496790000
7	-4.794853000	1.367598000	0.497399000
7	-9.602467000	-1.361426000	-0.451859000
7	-9.602483000	1.361775000	-0.450866000
6	-10.807884000	-0.703453000	-0.172187000
6	-10.807887000	0.703582000	-0.171651000
6	-11.994768000	-1.387234000	0.057516000
6	-11.994771000	1.387186000	0.058584000
6	-13.187007000	-0.693277000	0.265352000
6	-13.187008000	0.693070000	0.265894000
1	-9.602613000	2.351298000	-0.250065000
1	-9.602590000	-2.351096000	-0.251778000
1	-4.796211000	2.348692000	0.257733000
1	-4.796277000	-2.348844000	0.256693000
1	0.000045000	-2.348467000	-0.274760000
1	-0.000045000	2.348469000	-0.274733000
1	4.796212000	-2.348696000	0.257704000
1	4.796277000	2.348840000	0.256718000
1	9.602614000	-2.351295000	-0.250094000
1	9.602589000	2.351099000	-0.251755000
1	-11.984524000	2.473919000	0.063401000
1	-14.106700000	1.243785000	0.430674000
1	-14.106700000	-1.244121000	0.429708000
1	-11.984521000	-2.473971000	0.061498000

Table S16: Coordinates of pB₆ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-5.989108000	-0.698804000	0.232899000
6	-4.797342000	-1.383355000	0.011437000
6	-3.605402000	-0.699064000	-0.210226000
6	-3.605401000	0.699068000	-0.210255000
6	-4.797343000	1.383372000	0.011361000
6	-5.989109000	0.698832000	0.232852000
6	-1.192902000	0.698950000	-0.215720000
6	-1.192903000	-0.698957000	-0.215710000
6	0.000004000	-1.383323000	0.000299000
1	0.000005000	-2.470717000	0.000296000
6	1.192912000	-0.698956000	0.216308000
6	1.192910000	0.698949000	0.216317000
6	0.000004000	1.383316000	0.000299000
1	-4.797383000	-2.470735000	0.011770000
1	-4.797383000	2.470751000	0.011636000
1	0.000005000	2.470710000	0.000296000
6	3.605403000	0.699068000	0.210771000

6	3.605405000	-0.699063000	0.210742000
6	4.797329000	-1.383356000	-0.011002000
6	4.797330000	1.383372000	-0.010927000
6	5.989081000	0.698832000	-0.232500000
6	5.989079000	-0.698804000	-0.232547000
1	4.797369000	-2.470735000	-0.011341000
1	4.797369000	2.470751000	-0.011207000
6	-8.401801000	-0.699152000	0.240765000
6	-8.401803000	0.699170000	0.240704000
6	-9.595249000	1.384073000	0.026910000
6	-9.595247000	-1.384078000	0.027043000
6	-10.787287000	0.698476000	-0.186213000
6	-10.787287000	-0.698504000	-0.186140000
1	-9.595677000	-2.471350000	0.027210000
1	-9.595681000	2.471345000	0.026973000
6	8.401779000	-0.699153000	-0.240656000
6	8.401781000	0.699170000	-0.240594000
6	9.595256000	1.384072000	-0.026961000
6	9.595253000	-1.384078000	-0.027094000
6	10.787323000	0.698476000	0.185999000
6	10.787322000	-0.698504000	0.185926000
1	9.595688000	2.471344000	-0.027029000
1	9.595684000	-2.471350000	-0.027266000
7	7.194996000	-1.367425000	-0.515730000
7	7.195003000	1.367470000	-0.515623000
7	2.399937000	-1.367463000	0.493771000
7	2.399930000	1.367454000	0.493809000
7	-2.399921000	-1.367467000	-0.493187000
7	-2.399915000	1.367458000	-0.493225000
7	-7.195049000	-1.367422000	0.515988000
7	-7.195056000	1.367466000	0.515881000
7	-11.998049000	-1.361742000	-0.456236000
7	-11.998048000	1.361686000	-0.456386000
6	-13.205193000	-0.703553000	-0.184958000
6	-13.205193000	0.703527000	-0.185038000
6	-14.393676000	-1.387170000	0.036693000
6	-14.393677000	1.387169000	0.036531000
6	-15.587396000	-0.693150000	0.235731000
6	-15.587397000	0.693171000	0.235649000
1	-11.999371000	2.351219000	-0.255677000
1	-11.999372000	-2.351253000	-0.255420000
1	-7.195752000	2.348642000	0.276443000
1	-7.195742000	-2.348616000	0.276627000
1	-2.399341000	-2.348453000	-0.252911000
1	-2.399332000	2.348451000	-0.252977000
1	2.399348000	-2.348451000	0.253504000
1	2.399339000	2.348449000	0.253570000
1	7.195713000	-2.348617000	-0.276361000

1	7.195723000	2.348643000	-0.276176000
1	-14.383501000	2.473907000	0.040864000
1	-16.508212000	1.244003000	0.393654000
1	-16.508211000	-1.243964000	0.393801000
1	-14.383500000	-2.473907000	0.041152000
7	11.998124000	1.361683000	0.456002000
7	11.998125000	-1.361740000	0.455852000
6	13.205224000	0.703527000	0.184444000
6	13.205223000	-0.703553000	0.184363000
6	14.393667000	1.387169000	-0.037341000
6	14.393666000	-1.387170000	-0.037503000
6	15.587350000	0.693171000	-0.236678000
6	15.587350000	-0.693150000	-0.236760000
1	11.999415000	2.351217000	0.255296000
1	11.999416000	-2.351252000	0.255037000
1	14.383491000	2.473907000	-0.041674000
1	16.508136000	1.244003000	-0.394851000
1	16.508135000	-1.243964000	-0.394998000
1	14.383489000	-2.473908000	-0.041963000

Table S17: Coordinates of pN₁ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	6.087953000	0.703225000	-0.000022000
6	6.087953000	-0.703226000	-0.000021000
6	4.897827000	-1.395493000	-0.000011000
6	4.897827000	1.395493000	-0.000015000
6	3.661320000	0.714781000	-0.000006000
6	3.661319000	-0.714780000	-0.000004000
1	4.894620000	-2.482249000	-0.000010000
1	4.894622000	2.482249000	-0.000017000
6	1.227598000	-0.713983000	0.000017000
6	1.227599000	0.713982000	0.000018000
7	0.000000000	1.358638000	0.000035000
7	0.000000000	-1.358638000	0.000033000
6	-1.227599000	0.713983000	0.000017000
6	-1.227599000	-0.713982000	0.000017000
1	0.000000000	2.366464000	0.000113000
1	0.000000000	-2.366464000	0.000086000
6	2.420103000	-1.395822000	0.000002000
6	2.420103000	1.395822000	0.000000000
6	-2.420103000	-1.395822000	0.000001000
6	-2.420103000	1.395822000	0.000001000
6	-3.661320000	-0.714781000	-0.000005000
6	-3.661319000	0.714780000	-0.000005000
6	-4.897827000	-1.395493000	-0.000013000
6	-4.897827000	1.395493000	-0.000013000

6	-6.087953000	-0.703226000	-0.000021000
6	-6.087953000	0.703226000	-0.000022000
1	-4.894620000	-2.482249000	-0.000013000
1	-7.029679000	-1.242604000	-0.000028000
1	-7.029679000	1.242604000	-0.000028000
1	-4.894621000	2.482249000	-0.000014000
1	-2.413400000	2.482950000	-0.000003000
1	-2.413400000	-2.482950000	0.000000000
1	2.413399000	2.482950000	-0.000004000
1	2.413401000	-2.482950000	0.000001000
1	7.029679000	-1.242605000	-0.000026000
1	7.029679000	1.242604000	-0.000029000

Table S18: Coordinates of pN₂ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-9.751058000	0.702984000	0.000225000
6	-9.751058000	-0.702983000	0.000235000
6	-7.323847000	-0.714817000	0.000065000
6	-7.323847000	0.714817000	0.000056000
6	-6.082094000	1.395557000	-0.000034000
1	-6.075511000	2.482752000	-0.000032000
6	-4.888800000	0.714478000	-0.000124000
6	-4.888800000	-0.714478000	-0.000123000
6	-6.082094000	-1.395557000	-0.000023000
1	-6.075511000	-2.482752000	-0.000024000
6	-2.433742000	-0.711157000	-0.000165000
6	-2.433742000	0.711157000	-0.000164000
6	-1.238219000	1.393955000	-0.000111000
6	-1.238219000	-1.393955000	-0.000110000
6	0.000000000	-0.713996000	-0.000061000
6	0.000000000	0.713996000	-0.000064000
1	-1.246524000	2.481104000	-0.000108000
1	-1.246524000	-2.481104000	-0.000115000
6	2.433742000	0.711157000	0.000019000
6	2.433742000	-0.711157000	0.000013000
7	3.662028000	-1.359157000	0.000029000
7	3.662028000	1.359157000	0.000087000
6	4.888800000	-0.714478000	0.000048000
6	4.888799000	0.714478000	0.000051000
1	3.661889000	-2.366758000	0.000119000
1	3.661889000	2.366758000	-0.000014000
6	1.238219000	1.393955000	-0.000020000
6	1.238219000	-1.393955000	-0.000024000
7	-3.662028000	1.359157000	-0.000237000
7	-3.662028000	-1.359157000	-0.000268000
6	-8.560227000	1.395117000	0.000138000

6	-8.560227000	-1.395117000	0.000157000
6	6.082094000	1.395557000	0.000045000
6	6.082094000	-1.395557000	0.000048000
6	7.323847000	0.714817000	0.000042000
6	7.323847000	-0.714817000	0.000050000
6	8.560227000	1.395117000	0.000037000
6	8.560227000	-1.395117000	0.000052000
6	9.751058000	0.702984000	0.000039000
6	9.751058000	-0.702983000	0.000047000
1	8.557180000	2.481942000	0.000032000
1	10.692529000	1.242890000	0.000034000
1	10.692529000	-1.242890000	0.000049000
1	8.557180000	-2.481942000	0.000057000
1	6.075512000	-2.482752000	0.000040000
1	6.075511000	2.482752000	0.000051000
1	1.246524000	-2.481104000	-0.000035000
1	1.246524000	2.481104000	-0.000013000
1	-3.661889000	-2.366758000	-0.000088000
1	-3.661889000	2.366758000	-0.000174000
1	-8.557180000	2.481942000	0.000131000
1	-8.557180000	-2.481942000	0.000164000
1	-10.692529000	1.242890000	0.000288000
1	-10.692529000	-1.242890000	0.000306000

Table S19: Coordinates of pN₃ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-8.551888000	0.714646000	-0.000069000
7	-7.325336000	1.359456000	-0.000654000
6	-6.096521000	0.710773000	-0.000660000
6	-6.096521000	-0.710773000	-0.000667000
7	-7.325336000	-1.359456000	-0.000708000
6	-8.551888000	-0.714646000	-0.000075000
6	-3.662520000	-0.714047000	-0.000804000
6	-3.662520000	0.714047000	-0.000807000
6	-2.423663000	1.393903000	-0.000917000
1	-2.415404000	2.481156000	-0.000920000
6	-1.227520000	0.711761000	-0.001051000
6	-1.227520000	-0.711762000	-0.001040000
6	-2.423663000	-1.393903000	-0.000904000
1	-7.325026000	2.366982000	-0.000478000
1	-7.325026000	-2.366982000	-0.000386000
1	-2.415404000	-2.481156000	-0.000886000
6	1.227520000	-0.711762000	-0.000961000
6	1.227520000	0.711761000	-0.000972000
6	2.423663000	1.393903000	-0.000758000
6	2.423663000	-1.393903000	-0.000741000

6	3.662520000	-0.714047000	-0.000544000
6	3.662520000	0.714047000	-0.000550000
1	2.415404000	2.481156000	-0.000759000
1	2.415404000	-2.481156000	-0.000719000
6	-10.987459000	0.714849000	0.000938000
6	-10.987459000	-0.714849000	0.000940000
6	-12.224016000	-1.395238000	0.001436000
6	-12.224016000	1.395238000	0.001434000
6	-13.414958000	-0.703111000	0.001908000
6	-13.414958000	0.703111000	0.001907000
1	-12.221164000	2.482121000	0.001431000
1	-12.221164000	-2.482121000	0.001435000
6	6.096521000	0.710773000	-0.000157000
6	6.096521000	-0.710773000	-0.000157000
7	7.325336000	-1.359456000	0.000032000
7	7.325336000	1.359456000	0.000062000
6	8.551888000	-0.714646000	0.000293000
6	8.551888000	0.714646000	0.000293000
1	7.325026000	-2.366982000	0.000126000
1	7.325026000	2.366982000	0.000047000
6	4.900735000	1.393837000	-0.000349000
6	4.900735000	-1.393837000	-0.000345000
7	0.000000000	1.360069000	-0.001257000
7	0.000000000	-1.360069000	-0.001201000
6	-4.900735000	1.393837000	-0.000711000
6	-4.900735000	-1.393837000	-0.000716000
6	-9.745523000	1.395550000	0.000444000
6	-9.745523000	-1.395550000	0.000439000
6	9.745524000	1.395550000	0.000529000
6	9.745524000	-1.395550000	0.000536000
6	10.987459000	0.714849000	0.000779000
6	10.987459000	-0.714849000	0.000785000
6	12.224016000	1.395238000	0.001024000
6	12.224016000	-1.395238000	0.001036000
6	13.414958000	0.703111000	0.001266000
6	13.414958000	-0.703111000	0.001273000
1	12.221164000	2.482121000	0.001019000
1	14.356527000	1.242965000	0.001452000
1	14.356527000	-1.242965000	0.001463000
1	12.221164000	-2.482121000	0.001041000
1	9.738929000	-2.482812000	0.000535000
1	9.738929000	2.482812000	0.000533000
1	4.909386000	-2.481088000	-0.000339000
1	4.909386000	2.481088000	-0.000338000
1	0.000000000	-2.367420000	-0.001057000
1	0.000000000	2.367420000	-0.000994000
1	-4.909386000	2.481088000	-0.000694000

1	-4.909386000	-2.481088000	-0.000715000
1	-9.738929000	-2.482812000	0.000435000
1	-9.738929000	2.482812000	0.000456000
1	-14.356526000	1.242965000	0.002284000
1	-14.356526000	-1.242965000	0.002287000

Table S20: Coordinates of pN₄ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-4.890272000	0.711928000	-0.000001000
7	-3.663048000	1.360115000	0.000022000
6	-2.435109000	0.711366000	-0.000006000
6	-2.435109000	-0.711366000	-0.000012000
7	-3.663048000	-1.360115000	-0.000034000
6	-4.890272000	-0.711928000	-0.000005000
6	0.000000000	-0.713988000	-0.000067000
6	0.000000000	0.713988000	-0.000071000
6	1.238731000	1.393639000	-0.000140000
1	1.247135000	2.480950000	-0.000149000
6	2.435109000	0.711366000	-0.000233000
6	2.435109000	-0.711366000	-0.000228000
6	1.238731000	-1.393639000	-0.000131000
1	-3.662930000	2.367432000	-0.000047000
1	-3.662930000	-2.367432000	0.000072000
1	1.247135000	-2.480950000	-0.000130000
6	4.890272000	-0.711928000	-0.000254000
6	4.890272000	0.711928000	-0.000260000
6	6.086606000	1.393862000	-0.000193000
6	6.086606000	-1.393862000	-0.000186000
6	7.325577000	-0.714044000	-0.000153000
6	7.325577000	0.714044000	-0.000156000
1	6.078393000	2.481130000	-0.000202000
1	6.078393000	-2.481130000	-0.000185000
6	-7.325577000	0.714044000	-0.000052000
6	-7.325577000	-0.714044000	-0.000045000
6	-8.563786000	-1.393756000	-0.000095000
6	-8.563786000	1.393756000	-0.000110000
6	-9.759622000	-0.710645000	-0.000180000
6	-9.759622000	0.710645000	-0.000189000
1	-8.572481000	2.481028000	-0.000118000
1	-8.572481000	-2.481028000	-0.000091000
6	9.759622000	0.710645000	-0.000163000
6	9.759622000	-0.710645000	-0.000166000
7	10.988617000	-1.359457000	-0.000254000
7	10.988617000	1.359457000	-0.000217000
6	12.215044000	-0.714699000	-0.000021000
6	12.215044000	0.714699000	-0.000019000

1	10.988259000	-2.366971000	-0.000083000
1	10.988259000	2.366971000	-0.000157000
6	8.563786000	1.393756000	-0.000143000
6	8.563786000	-1.393756000	-0.000145000
7	3.663048000	1.360115000	-0.000389000
7	3.663048000	-1.360115000	-0.000366000
6	-1.238731000	1.393639000	-0.000027000
6	-1.238731000	-1.393639000	-0.000030000
6	-6.086606000	1.393862000	-0.000017000
6	-6.086606000	-1.393862000	-0.000015000
7	-10.988617000	1.359457000	-0.000339000
7	-10.988617000	-1.359457000	-0.000318000
6	-12.215044000	0.714699000	-0.000097000
6	-12.215044000	-0.714699000	-0.000086000
6	-13.408780000	1.395530000	0.000073000
6	-13.408780000	-1.395530000	0.000096000
6	-14.650742000	0.714855000	0.000236000
6	-14.650742000	-0.714855000	0.000249000
6	13.408780000	1.395530000	0.000145000
6	13.408780000	-1.395530000	0.000146000
6	14.650742000	0.714855000	0.000296000
6	14.650742000	-0.714855000	0.000300000
6	15.887309000	1.395200000	0.000443000
6	15.887309000	-1.395200000	0.000450000
6	17.078313000	0.703098000	0.000584000
6	17.078313000	-0.703098000	0.000588000
1	15.884436000	2.482094000	0.000439000
1	18.019881000	1.242970000	0.000695000
1	18.019881000	-1.242970000	0.000702000
1	15.884436000	-2.482094000	0.000452000
1	13.402191000	-2.482799000	0.000142000
1	13.402191000	2.482799000	0.000150000
1	8.572481000	-2.481028000	-0.000154000
1	8.572481000	2.481028000	-0.000141000
1	3.662930000	-2.367432000	-0.000260000
1	3.662930000	2.367432000	-0.000246000
1	-1.247135000	2.480950000	-0.000024000
1	-1.247135000	-2.480950000	-0.000043000
1	-6.078393000	-2.481130000	-0.000026000
1	-6.078393000	2.481130000	-0.000015000
1	-10.988259000	-2.366971000	-0.000168000
1	-10.988259000	2.366971000	-0.000197000
1	-13.402191000	-2.482799000	0.000106000
1	-13.402191000	2.482799000	0.000065000
6	-15.887309000	1.395200000	0.000385000
6	-15.887309000	-1.395200000	0.000410000
6	-17.078313000	0.703098000	0.000536000

6	-17.078313000	-0.703098000	0.000549000
1	-15.884436000	2.482094000	0.000374000
1	-15.884436000	-2.482094000	0.000419000
1	-18.019881000	-1.242970000	0.000673000
1	-18.019881000	1.242970000	0.000650000

Table S21: Coordinates of pN₅ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	8.553379000	-0.711814000	0.000461000
7	7.326270000	-1.359893000	0.000692000
6	6.098172000	-0.710959000	0.000632000
6	6.098214000	0.711516000	0.000547000
7	7.326371000	1.360362000	0.000494000
6	8.553441000	0.712185000	0.000375000
6	3.663064000	0.714327000	0.000615000
6	3.663038000	-0.713629000	0.000688000
6	2.424185000	-1.393237000	0.000777000
1	2.415815000	-2.480562000	0.000831000
6	1.227639000	-0.711161000	0.000833000
6	1.227649000	0.711917000	0.000766000
6	2.424218000	1.393964000	0.000640000
1	7.326062000	-2.367200000	0.000613000
1	7.326243000	2.367668000	0.000418000
1	2.415876000	2.481291000	0.000581000
6	-1.227647000	0.711917000	0.000693000
6	-1.227636000	-0.711162000	0.000746000
6	-2.424183000	-1.393236000	0.000599000
6	-2.424216000	1.393964000	0.000515000
6	-3.663062000	0.714328000	0.000418000
6	-3.663035000	-0.713628000	0.000450000
1	-2.415814000	-2.480562000	0.000639000
1	-2.415872000	2.481291000	0.000480000
6	10.988798000	-0.713981000	0.000142000
6	10.988871000	0.714110000	0.000062000
6	12.227128000	1.393712000	-0.000138000
6	12.226963000	-1.393737000	0.000021000
6	13.422940000	0.710504000	-0.000261000
6	13.422855000	-0.710678000	-0.000179000
1	12.235601000	-2.481017000	0.000082000
1	12.235912000	2.480992000	-0.000209000
6	-6.098169000	-0.710957000	0.000281000
6	-6.098212000	0.711517000	0.000272000
7	-7.326369000	1.360364000	0.000262000
7	-7.326268000	-1.359892000	0.000252000
6	-8.553438000	0.712187000	0.000078000
6	-8.553376000	-0.711813000	0.000054000

1	-7.326239000	2.367671000	0.000156000
1	-7.326058000	-2.367199000	0.000087000
6	-4.901737000	-1.393242000	0.000362000
6	-4.901812000	1.393872000	0.000318000
7	0.000001000	-1.359791000	0.001016000
7	0.000001000	1.360552000	0.000880000
6	4.901739000	-1.393244000	0.000687000
6	4.901814000	1.393870000	0.000531000
6	9.749757000	-1.393726000	0.000339000
6	9.749891000	1.393978000	0.000180000
7	14.651888000	-1.359623000	-0.000314000
7	14.652065000	1.359289000	-0.000503000
6	15.878296000	-0.714974000	-0.000460000
6	15.878393000	0.714474000	-0.000534000
6	17.072028000	-1.395861000	-0.000540000
6	17.072228000	1.395183000	-0.000665000
6	18.314051000	-0.715290000	-0.000692000
6	18.314152000	0.714427000	-0.000750000
6	-9.749756000	-1.393722000	-0.000119000
6	-9.749888000	1.393980000	-0.000043000
6	-10.988796000	-0.713976000	-0.000242000
6	-10.988868000	0.714113000	-0.000186000
6	-12.226958000	-1.393737000	-0.000396000
6	-12.227128000	1.393712000	-0.000267000
6	-13.422855000	-0.710685000	-0.000427000
6	-13.422934000	0.710499000	-0.000342000
1	-12.235587000	-2.481018000	-0.000467000
1	-12.235922000	2.480992000	-0.000226000
1	-9.741748000	2.481256000	-0.000014000
1	-9.741501000	-2.480996000	-0.000140000
1	-4.910294000	2.481203000	0.000308000
1	-4.910152000	-2.480574000	0.000386000
1	0.000002000	2.367835000	0.000764000
1	0.000002000	-2.367074000	0.000884000
1	4.910153000	-2.480575000	0.000750000
1	4.910298000	2.481202000	0.000464000
1	9.741751000	2.481253000	0.000106000
1	9.741500000	-2.481000000	0.000400000
1	14.651754000	2.366799000	-0.000484000
1	14.651437000	-2.367133000	-0.000294000
1	17.065726000	2.482456000	-0.000721000
1	17.065352000	-2.483132000	-0.000487000
6	19.550570000	-1.395713000	-0.000784000
6	19.550783000	1.394653000	-0.000895000
6	20.741657000	-0.703719000	-0.000925000
6	20.741763000	0.702467000	-0.000981000
1	19.547587000	-2.482612000	-0.000741000

1	19.547989000	2.481552000	-0.000938000
1	21.683368000	1.242283000	-0.001089000
1	21.683179000	-1.243679000	-0.000995000
7	-14.652065000	1.359284000	-0.000367000
7	-14.651884000	-1.359624000	-0.000551000
6	-15.878388000	0.714473000	-0.000450000
6	-15.878293000	-0.714970000	-0.000582000
6	-17.072234000	1.395178000	-0.000368000
6	-17.072025000	-1.395853000	-0.000741000
6	-18.314159000	0.714436000	-0.000439000
6	-18.314050000	-0.715295000	-0.000701000
1	-17.065711000	2.482451000	-0.000194000
1	-17.065361000	-2.483124000	-0.000862000
1	-14.651753000	2.366794000	0.000109000
1	-14.651441000	-2.367134000	-0.000089000
6	-20.741790000	0.702457000	-0.000251000
6	-20.741674000	-0.703726000	-0.000523000
6	-19.550574000	-1.395694000	-0.000833000
6	-19.550804000	1.394647000	-0.000255000
1	-19.547600000	-2.482592000	-0.001275000
1	-19.547962000	2.481543000	-0.000038000
1	-21.683175000	-1.243722000	-0.000540000
1	-21.683387000	1.242288000	0.000029000

Table S22: Coordinates of pN₆ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	4.890819000	-0.711624000	-0.000034000
7	3.663299000	-1.360183000	0.000109000
6	2.435452000	-0.711421000	0.000080000
6	2.435452000	0.711422000	0.000080000
7	3.663299000	1.360185000	0.000113000
6	4.890819000	0.711626000	-0.000030000
6	0.000000000	0.713968000	0.000055000
6	0.000000000	-0.713966000	0.000057000
6	-1.238854000	-1.393515000	0.000044000
1	-1.247274000	-2.480864000	0.000046000
6	-2.435452000	-0.711421000	0.000031000
6	-2.435452000	0.711422000	0.000028000
6	-1.238854000	1.393517000	0.000040000
1	3.663248000	-2.367465000	0.000050000
1	3.663248000	2.367466000	0.000056000
1	-1.247274000	2.480866000	0.000038000
6	-4.890819000	0.711626000	-0.000018000
6	-4.890819000	-0.711624000	-0.000012000
6	-6.087459000	-1.393586000	-0.000039000
6	-6.087459000	1.393588000	-0.000052000

6	-7.326360000	0.713978000	-0.000081000
6	-7.326360000	-0.713977000	-0.000073000
1	-6.079104000	-2.480920000	-0.000033000
1	-6.079104000	2.480921000	-0.000058000
6	7.326360000	-0.713977000	-0.000308000
6	7.326360000	0.713978000	-0.000303000
6	8.565097000	1.393523000	-0.000465000
6	8.565097000	-1.393522000	-0.000477000
6	9.761529000	0.711193000	-0.000672000
6	9.761529000	-0.711192000	-0.000679000
1	8.573582000	-2.480864000	-0.000481000
1	8.573582000	2.480865000	-0.000460000
6	-9.761529000	-0.711193000	-0.000133000
6	-9.761529000	0.711193000	-0.000142000
7	-10.989760000	1.360130000	-0.000196000
7	-10.989759000	-1.360130000	-0.000176000
6	-12.216795000	0.712045000	-0.000078000
6	-12.216795000	-0.712045000	-0.000066000
1	-10.989567000	2.367441000	-0.000146000
1	-10.989567000	-2.367440000	-0.000111000
6	-8.565097000	-1.393522000	-0.000096000
6	-8.565097000	1.393523000	-0.000114000
7	-3.663299000	-1.360183000	0.000024000
7	-3.663299000	1.360185000	0.000016000
6	1.238854000	-1.393515000	0.000066000
6	1.238854000	1.393517000	0.000065000
6	6.087459000	-1.393586000	-0.000165000
6	6.087460000	1.393588000	-0.000156000
7	10.989759000	-1.360130000	-0.000982000
7	10.989760000	1.360131000	-0.000969000
6	12.216795000	-0.712045000	-0.000637000
6	12.216795000	0.712045000	-0.000628000
6	13.413254000	-1.393846000	-0.000398000
6	13.413255000	1.393846000	-0.000377000
6	14.652290000	-0.714047000	-0.000189000
6	14.652290000	0.714047000	-0.000177000
6	-13.413254000	-1.393846000	0.000040000
6	-13.413255000	1.393846000	0.000014000
6	-14.652290000	-0.714047000	0.000140000
6	-14.652290000	0.714047000	0.000126000
6	-15.890514000	-1.393707000	0.000263000
6	-15.890514000	1.393706000	0.000237000
6	-17.086378000	-0.710578000	0.000398000
6	-17.086378000	0.710577000	0.000385000
1	-15.899248000	-2.480994000	0.000271000
1	-15.899249000	2.480993000	0.000229000
1	-13.405043000	2.481125000	0.000008000

1	-13.405042000	-2.481125000	0.000053000
1	-8.573582000	2.480865000	-0.000119000
1	-8.573582000	-2.480864000	-0.000088000
1	-3.663248000	2.367466000	0.000004000
1	-3.663248000	-2.367465000	0.000020000
1	1.247274000	-2.480864000	0.000064000
1	1.247274000	2.480866000	0.000063000
1	6.079104000	2.480921000	-0.000158000
1	6.079104000	-2.480920000	-0.000174000
1	10.989567000	2.367441000	-0.000712000
1	10.989567000	-2.367440000	-0.000743000
1	13.405043000	2.481125000	-0.000369000
1	13.405042000	-2.481125000	-0.000405000
6	15.890514000	-1.393707000	-0.000011000
6	15.890514000	1.393706000	0.000013000
6	17.086377000	-0.710578000	0.000158000
6	17.086378000	0.710577000	0.000171000
1	15.899248000	-2.480994000	-0.000025000
1	15.899249000	2.480993000	0.000018000
7	-18.315510000	1.359457000	0.000597000
7	-18.315510000	-1.359458000	0.000607000
6	-19.541856000	0.714745000	0.000328000
6	-19.541855000	-0.714746000	0.000343000
6	-20.735671000	1.395524000	0.000122000
6	-20.735671000	-1.395526000	0.000157000
6	-21.977641000	0.714857000	-0.000045000
6	-21.977641000	-0.714859000	-0.000024000
1	-20.729040000	2.482800000	0.000108000
1	-20.729039000	-2.482802000	0.000166000
1	-18.315117000	2.366973000	0.000392000
1	-18.315116000	-2.366974000	0.000464000
7	18.315510000	1.359457000	0.000353000
7	18.315510000	-1.359458000	0.000326000
6	19.541856000	0.714745000	0.000379000
6	19.541855000	-0.714746000	0.000364000
6	20.735671000	1.395524000	0.000429000
6	20.735671000	-1.395526000	0.000399000
6	21.977641000	0.714857000	0.000470000
6	21.977641000	-0.714859000	0.000453000
6	23.214243000	1.395171000	0.000521000
6	23.214243000	-1.395174000	0.000488000
6	24.405280000	0.703101000	0.000553000
6	24.405280000	-0.703104000	0.000536000
1	18.315117000	2.366973000	0.000315000
1	18.315116000	-2.366974000	0.000271000
1	20.729039000	-2.482802000	0.000384000
1	20.729040000	2.482800000	0.000439000

1	23.211297000	2.482075000	0.000533000
1	23.211296000	-2.482078000	0.000474000
1	25.346867000	-1.242957000	0.000562000
1	25.346868000	1.242953000	0.000592000
6	-23.214243000	-1.395174000	-0.000188000
6	-23.214243000	1.395171000	-0.000230000
6	-24.405280000	-0.703104000	-0.000362000
6	-24.405280000	0.703101000	-0.000384000
1	-23.211296000	-2.482078000	-0.000171000
1	-23.211297000	2.482076000	-0.000244000
1	-25.346867000	-1.242956000	-0.000488000
1	-25.346868000	1.242953000	-0.000526000

Table S23: Coordinates of pA₁ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-7.354012000	-1.400133000	-0.000091000
6	-6.106136000	-0.719813000	-0.000065000
6	-4.882206000	-1.398647000	-0.000166000
6	-6.106136000	0.719813000	0.000066000
6	-4.882206000	1.398647000	0.000087000
6	-3.664110000	0.721406000	-0.000017000
6	-3.664110000	-0.721406000	-0.000148000
6	-8.535333000	-0.708658000	0.000006000
6	-7.354012000	1.400133000	0.000166000
1	-4.883586000	2.486296000	0.000185000
6	-2.415841000	1.400205000	0.000009000
6	-2.415841000	-1.400205000	-0.000269000
6	-1.228015000	-0.717967000	-0.000266000
6	-1.228015000	0.717967000	-0.000108000
1	-2.408273000	2.487147000	0.000132000
1	-2.408273000	-2.487147000	-0.000391000
6	-8.535333000	0.708658000	0.000137000
1	-7.350087000	-2.486882000	-0.000191000
1	-4.883586000	-2.486296000	-0.000265000
1	-7.350087000	2.486882000	0.000265000
6	2.415832000	-1.400204000	-0.000205000
6	3.664119000	-0.721414000	-0.000050000
6	4.882194000	-1.398646000	-0.000034000
6	3.664119000	0.721414000	0.000081000
6	4.882194000	1.398646000	0.000219000
6	6.106148000	0.719809000	0.000231000
6	6.106148000	-0.719809000	0.000100000
6	1.228014000	-0.717975000	-0.000233000
6	2.415832000	1.400204000	0.000073000
1	4.883609000	2.486296000	0.000317000
6	7.354001000	1.400131000	0.000365000

6	7.354001000	-1.400131000	0.000108000
6	8.535340000	-0.708647000	0.000236000
6	8.535340000	0.708647000	0.000368000
1	7.350109000	2.486879000	0.000464000
1	7.350108000	-2.486880000	0.000008000
1	9.480140000	-1.242972000	0.000240000
1	9.480140000	1.242972000	0.000472000
6	1.228014000	0.717975000	-0.000076000
1	2.408278000	-2.487147000	-0.000328000
1	4.883609000	-2.486296000	-0.000134000
1	2.408278000	2.487147000	0.000196000
7	-0.000002000	1.356791000	-0.000069000
7	-0.000002000	-1.356791000	-0.000490000
1	-0.000004000	2.365209000	-0.000038000
1	-0.000004000	-2.365209000	-0.000365000
1	-9.480147000	-1.242952000	-0.000016000
1	-9.480147000	1.242952000	0.000215000

Table S24: Coordinates of pA₂ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	2.468239000	1.398803000	0.000368000
6	1.221560000	0.720246000	0.000223000
6	0.000000000	1.397728000	0.000109000
6	1.221560000	-0.720245000	0.000186000
6	0.000000000	-1.397727000	0.000052000
6	-1.221560000	-0.720246000	-0.000051000
6	-1.221560000	0.720246000	-0.000033000
6	3.657545000	0.716398000	0.000483000
6	2.468239000	-1.398804000	0.000296000
1	0.000000000	-2.485306000	0.000032000
6	-2.468239000	-1.398803000	-0.000154000
6	-2.468239000	1.398804000	-0.000188000
6	-3.657545000	0.716399000	-0.000330000
6	-3.657545000	-0.716398000	-0.000276000
1	-2.476044000	-2.485908000	-0.000111000
1	-2.476044000	2.485909000	-0.000233000
6	3.657545000	-0.716399000	0.000443000
1	2.476045000	2.485908000	0.000387000
1	0.000000000	2.485306000	0.000126000
1	2.476043000	-2.485909000	0.000276000
6	-7.302105000	1.400019000	-0.000274000
6	-8.550684000	0.721419000	-0.000140000
6	-9.768701000	1.398507000	-0.000067000
6	-8.550684000	-0.721419000	-0.000106000
6	-9.768701000	-1.398508000	0.000003000
6	-10.993009000	-0.719703000	0.000073000

6	-10.993009000	0.719702000	0.000033000
6	-6.113776000	0.718303000	-0.000366000
6	-7.302105000	-1.400019000	-0.000171000
1	-9.770180000	-2.486190000	0.000030000
6	-12.240799000	-1.399937000	0.000176000
6	-12.240799000	1.399936000	0.000092000
6	-13.422404000	0.708586000	0.000185000
6	-13.422403000	-0.708586000	0.000231000
1	-12.236733000	-2.486725000	0.000209000
1	-12.236733000	2.486724000	0.000058000
1	-14.367249000	1.242887000	0.000228000
1	-14.367249000	-1.242888000	0.000312000
6	-6.113776000	-0.718304000	-0.000293000
1	-7.294851000	2.487001000	-0.000347000
1	-9.770180000	2.486190000	-0.000098000
1	-7.294852000	-2.487001000	-0.000105000
7	-4.886366000	-1.356917000	-0.000317000
7	-4.886367000	1.356917000	-0.000682000
1	-4.886112000	-2.365192000	-0.000380000
1	-4.886113000	2.365192000	-0.000213000
6	12.240799000	1.399937000	-0.000256000
6	10.993009000	0.719702000	-0.000164000
6	9.768701000	1.398507000	0.000030000
6	10.993010000	-0.719703000	-0.000273000
6	9.768701000	-1.398508000	-0.000170000
6	8.550684000	-0.721419000	0.000037000
6	8.550684000	0.721418000	0.000133000
6	13.422403000	0.708586000	-0.000443000
6	12.240799000	-1.399937000	-0.000474000
1	9.770180000	-2.486190000	-0.000244000
6	7.302104000	-1.400019000	0.000173000
6	7.302105000	1.400019000	0.000327000
6	6.113776000	0.718304000	0.000452000
6	6.113777000	-0.718303000	0.000389000
1	7.294851000	-2.487001000	0.000126000
1	7.294853000	2.487001000	0.000376000
6	13.422403000	-0.708586000	-0.000557000
1	12.236732000	2.486724000	-0.000170000
1	9.770180000	2.486190000	0.000108000
1	14.367249000	1.242888000	-0.000510000
1	12.236733000	-2.486724000	-0.000558000
1	14.367249000	-1.242887000	-0.000712000
7	4.886367000	-1.356917000	0.000653000
7	4.886366000	1.356917000	0.000678000
1	4.886113000	-2.365192000	0.000266000
1	4.886112000	2.365192000	0.000568000

Table S25: Coordinates of pA₃ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-2.417809000	1.398737000	-0.000106000
6	-3.664767000	0.720348000	-0.000089000
6	-4.886212000	1.397539000	-0.000089000
6	-3.664767000	-0.720348000	-0.000076000
6	-4.886212000	-1.397539000	-0.000063000
6	-6.108139000	-0.720219000	-0.000072000
6	-6.108139000	0.720219000	-0.000085000
6	-1.228081000	0.716729000	-0.000125000
6	-2.417809000	-1.398737000	-0.000086000
1	-4.886259000	-2.485241000	-0.000055000
6	-7.354745000	-1.398710000	-0.000076000
6	-7.354745000	1.398710000	-0.000101000
6	-8.544089000	0.716115000	-0.000118000
6	-8.544089000	-0.716115000	-0.000105000
1	-7.363064000	-2.485856000	-0.000067000
1	-7.363064000	2.485856000	-0.000111000
6	-1.228081000	-0.716729000	-0.000117000
1	-2.409676000	2.485885000	-0.000112000
1	-4.886259000	2.485241000	-0.000100000
1	-2.409676000	-2.485885000	-0.000081000
6	-12.188655000	1.400013000	-0.000007000
6	-13.437367000	0.721496000	0.000063000
6	-14.655313000	1.398432000	0.000115000
6	-13.437367000	-0.721496000	0.000079000
6	-14.655313000	-1.398432000	0.000147000
6	-15.879897000	-0.719844000	0.000196000
6	-15.879897000	0.719844000	0.000179000
6	-11.000210000	0.718355000	-0.000070000
6	-12.188655000	-1.400013000	0.000022000
1	-14.656616000	-2.486185000	0.000159000
6	-17.127520000	-1.399826000	0.000258000
6	-17.127520000	1.399826000	0.000225000
6	-18.309503000	0.708384000	0.000283000
6	-18.309503000	-0.708384000	0.000300000
1	-17.124393000	-2.486639000	0.000271000
1	-17.124393000	2.486639000	0.000212000
1	-19.253778000	1.243735000	0.000318000
1	-19.253778000	-1.243734000	0.000348000
6	-11.000210000	-0.718355000	-0.000056000
1	-12.181004000	2.487001000	-0.000017000
1	-14.656616000	2.486185000	0.000102000
1	-12.181004000	-2.487001000	0.000033000
7	-9.773104000	-1.357551000	-0.000150000
7	-9.773104000	1.357551000	-0.000170000
1	-9.772768000	-2.365762000	-0.000089000

1	-9.772768000	2.365762000	-0.000140000
6	7.354745000	1.398710000	0.000002000
6	6.108139000	0.720219000	-0.000007000
6	4.886212000	1.397539000	-0.000033000
6	6.108139000	-0.720219000	0.000007000
6	4.886212000	-1.397539000	-0.000006000
6	3.664767000	-0.720348000	-0.000037000
6	3.664767000	0.720348000	-0.000050000
6	8.544089000	0.716115000	0.000023000
6	7.354745000	-1.398710000	0.000031000
1	4.886259000	-2.485241000	0.000004000
6	2.417809000	-1.398737000	-0.000062000
6	2.417809000	1.398737000	-0.000083000
6	1.228081000	0.716729000	-0.000113000
6	1.228081000	-0.716729000	-0.000105000
1	2.409676000	-2.485885000	-0.000057000
1	2.409676000	2.485885000	-0.000088000
6	8.544089000	-0.716115000	0.000038000
1	7.363064000	2.485856000	-0.000010000
1	4.886259000	2.485241000	-0.000044000
1	7.363064000	-2.485856000	0.000041000
7	0.000000000	-1.357747000	-0.000167000
7	0.000000000	1.357747000	-0.000162000
1	0.000000000	-2.365863000	-0.000100000
1	0.000000000	2.365863000	-0.000163000
6	17.127520000	1.399826000	0.000015000
6	15.879897000	0.719844000	0.000027000
6	14.655313000	1.398432000	0.000020000
6	15.879897000	-0.719844000	0.000045000
6	14.655313000	-1.398432000	0.000055000
6	13.437367000	-0.721496000	0.000048000
6	13.437367000	0.721496000	0.000031000
6	18.309503000	0.708384000	0.000022000
6	17.127520000	-1.399826000	0.000052000
1	14.656616000	-2.486185000	0.000069000
6	12.188655000	-1.400013000	0.000057000
6	12.188655000	1.400013000	0.000024000
6	11.000210000	0.718355000	0.000034000
6	11.000210000	-0.718355000	0.000050000
1	12.181004000	-2.487001000	0.000070000
1	12.181004000	2.487001000	0.000012000
6	18.309503000	-0.708384000	0.000040000
1	17.124393000	2.486639000	0.000001000
1	14.656616000	2.486185000	0.000007000
1	19.253778000	1.243735000	0.000013000
1	17.124393000	-2.486639000	0.000066000
1	19.253778000	-1.243734000	0.000046000

7	9.773104000	-1.357551000	0.000059000
7	9.773104000	1.357551000	0.000030000
1	9.772768000	-2.365762000	0.000066000
1	9.772768000	2.365762000	0.000016000

Table S26: Coordinates of pA₄ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	2.468721000	1.398552000	-0.000009000
6	1.221802000	0.720229000	-0.000046000
6	0.000000000	1.397379000	-0.000090000
6	1.221802000	-0.720262000	-0.000038000
6	0.000000000	-1.397411000	-0.000046000
6	-1.221803000	-0.720262000	-0.000078000
6	-1.221802000	0.720229000	-0.000114000
6	3.658510000	0.716492000	0.000019000
6	2.468723000	-1.398583000	-0.000026000
1	0.000000000	-2.485153000	-0.000030000
6	-2.468723000	-1.398583000	-0.000078000
6	-2.468722000	1.398552000	-0.000175000
6	-3.658510000	0.716492000	-0.000194000
6	-3.658511000	-0.716522000	-0.000132000
1	-2.476922000	-2.485767000	-0.000037000
1	-2.476920000	2.485736000	-0.000216000
6	3.658511000	-0.716522000	-0.000009000
1	2.476920000	2.485736000	0.000002000
1	0.000000000	2.485120000	-0.000107000
1	2.476922000	-2.485767000	-0.000038000
6	-7.304662000	1.398697000	-0.000221000
6	-8.551676000	0.720356000	-0.000141000
6	-9.773109000	1.397491000	-0.000171000
6	-8.551679000	-0.720375000	-0.000024000
6	-9.773113000	-1.397506000	0.000076000
6	-10.995130000	-0.720200000	0.000060000
6	-10.995128000	0.720190000	-0.000083000
6	-6.114789000	0.716827000	-0.000205000
6	-7.304666000	-1.398719000	-0.000016000
1	-9.773172000	-2.485221000	0.000172000
6	-12.241741000	-1.398660000	0.000180000
6	-12.241735000	1.398655000	-0.000130000
6	-13.431090000	0.716049000	-0.000034000
6	-13.431093000	-0.716048000	0.000163000
1	-12.250090000	-2.485820000	0.000304000
1	-12.250079000	2.485815000	-0.000255000
6	-6.114791000	-0.716852000	-0.000113000
1	-7.296552000	2.485852000	-0.000299000
1	-9.773164000	2.485206000	-0.000267000

1	-7.296558000	-2.485874000	0.000063000
7	-4.886926000	-1.357767000	-0.000140000
7	-4.886924000	1.357739000	-0.000293000
1	-4.886857000	-2.365865000	-0.000086000
1	-4.886852000	2.365837000	-0.000283000
6	12.241735000	1.398656000	0.000182000
6	10.995127000	0.720190000	0.000097000
6	9.773108000	1.397491000	0.000149000
6	10.995130000	-0.720201000	-0.000048000
6	9.773113000	-1.397506000	-0.000100000
6	8.551678000	-0.720375000	-0.000031000
6	8.551676000	0.720356000	0.000080000
6	13.431088000	0.716048000	0.000113000
6	12.241741000	-1.398661000	-0.000133000
1	9.773172000	-2.485221000	-0.000195000
6	7.304666000	-1.398719000	-0.000066000
6	7.304662000	1.398697000	0.000114000
6	6.114789000	0.716827000	0.000061000
6	6.114790000	-0.716853000	-0.000010000
1	7.296558000	-2.485875000	-0.000136000
1	7.296551000	2.485852000	0.000184000
6	13.431091000	-0.716048000	-0.000065000
1	12.250079000	2.485816000	0.000310000
1	9.773163000	2.485206000	0.000245000
1	12.250090000	-2.485821000	-0.000261000
7	4.886926000	-1.357767000	-0.000018000
7	4.886923000	1.357739000	0.000079000
1	4.886856000	-2.365865000	-0.000028000
1	4.886852000	2.365837000	0.000074000
6	22.014676000	1.399825000	0.000346000
6	20.767057000	0.719858000	0.000189000
6	19.542438000	1.398429000	0.000318000
6	20.767061000	-0.719819000	-0.000118000
6	19.542446000	-1.398397000	-0.000250000
6	18.324488000	-0.721493000	-0.000106000
6	18.324485000	0.721517000	0.000170000
6	23.196694000	0.708405000	0.000202000
6	22.014685000	-1.399779000	-0.000271000
1	19.543758000	-2.486155000	-0.000468000
6	17.075768000	-1.399991000	-0.000219000
6	17.075761000	1.400009000	0.000278000
6	15.887253000	0.718398000	0.000140000
6	15.887256000	-0.718387000	-0.000087000
1	17.068122000	-2.486983000	-0.000412000
1	17.068108000	2.487001000	0.000472000
6	23.196698000	-0.708351000	-0.000123000
1	22.011528000	2.486644000	0.000586000

1	19.543743000	2.486187000	0.000536000
1	24.140968000	1.243766000	0.000330000
1	22.011543000	-2.486597000	-0.000512000
1	24.140975000	-1.243706000	-0.000248000
7	14.660235000	-1.357537000	-0.000163000
7	14.660228000	1.357543000	0.000212000
6	-17.075761000	1.400007000	-0.000134000
6	-18.324484000	0.721517000	-0.000044000
6	-19.542438000	1.398429000	-0.000163000
6	-18.324488000	-0.721492000	0.000183000
6	-19.542446000	-1.398397000	0.000291000
6	-20.767060000	-0.719820000	0.000182000
6	-20.767056000	0.719858000	-0.000062000
6	-15.887251000	0.718399000	-0.000024000
6	-17.075768000	-1.399989000	0.000287000
1	-19.543757000	-2.486155000	0.000465000
6	-22.014684000	-1.399779000	0.000304000
6	-22.014676000	1.399825000	-0.000189000
6	-23.196693000	0.708405000	-0.000074000
6	-23.196697000	-0.708351000	0.000185000
1	-22.011542000	-2.486598000	0.000495000
1	-22.011527000	2.486644000	-0.000380000
1	-24.140967000	1.243765000	-0.000179000
1	-24.140975000	-1.243706000	0.000286000
6	-15.887254000	-0.718387000	0.000203000
1	-17.068109000	2.487000000	-0.000298000
1	-19.543743000	2.486187000	-0.000337000
1	-17.068121000	-2.486982000	0.000451000
7	-14.660235000	-1.357539000	0.000346000
7	-14.660228000	1.357545000	-0.000113000
1	14.659874000	-2.365744000	-0.000220000
1	14.659863000	2.365749000	0.000270000
1	-14.659874000	-2.365745000	0.000568000
1	-14.659863000	2.365751000	-0.000381000

Table S27: Coordinates of pA₅ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-2.418114000	1.398378000	-0.000602000
6	-3.665093000	0.720102000	-0.000529000
6	-4.886870000	1.397214000	-0.001060000
6	-3.665100000	-0.720417000	0.000136000
6	-4.886889000	-1.397512000	0.000601000
6	-6.108772000	-0.720359000	0.000258000
6	-6.108760000	0.720078000	-0.000786000
6	-1.228190000	0.716451000	-0.000244000
6	-2.418123000	-1.398701000	0.000274000

1	-4.886909000	-2.485263000	0.001241000
6	-7.355706000	-1.398646000	0.000903000
6	-7.355678000	1.398390000	-0.001504000
6	-8.545470000	0.716318000	-0.001068000
6	-8.545485000	-0.716550000	0.000380000
1	-7.363930000	-2.485842000	0.001876000
1	-7.363880000	2.485586000	-0.002473000
6	-1.228193000	-0.716781000	-0.000022000
1	-2.409947000	2.485570000	-0.000904000
1	-4.886875000	2.484965000	-0.001699000
1	-2.409963000	-2.485893000	0.000577000
6	-12.191699000	1.398631000	-0.002304000
6	-13.438738000	0.720324000	-0.001314000
6	-14.660153000	1.397462000	-0.002499000
6	-13.438762000	-0.720419000	0.001041000
6	-14.660202000	-1.397513000	0.002400000
6	-15.882239000	-0.720188000	0.001384000
6	-15.882213000	0.720181000	-0.001301000
6	-11.001780000	0.716796000	-0.001267000
6	-12.191740000	-1.398764000	0.001867000
1	-14.660282000	-2.485230000	0.004287000
6	-17.128864000	-1.398617000	0.002889000
6	-17.128809000	1.398661000	-0.002609000
6	-18.318173000	0.716064000	-0.001238000
6	-18.318202000	-0.715972000	0.001742000
1	-17.137228000	-2.485780000	0.005055000
1	-17.137127000	2.485823000	-0.004776000
6	-11.001799000	-0.716966000	0.000660000
1	-12.183591000	2.485787000	-0.003890000
1	-14.660193000	2.485178000	-0.004383000
1	-12.183667000	-2.485921000	0.003458000
7	-9.774037000	-1.357862000	0.001177000
7	-9.774003000	1.357661000	-0.001994000
1	-9.773953000	-2.365951000	0.002261000
1	-9.773893000	2.365750000	-0.002980000
6	7.355677000	1.398385000	0.001312000
6	6.108759000	0.720074000	0.000582000
6	4.886869000	1.397210000	0.000890000
6	6.108770000	-0.720363000	-0.000515000
6	4.886887000	-1.397515000	-0.000882000
6	3.665098000	-0.720419000	-0.000387000
6	3.665092000	0.720100000	0.000339000
6	8.545468000	0.716313000	0.000841000
6	7.355704000	-1.398650000	-0.001183000
1	4.886906000	-2.485267000	-0.001564000
6	2.418120000	-1.398703000	-0.000550000
6	2.418113000	1.398377000	0.000448000

6	1.228189000	0.716450000	0.000067000
6	1.228191000	-0.716782000	-0.000219000
1	2.409960000	-2.485894000	-0.000903000
1	2.409947000	2.485568000	0.000800000
6	8.545484000	-0.716555000	-0.000643000
1	7.363879000	2.485581000	0.002312000
1	4.886875000	2.484962000	0.001572000
1	7.363928000	-2.485846000	-0.002185000
7	-0.000001000	-1.357946000	-0.000134000
7	0.000000000	1.357613000	-0.000066000
1	-0.000002000	-2.366021000	-0.000142000
1	0.000000000	2.365688000	-0.000063000
6	17.128808000	1.398656000	0.002790000
6	15.882212000	0.720176000	0.001404000
6	14.660151000	1.397456000	0.002529000
6	15.882239000	-0.720193000	-0.001282000
6	14.660201000	-1.397518000	-0.002385000
6	13.438761000	-0.720424000	-0.001100000
6	13.438737000	0.720318000	0.001269000
6	18.318171000	0.716060000	0.001523000
6	17.128865000	-1.398621000	-0.002689000
1	14.660282000	-2.485235000	-0.004275000
6	12.191739000	-1.398770000	-0.002005000
6	12.191697000	1.398625000	0.002201000
6	11.001778000	0.716790000	0.001090000
6	11.001798000	-0.716971000	-0.000859000
1	12.183666000	-2.485926000	-0.003606000
1	12.183590000	2.485782000	0.003800000
6	18.318201000	-0.715976000	-0.001443000
1	17.137129000	2.485819000	0.004940000
1	14.660191000	2.485173000	0.004420000
1	17.137232000	-2.485784000	-0.004839000
7	9.774035000	-1.357867000	-0.001456000
7	9.774002000	1.357655000	0.001744000
6	-21.962868000	1.400115000	-0.003240000
6	-23.211612000	0.721660000	-0.001700000
6	-24.429549000	1.398586000	-0.003645000
6	-23.211645000	-0.721352000	0.002060000
6	-24.429615000	-1.398219000	0.003909000
6	-25.654233000	-0.719621000	0.002093000
6	-25.654199000	0.720047000	-0.001915000
6	-20.774346000	0.718504000	-0.001388000
6	-21.962931000	-1.399864000	0.003704000
1	-24.430959000	-2.485975000	0.006814000
6	-26.901866000	-1.399541000	0.004027000
6	-26.901797000	1.400029000	-0.003930000
6	-28.083850000	0.708643000	-0.002051000

6	-28.083884000	-0.708095000	0.002076000
1	-26.898756000	-2.486358000	0.007118000
1	-26.898630000	2.486845000	-0.007021000
1	-29.028104000	1.244039000	-0.003667000
1	-29.028165000	-1.243446000	0.003632000
6	-20.774377000	-0.718308000	0.001988000
1	-21.955209000	2.487105000	-0.005913000
1	-24.430838000	2.486342000	-0.006548000
1	-21.955323000	-2.486855000	0.006374000
7	-19.547408000	-1.357466000	0.003362000
7	-19.547351000	1.357611000	-0.002544000
1	9.773951000	-2.365956000	-0.002563000
1	9.773892000	2.365745000	0.002810000
1	-19.547054000	-2.365666000	0.005237000
1	-19.546954000	2.365810000	-0.004564000
6	26.901798000	1.400036000	0.003938000
6	25.654201000	0.720053000	0.002003000
6	24.429549000	1.398590000	0.003744000
6	25.654237000	-0.719616000	-0.001927000
6	24.429620000	-1.398216000	-0.003670000
6	23.211648000	-0.721351000	-0.001812000
6	23.211613000	0.721662000	0.001884000
6	28.083852000	0.708653000	0.002060000
6	26.901871000	-1.399533000	-0.003860000
1	24.430965000	-2.485972000	-0.006521000
6	21.962934000	-1.399864000	-0.003382000
6	21.962867000	1.400115000	0.003451000
6	20.774348000	0.718502000	0.001700000
6	20.774381000	-0.718309000	-0.001637000
1	21.955325000	-2.486855000	-0.006003000
1	21.955204000	2.487105000	0.006073000
6	28.083889000	-0.708086000	-0.001981000
1	26.898629000	2.486853000	0.006967000
1	24.430837000	2.486345000	0.006595000
1	29.028105000	1.244051000	0.003612000
1	26.898763000	-2.486350000	-0.006889000
1	29.028171000	-1.243434000	-0.003532000
7	19.547410000	-1.357469000	-0.002902000
7	19.547350000	1.357608000	0.002955000
1	19.547058000	-2.365670000	-0.004911000
1	19.546953000	2.365808000	0.004973000

Table S28: Coordinates of pA₆ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-2.468852000	-1.398482000	0.000104000
6	-1.221868000	-0.720224000	0.000319000

6	0.000000000	-1.397316000	0.000515000
6	-1.221868000	0.720243000	0.000331000
6	0.000000000	1.397334000	0.000529000
6	1.221868000	0.720243000	0.000714000
6	1.221868000	-0.720224000	0.000712000
6	-3.658776000	-0.716534000	-0.000090000
6	-2.468852000	1.398500000	0.000139000
1	0.000000000	2.485099000	0.000535000
6	2.468852000	1.398500000	0.000899000
6	2.468852000	-1.398482000	0.000904000
6	3.658776000	-0.716534000	0.001082000
6	3.658776000	0.716552000	0.001074000
1	2.477043000	2.485704000	0.000895000
1	2.477042000	-2.485686000	0.000905000
6	-3.658776000	0.716552000	-0.000067000
1	-2.477042000	-2.485686000	0.000093000
1	0.000000000	-2.485080000	0.000510000
1	-2.477043000	2.485704000	0.000155000
6	7.305177000	-1.398521000	0.001502000
6	8.552174000	-0.720260000	0.001577000
6	9.773949000	-1.397342000	0.001655000
6	8.552174000	0.720274000	0.001541000
6	9.773951000	1.397355000	0.001575000
6	10.995869000	0.720216000	0.001630000
6	10.995868000	-0.720204000	0.001676000
6	6.115193000	-0.716649000	0.001386000
6	7.305178000	1.398537000	0.001446000
1	9.773965000	2.485112000	0.001532000
6	12.242797000	1.398506000	0.001612000
6	12.242795000	-1.398496000	0.001709000
6	13.432577000	-0.716399000	0.001677000
6	13.432578000	0.716408000	0.001623000
1	12.251025000	2.485707000	0.001561000
1	12.251022000	-2.485697000	0.001731000
6	6.115194000	0.716666000	0.001364000
1	7.297019000	-2.485715000	0.001511000
1	9.773962000	-2.485099000	0.001673000
1	7.297021000	2.485730000	0.001415000
7	4.887098000	1.357801000	0.001246000
7	4.887097000	-1.357784000	0.001267000
1	4.887072000	2.365868000	0.001206000
1	4.887071000	-2.365851000	0.001266000
6	-12.242795000	-1.398496000	-0.001053000
6	-10.995868000	-0.720204000	-0.000919000
6	-9.773949000	-1.397342000	-0.000829000
6	-10.995868000	0.720216000	-0.000860000
6	-9.773951000	1.397355000	-0.000723000
6	-8.552174000	0.720274000	-0.000639000

6	-8.552174000	-0.720260000	-0.000688000
6	-13.432577000	-0.716399000	-0.001121000
6	-12.242797000	1.398506000	-0.000928000
1	-9.773965000	2.485112000	-0.000672000
6	-7.305178000	1.398537000	-0.000495000
6	-7.305177000	-1.398521000	-0.000579000
6	-6.115193000	-0.716649000	-0.000435000
6	-6.115193000	0.716666000	-0.000398000
1	-7.297021000	2.485730000	-0.000455000
1	-7.297019000	-2.485715000	-0.000600000
6	-13.432578000	0.716408000	-0.001052000
1	-12.251022000	-2.485697000	-0.001091000
1	-9.773962000	-2.485099000	-0.000859000
1	-12.251025000	2.485707000	-0.000867000
7	-4.887098000	1.357801000	-0.000265000
7	-4.887097000	-1.357784000	-0.000316000
1	-4.887072000	2.365868000	-0.000209000
1	-4.887070000	-2.365851000	-0.000310000
6	-22.015999000	-1.398633000	-0.000929000
6	-20.769385000	-0.720185000	-0.000947000
6	-19.547323000	-1.397483000	-0.001047000
6	-20.769386000	0.720182000	-0.000847000
6	-19.547326000	1.397482000	-0.000860000
6	-18.325899000	0.720377000	-0.000968000
6	-18.325898000	-0.720375000	-0.001060000
6	-23.205349000	-0.716008000	-0.000825000
6	-22.016001000	1.398628000	-0.000728000
1	-19.547389000	2.485203000	-0.000779000
6	-17.078863000	1.398696000	-0.000983000
6	-17.078861000	-1.398693000	-0.001151000
6	-15.888905000	-0.716895000	-0.001164000
6	-15.888906000	0.716900000	-0.001083000
1	-17.070771000	2.485855000	-0.000909000
1	-17.070767000	-2.485851000	-0.001207000
6	-23.205351000	0.716000000	-0.000718000
1	-22.024353000	-2.485800000	-0.000996000
1	-19.547385000	-2.485204000	-0.001109000
1	-22.024358000	2.485794000	-0.000638000
7	-14.661178000	1.357772000	-0.001116000
7	-14.661176000	-1.357765000	-0.001259000
6	17.078861000	-1.398693000	0.001297000
6	18.325898000	-0.720376000	0.001012000
6	19.547324000	-1.397483000	0.000756000
6	18.325899000	0.720377000	0.000929000
6	19.547326000	1.397482000	0.000584000
6	20.769386000	0.720181000	0.000282000
6	20.769385000	-0.720185000	0.000376000

6	15.888905000	-0.716895000	0.001466000
6	17.078864000	1.398696000	0.001150000
1	19.547389000	2.485203000	0.000498000
6	22.016001000	1.398627000	-0.000168000
6	22.015998000	-1.398634000	0.000026000
6	23.205349000	-0.716008000	-0.000476000
6	23.205351000	0.716000000	-0.000583000
1	22.024358000	2.485794000	-0.000261000
1	22.024353000	-2.485800000	0.000092000
6	15.888906000	0.716900000	0.001398000
1	17.070767000	-2.485851000	0.001332000
1	19.547385000	-2.485204000	0.000803000
1	17.070771000	2.485855000	0.001077000
7	14.661179000	1.357772000	0.001568000
7	14.661177000	-1.357765000	0.001668000
1	-14.661070000	2.365859000	-0.001013000
1	-14.661067000	-2.365852000	-0.001250000
1	14.661070000	2.365859000	0.001461000
1	14.661067000	-2.365852000	0.001680000
6	-31.789029000	-1.399801000	0.000732000
6	-30.541408000	-0.719851000	0.000542000
6	-29.316772000	-1.398416000	0.000234000
6	-30.541410000	0.719826000	0.000673000
6	-29.316776000	1.398393000	0.000484000
6	-28.098814000	0.721500000	0.000170000
6	-28.098812000	-0.721520000	0.000044000
6	-32.971068000	-0.708388000	0.001038000
6	-31.789032000	1.399772000	0.000991000
1	-29.318081000	2.486154000	0.000580000
6	-26.850087000	1.399983000	-0.000037000
6	-26.850084000	-1.399999000	-0.000271000
6	-25.661533000	-0.718418000	-0.000480000
6	-25.661534000	0.718405000	-0.000364000
1	-26.842438000	2.486977000	0.000054000
1	-26.842433000	-2.486994000	-0.000361000
6	-32.971070000	0.708357000	0.001172000
1	-31.785885000	-2.486623000	0.000630000
1	-29.318075000	-2.486177000	0.000138000
1	-33.915337000	-1.243765000	0.001179000
1	-31.785891000	2.486595000	0.001092000
1	-33.915340000	1.243732000	0.001415000
7	-24.434570000	1.357543000	-0.000632000
7	-24.434567000	-1.357554000	-0.000841000
1	-24.434191000	2.365744000	-0.000476000
1	-24.434186000	-2.365755000	-0.000831000
6	26.850084000	-1.399999000	-0.000896000
6	28.098812000	-0.721519000	-0.001017000

6	29.316772000	-1.398415000	-0.001044000
6	28.098813000	0.721500000	-0.001137000
6	29.316775000	1.398393000	-0.001284000
6	30.541410000	0.719826000	-0.001334000
6	30.541408000	-0.719851000	-0.001207000
6	25.661532000	-0.718418000	-0.000953000
6	26.850087000	1.399982000	-0.001127000
1	29.318080000	2.486154000	-0.001385000
6	31.789032000	1.399773000	-0.001522000
6	31.789028000	-1.399800000	-0.001273000
6	32.971068000	-0.708387000	-0.001461000
6	32.971070000	0.708357000	-0.001590000
1	31.785891000	2.486595000	-0.001620000
1	31.785885000	-2.486623000	-0.001177000
1	33.915337000	-1.243765000	-0.001509000
1	33.915339000	1.243732000	-0.001736000
6	25.661534000	0.718405000	-0.001069000
1	26.842432000	-2.486994000	-0.000808000
1	29.318075000	-2.486176000	-0.000960000
1	26.842438000	2.486977000	-0.001222000
7	24.434567000	-1.357554000	-0.001033000
7	24.434570000	1.357542000	-0.001268000
1	24.434186000	-2.365755000	-0.000776000
1	24.434191000	2.365744000	-0.001086000

Table S29: Coordinates of pT₁ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-1.228020000	-0.719803000	-0.000153000
7	0.000000000	-1.356537000	-0.000229000
6	1.228020000	-0.719803000	-0.000153000
6	1.228020000	0.719803000	-0.000153000
7	0.000000000	1.356537000	-0.000229000
6	-1.228020000	0.719803000	-0.000153000
6	3.664925000	0.724488000	-0.000056000
6	3.664925000	-0.724488000	-0.000056000
6	4.875858000	-1.401438000	-0.000016000
1	4.876941000	-2.488933000	-0.000016000
6	6.109931000	-0.723984000	0.000021000
6	6.109931000	0.723984000	0.000021000
6	4.875858000	1.401438000	-0.000016000
1	0.000000000	-2.365176000	-0.000190000
1	0.000000000	2.365176000	-0.000190000
1	4.876941000	2.488933000	-0.000016000
6	8.553592000	0.722847000	0.000089000
6	8.553592000	-0.722847000	0.000089000
6	9.806789000	-1.402546000	0.000121000

6	9.806789000	1.402546000	0.000121000
6	10.984042000	0.711178000	0.000150000
6	10.984042000	-0.711178000	0.000150000
1	9.803295000	-2.489240000	0.000121000
1	9.803295000	2.489240000	0.000121000
6	-3.664925000	-0.724488000	-0.000056000
6	-3.664925000	0.724488000	-0.000056000
6	-4.875858000	1.401438000	-0.000016000
6	-4.875858000	-1.401438000	-0.000016000
6	-6.109931000	0.723984000	0.000021000
6	-6.109931000	-0.723984000	0.000021000
1	-4.876941000	-2.488933000	-0.000016000
1	-4.876941000	2.488933000	-0.000016000
6	7.338580000	-1.401174000	0.000056000
6	7.338580000	1.401174000	0.000056000
6	2.413600000	-1.402243000	-0.000101000
6	2.413600000	1.402243000	-0.000101000
6	-2.413600000	-1.402243000	-0.000101000
6	-2.413600000	1.402243000	-0.000101000
6	-7.338579000	-1.401174000	0.000056000
6	-7.338579000	1.401174000	0.000056000
6	-8.553592000	-0.722847000	0.000089000
6	-8.553592000	0.722847000	0.000089000
6	-9.806789000	-1.402546000	0.000121000
6	-9.806789000	1.402546000	0.000121000
6	-10.984042000	-0.711178000	0.000150000
6	-10.984042000	0.711178000	0.000150000
1	-7.339139000	2.488913000	0.000056000
1	-7.339139000	-2.488913000	0.000056000
1	-2.406201000	2.489112000	-0.000100000
1	-2.406201000	-2.489112000	-0.000100000
1	2.406201000	-2.489112000	-0.000100000
1	2.406201000	2.489112000	-0.000100000
1	7.339139000	-2.488913000	0.000056000
1	7.339139000	2.488913000	0.000056000
1	-9.803295000	2.489240000	0.000121000
1	-11.929929000	1.243702000	0.000174000
1	-11.929929000	-1.243702000	0.000174000
1	-9.803295000	-2.489240000	0.000121000
1	11.929929000	1.243702000	0.000174000
1	11.929929000	-1.243702000	0.000174000

Table S30: Coordinates of pT₂ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	7.338379000	0.720068000	-0.000172000
7	6.110888000	1.356135000	-0.000259000

6	4.882167000	0.718860000	-0.000259000
6	4.882167000	-0.718860000	-0.000263000
7	6.110888000	-1.356135000	-0.000318000
6	7.338379000	-0.720068000	-0.000175000
6	2.445466000	-0.723868000	-0.000241000
6	2.445465000	0.723868000	-0.000250000
6	1.231783000	1.400426000	-0.000250000
1	1.230864000	2.488018000	-0.000255000
6	0.000001000	0.723609000	-0.000240000
6	0.000001000	-0.723609000	-0.000228000
6	1.231783000	-1.400427000	-0.000228000
1	6.110693000	2.364736000	-0.000272000
1	6.110693000	-2.364736000	-0.000235000
1	1.230864000	-2.488018000	-0.000218000
6	-2.445463000	-0.723870000	-0.000216000
6	-2.445463000	0.723870000	-0.000226000
6	-3.695615000	1.401384000	-0.000210000
6	-3.695615000	-1.401385000	-0.000214000
6	-4.882166000	-0.718861000	-0.000210000
6	-4.882166000	0.718861000	-0.000194000
1	-3.703625000	2.488373000	-0.000189000
1	-3.703625000	-2.488374000	-0.000221000
6	9.775746000	0.724738000	0.000005000
6	9.775746000	-0.724738000	0.000015000
6	10.986992000	-1.401365000	0.000107000
6	10.986992000	1.401365000	0.000086000
6	12.221125000	-0.724105000	0.000187000
6	12.221125000	0.724105000	0.000176000
1	10.988275000	2.488835000	0.000080000
1	10.988275000	-2.488835000	0.000115000
6	-1.231784000	1.400426000	-0.000239000
6	-1.231784000	-1.400426000	-0.000216000
6	3.695615000	1.401384000	-0.000254000
6	3.695615000	-1.401384000	-0.000247000
6	8.524631000	1.402094000	-0.000083000
6	8.524632000	-1.402094000	-0.000075000
6	13.449735000	1.401087000	0.000254000
6	13.449735000	-1.401087000	0.000276000
6	14.665063000	0.722939000	0.000341000
6	14.665063000	-0.722939000	0.000352000
6	15.918081000	1.402553000	0.000418000
6	15.918082000	-1.402552000	0.000440000
6	17.095443000	0.711167000	0.000501000
6	17.095444000	-0.711167000	0.000513000
1	13.450225000	-2.488810000	0.000285000
1	13.450225000	2.488810000	0.000247000
1	8.516907000	-2.488990000	-0.000076000

1	8.516907000	2.488990000	-0.000078000
1	3.703627000	2.488373000	-0.000251000
1	3.703627000	-2.488374000	-0.000250000
1	-1.230858000	2.488017000	-0.000243000
1	-1.230858000	-2.488018000	-0.000206000
1	15.914095000	-2.489231000	0.000448000
1	18.041438000	-1.243373000	0.000580000
1	18.041437000	1.243374000	0.000560000
1	15.914095000	2.489232000	0.000409000
7	-6.110887000	-1.356134000	-0.000268000
7	-6.110887000	1.356134000	-0.000122000
6	-7.338380000	-0.720069000	-0.000139000
6	-7.338380000	0.720069000	-0.000128000
6	-8.524631000	-1.402094000	-0.000070000
6	-8.524631000	1.402094000	-0.000086000
6	-9.775748000	-0.724739000	-0.000008000
6	-9.775748000	0.724739000	-0.000030000
6	-10.986991000	-1.401365000	0.000064000
6	-10.986990000	1.401365000	0.000015000
6	-12.221127000	-0.724105000	0.000113000
6	-12.221127000	0.724106000	0.000087000
6	-13.449734000	-1.401087000	0.000188000
6	-13.449734000	1.401087000	0.000136000
6	-14.665065000	-0.722938000	0.000239000
6	-14.665065000	0.722938000	0.000211000
6	-15.918081000	-1.402552000	0.000319000
6	-15.918081000	1.402552000	0.000264000
6	-17.095445000	-0.711165000	0.000370000
6	-17.095445000	0.711166000	0.000341000
1	-6.110693000	-2.364736000	-0.000139000
1	-6.110693000	2.364736000	-0.000183000
1	-8.516908000	-2.488990000	-0.000072000
1	-8.516908000	2.488990000	-0.000072000
1	-10.988279000	-2.488834000	0.000081000
1	-10.988278000	2.488834000	-0.000002000
1	-13.450230000	-2.488810000	0.000207000
1	-13.450230000	2.488810000	0.000115000
1	-15.914097000	-2.489231000	0.000340000
1	-18.041437000	-1.243375000	0.000433000
1	-18.041437000	1.243376000	0.000382000
1	-15.914097000	2.489231000	0.000242000

Table S31: Coordinates of pT₃ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
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6	-13.449532000	-0.720096000	0.000046000
7	-12.222262000	-1.356902000	0.000050000
6	-10.993386000	-0.718677000	0.000025000
6	-10.993386000	0.718677000	0.000051000
7	-12.222262000	1.356902000	0.000100000
6	-13.449532000	0.720096000	0.000077000
6	-8.556658000	0.723782000	-0.000001000
6	-8.556658000	-0.723782000	-0.000023000
6	-7.342788000	-1.400366000	-0.000052000
1	-7.342427000	-2.488048000	-0.000066000
6	-6.111098000	-0.723754000	-0.000062000
6	-6.111098000	0.723755000	-0.000043000
6	-7.342788000	1.400366000	-0.000013000
1	-12.222006000	-2.365464000	0.000023000
1	-12.222006000	2.365464000	0.000112000
1	-7.342427000	2.488048000	0.000004000
6	-3.665401000	0.723899000	-0.000082000
6	-3.665401000	-0.723899000	-0.000096000
6	-2.415045000	-1.401373000	-0.000120000
6	-2.415045000	1.401373000	-0.000094000
6	-1.228145000	0.719082000	-0.000122000
6	-1.228145000	-0.719082000	-0.000133000
1	-2.406612000	-2.488381000	-0.000129000
1	-2.406612000	2.488381000	-0.000082000
6	-15.887059000	-0.724741000	0.000034000
6	-15.887059000	0.724741000	0.000071000
6	-17.098295000	1.401330000	0.000088000
6	-17.098295000	-1.401330000	0.000013000
6	-18.332639000	0.724283000	0.000071000
6	-18.332639000	-0.724283000	0.000030000
1	-17.098980000	-2.488864000	-0.000016000
1	-17.098980000	2.488864000	0.000117000
6	-4.879028000	-1.400363000	-0.000087000
6	-4.879028000	1.400363000	-0.000055000
6	-9.806848000	-1.401385000	-0.000012000
6	-9.806848000	1.401385000	0.000034000
6	-14.635861000	-1.402180000	0.000022000
6	-14.635861000	1.402180000	0.000088000
6	-19.561138000	-1.401104000	0.000009000
6	-19.561138000	1.401104000	0.000091000
6	-20.776726000	-0.722987000	0.000029000
6	-20.776726000	0.722986000	0.000072000
6	-22.029624000	-1.402456000	0.000009000
6	-22.029624000	1.402456000	0.000095000
6	-23.207373000	-0.710962000	0.000030000
6	-23.207373000	0.710962000	0.000075000
1	-19.562015000	2.488873000	0.000122000

1	-19.562015000	-2.488873000	-0.000022000
1	-14.627658000	2.489073000	0.000112000
1	-14.627658000	-2.489073000	-0.000004000
1	-9.815386000	-2.488392000	-0.000029000
1	-9.815386000	2.488392000	0.000053000
1	-4.879437000	-2.488043000	-0.000098000
1	-4.879437000	2.488044000	-0.000042000
1	-22.026720000	2.489146000	0.000128000
1	-24.152793000	1.244253000	0.000093000
1	-24.152793000	-1.244253000	0.000014000
1	-22.026720000	-2.489146000	-0.000025000
7	0.000000000	1.356983000	-0.000140000
7	0.000000000	-1.356983000	-0.000169000
6	1.228145000	0.719082000	-0.000125000
6	1.228145000	-0.719082000	-0.000130000
6	2.415045000	1.401373000	-0.000108000
6	2.415045000	-1.401373000	-0.000109000
6	3.665401000	0.723899000	-0.000095000
6	3.665401000	-0.723899000	-0.000092000
6	4.879028000	1.400363000	-0.000086000
6	4.879028000	-1.400363000	-0.000075000
6	6.111098000	0.723755000	-0.000074000
6	6.111098000	-0.723755000	-0.000065000
6	7.342788000	1.400366000	-0.000071000
6	7.342787000	-1.400366000	-0.000050000
6	8.556658000	0.723782000	-0.000061000
6	8.556658000	-0.723782000	-0.000048000
6	9.806848000	1.401385000	-0.000071000
6	9.806848000	-1.401385000	-0.000029000
6	10.993386000	0.718677000	-0.000065000
6	10.993386000	-0.718677000	-0.000036000
1	0.000000000	2.365478000	-0.000147000
1	0.000000000	-2.365478000	-0.000156000
1	2.406612000	2.488381000	-0.000104000
1	2.406612000	-2.488381000	-0.000111000
1	4.879437000	2.488044000	-0.000090000
1	4.879437000	-2.488044000	-0.000070000
1	7.342427000	2.488048000	-0.000080000
1	7.342427000	-2.488048000	-0.000041000
1	9.815386000	2.488392000	-0.000093000
1	9.815386000	-2.488392000	-0.000006000
7	12.222262000	1.356902000	-0.000114000
7	12.222262000	-1.356902000	-0.000003000
6	13.449532000	0.720096000	-0.000033000
6	13.449532000	-0.720096000	0.000001000
6	14.635861000	1.402179000	-0.000012000
6	14.635861000	-1.402180000	0.000044000
6	15.887059000	0.724740000	0.000032000

6	15.887059000	-0.724741000	0.000057000
6	17.098295000	1.401330000	0.000045000
6	17.098295000	-1.401330000	0.000095000
6	18.332639000	0.724283000	0.000081000
6	18.332639000	-0.724283000	0.000108000
6	19.561138000	1.401104000	0.000089000
6	19.561138000	-1.401104000	0.000144000
6	20.776726000	0.722987000	0.000122000
6	20.776726000	-0.722987000	0.000152000
6	22.029624000	1.402456000	0.000128000
6	22.029624000	-1.402456000	0.000186000
6	23.207373000	0.710962000	0.000159000
6	23.207373000	-0.710962000	0.000190000
1	12.222006000	2.365464000	-0.000069000
1	12.222006000	-2.365464000	-0.000032000
1	14.627658000	2.489073000	-0.000040000
1	14.627658000	-2.489073000	0.000071000
1	17.098980000	2.488864000	0.000024000
1	17.098980000	-2.488864000	0.000114000
1	19.562015000	2.488873000	0.000067000
1	19.562015000	-2.488873000	0.000165000
1	22.026720000	2.489146000	0.000105000
1	22.026720000	-2.489146000	0.000208000
1	24.152793000	1.244253000	0.000163000
1	24.152793000	-1.244253000	0.000216000

Table S32: Coordinates of pT₄ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-7.339359000	-0.719148000	-0.000372000
7	-6.111393000	-1.356994000	-0.000339000
6	-4.883014000	-0.718944000	-0.000293000
6	-4.883014000	0.718943000	-0.000291000
7	-6.111393000	1.356994000	-0.000339000
6	-7.339359000	0.719148000	-0.000369000
6	-2.445761000	0.723820000	-0.000187000
6	-2.445761000	-0.723821000	-0.000188000
6	-1.231959000	-1.400275000	-0.000133000
1	-1.231560000	-2.487980000	-0.000133000
6	0.000000000	-0.723724000	-0.000079000
6	0.000000000	0.723724000	-0.000079000
6	-1.231959000	1.400275000	-0.000133000
1	-6.111350000	-2.365471000	-0.000340000
1	-6.111350000	2.365470000	-0.000326000
1	-1.231560000	2.487980000	-0.000133000
6	2.445761000	0.723820000	0.000026000
6	2.445761000	-0.723821000	0.000028000

6	3.696129000	-1.401270000	0.000081000
6	3.696129000	1.401270000	0.000075000
6	4.883014000	0.718943000	0.000120000
6	4.883014000	-0.718944000	0.000124000
1	3.704566000	-2.488302000	0.000082000
1	3.704566000	2.488301000	0.000071000
6	-9.776732000	-0.723914000	-0.000406000
6	-9.776732000	0.723913000	-0.000399000
6	-10.990351000	1.400351000	-0.000393000
6	-10.990351000	-1.400351000	-0.000408000
6	-12.222473000	0.723749000	-0.000387000
6	-12.222473000	-0.723749000	-0.000395000
1	-10.990783000	-2.488036000	-0.000406000
1	-10.990783000	2.488036000	-0.000380000
6	1.231959000	-1.400275000	-0.000024000
6	1.231959000	1.400275000	-0.000027000
6	-3.696129000	-1.401270000	-0.000243000
6	-3.696129000	1.401270000	-0.000241000
6	-8.526359000	-1.401350000	-0.000396000
6	-8.526359000	1.401350000	-0.000385000
6	-13.454135000	-1.400353000	-0.000375000
6	-13.454135000	1.400353000	-0.000357000
6	-14.668044000	-0.723763000	-0.000337000
6	-14.668044000	0.723763000	-0.000327000
6	-15.918238000	-1.401357000	-0.000292000
6	-15.918238000	1.401357000	-0.000272000
6	-17.104762000	-0.718631000	-0.000225000
6	-17.104762000	0.718631000	-0.000214000
1	-13.453763000	2.488040000	-0.000342000
1	-13.453764000	-2.488041000	-0.000374000
1	-8.517973000	2.488362000	-0.000376000
1	-8.517973000	-2.488362000	-0.000393000
1	-3.704566000	-2.488302000	-0.000241000
1	-3.704566000	2.488301000	-0.000238000
1	1.231559000	-2.487980000	-0.000023000
1	1.231559000	2.487980000	-0.000028000
1	-15.926757000	2.488370000	-0.000257000
1	-15.926757000	-2.488370000	-0.000293000
7	6.111393000	1.356994000	0.000152000
7	6.111393000	-1.356994000	0.000161000
6	7.339359000	0.719148000	0.000220000
6	7.339359000	-0.719148000	0.000226000
6	8.526359000	1.401350000	0.000264000
6	8.526359000	-1.401350000	0.000277000
6	9.776732000	0.723913000	0.000305000
6	9.776732000	-0.723914000	0.000313000
6	10.990351000	1.400351000	0.000326000

6	10.990351000	-1.400351000	0.000342000
6	12.222473000	0.723749000	0.000347000
6	12.222473000	-0.723749000	0.000356000
6	13.454135000	1.400353000	0.000344000
6	13.454135000	-1.400353000	0.000363000
6	14.668044000	0.723763000	0.000343000
6	14.668044000	-0.723763000	0.000353000
6	15.918238000	1.401357000	0.000317000
6	15.918238000	-1.401357000	0.000337000
6	17.104762000	0.718631000	0.000290000
6	17.104762000	-0.718631000	0.000301000
1	6.111350000	2.365470000	0.000157000
1	6.111350000	-2.365470000	0.000171000
1	8.517973000	2.488362000	0.000253000
1	8.517973000	-2.488362000	0.000277000
1	10.990783000	2.488036000	0.000312000
1	10.990783000	-2.488036000	0.000342000
1	13.453763000	2.488040000	0.000329000
1	13.453764000	-2.488041000	0.000363000
1	15.926757000	2.488370000	0.000303000
1	15.926757000	-2.488370000	0.000338000
7	18.333709000	1.356900000	0.000237000
7	18.333709000	-1.356900000	0.000253000
6	19.560910000	0.720115000	0.000203000
6	19.560910000	-0.720115000	0.000215000
6	20.747275000	1.402166000	0.000148000
6	20.747276000	-1.402166000	0.000176000
6	21.998479000	0.724747000	0.000100000
6	21.998480000	-0.724746000	0.000115000
6	23.209710000	1.401327000	0.000033000
6	23.209710000	-1.401326000	0.000065000
6	24.444077000	0.724281000	-0.000021000
6	24.444077000	-0.724280000	-0.000004000
6	25.672563000	1.401093000	-0.000097000
6	25.672564000	-1.401092000	-0.000062000
6	26.888182000	0.722980000	-0.000157000
6	26.888182000	-0.722979000	-0.000139000
6	28.141068000	1.402436000	-0.000241000
6	28.141068000	-1.402435000	-0.000204000
6	29.318846000	0.710951000	-0.000305000
6	29.318846000	-0.710951000	-0.000286000
1	18.333438000	2.365453000	0.000224000
1	18.333438000	-2.365453000	0.000267000
1	20.739112000	2.489062000	0.000135000
1	20.739112000	-2.489061000	0.000183000
1	23.210425000	2.488861000	0.000018000
1	23.210425000	-2.488860000	0.000074000

1	25.673447000	2.488862000	-0.000112000
1	25.673447000	-2.488862000	-0.000051000
1	28.138174000	2.489129000	-0.000255000
1	28.138174000	-2.489128000	-0.000191000
1	30.264250000	1.244275000	-0.000368000
1	30.264250000	-1.244275000	-0.000334000
7	-18.333709000	-1.356900000	-0.000141000
7	-18.333709000	1.356900000	-0.000118000
6	-19.560910000	-0.720115000	-0.000108000
6	-19.560910000	0.720115000	-0.000095000
6	-20.747276000	-1.402166000	-0.000069000
6	-20.747275000	1.402166000	-0.000041000
6	-21.998480000	-0.724746000	-0.000004000
6	-21.998479000	0.724747000	0.000011000
6	-23.209710000	-1.401326000	0.000051000
6	-23.209710000	1.401327000	0.000083000
6	-24.444077000	-0.724280000	0.000127000
6	-24.444077000	0.724281000	0.000143000
6	-25.672564000	-1.401092000	0.000192000
6	-25.672563000	1.401093000	0.000226000
6	-26.888182000	-0.722979000	0.000277000
6	-26.888182000	0.722980000	0.000295000
6	-28.141068000	-1.402435000	0.000351000
6	-28.141068000	1.402436000	0.000387000
6	-29.318846000	-0.710951000	0.000441000
6	-29.318846000	0.710951000	0.000459000
1	-28.138174000	-2.489128000	0.000338000
1	-30.264250000	-1.244275000	0.000496000
1	-30.264250000	1.244275000	0.000529000
1	-28.138174000	2.489129000	0.000401000
1	-25.673447000	2.488862000	0.000241000
1	-25.673447000	-2.488862000	0.000182000
1	-23.210425000	-2.488860000	0.000043000
1	-23.210425000	2.488861000	0.000098000
1	-20.739112000	-2.489061000	-0.000077000
1	-20.739112000	2.489062000	-0.000027000
1	-18.333438000	-2.365453000	-0.000161000
1	-18.333438000	2.365453000	-0.000123000

Table S33: Coordinates of pT₅ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	1.228217000	-0.719059000
7	0.000000000	0.000000000	-1.356880000
6	0.000000000	-1.228217000	-0.719059000
6	0.000000000	-1.228217000	0.719059000
7	0.000000000	0.000000000	1.356880000

6	0.000000000	1.228217000	0.719059000
6	0.000000000	-3.665526000	0.723871000
6	0.000000000	-3.665526000	-0.723871000
6	0.000000000	-4.879322000	-1.400242000
1	0.000000000	-4.879787000	-2.487962000
6	0.000000000	-6.111327000	-0.723705000
6	0.000000000	-6.111327000	0.723705000
6	0.000000000	-4.879322000	1.400242000
1	0.000000000	0.000000000	-2.365373000
1	0.000000000	0.000000000	2.365373000
1	0.000000000	-4.879787000	2.487962000
6	0.000000000	-8.557095000	0.723835000
6	0.000000000	-8.557095000	-0.723835000
6	0.000000000	-9.807439000	-1.401263000
6	0.000000000	-9.807439000	1.401263000
6	0.000000000	-10.994270000	0.718951000
6	0.000000000	-10.994270000	-0.718951000
1	0.000000000	-9.815960000	-2.488316000
1	0.000000000	-9.815960000	2.488316000
6	0.000000000	3.665526000	-0.723871000
6	0.000000000	3.665526000	0.723871000
6	0.000000000	4.879322000	1.400242000
6	0.000000000	4.879322000	-1.400242000
6	0.000000000	6.111327000	0.723705000
6	0.000000000	6.111327000	-0.723705000
1	0.000000000	4.879787000	-2.487962000
1	0.000000000	4.879787000	2.487962000
6	0.000000000	-7.343252000	-1.400240000
6	0.000000000	-7.343252000	1.400240000
6	0.000000000	-2.415168000	-1.401264000
6	0.000000000	-2.415168000	1.401264000
6	0.000000000	2.415168000	-1.401264000
6	0.000000000	2.415168000	1.401264000
6	0.000000000	7.343252000	-1.400240000
6	0.000000000	7.343252000	1.400240000
6	0.000000000	8.557095000	-0.723835000
6	0.000000000	8.557095000	0.723835000
6	0.000000000	9.807439000	-1.401263000
6	0.000000000	9.807439000	1.401263000
6	0.000000000	10.994270000	-0.718951000
6	0.000000000	10.994270000	0.718951000
1	0.000000000	7.342799000	2.487968000
1	0.000000000	7.342799000	-2.487968000
1	0.000000000	2.406673000	2.488322000
1	0.000000000	2.406673000	-2.488322000
1	0.000000000	-2.406673000	-2.488322000
1	0.000000000	-2.406673000	2.488322000

1	0.000000000	-7.342799000	-2.487968000
1	0.000000000	-7.342799000	2.487968000
1	0.000000000	9.815960000	2.488316000
1	0.000000000	9.815960000	-2.488316000
7	0.000000000	-12.222743000	1.356872000
7	0.000000000	-12.222743000	-1.356872000
6	0.000000000	-13.450653000	0.719221000
6	0.000000000	-13.450653000	-0.719221000
6	0.000000000	-14.637653000	1.401363000
6	0.000000000	-14.637653000	-1.401363000
6	0.000000000	-15.887992000	0.723947000
6	0.000000000	-15.887992000	-0.723947000
6	0.000000000	-17.101611000	1.400333000
6	0.000000000	-17.101611000	-1.400333000
6	0.000000000	-18.333736000	0.723735000
6	0.000000000	-18.333736000	-0.723735000
6	0.000000000	-19.565385000	1.400331000
6	0.000000000	-19.565385000	-1.400331000
6	0.000000000	-20.779303000	0.723784000
6	0.000000000	-20.779303000	-0.723784000
6	0.000000000	-22.029472000	1.401364000
6	0.000000000	-22.029472000	-1.401364000
6	0.000000000	-23.215949000	0.718661000
6	0.000000000	-23.215949000	-0.718661000
1	0.000000000	-12.222681000	2.365376000
1	0.000000000	-12.222681000	-2.365376000
1	0.000000000	-14.629201000	2.488391000
1	0.000000000	-14.629201000	-2.488391000
1	0.000000000	-17.102096000	2.488027000
1	0.000000000	-17.102096000	-2.488027000
1	0.000000000	-19.564959000	2.488028000
1	0.000000000	-19.564959000	-2.488028000
1	0.000000000	-22.038079000	2.488396000
1	0.000000000	-22.038079000	-2.488396000
7	0.000000000	-24.444940000	1.356769000
7	0.000000000	-24.444940000	-1.356769000
6	0.000000000	-25.672125000	0.720153000
6	0.000000000	-25.672125000	-0.720153000
6	0.000000000	-26.858483000	1.402167000
6	0.000000000	-26.858483000	-1.402167000
6	0.000000000	-28.109636000	0.724759000
6	0.000000000	-28.109636000	-0.724759000
6	0.000000000	-29.320913000	1.401308000
6	0.000000000	-29.320913000	-1.401308000
6	0.000000000	-30.555237000	0.724257000
6	0.000000000	-30.555237000	-0.724257000
6	0.000000000	-31.783785000	1.401075000

6	0.000000000	-31.783785000	-1.401075000
6	0.000000000	-32.999342000	0.722978000
6	0.000000000	-32.999342000	-0.722978000
6	0.000000000	-34.252311000	1.402458000
6	0.000000000	-34.252311000	-1.402458000
6	0.000000000	-35.429997000	0.711003000
6	0.000000000	-35.429997000	-0.711003000
1	0.000000000	-24.444673000	2.365352000
1	0.000000000	-24.444673000	-2.365352000
1	0.000000000	-26.850239000	2.489074000
1	0.000000000	-26.850239000	-2.489074000
1	0.000000000	-29.321664000	2.488845000
1	0.000000000	-29.321664000	-2.488845000
1	0.000000000	-31.784585000	2.488850000
1	0.000000000	-31.784585000	-2.488850000
1	0.000000000	-34.249176000	2.489154000
1	0.000000000	-34.249176000	-2.489154000
1	0.000000000	-36.375551000	1.244065000
1	0.000000000	-36.375551000	-1.244065000
7	0.000000000	12.222743000	-1.356872000
7	0.000000000	12.222743000	1.356872000
6	0.000000000	13.450653000	-0.719221000
6	0.000000000	13.450653000	0.719221000
6	0.000000000	14.637653000	-1.401363000
6	0.000000000	14.637653000	1.401363000
6	0.000000000	15.887992000	-0.723947000
6	0.000000000	15.887992000	0.723947000
6	0.000000000	17.101611000	-1.400333000
6	0.000000000	17.101611000	1.400333000
6	0.000000000	18.333736000	-0.723735000
6	0.000000000	18.333736000	0.723735000
6	0.000000000	19.565385000	-1.400331000
6	0.000000000	19.565385000	1.400331000
6	0.000000000	20.779303000	-0.723784000
6	0.000000000	20.779303000	0.723784000
6	0.000000000	22.029472000	-1.401364000
6	0.000000000	22.029472000	1.401364000
6	0.000000000	23.215949000	-0.718661000
6	0.000000000	23.215949000	0.718661000
1	0.000000000	22.038079000	-2.488396000
1	0.000000000	22.038079000	2.488396000
1	0.000000000	19.564959000	2.488028000
1	0.000000000	19.564959000	-2.488028000
1	0.000000000	17.102096000	-2.488027000
1	0.000000000	17.102096000	2.488027000
1	0.000000000	14.629201000	-2.488391000
1	0.000000000	14.629201000	2.488391000

1	0.000000000	12.222681000	-2.365376000
1	0.000000000	12.222681000	2.365376000
7	0.000000000	24.444940000	-1.356769000
1	0.000000000	24.444673000	-2.365352000
7	0.000000000	24.444940000	1.356769000
1	0.000000000	24.444673000	2.365352000
6	0.000000000	25.672125000	-0.720153000
6	0.000000000	25.672125000	0.720153000
6	0.000000000	26.858483000	-1.402167000
6	0.000000000	26.858483000	1.402167000
6	0.000000000	28.109636000	-0.724759000
6	0.000000000	28.109636000	0.724759000
6	0.000000000	29.320913000	-1.401308000
6	0.000000000	29.320913000	1.401308000
6	0.000000000	30.555237000	-0.724257000
6	0.000000000	30.555237000	0.724257000
6	0.000000000	31.783785000	-1.401075000
6	0.000000000	31.783785000	1.401075000
6	0.000000000	32.999342000	-0.722978000
6	0.000000000	32.999342000	0.722978000
6	0.000000000	34.252311000	-1.402458000
6	0.000000000	34.252311000	1.402458000
6	0.000000000	35.429997000	-0.711003000
6	0.000000000	35.429997000	0.711003000
1	0.000000000	26.850239000	-2.489074000
1	0.000000000	26.850239000	2.489074000
1	0.000000000	29.321664000	-2.488845000
1	0.000000000	29.321664000	2.488845000
1	0.000000000	31.784585000	-2.488850000
1	0.000000000	31.784585000	2.488850000
1	0.000000000	34.249176000	-2.489154000
1	0.000000000	36.375551000	-1.244065000
1	0.000000000	36.375551000	1.244065000
1	0.000000000	34.249176000	2.489154000

Table S34: Coordinates of pT₆ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	7.339578000	0.719109000
7	0.000000000	6.111420000	1.356901000
6	0.000000000	4.883116000	0.719034000
6	0.000000000	4.883116000	-0.719034000
7	0.000000000	6.111420000	-1.356901000
6	0.000000000	7.339578000	-0.719109000
6	0.000000000	2.445830000	-0.723837000
6	0.000000000	2.445830000	0.723837000
6	0.000000000	1.231984000	1.400219000

1	0.000000000	1.231507000	2.487945000
6	0.000000000	0.000000000	0.723693000
6	0.000000000	0.000000000	-0.723693000
6	0.000000000	1.231984000	-1.400219000
1	0.000000000	6.111401000	2.365388000
1	0.000000000	6.111401000	-2.365388000
1	0.000000000	1.231507000	-2.487945000
6	0.000000000	-2.445830000	-0.723837000
6	0.000000000	-2.445830000	0.723837000
6	0.000000000	-3.696190000	1.401235000
6	0.000000000	-3.696190000	-1.401235000
6	0.000000000	-4.883116000	-0.719034000
6	0.000000000	-4.883116000	0.719034000
1	0.000000000	-3.704698000	2.488290000
1	0.000000000	-3.704698000	-2.488290000
6	0.000000000	9.776929000	0.723884000
6	0.000000000	9.776929000	-0.723884000
6	0.000000000	10.990721000	-1.400226000
6	0.000000000	10.990721000	1.400226000
6	0.000000000	12.222742000	-0.723694000
6	0.000000000	12.222742000	0.723694000
1	0.000000000	10.991184000	2.487989000
1	0.000000000	10.991184000	-2.487989000
6	0.000000000	-1.231984000	1.400219000
6	0.000000000	-1.231984000	-1.400219000
6	0.000000000	3.696190000	1.401235000
6	0.000000000	3.696190000	-1.401235000
6	0.000000000	8.526565000	1.401279000
6	0.000000000	8.526565000	-1.401279000
6	0.000000000	13.454665000	1.400253000
6	0.000000000	13.454665000	-1.400253000
6	0.000000000	14.668523000	0.723841000
6	0.000000000	14.668523000	-0.723841000
6	0.000000000	15.918870000	1.401277000
6	0.000000000	15.918870000	-1.401277000
6	0.000000000	17.105689000	0.718957000
6	0.000000000	17.105689000	-0.718957000
1	0.000000000	13.454210000	-2.487931000
1	0.000000000	13.454210000	2.487931000
1	0.000000000	8.518086000	-2.488288000
1	0.000000000	8.518086000	2.488288000
1	0.000000000	3.704698000	2.488290000
1	0.000000000	3.704698000	-2.488290000
1	0.000000000	-1.231507000	2.487945000
1	0.000000000	-1.231507000	-2.487945000
1	0.000000000	15.927386000	-2.488288000
1	0.000000000	15.927386000	2.488288000
7	0.000000000	-6.111420000	-1.356901000

7	0.000000000	-6.111420000	1.356901000
6	0.000000000	-7.339578000	-0.719109000
6	0.000000000	-7.339578000	0.719109000
6	0.000000000	-8.526565000	-1.401279000
6	0.000000000	-8.526565000	1.401279000
6	0.000000000	-9.776929000	-0.723884000
6	0.000000000	-9.776929000	0.723884000
6	0.000000000	-10.990721000	-1.400226000
6	0.000000000	-10.990721000	1.400226000
6	0.000000000	-12.222742000	-0.723694000
6	0.000000000	-12.222742000	0.723694000
6	0.000000000	-13.454665000	-1.400253000
6	0.000000000	-13.454665000	1.400253000
6	0.000000000	-14.668523000	-0.723841000
6	0.000000000	-14.668523000	0.723841000
6	0.000000000	-15.918870000	-1.401277000
6	0.000000000	-15.918870000	1.401277000
6	0.000000000	-17.105689000	-0.718957000
6	0.000000000	-17.105689000	0.718957000
1	0.000000000	-6.111401000	-2.365388000
1	0.000000000	-6.111401000	2.365388000
1	0.000000000	-8.518086000	-2.488288000
1	0.000000000	-8.518086000	2.488288000
1	0.000000000	-10.991184000	-2.487989000
1	0.000000000	-10.991184000	2.487989000
1	0.000000000	-13.454210000	-2.487931000
1	0.000000000	-13.454210000	2.487931000
1	0.000000000	-15.927386000	-2.488288000
1	0.000000000	-15.927386000	2.488288000
7	0.000000000	-18.334198000	-1.356893000
7	0.000000000	-18.334198000	1.356893000
6	0.000000000	-19.562084000	-0.719249000
6	0.000000000	-19.562084000	0.719249000
6	0.000000000	-20.749093000	-1.401382000
6	0.000000000	-20.749093000	1.401382000
6	0.000000000	-21.999435000	-0.723961000
6	0.000000000	-21.999435000	0.723961000
6	0.000000000	-23.213055000	-1.400348000
6	0.000000000	-23.213055000	1.400348000
6	0.000000000	-24.445183000	-0.723740000
6	0.000000000	-24.445183000	0.723740000
6	0.000000000	-25.676832000	-1.400340000
6	0.000000000	-25.676832000	1.400340000
6	0.000000000	-26.890748000	-0.723788000
6	0.000000000	-26.890748000	0.723788000
6	0.000000000	-28.140921000	-1.401366000
6	0.000000000	-28.140921000	1.401366000
6	0.000000000	-29.327388000	-0.718661000

6	0.000000000	-29.327388000	0.718661000
1	0.000000000	-18.334132000	-2.365393000
1	0.000000000	-18.334132000	2.365393000
1	0.000000000	-20.740651000	-2.488409000
1	0.000000000	-20.740651000	2.488409000
1	0.000000000	-23.213551000	-2.488042000
1	0.000000000	-23.213551000	2.488042000
1	0.000000000	-25.676401000	-2.488036000
1	0.000000000	-25.676401000	2.488036000
1	0.000000000	-28.149526000	-2.488399000
1	0.000000000	-28.149526000	2.488399000
7	0.000000000	18.334198000	1.356893000
7	0.000000000	18.334198000	-1.356893000
6	0.000000000	19.562084000	0.719249000
6	0.000000000	19.562084000	-0.719249000
6	0.000000000	20.749093000	1.401382000
6	0.000000000	20.749093000	-1.401382000
6	0.000000000	21.999435000	0.723961000
6	0.000000000	21.999435000	-0.723961000
6	0.000000000	23.213055000	1.400348000
6	0.000000000	23.213055000	-1.400348000
6	0.000000000	24.445183000	0.723740000
6	0.000000000	24.445183000	-0.723740000
6	0.000000000	25.676832000	1.400340000
6	0.000000000	25.676832000	-1.400340000
6	0.000000000	26.890748000	0.723788000
6	0.000000000	26.890748000	-0.723788000
6	0.000000000	28.140921000	1.401366000
6	0.000000000	28.140921000	-1.401366000
6	0.000000000	29.327388000	0.718661000
6	0.000000000	29.327388000	-0.718661000
1	0.000000000	28.149526000	2.488399000
1	0.000000000	28.149526000	-2.488399000
1	0.000000000	25.676401000	-2.488036000
1	0.000000000	25.676401000	2.488036000
1	0.000000000	23.213551000	2.488042000
1	0.000000000	23.213551000	-2.488042000
1	0.000000000	20.740651000	2.488409000
1	0.000000000	20.740651000	-2.488409000
1	0.000000000	18.334132000	2.365393000
1	0.000000000	18.334132000	-2.365393000
7	0.000000000	30.556393000	1.356762000
1	0.000000000	30.556128000	2.365343000
7	0.000000000	30.556393000	-1.356762000
1	0.000000000	30.556128000	-2.365343000
6	0.000000000	31.783568000	0.720152000
6	0.000000000	31.783568000	-0.720152000
6	0.000000000	32.969932000	1.402153000

6	0.000000000	32.969932000	-1.402153000
6	0.000000000	34.221089000	0.724750000
6	0.000000000	34.221089000	-0.724750000
6	0.000000000	35.432370000	1.401291000
6	0.000000000	35.432370000	-1.401291000
6	0.000000000	36.666696000	0.724241000
6	0.000000000	36.666696000	-0.724241000
6	0.000000000	37.895254000	1.401050000
6	0.000000000	37.895254000	-1.401050000
6	0.000000000	39.110805000	0.722958000
6	0.000000000	39.110805000	-0.722958000
6	0.000000000	40.363787000	1.402426000
6	0.000000000	40.363787000	-1.402426000
6	0.000000000	41.541468000	0.710984000
6	0.000000000	41.541468000	-0.710984000
1	0.000000000	32.961697000	2.489060000
1	0.000000000	32.961697000	-2.489060000
1	0.000000000	35.433133000	2.488826000
1	0.000000000	35.433133000	-2.488826000
1	0.000000000	37.896052000	2.488824000
1	0.000000000	37.896052000	-2.488824000
1	0.000000000	40.360638000	2.489123000
1	0.000000000	42.487038000	1.244015000
1	0.000000000	42.487038000	-1.244015000
1	0.000000000	40.360638000	-2.489123000
7	0.000000000	-30.556393000	1.356762000
7	0.000000000	-30.556393000	-1.356762000
6	0.000000000	-31.783568000	0.720152000
6	0.000000000	-31.783568000	-0.720152000
6	0.000000000	-32.969932000	1.402153000
6	0.000000000	-32.969932000	-1.402153000
6	0.000000000	-34.221089000	0.724750000
6	0.000000000	-34.221089000	-0.724750000
6	0.000000000	-35.432370000	1.401291000
6	0.000000000	-35.432370000	-1.401291000
6	0.000000000	-36.666696000	0.724241000
6	0.000000000	-36.666696000	-0.724241000
6	0.000000000	-37.895254000	1.401050000
6	0.000000000	-37.895254000	-1.401050000
6	0.000000000	-39.110805000	0.722958000
6	0.000000000	-39.110805000	-0.722958000
6	0.000000000	-40.363787000	1.402426000
6	0.000000000	-40.363787000	-1.402426000
6	0.000000000	-41.541468000	0.710984000
6	0.000000000	-41.541468000	-0.710984000
1	0.000000000	-30.556128000	2.365343000
1	0.000000000	-30.556128000	-2.365343000
1	0.000000000	-32.961697000	2.489060000

1	0.000000000	-32.961697000	-2.489060000
1	0.000000000	-35.433133000	-2.488826000
1	0.000000000	-35.433133000	2.488826000
1	0.000000000	-37.896052000	2.488824000
1	0.000000000	-37.896052000	-2.488824000
1	0.000000000	-40.360638000	-2.489123000
1	0.000000000	-40.360638000	2.489123000
1	0.000000000	-42.487038000	1.244015000
1	0.000000000	-42.487038000	-1.244015000

Table S35: Coordinates of pB₁_1 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.710737000	3.557790000
6	0.000000000	1.410537000	2.384269000
6	0.000000000	0.722012000	1.139480000
6	0.000000000	-0.722012000	1.139480000
6	0.000000000	-1.410537000	2.384269000
6	0.000000000	-0.710737000	3.557790000
7	0.000000000	1.424892000	0.000000000
7	0.000000000	-1.424892000	0.000000000
6	0.000000000	-0.722012000	-1.139480000
6	0.000000000	0.722012000	-1.139480000
6	0.000000000	1.410537000	-2.384269000
1	0.000000000	2.495220000	-2.360151000
6	0.000000000	0.710737000	-3.557790000
6	0.000000000	-0.710737000	-3.557790000
6	0.000000000	-1.410537000	-2.384269000
1	0.000000000	1.240474000	4.505169000
1	0.000000000	2.495220000	2.360151000
1	0.000000000	-2.495220000	2.360151000
1	0.000000000	-1.240474000	4.505169000
1	0.000000000	-2.495220000	-2.360151000
1	0.000000000	1.240474000	-4.505169000
1	0.000000000	-1.240474000	-4.505169000

Table S36: Coordinates of pB₂_1 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.694674000	-5.992983000
6	0.000000000	1.390572000	-4.787781000
6	0.000000000	0.703202000	-3.578801000
6	0.000000000	-0.703202000	-3.578801000

6	0.000000000	-1.390572000	-4.787781000
6	0.000000000	-0.694674000	-5.992983000
7	0.000000000	1.357775000	-2.354143000
7	0.000000000	-1.357775000	-2.354143000
6	0.000000000	-0.721488000	-1.127862000
6	0.000000000	0.721488000	-1.127862000
6	0.000000000	1.407301000	0.056743000
1	0.000000000	2.492813000	0.070887000
6	0.000000000	0.724202000	1.302252000
6	0.000000000	-0.724202000	1.302252000
6	0.000000000	-1.407301000	0.056743000
1	0.000000000	1.243517000	-6.927849000
1	0.000000000	2.476731000	-4.777615000
1	0.000000000	-2.476731000	-4.777615000
1	0.000000000	-1.243517000	-6.927849000
1	0.000000000	-2.492813000	0.070887000
7	0.000000000	-1.425455000	2.434166000
7	0.000000000	1.425455000	2.434166000
6	0.000000000	-0.718459000	3.583250000
6	0.000000000	0.718459000	3.583250000
6	0.000000000	1.405356000	4.822686000
6	0.000000000	-1.405356000	4.822686000
6	0.000000000	-0.707603000	6.003165000
6	0.000000000	0.707603000	6.003165000
1	0.000000000	2.490421000	4.798337000
1	0.000000000	1.241271000	6.948461000
1	0.000000000	-1.241271000	6.948461000
1	0.000000000	-2.490421000	4.798337000
1	0.000000000	-2.366061000	-2.356376000
1	0.000000000	2.366061000	-2.356376000

Table S37: Coordinates of pB₂_2 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	5.916581000	0.714231000
6	0.000000000	4.748612000	1.414869000
6	0.000000000	3.496320000	0.727878000
6	0.000000000	3.496320000	-0.727878000
6	0.000000000	4.748612000	-1.414869000
6	0.000000000	5.916581000	-0.714231000
7	0.000000000	2.370437000	1.429782000
7	0.000000000	2.370437000	-1.429782000
6	0.000000000	1.213262000	-0.727766000
6	0.000000000	1.213262000	0.727766000
6	0.000000000	0.000000000	1.419430000
1	0.000000000	0.000000000	2.503675000
6	0.000000000	-1.213262000	0.727766000

6	0.000000000	-1.213262000	-0.727766000
6	0.000000000	0.000000000	-1.419430000
1	0.000000000	6.865728000	1.240714000
1	0.000000000	4.724868000	2.499389000
1	0.000000000	4.724868000	-2.499389000
1	0.000000000	6.865728000	-1.240714000
1	0.000000000	0.000000000	-2.503675000
7	0.000000000	-2.370437000	-1.429782000
7	0.000000000	-2.370437000	1.429782000
6	0.000000000	-3.496320000	-0.727878000
6	0.000000000	-3.496320000	0.727878000
6	0.000000000	-4.748612000	1.414869000
6	0.000000000	-4.748612000	-1.414869000
6	0.000000000	-5.916581000	-0.714231000
6	0.000000000	-5.916581000	0.714231000
1	0.000000000	-4.724868000	2.499389000
1	0.000000000	-6.865728000	1.240714000
1	0.000000000	-6.865728000	-1.240714000
1	0.000000000	-4.724868000	-2.499389000

Table S38: Coordinates of pB₃_1 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.310710000	-3.575314000	0.701944000
6	0.248025000	-2.369343000	1.388294000
6	0.206264000	-1.157306000	0.699320000
6	0.206264000	-1.157306000	-0.699320000
6	0.248025000	-2.369343000	-1.388294000
6	0.310710000	-3.575314000	-0.701944000
7	0.161177000	0.065905000	1.358075000
7	0.161177000	0.065905000	-1.358075000
6	0.105252000	1.289718000	-0.721436000
6	0.105252000	1.289718000	0.721436000
6	0.050398000	2.474717000	1.406772000
1	0.049578000	2.488953000	2.492372000
6	-0.005883000	3.718703000	0.724451000
6	-0.005883000	3.718703000	-0.724451000
6	0.050398000	2.474717000	-1.406772000
1	0.243922000	-2.368109000	2.474853000
1	0.243922000	-2.368109000	-2.474853000
1	0.049578000	2.488953000	-2.492372000
7	-0.056347000	4.849529000	-1.426066000
7	-0.056347000	4.849529000	1.426066000
6	-0.107254000	5.998555000	-0.717917000
6	-0.107254000	5.998555000	0.717917000
6	-0.162332000	7.236073000	1.404512000
6	-0.162332000	7.236073000	-1.404512000

6	-0.214505000	8.416667000	-0.707120000
6	-0.214505000	8.416667000	0.707120000
1	-0.161682000	7.211356000	2.489635000
1	-0.257297000	9.360893000	1.241068000
1	-0.257297000	9.360893000	-1.241068000
1	-0.161682000	7.211356000	-2.489635000
7	0.420098000	-4.806550000	1.360044000
7	0.420098000	-4.806550000	-1.360044000
6	0.033688000	-5.982038000	0.702775000
6	0.033688000	-5.982038000	-0.702775000
6	-0.303993000	-7.141466000	-1.388295000
6	-0.303993000	-7.141466000	1.388295000
6	-0.623455000	-8.307635000	-0.693231000
6	-0.623455000	-8.307635000	0.693231000
1	-0.305795000	-7.131156000	2.474837000
1	-0.305795000	-7.131156000	-2.474837000
1	-0.873189000	-9.207876000	-1.243462000
1	-0.873189000	-9.207876000	1.243462000
1	0.248511000	-4.789329000	-2.354483000
1	0.248511000	-4.789329000	2.354483000
1	0.159965000	0.065092000	-2.366000000
1	0.159965000	0.065092000	2.366000000

Table S39: Coordinates of pB₃_2 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.724899000	-3.485776000
6	0.000000000	1.411369000	-2.303813000
6	0.000000000	0.730277000	-1.055464000
6	0.000000000	-0.730277000	-1.055464000
6	0.000000000	-1.411369000	-2.303813000
6	0.000000000	-0.724899000	-3.485776000
7	0.000000000	1.431388000	0.065696000
7	0.000000000	-1.431388000	0.065696000
6	0.000000000	-0.727215000	1.230173000
6	0.000000000	0.727215000	1.230173000
6	0.000000000	1.416023000	2.438232000
1	0.000000000	2.500478000	2.438140000
6	0.000000000	0.727496000	3.659248000
6	0.000000000	-0.727496000	3.659248000
6	0.000000000	-1.416023000	2.438232000
1	0.000000000	2.496735000	-2.289816000
1	0.000000000	-2.496735000	-2.289816000
1	0.000000000	-2.500478000	2.438140000
7	0.000000000	-1.428737000	4.811366000
7	0.000000000	1.428737000	4.811366000
6	0.000000000	-0.725117000	5.942443000

6	0.000000000	0.725117000	5.942443000
6	0.000000000	1.411701000	7.192107000
6	0.000000000	-1.411701000	7.192107000
6	0.000000000	-0.712516000	8.363718000
6	0.000000000	0.712516000	8.363718000
1	0.000000000	2.496478000	7.167962000
1	0.000000000	1.241165000	9.311826000
1	0.000000000	-1.241165000	9.311826000
1	0.000000000	-2.496478000	7.167962000
7	0.000000000	1.356230000	-4.710932000
7	0.000000000	-1.356230000	-4.710932000
6	0.000000000	0.703224000	-5.934373000
6	0.000000000	-0.703224000	-5.934373000
6	0.000000000	-1.392184000	-7.143783000
6	0.000000000	1.392184000	-7.143783000
6	0.000000000	-0.695682000	-8.346321000
6	0.000000000	0.695682000	-8.346321000
1	0.000000000	2.478192000	-7.133632000
1	0.000000000	-2.478192000	-7.133632000
1	0.000000000	-1.243147000	-9.281882000
1	0.000000000	1.243147000	-9.281882000
1	0.000000000	-2.365214000	-4.713850000
1	0.000000000	2.365214000	-4.713850000

Table S40: Coordinates of pB₃_3 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	3.572377000	0.729378000
6	0.000000000	2.365681000	1.421726000
6	0.000000000	1.143012000	0.731693000
6	0.000000000	1.143012000	-0.731693000
6	0.000000000	2.365681000	-1.421726000
6	0.000000000	3.572377000	-0.729378000
7	0.000000000	0.000000000	1.433027000
7	0.000000000	0.000000000	-1.433027000
6	0.000000000	-1.143012000	-0.731693000
6	0.000000000	-1.143012000	0.731693000
6	0.000000000	-2.365681000	1.421726000
1	0.000000000	-2.366577000	2.505744000
6	0.000000000	-3.572377000	0.729378000
6	0.000000000	-3.572377000	-0.729378000
6	0.000000000	-2.365681000	-1.421726000
1	0.000000000	2.366577000	2.505744000
1	0.000000000	2.366577000	-2.505744000
1	0.000000000	-2.366577000	-2.505744000
7	0.000000000	-4.733736000	-1.431242000
7	0.000000000	-4.733736000	1.431242000

6	0.000000000	-5.856338000	-0.729588000
6	0.000000000	-5.856338000	0.729588000
6	0.000000000	-7.110199000	1.416154000
6	0.000000000	-7.110199000	-1.416154000
6	0.000000000	-8.276721000	-0.715017000
6	0.000000000	-8.276721000	0.715017000
1	0.000000000	-7.087350000	2.500462000
1	0.000000000	-9.225944000	1.240758000
1	0.000000000	-9.225944000	-1.240758000
1	0.000000000	-7.087350000	-2.500462000
7	0.000000000	4.733736000	1.431242000
7	0.000000000	4.733736000	-1.431242000
6	0.000000000	5.856338000	0.729588000
6	0.000000000	5.856338000	-0.729588000
6	0.000000000	7.110199000	-1.416154000
6	0.000000000	7.110199000	1.416154000
6	0.000000000	8.276721000	-0.715017000
6	0.000000000	8.276721000	0.715017000
1	0.000000000	7.087350000	2.500462000
1	0.000000000	7.087350000	-2.500462000
1	0.000000000	9.225944000	-1.240758000
1	0.000000000	9.225944000	1.240758000

Table S41: Coordinates of pB₄_1 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-0.383922000	-5.983802000	0.699359000
6	-0.514263000	-4.780014000	1.384667000
6	-0.682723000	-3.580035000	0.698368000
6	-0.682723000	-3.580035000	-0.698368000
6	-0.514263000	-4.780014000	-1.384667000
6	-0.383922000	-5.983802000	-0.699359000
6	-0.645407000	-1.159344000	-0.702652000
6	-0.645407000	-1.159344000	0.702652000
6	-0.445345000	0.033239000	1.387250000
1	-0.444472000	0.034953000	2.473936000
6	-0.266403000	1.232924000	0.699048000
6	-0.266403000	1.232924000	-0.699048000
6	-0.445345000	0.033239000	-1.387250000
1	-0.510314000	-4.779263000	2.471749000
1	-0.510314000	-4.779263000	-2.471749000
1	-0.444472000	0.034953000	-2.473936000
6	-0.000375000	3.666154000	-0.721303000
6	-0.000375000	3.666154000	0.721303000
6	0.080768000	4.849846000	1.406693000
6	0.080768000	4.849846000	-1.406693000
6	0.165843000	6.092082000	-0.724551000

6	0.165843000	6.092082000	0.724551000
1	0.078116000	4.864251000	2.492321000
1	0.078116000	4.864251000	-2.492321000
6	0.297532000	-8.305426000	0.703007000
6	0.297532000	-8.305426000	-0.703007000
6	0.837047000	-9.386608000	-1.387486000
6	0.837047000	-9.386608000	1.387486000
6	1.357080000	-10.479012000	-0.693094000
6	1.357080000	-10.479012000	0.693094000
1	0.837210000	-9.376092000	2.474172000
1	0.837210000	-9.376092000	-2.474172000
1	1.761877000	-11.321025000	-1.243706000
1	1.761877000	-11.321025000	1.243706000
6	0.305062000	8.370146000	0.717913000
6	0.305062000	8.370146000	-0.717913000
6	0.377962000	9.606738000	-1.404337000
6	0.377962000	9.606738000	1.404337000
6	0.446758000	10.786709000	-0.707038000
6	0.446758000	10.786709000	0.707038000
1	0.376605000	9.582100000	-2.489485000
1	0.376605000	9.582100000	2.489485000
1	0.502633000	11.730180000	1.241136000
1	0.502633000	11.730180000	-1.241136000
7	0.236579000	7.221972000	1.426213000
7	0.236579000	7.221972000	-1.426213000
7	-0.074665000	2.442789000	1.357507000
7	-0.074665000	2.442789000	-1.357507000
7	-0.904604000	-2.364082000	1.367062000
7	-0.904604000	-2.364082000	-1.367062000
7	-0.294909000	-7.218828000	1.361077000
7	-0.294909000	-7.218828000	-1.361077000
1	-0.692985000	-2.368500000	2.353916000
1	-0.692985000	-2.368500000	-2.353916000
1	-0.112188000	-7.167213000	2.352598000
1	-0.112188000	-7.167213000	-2.352598000
1	-0.110983000	2.446077000	2.364910000
1	-0.110983000	2.446077000	-2.364910000

Table S42: Coordinates of pB₄_2 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-0.267438000	-5.926174000	0.704318000
6	-0.233357000	-4.720817000	1.390488000
6	-0.218632000	-3.507587000	0.700021000
6	-0.218632000	-3.507587000	-0.700021000
6	-0.233357000	-4.720817000	-1.390488000
6	-0.267438000	-5.926174000	-0.704318000

6	-0.164734000	-1.061414000	-0.723997000
6	-0.164734000	-1.061414000	0.723997000
6	-0.130603000	0.121693000	1.410581000
1	-0.129787000	0.135583000	2.496088000
6	-0.093847000	1.368696000	0.730172000
6	-0.093847000	1.368696000	-0.730172000
6	-0.130603000	0.121693000	-1.410581000
1	-0.228464000	-4.719156000	2.476784000
1	-0.228464000	-4.719156000	-2.476784000
1	-0.129787000	0.135583000	-2.496088000
6	-0.024162000	3.654085000	-0.727455000
6	-0.024162000	3.654085000	0.727455000
6	0.012583000	4.861805000	1.415323000
6	0.012583000	4.861805000	-1.415323000
6	0.049325000	6.083576000	-0.727630000
6	0.049325000	6.083576000	0.727630000
1	0.012460000	4.861811000	2.499805000
1	0.012460000	4.861811000	-2.499805000
6	0.031887000	-8.334426000	0.702525000
6	0.031887000	-8.334426000	-0.702525000
6	0.361920000	-9.495493000	-1.388875000
6	0.361920000	-9.495493000	1.388875000
6	0.677058000	-10.662060000	-0.693352000
6	0.677058000	-10.662060000	0.693352000
1	0.363186000	-9.485455000	2.475273000
1	0.363186000	-9.485455000	-2.475273000
1	0.923454000	-11.563260000	-1.243303000
1	0.923454000	-11.563260000	1.243303000
6	0.116046000	8.366249000	0.724399000
6	0.116046000	8.366249000	-0.724399000
6	0.152222000	9.614729000	-1.410704000
6	0.152222000	9.614729000	1.410704000
6	0.185608000	10.787071000	-0.712007000
6	0.185608000	10.787071000	0.712007000
1	0.151871000	9.590331000	-2.495557000
1	0.151871000	9.590331000	2.495557000
1	0.213434000	11.734515000	1.241236000
1	0.213434000	11.734515000	-1.241236000
7	0.083313000	7.234330000	1.428741000
7	0.083313000	7.234330000	-1.428741000
7	-0.059830000	2.490184000	1.431925000
7	-0.059830000	2.490184000	-1.431925000
7	-0.199801000	-2.286077000	1.355468000
7	-0.199801000	-2.286077000	-1.355468000
7	-0.343595000	-7.156478000	1.359620000
7	-0.343595000	-7.156478000	-1.359620000
1	-0.198534000	-2.287101000	2.364165000
1	-0.198534000	-2.287101000	-2.364165000

1	-0.191495000	-7.140576000	2.356995000
1	-0.191495000	-7.140576000	-2.356995000

Table S43: Coordinates of pB₄_3optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-5.844808000	0.725998000	0.000000000
6	-4.663321000	1.412850000	0.000000000
6	-3.415187000	0.732044000	0.000000000
6	-3.415187000	-0.732044000	0.000000000
6	-4.663321000	-1.412850000	0.000000000
6	-5.844808000	-0.725998000	0.000000000
6	-1.128915000	-0.729878000	0.000000000
6	-1.128915000	0.729878000	0.000000000
6	0.073600000	1.418862000	0.000000000
1	0.073081000	2.503175000	0.000000000
6	1.302793000	0.732350000	0.000000000
6	1.302793000	-0.732349000	0.000000000
6	0.073600000	-1.418862000	0.000000000
1	-4.649784000	2.498176000	0.000000000
1	-4.649784000	-2.498176000	0.000000000
1	0.073081000	-2.503175000	0.000000000
6	3.589582000	-0.730346000	0.000000000
6	3.589582000	0.730346000	0.000000000
6	4.808635000	1.419613000	0.000000000
6	4.808635000	-1.419614000	0.000000000
6	6.019543000	-0.729101000	0.000000000
6	6.019543000	0.729101000	0.000000000
1	4.808689000	2.503900000	0.000000000
1	4.808689000	-2.503900000	0.000000000
6	-8.292232000	0.703436000	0.000000000
6	-8.292232000	-0.703436000	0.000000000
6	-9.501974000	-1.392976000	0.000000000
6	-9.501974000	1.392976000	0.000000000
6	-10.703145000	-0.696188000	0.000000000
6	-10.703145000	0.696188000	0.000000000
1	-9.491588000	2.478908000	0.000000000
1	-9.491588000	-2.478908000	0.000000000
1	-11.639079000	-1.242882000	0.000000000
1	-11.639079000	1.242882000	0.000000000
6	8.303633000	0.728134000	0.000000000
6	8.303633000	-0.728134000	0.000000000
6	9.556923000	-1.414351000	0.000000000
6	9.556923000	1.414351000	0.000000000
6	10.725210000	-0.714378000	0.000000000
6	10.725210000	0.714378000	0.000000000
1	9.532955000	-2.498989000	0.000000000

1	9.532955000	2.498989000	0.000000000
1	11.674301000	1.241124000	0.000000000
1	11.674301000	-1.241124000	0.000000000
7	7.178749000	1.430381000	0.000000000
7	7.178749000	-1.430381000	0.000000000
7	2.441188000	1.432957000	0.000000000
7	2.441188000	-1.432957000	0.000000000
7	-2.295993000	1.432917000	0.000000000
7	-2.295993000	-1.432917000	0.000000000
7	-7.069398000	1.355292000	0.000000000
7	-7.069398000	-1.355292000	0.000000000
1	-7.072431000	2.364680000	0.000000000
1	-7.072431000	-2.364680000	0.000000000

Table S44: Coordinates of pB₄_4 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	5.932493000	-0.730016000	0.000000000
6	4.728030000	-1.422746000	0.000000000
6	3.502596000	-0.733210000	0.000000000
6	3.502596000	0.733210000	0.000000000
6	4.728030000	1.422746000	0.000000000
6	5.932493000	0.730016000	0.000000000
6	1.215839000	0.732966000	0.000000000
6	1.215839000	-0.732966000	0.000000000
6	0.000000000	-1.423830000	0.000000000
1	0.000000000	-2.507782000	0.000000000
6	-1.215839000	-0.732966000	0.000000000
6	-1.215839000	0.732966000	0.000000000
6	0.000000000	1.423830000	0.000000000
1	4.729339000	-2.506730000	0.000000000
1	4.729339000	2.506730000	0.000000000
1	0.000000000	2.507782000	0.000000000
6	-3.502596000	0.733210000	0.000000000
6	-3.502596000	-0.733210000	0.000000000
6	-4.728030000	-1.422746000	0.000000000
6	-4.728030000	1.422746000	0.000000000
6	-5.932493000	0.730016000	0.000000000
6	-5.932493000	-0.730016000	0.000000000
1	-4.729339000	-2.506730000	0.000000000
1	-4.729339000	2.506730000	0.000000000
6	8.216691000	-0.730340000	0.000000000
6	8.216691000	0.730340000	0.000000000
6	9.471164000	1.416782000	0.000000000
6	9.471164000	-1.416782000	0.000000000
6	10.637048000	0.715406000	0.000000000
6	10.637048000	-0.715406000	0.000000000

1	9.448444000	-2.501056000	0.000000000
1	9.448444000	2.501056000	0.000000000
1	11.586469000	1.240743000	0.000000000
1	11.586469000	-1.240742000	0.000000000
6	-8.216691000	-0.730340000	0.000000000
6	-8.216691000	0.730340000	0.000000000
6	-9.471164000	1.416782000	0.000000000
6	-9.471164000	-1.416782000	0.000000000
6	-10.637048000	0.715406000	0.000000000
6	-10.637048000	-0.715406000	0.000000000
1	-9.448444000	2.501056000	0.000000000
1	-9.448444000	-2.501056000	0.000000000
1	-11.586469000	-1.240742000	0.000000000
1	-11.586469000	1.240742000	0.000000000
7	-7.095229000	-1.431825000	0.000000000
7	-7.095229000	1.431825000	0.000000000
7	-2.363543000	-1.434204000	0.000000000
7	-2.363543000	1.434204000	0.000000000
7	2.363543000	-1.434204000	0.000000000
7	2.363543000	1.434204000	0.000000000
7	7.095229000	-1.431825000	0.000000000
7	7.095229000	1.431825000	0.000000000

Table S45: Coordinates of pB₅_1 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-3.666169000	0.699118000	0.187304000
6	-2.456695000	1.387335000	0.279926000
6	-1.252840000	0.702736000	0.395142000
6	-1.252840000	-0.702740000	0.395142000
6	-2.456695000	-1.387338000	0.279923000
6	-3.666169000	-0.699120000	0.187302000
6	1.164392000	-0.698345000	0.260948000
6	1.164392000	0.698340000	0.260948000
6	2.350899000	1.384205000	0.015865000
1	2.350902000	2.471371000	0.019296000
6	3.537045000	0.699728000	-0.232650000
6	3.537045000	-0.699733000	-0.232648000
6	2.350900000	-1.384209000	0.015868000
1	-2.458410000	2.474019000	0.277800000
1	-2.458411000	-2.474022000	0.277794000
1	2.350903000	-2.471376000	0.019302000
6	5.948642000	-0.698573000	-0.281620000
6	5.948641000	0.698571000	-0.281625000
6	7.144199000	1.384381000	-0.083977000
6	7.144200000	-1.384381000	-0.083968000
6	8.338659000	-0.698959000	0.114833000

6	8.338659000	0.698961000	0.114828000
1	7.144366000	2.471580000	-0.083924000
1	7.144368000	-2.471580000	-0.083908000
6	-6.110669000	0.721379000	0.040668000
6	-6.110669000	-0.721379000	0.040664000
6	-7.296284000	-1.406658000	-0.009674000
6	-7.296283000	1.406659000	-0.009664000
6	-8.540349000	-0.724576000	-0.062544000
6	-8.540348000	0.724577000	-0.062538000
1	-7.310533000	2.492288000	-0.008629000
1	-7.310534000	-2.492287000	-0.008646000
6	10.757071000	0.703324000	0.093529000
6	10.757072000	-0.703319000	0.093535000
6	11.943851000	-1.387303000	-0.135211000
6	11.943849000	1.387307000	-0.135223000
6	13.136079000	-0.693160000	-0.341985000
6	13.136078000	0.693164000	-0.341991000
1	11.933702000	-2.474002000	-0.139152000
1	11.933699000	2.474006000	-0.139174000
1	14.055931000	1.243865000	-0.505598000
1	14.055932000	-1.243862000	-0.505586000
7	9.551219000	1.361687000	0.371778000
7	9.551220000	-1.361682000	0.371789000
7	4.736201000	1.366132000	-0.537944000
7	4.736202000	-1.366137000	-0.537937000
7	-0.033118000	1.367186000	0.569275000
7	-0.033119000	-1.367190000	0.569274000
7	-4.886546000	1.357736000	0.087464000
7	-4.886547000	-1.357737000	0.087458000
7	-9.671531000	1.426281000	-0.107111000
7	-9.671532000	-1.426279000	-0.107124000
6	-10.820989000	0.717860000	-0.150823000
6	-10.820989000	-0.717857000	-0.150830000
6	-12.058827000	1.404249000	-0.197676000
6	-12.058827000	-1.404245000	-0.197691000
6	-13.240110000	0.706998000	-0.241650000
6	-13.240110000	-0.706993000	-0.241658000
1	-4.886934000	-2.365514000	0.106466000
1	-4.886933000	2.365513000	0.106474000
1	-0.043912000	2.353424000	0.354982000
1	-0.043913000	-2.353429000	0.354981000
1	4.741313000	2.349371000	-0.307417000
1	4.741316000	-2.349375000	-0.307405000
1	9.551193000	2.351813000	0.174310000
1	9.551195000	-2.351809000	0.174328000
1	-12.034086000	-2.489402000	-0.197027000
1	-14.184524000	-1.241162000	-0.277707000

1	-14.184524000	1.241167000	-0.277692000
1	-12.034085000	2.489405000	-0.197000000

Table S46: Coordinates of pB₅_2 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-3.821687000	0.729784000	0.000054000
6	-2.574114000	1.409805000	0.000042000
6	-1.389864000	0.723057000	0.000022000
6	-1.389864000	-0.723057000	0.000022000
6	-2.574114000	-1.409805000	0.000042000
6	-3.821687000	-0.729784000	0.000054000
6	1.057010000	-0.699759000	-0.000049000
6	1.057010000	0.699759000	-0.000049000
6	2.271821000	1.390242000	-0.000102000
1	2.269784000	2.476462000	-0.000102000
6	3.479987000	0.706534000	-0.000183000
6	3.479987000	-0.706534000	-0.000183000
6	2.271821000	-1.390242000	-0.000102000
1	-2.588148000	2.495443000	0.000040000
1	-2.588148000	-2.495443000	0.000040000
1	2.269784000	-2.476462000	-0.000102000
6	5.925980000	-0.698643000	-0.000199000
6	5.925980000	0.698643000	-0.000199000
6	7.139232000	1.385336000	-0.000133000
6	7.139232000	-1.385336000	-0.000133000
6	8.351223000	-0.701577000	-0.000098000
6	8.351223000	0.701577000	-0.000098000
1	7.138640000	2.471929000	-0.000134000
1	7.138640000	-2.471929000	-0.000134000
6	-6.108704000	0.727502000	0.000064000
6	-6.108704000	-0.727502000	0.000064000
6	-7.317502000	-1.414702000	0.000060000
6	-7.317502000	1.414702000	0.000060000
6	-8.540598000	-0.727641000	0.000054000
6	-8.540598000	0.727641000	0.000054000
1	-7.317510000	2.499204000	0.000059000
1	-7.317510000	-2.499204000	0.000059000
6	10.800300000	0.704522000	0.000081000
6	10.800300000	-0.704522000	0.000081000
6	12.009104000	-1.387357000	0.000235000
6	12.009104000	1.387357000	0.000235000
6	13.220230000	-0.692383000	0.000378000
6	13.220230000	0.692383000	0.000378000
1	11.999704000	-2.473832000	0.000235000
1	11.999704000	2.473832000	0.000235000
1	14.153620000	1.243962000	0.000492000

1	14.153620000	-1.243961000	0.000492000
7	9.574793000	1.366431000	-0.000094000
7	9.574793000	-1.366431000	-0.000094000
7	4.700651000	1.366228000	-0.000303000
7	4.700651000	-1.366228000	-0.000303000
7	-0.163575000	1.354650000	-0.000005000
7	-0.163575000	-1.354650000	-0.000005000
7	-4.944355000	1.432369000	0.000061000
7	-4.944355000	-1.432369000	0.000061000
7	-9.691576000	1.429018000	0.000044000
7	-9.691576000	-1.429018000	0.000044000
6	-10.824773000	0.723940000	0.000034000
6	-10.824773000	-0.723940000	0.000034000
6	-12.073613000	1.409942000	0.000021000
6	-12.073613000	-1.409942000	0.000021000
6	-13.247376000	0.711690000	0.000008000
6	-13.247376000	-0.711690000	0.000008000
1	-0.162829000	2.363313000	-0.000020000
1	-0.162829000	-2.363313000	-0.000020000
1	4.702404000	2.372488000	-0.000224000
1	4.702404000	-2.372488000	-0.000224000
1	9.576798000	2.372656000	-0.000025000
1	9.576798000	-2.372656000	-0.000025000
1	-12.048819000	-2.494891000	0.000021000
1	-14.195150000	-1.241241000	-0.000002000
1	-14.195150000	1.241241000	-0.000002000
1	-12.048819000	2.494891000	0.000021000

Table S47: Coordinates of pB₅_3 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-3.744156000	0.732449000	-0.000016000
6	-2.514139000	1.417898000	-0.000012000
6	-1.310794000	0.730218000	-0.000009000
6	-1.310794000	-0.730218000	-0.000009000
6	-2.514139000	-1.417898000	-0.000012000
6	-3.744156000	-0.732449000	-0.000016000
6	0.976201000	-0.731384000	0.000026000
6	0.976201000	0.731384000	0.000026000
6	2.223664000	1.411651000	0.000014000
1	2.209538000	2.497173000	0.000012000
6	3.406589000	0.724250000	0.000013000
6	3.406589000	-0.724250000	0.000013000
6	2.223664000	-1.411651000	0.000014000
1	-2.513826000	2.502242000	-0.000010000
1	-2.513826000	-2.502242000	-0.000010000
1	2.209538000	-2.497173000	0.000012000

6	5.851804000	-0.700498000	0.000030000
6	5.851804000	0.700498000	0.000030000
6	7.066224000	1.391574000	0.000044000
6	7.066224000	-1.391574000	0.000044000
6	8.272383000	-0.706887000	0.000065000
6	8.272383000	0.706887000	0.000065000
1	7.064536000	2.477592000	0.000045000
1	7.064536000	-2.477592000	0.000045000
6	-6.031641000	0.730051000	-0.000022000
6	-6.031641000	-0.730051000	-0.000022000
6	-7.250023000	-1.418635000	-0.000018000
6	-7.250023000	1.418635000	-0.000018000
6	-8.462702000	-0.729001000	-0.000017000
6	-8.462702000	0.729001000	-0.000017000
1	-7.250002000	2.502969000	-0.000016000
1	-7.250002000	-2.502969000	-0.000016000
6	10.720194000	0.703598000	0.000010000
6	10.720194000	-0.703598000	0.000010000
6	11.928058000	-1.388956000	-0.000067000
6	11.928058000	1.388956000	-0.000067000
6	13.136457000	-0.693220000	-0.000139000
6	13.136457000	0.693220000	-0.000139000
1	11.918658000	-2.475186000	-0.000067000
1	11.918658000	2.475187000	-0.000067000
1	14.070423000	1.243483000	-0.000196000
1	14.070423000	-1.243483000	-0.000196000
7	9.493831000	1.363957000	0.000104000
7	9.493831000	-1.363957000	0.000104000
7	4.632530000	1.354253000	0.000016000
7	4.632530000	-1.354253000	0.000016000
7	-0.144212000	1.433561000	0.000010000
7	-0.144212000	-1.433561000	0.000010000
7	-4.882059000	1.433379000	-0.000018000
7	-4.882059000	-1.433379000	-0.000018000
7	-9.620896000	1.430422000	-0.000011000
7	-9.620896000	-1.430422000	-0.000011000
6	-10.747145000	0.727187000	-0.000006000
6	-10.747145000	-0.727187000	-0.000006000
6	-11.999903000	1.413296000	0.000003000
6	-11.999903000	-1.413296000	0.000003000
6	-13.169432000	0.713898000	0.000010000
6	-13.169432000	-0.713897000	0.000010000
1	4.633472000	2.363322000	0.000013000
1	4.633472000	-2.363322000	0.000013000
1	9.497049000	2.370910000	0.000042000
1	9.497049000	-2.370910000	0.000042000
1	-11.975664000	-2.498030000	0.000003000

1	-14.118382000	-1.241126000	0.000016000
1	-14.118382000	1.241126000	0.000016000
1	-11.975664000	2.498030000	0.000003000

Table S48: Coordinates of pB_s_4 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-0.000001000	3.663127000	0.732978000
6	-0.000001000	2.442989000	1.421960000
6	-0.000001000	1.230971000	0.731896000
6	-0.000001000	1.230971000	-0.731896000
6	-0.000001000	2.442989000	-1.421960000
6	-0.000001000	3.663127000	-0.732978000
6	-0.000002000	-1.056497000	-0.733867000
6	-0.000002000	-1.056497000	0.733867000
6	-0.000001000	-2.287976000	1.420052000
1	-0.000001000	-2.288727000	2.504262000
6	-0.000001000	-3.488495000	0.730686000
6	-0.000001000	-3.488495000	-0.730686000
6	-0.000001000	-2.287976000	-1.420052000
1	-0.000001000	2.442424000	2.506116000
1	-0.000001000	2.442424000	-2.506116000
1	-0.000001000	-2.288727000	-2.504262000
6	-0.000001000	-5.774791000	-0.732601000
6	-0.000001000	-5.774791000	0.732601000
6	0.000000000	-7.022867000	1.413480000
6	0.000000000	-7.022867000	-1.413480000
6	0.000001000	-8.204243000	-0.726338000
6	0.000001000	-8.204243000	0.726338000
1	0.000000000	-7.008592000	2.498734000
1	0.000000000	-7.008592000	-2.498734000
6	-0.000001000	5.950183000	0.731924000
6	-0.000001000	5.950183000	-0.731924000
6	-0.000001000	7.173715000	-1.421349000
6	-0.000001000	7.173715000	1.421349000
6	-0.000001000	8.380300000	-0.729680000
6	-0.000001000	8.380300000	0.729680000
1	-0.000001000	7.174286000	2.505537000
1	-0.000001000	7.174286000	-2.505537000
6	0.000003000	-10.650873000	0.703423000
6	0.000003000	-10.650873000	-0.703423000
6	0.000003000	-11.860689000	-1.393560000
6	0.000003000	-11.860689000	1.393560000
6	0.000004000	-13.061258000	-0.696450000
6	0.000004000	-13.061258000	0.696450000
1	0.000003000	-11.850872000	-2.479419000
1	0.000003000	-11.850872000	2.479419000

1	0.000004000	-13.997348000	1.242881000
1	0.000004000	-13.997348000	-1.242881000
7	0.000003000	-9.428396000	1.355335000
7	0.000003000	-9.428396000	-1.355335000
7	-0.000001000	-4.656364000	1.433766000
7	-0.000001000	-4.656364000	-1.433766000
7	-0.000001000	0.078066000	1.434456000
7	-0.000001000	0.078066000	-1.434456000
7	-0.000001000	4.808132000	1.433943000
7	-0.000001000	4.808132000	-1.433943000
7	-0.000001000	9.542254000	1.431496000
7	-0.000001000	9.542254000	-1.431496000
6	-0.000001000	10.664714000	0.729396000
6	-0.000001000	10.664714000	-0.729396000
6	0.000000000	11.919358000	1.415731000
6	0.000000000	11.919358000	-1.415731000
6	0.000001000	13.086197000	0.715211000
6	0.000001000	13.086197000	-0.715211000
1	0.000003000	-9.431749000	2.364819000
1	0.000003000	-9.431749000	-2.364819000
1	0.000001000	11.895655000	-2.500268000
1	0.000002000	14.035886000	-1.240861000
1	0.000002000	14.035886000	1.240861000
1	0.000001000	11.895655000	2.500268000

Table S49: Coordinates of pB₅_5 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-3.575717000	0.733405000	0.000019000
6	-2.362252000	1.424571000	0.000023000
6	-1.143728000	0.734425000	0.000020000
6	-1.143728000	-0.734425000	0.000012000
6	-2.362252000	-1.424572000	0.000007000
6	-3.575717000	-0.733405000	0.000011000
6	1.143728000	-0.734425000	0.000012000
6	1.143728000	0.734425000	0.000020000
6	2.362252000	1.424571000	0.000023000
1	2.362634000	2.508483000	0.000025000
6	3.575717000	0.733405000	0.000019000
6	3.575717000	-0.733405000	0.000011000
6	2.362252000	-1.424572000	0.000007000
1	-2.362634000	2.508483000	0.000025000
1	-2.362634000	-2.508483000	-0.000004000
1	2.362634000	-2.508483000	-0.000003000
6	5.862527000	-0.733998000	0.000003000
6	5.862527000	0.733998000	0.000011000
6	7.088906000	1.423161000	0.000015000

6	7.088906000	-1.423161000	-0.000001000
6	8.292212000	-0.730449000	-0.000001000
6	8.292212000	0.730449000	0.000007000
1	7.090228000	2.507153000	0.000023000
1	7.090228000	-2.507153000	-0.000004000
6	-5.862527000	0.733998000	0.000011000
6	-5.862527000	-0.733998000	0.000002000
6	-7.088906000	-1.423161000	-0.000002000
6	-7.088906000	1.423161000	0.000014000
6	-8.292212000	-0.730449000	-0.000002000
6	-8.292212000	0.730449000	0.000006000
1	-7.090228000	2.507153000	0.000023000
1	-7.090228000	-2.507153000	-0.000005000
6	10.576106000	0.730891000	-0.000005000
6	10.576106000	-0.730891000	-0.000013000
6	11.831124000	-1.417143000	-0.000027000
6	11.831124000	1.417143000	-0.000011000
6	12.996570000	-0.715764000	-0.000043000
6	12.996570000	0.715765000	-0.000034000
1	11.808045000	-2.501458000	-0.000025000
1	11.808045000	2.501458000	0.000004000
1	13.946211000	1.241090000	-0.000044000
1	13.946211000	-1.241090000	-0.000058000
7	9.455553000	1.432024000	0.000004000
7	9.455553000	-1.432024000	-0.000012000
7	4.725097000	1.434435000	0.000017000
7	4.725097000	-1.434435000	0.000001000
7	0.000000000	1.435225000	0.000022000
7	0.000000000	-1.435225000	0.000006000
7	-4.725097000	1.434435000	0.000017000
7	-4.725097000	-1.434435000	0.000001000
7	-9.455553000	1.432024000	0.000004000
7	-9.455553000	-1.432024000	-0.000013000
6	-10.576106000	0.730891000	-0.000006000
6	-10.576106000	-0.730891000	-0.000014000
6	-11.831124000	1.417143000	-0.000012000
6	-11.831124000	-1.417143000	-0.000029000
6	-12.996570000	0.715765000	-0.000036000
6	-12.996570000	-0.715764000	-0.000044000
1	-11.808045000	-2.501458000	-0.000026000
1	-13.946211000	-1.241090000	-0.000060000
1	-13.946211000	1.241090000	-0.000045000
1	-11.808045000	2.501458000	0.000003000

Table S50: Coordinates of pB₆_1 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
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6	6.001683000	0.700241000	0.000113000
6	4.786843000	1.382674000	0.000396000
6	3.572213000	0.698926000	0.000666000
6	3.572213000	-0.698926000	0.000666000
6	4.786843000	-1.382674000	0.000396000
6	6.001683000	-0.700241000	0.000113000
6	1.125003000	-0.701602000	0.000856000
6	1.125003000	0.701602000	0.000856000
6	-0.089268000	1.383603000	0.000777000
1	-0.090281000	2.470505000	0.000768000
6	-1.303424000	0.698102000	0.000694000
6	-1.303424000	-0.698102000	0.000694000
6	-0.089268000	-1.383603000	0.000777000
1	4.786511000	2.469698000	0.000387000
1	4.786511000	-2.469698000	0.000387000
1	-0.090281000	-2.470505000	0.000768000
6	-3.750721000	-0.705110000	0.000518000
6	-3.750721000	0.705110000	0.000518000
6	-4.960858000	1.387724000	0.000423000
6	-4.960858000	-1.387724000	0.000423000
6	-6.175596000	-0.698065000	0.000317000
6	-6.175596000	0.698065000	0.000317000
1	-4.962996000	2.474256000	0.000417000
1	-4.962996000	-2.474256000	0.000417000
6	8.449045000	0.699941000	-0.000272000
6	8.449045000	-0.699941000	-0.000272000
6	9.663669000	-1.382936000	-0.000373000
6	9.663669000	1.382936000	-0.000373000
6	10.877493000	-0.698810000	-0.000517000
6	10.877493000	0.698810000	-0.000517000
1	9.664178000	2.469924000	-0.000380000
1	9.664178000	-2.469924000	-0.000380000
6	-8.624685000	0.721021000	0.000047000
6	-8.624685000	-0.721021000	0.000047000
6	-9.811977000	-1.406381000	-0.000109000
6	-9.811977000	1.406381000	-0.000109000
6	-11.057283000	-0.724706000	-0.000272000
6	-11.057283000	0.724706000	-0.000272000
1	-9.826022000	-2.492070000	-0.000115000
1	-9.826022000	2.492070000	-0.000115000
7	-7.399436000	1.357062000	0.000204000
7	-7.399436000	-1.357063000	0.000204000
7	-2.529422000	1.367994000	0.000594000
7	-2.529422000	-1.367994000	0.000594000
7	2.347094000	1.370099000	0.000957000
7	2.347094000	-1.370099000	0.000957000
7	7.225074000	1.370498000	-0.000232000

7	7.225074000	-1.370498000	-0.000232000
7	12.103849000	1.367265000	-0.000717000
7	12.103849000	-1.367265000	-0.000717000
6	13.327583000	0.705538000	-0.000556000
6	13.327583000	-0.705538000	-0.000556000
6	14.537690000	1.386618000	-0.000435000
6	14.537690000	-1.386618000	-0.000435000
6	15.750215000	0.692057000	-0.000340000
6	15.750215000	-0.692056000	-0.000340000
1	12.104874000	-2.373183000	-0.000613000
1	12.104874000	2.373183000	-0.000613000
1	7.225293000	-2.375839000	0.000009000
1	7.225293000	2.375839000	0.000009000
1	2.347801000	2.375514000	0.000726000
1	2.347801000	-2.375514000	0.000726000
1	-2.527923000	2.373793000	0.000621000
1	-2.527923000	-2.373793000	0.000621000
1	-7.398698000	2.364966000	0.000175000
1	-7.398698000	-2.364966000	0.000175000
1	14.528146000	-2.473270000	-0.000432000
1	16.683385000	-1.244319000	-0.000260000
1	16.683385000	1.244320000	-0.000260000
1	14.528146000	2.473271000	-0.000432000
7	-12.189399000	-1.426786000	-0.000429000
7	-12.189399000	1.426786000	-0.000429000
6	-13.340194000	-0.717727000	-0.000589000
6	-13.340194000	0.717727000	-0.000589000
6	-14.578739000	-1.403658000	-0.000765000
6	-14.578739000	1.403658000	-0.000765000
6	-15.761707000	-0.706648000	-0.000933000
6	-15.761707000	0.706649000	-0.000933000
1	-14.553906000	-2.488876000	-0.000762000
1	-16.706591000	-1.241313000	-0.001067000
1	-16.706591000	1.241313000	-0.001067000
1	-14.553906000	2.488876000	-0.000762000

Table S51: Coordinates of pB₆_2 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-5.885812000	0.700799000	-0.213679000
6	-4.697168000	1.385024000	0.021689000
6	-3.507547000	0.698358000	0.249773000
6	-3.507547000	-0.698359000	0.249775000
6	-4.697168000	-1.385025000	0.021693000
6	-5.885813000	-0.700801000	-0.213676000
6	-1.085327000	-0.705116000	0.404773000
6	-1.085327000	0.705116000	0.404772000

6	0.119778000	1.389815000	0.325073000
1	0.121695000	2.476203000	0.321784000
6	1.332028000	0.700245000	0.266813000
6	1.332028000	-0.700246000	0.266813000
6	0.119778000	-1.389815000	0.325075000
1	-4.696739000	2.471997000	0.025026000
1	-4.696740000	-2.471998000	0.025032000
1	0.121695000	-2.476203000	0.321787000
6	3.776524000	-0.723401000	0.156435000
6	3.776524000	0.723400000	0.156435000
6	4.959636000	1.410061000	0.107619000
6	4.959636000	-1.410062000	0.107618000
6	6.205943000	-0.729958000	0.057838000
6	6.205943000	0.729958000	0.057838000
1	4.973344000	2.495654000	0.107755000
1	4.973344000	-2.495655000	0.107755000
6	-8.300464000	0.698315000	-0.269914000
6	-8.300465000	-0.698316000	-0.269911000
6	-9.498942000	-1.384594000	-0.092694000
6	-9.498941000	1.384595000	-0.092700000
6	-10.696293000	-0.699393000	0.087551000
6	-10.696293000	0.699394000	0.087548000
1	-9.499000000	2.471707000	-0.093905000
1	-9.499001000	-2.471707000	-0.093895000
6	8.491152000	0.727631000	-0.027780000
6	8.491152000	-0.727631000	-0.027780000
6	9.699130000	-1.414930000	-0.070165000
6	9.699130000	1.414930000	-0.070163000
6	10.921234000	-0.727786000	-0.111064000
6	10.921234000	0.727786000	-0.111063000
1	9.699146000	-2.499448000	-0.069592000
1	9.699145000	2.499448000	-0.069589000
7	7.327737000	1.432093000	0.014805000
7	7.327737000	-1.432093000	0.014804000
7	2.551862000	1.354972000	0.205687000
7	2.551862000	-1.354973000	0.205687000
7	-2.306608000	1.365542000	0.534359000
7	-2.306608000	-1.365542000	0.534362000
7	-7.084963000	1.366609000	-0.506280000
7	-7.084964000	-1.366612000	-0.506275000
7	-11.911861000	1.361437000	0.324742000
7	-11.911862000	-1.361434000	0.324748000
6	-13.114372000	0.703138000	0.030875000
6	-13.114373000	-0.703136000	0.030878000
6	-14.297512000	1.387486000	-0.214278000
6	-14.297513000	-1.387485000	-0.214272000
6	-15.486416000	0.693162000	-0.438376000

6	-15.486416000	-0.693161000	-0.438373000
1	-11.909280000	-2.352263000	0.131065000
1	-11.909279000	2.352265000	0.131055000
1	-7.091010000	-2.351285000	-0.283100000
1	-7.091009000	2.351283000	-0.283108000
1	-2.296439000	2.357535000	0.351446000
1	-2.296439000	-2.357535000	0.351450000
1	2.551447000	2.363644000	0.212130000
1	2.551448000	-2.363644000	0.212132000
1	-14.287354000	-2.474145000	-0.217951000
1	-16.403820000	-1.243780000	-0.615087000
1	-16.403820000	1.243780000	-0.615092000
1	-14.287353000	2.474146000	-0.217961000
7	12.071652000	-1.428874000	-0.147960000
7	12.071652000	1.428874000	-0.147958000
6	13.204090000	-0.724122000	-0.182930000
6	13.204090000	0.724123000	-0.182928000
6	14.452265000	-1.410125000	-0.221241000
6	14.452264000	1.410125000	-0.221239000
6	15.625251000	-0.711731000	-0.256438000
6	15.625251000	0.711732000	-0.256436000
1	14.427765000	-2.495043000	-0.220763000
1	16.572477000	-1.241350000	-0.285676000
1	16.572477000	1.241351000	-0.285673000
1	14.427765000	2.495044000	-0.220759000

Table S52: Coordinates of pB₆_3 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-5.853065000	0.706077000	-0.411744000
6	-4.647071000	1.391362000	-0.367831000
6	-3.433717000	0.701356000	-0.341923000
6	-3.433718000	-0.701356000	-0.341924000
6	-4.647071000	-1.391362000	-0.367832000
6	-5.853065000	-0.706077000	-0.411745000
6	-0.988939000	-0.723656000	-0.269930000
6	-0.988939000	0.723656000	-0.269930000
6	0.193395000	1.411274000	-0.229580000
1	0.207112000	2.496843000	-0.228916000
6	1.439724000	0.731024000	-0.186772000
6	1.439724000	-0.731024000	-0.186773000
6	0.193395000	-1.411275000	-0.229581000
1	-4.645241000	2.477547000	-0.362934000
1	-4.645241000	-2.477547000	-0.362936000
1	0.207112000	-2.496843000	-0.228918000
6	3.725340000	-0.730503000	-0.106762000
6	3.725340000	0.730503000	-0.106762000

6	4.928748000	1.417658000	-0.064661000
6	4.928748000	-1.417658000	-0.064661000
6	6.157689000	-0.732636000	-0.022261000
6	6.157689000	0.732636000	-0.022261000
1	4.928390000	2.502061000	-0.064918000
1	4.928390000	-2.502061000	-0.064919000
6	-8.273704000	0.698615000	-0.202931000
6	-8.273704000	-0.698614000	-0.202932000
6	-9.459658000	-1.386588000	0.042849000
6	-9.459658000	1.386588000	0.042851000
6	-10.642695000	-0.701350000	0.297912000
6	-10.642694000	0.701350000	0.297913000
1	-9.459191000	2.473287000	0.041086000
1	-9.459191000	-2.473288000	0.041083000
6	8.444317000	0.730334000	0.053545000
6	8.444317000	-0.730334000	0.053545000
6	9.661917000	-1.418420000	0.093011000
6	9.661917000	1.418420000	0.093011000
6	10.874688000	-0.729319000	0.130822000
6	10.874688000	0.729319000	0.130822000
1	9.662005000	-2.502808000	0.092754000
1	9.662005000	2.502808000	0.092754000
7	7.295248000	1.433475000	0.015921000
7	7.295248000	-1.433475000	0.015921000
7	2.560162000	1.433359000	-0.147721000
7	2.560162000	-1.433359000	-0.147722000
7	-2.214713000	1.354202000	-0.311429000
7	-2.214713000	-1.354202000	-0.311430000
7	-7.076706000	1.363801000	-0.496062000
7	-7.076706000	-1.363800000	-0.496063000
7	-11.836237000	1.362204000	0.608023000
7	-11.836237000	-1.362204000	0.608021000
6	-13.062308000	0.702796000	0.449374000
6	-13.062309000	-0.702796000	0.449373000
6	-14.264711000	1.388013000	0.337991000
6	-14.264712000	-1.388013000	0.337988000
6	-15.470335000	0.693211000	0.245699000
6	-15.470335000	-0.693211000	0.245698000
1	-11.849853000	-2.355933000	0.432685000
1	-11.849852000	2.355932000	0.432689000
1	-7.064839000	-2.359980000	-0.339115000
1	-7.064839000	2.359980000	-0.339112000
1	-2.215102000	2.363220000	-0.312716000
1	-2.215102000	-2.363220000	-0.312718000
1	-14.255151000	-2.474520000	0.335150000
1	-16.401606000	-1.243421000	0.170842000
1	-16.401606000	1.243422000	0.170844000

1	-14.255151000	2.474520000	0.335154000
7	12.031713000	-1.430338000	0.165404000
7	12.031713000	1.430338000	0.165404000
6	13.158221000	-0.726897000	0.197727000
6	13.158221000	0.726897000	0.197727000
6	14.409880000	-1.412811000	0.233729000
6	14.409880000	1.412811000	0.233729000
6	15.579550000	-0.713565000	0.266677000
6	15.579550000	0.713565000	0.266676000
1	14.385846000	-2.497580000	0.233354000
1	16.527780000	-1.241362000	0.294180000
1	16.527780000	1.241362000	0.294180000
1	14.385846000	2.497580000	0.233354000

Table S53: Coordinates of pB₆_4 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-5.771655000	-0.724408000	-0.167734000
6	-4.589344000	-1.412446000	-0.155592000
6	-3.342694000	-0.731752000	-0.141330000
6	-3.342694000	0.731752000	-0.141330000
6	-4.589344000	1.412446000	-0.155592000
6	-5.771655000	0.724408000	-0.167734000
6	-1.056243000	0.731401000	-0.110873000
6	-1.056243000	-0.731401000	-0.110873000
6	0.145925000	-1.419138000	-0.093774000
1	0.145403000	-2.503447000	-0.093674000
6	1.376842000	-0.734095000	-0.075276000
6	1.376842000	0.734095000	-0.075276000
6	0.145925000	1.419138000	-0.093774000
1	-4.575431000	-2.497908000	-0.154742000
1	-4.575431000	2.497908000	-0.154742000
1	0.145403000	2.503447000	-0.093674000
6	3.664793000	0.732351000	-0.039162000
6	3.664793000	-0.732351000	-0.039162000
6	4.876631000	-1.421156000	-0.019466000
6	4.876631000	1.421156000	-0.019466000
6	6.097880000	0.733499000	0.000295000
6	6.097880000	-0.733499000	0.000295000
1	4.876053000	-2.505398000	-0.019517000
1	4.876053000	2.505398000	-0.019517000
6	-8.216312000	-0.701522000	-0.174674000
6	-8.216312000	0.701522000	-0.174674000
6	-9.429772000	1.392545000	-0.165341000
6	-9.429772000	-1.392545000	-0.165341000
6	-10.634823000	0.706542000	-0.172622000
6	-10.634823000	-0.706542000	-0.172622000

1	-9.427982000	-2.478561000	-0.160326000
1	-9.427982000	2.478561000	-0.160326000
6	8.385268000	-0.731760000	0.035848000
6	8.385268000	0.731760000	0.035848000
6	9.607447000	1.420569000	0.054458000
6	9.607447000	-1.420569000	0.054459000
6	10.815805000	0.729866000	0.072075000
6	10.815806000	-0.729866000	0.072075000
1	9.607964000	2.504839000	0.054339000
1	9.607964000	-2.504839000	0.054339000
7	7.241812000	-1.434039000	0.018318000
7	7.241812000	1.434039000	0.018318000
7	2.511766000	-1.434733000	-0.057635000
7	2.511766000	1.434733000	-0.057635000
7	-2.222572000	-1.433771000	-0.127027000
7	-2.222572000	1.433771000	-0.127027000
7	-6.997557000	-1.354043000	-0.179185000
7	-6.997557000	1.354043000	-0.179185000
7	-11.861534000	-1.359921000	-0.214476000
7	-11.861534000	1.359921000	-0.214476000
6	-13.050969000	-0.702592000	0.112074000
6	-13.050969000	0.702592000	0.112074000
6	-14.222662000	-1.389657000	0.401667000
6	-14.222662000	1.389657000	0.401667000
6	-15.397601000	-0.693679000	0.678969000
6	-15.397601000	0.693679000	0.678969000
1	-11.850807000	2.361334000	-0.094526000
1	-11.850807000	-2.361334000	-0.094526000
1	-6.998246000	2.363321000	-0.178800000
1	-6.998246000	-2.363321000	-0.178800000
1	-14.212822000	2.475888000	0.402819000
1	-16.306602000	1.243095000	0.895761000
1	-16.306602000	-1.243095000	0.895761000
1	-14.212822000	-2.475888000	0.402819000
7	11.976339000	1.431120000	0.088226000
7	11.976339000	-1.431120000	0.088226000
6	13.100050000	0.728612000	0.103127000
6	13.100050000	-0.728611000	0.103127000
6	14.353781000	1.414722000	0.119777000
6	14.353781000	-1.414722000	0.119777000
6	15.521623000	0.714656000	0.134878000
6	15.521623000	-0.714656000	0.134878000
1	14.330100000	2.499346000	0.119623000
1	16.470784000	1.241178000	0.147556000
1	16.470784000	-1.241178000	0.147556000
1	14.330100000	-2.499346000	0.119623000

Table S54: Coordinates of pB₆_5 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	5.848574000	0.731327000	0.000513000
6	4.648358000	1.420620000	0.000581000
6	3.416672000	0.734647000	0.000657000
6	3.416672000	-0.734647000	0.000657000
6	4.648358000	-1.420620000	0.000581000
6	5.848574000	-0.731327000	0.000513000
6	1.128988000	-0.732827000	0.000567000
6	1.128988000	0.732827000	0.000567000
6	-0.080813000	1.422981000	0.000531000
1	-0.079973000	2.507122000	0.000530000
6	-1.303728000	0.734730000	0.000474000
6	-1.303728000	-0.734730000	0.000474000
6	-0.080813000	-1.422981000	0.000531000
1	4.649244000	2.504829000	0.000568000
1	4.649244000	-2.504829000	0.000568000
1	-0.079973000	-2.507122000	0.000531000
6	-3.591621000	-0.733409000	0.000287000
6	-3.591621000	0.733409000	0.000287000
6	-4.807680000	1.423487000	0.000177000
6	-4.807680000	-1.423487000	0.000177000
6	-6.023970000	-0.733539000	0.000060000
6	-6.023970000	0.733539000	0.000060000
1	-4.807532000	2.507610000	0.000182000
1	-4.807532000	-2.507610000	0.000182000
6	8.134670000	0.732844000	0.000324000
6	8.134670000	-0.732844000	0.000324000
6	9.382111000	-1.413863000	0.000070000
6	9.382111000	1.413863000	0.000070000
6	10.563445000	-0.726445000	-0.000233000
6	10.563445000	0.726445000	-0.000233000
1	9.368140000	2.499099000	0.000074000
1	9.368140000	-2.499099000	0.000074000
6	-8.311162000	0.732936000	-0.000147000
6	-8.311162000	-0.732936000	-0.000147000
6	-9.536130000	-1.422325000	-0.000220000
6	-9.536130000	1.422325000	-0.000220000
6	-10.741110000	-0.730206000	-0.000292000
6	-10.741110000	0.730206000	-0.000292000
1	-9.537147000	-2.506488000	-0.000205000
1	-9.537146000	2.506488000	-0.000205000
7	-7.171472000	1.434368000	-0.000050000
7	-7.171472000	-1.434368000	-0.000050000
7	-2.444536000	1.435120000	0.000409000
7	-2.444536000	-1.435120000	0.000409000
7	2.283061000	1.434946000	0.000605000

7	2.283061000	-1.434946000	0.000605000
7	7.016120000	1.433853000	0.000435000
7	7.016120000	-1.433853000	0.000435000
7	11.787367000	1.355173000	-0.000523000
7	11.787367000	-1.355173000	-0.000523000
6	13.009519000	0.703515000	-0.000626000
6	13.009519000	-0.703515000	-0.000626000
6	14.219375000	1.393829000	-0.000734000
6	14.219375000	-1.393829000	-0.000734000
6	15.419444000	0.696629000	-0.000877000
6	15.419444000	-0.696629000	-0.000877000
1	11.790661000	-2.364771000	-0.000735000
1	11.790661000	2.364772000	-0.000735000
1	14.209416000	-2.479658000	-0.000700000
1	16.355666000	-1.242752000	-0.000950000
1	16.355666000	1.242752000	-0.000950000
1	14.209416000	2.479658000	-0.000700000
7	-11.903733000	-1.431796000	-0.000344000
7	-11.903733000	1.431796000	-0.000344000
6	-13.025426000	-0.730026000	-0.000391000
6	-13.025426000	0.730026000	-0.000391000
6	-14.280220000	-1.416361000	-0.000455000
6	-14.280220000	1.416361000	-0.000455000
6	-15.446467000	-0.715453000	-0.000510000
6	-15.446467000	0.715453000	-0.000510000
1	-14.256885000	-2.500840000	-0.000458000
1	-16.396208000	-1.240894000	-0.000559000
1	-16.396208000	1.240895000	-0.000559000
1	-14.256885000	2.500840000	-0.000458000

Table S55: Coordinates of pB₆_6 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	5.935437000	0.733629000	0.000000000
6	4.723213000	1.425296000	0.000001000
6	3.503674000	0.734910000	0.000000000
6	3.503674000	-0.734910000	0.000000000
6	4.723213000	-1.425296000	0.000001000
6	5.935437000	-0.733629000	0.000000000
6	1.216105000	-0.734754000	-0.000005000
6	1.216105000	0.734754000	-0.000005000
6	-0.000001000	1.425681000	-0.000009000
1	-0.000003000	2.509732000	-0.000009000
6	-1.216103000	0.734752000	-0.000013000
6	-1.216103000	-0.734752000	-0.000013000
6	-0.000001000	-1.425682000	-0.000009000
1	4.723895000	2.509352000	0.000005000

1	4.723895000	-2.509352000	0.000005000
1	-0.000003000	-2.509732000	-0.000009000
6	-3.503671000	-0.734911000	-0.000016000
6	-3.503671000	0.734911000	-0.000016000
6	-4.723216000	1.425296000	-0.000014000
6	-4.723216000	-1.425296000	-0.000014000
6	-5.935433000	-0.733629000	-0.000011000
6	-5.935433000	0.733629000	-0.000011000
1	-4.723897000	2.509352000	-0.000017000
1	-4.723897000	-2.509352000	-0.000018000
6	8.222359000	0.734270000	0.000000000
6	8.222359000	-0.734270000	0.000000000
6	9.449191000	-1.423693000	0.000000000
6	9.449191000	1.423693000	0.000000000
6	10.651916000	-0.730606000	0.000004000
6	10.651916000	0.730606000	0.000004000
1	9.450841000	2.507801000	0.000000000
1	9.450841000	-2.507801000	0.000000000
6	-8.222356000	0.734272000	-0.000003000
6	-8.222356000	-0.734272000	-0.000003000
6	-9.449194000	-1.423694000	0.000002000
6	-9.449194000	1.423694000	0.000002000
6	-10.651914000	-0.730606000	0.000002000
6	-10.651914000	0.730606000	0.000002000
1	-9.450842000	-2.507801000	0.000002000
1	-9.450842000	2.507801000	0.000002000
7	-7.085463000	1.434903000	-0.000002000
7	-7.085463000	-1.434903000	-0.000002000
7	-2.361413000	1.435724000	-0.000018000
7	-2.361413000	-1.435724000	-0.000018000
7	2.361411000	1.435725000	0.000002000
7	2.361411000	-1.435725000	0.000002000
7	7.085460000	1.434903000	-0.000005000
7	7.085460000	-1.434903000	-0.000004000
7	11.815626000	1.432388000	0.000008000
7	11.815626000	-1.432388000	0.000008000
6	12.936182000	0.731108000	0.000007000
6	12.936183000	-0.731108000	0.000007000
6	14.191403000	1.417510000	0.000009000
6	14.191403000	-1.417510000	0.000009000
6	15.356663000	0.715923000	0.000009000
6	15.356663000	-0.715923000	0.000009000
1	14.168537000	-2.501890000	0.000013000
1	16.306559000	-1.240933000	0.000004000
1	16.306559000	1.240934000	0.000004000
1	14.168537000	2.501890000	0.000013000
7	-11.815627000	-1.432388000	0.000004000

7	-11.815627000	1.432388000	0.000004000
6	-12.936181000	-0.731109000	0.000010000
6	-12.936181000	0.731109000	0.000010000
6	-14.191404000	-1.417511000	0.000014000
6	-14.191404000	1.417511000	0.000014000
6	-15.356662000	-0.715923000	0.000020000
6	-15.356662000	0.715923000	0.000020000
1	-14.168537000	-2.501891000	0.000010000
1	-16.306559000	-1.240933000	0.000029000
1	-16.306559000	1.240933000	0.000029000
1	-14.168537000	2.501891000	0.000010000

Table S56: Coordinates of pN₁_1 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-6.007534000	0.712927000	0.000000000
6	-6.007534000	-0.712927000	-0.000001000
6	-4.834397000	-1.405954000	-0.000001000
6	-4.834397000	1.405954000	0.000001000
6	-3.577449000	0.726619000	0.000000000
6	-3.577449000	-0.726619000	-0.000001000
1	-4.831077000	-2.491966000	-0.000002000
1	-4.831077000	2.491966000	0.000002000
6	-1.141761000	-0.727920000	0.000000000
6	-1.141761000	0.727920000	0.000000000
7	0.000000000	1.430828000	0.000001000
7	0.000000000	-1.430828000	-0.000001000
6	1.141761000	0.727920000	0.000000000
6	1.141761000	-0.727920000	0.000000000
6	-2.372574000	-1.411653000	-0.000001000
6	-2.372574000	1.411653000	0.000001000
6	2.372574000	-1.411653000	-0.000001000
6	2.372574000	1.411653000	0.000001000
6	3.577449000	-0.726619000	0.000000000
6	3.577449000	0.726619000	0.000001000
6	4.834397000	-1.405954000	-0.000001000
6	4.834397000	1.405954000	0.000001000
6	6.007534000	-0.712927000	0.000000000
6	6.007534000	0.712927000	0.000001000
1	4.831077000	-2.491966000	-0.000002000
1	6.954157000	-1.243732000	-0.000001000
1	6.954157000	1.243732000	0.000001000

1	4.831077000	2.491966000	0.000002000
1	2.351236000	2.497353000	0.000002000
1	2.351236000	-2.497353000	-0.000002000
1	-2.351236000	2.497353000	0.000002000
1	-2.351236000	-2.497353000	-0.000002000
1	-6.954157000	-1.243732000	-0.000001000
1	-6.954157000	1.243732000	0.000001000

Table S57: Coordinates of pN₂_1 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	9.675744000	-0.711967000	0.000015000
6	9.675744000	0.711967000	0.000022000
6	7.245125000	0.725265000	0.000017000
6	7.245125000	-0.725265000	0.000011000
6	6.036330000	-1.409332000	0.000006000
1	6.014979000	-2.495244000	0.000001000
6	4.808712000	-0.726292000	0.000007000
6	4.808712000	0.726292000	0.000013000
6	6.036330000	1.409332000	0.000018000
1	6.014979000	2.495244000	0.000023000
6	2.524014000	0.728751000	0.000009000
6	2.524014000	-0.728751000	0.000004000
6	1.289025000	-1.410134000	0.000000000
6	1.289025000	1.410134000	0.000010000
6	0.085079000	0.728001000	0.000007000
6	0.085079000	-0.728001000	0.000002000
1	1.311209000	-2.495819000	-0.000004000
1	1.311209000	2.495819000	0.000014000
6	-2.352373000	-0.722183000	0.000003000
6	-2.352373000	0.722183000	0.000005000
7	-3.578812000	1.356685000	0.000004000
7	-3.578812000	-1.356685000	0.000011000
6	-4.805802000	0.713154000	-0.000004000
6	-4.805802000	-0.713154000	-0.000004000
1	-3.580495000	2.365462000	0.000014000
1	-3.580495000	-2.365462000	-0.000007000
6	-1.167579000	-1.404064000	0.000000000
6	-1.167579000	1.404064000	0.000007000
7	3.661677000	-1.430798000	0.000002000
7	3.661677000	1.430798000	0.000014000
6	8.500468000	-1.404351000	0.000010000
6	8.500468000	1.404351000	0.000023000
6	-5.998773000	-1.397415000	-0.000015000
6	-5.998773000	1.397415000	-0.000012000
6	-7.236453000	-0.715654000	-0.000023000
6	-7.236453000	0.715654000	-0.000021000

6	-8.474704000	-1.397016000	-0.000033000
6	-8.474704000	1.397016000	-0.000028000
6	-9.662388000	-0.704361000	-0.000040000
6	-9.662388000	0.704361000	-0.000037000
1	-8.471835000	-2.483593000	-0.000035000
1	-10.604731000	-1.242489000	-0.000047000
1	-10.604731000	1.242489000	-0.000043000
1	-8.471835000	2.483593000	-0.000026000
1	-5.991462000	2.484407000	-0.000012000
1	-5.991462000	-2.484407000	-0.000015000
1	-1.175078000	2.490564000	0.000008000
1	-1.175078000	-2.490564000	-0.000001000
1	8.496901000	-2.490593000	0.000005000
1	8.496901000	2.490593000	0.000028000
1	10.621907000	-1.243838000	0.000014000
1	10.621907000	1.243838000	0.000026000

Table S58: Coordinates of pN₂_2 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-9.592651000	-0.714000000	-0.000026000
6	-9.592651000	0.714000000	-0.000025000
6	-7.162256000	0.728400000	-0.000019000
6	-7.162256000	-0.728400000	-0.000020000
6	-5.961179000	-1.413728000	-0.000017000
1	-5.940460000	-2.499356000	-0.000017000
6	-4.725025000	-0.731224000	-0.000013000
6	-4.725025000	0.731224000	-0.000013000
6	-5.961179000	1.413728000	-0.000016000
1	-5.940460000	2.499356000	-0.000015000
6	-2.439867000	0.730513000	-0.000007000
6	-2.439867000	-0.730513000	-0.000007000
6	-1.223747000	-1.415449000	-0.000004000
6	-1.223747000	1.415449000	-0.000003000
6	0.000000000	0.732892000	0.000000000
6	0.000000000	-0.732892000	0.000000000
1	-1.246122000	-2.500639000	-0.000005000
1	-1.246122000	2.500639000	-0.000002000
6	2.439867000	-0.730513000	0.000007000
6	2.439867000	0.730513000	0.000007000
7	3.591357000	1.433229000	0.000011000
7	3.591357000	-1.433229000	0.000009000
6	4.725025000	0.731224000	0.000013000
6	4.725025000	-0.731224000	0.000013000
6	1.223747000	-1.415449000	0.000003000
6	1.223747000	1.415449000	0.000004000
7	-3.591357000	-1.433229000	-0.000011000

7	-3.591357000	1.433229000	-0.000009000
6	-8.421160000	-1.407285000	-0.000023000
6	-8.421160000	1.407285000	-0.000022000
6	5.961179000	-1.413728000	0.000016000
6	5.961179000	1.413728000	0.000017000
6	7.162256000	-0.728400000	0.000019000
6	7.162256000	0.728400000	0.000020000
6	8.421160000	-1.407285000	0.000022000
6	8.421160000	1.407285000	0.000023000
6	9.592651000	-0.714000000	0.000025000
6	9.592651000	0.714000000	0.000026000
1	8.418210000	-2.493189000	0.000021000
1	10.539578000	-1.244151000	0.000027000
1	10.539578000	1.244151000	0.000028000
1	8.418210000	2.493189000	0.000024000
1	5.940460000	2.499356000	0.000017000
1	5.940460000	-2.499356000	0.000015000
1	1.246122000	2.500639000	0.000005000
1	1.246122000	-2.500639000	0.000002000
1	-8.418210000	-2.493189000	-0.000024000
1	-8.418210000	2.493189000	-0.000021000
1	-10.539578000	-1.244151000	-0.000028000
1	-10.539578000	1.244151000	-0.000027000

Table S59: Coordinates of pN₃_1 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-8.462864000	0.713974000	-0.000149000
7	-7.235009000	1.358916000	-0.000463000
6	-6.008297000	0.713072000	-0.000356000
6	-6.008297000	-0.713072000	-0.000363000
7	-7.235009000	-1.358916000	-0.000505000
6	-8.462864000	-0.713974000	-0.000157000
6	-3.574472000	-0.715482000	-0.000277000
6	-3.574472000	0.715482000	-0.000278000
6	-2.340163000	1.395910000	-0.000275000
1	-2.331074000	2.482877000	-0.000279000
6	-1.143740000	0.710435000	-0.000288000
6	-1.143740000	-0.710435000	-0.000284000
6	-2.340163000	-1.395910000	-0.000269000
1	-7.235341000	2.366743000	-0.000337000
1	-7.235341000	-2.366743000	-0.000294000
1	-2.331074000	-2.482877000	-0.000267000
6	1.309187000	-0.722405000	-0.000226000
6	1.309187000	0.722405000	-0.000230000
6	2.495059000	1.403885000	-0.000152000
6	2.495059000	-1.403885000	-0.000146000

6	3.747436000	-0.728163000	-0.000084000
6	3.747436000	0.728163000	-0.000085000
1	2.487665000	2.490468000	-0.000153000
1	2.487665000	-2.490468000	-0.000139000
6	-10.896569000	0.714899000	0.000347000
6	-10.896569000	-0.714899000	0.000345000
6	-12.133312000	-1.395808000	0.000582000
6	-12.133312000	1.395808000	0.000587000
6	-13.323200000	-0.703416000	0.000808000
6	-13.323200000	0.703416000	0.000810000
1	-12.130353000	2.482558000	0.000587000
1	-12.130353000	-2.482558000	0.000579000
6	6.187285000	0.728990000	0.000020000
6	6.187285000	-0.728990000	0.000022000
7	7.324750000	-1.430991000	0.000069000
7	7.324750000	1.430991000	0.000065000
6	8.472514000	-0.726084000	0.000109000
6	8.472514000	0.726084000	0.000107000
6	4.951907000	1.409756000	-0.000029000
6	4.951907000	-1.409756000	-0.000026000
7	0.083393000	1.356215000	-0.000342000
7	0.083393000	-1.356215000	-0.000320000
6	-4.813901000	1.395602000	-0.000297000
6	-4.813901000	-1.395602000	-0.000303000
6	-9.655510000	1.396007000	0.000109000
6	-9.655510000	-1.396007000	0.000100000
6	9.699776000	1.408796000	0.000151000
6	9.699776000	-1.408796000	0.000155000
6	10.909404000	0.725005000	0.000194000
6	10.909404000	-0.725005000	0.000196000
6	12.164475000	1.403942000	0.000235000
6	12.164475000	-1.403942000	0.000240000
6	13.340294000	0.711764000	0.000276000
6	13.340294000	-0.711764000	0.000279000
1	12.160812000	2.490253000	0.000233000
1	14.286355000	1.243902000	0.000307000
1	14.286355000	-1.243902000	0.000312000
1	12.160812000	-2.490253000	0.000242000
1	9.678408000	-2.494765000	0.000157000
1	9.678408000	2.494765000	0.000148000
1	4.974051000	-2.495493000	-0.000024000
1	4.974051000	2.495493000	-0.000030000
1	0.081608000	-2.364898000	-0.000281000
1	0.081608000	2.364898000	-0.000270000
1	-4.822230000	2.482556000	-0.000289000
1	-4.822230000	-2.482556000	-0.000307000
1	-9.648621000	-2.483179000	0.000093000

1	-9.648621000	2.483179000	0.000118000
1	-14.265079000	1.242536000	0.000993000
1	-14.265079000	-1.242536000	0.000989000

Table S60: Coordinates of pN₃_2 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-8.387515000	0.713012000	0.000040000
7	-7.160824000	1.356435000	0.000038000
6	-5.935243000	0.723484000	0.000032000
6	-5.935243000	-0.723484000	0.000033000
7	-7.160824000	-1.356435000	0.000040000
6	-8.387515000	-0.713012000	0.000041000
6	-3.498132000	-0.729927000	0.000021000
6	-3.498132000	0.729927000	0.000020000
6	-2.296857000	1.412190000	0.000014000
1	-2.274937000	2.497754000	0.000013000
6	-1.057978000	0.732036000	0.000008000
6	-1.057978000	-0.732036000	0.000009000
6	-2.296857000	-1.412190000	0.000015000
1	-7.162886000	2.365428000	0.000038000
1	-7.162886000	-2.365428000	0.000041000
1	-2.274937000	-2.497754000	0.000016000
6	1.228435000	-0.729746000	-0.000003000
6	1.228435000	0.729746000	-0.000004000
6	2.441460000	1.413536000	-0.000011000
6	2.441460000	-1.413536000	-0.000009000
6	3.669216000	-0.732245000	-0.000016000
6	3.669216000	0.732245000	-0.000017000
1	2.419314000	2.498899000	-0.000011000
1	2.419314000	-2.498899000	-0.000009000
6	-10.817340000	0.715874000	0.000044000
6	-10.817340000	-0.715874000	0.000044000
6	-12.055928000	-1.397582000	0.000047000
6	-12.055928000	1.397582000	0.000045000
6	-13.242897000	-0.704658000	0.000049000
6	-13.242897000	0.704658000	0.000048000
1	-12.053297000	2.484073000	0.000045000
1	-12.053297000	-2.484073000	0.000048000
6	6.109558000	0.730448000	-0.000029000
6	6.109558000	-0.730448000	-0.000028000
7	7.259421000	-1.433092000	-0.000034000
7	7.259421000	1.433092000	-0.000035000
6	8.395008000	-0.730014000	-0.000039000
6	8.395008000	0.730014000	-0.000040000
6	4.890690000	1.414472000	-0.000023000
6	4.890690000	-1.414472000	-0.000022000

7	0.072474000	1.433977000	0.000002000
7	0.072474000	-1.433977000	0.000003000
6	-4.751043000	1.405634000	0.000026000
6	-4.751043000	-1.405634000	0.000027000
6	-9.580588000	1.398020000	0.000041000
6	-9.580588000	-1.398020000	0.000043000
6	9.630239000	1.412642000	-0.000046000
6	9.630239000	-1.412642000	-0.000045000
6	10.832639000	0.727749000	-0.000051000
6	10.832639000	-0.727749000	-0.000050000
6	12.091274000	1.406608000	-0.000057000
6	12.091274000	-1.406608000	-0.000055000
6	13.263557000	0.713789000	-0.000061000
6	13.263557000	-0.713789000	-0.000060000
1	12.087931000	2.492674000	-0.000057000
1	14.210429000	1.244234000	-0.000065000
1	14.210429000	-1.244234000	-0.000064000
1	12.087931000	-2.492674000	-0.000055000
1	9.609154000	-2.498361000	-0.000044000
1	9.609154000	2.498361000	-0.000046000
1	4.912689000	-2.499804000	-0.000022000
1	4.912689000	2.499804000	-0.000024000
1	-4.758207000	2.492025000	0.000025000
1	-4.758207000	-2.492025000	0.000028000
1	-9.573625000	-2.484913000	0.000043000
1	-9.573625000	2.484913000	0.000040000
1	-14.185376000	1.242467000	0.000049000
1	-14.185376000	-1.242467000	0.000051000

Table S61: Coordinates of pN₃_3 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-8.336945000	0.724110000	0.000021000
7	-7.179485000	1.432397000	-0.000032000
6	-6.052511000	0.728819000	-0.000049000
6	-6.052511000	-0.728819000	0.000048000
7	-7.179485000	-1.432397000	0.000032000
6	-8.336945000	-0.724110000	-0.000020000
6	-3.600081000	-0.729803000	0.000045000
6	-3.600081000	0.729803000	-0.000046000
6	-2.363237000	1.405610000	-0.000067000
1	-2.341627000	2.491598000	-0.000125000
6	-1.143310000	0.730589000	-0.000033000
6	-1.143310000	-0.730589000	0.000032000
6	-2.363237000	-1.405610000	0.000066000
1	-2.341627000	-2.491598000	0.000124000
6	1.143310000	-0.730589000	0.000031000

6	1.143310000	0.730589000	-0.000033000
6	2.363237000	1.405610000	-0.000064000
6	2.363237000	-1.405610000	0.000063000
6	3.600081000	-0.729803000	0.000043000
6	3.600081000	0.729803000	-0.000044000
1	2.341627000	2.491598000	-0.000119000
1	2.341627000	-2.491598000	0.000118000
6	-10.774524000	0.721565000	0.000049000
6	-10.774524000	-0.721565000	-0.000048000
6	-12.020391000	-1.401778000	-0.000117000
6	-12.020391000	1.401778000	0.000118000
6	-13.202328000	-0.707667000	-0.000063000
6	-13.202328000	0.707667000	0.000065000
1	-12.017365000	2.487838000	0.000209000
1	-12.017365000	-2.487838000	-0.000208000
6	6.052511000	0.728819000	-0.000045000
6	6.052511000	-0.728819000	0.000044000
7	7.179485000	-1.432397000	0.000023000
7	7.179485000	1.432397000	-0.000024000
6	8.336945000	-0.724110000	-0.000025000
6	8.336945000	0.724110000	0.000025000
6	4.809575000	1.408418000	-0.000100000
6	4.809575000	-1.408418000	0.000099000
7	0.000000000	1.437609000	-0.000061000
7	0.000000000	-1.437609000	0.000060000
6	-4.809575000	1.408418000	-0.000105000
6	-4.809575000	-1.408418000	0.000105000
6	-9.553746000	1.406594000	0.000071000
6	-9.553746000	-1.406594000	-0.000070000
6	9.553746000	1.406594000	0.000081000
6	9.553746000	-1.406594000	-0.000081000
6	10.774524000	0.721565000	0.000055000
6	10.774524000	-0.721565000	-0.000054000
6	12.020391000	1.401778000	0.000130000
6	12.020391000	-1.401778000	-0.000128000
6	13.202328000	0.707667000	0.000071000
6	13.202328000	-0.707667000	-0.000069000
1	12.017365000	2.487838000	0.000229000
1	14.146659000	1.242277000	0.000130000
1	14.146659000	-1.242277000	-0.000128000
1	12.017365000	-2.487838000	-0.000228000
1	9.532088000	-2.492465000	-0.000133000
1	9.532088000	2.492465000	0.000133000
1	4.830567000	-2.494245000	0.000177000
1	4.830567000	2.494245000	-0.000178000
1	-4.830567000	2.494245000	-0.000188000
1	-4.830567000	-2.494245000	0.000188000

1	-9.532088000	-2.492465000	-0.000114000
1	-9.532088000	2.492465000	0.000115000
1	-14.146659000	1.242277000	0.000119000
1	-14.146659000	-1.242277000	-0.000117000

Table S62: Coordinates of pN₄_1 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-4.801196000	0.711051000	0.000127000
7	-3.572666000	1.359480000	0.000183000
6	-2.347036000	0.713656000	0.000187000
6	-2.347036000	-0.713656000	0.000189000
7	-3.572666000	-1.359480000	0.000179000
6	-4.801196000	-0.711051000	0.000129000
6	0.087958000	-0.715526000	0.000189000
6	0.087958000	0.715526000	0.000185000
6	1.322114000	1.395725000	0.000166000
1	1.331238000	2.482738000	0.000160000
6	2.518903000	0.710068000	0.000144000
6	2.518903000	-0.710068000	0.000148000
6	1.322114000	-1.395725000	0.000175000
1	-3.573236000	2.367070000	0.000156000
1	-3.573236000	-2.367070000	0.000184000
1	1.331238000	-2.482738000	0.000175000
6	4.971757000	-0.722344000	0.000114000
6	4.971757000	0.722344000	0.000109000
6	6.157924000	1.403799000	0.000099000
6	6.157924000	-1.403799000	0.000108000
6	7.410202000	-0.728147000	0.000088000
6	7.410202000	0.728147000	0.000083000
1	6.150622000	2.490391000	0.000094000
1	6.150622000	-2.490391000	0.000111000
6	-7.234743000	0.714248000	0.000000000
6	-7.234743000	-0.714248000	0.000004000
6	-8.473056000	-1.394323000	-0.000078000
6	-8.473056000	1.394323000	-0.000085000
6	-9.668613000	-0.711485000	-0.000181000
6	-9.668613000	0.711485000	-0.000184000
1	-8.481512000	2.481460000	-0.000089000
1	-8.481512000	-2.481460000	-0.000077000
6	9.850199000	0.729037000	0.000029000
6	9.850199000	-0.729037000	0.000035000
7	10.987646000	-1.431091000	0.000003000
7	10.987646000	1.431091000	-0.000008000
6	12.135496000	-0.726068000	-0.000036000
6	12.135496000	0.726068000	-0.000042000
6	8.614856000	1.409692000	0.000056000

6	8.614856000	-1.409692000	0.000067000
7	3.746196000	1.356207000	0.000100000
7	3.746196000	-1.356207000	0.000110000
6	-1.151881000	1.395477000	0.000188000
6	-1.151881000	-1.395477000	0.000194000
6	-5.996766000	1.394280000	0.000069000
6	-5.996766000	-1.394280000	0.000074000
7	-10.896405000	1.359399000	-0.000329000
7	-10.896405000	-1.359399000	-0.000321000
6	-12.123619000	0.714329000	-0.000219000
6	-12.123619000	-0.714329000	-0.000215000
6	-13.316752000	1.395677000	-0.000153000
6	-13.316752000	-1.395677000	-0.000145000
6	-14.558461000	0.714820000	-0.000098000
6	-14.558461000	-0.714820000	-0.000094000
6	13.362650000	1.408656000	-0.000089000
6	13.362650000	-1.408656000	-0.000077000
6	14.572523000	0.724931000	-0.000130000
6	14.572523000	-0.724931000	-0.000124000
6	15.827472000	1.403781000	-0.000181000
6	15.827472000	-1.403781000	-0.000169000
6	17.003543000	0.711670000	-0.000223000
6	17.003543000	-0.711670000	-0.000217000
1	15.824027000	2.490115000	-0.000186000
1	17.949405000	1.244186000	-0.000262000
1	17.949405000	-1.244186000	-0.000251000
1	15.824027000	-2.490115000	-0.000164000
1	13.341450000	-2.494646000	-0.000072000
1	13.341450000	2.494646000	-0.000093000
1	8.636777000	-2.495441000	0.000068000
1	8.636777000	2.495441000	0.000049000
1	3.744330000	-2.364820000	0.000128000
1	3.744330000	2.364820000	0.000115000
1	-1.159859000	2.482481000	0.000184000
1	-1.159859000	-2.482481000	0.000192000
1	-5.988297000	-2.481450000	0.000071000
1	-5.988297000	2.481450000	0.000064000
1	-10.896360000	-2.366996000	-0.000231000
1	-10.896360000	2.366996000	-0.000242000
1	-13.310115000	-2.482900000	-0.000141000
1	-13.310115000	2.482900000	-0.000156000
6	-15.795006000	1.395465000	-0.000048000
6	-15.795006000	-1.395465000	-0.000040000
6	-16.985549000	0.703208000	0.000001000
6	-16.985549000	-0.703208000	0.000005000
1	-15.792173000	2.482291000	-0.000052000
1	-15.792173000	-2.482291000	-0.000037000

1	-17.927202000	-1.242822000	0.000046000
1	-17.927202000	1.242822000	0.000038000

Table S63: Coordinates of pN₄_2 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-4.723683000	0.710619000	-0.000219000
7	-3.497593000	1.355646000	-0.000233000
6	-2.272242000	0.723360000	-0.000246000
6	-2.272242000	-0.723360000	-0.000242000
7	-3.497593000	-1.355646000	-0.000227000
6	-4.723683000	-0.710619000	-0.000215000
6	0.165151000	-0.729972000	-0.000249000
6	0.165151000	0.729972000	-0.000254000
6	1.367443000	1.411636000	-0.000250000
1	1.389049000	2.497281000	-0.000250000
6	2.605956000	0.732196000	-0.000236000
6	2.605956000	-0.732196000	-0.000231000
6	1.367443000	-1.411636000	-0.000240000
1	-3.499551000	2.364615000	-0.000238000
1	-3.499551000	-2.364615000	-0.000222000
1	1.389049000	-2.497281000	-0.000233000
6	4.892839000	-0.730062000	-0.000180000
6	4.892839000	0.730062000	-0.000185000
6	6.105884000	1.413068000	-0.000149000
6	6.105884000	-1.413068000	-0.000139000
6	7.334331000	-0.732309000	-0.000095000
6	7.334331000	0.732309000	-0.000100000
1	6.083910000	2.498493000	-0.000150000
1	6.083910000	-2.498493000	-0.000133000
6	-7.153526000	0.716088000	-0.000182000
6	-7.153526000	-0.716088000	-0.000177000
6	-8.392885000	-1.396287000	-0.000152000
6	-8.392885000	1.396287000	-0.000162000
6	-9.587113000	-0.713741000	-0.000142000
6	-9.587113000	0.713741000	-0.000146000
1	-8.400997000	2.483121000	-0.000162000
1	-8.400997000	-2.483121000	-0.000145000
6	9.775198000	0.730790000	0.000011000
6	9.775198000	-0.730790000	0.000017000
7	10.924349000	-1.432944000	0.000081000
7	10.924349000	1.432944000	0.000070000
6	12.060850000	-0.729744000	0.000142000
6	12.060850000	0.729744000	0.000137000
6	8.555417000	1.414166000	-0.000049000
6	8.555417000	-1.414166000	-0.000039000
7	3.736797000	1.434111000	-0.000216000

7	3.736797000	-1.434111000	-0.000206000
6	-1.087022000	1.405391000	-0.000255000
6	-1.087022000	-1.405391000	-0.000246000
6	-5.920450000	1.396718000	-0.000203000
6	-5.920450000	-1.396718000	-0.000195000
7	-10.812757000	1.358885000	-0.000156000
7	-10.812757000	-1.358885000	-0.000146000
6	-12.040946000	0.713693000	0.000019000
6	-12.040946000	-0.713693000	0.000024000
6	-13.233253000	1.396246000	0.000163000
6	-13.233253000	-1.396246000	0.000173000
6	-14.473929000	0.714941000	0.000309000
6	-14.473929000	-0.714941000	0.000315000
6	13.295401000	1.412157000	0.000208000
6	13.295401000	-1.412157000	0.000219000
6	14.498561000	0.727469000	0.000285000
6	14.498561000	-0.727469000	0.000291000
6	15.756849000	1.406152000	0.000362000
6	15.756849000	-1.406152000	0.000372000
6	16.929648000	0.713515000	0.000438000
6	16.929648000	-0.713515000	0.000444000
1	15.753627000	2.492256000	0.000358000
1	17.876318000	1.244374000	0.000496000
1	17.876318000	-1.244374000	0.000505000
1	15.753627000	-2.492256000	0.000376000
1	13.274520000	-2.497938000	0.000222000
1	13.274520000	2.497938000	0.000204000
1	8.577298000	-2.499550000	-0.000032000
1	8.577298000	2.499550000	-0.000049000
1	-1.094454000	2.491870000	-0.000256000
1	-1.094454000	-2.491870000	-0.000240000
1	-5.911427000	-2.483573000	-0.000190000
1	-5.911427000	2.483573000	-0.000205000
1	-10.813310000	-2.366793000	-0.000084000
1	-10.813310000	2.366793000	-0.000100000
1	-13.226490000	-2.483355000	0.000178000
1	-13.226490000	2.483355000	0.000160000
6	-15.710683000	1.396118000	0.000451000
6	-15.710683000	-1.396118000	0.000461000
6	-16.900146000	0.703531000	0.000591000
6	-16.900146000	-0.703531000	0.000596000
1	-15.707965000	2.482799000	0.000447000
1	-15.707965000	-2.482799000	0.000465000
1	-17.842005000	-1.242584000	0.000709000
1	-17.842005000	1.242584000	0.000699000

Table S64: Coordinates of pN₄_3 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-4.814363000	0.732146000	0.000003000
7	-3.668962000	1.435299000	0.000001000
6	-2.527426000	0.733228000	0.000003000
6	-2.527426000	-0.733228000	0.000007000
7	-3.668962000	-1.435299000	0.000009000
6	-4.814363000	-0.732146000	0.000007000
6	-0.085607000	-0.733550000	0.000007000
6	-0.085607000	0.733550000	0.000003000
6	1.144825000	1.414428000	0.000001000
1	1.167070000	2.499708000	-0.000002000
6	2.355605000	0.730535000	0.000002000
6	2.355605000	-0.730535000	0.000006000
6	1.144825000	-1.414428000	0.000008000
1	1.167070000	-2.499708000	0.000011000
6	4.642181000	-0.732733000	0.000004000
6	4.642181000	0.732733000	0.000000000
6	5.881426000	1.412681000	-0.000003000
6	5.881426000	-1.412681000	0.000005000
6	7.082359000	-0.730370000	0.000001000
6	7.082359000	0.730370000	-0.000003000
1	5.859523000	2.498191000	-0.000006000
1	5.859523000	-2.498191000	0.000007000
6	-7.256019000	0.733501000	0.000002000
6	-7.256019000	-0.733501000	0.000006000
6	-8.481783000	-1.415731000	0.000007000
6	-8.481783000	1.415731000	-0.000001000
6	-9.696541000	-0.730901000	0.000004000
6	-9.696541000	0.730901000	0.000000000
1	-8.504104000	2.500937000	-0.000004000
1	-8.504104000	-2.500937000	0.000010000
6	9.519122000	0.723812000	-0.000007000
6	9.519122000	-0.723812000	-0.000003000
7	10.744313000	-1.356241000	-0.000005000
7	10.744313000	1.356241000	-0.000012000
6	11.970880000	-0.712997000	-0.000005000
6	11.970880000	0.712997000	-0.000009000
1	10.746455000	-2.365350000	-0.000002000
1	10.746455000	2.365350000	-0.000016000
6	8.334944000	1.406108000	-0.000007000
6	8.334944000	-1.406108000	0.000001000
7	3.512823000	1.434586000	-0.000001000
7	3.512823000	-1.434586000	0.000007000
6	-1.302822000	1.416150000	0.000001000
6	-1.302822000	-1.416150000	0.000009000
6	-6.034811000	1.416020000	0.000000000
6	-6.034811000	-1.416020000	0.000008000

7	-10.849157000	1.433766000	-0.000002000
7	-10.849157000	-1.433766000	0.000005000
6	-11.982073000	0.731179000	-0.000002000
6	-11.982073000	-0.731179000	0.000002000
6	-13.218964000	1.413708000	-0.000004000
6	-13.218964000	-1.413708000	0.000003000
6	-14.419750000	0.728434000	-0.000004000
6	-14.419750000	-0.728434000	0.000000000
6	13.163971000	1.398294000	-0.000010000
6	13.163971000	-1.398294000	-0.000001000
6	14.400267000	0.715990000	-0.000007000
6	14.400267000	-0.715990000	-0.000003000
6	15.638981000	1.397817000	-0.000009000
6	15.638981000	-1.397817000	0.000000000
6	16.825614000	0.704770000	-0.000006000
6	16.825614000	-0.704770000	-0.000001000
1	15.636394000	2.484250000	-0.000012000
1	17.768160000	1.242404000	-0.000007000
1	17.768160000	-1.242404000	0.000001000
1	15.636394000	-2.484250000	0.000003000
1	13.156995000	-2.485140000	0.000002000
1	13.156995000	2.485140000	-0.000013000
1	8.342118000	-2.492446000	0.000004000
1	8.342118000	2.492446000	-0.000010000
1	-1.324453000	2.501402000	-0.000002000
1	-1.324453000	-2.501402000	0.000012000
1	-6.012769000	-2.501250000	0.000011000
1	-6.012769000	2.501250000	-0.000003000
1	-13.197988000	-2.499335000	0.000006000
1	-13.197988000	2.499335000	-0.000007000
6	-15.679059000	1.407317000	-0.000007000
6	-15.679059000	-1.407317000	0.000001000
6	-16.850484000	0.714227000	-0.000006000
6	-16.850484000	-0.714227000	-0.000002000
1	-15.675806000	2.493284000	-0.000010000
1	-15.675806000	-2.493284000	0.000004000
1	-17.797563000	-1.244199000	-0.000001000
1	-17.797563000	1.244199000	-0.000008000

Table S65: Coordinates of pN₄_4 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	4.738803000	0.729934000	-0.000058000
7	3.585987000	1.436662000	-0.000064000
6	2.453194000	0.731965000	-0.000072000
6	2.453194000	-0.731965000	-0.000075000
7	3.585987000	-1.436662000	-0.000070000

6	4.738803000	-0.729934000	-0.000061000
6	0.000000000	-0.731349000	-0.000080000
6	0.000000000	0.731349000	-0.000077000
6	-1.222004000	1.408139000	-0.000074000
1	-1.243083000	2.493996000	-0.000070000
6	-2.453194000	0.731965000	-0.000073000
6	-2.453194000	-0.731965000	-0.000076000
6	-1.222004000	-1.408139000	-0.000079000
1	-1.243083000	-2.493996000	-0.000080000
6	-4.738803000	-0.729934000	-0.000062000
6	-4.738803000	0.729934000	-0.000059000
6	-5.950838000	1.408928000	-0.000046000
6	-5.950838000	-1.408928000	-0.000052000
6	-7.187948000	-0.730415000	-0.000038000
6	-7.187948000	0.730415000	-0.000035000
1	-5.928550000	2.494630000	-0.000043000
1	-5.928550000	-2.494630000	-0.000053000
6	7.187948000	0.730415000	-0.000033000
6	7.187948000	-0.730415000	-0.000036000
6	8.398376000	-1.411288000	-0.000022000
6	8.398376000	1.411288000	-0.000016000
6	9.633650000	-0.728782000	-0.000004000
6	9.633650000	0.728782000	-0.000001000
1	8.419859000	2.496847000	-0.000013000
1	8.419859000	-2.496847000	-0.000022000
6	-9.633650000	0.728782000	-0.000003000
6	-9.633650000	-0.728782000	-0.000006000
7	-10.768075000	-1.431884000	0.000010000
7	-10.768075000	1.431884000	0.000016000
6	-11.917312000	-0.726365000	0.000031000
6	-11.917312000	0.726365000	0.000034000
6	-8.398376000	1.411288000	-0.000018000
6	-8.398376000	-1.411288000	-0.000024000
7	-3.585987000	1.436662000	-0.000065000
7	-3.585987000	-1.436662000	-0.000071000
6	1.222004000	1.408139000	-0.000073000
6	1.222004000	-1.408139000	-0.000079000
6	5.950838000	1.408928000	-0.000045000
6	5.950838000	-1.408928000	-0.000050000
7	10.768075000	1.431884000	0.000018000
7	10.768075000	-1.431884000	0.000013000
6	11.917312000	0.726365000	0.000036000
6	11.917312000	-0.726365000	0.000033000
6	13.140873000	1.409489000	0.000060000
6	13.140873000	-1.409489000	0.000054000
6	14.353408000	0.724184000	0.000081000
6	14.353408000	-0.724184000	0.000078000

6	-13.140873000	1.409489000	0.000057000
6	-13.140873000	-1.409489000	0.000051000
6	-14.353408000	0.724184000	0.000077000
6	-14.353408000	-0.724184000	0.000075000
6	-15.604684000	1.404115000	0.000103000
6	-15.604684000	-1.404115000	0.000097000
6	-16.781945000	0.710359000	0.000124000
6	-16.781945000	-0.710359000	0.000121000
1	-15.601572000	2.490082000	0.000105000
1	-17.727481000	1.242898000	0.000143000
1	-17.727481000	-1.242898000	0.000138000
1	-15.601572000	-2.490082000	0.000095000
1	-13.119366000	-2.495217000	0.000049000
1	-13.119366000	2.495217000	0.000059000
1	-8.419859000	-2.496847000	-0.000024000
1	-8.419859000	2.496847000	-0.000014000
1	1.243083000	2.493996000	-0.000070000
1	1.243083000	-2.493996000	-0.000080000
1	5.928550000	-2.494630000	-0.000051000
1	5.928550000	2.494630000	-0.000041000
1	13.119366000	-2.495217000	0.000052000
1	13.119366000	2.495217000	0.000062000
6	15.604684000	1.404115000	0.000106000
6	15.604684000	-1.404115000	0.000100000
6	16.781945000	0.710359000	0.000127000
6	16.781945000	-0.710359000	0.000125000
1	15.601572000	2.490082000	0.000108000
1	15.601572000	-2.490082000	0.000098000
1	17.727481000	-1.242898000	0.000141000
1	17.727481000	1.242898000	0.000147000

Table S66: Coordinates of pN₅_1 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-8.462203000	-0.711510000	0.000645000
7	-7.234225000	-1.359923000	0.000797000
6	-6.007397000	-0.712129000	0.000953000
6	-6.007397000	0.712129000	0.000950000
7	-7.234225000	1.359923000	0.000793000
6	-8.462203000	0.711510000	0.000642000
6	-3.572406000	0.714232000	0.001150000
6	-3.572406000	-0.714232000	0.001153000
6	-2.334612000	-1.394079000	0.001202000
1	-2.325979000	-2.481280000	0.001187000
6	-1.138785000	-0.710637000	0.001217000
6	-1.138785000	0.710637000	0.001214000
6	-2.334612000	1.394079000	0.001196000

1	-7.234400000	-2.367311000	0.000795000
1	-7.234400000	2.367311000	0.000785000
1	-2.325979000	2.481280000	0.001177000
6	1.315486000	0.713824000	0.001182000
6	1.315486000	-0.713824000	0.001185000
6	2.510848000	-1.395505000	0.001139000
6	2.510848000	1.395505000	0.001133000
6	3.750734000	0.715562000	0.001057000
6	3.750734000	-0.715562000	0.001060000
1	2.502895000	-2.482500000	0.001125000
1	2.502895000	2.482500000	0.001115000
6	-10.896759000	-0.714064000	0.000264000
6	-10.896759000	0.714064000	0.000261000
6	-12.134966000	1.394001000	0.000031000
6	-12.134966000	-1.394001000	0.000037000
6	-13.330703000	0.710996000	-0.000207000
6	-13.330703000	-0.710996000	-0.000204000
1	-12.143559000	-2.481194000	0.000026000
1	-12.143559000	2.481194000	0.000016000
6	6.181712000	-0.709980000	0.000814000
6	6.181712000	0.709980000	0.000811000
7	7.409112000	1.356073000	0.000639000
7	7.409112000	-1.356073000	0.000645000
6	8.634624000	0.722333000	0.000469000
6	8.634624000	-0.722333000	0.000472000
1	7.407235000	2.364680000	0.000629000
1	7.407235000	-2.364680000	0.000638000
6	4.984857000	-1.395716000	0.000949000
6	4.984857000	1.395716000	0.000944000
7	0.090173000	-1.359395000	0.001193000
7	0.090173000	1.359395000	0.001188000
6	-4.811207000	-1.394202000	0.001068000
6	-4.811207000	1.394202000	0.001062000
6	-9.658101000	-1.393997000	0.000469000
6	-9.658101000	1.393997000	0.000464000
7	-14.559153000	-1.359409000	-0.000471000
7	-14.559153000	1.359409000	-0.000477000
6	-15.785981000	-0.714524000	-0.000758000
6	-15.785981000	0.714524000	-0.000761000
6	-16.979405000	-1.395609000	-0.001041000
6	-16.979405000	1.395609000	-0.001047000
6	-18.221266000	-0.714819000	-0.001340000
6	-18.221266000	0.714819000	-0.001343000
6	9.820901000	-1.403789000	0.000282000
6	9.820901000	1.403789000	0.000276000
6	11.073115000	-0.728145000	0.000072000
6	11.073115000	0.728145000	0.000069000

6	12.277874000	-1.409654000	-0.000145000
6	12.277874000	1.409654000	-0.000151000
6	13.513212000	-0.729062000	-0.000370000
6	13.513212000	0.729062000	-0.000373000
1	12.299823000	-2.495394000	-0.000158000
1	12.299823000	2.495394000	-0.000168000
1	9.813588000	2.490375000	0.000265000
1	9.813588000	-2.490375000	0.000275000
1	4.994035000	2.482727000	0.000925000
1	4.994035000	-2.482727000	0.000935000
1	0.089478000	2.366957000	0.001183000
1	0.089478000	-2.366957000	0.001193000
1	-4.819424000	-2.481373000	0.001052000
1	-4.819424000	2.481373000	0.001042000
1	-9.649783000	2.481208000	0.000451000
1	-9.649783000	-2.481208000	0.000461000
1	-14.558945000	2.366947000	-0.000489000
1	-14.558945000	-2.366947000	-0.000478000
1	-16.972784000	2.482841000	-0.001051000
1	-16.972784000	-2.482841000	-0.001040000
6	-19.457812000	-1.395330000	-0.001638000
6	-19.457812000	1.395330000	-0.001644000
6	-20.648593000	-0.703140000	-0.001930000
6	-20.648593000	0.703140000	-0.001934000
1	-19.454940000	-2.482172000	-0.001636000
1	-19.454940000	2.482172000	-0.001647000
1	-21.590204000	1.242872000	-0.002161000
1	-21.590204000	-1.242872000	-0.002155000
7	14.650670000	1.431124000	-0.000605000
7	14.650670000	-1.431124000	-0.000599000
6	15.798578000	0.726045000	-0.000839000
6	15.798578000	-0.726046000	-0.000836000
6	17.025693000	1.408590000	-0.001103000
6	17.025693000	-1.408590000	-0.001097000
6	18.235678000	0.724892000	-0.001365000
6	18.235678000	-0.724892000	-0.001362000
1	17.004436000	2.494577000	-0.001104000
1	17.004436000	-2.494577000	-0.001093000
6	20.666751000	0.711632000	-0.001915000
6	20.666751000	-0.711632000	-0.001912000
6	19.490595000	-1.403714000	-0.001642000
6	19.490595000	1.403714000	-0.001648000
1	19.487124000	-2.490047000	-0.001640000
1	19.487124000	2.490047000	-0.001651000
1	21.612597000	-1.244186000	-0.002122000
1	21.612597000	1.244186000	-0.002128000

Table S67: Coordinates of pN₅_2 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-8.395342000	-0.711071000	0.000012000
7	-7.166397000	-1.359820000	0.000004000
6	-5.941486000	-0.712446000	0.000006000
6	-5.941486000	0.712446000	0.000004000
7	-7.166397000	1.359820000	0.000002000
6	-8.395342000	0.711071000	0.000011000
6	-3.506511000	0.714161000	0.000003000
6	-3.506511000	-0.714160000	0.000004000
6	-2.268660000	-1.394506000	0.000003000
1	-2.260052000	-2.481557000	0.000004000
6	-1.073511000	-0.710272000	-0.000002000
6	-1.073511000	0.710272000	-0.000004000
6	-2.268660000	1.394506000	-0.000001000
1	-7.166666000	-2.367324000	0.000008000
1	-7.166666000	2.367324000	0.000002000
1	-2.260052000	2.481557000	-0.000002000
6	1.376813000	0.713212000	-0.000006000
6	1.376813000	-0.713212000	-0.000004000
6	2.576374000	-1.396120000	-0.000001000
6	2.576374000	1.396120000	-0.000006000
6	3.813630000	0.718023000	-0.000004000
6	3.813630000	-0.718023000	-0.000002000
1	2.569633000	-2.482964000	0.000001000
1	2.569633000	2.482965000	-0.000008000
6	-10.829288000	-0.714021000	0.000025000
6	-10.829288000	0.714021000	0.000024000
6	-12.067330000	1.394255000	0.000029000
6	-12.067330000	-1.394255000	0.000031000
6	-13.263257000	0.711341000	0.000035000
6	-13.263257000	-0.711341000	0.000036000
1	-12.075660000	-2.481374000	0.000031000
1	-12.075660000	2.481374000	0.000028000
6	6.258629000	-0.720913000	-0.000003000
6	6.258629000	0.720913000	-0.000006000
7	7.420585000	1.433865000	-0.000010000
7	7.420585000	-1.433864000	-0.000003000
6	8.545884000	0.728076000	-0.000010000
6	8.545884000	-0.728076000	-0.000007000
6	5.043882000	-1.400194000	-0.000001000
6	5.043882000	1.400195000	-0.000006000
7	0.156224000	-1.359268000	-0.000007000
7	0.156224000	1.359269000	-0.000011000
6	-4.744329000	-1.394529000	0.000007000
6	-4.744329000	1.394529000	0.000004000
6	-9.590729000	-1.394156000	0.000019000

6	-9.590729000	1.394156000	0.000018000
7	-14.490923000	-1.359335000	0.000042000
7	-14.490923000	1.359335000	0.000041000
6	-15.718264000	-0.714330000	0.000037000
6	-15.718264000	0.714330000	0.000036000
6	-16.911410000	-1.395720000	0.000033000
6	-16.911410000	1.395720000	0.000032000
6	-18.153230000	-0.714776000	0.000029000
6	-18.153231000	0.714775000	0.000029000
6	9.791055000	-1.401950000	-0.000008000
6	9.791055000	1.401950000	-0.000015000
6	11.012761000	-0.728445000	-0.000013000
6	11.012761000	0.728445000	-0.000017000
6	12.237429000	-1.401826000	-0.000014000
6	12.237429000	1.401826000	-0.000022000
6	13.481977000	-0.729682000	-0.000020000
6	13.481977000	0.729682000	-0.000024000
1	12.258169000	-2.488176000	-0.000011000
1	12.258169000	2.488176000	-0.000025000
1	9.770298000	2.488307000	-0.000018000
1	9.770298000	-2.488307000	-0.000005000
1	5.066605000	2.486423000	-0.000009000
1	5.066605000	-2.486423000	0.000001000
1	0.156765000	2.367306000	-0.000012000
1	0.156765000	-2.367306000	-0.000004000
1	-4.752129000	-2.481548000	0.000007000
1	-4.752129000	2.481548000	0.000003000
1	-9.582431000	2.481315000	0.000017000
1	-9.582430000	-2.481315000	0.000020000
1	-14.490855000	2.366918000	0.000038000
1	-14.490855000	-2.366918000	0.000042000
1	-16.904889000	2.482926000	0.000031000
1	-16.904889000	-2.482926000	0.000033000
6	-19.389793000	-1.395509000	0.000026000
6	-19.389793000	1.395509000	0.000025000
6	-20.580341000	-0.703214000	0.000022000
6	-20.580341000	0.703214000	0.000022000
1	-19.386878000	-2.482329000	0.000027000
1	-19.386878000	2.482329000	0.000024000
1	-21.522081000	1.242701000	0.000019000
1	-21.522081000	-1.242701000	0.000020000
7	14.605288000	1.436239000	-0.000030000
7	14.605288000	-1.436239000	-0.000021000
6	15.771477000	0.722373000	-0.000031000
6	15.771477000	-0.722373000	-0.000027000
6	16.980502000	1.400909000	-0.000038000
6	16.980502000	-1.400910000	-0.000029000

6	18.218060000	0.717223000	-0.000040000
6	18.218060000	-0.717224000	-0.000035000
1	16.959130000	2.487175000	-0.000041000
1	16.959130000	-2.487176000	-0.000026000
6	20.646382000	0.702150000	-0.000048000
6	20.646382000	-0.702151000	-0.000044000
6	19.453467000	-1.396976000	-0.000037000
6	19.453467000	1.396975000	-0.000046000
1	19.450344000	-2.483361000	-0.000034000
1	19.450345000	2.483360000	-0.000050000
1	21.588223000	-1.241243000	-0.000045000
1	21.588223000	1.241242000	-0.000053000

Table S68: Coordinates of pN₅_3 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-8.305853000	-0.710893000	0.000043000
7	-7.080335000	-1.355324000	0.000048000
6	-5.854973000	-0.723561000	0.000052000
6	-5.854973000	0.723561000	0.000049000
7	-7.080335000	1.355324000	0.000041000
6	-8.305853000	0.710893000	0.000040000
6	-3.418005000	0.730347000	0.000055000
6	-3.418005000	-0.730347000	0.000058000
6	-2.215998000	-1.412065000	0.000061000
1	-2.194058000	-2.497657000	0.000063000
6	-0.977104000	-0.732669000	0.000059000
6	-0.977104000	0.732669000	0.000055000
6	-2.215998000	1.412065000	0.000054000
1	-7.082393000	-2.364426000	0.000050000
1	-7.082393000	2.364426000	0.000038000
1	-2.194058000	2.497657000	0.000050000
6	1.309924000	0.730766000	0.000051000
6	1.309924000	-0.730766000	0.000055000
6	2.521003000	-1.413966000	0.000052000
6	2.521003000	1.413966000	0.000044000
6	3.751771000	0.733587000	0.000040000
6	3.751771000	-0.733587000	0.000044000
1	2.498952000	-2.499299000	0.000054000
1	2.498952000	2.499299000	0.000041000
6	-10.735403000	-0.716410000	0.000033000
6	-10.735403000	0.716410000	0.000029000
6	-11.974542000	1.396770000	0.000021000
6	-11.974542000	-1.396770000	0.000028000
6	-13.168829000	0.714084000	0.000016000
6	-13.168829000	-0.714084000	0.000020000
1	-11.982481000	-2.483507000	0.000030000

1	-11.982481000	2.483507000	0.000018000
6	6.194146000	-0.733415000	0.000030000
6	6.194146000	0.733415000	0.000026000
7	7.335466000	1.435411000	0.000015000
7	7.335466000	-1.435411000	0.000023000
6	8.481446000	0.732051000	0.000008000
6	8.481446000	-0.732051000	0.000012000
6	4.969063000	-1.415732000	0.000039000
6	4.969063000	1.415732000	0.000031000
7	0.152746000	-1.434769000	0.000059000
7	0.152746000	1.434769000	0.000052000
6	-4.669914000	-1.405896000	0.000058000
6	-4.669914000	1.405896000	0.000051000
6	-9.502762000	-1.397262000	0.000040000
6	-9.502762000	1.397262000	0.000033000
7	-14.393927000	-1.358663000	0.000015000
7	-14.393927000	1.358663000	0.000008000
6	-15.622280000	-0.713598000	-0.000002000
6	-15.622280000	0.713598000	-0.000006000
6	-16.814505000	-1.396524000	-0.000015000
6	-16.814505000	1.396524000	-0.000022000
6	-18.054878000	-0.714988000	-0.000031000
6	-18.054878000	0.714988000	-0.000035000
6	9.701572000	-1.415545000	0.000003000
6	9.701572000	1.415545000	-0.000005000
6	10.923541000	-0.733427000	-0.000010000
6	10.923541000	0.733427000	-0.000015000
6	12.148950000	-1.415446000	-0.000021000
6	12.148950000	1.415446000	-0.000029000
6	13.364386000	-0.730992000	-0.000036000
6	13.364386000	0.730992000	-0.000040000
1	12.171135000	-2.500692000	-0.000018000
1	12.171135000	2.500692000	-0.000033000
1	9.679540000	2.500821000	-0.000008000
1	9.679540000	-2.500821000	0.000006000
1	4.990601000	2.501032000	0.000028000
1	4.990601000	-2.501032000	0.000042000
1	-4.677126000	-2.492343000	0.000060000
1	-4.677126000	2.492343000	0.000047000
1	-9.493957000	2.484017000	0.000030000
1	-9.493957000	-2.484017000	0.000043000
1	-14.394558000	2.366654000	0.000003000
1	-14.394558000	-2.366654000	0.000017000
1	-16.807892000	2.483574000	-0.000025000
1	-16.807892000	-2.483574000	-0.000012000
6	-19.291757000	-1.396387000	-0.000043000
6	-19.291757000	1.396387000	-0.000051000

6	-20.480886000	-0.703653000	-0.000059000
6	-20.480886000	0.703653000	-0.000063000
1	-19.289053000	-2.483016000	-0.000040000
1	-19.289053000	2.483016000	-0.000054000
1	-21.422886000	1.242428000	-0.000076000
1	-21.422886000	-1.242428000	-0.000069000
7	14.516656000	1.433684000	-0.000055000
7	14.516656000	-1.433684000	-0.000047000
6	15.650082000	0.730896000	-0.000066000
6	15.650082000	-0.730896000	-0.000062000
6	16.886742000	1.413304000	-0.000083000
6	16.886742000	-1.413304000	-0.000074000
6	18.087995000	0.728239000	-0.000095000
6	18.087995000	-0.728239000	-0.000091000
1	16.865715000	2.498982000	-0.000086000
1	16.865715000	-2.498982000	-0.000071000
6	20.518944000	0.714109000	-0.000125000
6	20.518944000	-0.714109000	-0.000121000
6	19.347192000	-1.407025000	-0.000104000
6	19.347192000	1.407025000	-0.000113000
1	19.343855000	-2.493044000	-0.000101000
1	19.343855000	2.493044000	-0.000116000
1	21.465957000	-1.244264000	-0.000131000
1	21.465957000	1.244264000	-0.000138000

Table S69: Coordinates of pN₅_4 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-8.243917000	-0.727384000	-0.000028000
7	-7.100059000	-1.431534000	-0.000040000
6	-5.959951000	-0.727302000	-0.000053000
6	-5.959951000	0.727302000	-0.000056000
7	-7.100059000	1.431534000	-0.000045000
6	-8.243917000	0.727384000	-0.000031000
6	-3.514805000	0.729327000	-0.000074000
6	-3.514805000	-0.729327000	-0.000071000
6	-2.279188000	-1.408230000	-0.000075000
1	-2.256953000	-2.494019000	-0.000072000
6	-1.066430000	-0.729044000	-0.000082000
6	-1.066430000	0.729044000	-0.000085000
6	-2.279188000	1.408230000	-0.000081000
1	-2.256953000	2.494019000	-0.000082000
6	1.219335000	0.731692000	-0.000088000
6	1.219335000	-0.731692000	-0.000085000
6	2.452280000	-1.407826000	-0.000082000
6	2.452280000	1.407826000	-0.000088000
6	3.672769000	0.731110000	-0.000084000

6	3.672769000	-0.731110000	-0.000081000
1	2.431374000	-2.493742000	-0.000078000
1	2.431374000	2.493742000	-0.000089000
6	-10.682302000	-0.726052000	0.000005000
6	-10.682302000	0.726052000	0.000002000
6	-11.929917000	1.402971000	0.000020000
6	-11.929917000	-1.402971000	0.000025000
6	-13.118189000	0.720518000	0.000041000
6	-13.118189000	-0.720518000	0.000044000
1	-11.936992000	-2.489365000	0.000028000
1	-11.936992000	2.489365000	0.000019000
6	6.126882000	-0.731818000	-0.000071000
6	6.126882000	0.731818000	-0.000074000
7	7.261248000	1.436818000	-0.000068000
7	7.261248000	-1.436818000	-0.000061000
6	8.413062000	0.730164000	-0.000058000
6	8.413062000	-0.730164000	-0.000054000
6	4.897060000	-1.407348000	-0.000075000
6	4.897060000	1.407348000	-0.000081000
7	0.087180000	-1.436075000	-0.000082000
7	0.087180000	1.436075000	-0.000088000
6	-4.728720000	-1.409582000	-0.000061000
6	-4.728720000	1.409582000	-0.000066000
6	-9.472312000	-1.408687000	-0.000011000
6	-9.472312000	1.408687000	-0.000016000
7	-14.341832000	-1.356974000	0.000067000
7	-14.341832000	1.356974000	0.000062000
6	-15.569805000	-0.712936000	0.000088000
6	-15.569805000	0.712936000	0.000085000
6	-16.761918000	-1.397676000	0.000111000
6	-16.761918000	1.397676000	0.000106000
6	-17.999770000	-0.715551000	0.000133000
6	-17.999770000	0.715551000	0.000130000
6	9.626188000	-1.408180000	-0.000041000
6	9.626188000	1.408180000	-0.000048000
6	10.863607000	-0.730397000	-0.000031000
6	10.863607000	0.730397000	-0.000035000
6	12.074049000	-1.410599000	-0.000016000
6	12.074049000	1.410599000	-0.000023000
6	13.310562000	-0.729025000	-0.000004000
6	13.310562000	0.729025000	-0.000008000
1	12.095388000	-2.496236000	-0.000013000
1	12.095388000	2.496236000	-0.000025000
1	9.604175000	2.493955000	-0.000050000
1	9.604175000	-2.493955000	-0.000038000
1	4.918139000	2.493282000	-0.000082000
1	4.918139000	-2.493282000	-0.000071000

1	-4.750289000	-2.495282000	-0.000057000
1	-4.750289000	2.495282000	-0.000067000
1	-9.450023000	2.494328000	-0.000017000
1	-9.450023000	-2.494328000	-0.000008000
1	-14.343088000	2.365815000	0.000061000
1	-14.343088000	-2.365815000	0.000069000
1	-16.754827000	2.484580000	0.000104000
1	-16.754827000	-2.484580000	0.000113000
6	-19.237512000	-1.397329000	0.000157000
6	-19.237512000	1.397329000	0.000152000
6	-20.425011000	-0.704279000	0.000178000
6	-20.425011000	0.704279000	0.000176000
1	-19.234923000	-2.483799000	0.000159000
1	-19.234923000	2.483799000	0.000150000
1	-21.367289000	1.242363000	0.000192000
1	-21.367289000	-1.242363000	0.000197000
7	14.444095000	1.432027000	0.000005000
7	14.444095000	-1.432027000	0.000012000
6	15.594771000	0.725891000	0.000023000
6	15.594771000	-0.725891000	0.000026000
6	16.817435000	1.408724000	0.000038000
6	16.817435000	-1.408724000	0.000046000
6	18.031315000	0.723732000	0.000058000
6	18.031315000	-0.723732000	0.000062000
1	16.795972000	2.494519000	0.000036000
1	16.795972000	-2.494519000	0.000048000
6	20.460136000	0.710015000	0.000096000
6	20.460136000	-0.710015000	0.000100000
6	19.282065000	-1.403504000	0.000083000
6	19.282065000	1.403504000	0.000076000
1	19.278859000	-2.489564000	0.000086000
1	19.278859000	2.489564000	0.000073000
1	21.405455000	-1.243037000	0.000116000
1	21.405455000	1.243037000	0.000109000

Table S70: Coordinates of pN₅_5 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	8.326815000	-0.730134000	0.000069000
7	7.173058000	-1.435809000	0.000089000
6	6.041483000	-0.732326000	0.000114000
6	6.041483000	0.732326000	0.000123000
7	7.173058000	1.435809000	0.000106000
6	8.326815000	0.730134000	0.000078000
6	3.592405000	0.731899000	0.000158000
6	3.592405000	-0.731899000	0.000149000
6	2.363580000	-1.409334000	0.000156000

1	2.341931000	-2.495074000	0.000148000
6	1.142508000	-0.731690000	0.000169000
6	1.142508000	0.731690000	0.000179000
6	2.363580000	1.409334000	0.000175000
1	2.341931000	2.495074000	0.000180000
6	-1.142509000	0.731690000	0.000182000
6	-1.142509000	-0.731690000	0.000173000
6	-2.363580000	-1.409334000	0.000164000
6	-2.363580000	1.409334000	0.000183000
6	-3.592405000	0.731899000	0.000170000
6	-3.592405000	-0.731899000	0.000161000
1	-2.341931000	-2.495074000	0.000156000
1	-2.341931000	2.495074000	0.000189000
6	10.771998000	-0.731152000	0.000007000
6	10.771998000	0.731152000	0.000016000
6	11.986036000	1.412876000	-0.000016000
6	11.986036000	-1.412876000	-0.000032000
6	13.214822000	0.729217000	-0.000057000
6	13.214822000	-0.729217000	-0.000065000
1	12.007857000	-2.498301000	-0.000040000
1	12.007857000	2.498301000	-0.000011000
6	-6.041483000	-0.732326000	0.000134000
6	-6.041483000	0.732326000	0.000143000
7	-7.173058000	1.435809000	0.000130000
7	-7.173058000	-1.435809000	0.000111000
6	-8.326815000	0.730134000	0.000104000
6	-8.326815000	-0.730134000	0.000095000
6	-4.808120000	-1.410844000	0.000144000
6	-4.808120000	1.410844000	0.000163000
7	0.000000000	-1.436652000	0.000168000
7	0.000000000	1.436652000	0.000187000
6	4.808120000	-1.410844000	0.000129000
6	4.808120000	1.410844000	0.000147000
6	9.538582000	-1.411463000	0.000035000
6	9.538582000	1.411463000	0.000052000
7	14.354919000	-1.432156000	-0.000107000
7	14.354919000	1.432156000	-0.000090000
6	15.498589000	-0.728021000	-0.000141000
6	15.498589000	0.728021000	-0.000132000
6	16.726552000	-1.411219000	-0.000187000
6	16.726552000	1.411219000	-0.000171000
6	17.934554000	-0.725762000	-0.000226000
6	17.934554000	0.725762000	-0.000217000
6	-9.538582000	-1.411463000	0.000064000
6	-9.538582000	1.411463000	0.000083000
6	-10.771998000	-0.731152000	0.000039000
6	-10.771998000	0.731152000	0.000049000

6	-11.986036000	-1.412876000	0.000003000
6	-11.986036000	1.412876000	0.000021000
6	-13.214822000	-0.729217000	-0.000027000
6	-13.214822000	0.729217000	-0.000017000
1	-12.007857000	-2.498301000	-0.000006000
1	-12.007857000	2.498301000	0.000027000
1	-9.516261000	2.496970000	0.000089000
1	-9.516261000	-2.496970000	0.000056000
1	-4.829119000	2.496526000	0.000169000
1	-4.829119000	-2.496526000	0.000136000
1	4.829119000	-2.496526000	0.000121000
1	4.829119000	2.496526000	0.000152000
1	9.516261000	2.496970000	0.000058000
1	9.516261000	-2.496970000	0.000028000
1	16.705355000	2.496871000	-0.000164000
1	16.705355000	-2.496871000	-0.000193000
6	19.188749000	-1.405427000	-0.000274000
6	19.188749000	1.405427000	-0.000257000
6	20.363611000	-0.711821000	-0.000311000
6	20.363611000	0.711821000	-0.000303000
1	19.185671000	-2.491353000	-0.000280000
1	19.185671000	2.491353000	-0.000251000
1	21.309722000	1.243343000	-0.000333000
1	21.309722000	-1.243343000	-0.000348000
7	-14.354919000	1.432156000	-0.000047000
7	-14.354919000	-1.432156000	-0.000066000
6	-15.498589000	0.728021000	-0.000087000
6	-15.498589000	-0.728021000	-0.000097000
6	-16.726552000	1.411219000	-0.000123000
6	-16.726552000	-1.411219000	-0.000142000
6	-17.934554000	0.725762000	-0.000167000
6	-17.934554000	-0.725762000	-0.000177000
1	-16.705355000	2.496871000	-0.000115000
1	-16.705355000	-2.496871000	-0.000149000
6	-20.363611000	0.711821000	-0.000249000
6	-20.363611000	-0.711821000	-0.000258000
6	-19.188749000	-1.405427000	-0.000224000
6	-19.188749000	1.405427000	-0.000205000
1	-19.185671000	-2.491353000	-0.000231000
1	-19.185671000	2.491353000	-0.000197000
1	-21.309722000	-1.243343000	-0.000294000
1	-21.309722000	1.243343000	-0.000277000

Table S71: Coordinates of pN₆_1 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-4.978368000	-0.713898000	0.000225000

7	-3.753213000	-1.359410000	0.000227000
6	-2.524100000	-0.710512000	0.000247000
6	-2.524100000	0.710512000	0.000249000
7	-3.753213000	1.359410000	0.000230000
6	-4.978368000	0.713898000	0.000227000
6	-0.090431000	0.714263000	0.000269000
6	-0.090431000	-0.714263000	0.000267000
6	1.148485000	-1.394155000	0.000269000
1	1.156649000	-2.481362000	0.000266000
6	2.344898000	-0.712322000	0.000267000
6	2.344898000	0.712322000	0.000269000
6	1.148485000	1.394155000	0.000272000
1	-3.752469000	-2.366980000	0.000232000
1	-3.752469000	2.366980000	0.000236000
1	1.156649000	2.481362000	0.000272000
6	4.799781000	0.711103000	0.000253000
6	4.799781000	-0.711102000	0.000251000
6	5.995939000	-1.393718000	0.000238000
6	5.995939000	1.393718000	0.000241000
6	7.234458000	0.714037000	0.000224000
6	7.234458000	-0.714037000	0.000222000
1	5.987472000	-2.481010000	0.000236000
1	5.987472000	2.481010000	0.000242000
6	-7.413756000	-0.715601000	0.000197000
6	-7.413756000	0.715601000	0.000199000
6	-8.647879000	1.395677000	0.000176000
6	-8.647879000	-1.395677000	0.000173000
6	-9.844791000	0.709952000	0.000150000
6	-9.844791000	-0.709952000	0.000148000
1	-8.657067000	-2.482713000	0.000170000
1	-8.657067000	2.482713000	0.000175000
6	9.669566000	-0.711621000	0.000181000
6	9.669566000	0.711621000	0.000183000
7	10.897079000	1.360078000	0.000165000
7	10.897079000	-1.360078000	0.000162000
6	12.124607000	0.711766000	0.000110000
6	12.124607000	-0.711766000	0.000108000
1	10.897078000	2.367419000	0.000156000
1	10.897078000	-2.367419000	0.000150000
6	8.473193000	-1.393791000	0.000200000
6	8.473193000	1.393791000	0.000204000
7	3.571379000	-1.359984000	0.000260000
7	3.571379000	1.359984000	0.000263000
6	-1.328202000	-1.393989000	0.000259000
6	-1.328202000	1.393989000	0.000262000
6	-6.173845000	-1.395480000	0.000214000
6	-6.173845000	1.395480000	0.000217000
7	-11.072213000	-1.356074000	0.000119000

7	-11.072213000	1.356074000	0.000122000
6	-12.297682000	-0.722330000	0.000073000
6	-12.297682000	0.722330000	0.000075000
6	-13.484033000	-1.403759000	0.000025000
6	-13.484033000	1.403759000	0.000028000
6	-14.736219000	-0.728159000	-0.000030000
6	-14.736219000	0.728159000	-0.000028000
6	13.320778000	-1.393888000	0.000054000
6	13.320778000	1.393888000	0.000057000
6	14.559655000	-0.714049000	-0.000004000
6	14.559655000	0.714049000	-0.000002000
6	15.797864000	-1.393832000	-0.000067000
6	15.797864000	1.393832000	-0.000063000
6	16.993681000	-0.710782000	-0.000129000
6	16.993681000	0.710782000	-0.000127000
1	15.806520000	-2.481083000	-0.000068000
1	15.806520000	2.481083000	-0.000062000
1	13.312529000	2.481148000	0.000057000
1	13.312529000	-2.481148000	0.000051000
1	8.481535000	2.481065000	0.000204000
1	8.481535000	-2.481065000	0.000198000
1	3.571683000	2.367356000	0.000264000
1	3.571683000	-2.367356000	0.000259000
1	-1.336885000	-2.481232000	0.000257000
1	-1.336885000	2.481232000	0.000262000
1	-6.165913000	2.482500000	0.000217000
1	-6.165913000	-2.482500000	0.000211000
1	-11.070316000	2.364689000	0.000119000
1	-11.070316000	-2.364689000	0.000114000
1	-13.476715000	2.490365000	0.000027000
1	-13.476715000	-2.490365000	0.000022000
6	-15.941040000	-1.409608000	-0.000089000
6	-15.941040000	1.409608000	-0.000086000
6	-17.176398000	-0.729083000	-0.000151000
6	-17.176398000	0.729083000	-0.000150000
1	-15.962945000	-2.495370000	-0.000093000
1	-15.962945000	2.495370000	-0.000088000
7	18.222450000	1.359456000	-0.000199000
7	18.222450000	-1.359456000	-0.000202000
6	19.449039000	0.714627000	-0.000219000
6	19.449039000	-0.714627000	-0.000221000
6	20.642657000	1.395549000	-0.000247000
6	20.642657000	-1.395549000	-0.000251000
6	21.884582000	0.714843000	-0.000283000
6	21.884582000	-0.714844000	-0.000285000
1	20.636061000	2.482811000	-0.000245000
1	20.636061000	-2.482811000	-0.000252000

1	18.222157000	2.366982000	-0.000181000
1	18.222157000	-2.366982000	-0.000188000
7	-18.313870000	1.431156000	-0.000210000
7	-18.313870000	-1.431156000	-0.000213000
6	-19.461821000	0.726046000	-0.000274000
6	-19.461821000	-0.726046000	-0.000275000
6	-20.688936000	1.408540000	-0.000344000
6	-20.688936000	-1.408540000	-0.000347000
6	-21.898990000	0.724883000	-0.000415000
6	-21.898990000	-0.724883000	-0.000417000
6	-23.153884000	1.403683000	-0.000488000
6	-23.153884000	-1.403683000	-0.000491000
6	-24.330092000	0.711621000	-0.000557000
6	-24.330092000	-0.711621000	-0.000559000
1	-20.667724000	-2.494545000	-0.000347000
1	-20.667724000	2.494545000	-0.000342000
1	-23.150420000	2.490036000	-0.000487000
1	-23.150420000	-2.490036000	-0.000492000
1	-25.275924000	-1.244217000	-0.000616000
1	-25.275924000	1.244217000	-0.000613000
6	23.121142000	-1.395250000	-0.000322000
6	23.121142000	1.395250000	-0.000318000
6	24.312057000	-0.703119000	-0.000356000
6	24.312057000	0.703119000	-0.000353000
1	23.118267000	-2.482132000	-0.000324000
1	23.118267000	2.482132000	-0.000317000
1	25.253644000	-1.242933000	-0.000384000
1	25.253644000	1.242933000	-0.000380000

Table S72: Coordinates of pN₆_2 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	5.054127000	-0.723002000	-0.000027000
7	3.828361000	-1.355275000	-0.000026000
6	2.602517000	-0.710585000	-0.000026000
6	2.602517000	0.710585000	-0.000028000
7	3.828361000	1.355275000	-0.000030000
6	5.054127000	0.723002000	-0.000028000
6	0.172169000	0.716354000	-0.000025000
6	0.172169000	-0.716354000	-0.000023000
6	-1.067297000	-1.396254000	-0.000020000
1	-1.075234000	-2.483151000	-0.000018000
6	-2.262549000	-0.714346000	-0.000019000
6	-2.262549000	0.714346000	-0.000021000
6	-1.067297000	1.396254000	-0.000024000
1	3.826501000	-2.364232000	-0.000025000
1	3.826501000	2.364232000	-0.000030000

1	-1.075234000	2.483151000	-0.000025000
6	-4.715839000	0.710633000	-0.000017000
6	-4.715839000	-0.710633000	-0.000014000
6	-5.911627000	-1.394575000	-0.000011000
6	-5.911627000	1.394575000	-0.000016000
6	-7.148693000	0.714665000	-0.000013000
6	-7.148693000	-0.714665000	-0.000011000
1	-5.902916000	-2.481712000	-0.000010000
1	-5.902916000	2.481712000	-0.000018000
6	7.491593000	-0.729803000	-0.000023000
6	7.491593000	0.729803000	-0.000024000
6	8.694563000	1.411195000	-0.000021000
6	8.694563000	-1.411195000	-0.000018000
6	9.932806000	0.732049000	-0.000015000
6	9.932806000	-0.732049000	-0.000014000
1	8.716173000	-2.496900000	-0.000015000
1	8.716173000	2.496900000	-0.000021000
6	-9.583469000	-0.712655000	-0.000012000
6	-9.583469000	0.712655000	-0.000015000
7	-10.809415000	1.359694000	-0.000019000
7	-10.809415000	-1.359694000	-0.000014000
6	-12.037669000	0.711302000	-0.000016000
6	-12.037669000	-0.711302000	-0.000013000
1	-10.809763000	2.367216000	-0.000020000
1	-10.809763000	-2.367216000	-0.000012000
6	-8.387281000	-1.394692000	-0.000010000
6	-8.387281000	1.394692000	-0.000015000
7	-3.487091000	-1.358866000	-0.000017000
7	-3.487091000	1.358866000	-0.000021000
6	1.405186000	-1.396603000	-0.000024000
6	1.405186000	1.396603000	-0.000027000
6	6.239622000	-1.405134000	-0.000024000
6	6.239622000	1.405134000	-0.000028000
7	11.064135000	-1.434220000	-0.000006000
7	11.064135000	1.434220000	-0.000009000
6	12.220018000	-0.730214000	0.000000000
6	12.220018000	0.730214000	-0.000001000
6	13.433407000	-1.412766000	0.000011000
6	13.433407000	1.412766000	0.000008000
6	14.662063000	-0.732344000	0.000021000
6	14.662063000	0.732344000	0.000020000
6	-13.233389000	-1.394214000	-0.000011000
6	-13.233389000	1.394214000	-0.000016000
6	-14.471604000	-0.714244000	-0.000013000
6	-14.471604000	0.714244000	-0.000016000
6	-15.709788000	-1.394256000	-0.000014000
6	-15.709788000	1.394256000	-0.000019000

6	-16.905483000	-0.711383000	-0.000017000
6	-16.905483000	0.711383000	-0.000020000
1	-15.718303000	-2.481408000	-0.000013000
1	-15.718303000	2.481408000	-0.000022000
1	-13.224990000	2.481400000	-0.000019000
1	-13.224990000	-2.481400000	-0.000010000
1	-8.395416000	2.481788000	-0.000017000
1	-8.395416000	-2.481788000	-0.000009000
1	-3.487886000	2.366656000	-0.000022000
1	-3.487886000	-2.366656000	-0.000015000
1	1.414358000	-2.483505000	-0.000022000
1	1.414358000	2.483505000	-0.000028000
1	6.232078000	2.491677000	-0.000028000
1	6.232078000	-2.491677000	-0.000022000
1	13.411539000	2.498230000	0.000008000
1	13.411539000	-2.498230000	0.000013000
6	15.883235000	-1.413890000	0.000034000
6	15.883235000	1.413890000	0.000031000
6	17.103457000	-0.730946000	0.000046000
6	17.103457000	0.730946000	0.000045000
1	15.905023000	-2.499310000	0.000037000
1	15.905023000	2.499310000	0.000031000
7	-18.133314000	1.359390000	-0.000024000
7	-18.133314000	-1.359390000	-0.000019000
6	-19.360474000	0.714360000	-0.000032000
6	-19.360474000	-0.714360000	-0.000029000
6	-20.553656000	1.395681000	-0.000042000
6	-20.553656000	-1.395681000	-0.000037000
6	-21.795352000	0.714833000	-0.000050000
6	-21.795352000	-0.714833000	-0.000047000
1	-20.547017000	2.482906000	-0.000045000
1	-20.547017000	-2.482906000	-0.000035000
1	-18.133249000	2.366990000	-0.000027000
1	-18.133249000	-2.366990000	-0.000019000
7	18.252371000	1.433030000	0.000059000
7	18.252371000	-1.433030000	0.000061000
6	19.389417000	0.729543000	0.000074000
6	19.389417000	-0.729543000	0.000075000
6	20.623671000	1.411730000	0.000090000
6	20.623671000	-1.411730000	0.000093000
6	21.827458000	0.727262000	0.000108000
6	21.827458000	-0.727262000	0.000109000
6	23.085542000	1.405817000	0.000125000
6	23.085542000	-1.405817000	0.000128000
6	24.258775000	0.713347000	0.000143000
6	24.258775000	-0.713347000	0.000144000
1	20.602754000	-2.497561000	0.000094000
1	20.602754000	2.497561000	0.000089000

1	23.082263000	2.491977000	0.000124000
1	23.082263000	-2.491977000	0.000129000
1	25.205347000	-1.244455000	0.000158000
1	25.205347000	1.244455000	0.000156000
6	-23.031907000	-1.395465000	-0.000055000
6	-23.031907000	1.395465000	-0.000060000
6	-24.222453000	-0.703208000	-0.000065000
6	-24.222453000	0.703208000	-0.000068000
1	-23.029079000	-2.482290000	-0.000052000
1	-23.029079000	2.482290000	-0.000063000
1	-25.164105000	-1.242817000	-0.000071000
1	-25.164105000	1.242817000	-0.000076000

Table S73: Coordinates of pN₆_3 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	4.973971000	-0.731112000	0.000123000
7	3.817384000	-1.434645000	0.000125000
6	2.686842000	-0.732459000	0.000123000
6	2.686842000	0.732459000	0.000121000
7	3.817384000	1.434645000	0.000121000
6	4.973971000	0.731112000	0.000121000
6	0.245958000	0.730126000	0.000116000
6	0.245958000	-0.730126000	0.000118000
6	-1.005768000	-1.405617000	0.000113000
1	-1.013346000	-2.492113000	0.000114000
6	-2.190847000	-0.723116000	0.000105000
6	-2.190847000	0.723116000	0.000103000
6	-1.005768000	1.405617000	0.000109000
1	-1.013346000	2.492113000	0.000107000
6	-4.641800000	0.711049000	0.000085000
6	-4.641800000	-0.711049000	0.000087000
6	-5.839131000	-1.397111000	0.000077000
6	-5.839131000	1.397111000	0.000073000
6	-7.071746000	0.716704000	0.000060000
6	-7.071746000	-0.716704000	0.000062000
1	-5.830029000	-2.483926000	0.000078000
1	-5.830029000	2.483926000	0.000070000
6	7.416185000	-0.733653000	0.000115000
6	7.416185000	0.733653000	0.000113000
6	8.633905000	1.415462000	0.000104000
6	8.633905000	-1.415462000	0.000109000
6	9.858928000	0.733629000	0.000096000
6	9.858928000	-0.733629000	0.000098000
1	8.655289000	-2.500807000	0.000109000
1	8.655289000	2.500807000	0.000102000
6	-9.505786000	-0.714475000	0.000027000

6	-9.505786000	0.714475000	0.000024000
7	-10.730109000	1.358677000	0.000000000
7	-10.730109000	-1.358677000	0.000004000
6	-11.958346000	0.711024000	-0.000007000
6	-11.958346000	-0.711024000	-0.000005000
1	-10.730850000	2.366622000	0.000002000
1	-10.730850000	-2.366622000	0.000009000
6	-8.310750000	-1.396713000	0.000046000
6	-8.310750000	1.396713000	0.000042000
7	-3.416792000	-1.355153000	0.000097000
7	-3.416792000	1.355153000	0.000093000
6	1.448530000	-1.411696000	0.000122000
6	1.448530000	1.411696000	0.000118000
6	6.185709000	-1.413757000	0.000121000
6	6.185709000	1.413757000	0.000117000
7	11.000321000	-1.435433000	0.000088000
7	11.000321000	1.435433000	0.000084000
6	12.146514000	-0.732255000	0.000075000
6	12.146514000	0.732255000	0.000073000
6	13.366446000	-1.415280000	0.000060000
6	13.366446000	1.415280000	0.000055000
6	14.588953000	-0.733485000	0.000040000
6	14.588953000	0.733485000	0.000038000
6	-13.153829000	-1.395128000	-0.000016000
6	-13.153829000	1.395128000	-0.000020000
6	-14.390555000	-0.714897000	-0.000032000
6	-14.390555000	0.714897000	-0.000035000
6	-15.628602000	-1.395154000	-0.000049000
6	-15.628602000	1.395154000	-0.000053000
6	-16.824066000	-0.712405000	-0.000065000
6	-16.824066000	0.712405000	-0.000067000
1	-15.636916000	-2.482131000	-0.000048000
1	-15.636916000	2.482131000	-0.000056000
1	-13.145230000	2.482157000	-0.000023000
1	-13.145230000	-2.482157000	-0.000015000
1	-8.318715000	2.483526000	0.000040000
1	-8.318715000	-2.483526000	0.000047000
1	-3.418561000	2.364255000	0.000091000
1	-3.418561000	-2.364255000	0.000098000
1	1.470166000	-2.497357000	0.000123000
1	1.470166000	2.497357000	0.000116000
1	6.163774000	2.499141000	0.000114000
1	6.163774000	-2.499141000	0.000121000
1	13.344615000	2.500600000	0.000053000
1	13.344615000	-2.500600000	0.000061000
6	15.813979000	-1.415256000	0.000020000
6	15.813979000	1.415256000	0.000016000

6	17.030142000	-0.731294000	-0.000004000
6	17.030142000	0.731294000	-0.000006000
1	15.836098000	-2.500545000	0.000020000
1	15.836098000	2.500545000	0.000013000
7	-18.050370000	1.359165000	-0.000079000
7	-18.050370000	-1.359165000	-0.000075000
6	-19.278221000	0.713978000	-0.000128000
6	-19.278221000	-0.713978000	-0.000125000
6	-20.470835000	1.396025000	-0.000174000
6	-20.470835000	-1.396025000	-0.000169000
6	-21.711945000	0.714891000	-0.000218000
6	-21.711945000	-0.714891000	-0.000216000
1	-20.464132000	2.483176000	-0.000176000
1	-20.464132000	-2.483176000	-0.000168000
1	-18.050627000	2.366939000	-0.000092000
1	-18.050627000	-2.366939000	-0.000083000
7	18.181771000	1.433559000	-0.000029000
7	18.181771000	-1.433559000	-0.000025000
6	19.315947000	0.730710000	-0.000050000
6	19.315947000	-0.730710000	-0.000048000
6	20.551979000	1.412978000	-0.000076000
6	20.551979000	-1.412978000	-0.000072000
6	21.753809000	0.728034000	-0.000100000
6	21.753809000	-0.728034000	-0.000098000
6	23.012708000	1.406676000	-0.000126000
6	23.012708000	-1.406676000	-0.000122000
6	24.184853000	0.713881000	-0.000148000
6	24.184853000	-0.713881000	-0.000146000
1	20.531202000	-2.498705000	-0.000070000
1	20.531202000	2.498705000	-0.000077000
1	23.009544000	2.492722000	-0.000127000
1	23.009544000	-2.492722000	-0.000120000
1	25.131679000	-1.244403000	-0.000165000
1	25.131679000	1.244403000	-0.000169000
6	-22.948578000	-1.395884000	-0.000260000
6	-22.948578000	1.395884000	-0.000265000
6	-24.138445000	-0.703397000	-0.000304000
6	-24.138445000	0.703397000	-0.000307000
1	-22.945834000	-2.482611000	-0.000258000
1	-22.945834000	2.482611000	-0.000267000
1	-25.080224000	-1.242640000	-0.000338000
1	-25.080224000	1.242640000	-0.000343000

Table S74: Coordinates of pN₆_4 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	4.897589000	-0.732808000	0.000105000

7	3.750144000	-1.435817000	0.000103000
6	2.610083000	-0.734139000	0.000098000
6	2.610083000	0.734139000	0.000096000
7	3.750144000	1.435817000	0.000099000
6	4.897589000	0.732808000	0.000103000
6	0.167598000	0.733962000	0.000082000
6	0.167598000	-0.733962000	0.000084000
6	-1.063164000	-1.414254000	0.000076000
1	-1.085190000	-2.499580000	0.000076000
6	-2.274216000	-0.731245000	0.000065000
6	-2.274216000	0.731245000	0.000063000
6	-1.063164000	1.414254000	0.000072000
1	-1.085190000	2.499580000	0.000069000
6	-4.561075000	0.732747000	0.000040000
6	-4.561075000	-0.732747000	0.000042000
6	-5.799457000	-1.412193000	0.000030000
6	-5.799457000	1.412193000	0.000026000
6	-7.001569000	0.730397000	0.000014000
6	-7.001569000	-0.730397000	0.000016000
1	-5.777800000	-2.497792000	0.000032000
1	-5.777800000	2.497792000	0.000025000
6	7.340149000	-0.734615000	0.000105000
6	7.340149000	0.734615000	0.000102000
6	8.561204000	1.416963000	0.000098000
6	8.561204000	-1.416963000	0.000102000
6	9.782542000	0.733765000	0.000095000
6	9.782542000	-0.733765000	0.000097000
1	8.582929000	-2.502165000	0.000102000
1	8.582929000	2.502165000	0.000096000
6	-9.438048000	-0.723455000	-0.000012000
6	-9.438048000	0.723455000	-0.000014000
7	-10.663526000	1.355285000	-0.000029000
7	-10.663526000	-1.355285000	-0.000025000
6	-11.888503000	0.711173000	-0.000042000
6	-11.888503000	-0.711173000	-0.000039000
1	-10.665384000	2.364485000	-0.000030000
1	-10.665384000	-2.364485000	-0.000023000
6	-8.253131000	-1.406036000	0.000003000
6	-8.253131000	1.406036000	-0.000001000
7	-3.431033000	-1.434748000	0.000055000
7	-3.431033000	1.434748000	0.000051000
6	1.384389000	-1.416119000	0.000092000
6	1.384389000	1.416119000	0.000088000
6	6.115316000	-1.416275000	0.000106000
6	6.115316000	1.416275000	0.000102000
7	10.926365000	-1.435656000	0.000091000
7	10.926365000	1.435656000	0.000087000

6	12.069722000	-0.732949000	0.000082000
6	12.069722000	0.732949000	0.000080000
6	13.291528000	-1.416497000	0.000071000
6	13.291528000	1.416496000	0.000068000
6	14.511671000	-0.733848000	0.000058000
6	14.511671000	0.733848000	0.000056000
6	-13.085470000	-1.397442000	-0.000051000
6	-13.085470000	1.397442000	-0.000056000
6	-14.317829000	-0.716716000	-0.000065000
6	-14.317829000	0.716716000	-0.000068000
6	-15.556663000	-1.396966000	-0.000077000
6	-15.556663000	1.396966000	-0.000082000
6	-16.750958000	-0.714297000	-0.000090000
6	-16.750958000	0.714297000	-0.000093000
1	-15.564750000	-2.483692000	-0.000075000
1	-15.564750000	2.483692000	-0.000084000
1	-13.076463000	2.484191000	-0.000057000
1	-13.076463000	-2.484191000	-0.000049000
1	-8.260645000	2.492461000	-0.000003000
1	-8.260645000	-2.492461000	0.000005000
1	1.405756000	-2.501408000	0.000093000
1	1.405756000	2.501408000	0.000086000
1	6.093302000	2.501503000	0.000100000
1	6.093302000	-2.501503000	0.000106000
1	13.269712000	2.501720000	0.000065000
1	13.269712000	-2.501720000	0.000072000
6	15.738016000	-1.415941000	0.000043000
6	15.738016000	1.415941000	0.000040000
6	16.952359000	-0.731239000	0.000026000
6	16.952359000	0.731239000	0.000024000
1	15.760352000	-2.501146000	0.000043000
1	15.760352000	2.501146000	0.000037000
7	-17.975614000	1.358637000	-0.000106000
7	-17.975614000	-1.358637000	-0.000101000
6	-19.203919000	0.713553000	-0.000118000
6	-19.203919000	-0.713553000	-0.000115000
6	-20.396063000	1.396639000	-0.000131000
6	-20.396063000	-1.396639000	-0.000126000
6	-21.636060000	0.715092000	-0.000143000
6	-21.636060000	-0.715092000	-0.000140000
1	-20.389253000	2.483684000	-0.000133000
1	-20.389253000	-2.483684000	-0.000124000
1	-17.976318000	2.366730000	-0.000107000
1	-17.976318000	-2.366730000	-0.000100000
7	18.105069000	1.433782000	0.000005000
7	18.105069000	-1.433782000	0.000009000
6	19.237880000	0.731385000	-0.000012000

6	19.237880000	-0.731385000	-0.000011000
6	20.474673000	1.413804000	-0.000035000
6	20.474673000	-1.413804000	-0.000032000
6	21.675405000	0.728482000	-0.000057000
6	21.675405000	-0.728482000	-0.000055000
6	22.934652000	1.407275000	-0.000082000
6	22.934652000	-1.407275000	-0.000079000
6	24.106094000	0.714176000	-0.000105000
6	24.106094000	-0.714176000	-0.000103000
1	20.453979000	-2.499444000	-0.000031000
1	20.453979000	2.499444000	-0.000037000
1	22.931579000	2.493225000	-0.000084000
1	22.931579000	-2.493225000	-0.000077000
1	25.053090000	-1.244274000	-0.000120000
1	25.053090000	1.244274000	-0.000124000
6	-22.872981000	-1.396507000	-0.000152000
6	-22.872981000	1.396507000	-0.000157000
6	-24.061855000	-0.703725000	-0.000165000
6	-24.061855000	0.703725000	-0.000168000
1	-22.870331000	-2.483107000	-0.000150000
1	-22.870331000	2.483107000	-0.000159000
1	-25.003837000	-1.242450000	-0.000174000
1	-25.003837000	1.242450000	-0.000179000

Table S75: Coordinates of pN₆_5 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	4.816492000	-0.733474000	0.000040000
7	3.672006000	-1.436015000	0.000038000
6	2.529409000	-0.734161000	0.000034000
6	2.529409000	0.734161000	0.000032000
7	3.672006000	1.436015000	0.000035000
6	4.816492000	0.733474000	0.000038000
6	0.087256000	0.734863000	0.000023000
6	0.087256000	-0.734863000	0.000025000
6	-1.137585000	-1.416924000	0.000021000
1	-1.159717000	-2.502088000	0.000022000
6	-2.354858000	-0.732865000	0.000014000
6	-2.354858000	0.732865000	0.000012000
6	-1.137585000	1.416924000	0.000017000
1	-1.159717000	2.502088000	0.000016000
6	-4.641971000	0.734215000	0.000001000
6	-4.641971000	-0.734215000	0.000002000
6	-5.867668000	-1.416744000	-0.000004000
6	-5.867668000	1.416744000	-0.000007000
6	-7.083901000	0.734027000	-0.000013000
6	-7.083901000	-0.734027000	-0.000011000

1	-5.846260000	-2.501971000	-0.000002000
1	-5.846260000	2.501971000	-0.000009000
6	7.258590000	-0.734905000	0.000044000
6	7.258590000	0.734905000	0.000043000
6	8.480978000	1.417678000	0.000043000
6	8.480978000	-1.417678000	0.000046000
6	9.700483000	0.733547000	0.000045000
6	9.700483000	-0.733547000	0.000047000
1	8.502944000	-2.502796000	0.000047000
1	8.502944000	2.502796000	0.000042000
6	-9.525102000	-0.731034000	-0.000025000
6	-9.525102000	0.731034000	-0.000027000
7	-10.682162000	1.434665000	-0.000035000
7	-10.682162000	-1.434665000	-0.000031000
6	-11.811545000	0.733024000	-0.000040000
6	-11.811545000	-0.733024000	-0.000038000
6	-8.314677000	-1.414773000	-0.000018000
6	-8.314677000	1.414773000	-0.000021000
7	-3.502283000	-1.435794000	0.000009000
7	-3.502283000	1.435794000	0.000006000
6	1.307565000	-1.417698000	0.000031000
6	1.307565000	1.417698000	0.000027000
6	6.036186000	-1.417572000	0.000043000
6	6.036186000	1.417572000	0.000040000
7	10.845409000	-1.435733000	0.000047000
7	10.845409000	1.435733000	0.000044000
6	11.987285000	-0.733458000	0.000046000
6	11.987285000	0.733458000	0.000045000
6	13.210075000	-1.417305000	0.000046000
6	13.210075000	1.417305000	0.000043000
6	14.428804000	-0.734079000	0.000045000
6	14.428804000	0.734079000	0.000043000
6	-13.050351000	-1.412905000	-0.000044000
6	-13.050351000	1.412905000	-0.000047000
6	-14.251374000	-0.730551000	-0.000050000
6	-14.251374000	0.730551000	-0.000052000
6	-15.503473000	-1.406310000	-0.000054000
6	-15.503473000	1.406310000	-0.000058000
6	-16.687726000	-0.723905000	-0.000060000
6	-16.687726000	0.723905000	-0.000061000
1	-15.510940000	-2.492619000	-0.000053000
1	-15.510940000	2.492619000	-0.000059000
1	-13.028759000	2.498413000	-0.000048000
1	-13.028759000	-2.498413000	-0.000042000
1	-8.336903000	2.500035000	-0.000023000
1	-8.336903000	-2.500035000	-0.000016000
1	1.329306000	-2.502838000	0.000032000

1	1.329306000	2.502838000	0.000026000
1	6.014181000	2.502701000	0.000038000
1	6.014181000	-2.502701000	0.000044000
1	13.188318000	2.502457000	0.000042000
1	13.188318000	-2.502457000	0.000047000
6	15.655893000	-1.416363000	0.000044000
6	15.655893000	1.416363000	0.000041000
6	16.869155000	-0.731182000	0.000041000
6	16.869155000	0.731182000	0.000040000
1	15.678384000	-2.501509000	0.000045000
1	15.678384000	2.501509000	0.000039000
7	-17.912591000	1.356186000	-0.000067000
7	-17.912591000	-1.356186000	-0.000064000
6	-19.138980000	0.713014000	-0.000071000
6	-19.138980000	-0.713014000	-0.000069000
6	-20.332091000	1.398425000	-0.000076000
6	-20.332091000	-1.398425000	-0.000072000
6	-21.567955000	0.716129000	-0.000079000
6	-21.567955000	-0.716129000	-0.000077000
1	-20.324885000	2.485271000	-0.000077000
1	-20.324885000	-2.485271000	-0.000070000
1	-17.914708000	2.365402000	-0.000068000
1	-17.914708000	-2.365402000	-0.000062000
7	18.022408000	1.433964000	0.000036000
7	18.022408000	-1.433964000	0.000040000
6	19.154486000	0.731858000	0.000034000
6	19.154486000	-0.731858000	0.000036000
6	20.391622000	1.414358000	0.000030000
6	20.391622000	-1.414358000	0.000033000
6	21.591739000	0.728764000	0.000027000
6	21.591739000	-0.728764000	0.000029000
6	22.851116000	1.407678000	0.000023000
6	22.851116000	-1.407678000	0.000026000
6	24.022127000	0.714342000	0.000020000
6	24.022127000	-0.714342000	0.000021000
1	20.371006000	-2.499934000	0.000034000
1	20.371006000	2.499934000	0.000029000
1	22.848123000	2.493557000	0.000021000
1	22.848123000	-2.493557000	0.000027000
1	24.969226000	-1.244163000	0.000019000
1	24.969226000	1.244163000	0.000016000
6	-22.806740000	-1.397963000	-0.000079000
6	-22.806740000	1.397963000	-0.000083000
6	-23.993096000	-0.704860000	-0.000084000
6	-23.993096000	0.704860000	-0.000086000
1	-22.804190000	-2.484368000	-0.000078000
1	-22.804190000	2.484368000	-0.000085000

1	-24.935638000	-1.242420000	-0.000086000
1	-24.935638000	1.242420000	-0.000090000

Table S76: Coordinates of pN₆_6 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	4.733381000	-0.731508000	-0.000065000
7	3.585982000	-1.436362000	-0.000074000
6	2.448423000	-0.732390000	-0.000083000
6	2.448423000	0.732390000	-0.000084000
7	3.585982000	1.436362000	-0.000076000
6	4.733381000	0.731508000	-0.000066000
6	0.000000000	0.732284000	-0.000098000
6	0.000000000	-0.732284000	-0.000096000
6	-1.222109000	-1.410625000	-0.000100000
1	-1.243450000	-2.496296000	-0.000098000
6	-2.448422000	-0.732390000	-0.000103000
6	-2.448422000	0.732390000	-0.000104000
6	-1.222109000	1.410625000	-0.000102000
1	-1.243450000	2.496296000	-0.000102000
6	-4.733380000	0.731508000	-0.000104000
6	-4.733380000	-0.731508000	-0.000103000
6	-5.949920000	-1.411122000	-0.000099000
6	-5.949920000	1.411122000	-0.000102000
6	-7.180489000	0.732418000	-0.000097000
6	-7.180489000	-0.732418000	-0.000096000
1	-5.927913000	-2.496704000	-0.000098000
1	-5.927913000	2.496704000	-0.000101000
6	7.180489000	-0.732418000	-0.000038000
6	7.180489000	0.732418000	-0.000039000
6	8.394842000	1.412848000	-0.000024000
6	8.394842000	-1.412848000	-0.000022000
6	9.626845000	0.732485000	-0.000007000
6	9.626845000	-0.732485000	-0.000006000
1	8.416004000	-2.498371000	-0.000020000
1	8.416004000	2.498371000	-0.000023000
6	-9.626845000	-0.732485000	-0.000081000
6	-9.626845000	0.732485000	-0.000082000
7	-10.760031000	1.435431000	-0.000075000
7	-10.760031000	-1.435431000	-0.000073000
6	-11.912190000	0.730675000	-0.000066000
6	-11.912190000	-0.730675000	-0.000065000
6	-8.394842000	-1.412848000	-0.000089000
6	-8.394842000	1.412848000	-0.000091000
7	-3.585982000	-1.436362000	-0.000103000
7	-3.585982000	1.436362000	-0.000106000
6	1.222109000	-1.410625000	-0.000090000

6	1.222109000	1.410625000	-0.000092000
6	5.949920000	-1.411122000	-0.000051000
6	5.949920000	1.411122000	-0.000053000
7	10.760031000	-1.435431000	0.000010000
7	10.760031000	1.435431000	0.000008000
6	11.912190000	-0.730675000	0.000026000
6	11.912190000	0.730675000	0.000025000
6	13.125607000	-1.413206000	0.000045000
6	13.125607000	1.413206000	0.000043000
6	14.355445000	-0.731821000	0.000064000
6	14.355445000	0.731821000	0.000063000
6	-13.125607000	-1.413206000	-0.000053000
6	-13.125607000	1.413206000	-0.000056000
6	-14.355445000	-0.731821000	-0.000042000
6	-14.355445000	0.731821000	-0.000043000
6	-15.572707000	-1.413936000	-0.000029000
6	-15.572707000	1.413936000	-0.000031000
6	-16.796948000	-0.729617000	-0.000016000
6	-16.796948000	0.729617000	-0.000017000
1	-15.594751000	-2.499264000	-0.000028000
1	-15.594751000	2.499264000	-0.000032000
1	-13.103341000	2.498586000	-0.000056000
1	-13.103341000	-2.498586000	-0.000052000
1	-8.416004000	2.498371000	-0.000091000
1	-8.416004000	-2.498371000	-0.000087000
1	1.243450000	-2.496296000	-0.000088000
1	1.243450000	2.496296000	-0.000092000
1	5.927913000	2.496704000	-0.000053000
1	5.927913000	-2.496704000	-0.000049000
1	13.103341000	2.498586000	0.000042000
1	13.103341000	-2.498586000	0.000046000
6	15.572707000	-1.413936000	0.000083000
6	15.572707000	1.413936000	0.000082000
6	16.796948000	-0.729617000	0.000104000
6	16.796948000	0.729617000	0.000103000
1	15.594751000	-2.499264000	0.000085000
1	15.594751000	2.499264000	0.000081000
7	-17.940895000	1.432548000	-0.000004000
7	-17.940895000	-1.432548000	-0.000002000
6	-19.080963000	0.729187000	0.000010000
6	-19.080963000	-0.729187000	0.000011000
6	-20.311745000	1.412293000	0.000024000
6	-20.311745000	-1.412293000	0.000026000
6	-21.517087000	0.726741000	0.000040000
6	-21.517087000	-0.726741000	0.000041000
1	-20.290713000	2.497903000	0.000023000
1	-20.290713000	-2.497903000	0.000027000

7	17.940895000	1.432548000	0.000121000
7	17.940895000	-1.432548000	0.000122000
6	19.080963000	0.729187000	0.000140000
6	19.080963000	-0.729187000	0.000141000
6	20.311745000	1.412293000	0.000160000
6	20.311745000	-1.412293000	0.000162000
6	21.517087000	0.726741000	0.000181000
6	21.517087000	-0.726741000	0.000182000
6	22.772978000	1.406226000	0.000202000
6	22.772978000	-1.406226000	0.000204000
6	23.946473000	0.712669000	0.000222000
6	23.946473000	-0.712669000	0.000223000
1	20.290713000	-2.497903000	0.000162000
1	20.290713000	2.497903000	0.000159000
1	22.769931000	2.492122000	0.000201000
1	22.769931000	-2.492122000	0.000204000
1	24.892931000	-1.243575000	0.000240000
1	24.892931000	1.243575000	0.000238000
6	-22.772978000	-1.406226000	0.000058000
6	-22.772978000	1.406226000	0.000055000
6	-23.946473000	-0.712669000	0.000072000
6	-23.946473000	0.712669000	0.000071000
1	-22.769931000	-2.492122000	0.000059000
1	-22.769931000	2.492122000	0.000055000
1	-24.892931000	-1.243575000	0.000085000
1	-24.892931000	1.243575000	0.000083000

Table S77: Coordinates of pA₁_1 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-7.285225000	-1.406249000	-0.000236000
6	-6.027524000	-0.726675000	-0.000153000
6	-4.822133000	-1.405769000	-0.000203000
6	-6.027524000	0.726675000	-0.000011000
6	-4.822133000	1.405769000	0.000070000
6	-3.582012000	0.729966000	0.000021000
6	-3.582012000	-0.729966000	-0.000120000
6	-8.457867000	-0.713736000	-0.000184000
6	-7.285225000	1.406249000	0.000040000
1	-4.822512000	2.492842000	0.000175000
6	-2.368722000	1.414101000	0.000103000
6	-2.368722000	-1.414101000	-0.000169000
6	-1.142875000	-0.730859000	-0.000086000
6	-1.142875000	0.730859000	0.000054000
1	-2.346716000	2.499654000	0.000208000
1	-2.346716000	-2.499654000	-0.000274000
6	-8.457867000	0.713736000	-0.000042000

1	-7.282414000	-2.492526000	-0.000343000
1	-4.822512000	-2.492842000	-0.000308000
1	-7.282414000	2.492526000	0.000147000
6	2.368721000	-1.414101000	-0.000103000
6	3.582013000	-0.729966000	-0.000021000
6	4.822133000	-1.405769000	-0.000070000
6	3.582013000	0.729966000	0.000120000
6	4.822133000	1.405769000	0.000203000
6	6.027524000	0.726675000	0.000153000
6	6.027524000	-0.726675000	0.000011000
6	1.142876000	-0.730859000	-0.000054000
6	2.368721000	1.414101000	0.000170000
1	4.822512000	2.492842000	0.000308000
6	7.285225000	1.406249000	0.000236000
6	7.285225000	-1.406249000	-0.000040000
6	8.457867000	-0.713736000	0.000042000
6	8.457867000	0.713736000	0.000184000
1	7.282414000	2.492526000	0.000343000
1	7.282414000	-2.492526000	-0.000147000
1	9.404608000	-1.244317000	0.000000000
1	9.404608000	1.244317000	0.000250000
6	1.142876000	0.730859000	0.000086000
1	2.346716000	-2.499654000	-0.000208000
1	4.822512000	-2.492842000	-0.000175000
1	2.346716000	2.499654000	0.000274000
7	0.000000000	1.433275000	0.000137000
7	0.000000000	-1.433275000	-0.000137000
1	-9.404608000	-1.244317000	-0.000250000
1	-9.404608000	1.244317000	0.000000000

Table S78: Coordinates of pA₂_1 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-2.392990000	1.404762000	-0.000122000
6	-1.140482000	0.728131000	-0.000097000
6	0.064811000	1.404698000	-0.000089000
6	-1.140482000	-0.728131000	-0.000077000
6	0.064811000	-1.404698000	-0.000052000
6	1.307269000	-0.730214000	-0.000047000
6	1.307269000	0.730214000	-0.000067000
6	-3.577379000	0.722487000	-0.000140000
6	-2.392990000	-1.404762000	-0.000088000
1	0.065750000	-2.491711000	-0.000037000
6	2.518724000	-1.412896000	-0.000026000
6	2.518724000	1.412896000	-0.000065000
6	3.747960000	0.731358000	-0.000047000
6	3.747960000	-0.731358000	-0.000027000

1	2.540627000	-2.498597000	-0.000011000
1	2.540627000	2.498597000	-0.000079000
6	-3.577379000	-0.722487000	-0.000124000
1	-2.401352000	2.491445000	-0.000132000
1	0.065750000	2.491711000	-0.000103000
1	-2.401352000	-2.491445000	-0.000074000
6	7.258289000	1.412702000	-0.000028000
6	8.474087000	0.729286000	-0.000009000
6	9.713037000	1.404962000	-0.000009000
6	8.474087000	-0.729286000	0.000012000
6	9.713037000	-1.404962000	0.000032000
6	10.919812000	-0.726165000	0.000032000
6	10.919812000	0.726165000	0.000011000
6	6.034431000	0.729863000	-0.000028000
6	7.258289000	-1.412702000	0.000012000
1	9.713424000	-2.492174000	0.000048000
6	12.177087000	-1.405513000	0.000052000
6	12.177087000	1.405513000	0.000011000
6	13.350602000	0.713391000	0.000031000
6	13.350602000	-0.713391000	0.000052000
1	12.174125000	-2.491917000	0.000068000
1	12.174125000	2.491917000	-0.000005000
1	14.297168000	1.244436000	0.000031000
1	14.297168000	-1.244436000	0.000068000
6	6.034431000	-0.729863000	-0.000008000
1	7.236277000	2.498382000	-0.000043000
1	9.713424000	2.492174000	-0.000024000
1	7.236277000	-2.498382000	0.000028000
7	4.888361000	-1.433174000	-0.000007000
7	4.888361000	1.433173000	-0.000047000
6	-12.155746000	1.400830000	0.000190000
6	-10.907469000	0.720353000	0.000144000
6	-9.684930000	1.399212000	0.000078000
6	-10.907469000	-0.720353000	0.000163000
6	-9.684930000	-1.399212000	0.000116000
6	-8.465951000	-0.721749000	0.000047000
6	-8.465951000	0.721749000	0.000028000
6	-13.336250000	0.708913000	0.000252000
6	-12.155746000	-1.400830000	0.000229000
1	-9.686120000	-2.486794000	0.000130000
6	-7.219654000	-1.401176000	-0.000008000
6	-7.219654000	1.401176000	-0.000042000
6	-6.031856000	0.717404000	-0.000099000
6	-6.031856000	-0.717404000	-0.000083000
1	-7.211365000	-2.488008000	0.000004000
1	-7.211365000	2.488008000	-0.000053000
6	-13.336250000	-0.708913000	0.000272000

1	-12.152677000	2.487467000	0.000175000
1	-9.686120000	2.486794000	0.000064000
1	-14.280862000	1.243427000	0.000286000
1	-12.152677000	-2.487467000	0.000244000
1	-14.280862000	-1.243427000	0.000322000
7	-4.804114000	-1.356318000	-0.000170000
7	-4.804114000	1.356318000	-0.000190000
1	-4.805147000	-2.365289000	-0.000110000
1	-4.805147000	2.365289000	-0.000174000

Table S79: Coordinates of pA₂_2 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	2.448259000	-1.416130000	0.000000000
6	1.225200000	-0.733053000	0.000000000
6	0.000000000	-1.409763000	-0.000014000
6	1.225200000	0.733053000	0.000015000
6	0.000000000	1.409763000	0.000015000
6	-1.225200000	0.733053000	0.000000000
6	-1.225200000	-0.733053000	-0.000015000
6	3.666158000	-0.732133000	0.000014000
6	2.448259000	1.416130000	0.000029000
1	0.000000000	2.496317000	0.000026000
6	-2.448259000	1.416130000	0.000000000
6	-2.448259000	-1.416130000	-0.000029000
6	-3.666158000	-0.732133000	-0.000029000
6	-3.666158000	0.732133000	-0.000014000
1	-2.470983000	2.501537000	0.000011000
1	-2.470983000	-2.501537000	-0.000040000
6	3.666158000	0.732133000	0.000029000
1	2.470983000	-2.501537000	-0.000011000
1	0.000000000	-2.496317000	-0.000025000
1	2.470983000	2.501537000	0.000040000
6	-7.182136000	-1.415274000	-0.000055000
6	-8.392936000	-0.730970000	-0.000054000
6	-9.634492000	-1.406444000	-0.000067000
6	-8.392936000	0.730970000	-0.000039000
6	-9.634492000	1.406444000	-0.000039000
6	-10.838798000	0.727294000	-0.000051000
6	-10.838798000	-0.727294000	-0.000066000
6	-5.952819000	-0.732770000	-0.000041000
6	-7.182136000	1.415274000	-0.000026000
1	-9.635377000	2.493466000	-0.000028000
6	-12.096998000	1.406694000	-0.000050000
6	-12.096998000	-1.406694000	-0.000078000
6	-13.269199000	-0.714009000	-0.000076000
6	-13.269199000	0.714009000	-0.000062000

1	-12.094748000	2.492921000	-0.000039000
1	-12.094748000	-2.492921000	-0.000089000
1	-14.215812000	-1.244768000	-0.000086000
1	-14.215812000	1.244768000	-0.000061000
6	-5.952819000	0.732770000	-0.000027000
1	-7.160586000	-2.500801000	-0.000066000
1	-9.635377000	-2.493466000	-0.000078000
1	-7.160585000	2.500801000	-0.000015000
7	-4.814787000	1.434441000	-0.000013000
7	-4.814787000	-1.434441000	-0.000042000
6	12.096998000	-1.406694000	0.000050000
6	10.838798000	-0.727294000	0.000051000
6	9.634492000	-1.406444000	0.000039000
6	10.838798000	0.727294000	0.000065000
6	9.634492000	1.406444000	0.000067000
6	8.392936000	0.730970000	0.000054000
6	8.392936000	-0.730970000	0.000039000
6	13.269199000	-0.714009000	0.000061000
6	12.096998000	1.406694000	0.000078000
1	9.635377000	2.493466000	0.000077000
6	7.182136000	1.415274000	0.000055000
6	7.182136000	-1.415274000	0.000027000
6	5.952819000	-0.732770000	0.000027000
6	5.952819000	0.732770000	0.000041000
1	7.160585000	2.500801000	0.000065000
1	7.160585000	-2.500801000	0.000016000
6	13.269199000	0.714009000	0.000076000
1	12.094748000	-2.492921000	0.000039000
1	9.635377000	-2.493466000	0.000028000
1	14.215812000	-1.244768000	0.000060000
1	12.094748000	2.492921000	0.000089000
1	14.215812000	1.244768000	0.000085000
7	4.814787000	1.434441000	0.000043000
7	4.814787000	-1.434441000	0.000014000

Table S80: Coordinates of pA₃_1 optimized at M06L/6-311++g(d,p) level

atom	X	Y	Z
6	2.494742000	1.404720000	0.000012000
6	3.747246000	0.728236000	0.000002000
6	4.952702000	1.404689000	0.000005000
6	3.747246000	-0.728236000	-0.000012000
6	4.952702000	-1.404689000	-0.000022000
6	6.195267000	-0.730228000	-0.000020000
6	6.195267000	0.730228000	-0.000006000
6	1.309640000	0.722723000	0.000008000
6	2.494742000	-1.404720000	-0.000015000

1	4.953849000	-2.491739000	-0.000033000
6	7.406793000	-1.412743000	-0.000030000
6	7.406793000	1.412743000	-0.000003000
6	8.636246000	0.731312000	-0.000013000
6	8.636246000	-0.731312000	-0.000028000
1	7.428586000	-2.498454000	-0.000041000
1	7.428586000	2.498454000	0.000008000
6	1.309640000	-0.722723000	-0.000005000
1	2.486910000	2.491429000	0.000022000
1	4.953849000	2.491739000	0.000015000
1	2.486910000	-2.491429000	-0.000025000
6	12.146479000	1.412451000	-0.000018000
6	13.362597000	0.729147000	-0.000028000
6	14.601477000	1.404912000	-0.000025000
6	13.362597000	-0.729147000	-0.000043000
6	14.601477000	-1.404912000	-0.000054000
6	15.808408000	-0.726096000	-0.000051000
6	15.808408000	0.726096000	-0.000036000
6	10.922740000	0.729644000	-0.000021000
6	12.146479000	-1.412451000	-0.000046000
1	14.601753000	-2.492158000	-0.000065000
6	17.065744000	-1.405441000	-0.000062000
6	17.065744000	1.405441000	-0.000032000
6	18.239423000	0.713397000	-0.000043000
6	18.239423000	-0.713397000	-0.000058000
1	17.062754000	-2.491880000	-0.000073000
1	17.062754000	2.491880000	-0.000021000
1	19.186009000	1.244485000	-0.000040000
1	19.186009000	-1.244485000	-0.000067000
6	10.922740000	-0.729644000	-0.000035000
1	12.124478000	2.498158000	-0.000007000
1	14.601753000	2.492158000	-0.000014000
1	12.124478000	-2.498158000	-0.000057000
7	9.776484000	-1.433404000	-0.000039000
7	9.776484000	1.433404000	-0.000010000
6	-7.268406000	1.399649000	0.000035000
6	-6.021541000	0.720926000	0.000026000
6	-4.801438000	1.398429000	0.000030000
6	-6.021541000	-0.720926000	0.000011000
6	-4.801438000	-1.398429000	0.000002000
6	-3.578747000	-0.720739000	0.000006000
6	-3.578747000	0.720739000	0.000020000
6	-8.457491000	0.717205000	0.000030000
6	-7.268406000	-1.399649000	0.000007000
1	-4.801385000	-2.485947000	-0.000008000
6	-2.334376000	-1.399950000	-0.000003000
6	-2.334376000	1.399950000	0.000024000

6	-1.144784000	0.715796000	0.000015000
6	-1.144784000	-0.715796000	0.000001000
1	-2.326143000	-2.486929000	-0.000013000
1	-2.326143000	2.486929000	0.000034000
6	-8.457491000	-0.717205000	0.000016000
1	-7.276266000	2.486624000	0.000046000
1	-4.801385000	2.485947000	0.000041000
1	-7.276266000	-2.486624000	-0.000004000
7	0.083544000	-1.356273000	-0.000008000
7	0.083544000	1.356273000	0.000018000
1	0.082210000	-2.365112000	-0.000017000
1	0.082210000	2.365112000	0.000027000
6	-17.039308000	1.400188000	0.000051000
6	-15.791524000	0.719893000	0.000042000
6	-14.567391000	1.398718000	0.000047000
6	-15.791524000	-0.719893000	0.000025000
6	-14.567391000	-1.398718000	0.000016000
6	-13.349424000	-0.721419000	0.000022000
6	-13.349424000	0.721419000	0.000038000
6	-18.220817000	0.708557000	0.000045000
6	-17.039308000	-1.400188000	0.000019000
1	-14.568721000	-2.486402000	0.000004000
6	-12.100926000	-1.400302000	0.000014000
6	-12.100926000	1.400302000	0.000043000
6	-10.913121000	0.717963000	0.000034000
6	-10.913121000	-0.717963000	0.000019000
1	-12.093422000	-2.487235000	0.000002000
1	-12.093422000	2.487235000	0.000055000
6	-18.220817000	-0.708557000	0.000028000
1	-17.036098000	2.486940000	0.000063000
1	-14.568721000	2.486402000	0.000059000
1	-19.165294000	1.243481000	0.000052000
1	-17.036098000	-2.486940000	0.000007000
1	-19.165294000	-1.243480000	0.000023000
7	-9.685086000	-1.357411000	0.000011000
7	-9.685086000	1.357411000	0.000039000
1	-9.685072000	-2.365743000	0.000002000
1	-9.685072000	2.365743000	0.000049000

Table S81: Coordinates of pA₃_2 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	2.443522000	-1.414963000	-0.000051000
6	3.669202000	-0.732585000	-0.000038000
6	4.892847000	-1.409240000	-0.000037000
6	3.669202000	0.732585000	-0.000023000
6	4.892847000	1.409240000	-0.000008000

6	6.119680000	0.732785000	-0.000006000
6	6.119680000	-0.732785000	-0.000021000
6	1.227747000	-0.731478000	-0.000050000
6	2.443522000	1.414963000	-0.000023000
1	4.892924000	2.495899000	0.000004000
6	7.341787000	1.415792000	0.000011000
6	7.341787000	-1.415792000	-0.000018000
6	8.560935000	-0.732229000	0.000000000
6	8.560935000	0.732229000	0.000015000
1	7.364190000	2.501239000	0.000023000
1	7.364190000	-2.501239000	-0.000028000
6	1.227747000	0.731478000	-0.000036000
1	2.421052000	-2.500451000	-0.000061000
1	4.892924000	-2.495899000	-0.000047000
1	2.421052000	2.500451000	-0.000011000
6	12.076309000	-1.414762000	0.000029000
6	13.287784000	-0.730532000	0.000049000
6	14.529208000	-1.406230000	0.000056000
6	13.287784000	0.730532000	0.000064000
6	14.529208000	1.406230000	0.000086000
6	15.733679000	0.727095000	0.000093000
6	15.733679000	-0.727095000	0.000078000
6	10.847656000	-0.732007000	0.000022000
6	12.076309000	1.414762000	0.000058000
1	14.529548000	2.493300000	0.000097000
6	16.992043000	1.406578000	0.000115000
6	16.992043000	-1.406578000	0.000086000
6	18.164338000	-0.714088000	0.000107000
6	18.164338000	0.714088000	0.000122000
1	16.989250000	2.492864000	0.000127000
1	16.989250000	-2.492864000	0.000074000
1	19.111247000	-1.244431000	0.000112000
1	19.111247000	1.244431000	0.000139000
6	10.847656000	0.732007000	0.000037000
1	12.054638000	-2.500304000	0.000018000
1	14.529548000	-2.493300000	0.000045000
1	12.054638000	2.500304000	0.000069000
7	9.708639000	1.434630000	0.000033000
7	9.708639000	-1.434630000	0.000004000
6	-7.201136000	-1.405501000	-0.000056000
6	-5.948656000	-0.728872000	-0.000054000
6	-4.744281000	-1.405568000	-0.000063000
6	-5.948656000	0.728872000	-0.000040000
6	-4.744281000	1.405568000	-0.000036000
6	-3.500872000	0.731191000	-0.000044000
6	-3.500872000	-0.731191000	-0.000058000
6	-8.385403000	-0.723020000	-0.000044000

6	-7.201136000	1.405501000	-0.000029000
1	-4.743144000	2.492503000	-0.000025000
6	-2.291602000	1.414120000	-0.000037000
6	-2.291602000	-1.414120000	-0.000064000
6	-1.059499000	-0.733128000	-0.000057000
6	-1.059499000	0.733128000	-0.000042000
1	-2.269947000	2.499735000	-0.000025000
1	-2.269947000	-2.499735000	-0.000074000
6	-8.385403000	0.723020000	-0.000030000
1	-7.209045000	-2.492103000	-0.000065000
1	-4.743144000	-2.492503000	-0.000072000
1	-7.209045000	2.492103000	-0.000018000
7	0.076316000	1.434936000	-0.000032000
7	0.076316000	-1.434937000	-0.000061000
6	-16.962858000	-1.401081000	0.000004000
6	-15.714418000	-0.720381000	0.000002000
6	-14.492189000	-1.399529000	-0.000014000
6	-15.714418000	0.720381000	0.000017000
6	-14.492189000	1.399529000	0.000015000
6	-13.273130000	0.721746000	-0.000001000
6	-13.273130000	-0.721746000	-0.000015000
6	-18.143092000	-0.709047000	0.000020000
6	-16.962858000	1.401081000	0.000034000
1	-14.493509000	2.487047000	0.000026000
6	-12.027084000	1.401483000	-0.000002000
6	-12.027084000	-1.401483000	-0.000030000
6	-10.839353000	-0.717301000	-0.000031000
6	-10.839353000	0.717301000	-0.000017000
1	-12.019345000	2.488256000	0.000009000
1	-12.019345000	-2.488256000	-0.000040000
6	-18.143092000	0.709047000	0.000035000
1	-16.959788000	-2.487675000	-0.000007000
1	-14.493509000	-2.487047000	-0.000025000
1	-19.087839000	-1.243309000	0.000022000
1	-16.959788000	2.487675000	0.000045000
1	-19.087839000	1.243309000	0.000048000
7	-9.611584000	1.356334000	-0.000018000
7	-9.611584000	-1.356334000	-0.000043000
1	-9.612804000	2.365365000	-0.000008000
1	-9.612804000	-2.365365000	-0.000052000

Table S82: Coordinates of pA₃_3 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-2.364533000	1.407659000	-0.000007000
6	-3.594353000	0.730483000	0.000003000
6	-4.812171000	1.403957000	0.000000000

6	-3.594353000	-0.730483000	0.000018000
6	-4.812171000	-1.403957000	0.000028000
6	-6.050330000	-0.730431000	0.000025000
6	-6.050330000	0.730431000	0.000010000
6	-1.143078000	0.731448000	-0.000004000
6	-2.364533000	-1.407659000	0.000021000
1	-4.812592000	-2.490978000	0.000038000
6	-7.260717000	-1.410742000	0.000034000
6	-7.260717000	1.410742000	0.000007000
6	-8.497955000	0.730851000	0.000017000
6	-8.497955000	-0.730851000	0.000031000
1	-7.282597000	-2.496567000	0.000045000
1	-7.282597000	2.496567000	-0.000004000
6	-1.143078000	-0.731448000	0.000010000
1	-2.342909000	2.493704000	-0.000018000
1	-4.812592000	2.490978000	-0.000011000
1	-2.342909000	-2.493704000	0.000031000
6	-11.998847000	1.410263000	0.000018000
6	-13.224172000	0.726951000	0.000028000
6	-14.454706000	1.403320000	0.000024000
6	-13.224172000	-0.726951000	0.000042000
6	-14.454706000	-1.403320000	0.000052000
6	-15.668879000	-0.723542000	0.000048000
6	-15.668879000	0.723542000	0.000033000
6	-10.783499000	0.727999000	0.000022000
6	-11.998847000	-1.410263000	0.000046000
1	-14.454905000	-2.490475000	0.000062000
6	-16.920632000	-1.403917000	0.000057000
6	-16.920632000	1.403917000	0.000029000
6	-18.097701000	0.710897000	0.000038000
6	-18.097701000	-0.710897000	0.000052000
1	-16.917638000	-2.490193000	0.000068000
1	-16.917638000	2.490193000	0.000018000
1	-19.043419000	1.243213000	0.000034000
1	-19.043419000	-1.243213000	0.000060000
6	-10.783499000	-0.727999000	0.000037000
1	-11.976500000	2.495966000	0.000008000
1	-14.454905000	2.490475000	0.000013000
1	-11.976500000	-2.495966000	0.000057000
7	-9.628880000	-1.434070000	0.000041000
7	-9.628880000	1.434070000	0.000013000
6	7.260717000	1.410742000	-0.000035000
6	6.050330000	0.730431000	-0.000025000
6	4.812171000	1.403957000	-0.000028000
6	6.050330000	-0.730431000	-0.000011000
6	4.812171000	-1.403957000	0.000000000
6	3.594353000	-0.730483000	-0.000004000

6	3.594353000	0.730483000	-0.000018000
6	8.497955000	0.730851000	-0.000031000
6	7.260717000	-1.410742000	-0.000007000
1	4.812592000	-2.490978000	0.000010000
6	2.364533000	-1.407659000	0.000007000
6	2.364533000	1.407659000	-0.000021000
6	1.143078000	0.731448000	-0.000011000
6	1.143078000	-0.731448000	0.000004000
1	2.342909000	-2.493704000	0.000018000
1	2.342909000	2.493704000	-0.000032000
6	8.497955000	-0.730851000	-0.000017000
1	7.282597000	2.496567000	-0.000046000
1	4.812592000	2.490978000	-0.000039000
1	7.282597000	-2.496567000	0.000004000
7	0.000000000	-1.437033000	0.000014000
7	0.000000000	1.437033000	-0.000015000
6	16.920632000	1.403917000	-0.000056000
6	15.668879000	0.723542000	-0.000047000
6	14.454706000	1.403320000	-0.000051000
6	15.668879000	-0.723542000	-0.000032000
6	14.454706000	-1.403320000	-0.000023000
6	13.224172000	-0.726951000	-0.000027000
6	13.224172000	0.726951000	-0.000042000
6	18.097701000	0.710897000	-0.000051000
6	16.920632000	-1.403917000	-0.000028000
1	14.454905000	-2.490475000	-0.000012000
6	11.998847000	-1.410263000	-0.000018000
6	11.998847000	1.410263000	-0.000046000
6	10.783499000	0.727999000	-0.000037000
6	10.783499000	-0.727999000	-0.000022000
1	11.976500000	-2.495966000	-0.000007000
1	11.976500000	2.495966000	-0.000057000
6	18.097701000	-0.710897000	-0.000037000
1	16.917638000	2.490193000	-0.000067000
1	14.454905000	2.490475000	-0.000062000
1	19.043419000	1.243213000	-0.000059000
1	16.917638000	-2.490193000	-0.000017000
1	19.043419000	-1.243213000	-0.000033000
7	9.628880000	-1.434070000	-0.000013000
7	9.628880000	1.434070000	-0.000041000

Table S83: Coordinates of pA₄_1 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-2.552818000	-1.399822000	0.000104000
6	-1.308588000	-0.720690000	0.000110000
6	-0.085511000	-1.398340000	0.000107000

6	-1.308588000	0.720690000	0.000116000
6	-0.085511000	1.398340000	0.000119000
6	1.134491000	0.721008000	0.000115000
6	1.134491000	-0.721008000	0.000109000
6	-3.742552000	-0.715580000	0.000102000
6	-2.552818000	1.399822000	0.000115000
1	-0.085608000	2.485876000	0.000122000
6	2.381566000	1.399550000	0.000113000
6	2.381566000	-1.399550000	0.000102000
6	3.571194000	-0.717618000	0.000098000
6	3.571194000	0.717618000	0.000104000
1	2.389331000	2.486535000	0.000117000
1	2.389331000	-2.486535000	0.000096000
6	-3.742552000	0.715580000	0.000108000
1	-2.561152000	-2.486814000	0.000098000
1	-0.085608000	-2.485876000	0.000102000
1	-2.561152000	2.486814000	0.000119000
6	7.216247000	-1.398980000	0.000072000
6	8.462920000	-0.720308000	0.000064000
6	9.684508000	-1.397815000	0.000049000
6	8.462920000	0.720308000	0.000071000
6	9.684508000	1.397815000	0.000061000
6	10.906061000	0.720319000	0.000045000
6	10.906061000	-0.720319000	0.000038000
6	6.026931000	-0.716358000	0.000083000
6	7.216247000	1.398980000	0.000084000
1	9.684522000	2.485445000	0.000065000
6	12.152724000	1.398986000	0.000031000
6	12.152724000	-1.398986000	0.000019000
6	13.342092000	-0.716444000	0.000005000
6	13.342092000	0.716444000	0.000011000
1	12.160756000	2.486049000	0.000035000
1	12.160756000	-2.486049000	0.000013000
6	6.026931000	0.716358000	0.000089000
1	7.208240000	-2.486063000	0.000067000
1	9.684522000	-2.485445000	0.000044000
1	7.208240000	2.486063000	0.000088000
7	4.798074000	1.357491000	0.000096000
7	4.798074000	-1.357491000	0.000085000
1	4.798336000	2.365712000	0.000099000
1	4.798336000	-2.365712000	0.000081000
6	-12.294465000	-1.412682000	0.000008000
6	-11.082881000	-0.730246000	0.000028000
6	-9.840323000	-1.404659000	0.000042000
6	-11.082881000	0.730246000	0.000035000
6	-9.840323000	1.404659000	0.000054000
6	-8.634749000	0.728258000	0.000065000

6	-8.634749000	-0.728258000	0.000059000
6	-13.523985000	-0.731361000	-0.000008000
6	-12.294465000	1.412682000	0.000020000
1	-9.841473000	2.491707000	0.000057000
6	-7.382332000	1.404691000	0.000082000
6	-7.382332000	-1.404691000	0.000070000
6	-6.197020000	-0.722772000	0.000084000
6	-6.197020000	0.722772000	0.000090000
1	-7.374482000	2.491390000	0.000085000
1	-7.374482000	-2.491390000	0.000065000
6	-13.523985000	0.731361000	-0.000001000
1	-12.316281000	-2.498387000	0.000002000
1	-9.841473000	-2.491707000	0.000036000
1	-12.316281000	2.498387000	0.000024000
7	-4.971122000	1.356151000	0.000103000
7	-4.971122000	-1.356151000	0.000092000
1	-4.969736000	2.364976000	0.000107000
1	-4.969736000	-2.364976000	0.000087000
6	-21.953617000	-1.405374000	-0.000167000
6	-20.696310000	-0.726054000	-0.000139000
6	-19.489277000	-1.404862000	-0.000118000
6	-20.696310000	0.726054000	-0.000132000
6	-19.489277000	1.404862000	-0.000105000
6	-18.250458000	0.729104000	-0.000084000
6	-18.250458000	-0.729104000	-0.000091000
6	-23.127371000	-0.713365000	-0.000188000
6	-21.953617000	1.405374000	-0.000153000
1	-19.489537000	2.492109000	-0.000100000
6	-17.034195000	1.412364000	-0.000059000
6	-17.034195000	-1.412364000	-0.000072000
6	-15.810519000	-0.729609000	-0.000046000
6	-15.810519000	0.729609000	-0.000040000
1	-17.012170000	2.498067000	-0.000053000
1	-17.012170000	-2.498067000	-0.000077000
6	-23.127371000	0.713365000	-0.000180000
1	-21.950636000	-2.491807000	-0.000173000
1	-19.489537000	-2.492109000	-0.000124000
1	-24.073936000	-1.244499000	-0.000209000
1	-21.950636000	2.491807000	-0.000148000
1	-24.073936000	1.244499000	-0.000197000
7	-14.664174000	1.433425000	-0.000017000
7	-14.664174000	-1.433425000	-0.000030000
6	16.986334000	-1.400135000	-0.000066000
6	18.235055000	-0.721429000	-0.000088000
6	19.453002000	-1.398580000	-0.000117000
6	18.235055000	0.721429000	-0.000082000
6	19.453002000	1.398580000	-0.000104000

6	20.677448000	0.719834000	-0.000133000
6	20.677448000	-0.719834000	-0.000140000
6	15.798135000	-0.718209000	-0.000038000
6	16.986334000	1.400135000	-0.000053000
1	19.454308000	2.486288000	-0.000099000
6	21.925179000	1.399984000	-0.000157000
6	21.925179000	-1.399984000	-0.000170000
6	23.106969000	-0.708474000	-0.000193000
6	23.106969000	0.708474000	-0.000186000
1	21.921954000	2.486761000	-0.000152000
1	21.921954000	-2.486761000	-0.000176000
1	24.051385000	-1.243556000	-0.000216000
1	24.051385000	1.243556000	-0.000203000
6	15.798135000	0.718209000	-0.000032000
1	16.978856000	-2.487082000	-0.000071000
1	19.454308000	-2.486288000	-0.000123000
1	16.978856000	2.487082000	-0.000049000
7	14.570598000	1.357472000	-0.000004000
7	14.570598000	-1.357472000	-0.000016000
1	14.570389000	2.365702000	0.000000000
1	14.570389000	-2.365702000	-0.000022000

Table S84: Coordinates of pA₄_2 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-2.598274000	-1.413837000	0.000109000
6	-1.388641000	-0.731230000	0.000115000
6	-0.145390000	-1.405385000	0.000113000
6	-1.388641000	0.731230000	0.000123000
6	-0.145390000	1.405385000	0.000127000
6	1.059469000	0.728965000	0.000122000
6	1.059469000	-0.728965000	0.000115000
6	-3.830388000	-0.733212000	0.000107000
6	-2.598274000	1.413837000	0.000123000
1	-0.146527000	2.492350000	0.000131000
6	2.311604000	1.405398000	0.000122000
6	2.311604000	-1.405398000	0.000108000
6	3.496617000	-0.723190000	0.000106000
6	3.496617000	0.723190000	0.000113000
1	2.319502000	2.492033000	0.000126000
1	2.319502000	-2.492033000	0.000102000
6	-3.830388000	0.733212000	0.000115000
1	-2.619878000	-2.499471000	0.000102000
1	-0.146527000	-2.492350000	0.000106000
1	-2.619878000	2.499471000	0.000127000
6	7.140054000	-1.400317000	0.000077000
6	8.383748000	-0.720940000	0.000068000

6	9.606634000	-1.398713000	0.000050000
6	8.383748000	0.720940000	0.000075000
6	9.606634000	1.398713000	0.000064000
6	10.826397000	0.721157000	0.000045000
6	10.826397000	-0.721157000	0.000038000
6	5.950339000	-0.715793000	0.000090000
6	7.140054000	1.400317000	0.000090000
1	9.606566000	2.486158000	0.000068000
6	12.073102000	1.399926000	0.000030000
6	12.073102000	-1.399926000	0.000017000
6	13.262223000	-0.717481000	0.000002000
6	13.262223000	0.717481000	0.000009000
1	12.080952000	2.486824000	0.000034000
1	12.080952000	-2.486824000	0.000011000
6	5.950339000	0.715793000	0.000096000
1	7.131767000	-2.487223000	0.000071000
1	9.606566000	-2.486158000	0.000044000
1	7.131767000	2.487223000	0.000094000
7	4.722283000	1.355956000	0.000107000
7	4.722283000	-1.355956000	0.000094000
1	4.723731000	2.364951000	0.000110000
1	4.723731000	-2.364951000	0.000089000
6	-12.232370000	-1.415645000	0.000010000
6	-11.010257000	-0.732767000	0.000033000
6	-9.783219000	-1.409080000	0.000046000
6	-11.010257000	0.732767000	0.000041000
6	-9.783219000	1.409080000	0.000062000
6	-8.559627000	0.732546000	0.000073000
6	-8.559627000	-0.732546000	0.000065000
6	-13.451667000	-0.732268000	-0.000006000
6	-12.232370000	1.415645000	0.000026000
1	-9.783240000	2.495760000	0.000067000
6	-7.333636000	1.414685000	0.000091000
6	-7.333636000	-1.414685000	0.000075000
6	-6.117869000	-0.731473000	0.000091000
6	-6.117869000	0.731473000	0.000099000
1	-7.311129000	2.500187000	0.000096000
1	-7.311129000	-2.500187000	0.000068000
6	-13.451667000	0.732268000	0.000003000
1	-12.254677000	-2.501097000	0.000002000
1	-9.783240000	-2.495760000	0.000039000
1	-12.254677000	2.501097000	0.000031000
7	-4.966300000	1.435021000	0.000111000
7	-4.966300000	-1.435021000	0.000096000
6	-21.883175000	-1.406462000	-0.000181000
6	-20.624795000	-0.727047000	-0.000149000
6	-19.420214000	-1.406126000	-0.000127000

6	-20.624795000	0.727047000	-0.000140000
6	-19.420214000	1.406126000	-0.000110000
6	-18.178796000	0.730463000	-0.000088000
6	-18.178796000	-0.730463000	-0.000097000
6	-23.055580000	-0.714057000	-0.000203000
6	-21.883175000	1.406461000	-0.000164000
1	-19.420486000	2.493212000	-0.000104000
6	-16.967158000	1.414569000	-0.000059000
6	-16.967158000	-1.414569000	-0.000076000
6	-15.738481000	-0.731924000	-0.000048000
6	-15.738481000	0.731924000	-0.000039000
1	-16.945374000	2.500126000	-0.000053000
1	-16.945374000	-2.500126000	-0.000082000
6	-23.055580000	0.714057000	-0.000194000
1	-21.880368000	-2.492757000	-0.000188000
1	-19.420486000	-2.493212000	-0.000134000
1	-24.002461000	-1.244474000	-0.000227000
1	-21.880368000	2.492757000	-0.000157000
1	-24.002461000	1.244474000	-0.000211000
7	-14.599378000	1.434600000	-0.000014000
7	-14.599378000	-1.434600000	-0.000030000
6	16.905201000	-1.400418000	-0.000072000
6	18.153536000	-0.721410000	-0.000095000
6	19.371519000	-1.398833000	-0.000125000
6	18.153536000	0.721410000	-0.000088000
6	19.371519000	1.398833000	-0.000110000
6	20.595473000	0.719921000	-0.000140000
6	20.595473000	-0.719921000	-0.000148000
6	15.717579000	-0.717841000	-0.000044000
6	16.905201000	1.400418000	-0.000058000
1	19.372830000	2.486472000	-0.000105000
6	21.843276000	1.400298000	-0.000164000
6	21.843276000	-1.400298000	-0.000179000
6	23.024624000	-0.708586000	-0.000202000
6	23.024624000	0.708586000	-0.000194000
1	21.840148000	2.487001000	-0.000158000
1	21.840148000	-2.487001000	-0.000185000
1	23.969112000	-1.243442000	-0.000225000
1	23.969112000	1.243442000	-0.000212000
6	15.717579000	0.717841000	-0.000037000
1	16.897649000	-2.487311000	-0.000078000
1	19.372830000	-2.486472000	-0.000131000
1	16.897649000	2.487311000	-0.000053000
7	14.489306000	1.357321000	-0.000009000
7	14.489306000	-1.357321000	-0.000022000
1	14.489377000	2.365700000	-0.000004000
1	14.489377000	-2.365700000	-0.000027000

Table S85: Coordinates of pA₄_3 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-2.530094000	-1.416803000	-0.000139000
6	-1.310554000	-0.733454000	-0.000141000
6	-0.082065000	-1.409730000	-0.000145000
6	-1.310554000	0.733505000	-0.000135000
6	-0.082064000	1.409776000	-0.000133000
6	1.140197000	0.732995000	-0.000136000
6	1.140196000	-0.732951000	-0.000142000
6	-3.752582000	-0.733796000	-0.000130000
6	-2.530096000	1.416855000	-0.000127000
1	-0.082078000	2.496376000	-0.000128000
6	2.366740000	1.415296000	-0.000130000
6	2.366737000	-1.415258000	-0.000141000
6	3.581720000	-0.731668000	-0.000134000
6	3.581722000	0.731702000	-0.000128000
1	2.389340000	2.500734000	-0.000124000
1	2.389334000	-2.500697000	-0.000144000
6	-3.752583000	0.733852000	-0.000124000
1	-2.552193000	-2.502184000	-0.000142000
1	-0.082081000	-2.496329000	-0.000148000
1	-2.552195000	2.502237000	-0.000121000
6	7.101237000	-1.414306000	-0.000105000
6	8.310347000	-0.731329000	-0.000087000
6	9.553680000	-1.405724000	-0.000071000
6	8.310350000	0.731337000	-0.000082000
6	9.553685000	1.405726000	-0.000061000
6	10.758048000	0.728976000	-0.000043000
6	10.758045000	-0.728981000	-0.000048000
6	5.869001000	-0.733374000	-0.000116000
6	7.101242000	1.414321000	-0.000094000
1	9.552579000	2.492623000	-0.000056000
6	12.010315000	1.405651000	-0.000018000
6	12.010310000	-1.405662000	-0.000028000
6	13.194633000	-0.723128000	-0.000002000
6	13.194635000	0.723111000	0.000004000
1	12.018252000	2.492212000	-0.000013000
1	12.018242000	-2.492223000	-0.000030000
6	5.869004000	0.733396000	-0.000111000
1	7.079616000	-2.499883000	-0.000108000
1	9.552568000	-2.492622000	-0.000073000
1	7.079626000	2.499898000	-0.000089000
7	4.733579000	1.435137000	-0.000117000
7	4.733575000	-1.435109000	-0.000128000
6	-12.156573000	-1.416337000	-0.000028000
6	-10.932711000	-0.733179000	-0.000046000
6	-9.708565000	-1.410090000	-0.000068000

6	-10.932715000	0.733204000	-0.000039000
6	-9.708575000	1.410122000	-0.000055000
6	-8.482051000	0.733410000	-0.000076000
6	-8.482048000	-0.733369000	-0.000082000
6	-13.373820000	-0.732249000	-0.000002000
6	-12.156585000	1.416353000	-0.000015000
1	-9.708601000	2.496673000	-0.000049000
6	-7.260821000	1.416745000	-0.000088000
6	-7.260813000	-1.416700000	-0.000100000
6	-6.040114000	-0.733187000	-0.000111000
6	-6.040117000	0.733238000	-0.000105000
1	-7.238472000	2.502116000	-0.000083000
1	-7.238459000	-2.502071000	-0.000104000
6	-13.373826000	0.732256000	0.000004000
1	-12.179140000	-2.501701000	-0.000031000
1	-9.708584000	-2.496641000	-0.000071000
1	-12.179160000	2.501717000	-0.000009000
7	-4.895564000	1.435872000	-0.000112000
7	-4.895558000	-1.435819000	-0.000124000
6	-21.804903000	-1.406897000	0.000186000
6	-20.546396000	-0.727330000	0.000158000
6	-19.342415000	-1.406576000	0.000125000
6	-20.546403000	0.727267000	0.000164000
6	-19.342429000	1.406526000	0.000138000
6	-18.100571000	0.730808000	0.000106000
6	-18.100564000	-0.730845000	0.000099000
6	-22.976874000	-0.714259000	0.000218000
6	-21.804917000	1.406822000	0.000198000
1	-19.342720000	2.493532000	0.000143000
6	-16.890025000	1.415291000	0.000081000
6	-16.890011000	-1.415316000	0.000069000
6	-15.660486000	-0.732581000	0.000044000
6	-15.660493000	0.732568000	0.000051000
1	-16.868336000	2.500774000	0.000086000
1	-16.868312000	-2.500799000	0.000064000
6	-22.976881000	0.714172000	0.000224000
1	-21.802179000	-2.493118000	0.000181000
1	-19.342694000	-2.493582000	0.000121000
1	-23.923849000	-1.244419000	0.000239000
1	-21.802204000	2.493043000	0.000203000
1	-23.923861000	1.244322000	0.000250000
7	-14.522801000	1.434865000	0.000030000
7	-14.522788000	-1.434868000	0.000018000
6	16.836073000	-1.401599000	0.000075000
6	18.081950000	-0.721781000	0.000106000
6	19.301050000	-1.399636000	0.000133000
6	18.081952000	0.721750000	0.000112000

6	19.301053000	1.399602000	0.000143000
6	20.523158000	0.720395000	0.000170000
6	20.523157000	-0.720431000	0.000164000
6	15.648369000	-0.717284000	0.000051000
6	16.836077000	1.401571000	0.000085000
1	19.302353000	2.487088000	0.000147000
6	21.771613000	1.401129000	0.000203000
6	21.771610000	-1.401169000	0.000192000
6	22.951750000	-0.709086000	0.000224000
6	22.951751000	0.709043000	0.000229000
1	21.768614000	2.487687000	0.000207000
1	21.768608000	-2.487727000	0.000188000
1	23.896494000	-1.243322000	0.000245000
1	23.896497000	1.243277000	0.000255000
6	15.648371000	0.717258000	0.000056000
1	16.828304000	-2.488339000	0.000072000
1	19.302347000	-2.487122000	0.000129000
1	16.828311000	2.488311000	0.000090000
7	14.420596000	1.356248000	0.000033000
7	14.420592000	-1.356270000	0.000023000
1	14.421847000	2.365315000	0.000037000
1	14.421840000	-2.365337000	0.000020000

Table S86: Coordinates of pA₄_4 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	2.446997000	-1.409915000	0.000116000
6	1.227509000	-0.731180000	0.000121000
6	0.000000000	-1.404271000	0.000119000
6	1.227509000	0.731180000	0.000126000
6	0.000000000	1.404271000	0.000130000
6	-1.227509000	0.731180000	0.000126000
6	-1.227509000	-0.731180000	0.000121000
6	3.675939000	-0.732425000	0.000113000
6	2.446997000	1.409915000	0.000125000
1	0.000000000	2.491241000	0.000133000
6	-2.446997000	1.409915000	0.000126000
6	-2.446997000	-1.409915000	0.000115000
6	-3.675939000	-0.732425000	0.000112000
6	-3.675939000	0.732425000	0.000118000
1	-2.468476000	2.495829000	0.000129000
1	-2.468476000	-2.495829000	0.000109000
6	3.675939000	0.732425000	0.000117000
1	2.468476000	-2.495829000	0.000111000
1	0.000000000	-2.491241000	0.000115000
1	2.468476000	2.495829000	0.000127000
6	-7.177113000	-1.410554000	0.000079000

6	-8.408117000	-0.731038000	0.000068000
6	-9.625343000	-1.406121000	0.000049000
6	-8.408117000	0.731038000	0.000076000
6	-9.625343000	1.406121000	0.000063000
6	-10.861020000	0.731082000	0.000042000
6	-10.861020000	-0.731082000	0.000034000
6	-5.961713000	-0.731213000	0.000095000
6	-7.177113000	1.410554000	0.000093000
1	-9.625255000	2.492937000	0.000068000
6	-12.074052000	1.413003000	0.000026000
6	-12.074052000	-1.413003000	0.000012000
6	-13.304801000	-0.731091000	-0.000005000
6	-13.304801000	0.731091000	0.000003000
1	-12.095812000	2.498648000	0.000031000
1	-12.095812000	-2.498648000	0.000005000
6	-5.961713000	0.731213000	0.000102000
1	-7.154708000	-2.496361000	0.000073000
1	-9.625255000	-2.492937000	0.000042000
1	-7.154708000	2.496361000	0.000097000
7	-4.811929000	1.436389000	0.000114000
7	-4.811929000	-1.436389000	0.000101000
6	12.074052000	-1.413003000	0.000017000
6	10.861020000	-0.731082000	0.000037000
6	9.625343000	-1.406121000	0.000053000
6	10.861020000	0.731082000	0.000039000
6	9.625343000	1.406121000	0.000058000
6	8.408117000	0.731038000	0.000073000
6	8.408117000	-0.731038000	0.000070000
6	13.304801000	-0.731091000	-0.000002000
6	12.074052000	1.413003000	0.000021000
1	9.625255000	2.492937000	0.000059000
6	7.177113000	1.410554000	0.000089000
6	7.177113000	-1.410554000	0.000083000
6	5.961713000	-0.731213000	0.000097000
6	5.961713000	0.731213000	0.000100000
1	7.154708000	2.496361000	0.000091000
1	7.154708000	-2.496361000	0.000080000
6	13.304801000	0.731091000	0.000000000
1	12.095812000	-2.498648000	0.000014000
1	9.625255000	-2.492937000	0.000051000
1	12.095812000	2.498648000	0.000022000
7	4.811929000	1.436389000	0.000111000
7	4.811929000	-1.436389000	0.000104000
6	21.728997000	-1.405171000	-0.000175000
6	20.474505000	-0.725084000	-0.000147000
6	19.264728000	-1.404630000	-0.000121000
6	20.474505000	0.725084000	-0.000146000

6	19.264728000	1.404630000	-0.000119000
6	18.029692000	0.728493000	-0.000093000
6	18.029692000	-0.728493000	-0.000094000
6	22.903804000	-0.712257000	-0.000201000
6	21.728997000	1.405171000	-0.000173000
1	19.265146000	2.491695000	-0.000119000
6	16.810458000	1.412417000	-0.000067000
6	16.810458000	-1.412417000	-0.000070000
6	15.590153000	-0.729715000	-0.000045000
6	15.590153000	0.729715000	-0.000043000
1	16.788424000	2.498021000	-0.000066000
1	16.788424000	-2.498021000	-0.000071000
6	22.903804000	0.712257000	-0.000200000
1	21.726325000	-2.491402000	-0.000176000
1	19.265146000	-2.491695000	-0.000122000
1	23.849943000	-1.243805000	-0.000222000
1	21.726325000	2.491402000	-0.000173000
1	23.849943000	1.243805000	-0.000220000
7	14.441616000	1.433860000	-0.000020000
7	14.441616000	-1.433860000	-0.000024000
6	-16.810458000	-1.412417000	-0.000077000
6	-18.029692000	-0.728493000	-0.000098000
6	-19.264728000	-1.404630000	-0.000129000
6	-18.029692000	0.728493000	-0.000090000
6	-19.264728000	1.404630000	-0.000112000
6	-20.474505000	0.725084000	-0.000142000
6	-20.474505000	-0.725084000	-0.000151000
6	-15.590153000	-0.729715000	-0.000048000
6	-16.810458000	1.412417000	-0.000061000
1	-19.265146000	2.491695000	-0.000106000
6	-21.728997000	1.405171000	-0.000166000
6	-21.728997000	-1.405171000	-0.000183000
6	-22.903804000	-0.712257000	-0.000205000
6	-22.903804000	0.712257000	-0.000196000
1	-21.726325000	2.491402000	-0.000159000
1	-21.726325000	-2.491402000	-0.000190000
1	-23.849943000	-1.243805000	-0.000229000
1	-23.849943000	1.243805000	-0.000214000
6	-15.590153000	0.729715000	-0.000040000
1	-16.788424000	-2.498021000	-0.000083000
1	-19.265146000	-2.491695000	-0.000136000
1	-16.788424000	2.498021000	-0.000054000
7	-14.441616000	1.433860000	-0.000014000
7	-14.441616000	-1.433860000	-0.000030000

Table S87: Coordinates of pA₅_1 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	2.505617000	-1.399475000	-0.000006000
6	3.752642000	-0.721086000	-0.000041000
6	4.972605000	-1.398216000	-0.000008000
6	3.752642000	0.721085000	-0.000112000
6	4.972605000	1.398215000	-0.000145000
6	6.195781000	0.720722000	-0.000112000
6	6.195781000	-0.720722000	-0.000042000
6	1.315846000	-0.717729000	-0.000037000
6	2.505617000	1.399475000	-0.000144000
1	4.972740000	2.485782000	-0.000198000
6	7.439878000	1.399721000	-0.000142000
6	7.439878000	-1.399722000	-0.000008000
6	8.629642000	-0.715505000	-0.000039000
6	8.629642000	0.715505000	-0.000107000
1	7.448491000	2.486754000	-0.000194000
1	7.448491000	-2.486754000	0.000044000
6	1.315846000	0.717729000	-0.000109000
1	2.497660000	-2.486497000	0.000048000
1	4.972740000	-2.485782000	0.000045000
1	2.497660000	2.486497000	-0.000198000
6	12.269404000	-1.404611000	0.000005000
6	13.521664000	-0.728261000	-0.000019000
6	14.727357000	-1.404534000	0.000023000
6	13.521664000	0.728261000	-0.000088000
6	14.727357000	1.404534000	-0.000111000
6	15.969828000	0.730288000	-0.000068000
6	15.969828000	-0.730288000	0.000002000
6	11.084012000	-0.722756000	-0.000032000
6	12.269404000	1.404611000	-0.000126000
1	14.728278000	2.491591000	-0.000162000
6	17.181462000	1.412656000	-0.000088000
6	17.181462000	-1.412656000	0.000048000
6	18.410944000	-0.731513000	0.000030000
6	18.410944000	0.731513000	-0.000041000
1	17.203071000	2.498388000	-0.000140000
1	17.203071000	-2.498388000	0.000102000
6	11.084012000	0.722755000	-0.000100000
1	12.261268000	-2.491338000	0.000057000
1	14.728278000	-2.491591000	0.000075000
1	12.261268000	2.491338000	-0.000176000
7	9.858237000	1.356181000	-0.000133000
7	9.858238000	-1.356181000	-0.000007000
1	9.856857000	2.365023000	-0.000176000
1	9.856857000	-2.365024000	0.000037000
6	-7.265983000	-1.398802000	0.000024000
6	-6.019110000	-0.720405000	-0.000019000

6	-4.797705000	-1.397584000	0.000014000
6	-6.019110000	0.720405000	-0.000099000
6	-4.797705000	1.397584000	-0.000139000
6	-3.575745000	0.720253000	-0.000104000
6	-3.575745000	-0.720253000	-0.000027000
6	-8.455807000	-0.716842000	-0.000008000
6	-7.265983000	1.398802000	-0.000133000
1	-4.797669000	2.485271000	-0.000198000
6	-2.329238000	1.398763000	-0.000142000
6	-2.329238000	-1.398764000	0.000006000
6	-1.139868000	-0.716102000	-0.000033000
6	-1.139868000	0.716102000	-0.000107000
1	-2.320931000	2.485912000	-0.000198000
1	-2.320931000	-2.485912000	0.000063000
6	-8.455807000	0.716842000	-0.000090000
1	-7.274102000	-2.485930000	0.000086000
1	-4.797669000	-2.485272000	0.000073000
1	-7.274102000	2.485930000	-0.000193000
7	0.089271000	1.357542000	-0.000139000
7	0.089271000	-1.357542000	-0.000003000
1	0.088917000	2.365766000	-0.000186000
1	0.088917000	-2.365766000	0.000044000
6	-17.038344000	-1.398748000	0.000097000
6	-15.791749000	-0.720242000	0.000041000
6	-14.569889000	-1.397565000	0.000073000
6	-15.791749000	0.720242000	-0.000052000
6	-14.569889000	1.397565000	-0.000105000
6	-13.348424000	0.720337000	-0.000070000
6	-13.348424000	-0.720337000	0.000020000
6	-18.227706000	-0.716192000	0.000066000
6	-17.038344000	1.398748000	-0.000085000
1	-14.569931000	2.485257000	-0.000172000
6	-12.101510000	1.398755000	-0.000117000
6	-12.101510000	-1.398755000	0.000053000
6	-10.911888000	-0.716641000	0.000005000
6	-10.911888000	0.716641000	-0.000081000
1	-12.093357000	2.485898000	-0.000182000
1	-12.093357000	-2.485899000	0.000119000
6	-18.227706000	0.716192000	-0.000029000
1	-17.046650000	-2.485883000	0.000169000
1	-14.569931000	-2.485257000	0.000142000
1	-17.046650000	2.485883000	-0.000156000
7	-9.683600000	1.357717000	-0.000121000
7	-9.683600000	-1.357717000	0.000035000
6	21.921181000	-1.412311000	0.000121000
6	23.137545000	-0.729117000	0.000110000
6	24.376246000	-1.404755000	0.000170000

6	23.137545000	0.729118000	0.000036000
6	24.376246000	1.404756000	0.000026000
6	25.583392000	0.726021000	0.000085000
6	25.583392000	-0.726020000	0.000160000
6	20.697599000	-0.729723000	0.000064000
6	21.921181000	1.412311000	-0.000022000
1	24.376696000	2.492006000	-0.000030000
6	26.840555000	1.405260000	0.000074000
6	26.840555000	-1.405259000	0.000221000
6	28.014415000	-0.713275000	0.000209000
6	28.014415000	0.713276000	0.000133000
1	26.837740000	2.491704000	0.000018000
1	26.837740000	-2.491704000	0.000278000
1	28.960830000	-1.244658000	0.000257000
1	28.960830000	1.244659000	0.000124000
6	20.697599000	0.729723000	-0.000009000
1	21.899324000	-2.498042000	0.000176000
1	24.376696000	-2.492006000	0.000226000
1	21.899324000	2.498043000	-0.000076000
7	19.551165000	1.433316000	-0.000060000
7	19.551165000	-1.433316000	0.000081000
1	-9.683662000	2.365852000	-0.000175000
1	-9.683662000	-2.365852000	0.000089000
6	-26.810971000	-1.399854000	0.000259000
6	-25.563347000	-0.719845000	0.000184000
6	-24.338799000	-1.398447000	0.000212000
6	-25.563347000	0.719846000	0.000074000
6	-24.338799000	1.398448000	0.000002000
6	-23.120865000	0.721486000	0.000033000
6	-23.120865000	-0.721486000	0.000139000
6	-27.992910000	-0.708393000	0.000227000
6	-26.810971000	1.399855000	0.000042000
1	-24.340107000	2.486194000	-0.000078000
6	-21.872160000	1.400023000	-0.000034000
6	-21.872160000	-1.400022000	0.000166000
6	-20.683792000	-0.718316000	0.000099000
6	-20.683792000	0.718317000	-0.000001000
1	-21.864493000	2.487009000	-0.000110000
1	-21.864493000	-2.487009000	0.000243000
6	-27.992910000	0.708393000	0.000115000
1	-26.807848000	-2.486658000	0.000343000
1	-24.340107000	-2.486193000	0.000293000
1	-28.937195000	-1.243711000	0.000286000
1	-26.807848000	2.486659000	-0.000042000
1	-28.937195000	1.243712000	0.000089000
7	-19.456573000	1.357545000	-0.000058000
7	-19.456573000	-1.357545000	0.000124000

1	-19.456268000	2.365766000	-0.000121000
1	-19.456269000	-2.365765000	0.000188000

Table S88: Coordinates of pA₅_2 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	2.577016000	-1.405290000	0.000406000
6	3.828887000	-0.728946000	0.000349000
6	5.034030000	-1.405204000	0.000398000
6	3.828887000	0.728946000	0.000230000
6	5.034029000	1.405204000	0.000165000
6	6.277044000	0.731245000	0.000208000
6	6.277044000	-0.731245000	0.000332000
6	1.391824000	-0.723131000	0.000351000
6	2.577016000	1.405290000	0.000180000
1	5.034893000	2.492190000	0.000074000
6	7.486943000	1.413739000	0.000134000
6	7.486943000	-1.413739000	0.000375000
6	8.718795000	-0.733327000	0.000299000
6	8.718795000	0.733327000	0.000172000
1	7.508287000	2.499412000	0.000039000
1	7.508287000	-2.499412000	0.000466000
6	1.391824000	0.723131000	0.000236000
1	2.568803000	-2.491964000	0.000491000
1	5.034893000	-2.492190000	0.000485000
1	2.568803000	2.491964000	0.000092000
6	12.222229000	-1.414580000	0.000284000
6	13.448267000	-0.732598000	0.000186000
6	14.671818000	-1.408941000	0.000210000
6	13.448267000	0.732598000	0.000050000
6	14.671818000	1.408941000	-0.000055000
6	15.899058000	0.732820000	-0.000036000
6	15.899058000	-0.732820000	0.000103000
6	11.006358000	-0.731692000	0.000253000
6	12.222229000	1.414580000	0.000025000
1	14.671886000	2.495622000	-0.000158000
6	17.120972000	1.415584000	-0.000149000
6	17.120972000	-1.415584000	0.000121000
6	18.340582000	-0.732503000	0.000006000
6	18.340582000	0.732503000	-0.000134000
1	17.143211000	2.501076000	-0.000255000
1	17.143211000	-2.501076000	0.000222000
6	11.006358000	0.731692000	0.000122000
1	12.199855000	-2.500127000	0.000382000
1	14.671886000	-2.495622000	0.000310000
1	12.199855000	2.500127000	-0.000076000
7	9.854936000	1.434961000	0.000086000

7	9.854936000	-1.434961000	0.000339000
6	-7.184743000	-1.399821000	0.000326000
6	-5.938021000	-0.721338000	0.000292000
6	-4.718343000	-1.398529000	0.000363000
6	-5.938021000	0.721338000	0.000176000
6	-4.718343000	1.398529000	0.000139000
6	-3.495108000	0.720997000	0.000208000
6	-3.495108000	-0.720997000	0.000323000
6	-8.374417000	-0.717903000	0.000250000
6	-7.184743000	1.399821000	0.000101000
1	-4.718204000	2.486024000	0.000051000
6	-2.251706000	1.400163000	0.000166000
6	-2.251706000	-1.400163000	0.000388000
6	-1.061785000	-0.715657000	0.000342000
6	-1.061785000	0.715657000	0.000228000
1	-2.243073000	2.487131000	0.000078000
1	-2.243073000	-2.487131000	0.000473000
6	-8.374417000	0.717903000	0.000134000
1	-7.192705000	-2.486781000	0.000412000
1	-4.718204000	-2.486024000	0.000449000
1	-7.192705000	2.486781000	0.000013000
7	0.166271000	1.355901000	0.000184000
7	0.166271000	-1.355901000	0.000396000
1	0.164853000	2.364918000	0.000109000
1	0.164853000	-2.364918000	0.000469000
6	-16.954607000	-1.399087000	0.000087000
6	-15.708100000	-0.720475000	0.000068000
6	-14.486780000	-1.397850000	0.000163000
6	-15.708100000	0.720475000	-0.000057000
6	-14.486780000	1.397850000	-0.000077000
6	-13.265109000	0.720406000	0.000017000
6	-13.265109000	-0.720406000	0.000140000
6	-18.143972000	-0.716623000	-0.000013000
6	-16.954607000	1.399087000	-0.000158000
1	-14.486776000	2.485466000	-0.000171000
6	-12.018840000	1.399092000	-0.000006000
6	-12.018840000	-1.399092000	0.000228000
6	-10.829648000	-0.716229000	0.000199000
6	-10.829648000	0.716229000	0.000081000
1	-12.010546000	2.486178000	-0.000097000
1	-12.010546000	-2.486178000	0.000317000
6	-18.143972000	0.716623000	-0.000140000
1	-16.962825000	-2.486145000	0.000181000
1	-14.486776000	-2.485466000	0.000255000
1	-16.962825000	2.486145000	-0.000254000
7	-9.600693000	1.357422000	0.000058000
7	-9.600693000	-1.357422000	0.000276000
6	21.855740000	-1.414461000	-0.000090000

6	23.067663000	-0.730420000	-0.000219000
6	24.308850000	-1.405972000	-0.000218000
6	23.067663000	0.730420000	-0.000363000
6	24.308850000	1.405972000	-0.000497000
6	25.513636000	0.726970000	-0.000496000
6	25.513636000	-0.726970000	-0.000350000
6	20.627425000	-0.731941000	-0.000097000
6	21.855740000	1.414461000	-0.000367000
1	24.309320000	2.493071000	-0.000605000
6	26.771833000	1.406297000	-0.000633000
6	26.771833000	-1.406297000	-0.000350000
6	27.944402000	-0.713944000	-0.000482000
6	27.944402000	0.713944000	-0.000628000
1	26.769170000	2.492610000	-0.000742000
1	26.769170000	-2.492610000	-0.000240000
1	28.891124000	-1.244634000	-0.000479000
1	28.891124000	1.244634000	-0.000735000
6	20.627425000	0.731941000	-0.000238000
1	21.834166000	-2.500050000	0.000016000
1	24.309320000	-2.493071000	-0.000111000
1	21.834166000	2.500051000	-0.000473000
7	19.487964000	1.434504000	-0.000253000
7	19.487964000	-1.434504000	0.000023000
1	-9.601060000	2.365744000	-0.000019000
1	-9.601060000	-2.365744000	0.000351000
6	-26.726232000	-1.400012000	-0.000282000
6	-25.478587000	-0.719876000	-0.000297000
6	-24.254264000	-1.398562000	-0.000179000
6	-25.478587000	0.719877000	-0.000442000
6	-24.254264000	1.398562000	-0.000455000
6	-23.036354000	0.721456000	-0.000334000
6	-23.036354000	-0.721455000	-0.000195000
6	-27.907944000	-0.708445000	-0.000402000
6	-26.726232000	1.400012000	-0.000566000
1	-24.255570000	2.486274000	-0.000561000
6	-21.787771000	1.400134000	-0.000345000
6	-21.787771000	-1.400134000	-0.000081000
6	-20.599758000	-0.718116000	-0.000100000
6	-20.599758000	0.718116000	-0.000232000
1	-21.780058000	2.487097000	-0.000447000
1	-21.780059000	-2.487097000	0.000019000
6	-27.907944000	0.708445000	-0.000549000
1	-26.723154000	-2.486777000	-0.000171000
1	-24.255570000	-2.486274000	-0.000074000
1	-28.852267000	-1.243639000	-0.000387000
1	-26.723154000	2.486777000	-0.000676000
1	-28.852267000	1.243639000	-0.000646000

7	-19.372066000	1.357512000	-0.000242000
7	-19.372066000	-1.357512000	0.000000000
1	-19.371914000	2.365790000	-0.000326000
1	-19.371914000	-2.365790000	0.000083000

Table S89: Coordinates of pA₅_3 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	2.529751000	-1.409808000	0.000145000
6	3.742105000	-0.729767000	0.000083000
6	4.979691000	-1.403462000	0.000180000
6	3.742105000	0.729767000	-0.000090000
6	4.979691000	1.403462000	-0.000180000
6	6.197761000	0.729991000	-0.000096000
6	6.197761000	-0.729992000	0.000104000
6	1.295182000	-0.729785000	0.000058000
6	2.529751000	1.409808000	-0.000161000
1	4.979817000	2.490541000	-0.000319000
6	7.428511000	1.407279000	-0.000199000
6	7.428511000	-1.407279000	0.000214000
6	8.648857000	-0.731069000	0.000125000
6	8.648857000	0.731069000	-0.000103000
1	7.450478000	2.493376000	-0.000359000
1	7.450478000	-2.493377000	0.000373000
6	1.295182000	0.729785000	-0.000083000
1	2.508309000	-2.495739000	0.000263000
1	4.979817000	-2.490541000	0.000318000
1	2.508309000	2.495739000	-0.000280000
6	12.158530000	-1.407276000	0.000279000
6	13.387310000	-0.730446000	0.000161000
6	14.606535000	-1.403375000	0.000301000
6	13.387310000	0.730446000	-0.000123000
6	14.606535000	1.403375000	-0.000262000
6	15.844145000	0.730443000	-0.000131000
6	15.844145000	-0.730443000	0.000170000
6	10.935361000	-0.731634000	0.000144000
6	12.158530000	1.407276000	-0.000245000
1	14.606423000	2.490435000	-0.000478000
6	17.055407000	1.410071000	-0.000278000
6	17.055407000	-1.410070000	0.000316000
6	18.292799000	-0.731083000	0.000175000
6	18.292799000	0.731083000	-0.000140000
1	17.076643000	2.495972000	-0.000507000
1	17.076643000	-2.495972000	0.000543000
6	10.935361000	0.731634000	-0.000112000
1	12.136807000	-2.493375000	0.000479000
1	14.606423000	-2.490435000	0.000516000

1	12.136807000	2.493375000	-0.000446000
7	9.793638000	1.436981000	-0.000225000
7	9.793638000	-1.436981000	0.000252000
6	-7.126253000	-1.402681000	0.000013000
6	-5.878749000	-0.725238000	-0.000003000
6	-4.666067000	-1.402373000	0.000040000
6	-5.878749000	0.725238000	-0.000064000
6	-4.666067000	1.402373000	-0.000100000
6	-3.431796000	0.727272000	-0.000069000
6	-3.431796000	-0.727272000	0.000015000
6	-8.315072000	-0.720433000	-0.000018000
6	-7.126253000	1.402681000	-0.000083000
1	-4.665127000	2.489456000	-0.000153000
6	-2.210117000	1.409319000	-0.000118000
6	-2.210117000	-1.409319000	0.000070000
6	-0.990254000	-0.728424000	0.000035000
6	-0.990254000	0.728424000	-0.000076000
1	-2.187882000	2.495179000	-0.000191000
1	-2.187882000	-2.495179000	0.000144000
6	-8.315072000	0.720432000	-0.000056000
1	-7.133960000	-2.489361000	0.000048000
1	-4.665127000	-2.489456000	0.000093000
1	-7.133960000	2.489361000	-0.000118000
7	0.160503000	1.433434000	-0.000141000
7	0.160503000	-1.433434000	0.000108000
6	-16.890828000	-1.399592000	-0.000034000
6	-15.644556000	-0.720826000	-0.000028000
6	-14.424046000	-1.398338000	-0.000033000
6	-15.644556000	0.720826000	-0.000016000
6	-14.424046000	1.398338000	-0.000022000
6	-13.201961000	0.720594000	-0.000032000
6	-13.201961000	-0.720594000	-0.000031000
6	-18.080269000	-0.717203000	-0.000021000
6	-16.890828000	1.399592000	0.000002000
1	-14.423959000	2.485826000	-0.000016000
6	-11.957086000	1.399802000	-0.000043000
6	-11.957086000	-1.399802000	-0.000026000
6	-10.768224000	-0.715642000	-0.000028000
6	-10.768224000	0.715642000	-0.000045000
1	-11.948604000	2.486774000	-0.000049000
1	-11.948604000	-2.486774000	-0.000018000
6	-18.080269000	0.717203000	0.000003000
1	-16.898844000	-2.486532000	-0.000047000
1	-14.423959000	-2.485826000	-0.000037000
1	-16.898844000	2.486532000	0.000017000
7	-9.538860000	1.356671000	-0.000062000
7	-9.538860000	-1.356671000	-0.000013000

6	21.793735000	-1.409614000	0.000336000
6	23.020318000	-0.726780000	0.000177000
6	24.250170000	-1.402823000	0.000338000
6	23.020318000	0.726780000	-0.000168000
6	24.250170000	1.402823000	-0.000338000
6	25.465312000	0.723251000	-0.000182000
6	25.465312000	-0.723251000	0.000171000
6	20.578905000	-0.728042000	0.000177000
6	21.793735000	1.409614000	-0.000319000
1	24.250615000	2.490047000	-0.000598000
6	26.716633000	1.403359000	-0.000357000
6	26.716633000	-1.403359000	0.000335000
6	27.894408000	-0.710576000	0.000161000
6	27.894408000	0.710576000	-0.000195000
1	26.713796000	2.489715000	-0.000625000
1	26.713796000	-2.489714000	0.000603000
1	28.839812000	-1.243526000	0.000292000
1	28.839812000	1.243526000	-0.000334000
6	20.578905000	0.728042000	-0.000152000
1	21.771476000	-2.495407000	0.000587000
1	24.250615000	-2.490047000	0.000597000
1	21.771476000	2.495407000	-0.000571000
7	19.423626000	1.434341000	-0.000302000
7	19.423626000	-1.434341000	0.000331000
1	-9.539560000	2.365474000	-0.000077000
1	-9.539560000	-2.365475000	0.000003000
6	-26.661019000	-1.400227000	0.000018000
6	-25.413363000	-0.719907000	0.000029000
6	-24.189323000	-1.398730000	-0.000002000
6	-25.413363000	0.719908000	0.000075000
6	-24.189323000	1.398730000	0.000084000
6	-22.971472000	0.721408000	0.000051000
6	-22.971472000	-0.721408000	0.000009000
6	-27.842438000	-0.708511000	0.000051000
6	-26.661019000	1.400227000	0.000109000
1	-24.190627000	2.486395000	0.000117000
6	-21.723046000	1.400305000	0.000056000
6	-21.723047000	-1.400305000	-0.000018000
6	-20.535545000	-0.717831000	-0.000008000
6	-20.535545000	0.717831000	0.000026000
1	-21.715305000	2.487232000	0.000084000
1	-21.715305000	-2.487232000	-0.000046000
6	-27.842438000	0.708512000	0.000098000
1	-26.657977000	-2.486941000	-0.000018000
1	-24.190627000	-2.486395000	-0.000035000
1	-28.786822000	-1.243524000	0.000042000
1	-26.657977000	2.486942000	0.000145000

1	-28.786822000	1.243525000	0.000125000
7	-19.307184000	1.357452000	0.000027000
7	-19.307184000	-1.357452000	-0.000029000
1	-19.307207000	2.365818000	0.000050000
1	-19.307207000	-2.365818000	-0.000051000

Table S90: Coordinates of pA_s_4 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	2.451890000	-1.409790000	0.000185000
6	3.670647000	-0.731139000	0.000090000
6	4.899277000	-1.404044000	0.000201000
6	3.670647000	0.731139000	-0.000134000
6	4.899277000	1.404044000	-0.000246000
6	6.125983000	0.731122000	-0.000143000
6	6.125983000	-0.731122000	0.000097000
6	1.221998000	-0.732416000	0.000080000
6	2.451890000	1.409790000	-0.000226000
1	4.899295000	2.491052000	-0.000417000
6	7.346607000	1.409442000	-0.000262000
6	7.346607000	-1.409442000	0.000216000
6	8.574988000	-0.732374000	0.000104000
6	8.574988000	0.732374000	-0.000150000
1	7.368077000	2.495399000	-0.000445000
1	7.368077000	-2.495399000	0.000400000
6	1.221998000	0.732416000	-0.000119000
1	2.430521000	-2.495729000	0.000343000
1	4.899295000	-2.491052000	0.000373000
1	2.430521000	2.495729000	-0.000383000
6	12.076980000	-1.410084000	0.000249000
6	13.308180000	-0.731019000	0.000125000
6	14.525467000	-1.405774000	0.000262000
6	13.308180000	0.731019000	-0.000158000
6	14.525467000	1.405774000	-0.000290000
6	15.761566000	0.731067000	-0.000156000
6	15.761566000	-0.731067000	0.000134000
6	10.861067000	-0.731305000	0.000114000
6	12.076980000	1.410084000	-0.000285000
1	14.525379000	2.492635000	-0.000501000
6	16.974464000	1.412639000	-0.000291000
6	16.974464000	-1.412639000	0.000276000
6	18.205921000	-0.731185000	0.000144000
6	18.205921000	0.731185000	-0.000152000
1	16.996116000	2.498321000	-0.000509000
1	16.996116000	-2.498321000	0.000494000
6	10.861067000	0.731305000	-0.000155000
1	12.054668000	-2.495938000	0.000453000

1	14.525379000	-2.492635000	0.000474000
1	12.054668000	2.495938000	-0.000489000
7	9.711668000	1.436497000	-0.000279000
7	9.711668000	-1.436497000	0.000235000
6	-7.178111000	-1.412068000	0.000119000
6	-5.962855000	-0.730526000	0.000063000
6	-4.728356000	-1.405722000	0.000132000
6	-5.962855000	0.730526000	-0.000073000
6	-4.728356000	1.405722000	-0.000147000
6	-3.510220000	0.730657000	-0.000088000
6	-3.510220000	-0.730657000	0.000067000
6	-8.406394000	-0.730153000	0.000058000
6	-7.178111000	1.412068000	-0.000123000
1	-4.728247000	2.492610000	-0.000255000
6	-2.279283000	1.410297000	-0.000172000
6	-2.279283000	-1.410297000	0.000146000
6	-1.063991000	-0.730876000	0.000072000
6	-1.063991000	0.730876000	-0.000103000
1	-2.256851000	2.496143000	-0.000295000
1	-2.256851000	-2.496143000	0.000270000
6	-8.406394000	0.730153000	-0.000056000
1	-7.199967000	-2.497795000	0.000212000
1	-4.728247000	-2.492610000	0.000240000
1	-7.199967000	2.497795000	-0.000216000
7	0.086508000	1.436247000	-0.000202000
7	0.086508000	-1.436247000	0.000167000
6	-16.828664000	-1.404062000	0.000070000
6	-15.579162000	-0.726771000	0.000046000
6	-14.370241000	-1.403888000	0.000080000
6	-15.579162000	0.726771000	-0.000017000
6	-14.370241000	1.403888000	-0.000054000
6	-13.132379000	0.728896000	-0.000027000
6	-13.132379000	-0.728896000	0.000049000
6	-18.015130000	-0.721502000	0.000043000
6	-16.828664000	1.404062000	-0.000038000
1	-14.369311000	2.490845000	-0.000105000
6	-11.915988000	1.411608000	-0.000073000
6	-11.915988000	-1.411608000	0.000090000
6	-10.691867000	-0.730210000	0.000053000
6	-10.691867000	0.730210000	-0.000040000
1	-11.894021000	2.497313000	-0.000137000
1	-11.894021000	-2.497313000	0.000153000
6	-18.015130000	0.721502000	-0.000008000
1	-16.836575000	-2.490652000	0.000111000
1	-14.369311000	-2.490845000	0.000130000
1	-16.836575000	2.490652000	-0.000079000
7	-9.546595000	1.433535000	-0.000098000

7	-9.546595000	-1.433535000	0.000106000
6	21.711396000	-1.411996000	0.000307000
6	22.931400000	-0.728312000	0.000169000
6	24.166099000	-1.404362000	0.000321000
6	22.931400000	0.728312000	-0.000143000
6	24.166099000	1.404362000	-0.000286000
6	25.376339000	0.724924000	-0.000136000
6	25.376339000	-0.724924000	0.000181000
6	20.491562000	-0.729508000	0.000156000
6	21.711396000	1.411996000	-0.000290000
1	24.166511000	2.491475000	-0.000519000
6	26.630716000	1.404897000	-0.000281000
6	26.630716000	-1.404897000	0.000336000
6	27.805843000	-0.712142000	0.000191000
6	27.805843000	0.712142000	-0.000127000
1	26.627983000	2.491176000	-0.000520000
1	26.627983000	-2.491176000	0.000575000
1	28.751907000	-1.243889000	0.000315000
1	28.751907000	1.243889000	-0.000243000
6	20.491562000	0.729508000	-0.000147000
1	21.689339000	-2.497640000	0.000535000
1	24.166511000	-2.491475000	0.000554000
1	21.689339000	2.497640000	-0.000519000
7	19.342275000	1.433924000	-0.000294000
7	19.342275000	-1.433924000	0.000294000
6	-26.591367000	-1.400999000	0.000045000
6	-25.343295000	-0.720274000	0.000030000
6	-24.120753000	-1.399430000	0.000049000
6	-25.343295000	0.720274000	-0.000005000
6	-24.120753000	1.399430000	-0.000021000
6	-22.902185000	0.721632000	-0.000003000
6	-22.902185000	-0.721632000	0.000034000
6	-27.771728000	-0.708881000	0.000026000
6	-26.591367000	1.400999000	-0.000023000
1	-24.122021000	2.486942000	-0.000048000
6	-21.655669000	1.401315000	-0.000021000
6	-21.655669000	-1.401315000	0.000054000
6	-20.468512000	-0.717215000	0.000038000
6	-20.468512000	0.717215000	-0.000003000
1	-21.647703000	2.488096000	-0.000051000
1	-21.647704000	-2.488096000	0.000084000
6	-27.771728000	0.708881000	-0.000009000
1	-26.588431000	-2.487565000	0.000071000
1	-24.122021000	-2.486942000	0.000076000
1	-28.716341000	-1.243311000	0.000038000
1	-26.588431000	2.487566000	-0.000050000
1	-28.716341000	1.243311000	-0.000023000

7	-19.239994000	1.356585000	-0.000023000
7	-19.239994000	-1.356585000	0.000059000
1	-19.240794000	2.365558000	-0.000051000
1	-19.240794000	-2.365558000	0.000086000

Table S91: Coordinates of pA₅_5 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-2.364739000	1.410700000	0.000375000
6	-3.589351000	0.731519000	0.000353000
6	-4.811913000	1.405627000	0.000310000
6	-3.589351000	-0.731519000	0.000373000
6	-4.811913000	-1.405626000	0.000359000
6	-6.042869000	-0.731714000	0.000318000
6	-6.042869000	0.731714000	0.000287000
6	-1.142732000	0.732124000	0.000406000
6	-2.364739000	-1.410700000	0.000400000
1	-4.811835000	-2.492487000	0.000376000
6	-7.259100000	-1.412147000	0.000303000
6	-7.259100000	1.412147000	0.000232000
6	-8.488856000	0.732813000	0.000208000
6	-8.488856000	-0.732813000	0.000251000
1	-7.280593000	-2.497893000	0.000328000
1	-7.280593000	2.497893000	0.000202000
6	-1.142732000	-0.732124000	0.000412000
1	-2.342764000	2.496525000	0.000364000
1	-4.811835000	2.492487000	0.000290000
1	-2.342764000	-2.496525000	0.000408000
6	-11.989751000	1.412689000	0.000037000
6	-13.218875000	0.731655000	0.000014000
6	-14.437907000	1.407516000	-0.000072000
6	-13.218875000	-0.731655000	0.000082000
6	-14.437907000	-1.407516000	0.000066000
6	-15.670483000	-0.731655000	-0.000018000
6	-15.670483000	0.731655000	-0.000093000
6	-10.774804000	0.731551000	0.000117000
6	-11.989751000	-1.412689000	0.000158000
1	-14.437866000	-2.494215000	0.000118000
6	-16.886391000	-1.414259000	-0.000033000
6	-16.886391000	1.414259000	-0.000185000
6	-18.112767000	0.731372000	-0.000205000
6	-18.112767000	-0.731372000	-0.000123000
1	-16.908440000	-2.499796000	0.000024000
1	-16.908440000	2.499796000	-0.000245000
6	-10.774804000	-0.731551000	0.000173000
1	-11.967241000	2.498329000	-0.000008000
1	-14.437866000	2.494215000	-0.000125000

1	-11.967241000	-2.498329000	0.000203000
7	-9.624351000	-1.436018000	0.000237000
7	-9.624351000	1.436018000	0.000139000
6	7.259106000	1.412148000	0.000439000
6	6.042886000	0.731712000	0.000434000
6	4.811918000	1.405637000	0.000457000
6	6.042886000	-0.731712000	0.000397000
6	4.811918000	-1.405637000	0.000397000
6	3.589390000	-0.731512000	0.000421000
6	3.589390000	0.731512000	0.000446000
6	8.488869000	0.732818000	0.000401000
6	7.259106000	-1.412148000	0.000356000
1	4.811838000	-2.492495000	0.000371000
6	2.364742000	-1.410700000	0.000416000
6	2.364742000	1.410700000	0.000452000
6	1.142773000	0.732127000	0.000437000
6	1.142773000	-0.732126000	0.000427000
1	2.342794000	-2.496525000	0.000400000
1	2.342794000	2.496525000	0.000462000
6	8.488869000	-0.732818000	0.000352000
1	7.280578000	2.497896000	0.000467000
1	4.811838000	2.492495000	0.000476000
1	7.280578000	-2.497896000	0.000320000
7	0.000004000	-1.436337000	0.000419000
7	0.000004000	1.436337000	0.000424000
6	16.886403000	1.414260000	0.000106000
6	15.670463000	0.731648000	0.000134000
6	14.437915000	1.407523000	0.000230000
6	15.670463000	-0.731648000	0.000053000
6	14.437915000	-1.407523000	0.000081000
6	13.218866000	-0.731650000	0.000176000
6	13.218866000	0.731650000	0.000249000
6	18.112735000	0.731368000	-0.000004000
6	16.886403000	-1.414260000	-0.000057000
1	14.437869000	-2.494220000	0.000020000
6	11.989753000	-1.412694000	0.000197000
6	11.989753000	1.412694000	0.000329000
6	10.774807000	0.731550000	0.000340000
6	10.774807000	-0.731550000	0.000279000
1	11.967254000	-2.498334000	0.000145000
1	11.967254000	2.498334000	0.000375000
6	18.112735000	-0.731368000	-0.000091000
1	16.908434000	2.499795000	0.000162000
1	14.437869000	2.494220000	0.000282000
1	16.908434000	-2.499795000	-0.000126000
7	9.624352000	-1.436019000	0.000290000
7	9.624352000	1.436019000	0.000398000

6	-21.621663000	1.413599000	-0.000413000
6	-22.837611000	0.729356000	-0.000427000
6	-24.075116000	1.405391000	-0.000529000
6	-22.837611000	-0.729356000	-0.000331000
6	-24.075116000	-1.405391000	-0.000342000
6	-25.282615000	-0.725926000	-0.000441000
6	-25.282615000	0.725926000	-0.000540000
6	-20.398293000	0.730734000	-0.000313000
6	-21.621663000	-1.413599000	-0.000234000
1	-24.075539000	-2.492411000	-0.000270000
6	-26.538580000	-1.405867000	-0.000451000
6	-26.538580000	1.405867000	-0.000645000
6	-27.712217000	0.713000000	-0.000652000
6	-27.712217000	-0.713000000	-0.000552000
1	-26.535953000	-2.492075000	-0.000376000
1	-26.535953000	2.492075000	-0.000720000
1	-28.658657000	1.244014000	-0.000734000
1	-28.658657000	-1.244014000	-0.000557000
6	-20.398293000	-0.730734000	-0.000224000
1	-21.599831000	2.499142000	-0.000481000
1	-24.075539000	2.492411000	-0.000601000
1	-21.599831000	-2.499142000	-0.000165000
7	-19.253451000	-1.434011000	-0.000132000
7	-19.253451000	1.434011000	-0.000299000
6	26.538573000	1.405872000	-0.000616000
6	25.282593000	0.725933000	-0.000555000
6	24.075115000	1.405393000	-0.000404000
6	25.282593000	-0.725933000	-0.000658000
6	24.075115000	-1.405393000	-0.000601000
6	22.837585000	-0.729363000	-0.000449000
6	22.837585000	0.729363000	-0.000349000
6	27.712199000	0.713007000	-0.000771000
6	26.538573000	-1.405872000	-0.000819000
1	24.075523000	-2.492413000	-0.000678000
6	21.621669000	-1.413602000	-0.000396000
6	21.621669000	1.413602000	-0.000207000
6	20.398262000	0.730745000	-0.000159000
6	20.398262000	-0.730745000	-0.000253000
1	21.599821000	-2.499145000	-0.000469000
1	21.599821000	2.499144000	-0.000136000
6	27.712199000	-0.713007000	-0.000876000
1	26.535936000	2.492079000	-0.000538000
1	24.075523000	2.492413000	-0.000331000
1	28.658646000	1.244008000	-0.000815000
1	26.535935000	-2.492079000	-0.000898000
1	28.658646000	-1.244008000	-0.000999000
7	19.253459000	-1.434011000	-0.000214000

7	19.253459000	1.434011000	-0.000037000
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Table S92: Coordinates of pA₆_1 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-2.378939000	-1.398779000	-0.000222000
6	-1.132019000	-0.720429000	-0.000224000
6	0.089367000	-1.397551000	-0.000230000
6	-1.132019000	0.720428000	-0.000217000
6	0.089367000	1.397550000	-0.000218000
6	1.311419000	0.720234000	-0.000223000
6	1.311419000	-0.720234000	-0.000229000
6	-3.568916000	-0.716959000	-0.000213000
6	-2.378939000	1.398779000	-0.000209000
1	0.089415000	2.485249000	-0.000213000
6	2.557916000	1.398719000	-0.000222000
6	2.557916000	-1.398720000	-0.000233000
6	3.747290000	-0.716029000	-0.000230000
6	3.747290000	0.716028000	-0.000224000
1	2.566247000	2.485879000	-0.000217000
1	2.566247000	-2.485880000	-0.000237000
6	-3.568916000	0.716958000	-0.000207000
1	-2.387031000	-2.485914000	-0.000226000
1	0.089415000	-2.485250000	-0.000235000
1	-2.387031000	2.485913000	-0.000204000
6	7.392864000	-1.399472000	-0.000224000
6	8.639891000	-0.721102000	-0.000213000
6	9.859854000	-1.398207000	-0.000205000
6	8.639891000	0.721101000	-0.000208000
6	9.859854000	1.398206000	-0.000195000
6	11.083063000	0.720723000	-0.000185000
6	11.083063000	-0.720724000	-0.000190000
6	6.203027000	-0.717773000	-0.000226000
6	7.392864000	1.399471000	-0.000213000
1	9.859991000	2.485776000	-0.000190000
6	12.327147000	1.399711000	-0.000166000
6	12.327147000	-1.399712000	-0.000176000
6	13.516921000	-0.715482000	-0.000156000
6	13.516921000	0.715482000	-0.000151000
1	12.335772000	2.486748000	-0.000161000
1	12.335772000	-2.486748000	-0.000179000
6	6.203027000	0.717772000	-0.000220000
1	7.384911000	-2.486496000	-0.000227000
1	9.859991000	-2.485777000	-0.000209000
1	7.384911000	2.486495000	-0.000208000
7	4.976557000	1.357538000	-0.000221000
7	4.976557000	-1.357539000	-0.000231000

1	4.976174000	2.365758000	-0.000217000
1	4.976174000	-2.365759000	-0.000235000
6	-12.152103000	-1.398612000	-0.000146000
6	-10.905199000	-0.720276000	-0.000156000
6	-9.683469000	-1.397426000	-0.000172000
6	-10.905199000	0.720276000	-0.000148000
6	-9.683469000	1.397426000	-0.000157000
6	-8.461641000	0.720236000	-0.000172000
6	-8.461641000	-0.720236000	-0.000180000
6	-13.341918000	-0.716590000	-0.000128000
6	-12.152103000	1.398612000	-0.000131000
1	-9.683464000	2.485156000	-0.000152000
6	-7.214775000	1.398586000	-0.000180000
6	-7.214775000	-1.398587000	-0.000193000
6	-6.025095000	-0.716409000	-0.000199000
6	-6.025095000	0.716408000	-0.000192000
1	-7.206553000	2.485766000	-0.000174000
1	-7.206553000	-2.485767000	-0.000198000
6	-13.341918000	0.716589000	-0.000120000
1	-12.160290000	-2.485784000	-0.000151000
1	-9.683464000	-2.485157000	-0.000177000
1	-12.160290000	2.485783000	-0.000125000
7	-4.796468000	1.357732000	-0.000198000
7	-4.796468000	-1.357733000	-0.000210000
1	-4.796603000	2.365847000	-0.000193000
1	-4.796603000	-2.365848000	-0.000214000
6	-21.924975000	-1.398679000	0.000018000
6	-20.678370000	-0.720207000	-0.000005000
6	-19.456393000	-1.397512000	-0.000035000
6	-20.678370000	0.720207000	0.000004000
6	-19.456393000	1.397513000	-0.000018000
6	-18.234951000	0.720354000	-0.000047000
6	-18.234951000	-0.720354000	-0.000055000
6	-23.114334000	-0.716091000	0.000051000
6	-21.924975000	1.398679000	0.000036000
1	-19.456447000	2.485221000	-0.000011000
6	-16.987957000	1.398712000	-0.000065000
6	-16.987957000	-1.398712000	-0.000081000
6	-15.798154000	-0.716783000	-0.000096000
6	-15.798154000	0.716782000	-0.000088000
1	-16.979833000	2.485865000	-0.000058000
1	-16.979833000	-2.485865000	-0.000087000
6	-23.114334000	0.716091000	0.000060000
1	-21.933313000	-2.485832000	0.000012000
1	-19.456447000	-2.485221000	-0.000041000
1	-21.933313000	2.485832000	0.000044000
7	-14.570162000	1.357753000	-0.000102000

7	-14.570162000	-1.357753000	-0.000117000
6	17.156721000	-1.404605000	-0.000088000
6	18.408964000	-0.728266000	-0.000052000
6	19.614679000	-1.404526000	-0.000018000
6	18.408964000	0.728266000	-0.000047000
6	19.614679000	1.404526000	-0.000008000
6	20.857145000	0.730291000	0.000032000
6	20.857145000	-0.730291000	0.000027000
6	15.971295000	-0.722762000	-0.000112000
6	17.156721000	1.404605000	-0.000078000
1	19.615598000	2.491584000	-0.000002000
6	22.068793000	1.412644000	0.000080000
6	22.068794000	-1.412644000	0.000070000
6	23.298282000	-0.731520000	0.000121000
6	23.298282000	0.731520000	0.000127000
1	22.090401000	2.498378000	0.000087000
1	22.090401000	-2.498378000	0.000068000
6	15.971295000	0.722762000	-0.000107000
1	17.148586000	-2.491334000	-0.000090000
1	19.615598000	-2.491584000	-0.000020000
1	17.148586000	2.491333000	-0.000072000
7	14.745553000	1.356168000	-0.000128000
7	14.745553000	-1.356168000	-0.000138000
1	-14.570132000	2.365858000	-0.000097000
1	-14.570132000	-2.365858000	-0.000122000
1	14.744165000	2.365011000	-0.000124000
1	14.744165000	-2.365011000	-0.000140000
6	-31.697827000	-1.399817000	0.000322000
6	-30.450206000	-0.719841000	0.000282000
6	-29.225610000	-1.398422000	0.000233000
6	-30.450206000	0.719842000	0.000293000
6	-29.225610000	1.398422000	0.000254000
6	-28.007662000	0.721499000	0.000205000
6	-28.007662000	-0.721498000	0.000195000
6	-32.879820000	-0.708380000	0.000370000
6	-31.697827000	1.399818000	0.000343000
1	-29.226917000	2.486176000	0.000262000
6	-26.758942000	1.400002000	0.000167000
6	-26.758943000	-1.400002000	0.000148000
6	-25.570478000	-0.718368000	0.000116000
6	-25.570478000	0.718369000	0.000126000
1	-26.751280000	2.486994000	0.000176000
1	-26.751280000	-2.486993000	0.000142000
6	-32.879820000	0.708381000	0.000380000
1	-31.694696000	-2.486630000	0.000314000
1	-29.226917000	-2.486175000	0.000226000
1	-33.824094000	-1.243732000	0.000400000

1	-31.694696000	2.486631000	0.000351000
1	-33.824094000	1.243733000	0.000419000
7	-24.343390000	1.357547000	0.000094000
7	-24.343390000	-1.357547000	0.000077000
1	-24.343046000	2.365758000	0.000102000
1	-24.343046000	-2.365758000	0.000072000
6	26.808523000	-1.412294000	0.000279000
6	28.024914000	-0.729112000	0.000345000
6	29.263605000	-1.404746000	0.000408000
6	28.024914000	0.729113000	0.000350000
6	29.263605000	1.404747000	0.000419000
6	30.470768000	0.726015000	0.000481000
6	30.470768000	-0.726014000	0.000475000
6	25.584950000	-0.729719000	0.000222000
6	26.808523000	1.412294000	0.000290000
1	29.264054000	2.491999000	0.000423000
6	31.727927000	1.405246000	0.000550000
6	31.727928000	-1.405245000	0.000539000
6	32.901804000	-0.713270000	0.000604000
6	32.901804000	0.713271000	0.000610000
1	31.725111000	2.491693000	0.000554000
1	31.725112000	-2.491692000	0.000535000
1	33.848213000	-1.244665000	0.000652000
1	33.848213000	1.244666000	0.000662000
6	25.584950000	0.729719000	0.000227000
1	26.786666000	-2.498027000	0.000276000
1	29.264054000	-2.491998000	0.000404000
1	26.786666000	2.498028000	0.000295000
7	24.438502000	-1.433324000	0.000168000
7	24.438502000	1.433324000	0.000178000

Table S93: Coordinates of pA₆_2 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	2.305916000	-1.399025000	-0.000763000
6	1.059808000	-0.720470000	-0.000812000
6	-0.161629000	-1.397785000	-0.000855000
6	1.059808000	0.720470000	-0.000815000
6	-0.161629000	1.397785000	-0.000865000
6	-1.383381000	0.720170000	-0.000904000
6	-1.383381000	-0.720170000	-0.000896000
6	3.496511000	-0.717251000	-0.000714000
6	2.305916000	1.399025000	-0.000763000
1	-0.161751000	2.485368000	-0.000868000
6	-2.629410000	1.399050000	-0.000944000
6	-2.629410000	-1.399050000	-0.000923000
6	-3.818217000	-0.715597000	-0.000953000

6	-3.818217000	0.715596000	-0.000966000
1	-2.637832000	2.486113000	-0.000951000
1	-2.637832000	-2.486113000	-0.000913000
6	3.496511000	0.717251000	-0.000712000
1	2.313801000	-2.486046000	-0.000764000
1	-0.161751000	-2.485368000	-0.000850000
1	2.313801000	2.486046000	-0.000762000
6	-7.463786000	-1.399818000	-0.000960000
6	-8.707095000	-0.721777000	-0.000955000
6	-9.927827000	-1.399616000	-0.000912000
6	-8.707095000	0.721777000	-0.000982000
6	-9.927827000	1.399616000	-0.000970000
6	-11.154532000	0.724275000	-0.000917000
6	-11.154532000	-0.724275000	-0.000884000
6	-6.271019000	-0.717407000	-0.000975000
6	-7.463786000	1.399817000	-0.001005000
1	-9.928654000	2.486929000	-0.000989000
6	-12.386787000	1.405095000	-0.000879000
6	-12.386787000	-1.405095000	-0.000810000
6	-13.600255000	-0.726072000	-0.000756000
6	-13.600255000	0.726072000	-0.000795000
1	-12.409340000	2.491264000	-0.000902000
1	-12.409340000	-2.491264000	-0.000778000
6	-6.271019000	0.717407000	-0.000995000
1	-7.456270000	-2.486644000	-0.000940000
1	-9.928654000	-2.486929000	-0.000887000
1	-7.456270000	2.486644000	-0.001020000
7	-5.048213000	1.357537000	-0.000997000
7	-5.048213000	-1.357537000	-0.000966000
1	-5.048284000	2.366070000	-0.001006000
1	-5.048284000	-2.366070000	-0.000952000
6	12.077987000	-1.398772000	-0.000269000
6	10.831254000	-0.720341000	-0.000333000
6	9.609700000	-1.397549000	-0.000413000
6	10.831254000	0.720341000	-0.000315000
6	9.609700000	1.397549000	-0.000382000
6	8.387895000	0.720174000	-0.000463000
6	8.387895000	-0.720175000	-0.000476000
6	13.267950000	-0.716823000	-0.000190000
6	12.077987000	1.398772000	-0.000230000
1	9.609664000	2.485233000	-0.000370000
6	7.141200000	1.398687000	-0.000528000
6	7.141200000	-1.398687000	-0.000549000
6	5.951982000	-0.716040000	-0.000605000
6	5.951982000	0.716040000	-0.000596000
1	7.132909000	2.485837000	-0.000519000
1	7.132909000	-2.485837000	-0.000557000

6	13.267950000	0.716823000	-0.000168000
1	12.086079000	-2.485891000	-0.000284000
1	9.609664000	-2.485233000	-0.000425000
1	12.086079000	2.485891000	-0.000215000
7	4.722587000	1.357702000	-0.000657000
7	4.722587000	-1.357702000	-0.000667000
1	4.722844000	2.365901000	-0.000651000
1	4.722844000	-2.365901000	-0.000670000
6	21.850310000	-1.398763000	0.000366000
6	20.603744000	-0.720240000	0.000293000
6	19.381885000	-1.397575000	0.000190000
6	20.603744000	0.720240000	0.000326000
6	19.381885000	1.397575000	0.000251000
6	18.160443000	0.720320000	0.000148000
6	18.160443000	-0.720320000	0.000118000
6	23.039699000	-0.716213000	0.000466000
6	21.850310000	1.398763000	0.000433000
1	19.381925000	2.485264000	0.000276000
6	16.913514000	1.398754000	0.000075000
6	16.913514000	-1.398754000	0.000020000
6	15.723958000	-0.716595000	-0.000044000
6	15.723958000	0.716595000	-0.000017000
1	16.905361000	2.485896000	0.000097000
1	16.905361000	-2.485896000	0.000000000
6	23.039699000	0.716213000	0.000502000
1	21.858602000	-2.485892000	0.000340000
1	19.381925000	-2.485264000	0.000166000
1	21.858602000	2.485892000	0.000459000
7	14.495558000	1.357740000	-0.000086000
7	14.495558000	-1.357740000	-0.000131000
6	-17.126921000	-1.405703000	-0.000436000
6	-18.343092000	-0.729391000	-0.000318000
6	-19.575387000	-1.400466000	-0.000135000
6	-18.343092000	0.729391000	-0.000372000
6	-19.575387000	1.400466000	-0.000243000
6	-20.805632000	0.729628000	-0.000049000
6	-20.805632000	-0.729628000	0.000010000
6	-15.887034000	-0.730301000	-0.000581000
6	-17.126921000	1.405703000	-0.000532000
1	-19.575377000	2.487747000	-0.000283000
6	-22.023367000	1.405574000	0.000094000
6	-22.023367000	-1.405574000	0.000212000
6	-23.263224000	-0.731185000	0.000370000
6	-23.263224000	0.731185000	0.000307000
1	-22.044313000	2.491827000	0.000050000
1	-22.044313000	-2.491827000	0.000258000
6	-15.887034000	0.730301000	-0.000627000

1	-17.105956000	-2.491960000	-0.000396000
1	-19.575377000	-2.487748000	-0.000092000
1	-17.105956000	2.491960000	-0.000567000
7	-14.758407000	1.434879000	-0.000739000
7	-14.758407000	-1.434880000	-0.000655000
1	14.495630000	2.365876000	-0.000068000
1	14.495630000	-2.365876000	-0.000147000
6	31.622859000	-1.399870000	0.001139000
6	30.375241000	-0.719846000	0.001053000
6	29.150706000	-1.398461000	0.000927000
6	30.375241000	0.719847000	0.001095000
6	29.150706000	1.398461000	0.001007000
6	27.932786000	0.721481000	0.000882000
6	27.932786000	-0.721481000	0.000841000
6	32.804780000	-0.708395000	0.001260000
6	31.622859000	1.399870000	0.001222000
1	29.152018000	2.486204000	0.001039000
6	26.684079000	1.400032000	0.000796000
6	26.684079000	-1.400032000	0.000719000
6	25.495753000	-0.718295000	0.000645000
6	25.495753000	0.718295000	0.000683000
1	26.676417000	2.487017000	0.000826000
1	26.676417000	-2.487017000	0.000690000
6	32.804780000	0.708395000	0.001302000
1	31.619749000	-2.486671000	0.001107000
1	29.152018000	-2.486204000	0.000896000
1	33.749065000	-1.243707000	0.001326000
1	31.619749000	2.486671000	0.001254000
1	33.749065000	1.243707000	0.001401000
7	24.268479000	1.357553000	0.000606000
7	24.268479000	-1.357553000	0.000536000
1	24.268188000	2.365775000	0.000632000
1	24.268188000	-2.365775000	0.000512000
6	-26.760880000	-1.405787000	0.000941000
6	-27.998015000	-0.724741000	0.001117000
6	-29.219637000	-1.400377000	0.001363000
6	-27.998015000	0.724742000	0.001046000
6	-29.219637000	1.400377000	0.001222000
6	-30.444314000	0.720384000	0.001467000
6	-30.444314000	-0.720384000	0.001541000
6	-25.551097000	-0.726933000	0.000713000
6	-26.760880000	1.405787000	0.000805000
1	-29.220215000	2.487767000	0.001167000
6	-31.689479000	1.400622000	0.001642000
6	-31.689479000	-1.400621000	0.001787000
6	-32.872664000	-0.707464000	0.001948000
6	-32.872664000	0.707465000	0.001874000

1	-31.686592000	2.487077000	0.001585000
1	-31.686592000	-2.487076000	0.001842000
1	-33.816744000	-1.242741000	0.002138000
1	-33.816744000	1.242741000	0.002008000
6	-25.551097000	0.726933000	0.000645000
1	-26.738574000	-2.491852000	0.000991000
1	-29.220215000	-2.487767000	0.001417000
1	-26.738574000	2.491852000	0.000752000
7	-24.390579000	-1.436089000	0.000567000
7	-24.390579000	1.436089000	0.000437000

Table S94: Coordinates of pA₆_3 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	2.229545000	-1.405452000	-0.000176000
6	0.977849000	-0.729021000	-0.000192000
6	-0.227293000	-1.405332000	-0.000197000
6	0.977849000	0.729021000	-0.000202000
6	-0.227293000	1.405331000	-0.000217000
6	-1.470183000	0.731340000	-0.000221000
6	-1.470183000	-0.731341000	-0.000210000
6	3.414632000	-0.723114000	-0.000167000
6	2.229545000	1.405451000	-0.000194000
1	-0.228166000	2.492298000	-0.000223000
6	-2.680014000	1.413872000	-0.000232000
6	-2.680014000	-1.413873000	-0.000210000
6	-3.911879000	-0.733465000	-0.000219000
6	-3.911879000	0.733464000	-0.000231000
1	-2.701383000	2.499532000	-0.000239000
1	-2.701383000	-2.499533000	-0.000200000
6	3.414632000	0.723114000	-0.000176000
1	2.237767000	-2.492111000	-0.000168000
1	-0.228166000	-2.492299000	-0.000188000
1	2.237767000	2.492111000	-0.000200000
6	-7.414742000	-1.414899000	-0.000206000
6	-8.641453000	-0.733036000	-0.000206000
6	-9.863831000	-1.409404000	-0.000189000
6	-8.641453000	0.733034000	-0.000220000
6	-9.863831000	1.409402000	-0.000217000
6	-11.092552000	0.733536000	-0.000199000
6	-11.092552000	-0.733538000	-0.000184000
6	-6.199459000	-0.731994000	-0.000218000
6	-7.414742000	1.414897000	-0.000232000
1	-9.863876000	2.496039000	-0.000226000
6	-12.312140000	1.416515000	-0.000192000
6	-12.312141000	-1.416518000	-0.000163000
6	-13.534951000	-0.734111000	-0.000154000

6	-13.534951000	0.734109000	-0.000169000
1	-12.334070000	2.501964000	-0.000201000
1	-12.334070000	-2.501967000	-0.000150000
6	-6.199459000	0.731992000	-0.000230000
1	-7.392343000	-2.500416000	-0.000195000
1	-9.863876000	-2.496041000	-0.000177000
1	-7.392343000	2.500414000	-0.000241000
7	-5.047769000	1.435148000	-0.000237000
7	-5.047769000	-1.435150000	-0.000213000
6	11.990364000	-1.400032000	-0.000038000
6	10.743936000	-0.721481000	-0.000062000
6	9.524269000	-1.398697000	-0.000077000
6	10.743936000	0.721481000	-0.000069000
6	9.524269000	1.398697000	-0.000092000
6	8.301127000	0.721162000	-0.000108000
6	8.301127000	-0.721162000	-0.000100000
6	13.180078000	-0.717991000	-0.000022000
6	11.990364000	1.400032000	-0.000052000
1	9.524134000	2.486154000	-0.000098000
6	7.057964000	1.400384000	-0.000130000
6	7.057964000	-1.400384000	-0.000115000
6	5.867957000	-0.715841000	-0.000136000
6	5.867957000	0.715841000	-0.000144000
1	7.049369000	2.487317000	-0.000136000
1	7.049369000	-2.487317000	-0.000108000
6	13.180078000	0.717991000	-0.000029000
1	11.998315000	-2.486962000	-0.000032000
1	9.524134000	-2.486154000	-0.000071000
1	11.998315000	2.486962000	-0.000057000
7	4.640287000	1.355820000	-0.000165000
7	4.640287000	-1.355820000	-0.000148000
1	4.641661000	2.364900000	-0.000170000
1	4.641661000	-2.364900000	-0.000142000
6	21.759416000	-1.399255000	0.000120000
6	20.513049000	-0.720604000	0.000099000
6	19.291865000	-1.397994000	0.000083000
6	20.513049000	0.720604000	0.000092000
6	19.291865000	1.397994000	0.000070000
6	18.070154000	0.720515000	0.000054000
6	18.070154000	-0.720515000	0.000061000
6	22.948823000	-0.716782000	0.000133000
6	21.759416000	1.399256000	0.000107000
1	19.291854000	2.485577000	0.000064000
6	16.824177000	1.399279000	0.000030000
6	16.824177000	-1.399279000	0.000043000
6	15.634960000	-0.716265000	0.000020000
6	15.634960000	0.716265000	0.000013000

1	16.815887000	2.486338000	0.000024000
1	16.815887000	-2.486338000	0.000048000
6	22.948823000	0.716783000	0.000127000
1	21.767596000	-2.486283000	0.000125000
1	19.291854000	-2.485577000	0.000088000
1	21.767596000	2.486284000	0.000102000
7	14.406140000	1.357325000	-0.000012000
7	14.406140000	-1.357325000	0.000001000
6	-17.043137000	-1.416349000	-0.000082000
6	-18.264943000	-0.733364000	-0.000063000
6	-19.491159000	-1.409818000	-0.000026000
6	-18.264942000	0.733363000	-0.000080000
6	-19.491158000	1.409816000	-0.000059000
6	-20.715859000	0.733217000	-0.000021000
6	-20.715860000	-0.733218000	-0.000003000
6	-15.822718000	-0.733271000	-0.000115000
6	-17.043137000	1.416347000	-0.000114000
1	-19.491216000	2.496393000	-0.000070000
6	-21.939355000	1.416169000	0.000005000
6	-21.939355000	-1.416170000	0.000038000
6	-23.157206000	-0.732535000	0.000065000
6	-23.157206000	0.732535000	0.000047000
1	-21.961777000	2.501592000	-0.000006000
1	-21.961778000	-2.501592000	0.000053000
6	-15.822718000	0.733268000	-0.000131000
1	-17.020929000	-2.501785000	-0.000069000
1	-19.491217000	-2.496394000	-0.000013000
1	-17.020928000	2.501783000	-0.000126000
7	-14.677758000	1.435846000	-0.000158000
7	-14.677758000	-1.435849000	-0.000128000
1	14.406515000	2.365718000	-0.000017000
1	14.406516000	-2.365717000	0.000005000
6	31.530592000	-1.400099000	0.000261000
6	30.282921000	-0.719901000	0.000240000
6	29.058729000	-1.398632000	0.000226000
6	30.282921000	0.719902000	0.000233000
6	29.058729000	1.398633000	0.000213000
6	27.840794000	0.721461000	0.000199000
6	27.840794000	-0.721460000	0.000206000
6	32.712185000	-0.708480000	0.000274000
6	31.530592000	1.400100000	0.000247000
1	29.060036000	2.486327000	0.000207000
6	26.592331000	1.400220000	0.000177000
6	26.592331000	-1.400219000	0.000190000
6	25.404413000	-0.718056000	0.000169000
6	25.404413000	0.718057000	0.000162000
1	26.584615000	2.487168000	0.000171000

1	26.584615000	-2.487168000	0.000195000
6	32.712185000	0.708481000	0.000267000
1	31.527524000	-2.486845000	0.000267000
1	29.060036000	-2.486326000	0.000231000
1	33.656537000	-1.243596000	0.000290000
1	31.527524000	2.486846000	0.000242000
1	33.656536000	1.243597000	0.000277000
7	24.176605000	1.357480000	0.000139000
7	24.176605000	-1.357479000	0.000151000
1	24.176500000	2.365797000	0.000135000
1	24.176500000	-2.365796000	0.000156000
6	-26.673030000	-1.415024000	0.000188000
6	-27.884051000	-0.730706000	0.000222000
6	-29.125640000	-1.406297000	0.000276000
6	-27.884051000	0.730709000	0.000204000
6	-29.125639000	1.406300000	0.000241000
6	-30.329926000	0.727177000	0.000294000
6	-30.329927000	-0.727174000	0.000312000
6	-25.443949000	-0.732455000	0.000138000
6	-26.673029000	1.415026000	0.000153000
1	-29.126094000	2.493341000	0.000228000
6	-31.588266000	1.406601000	0.000333000
6	-31.588266000	-1.406597000	0.000368000
6	-32.760493000	-0.714080000	0.000404000
6	-32.760492000	0.714085000	0.000386000
1	-31.585638000	2.492864000	0.000319000
1	-31.585640000	-2.492860000	0.000382000
1	-33.707300000	-1.244555000	0.000447000
1	-33.707300000	1.244560000	0.000415000
6	-25.443949000	0.732457000	0.000120000
1	-26.651500000	-2.500562000	0.000201000
1	-29.126095000	-2.493338000	0.000290000
1	-26.651499000	2.500564000	0.000140000
7	-24.305708000	-1.434741000	0.000109000
7	-24.305707000	1.434741000	0.000075000

Table S95: Coordinates of pA₆_4 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	2.284073000	-1.415087000	-0.000147000
6	1.057328000	-0.733101000	-0.000164000
6	-0.164786000	-1.409595000	-0.000170000
6	1.057328000	0.733101000	-0.000173000
6	-0.164786000	1.409595000	-0.000188000
6	-1.393644000	0.733650000	-0.000194000
6	-1.393644000	-0.733650000	-0.000184000
6	3.499125000	-0.731999000	-0.000138000

6	2.284073000	1.415087000	-0.000164000
1	-0.164830000	2.496200000	-0.000194000
6	-2.612814000	1.416818000	-0.000205000
6	-2.612814000	-1.416819000	-0.000186000
6	-3.835899000	-0.734318000	-0.000197000
6	-3.835899000	0.734317000	-0.000207000
1	-2.634739000	2.502240000	-0.000212000
1	-2.634739000	-2.502240000	-0.000178000
6	3.499125000	0.731999000	-0.000146000
1	2.306516000	-2.500580000	-0.000140000
1	-0.164830000	-2.496201000	-0.000162000
1	2.306516000	2.500579000	-0.000169000
6	-7.343171000	-1.416746000	-0.000192000
6	-8.565749000	-0.733719000	-0.000193000
6	-9.790601000	-1.410363000	-0.000181000
6	-8.565749000	0.733718000	-0.000205000
6	-9.790601000	1.410363000	-0.000203000
6	-11.016876000	0.733863000	-0.000190000
6	-11.016876000	-0.733863000	-0.000178000
6	-6.123585000	-0.733410000	-0.000200000
6	-7.343171000	1.416746000	-0.000214000
1	-9.790630000	2.496880000	-0.000210000
6	-12.237839000	1.417238000	-0.000184000
6	-12.237839000	-1.417238000	-0.000160000
6	-13.458911000	-0.734027000	-0.000153000
6	-13.458911000	0.734027000	-0.000165000
1	-12.259983000	2.502605000	-0.000191000
1	-12.259983000	-2.502606000	-0.000150000
6	-6.123585000	0.733410000	-0.000211000
1	-7.320870000	-2.502142000	-0.000182000
1	-9.790630000	-2.496880000	-0.000171000
1	-7.320870000	2.502142000	-0.000221000
7	-4.978171000	1.435971000	-0.000215000
7	-4.978171000	-1.435972000	-0.000194000
6	11.927623000	-1.405595000	-0.000009000
6	10.675980000	-0.729086000	-0.000032000
6	9.470993000	-1.405478000	-0.000048000
6	10.675980000	0.729086000	-0.000038000
6	9.470993000	1.405478000	-0.000061000
6	8.228083000	0.731413000	-0.000078000
6	8.228083000	-0.731414000	-0.000071000
6	13.112611000	-0.723201000	0.000007000
6	11.927623000	1.405595000	-0.000020000
1	9.470113000	2.492413000	-0.000066000
6	7.018482000	1.414081000	-0.000100000
6	7.018483000	-1.414081000	-0.000086000
6	5.786573000	-0.733557000	-0.000107000

6	5.786573000	0.733556000	-0.000115000
1	6.997105000	2.499715000	-0.000105000
1	6.997105000	-2.499715000	-0.000081000
6	13.112611000	0.723200000	0.000002000
1	11.935820000	-2.492225000	-0.000005000
1	9.470113000	-2.492413000	-0.000044000
1	11.935820000	2.492224000	-0.000025000
7	4.650874000	1.435166000	-0.000134000
7	4.650874000	-1.435166000	-0.000119000
6	21.687594000	-1.400140000	0.000124000
6	20.441255000	-0.721405000	0.000109000
6	19.221645000	-1.398839000	0.000097000
6	20.441255000	0.721405000	0.000105000
6	19.221645000	1.398839000	0.000088000
6	17.998762000	0.721180000	0.000075000
6	17.998762000	-0.721180000	0.000080000
6	22.876765000	-0.717693000	0.000133000
6	21.687594000	1.400140000	0.000115000
1	19.221552000	2.486257000	0.000083000
6	16.755574000	1.400545000	0.000055000
6	16.755574000	-1.400545000	0.000065000
6	15.565761000	-0.715943000	0.000046000
6	15.565761000	0.715943000	0.000041000
1	16.747030000	2.487444000	0.000051000
1	16.747030000	-2.487444000	0.000068000
6	22.876765000	0.717693000	0.000129000
1	21.695627000	-2.487028000	0.000127000
1	19.221552000	-2.486257000	0.000100000
1	21.695627000	2.487028000	0.000111000
7	14.338150000	1.355901000	0.000019000
7	14.338150000	-1.355902000	0.000029000
6	-16.967697000	-1.417035000	-0.000090000
6	-18.188292000	-0.733558000	-0.000073000
6	-19.415130000	-1.410179000	-0.000040000
6	-18.188292000	0.733558000	-0.000086000
6	-19.415130000	1.410179000	-0.000065000
6	-20.639008000	0.733291000	-0.000031000
6	-20.639008000	-0.733291000	-0.000018000
6	-15.746396000	-0.733685000	-0.000119000
6	-16.967697000	1.417035000	-0.000115000
1	-19.415164000	2.496695000	-0.000074000
6	-21.862915000	1.416439000	-0.000007000
6	-21.862915000	-1.416439000	0.000019000
6	-23.080073000	-0.732437000	0.000045000
6	-23.080073000	0.732438000	0.000032000
1	-21.885438000	2.501821000	-0.000015000
1	-21.885438000	-2.501821000	0.000031000

6	-15.746396000	0.733685000	-0.000131000
1	-16.945506000	-2.502411000	-0.000080000
1	-19.415164000	-2.496695000	-0.000029000
1	-16.945506000	2.502411000	-0.000124000
7	-14.602786000	1.435936000	-0.000155000
7	-14.602786000	-1.435936000	-0.000130000
1	14.339530000	2.365012000	0.000015000
1	14.339530000	-2.365012000	0.000032000
6	31.456680000	-1.400401000	0.000189000
6	30.208914000	-0.719998000	0.000181000
6	28.985211000	-1.398881000	0.000176000
6	30.208914000	0.719998000	0.000176000
6	28.985211000	1.398881000	0.000167000
6	27.767184000	0.721475000	0.000162000
6	27.767184000	-0.721474000	0.000167000
6	32.637854000	-0.708602000	0.000192000
6	31.456680000	1.400401000	0.000180000
1	28.986510000	2.486512000	0.000163000
6	26.519174000	1.400525000	0.000152000
6	26.519174000	-1.400525000	0.000161000
6	25.331671000	-0.717778000	0.000152000
6	25.331671000	0.717778000	0.000147000
1	26.511395000	2.487422000	0.000148000
1	26.511395000	-2.487421000	0.000164000
6	32.637854000	0.708603000	0.000188000
1	31.453660000	-2.487081000	0.000193000
1	28.986510000	-2.486512000	0.000179000
1	33.582294000	-1.243474000	0.000199000
1	31.453660000	2.487082000	0.000176000
1	33.582293000	1.243475000	0.000190000
7	24.103364000	1.357319000	0.000136000
7	24.103364000	-1.357318000	0.000144000
1	24.103495000	2.365789000	0.000132000
1	24.103495000	-2.365789000	0.000147000
6	-26.596023000	-1.415393000	0.000157000
6	-27.806555000	-0.730871000	0.000190000
6	-29.048306000	-1.406519000	0.000238000
6	-27.806555000	0.730872000	0.000176000
6	-29.048306000	1.406519000	0.000211000
6	-30.252303000	0.727295000	0.000259000
6	-30.252303000	-0.727295000	0.000272000
6	-25.366654000	-0.732740000	0.000112000
6	-26.596023000	1.415393000	0.000131000
1	-29.048757000	2.493516000	0.000202000
6	-31.510684000	1.406819000	0.000295000
6	-31.510684000	-1.406819000	0.000322000
6	-32.682674000	-0.714159000	0.000356000

6	-32.682674000	0.714159000	0.000342000
1	-31.508096000	2.493038000	0.000285000
1	-31.508096000	-2.493037000	0.000333000
1	-33.629540000	-1.244472000	0.000394000
1	-33.629540000	1.244473000	0.000370000
6	-25.366654000	0.732740000	0.000099000
1	-26.574531000	-2.500889000	0.000167000
1	-29.048757000	-2.493515000	0.000248000
1	-26.574531000	2.500890000	0.000120000
7	-24.228935000	-1.434811000	0.000085000
7	-24.228935000	1.434811000	0.000058000

Table S96: Coordinates of pA₆_5 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-2.360437000	1.417036000	-0.000171000
6	-1.138046000	0.733782000	-0.000177000
6	0.086695000	1.410592000	-0.000174000
6	-1.138046000	-0.733783000	-0.000185000
6	0.086695000	-1.410592000	-0.000189000
6	1.312957000	-0.733951000	-0.000184000
6	1.312957000	0.733951000	-0.000176000
6	-3.579973000	0.733441000	-0.000171000
6	-2.360437000	-1.417036000	-0.000185000
1	0.086717000	-2.497074000	-0.000193000
6	2.533613000	-1.417551000	-0.000185000
6	2.533613000	1.417551000	-0.000170000
6	3.754856000	0.734175000	-0.000170000
6	3.754856000	-0.734176000	-0.000178000
1	2.555774000	-2.502889000	-0.000190000
1	2.555774000	2.502889000	-0.000163000
6	-3.579973000	-0.733441000	-0.000179000
1	-2.382783000	2.502400000	-0.000165000
1	0.086717000	2.497073000	-0.000167000
1	-2.382783000	-2.502400000	-0.000190000
6	7.262798000	1.417464000	-0.000142000
6	8.484123000	0.733901000	-0.000136000
6	9.709623000	1.410728000	-0.000119000
6	8.484123000	-0.733901000	-0.000144000
6	9.709623000	-1.410728000	-0.000136000
6	10.935071000	-0.733907000	-0.000118000
6	10.935071000	0.733907000	-0.000109000
6	6.042265000	0.733847000	-0.000156000
6	7.262798000	-1.417464000	-0.000159000
1	9.709627000	-2.497186000	-0.000141000
6	12.156445000	-1.417500000	-0.000107000
6	12.156445000	1.417500000	-0.000090000

6	13.376836000	0.733869000	-0.000079000
6	13.376836000	-0.733869000	-0.000087000
1	12.178704000	-2.502828000	-0.000113000
1	12.178704000	2.502828000	-0.000083000
6	6.042265000	-0.733847000	-0.000164000
1	7.240525000	2.502798000	-0.000136000
1	9.709627000	2.497186000	-0.000112000
1	7.240525000	-2.502798000	-0.000164000
7	4.898268000	-1.436060000	-0.000175000
7	4.898268000	1.436060000	-0.000159000
6	-11.986765000	1.415363000	-0.000094000
6	-10.760216000	0.733095000	-0.000112000
6	-9.538176000	1.409811000	-0.000123000
6	-10.760216000	-0.733095000	-0.000118000
6	-9.538176000	-1.409811000	-0.000135000
6	-8.309442000	-0.733657000	-0.000145000
6	-8.309442000	0.733657000	-0.000139000
6	-13.201688000	0.731909000	-0.000080000
6	-11.986765000	-1.415364000	-0.000105000
1	-9.538141000	-2.496379000	-0.000139000
6	-7.090420000	-1.417089000	-0.000159000
6	-7.090420000	1.417089000	-0.000146000
6	-5.867462000	0.734294000	-0.000159000
6	-5.867462000	-0.734294000	-0.000166000
1	-7.068450000	-2.502479000	-0.000163000
1	-7.068450000	2.502479000	-0.000140000
6	-13.201688000	-0.731909000	-0.000086000
1	-12.009283000	2.500821000	-0.000088000
1	-9.538141000	2.496379000	-0.000117000
1	-12.009283000	-2.500822000	-0.000109000
7	-4.725242000	-1.435944000	-0.000176000
7	-4.725242000	1.435944000	-0.000162000
6	-21.629622000	1.405681000	0.000070000
6	-20.377637000	0.729018000	0.000044000
6	-19.173162000	1.405693000	0.000023000
6	-20.377637000	-0.729018000	0.000039000
6	-19.173162000	-1.405693000	0.000013000
6	-17.930035000	-0.731411000	-0.000007000
6	-17.930035000	0.731411000	-0.000002000
6	-22.813996000	0.723143000	0.000091000
6	-21.629622000	-1.405681000	0.000061000
1	-19.172288000	-2.492581000	0.000010000
6	-16.720884000	-1.414415000	-0.000031000
6	-16.720884000	1.414415000	-0.000021000
6	-15.488885000	0.733570000	-0.000045000
6	-15.488885000	-0.733570000	-0.000050000
1	-16.699495000	-2.500008000	-0.000035000

1	-16.699495000	2.500008000	-0.000017000
6	-22.813997000	-0.723143000	0.000086000
1	-21.637820000	2.492254000	0.000074000
1	-19.172288000	2.492581000	0.000027000
1	-21.637820000	-2.492254000	0.000057000
7	-14.353390000	-1.435083000	-0.000071000
7	-14.353390000	1.435083000	-0.000060000
6	16.885793000	1.417388000	-0.000020000
6	18.105834000	0.733662000	-0.000004000
6	19.332934000	1.410358000	0.000022000
6	18.105834000	-0.733662000	-0.000013000
6	19.332934000	-1.410358000	0.000005000
6	20.556428000	-0.733324000	0.000031000
6	20.556428000	0.733324000	0.000040000
6	15.664143000	0.733925000	-0.000044000
6	16.885793000	-1.417388000	-0.000038000
1	19.332957000	-2.496842000	-0.000002000
6	21.780516000	-1.416561000	0.000050000
6	21.780516000	1.416561000	0.000067000
6	22.997352000	0.732375000	0.000087000
6	22.997352000	-0.732375000	0.000077000
1	21.803097000	-2.501921000	0.000044000
1	21.803097000	2.501921000	0.000075000
6	15.664143000	-0.733925000	-0.000053000
1	16.863632000	2.502729000	-0.000014000
1	19.332957000	2.496842000	0.000029000
1	16.863632000	-2.502729000	-0.000045000
7	14.521069000	-1.435961000	-0.000075000
7	14.521069000	1.435961000	-0.000058000
6	-31.390347000	1.401173000	0.000271000
6	-30.141938000	0.720465000	0.000242000
6	-28.919969000	1.399600000	0.000219000
6	-30.141938000	-0.720465000	0.000237000
6	-28.919969000	-1.399600000	0.000210000
6	-27.700838000	-0.721817000	0.000186000
6	-27.700838000	0.721817000	0.000191000
6	-32.570415000	0.709058000	0.000292000
6	-31.390347000	-1.401173000	0.000261000
1	-28.921232000	-2.487096000	0.000206000
6	-26.455162000	-1.401593000	0.000158000
6	-26.455162000	1.401593000	0.000168000
6	-25.267478000	0.717269000	0.000141000
6	-25.267478000	-0.717269000	0.000136000
1	-26.447154000	-2.488354000	0.000154000
1	-26.447154000	2.488354000	0.000171000
6	-32.570415000	-0.709058000	0.000287000
1	-31.387410000	2.487728000	0.000275000

1	-28.921232000	2.487096000	0.000223000
1	-33.515105000	1.243346000	0.000314000
1	-31.387410000	-2.487728000	0.000257000
1	-33.515105000	-1.243346000	0.000305000
7	-24.039767000	-1.356296000	0.000108000
7	-24.039767000	1.356296000	0.000117000
1	-24.040992000	-2.365412000	0.000105000
1	-24.040992000	2.365412000	0.000120000
6	26.513328000	1.415583000	0.000162000
6	27.723644000	0.730956000	0.000183000
6	28.965444000	1.406635000	0.000213000
6	27.723644000	-0.730956000	0.000173000
6	28.965444000	-1.406635000	0.000195000
6	30.169313000	-0.727354000	0.000225000
6	30.169313000	0.727354000	0.000234000
6	25.283852000	0.732899000	0.000132000
6	26.513328000	-1.415583000	0.000144000
1	28.965893000	-2.493607000	0.000188000
6	31.427694000	-1.406938000	0.000247000
6	31.427694000	1.406938000	0.000264000
6	32.599563000	0.714194000	0.000284000
6	32.599563000	-0.714194000	0.000275000
1	31.425129000	-2.493131000	0.000240000
1	31.425129000	2.493131000	0.000272000
1	33.546463000	1.244416000	0.000307000
1	33.546463000	-1.244416000	0.000291000
6	25.283852000	-0.732899000	0.000123000
1	26.491860000	2.501056000	0.000168000
1	28.965893000	2.493607000	0.000220000
1	26.491860000	-2.501056000	0.000136000
7	24.146353000	1.434859000	0.000113000
7	24.146353000	-1.434859000	0.000096000

Table S97: Coordinates of pA₆ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	2.450561000	-1.410117000	0.000096000
6	1.225762000	-0.729268000	0.000101000
6	0.000000000	-1.404783000	0.000105000
6	1.225762000	0.729268000	0.000100000
6	0.000000000	1.404783000	0.000095000
6	-1.225762000	0.729268000	0.000094000
6	-1.225762000	-0.729268000	0.000103000
6	3.669827000	-0.729393000	0.000094000
6	2.450561000	1.410117000	0.000105000
1	0.000000000	2.491650000	0.000091000
6	-2.450561000	1.410117000	0.000082000

6	-2.450561000	-1.410117000	0.000110000
6	-3.669828000	-0.729393000	0.000104000
6	-3.669827000	0.729393000	0.000083000
1	-2.472828000	2.495887000	0.000069000
1	-2.472828000	-2.495887000	0.000121000
6	3.669827000	0.729393000	0.000105000
1	2.472828000	-2.495887000	0.000091000
1	0.000000000	-2.491650000	0.000108000
1	2.472828000	2.495887000	0.000108000
6	-7.185716000	-1.409922000	0.000116000
6	-8.401615000	-0.730086000	0.000094000
6	-9.634383000	-1.403800000	0.000111000
6	-8.401615000	0.730086000	0.000050000
6	-9.634383000	1.403800000	0.000018000
6	-10.856416000	0.730215000	0.000030000
6	-10.856416000	-0.730215000	0.000083000
6	-5.954829000	-0.730693000	0.000100000
6	-7.185716000	1.409922000	0.000041000
1	-9.634405000	2.490771000	-0.000019000
6	-12.082365000	1.408435000	-0.000008000
6	-12.082365000	-1.408435000	0.000104000
6	-13.305813000	-0.731364000	0.000071000
6	-13.305813000	0.731364000	0.000008000
1	-12.104165000	2.494409000	-0.000051000
1	-12.104165000	-2.494409000	0.000146000
6	-5.954829000	0.730693000	0.000068000
1	-7.164107000	-2.495774000	0.000144000
1	-9.634405000	-2.490771000	0.000147000
1	-7.164106000	2.495774000	0.000012000
7	-4.818402000	1.434687000	0.000063000
7	-4.818402000	-1.434687000	0.000115000
6	12.082365000	-1.408435000	0.000016000
6	10.856416000	-0.730215000	0.000048000
6	9.634383000	-1.403800000	0.000040000
6	10.856416000	0.730215000	0.000092000
6	9.634383000	1.403800000	0.000115000
6	8.401615000	0.730086000	0.000101000
6	8.401615000	-0.730086000	0.000067000
6	13.305813000	-0.731364000	0.000027000
6	12.082365000	1.408435000	0.000108000
1	9.634405000	2.490771000	0.000143000
6	7.185716000	1.409922000	0.000117000
6	7.185716000	-1.409922000	0.000062000
6	5.954829000	-0.730693000	0.000083000
6	5.954829000	0.730693000	0.000105000
1	7.164106000	2.495774000	0.000138000
1	7.164106000	-2.495774000	0.000040000

6	13.305813000	0.731364000	0.000080000
1	12.104165000	-2.494409000	-0.000020000
1	9.634405000	-2.490771000	0.000011000
1	12.104165000	2.494409000	0.000143000
7	4.818402000	1.434687000	0.000113000
7	4.818402000	-1.434687000	0.000081000
6	21.708139000	-1.411333000	-0.000112000
6	20.496290000	-0.730600000	-0.000059000
6	19.259839000	-1.404540000	-0.000078000
6	20.496290000	0.730600000	0.000018000
6	19.259839000	1.404540000	0.000065000
6	18.041077000	0.730557000	0.000042000
6	18.041077000	-0.730557000	-0.000029000
6	22.942987000	-0.730963000	-0.000090000
6	21.708139000	1.411333000	0.000042000
1	19.259717000	2.491467000	0.000119000
6	16.812186000	1.408715000	0.000084000
6	16.812186000	-1.408715000	-0.000046000
6	15.591569000	-0.731233000	0.000000000
6	15.591569000	0.731233000	0.000063000
1	16.790100000	2.494663000	0.000134000
1	16.790100000	-2.494663000	-0.000095000
6	22.942987000	0.730963000	-0.000008000
1	21.729629000	-2.497114000	-0.000171000
1	19.259717000	-2.491467000	-0.000133000
1	21.729629000	2.497114000	0.000100000
7	14.447358000	1.436563000	0.000099000
7	14.447358000	-1.436563000	-0.000015000
6	-16.812186000	-1.408715000	0.000083000
6	-18.041077000	-0.730557000	0.000039000
6	-19.259839000	-1.404540000	0.000068000
6	-18.041077000	0.730557000	-0.000042000
6	-19.259839000	1.404540000	-0.000093000
6	-20.496290000	0.730600000	-0.000067000
6	-20.496290000	-0.730600000	0.000020000
6	-15.591569000	-0.731233000	0.000056000
6	-16.812186000	1.408715000	-0.000065000
1	-19.259717000	2.491467000	-0.000154000
6	-21.708139000	1.411333000	-0.000120000
6	-21.708139000	-1.411333000	0.000051000
6	-22.942987000	-0.730963000	0.000000000
6	-22.942987000	0.730963000	-0.000091000
1	-21.729629000	2.497114000	-0.000186000
1	-21.729629000	-2.497114000	0.000116000
6	-15.591569000	0.731233000	-0.000016000
1	-16.790100000	-2.494663000	0.000140000
1	-19.259717000	-2.491467000	0.000130000

1	-16.790100000	2.494663000	-0.000121000
7	-14.447358000	1.436563000	-0.000037000
7	-14.447358000	-1.436563000	0.000096000
6	31.365683000	-1.404136000	-0.000255000
6	30.113713000	-0.723806000	-0.000192000
6	28.900255000	-1.403573000	-0.000218000
6	30.113713000	0.723806000	-0.000099000
6	28.900255000	1.403573000	-0.000039000
6	27.668966000	0.727347000	-0.000066000
6	27.668966000	-0.727347000	-0.000158000
6	32.542443000	-0.711022000	-0.000227000
6	31.365683000	1.404136000	-0.000071000
1	28.900711000	2.490685000	0.000029000
6	26.445044000	1.410809000	-0.000009000
6	26.445044000	-1.410809000	-0.000182000
6	25.228403000	-0.728623000	-0.000123000
6	25.228403000	0.728623000	-0.000036000
1	26.422822000	2.496501000	0.000057000
1	26.422822000	-2.496501000	-0.000249000
6	32.542443000	0.711022000	-0.000133000
1	31.363006000	-2.490378000	-0.000326000
1	28.900711000	-2.490685000	-0.000288000
1	33.488084000	-1.243407000	-0.000276000
1	31.363006000	2.490378000	0.000000000
1	33.488084000	1.243407000	-0.000110000
7	24.075746000	1.434137000	0.000019000
7	24.075746000	-1.434137000	-0.000147000
6	-26.445044000	-1.410809000	0.000016000
6	-27.668966000	-0.727347000	-0.000040000
6	-28.900255000	-1.403573000	-0.000004000
6	-27.668966000	0.727347000	-0.000140000
6	-28.900255000	1.403573000	-0.000200000
6	-30.113713000	0.723806000	-0.000164000
6	-30.113713000	-0.723806000	-0.000062000
6	-25.228403000	-0.728623000	-0.000020000
6	-26.445044000	1.410809000	-0.000174000
1	-28.900711000	2.490685000	-0.000276000
6	-31.365683000	1.404136000	-0.000225000
6	-31.365683000	-1.404136000	-0.000024000
6	-32.542443000	-0.711022000	-0.000084000
6	-32.542443000	0.711022000	-0.000187000
1	-31.363006000	2.490378000	-0.000303000
1	-31.363006000	-2.490378000	0.000053000
1	-33.488084000	-1.243407000	-0.000054000
1	-33.488084000	1.243407000	-0.000235000
6	-25.228403000	0.728623000	-0.000116000
1	-26.422822000	-2.496501000	0.000089000

1	-28.900711000	-2.490685000	0.000072000
1	-26.422822000	2.496501000	-0.000247000
7	-24.075746000	-1.434137000	0.000035000
7	-24.075746000	1.434137000	-0.000148000

Table S98: Coordinates of pT₁_1 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	1.143139000	0.732531000	0.000011000
7	0.000000000	1.434820000	0.000013000
6	-1.143139000	0.732531000	0.000011000
6	-1.143139000	-0.732531000	0.000011000
7	0.000000000	-1.434820000	0.000013000
6	1.143139000	-0.732531000	0.000011000
6	-3.584313000	-0.731876000	0.000006000
6	-3.584313000	0.731876000	0.000006000
6	-4.817621000	1.407701000	0.000004000
1	-4.817887000	2.494614000	0.000003000
6	-6.032612000	0.729311000	0.000001000
6	-6.032612000	-0.729311000	0.000001000
6	-4.817621000	-1.407701000	0.000004000
1	-4.817887000	-2.494614000	0.000003000
6	-8.477964000	-0.726951000	-0.000007000
6	-8.477964000	0.726951000	-0.000007000
6	-9.736031000	1.406209000	-0.000011000
6	-9.736031000	-1.406209000	-0.000011000
6	-10.908712000	-0.713833000	-0.000014000
6	-10.908712000	0.713833000	-0.000014000
1	-9.733837000	2.492538000	-0.000011000
1	-9.733837000	-2.492538000	-0.000011000
6	3.584313000	0.731876000	0.000006000
6	3.584313000	-0.731876000	0.000006000
6	4.817621000	-1.407701000	0.000004000
6	4.817621000	1.407701000	0.000004000
6	6.032612000	-0.729311000	0.000001000
6	6.032612000	0.729311000	0.000001000
1	4.817887000	2.494614000	0.000003000
1	4.817887000	-2.494614000	0.000003000
6	-7.272757000	1.405777000	-0.000003000
6	-7.272757000	-1.405777000	-0.000003000
6	-2.367162000	1.415220000	0.000009000
6	-2.367162000	-1.415220000	0.000009000
6	2.367162000	1.415220000	0.000009000
6	2.367162000	-1.415220000	0.000009000
6	7.272757000	1.405777000	-0.000003000

6	7.272757000	-1.405777000	-0.000003000
6	8.477964000	0.726951000	-0.000007000
6	8.477964000	-0.726951000	-0.000007000
6	9.736031000	1.406209000	-0.000011000
6	9.736031000	-1.406209000	-0.000011000
6	10.908712000	0.713833000	-0.000014000
6	10.908712000	-0.713833000	-0.000014000
1	7.274033000	-2.493068000	-0.000003000
1	7.274033000	2.493068000	-0.000003000
1	2.345066000	-2.500773000	0.000008000
1	2.345066000	2.500773000	0.000008000
1	-2.345066000	2.500773000	0.000008000
1	-2.345066000	-2.500773000	0.000008000
1	-7.274033000	2.493068000	-0.000003000
1	-7.274033000	-2.493068000	-0.000003000
1	9.733837000	-2.492538000	-0.000011000
1	11.855305000	-1.244710000	-0.000017000
1	11.855305000	1.244710000	-0.000017000
1	9.733837000	2.492538000	-0.000011000
1	-11.855305000	-1.244710000	-0.000017000
1	-11.855305000	1.244710000	-0.000017000

Table S99: Coordinates of pT₂_1 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	7.259918000	0.731542000	0.000020000
7	6.114680000	1.434583000	0.000011000
6	4.972828000	0.732459000	0.000011000
6	4.972828000	-0.732459000	0.000020000
7	6.114680000	-1.434583000	0.000029000
6	7.259918000	-0.731542000	0.000029000
6	2.531225000	-0.731796000	0.000010000
6	2.531225000	0.731796000	0.000001000
6	1.295340000	1.406775000	-0.000008000
1	1.295864000	2.493842000	-0.000015000
6	0.082044000	0.729543000	-0.000009000
6	0.082044000	-0.729543000	0.000000000
6	1.295340000	-1.406775000	0.000009000
1	1.295864000	-2.493842000	0.000015000
6	-2.365409000	-0.728420000	-0.000010000
6	-2.365409000	0.728419000	-0.000018000
6	-3.618295000	1.405000000	-0.000027000
6	-3.618295000	-1.405000000	-0.000011000
6	-4.802547000	-0.722385000	-0.000019000
6	-4.802547000	0.722385000	-0.000027000
1	-3.626507000	2.491690000	-0.000033000
1	-3.626507000	-2.491691000	-0.000004000

6	9.701109000	0.731384000	0.000029000
6	9.701109000	-0.731384000	0.000039000
6	10.933771000	-1.407245000	0.000048000
6	10.933771000	1.407245000	0.000029000
6	12.149510000	-0.729021000	0.000048000
6	12.149510000	0.729021000	0.000038000
1	10.933571000	2.494259000	0.000022000
1	10.933571000	-2.494259000	0.000055000
6	-1.160315000	1.404988000	-0.000018000
6	-1.160315000	-1.404988000	-0.000001000
6	3.746940000	1.414589000	0.000001000
6	3.746940000	-1.414589000	0.000019000
6	8.482373000	1.414458000	0.000020000
6	8.482373000	-1.414458000	0.000039000
6	13.389596000	1.405463000	0.000038000
6	13.389596000	-1.405463000	0.000057000
6	14.595127000	0.726823000	0.000046000
6	14.595127000	-0.726823000	0.000056000
6	15.853368000	1.405968000	0.000046000
6	15.853368000	-1.405968000	0.000065000
6	17.026301000	0.713864000	0.000054000
6	17.026301000	-0.713864000	0.000064000
1	13.390352000	-2.492845000	0.000064000
1	13.390352000	2.492845000	0.000030000
1	8.460155000	-2.500044000	0.000046000
1	8.460154000	2.500044000	0.000013000
1	3.768942000	2.500190000	-0.000005000
1	3.768942000	-2.500190000	0.000026000
1	-1.159675000	2.492208000	-0.000024000
1	-1.159675000	-2.492208000	0.000005000
1	15.850697000	-2.492381000	0.000073000
1	17.973033000	-1.244600000	0.000071000
1	17.973033000	1.244600000	0.000054000
1	15.850697000	2.492382000	0.000038000
7	-6.029429000	-1.356380000	-0.000021000
7	-6.029429000	1.356380000	-0.000035000
6	-7.257467000	-0.719440000	-0.000025000
6	-7.257467000	0.719440000	-0.000033000
6	-8.443140000	-1.402986000	-0.000023000
6	-8.443140000	1.402986000	-0.000039000
6	-9.693196000	-0.724772000	-0.000029000
6	-9.693196000	0.724772000	-0.000037000
6	-10.904860000	-1.401931000	-0.000026000
6	-10.904860000	1.401931000	-0.000043000
6	-12.138004000	-0.724392000	-0.000033000
6	-12.138004000	0.724392000	-0.000041000
6	-13.366996000	-1.401645000	-0.000030000

6	-13.366996000	1.401646000	-0.000048000
6	-14.581646000	-0.723219000	-0.000036000
6	-14.581646000	0.723219000	-0.000046000
6	-15.834878000	-1.403051000	-0.000034000
6	-15.834878000	1.403051000	-0.000052000
6	-17.011886000	-0.711239000	-0.000040000
6	-17.011886000	0.711240000	-0.000049000
1	-6.030059000	-2.365366000	-0.000014000
1	-6.030059000	2.365366000	-0.000041000
1	-8.435048000	-2.489762000	-0.000017000
1	-8.435048000	2.489762000	-0.000045000
1	-10.905664000	-2.489343000	-0.000020000
1	-10.905664000	2.489343000	-0.000050000
1	-13.367791000	-2.489294000	-0.000024000
1	-13.367791000	2.489294000	-0.000054000
1	-15.831929000	-2.489638000	-0.000027000
1	-17.957558000	-1.243969000	-0.000038000
1	-17.957558000	1.243969000	-0.000054000
1	-15.831929000	2.489638000	-0.000059000

Table S100: Coordinates of pT₂_2 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-7.196445000	-0.728955000	0.000021000
7	-6.039498000	-1.435834000	0.000014000
6	-4.909512000	-0.732026000	0.000015000
6	-4.909512000	0.732026000	0.000024000
7	-6.039498000	1.435834000	0.000031000
6	-7.196445000	0.728955000	0.000030000
6	-2.457419000	0.730555000	0.000016000
6	-2.457419000	-0.730555000	0.000007000
6	-1.224655000	-1.402265000	-0.000001000
1	-1.224761000	-2.489562000	-0.000008000
6	0.000000000	-0.729639000	-0.000002000
6	0.000000000	0.729639000	0.000007000
6	-1.224655000	1.402265000	0.000016000
1	-1.224761000	2.489562000	0.000023000
6	2.457419000	0.730555000	-0.000002000
6	2.457419000	-0.730555000	-0.000011000
6	3.672889000	-1.408126000	-0.000019000
6	3.672889000	1.408126000	-0.000002000
6	4.909512000	0.732026000	-0.000011000
6	4.909512000	-0.732026000	-0.000019000
1	3.694033000	-2.494204000	-0.000026000
1	3.694033000	2.494204000	0.000004000
6	-9.642330000	-0.728282000	0.000027000
6	-9.642330000	0.728282000	0.000036000

6	-10.861178000	1.403719000	0.000043000
6	-10.861178000	-1.403719000	0.000026000
6	-12.091766000	0.725606000	0.000042000
6	-12.091766000	-0.725606000	0.000033000
1	-10.860890000	-2.490888000	0.000019000
1	-10.860890000	2.490888000	0.000050000
6	1.224655000	-1.402265000	-0.000010000
6	1.224655000	1.402265000	0.000007000
6	-3.672889000	-1.408126000	0.000007000
6	-3.672889000	1.408126000	0.000024000
6	-8.407831000	-1.408691000	0.000020000
6	-8.407831000	1.408691000	0.000037000
6	-13.319575000	-1.402228000	0.000031000
6	-13.319575000	1.402228000	0.000048000
6	-14.536308000	-0.722900000	0.000037000
6	-14.536308000	0.722900000	0.000046000
6	-15.786601000	-1.403043000	0.000035000
6	-15.786601000	1.403043000	0.000053000
6	-16.965008000	-0.710099000	0.000041000
6	-16.965008000	0.710099000	0.000050000
1	-13.320392000	2.489670000	0.000055000
1	-13.320392000	-2.489670000	0.000024000
1	-8.385112000	2.494573000	0.000044000
1	-8.385112000	-2.494573000	0.000013000
1	-3.694033000	-2.494204000	0.000000000
1	-3.694033000	2.494204000	0.000031000
1	1.224761000	-2.489562000	-0.000017000
1	1.224761000	2.489562000	0.000014000
1	-15.783907000	2.489396000	0.000060000
1	-17.910213000	1.243280000	0.000055000
1	-17.910213000	-1.243280000	0.000039000
1	-15.783907000	-2.489396000	0.000028000
7	6.039498000	1.435834000	-0.000011000
7	6.039498000	-1.435834000	-0.000027000
6	7.196445000	0.728955000	-0.000019000
6	7.196445000	-0.728955000	-0.000027000
6	8.407831000	1.408691000	-0.000019000
6	8.407831000	-1.408691000	-0.000035000
6	9.642330000	0.728282000	-0.000027000
6	9.642330000	-0.728282000	-0.000036000
6	10.861178000	1.403719000	-0.000028000
6	10.861178000	-1.403719000	-0.000043000
6	12.091766000	0.725606000	-0.000036000
6	12.091766000	-0.725606000	-0.000044000
6	13.319575000	1.402228000	-0.000036000
6	13.319575000	-1.402228000	-0.000052000
6	14.536308000	0.722900000	-0.000044000

6	14.536308000	-0.722900000	-0.000052000
6	15.786601000	1.403043000	-0.000044000
6	15.786601000	-1.403043000	-0.000059000
6	16.965008000	0.710099000	-0.000051000
6	16.965008000	-0.710099000	-0.000059000
1	8.385112000	2.494573000	-0.000013000
1	8.385112000	-2.494573000	-0.000041000
1	10.860890000	2.490888000	-0.000022000
1	10.860890000	-2.490888000	-0.000050000
1	13.320392000	2.489670000	-0.000030000
1	13.320392000	-2.489670000	-0.000058000
1	15.783907000	2.489396000	-0.000038000
1	17.910213000	1.243280000	-0.000051000
1	17.910213000	-1.243280000	-0.000065000
1	15.783907000	-2.489396000	-0.000065000

Table S101: Coordinates of pT₃_1 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-13.363289000	-0.719844000	-0.000004000
7	-12.135419000	-1.356858000	0.000005000
6	-10.907522000	-0.719223000	0.000010000
6	-10.907522000	0.719223000	0.000015000
7	-12.135419000	1.356858000	0.000015000
6	-13.363289000	0.719844000	0.000002000
6	-8.470878000	0.724163000	0.000022000
6	-8.470878000	-0.724163000	0.000017000
6	-7.257788000	-1.400837000	0.000018000
1	-7.257346000	-2.488408000	0.000014000
6	-6.025578000	-0.724022000	0.000023000
6	-6.025578000	0.724022000	0.000028000
6	-7.257788000	1.400836000	0.000028000
1	-12.135337000	-2.365486000	0.000000000
1	-12.135337000	2.365486000	0.000016000
1	-7.257346000	2.488408000	0.000032000
6	-3.580523000	0.724017000	0.000031000
6	-3.580523000	-0.724017000	0.000026000
6	-2.331710000	-1.402116000	0.000024000
6	-2.331710000	1.402115000	0.000033000
6	-1.145163000	0.718409000	0.000030000
6	-1.145163000	-0.718409000	0.000025000
1	-2.323072000	-2.489024000	0.000020000
1	-2.323072000	2.489024000	0.000037000
6	-15.800270000	-0.724691000	-0.000024000
6	-15.800270000	0.724691000	-0.000019000
6	-17.011439000	1.401467000	-0.000026000
6	-17.011439000	-1.401467000	-0.000037000

6	-18.245550000	0.724279000	-0.000039000
6	-18.245550000	-0.724279000	-0.000045000
1	-17.012144000	-2.488965000	-0.000042000
1	-17.012144000	2.488965000	-0.000022000
6	-4.794876000	-1.400882000	0.000023000
6	-4.794876000	1.400882000	0.000032000
6	-9.720975000	-1.401829000	0.000011000
6	-9.720975000	1.401829000	0.000021000
6	-14.549162000	-1.402310000	-0.000016000
6	-14.549162000	1.402310000	-0.000006000
6	-19.474069000	-1.401236000	-0.000059000
6	-19.474069000	1.401236000	-0.000047000
6	-20.689441000	-0.723025000	-0.000066000
6	-20.689441000	0.723025000	-0.000060000
6	-21.942351000	-1.402610000	-0.000080000
6	-21.942351000	1.402610000	-0.000068000
6	-23.119898000	-0.711002000	-0.000088000
6	-23.119898000	0.711002000	-0.000082000
1	-19.474951000	2.488964000	-0.000043000
1	-19.474952000	-2.488964000	-0.000063000
1	-14.540949000	2.489178000	-0.000002000
1	-14.540949000	-2.489178000	-0.000021000
1	-9.729361000	-2.488743000	0.000007000
1	-9.729361000	2.488743000	0.000025000
1	-4.795232000	-2.488453000	0.000019000
1	-4.795232000	2.488453000	0.000036000
1	-21.939502000	2.489261000	-0.000064000
1	-24.065344000	1.244191000	-0.000088000
1	-24.065344000	-1.244191000	-0.000098000
1	-21.939502000	-2.489261000	-0.000085000
7	0.083454000	1.356313000	0.000029000
7	0.083454000	-1.356313000	0.000019000
6	1.309703000	0.722589000	0.000032000
6	1.309703000	-0.722589000	0.000028000
6	2.494494000	1.404860000	0.000038000
6	2.494494000	-1.404860000	0.000029000
6	3.747114000	0.728498000	0.000037000
6	3.747114000	-0.728499000	0.000032000
6	4.952477000	1.404793000	0.000039000
6	4.952477000	-1.404793000	0.000030000
6	6.194769000	0.729613000	0.000036000
6	6.194769000	-0.729613000	0.000032000
6	7.408181000	1.406604000	0.000037000
6	7.408181000	-1.406604000	0.000027000
6	8.644140000	0.731866000	0.000032000
6	8.644140000	-0.731866000	0.000027000
6	9.859837000	1.414478000	0.000030000
6	9.859837000	-1.414478000	0.000021000

6	11.085911000	0.732679000	0.000023000
6	11.085911000	-0.732679000	0.000019000
1	0.082619000	2.365258000	0.000033000
1	0.082619000	-2.365258000	0.000019000
1	2.486030000	2.491584000	0.000041000
1	2.486030000	-2.491584000	0.000025000
1	4.952906000	2.492042000	0.000042000
1	4.952906000	-2.492042000	0.000026000
1	7.408619000	2.493686000	0.000039000
1	7.408620000	-2.493686000	0.000023000
1	9.881715000	2.500106000	0.000033000
1	9.881715000	-2.500107000	0.000017000
7	12.227643000	1.434472000	0.000021000
7	12.227643000	-1.434472000	0.000012000
6	13.373142000	0.731576000	0.000014000
6	13.373142000	-0.731576000	0.000009000
6	14.595396000	1.414290000	0.000010000
6	14.595396000	-1.414289000	0.000001000
6	15.814415000	0.731342000	0.000002000
6	15.814415000	-0.731342000	-0.000003000
6	17.046883000	1.407083000	-0.000002000
6	17.046883000	-1.407083000	-0.000012000
6	18.262879000	0.728972000	-0.000012000
6	18.262879000	-0.728972000	-0.000017000
6	19.502753000	1.405316000	-0.000017000
6	19.502753000	-1.405316000	-0.000027000
6	20.708482000	0.726755000	-0.000027000
6	20.708482000	-0.726755000	-0.000032000
6	21.966544000	1.405818000	-0.000033000
6	21.966544000	-1.405818000	-0.000043000
6	23.139629000	0.713755000	-0.000043000
6	23.139629000	-0.713754000	-0.000048000
1	14.573276000	2.499901000	0.000014000
1	14.573276000	-2.499901000	-0.000003000
1	17.046794000	2.494106000	0.000001000
1	17.046794000	-2.494106000	-0.000016000
1	19.503679000	2.492716000	-0.000013000
1	19.503679000	-2.492715000	-0.000030000
1	21.964042000	2.492238000	-0.000029000
1	21.964043000	-2.492238000	-0.000047000
1	24.086208000	1.244756000	-0.000048000
1	24.086208000	-1.244756000	-0.000057000

Table S103: Coordinates of pT₃_2 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-13.303644000	-0.719493000	0.000008000

7	-12.074751000	-1.356891000	0.000009000
6	-10.849882000	-0.718991000	0.000009000
6	-10.849881000	0.718991000	0.000013000
7	-12.074751000	1.356891000	0.000016000
6	-13.303644000	0.719493000	0.000012000
6	-8.414301000	0.724135000	0.000012000
6	-8.414301000	-0.724135000	0.000008000
6	-7.199382000	-1.401543000	0.000004000
1	-7.198872000	-2.488890000	0.000001000
6	-5.968157000	-0.725374000	0.000005000
6	-5.968157000	0.725374000	0.000009000
6	-7.199382000	1.401543000	0.000013000
1	-12.074441000	-2.365731000	0.000005000
1	-12.074441000	2.365731000	0.000018000
1	-7.198872000	2.488890000	0.000017000
6	-3.518505000	0.727764000	0.000006000
6	-3.518505000	-0.727764000	0.000001000
6	-2.286128000	-1.408117000	-0.000004000
6	-2.286128000	1.408117000	0.000006000
6	-1.072944000	0.728604000	0.000002000
6	-1.072944000	-0.728604000	-0.000003000
1	-2.263499000	-2.494118000	-0.000008000
1	-2.263499000	2.494118000	0.000009000
6	-15.739631000	-0.724595000	-0.000001000
6	-15.739631000	0.724595000	0.000003000
6	-16.950458000	1.401720000	-0.000002000
6	-16.950458000	-1.401720000	-0.000010000
6	-18.184428000	0.724221000	-0.000012000
6	-18.184428000	-0.724221000	-0.000016000
1	-16.951131000	-2.489134000	-0.000015000
1	-16.951131000	2.489135000	-0.000001000
6	-4.740549000	-1.402755000	0.000000000
6	-4.740549000	1.402755000	0.000010000
6	-9.661058000	-1.401966000	0.000006000
6	-9.661058000	1.401966000	0.000015000
6	-14.488696000	-1.402638000	0.000002000
6	-14.488696000	1.402638000	0.000010000
6	-19.412612000	-1.401459000	-0.000027000
6	-19.412612000	1.401459000	-0.000019000
6	-20.627905000	-0.722990000	-0.000034000
6	-20.627905000	0.722991000	-0.000030000
6	-21.880543000	-1.402864000	-0.000046000
6	-21.880543000	1.402864000	-0.000037000
6	-23.057859000	-0.710959000	-0.000053000
6	-23.057859000	0.710959000	-0.000048000
1	-19.413476000	2.489099000	-0.000016000
1	-19.413476000	-2.489099000	-0.000031000

1	-14.480424000	2.489433000	0.000012000
1	-14.480424000	-2.489433000	-0.000002000
1	-9.669057000	-2.488694000	0.000004000
1	-9.669057000	2.488694000	0.000018000
1	-4.740102000	-2.490071000	-0.000003000
1	-4.740102000	2.490071000	0.000013000
1	-21.877752000	2.489426000	-0.000034000
1	-24.003340000	1.243963000	-0.000054000
1	-24.003340000	-1.243963000	-0.000062000
1	-21.877752000	-2.489426000	-0.000049000
7	0.082835000	1.435563000	0.000002000
7	0.082835000	-1.435563000	-0.000008000
6	1.213778000	0.731542000	-0.000002000
6	1.213778000	-0.731542000	-0.000007000
6	2.450106000	1.408031000	0.000001000
6	2.450106000	-1.408031000	-0.000010000
6	3.665376000	0.730362000	-0.000002000
6	3.665376000	-0.730362000	-0.000007000
6	4.898849000	1.402155000	0.000001000
6	4.898849000	-1.402156000	-0.000010000
6	6.123019000	0.729659000	-0.000001000
6	6.123019000	-0.729659000	-0.000006000
6	7.348497000	1.402125000	0.000003000
6	7.348497000	-1.402125000	-0.000008000
6	8.580871000	0.730511000	0.000002000
6	8.580871000	-0.730511000	-0.000004000
6	9.796913000	1.407899000	0.000006000
6	9.796913000	-1.407899000	-0.000006000
6	11.033269000	0.731958000	0.000003000
6	11.033269000	-0.731958000	-0.000003000
1	2.428927000	2.494130000	0.000004000
1	2.428927000	-2.494131000	-0.000015000
1	4.898481000	2.489509000	0.000005000
1	4.898481000	-2.489509000	-0.000015000
1	7.348878000	2.489478000	0.000007000
1	7.348878000	-2.489478000	-0.000013000
1	9.818077000	2.494002000	0.000010000
1	9.818077000	-2.494002000	-0.000011000
7	12.163566000	1.436144000	0.000010000
7	12.163566000	-1.436144000	-0.000002000
6	13.320456000	0.729070000	0.000011000
6	13.320456000	-0.729070000	0.000004000
6	14.531762000	1.408439000	0.000015000
6	14.531762000	-1.408439000	0.000003000
6	15.766809000	0.728223000	0.000014000
6	15.766809000	-0.728223000	0.000008000
6	16.985437000	1.403542000	0.000018000

6	16.985437000	-1.403541000	0.000006000
6	18.216505000	0.725486000	0.000016000
6	18.216505000	-0.725486000	0.000010000
6	19.444206000	1.402129000	0.000020000
6	19.444206000	-1.402129000	0.000008000
6	20.661170000	0.722790000	0.000018000
6	20.661170000	-0.722790000	0.000011000
6	21.911542000	1.402843000	0.000021000
6	21.911542000	-1.402842000	0.000008000
6	23.090184000	0.710075000	0.000018000
6	23.090184000	-0.710075000	0.000012000
1	14.509209000	2.494384000	0.000019000
1	14.509210000	-2.494384000	-0.000002000
1	16.985279000	2.490755000	0.000023000
1	16.985279000	-2.490755000	0.000001000
1	19.445049000	2.489595000	0.000025000
1	19.445049000	-2.489595000	0.000003000
1	21.908872000	2.489244000	0.000026000
1	21.908872000	-2.489244000	0.000003000
1	24.035353000	1.243419000	0.000021000
1	24.035353000	-1.243419000	0.000010000

Table S103: Coordinates of pT₃_3 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-13.215450000	0.733531000	0.000013000
7	-12.075137000	1.435302000	0.000013000
6	-10.928328000	0.733005000	0.000008000
6	-10.928328000	-0.733005000	0.000004000
7	-12.075137000	-1.435302000	0.000004000
6	-13.215450000	-0.733531000	0.000009000
6	-8.486712000	-0.733609000	-0.000001000
6	-8.486712000	0.733609000	0.000004000
6	-7.261670000	1.410131000	0.000003000
1	-7.262218000	2.496875000	0.000007000
6	-6.036327000	0.732539000	-0.000001000
6	-6.036327000	-0.732539000	-0.000005000
6	-7.261670000	-1.410131000	-0.000005000
1	-7.262218000	-2.496875000	-0.000009000
6	-3.585815000	-0.733934000	-0.000009000
6	-3.585815000	0.733933000	-0.000005000
6	-2.364784000	1.417281000	-0.000004000
6	-2.364784000	-1.417281000	-0.000013000
6	-1.143729000	-0.733988000	-0.000012000
6	-1.143729000	0.733987000	-0.000008000
1	-2.342544000	2.502705000	-0.000001000
1	-2.342544000	-2.502705000	-0.000016000

6	-15.656683000	0.732382000	0.000019000
6	-15.656683000	-0.732382000	0.000015000
6	-16.891002000	-1.408151000	0.000016000
6	-16.891002000	1.408151000	0.000024000
6	-18.105068000	-0.729641000	0.000021000
6	-18.105068000	0.729641000	0.000025000
1	-16.891078000	2.495035000	0.000028000
1	-16.891078000	-2.495035000	0.000013000
6	-4.812230000	1.410268000	-0.000001000
6	-4.812230000	-1.410269000	-0.000009000
6	-9.709567000	1.416728000	0.000008000
6	-9.709567000	-1.416729000	-0.000001000
6	-14.441227000	1.416227000	0.000018000
6	-14.441227000	-1.416227000	0.000010000
6	-19.345734000	1.406137000	0.000031000
6	-19.345734000	-1.406137000	0.000022000
6	-20.550427000	0.727230000	0.000032000
6	-20.550427000	-0.727230000	0.000027000
6	-21.808726000	1.406528000	0.000037000
6	-21.808726000	-1.406528000	0.000029000
6	-22.981108000	0.714003000	0.000038000
6	-22.981108000	-0.714003000	0.000034000
1	-19.346921000	-2.493408000	0.000019000
1	-19.346921000	2.493408000	0.000034000
1	-14.419420000	-2.501720000	0.000007000
1	-14.419420000	2.501720000	0.000022000
1	-9.732260000	2.502162000	0.000011000
1	-9.732260000	-2.502162000	-0.000004000
1	-4.812091000	2.497001000	0.000003000
1	-4.812091000	-2.497001000	-0.000013000
1	-21.806579000	-2.492825000	0.000025000
1	-23.927761000	-1.244735000	0.000035000
1	-23.927761000	1.244736000	0.000042000
1	-21.806579000	2.492825000	0.000041000
7	0.000000000	-1.436040000	-0.000016000
7	0.000000000	1.436040000	-0.000007000
6	1.143729000	-0.733988000	-0.000014000
6	1.143729000	0.733987000	-0.000010000
6	2.364785000	-1.417281000	-0.000017000
6	2.364784000	1.417281000	-0.000009000
6	3.585815000	-0.733934000	-0.000016000
6	3.585815000	0.733933000	-0.000011000
6	4.812230000	-1.410269000	-0.000018000
6	4.812230000	1.410268000	-0.000010000
6	6.036327000	-0.732539000	-0.000017000
6	6.036327000	0.732539000	-0.000012000
6	7.261670000	-1.410131000	-0.000019000

6	7.261670000	1.410131000	-0.000010000
6	8.486712000	-0.733609000	-0.000017000
6	8.486712000	0.733609000	-0.000012000
6	9.709567000	-1.416729000	-0.000018000
6	9.709567000	1.416728000	-0.000010000
6	10.928328000	-0.733005000	-0.000016000
6	10.928328000	0.733005000	-0.000011000
1	2.342544000	-2.502705000	-0.000020000
1	2.342544000	2.502705000	-0.000005000
1	4.812091000	-2.497001000	-0.000022000
1	4.812091000	2.497001000	-0.000006000
1	7.262218000	-2.496875000	-0.000022000
1	7.262218000	2.496875000	-0.000007000
1	9.732260000	-2.502162000	-0.000021000
1	9.732260000	2.502162000	-0.000006000
7	12.075137000	-1.435302000	-0.000017000
7	12.075137000	1.435302000	-0.000008000
6	13.215450000	-0.733531000	-0.000014000
6	13.215450000	0.733531000	-0.000010000
6	14.441227000	-1.416227000	-0.000015000
6	14.441227000	1.416227000	-0.000006000
6	15.656683000	-0.732382000	-0.000012000
6	15.656683000	0.732382000	-0.000007000
6	16.891002000	-1.408151000	-0.000012000
6	16.891002000	1.408151000	-0.000004000
6	18.105068000	-0.729641000	-0.000009000
6	18.105068000	0.729641000	-0.000004000
6	19.345734000	-1.406137000	-0.000009000
6	19.345734000	1.406137000	0.000000000
6	20.550427000	-0.727230000	-0.000005000
6	20.550427000	0.727230000	-0.000001000
6	21.808726000	-1.406528000	-0.000005000
6	21.808726000	1.406528000	0.000003000
6	22.981108000	-0.714003000	-0.000001000
6	22.981108000	0.714003000	0.000003000
1	14.419420000	-2.501720000	-0.000018000
1	14.419420000	2.501720000	-0.000003000
1	16.891078000	-2.495035000	-0.000015000
1	16.891078000	2.495035000	0.000000000
1	19.346921000	-2.493408000	-0.000012000
1	19.346921000	2.493408000	0.000003000
1	21.806579000	-2.492825000	-0.000008000
1	21.806579000	2.492825000	0.000007000
1	23.927761000	-1.244735000	-0.000001000
1	23.927761000	1.244736000	0.000006000

Table S104: Coordinates of pT₄_1 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	7.252146000	-0.718856000	0.000028000
7	6.023522000	-1.356906000	0.000033000
6	4.796178000	-0.719518000	0.000037000
6	4.796178000	0.719518000	0.000037000
7	6.023522000	1.356906000	0.000033000
6	7.252146000	0.718855000	0.000028000
6	2.358995000	0.724231000	0.000045000
6	2.358995000	-0.724232000	0.000045000
6	1.145936000	-1.400739000	0.000048000
1	1.145466000	-2.488334000	0.000047000
6	-0.086548000	-0.724022000	0.000050000
6	-0.086548000	0.724021000	0.000050000
6	1.145936000	1.400739000	0.000048000
1	6.023665000	-2.365461000	0.000033000
1	6.023665000	2.365460000	0.000033000
1	1.145466000	2.488334000	0.000048000
6	-2.531704000	0.723965000	0.000053000
6	-2.531704000	-0.723966000	0.000053000
6	-3.780468000	-1.402028000	0.000053000
6	-3.780468000	1.402028000	0.000053000
6	-4.967053000	0.718281000	0.000053000
6	-4.967053000	-0.718281000	0.000053000
1	-3.789147000	-2.488960000	0.000053000
1	-3.789147000	2.488960000	0.000053000
6	9.688945000	-0.723863000	0.000018000
6	9.688945000	0.723863000	0.000018000
6	10.902605000	1.400461000	0.000014000
6	10.902606000	-1.400461000	0.000014000
6	12.134438000	0.723775000	0.000010000
6	12.134438000	-0.723776000	0.000010000
1	10.903013000	-2.488116000	0.000015000
1	10.903013000	2.488116000	0.000015000
6	-1.317126000	-1.400789000	0.000052000
6	-1.317126000	1.400789000	0.000052000
6	3.609220000	-1.401731000	0.000041000
6	3.609220000	1.401731000	0.000041000
6	8.438734000	-1.401471000	0.000023000
6	8.438734000	1.401471000	0.000023000
6	13.366193000	-1.400467000	0.000007000
6	13.366193000	1.400467000	0.000007000
6	14.579903000	-0.723851000	0.000004000
6	14.579903000	0.723851000	0.000004000
6	15.830043000	-1.401481000	0.000001000
6	15.830043000	1.401481000	0.000002000
6	17.016612000	-0.718819000	0.000000000
6	17.016612000	0.718819000	0.000000000

1	13.365799000	2.488119000	0.000008000
1	13.365799000	-2.488119000	0.000007000
1	8.430277000	2.488462000	0.000023000
1	8.430277000	-2.488463000	0.000023000
1	3.617538000	-2.488667000	0.000041000
1	3.617537000	2.488667000	0.000041000
1	-1.316794000	-2.488386000	0.000051000
1	-1.316794000	2.488385000	0.000052000
1	15.838516000	2.488460000	0.000002000
1	15.838516000	-2.488460000	0.000002000
7	-6.195881000	1.356273000	0.000051000
7	-6.195881000	-1.356273000	0.000051000
6	-7.421961000	0.722649000	0.000049000
6	-7.421961000	-0.722649000	0.000049000
6	-8.606895000	1.404844000	0.000046000
6	-8.606895000	-1.404845000	0.000046000
6	-9.859462000	0.728526000	0.000042000
6	-9.859462000	-0.728527000	0.000042000
6	-11.064895000	1.404761000	0.000036000
6	-11.064895000	-1.404762000	0.000036000
6	-12.307187000	0.729631000	0.000030000
6	-12.307187000	-0.729631000	0.000029000
6	-13.520632000	1.406577000	0.000022000
6	-13.520632000	-1.406577000	0.000022000
6	-14.756610000	0.731882000	0.000013000
6	-14.756610000	-0.731882000	0.000013000
6	-15.972324000	1.414450000	0.000004000
6	-15.972324000	-1.414450000	0.000004000
6	-17.198428000	0.732705000	-0.000006000
6	-17.198428000	-0.732705000	-0.000006000
1	-6.195009000	2.365216000	0.000051000
1	-6.195009000	-2.365216000	0.000051000
1	-8.598428000	2.491574000	0.000046000
1	-8.598428000	-2.491575000	0.000045000
1	-11.065333000	2.492017000	0.000036000
1	-11.065333000	-2.492017000	0.000035000
1	-13.521074000	2.493665000	0.000021000
1	-13.521075000	-2.493665000	0.000021000
1	-15.994199000	2.500084000	0.000003000
1	-15.994199000	-2.500084000	0.000003000
7	-18.340153000	1.434479000	-0.000017000
7	-18.340153000	-1.434479000	-0.000017000
6	-19.485688000	0.731559000	-0.000028000
6	-19.485688000	-0.731559000	-0.000028000
6	-20.707926000	1.414243000	-0.000041000
6	-20.707926000	-1.414243000	-0.000042000
6	-21.926996000	0.731330000	-0.000055000

6	-21.926996000	-0.731330000	-0.000055000
6	-23.159455000	1.407053000	-0.000070000
6	-23.159455000	-1.407053000	-0.000070000
6	-24.375485000	0.728963000	-0.000085000
6	-24.375485000	-0.728963000	-0.000085000
6	-25.615360000	1.405290000	-0.000101000
6	-25.615360000	-1.405289000	-0.000101000
6	-26.821111000	0.726749000	-0.000117000
6	-26.821111000	-0.726748000	-0.000117000
6	-28.079179000	1.405794000	-0.000133000
6	-28.079179000	-1.405793000	-0.000133000
6	-29.252285000	0.713753000	-0.000149000
6	-29.252285000	-0.713752000	-0.000149000
1	-20.685786000	2.499862000	-0.000041000
1	-20.685786000	-2.499862000	-0.000042000
1	-23.159352000	2.494083000	-0.000070000
1	-23.159352000	-2.494083000	-0.000070000
1	-25.616271000	2.492696000	-0.000101000
1	-25.616272000	-2.492696000	-0.000101000
1	-28.076657000	2.492220000	-0.000133000
1	-28.076657000	-2.492219000	-0.000133000
1	-30.198866000	1.244757000	-0.000161000
1	-30.198867000	-1.244756000	-0.000161000
7	18.245175000	-1.356889000	-0.000001000
7	18.245175000	1.356889000	-0.000001000
6	19.472653000	-0.720016000	-0.000003000
6	19.472653000	0.720016000	-0.000003000
6	20.658824000	-1.402204000	-0.000004000
6	20.658824000	1.402205000	-0.000004000
6	21.910019000	-0.724721000	-0.000005000
6	21.910019000	0.724721000	-0.000005000
6	23.121213000	-1.401370000	-0.000006000
6	23.121213000	1.401371000	-0.000006000
6	24.355501000	-0.724276000	-0.000007000
6	24.355501000	0.724276000	-0.000007000
6	25.583992000	-1.401141000	-0.000007000
6	25.583992000	1.401142000	-0.000007000
6	26.799524000	-0.722993000	-0.000008000
6	26.799524000	0.722994000	-0.000008000
6	28.052417000	-1.402499000	-0.000008000
6	28.052417000	1.402500000	-0.000007000
6	29.230108000	-0.710968000	-0.000007000
6	29.230108000	0.710969000	-0.000007000
1	28.049534000	-2.489175000	-0.000008000
1	30.175531000	-1.244233000	-0.000007000
1	30.175531000	1.244234000	-0.000007000
1	28.049534000	2.489176000	-0.000007000

1	25.584875000	2.488896000	-0.000007000
1	25.584875000	-2.488895000	-0.000007000
1	23.121926000	-2.488892000	-0.000006000
1	23.121926000	2.488893000	-0.000005000
1	20.650636000	-2.489092000	-0.000004000
1	20.650636000	2.489093000	-0.000003000
1	18.244975000	-2.365464000	-0.000001000
1	18.244975000	2.365464000	-0.000001000

Table S105: Coordinates of pT₄_2 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	7.175869000	0.718356000	0.000319000
7	5.947285000	1.356188000	0.000280000
6	4.721384000	0.722807000	0.000234000
6	4.721378000	-0.722825000	0.000234000
7	5.947277000	-1.356218000	0.000279000
6	7.175866000	-0.718393000	0.000318000
6	2.284211000	-0.728789000	0.000132000
6	2.284219000	0.728811000	0.000133000
6	1.079002000	1.405115000	0.000080000
1	1.078595000	2.492323000	0.000080000
6	-0.163370000	0.730027000	0.000025000
6	-0.163379000	-0.729956000	0.000025000
6	1.078987000	-1.405070000	0.000080000
1	5.948172000	2.365214000	0.000278000
1	5.948156000	-2.365243000	0.000276000
1	1.078561000	-2.492278000	0.000080000
6	-2.612805000	-0.732356000	-0.000079000
6	-2.612797000	0.732477000	-0.000080000
6	-3.827215000	1.415236000	-0.000128000
6	-3.827222000	-1.415098000	-0.000127000
6	-5.054938000	-0.733678000	-0.000175000
6	-5.054932000	0.733843000	-0.000176000
1	-3.848909000	2.500820000	-0.000127000
1	-3.848933000	-2.500682000	-0.000125000
6	9.610916000	0.724065000	0.000369000
6	9.610914000	-0.724103000	0.000367000
6	10.825389000	-1.401019000	0.000376000
6	10.825392000	1.400984000	0.000379000
6	12.055856000	-0.724117000	0.000379000
6	12.055857000	0.724082000	0.000381000
1	10.825743000	2.488529000	0.000374000
1	10.825742000	-2.488565000	0.000369000
6	-1.376218000	1.407045000	-0.000027000
6	-1.376231000	-1.406952000	-0.000027000
6	3.536542000	1.405176000	0.000186000

6	3.536529000	-1.405174000	0.000185000
6	8.362425000	1.402273000	0.000348000
6	8.362420000	-1.402310000	0.000345000
6	13.288112000	1.400926000	0.000371000
6	13.288111000	-1.400959000	0.000368000
6	14.501095000	0.724239000	0.000354000
6	14.501094000	-0.724270000	0.000353000
6	15.751100000	1.401928000	0.000326000
6	15.751098000	-1.401960000	0.000322000
6	16.937685000	0.719328000	0.000290000
6	16.937684000	-0.719360000	0.000288000
1	13.287651000	-2.488505000	0.000361000
1	13.287652000	2.488472000	0.000366000
1	8.353774000	-2.489196000	0.000340000
1	8.353779000	2.489159000	0.000343000
1	3.545016000	2.491866000	0.000185000
1	3.544985000	-2.491865000	0.000184000
1	-1.376621000	2.494079000	-0.000026000
1	-1.376653000	-2.493987000	-0.000025000
1	15.759455000	-2.488849000	0.000314000
1	15.759457000	2.488817000	0.000321000
7	-6.194111000	-1.435263000	-0.000209000
7	-6.194111000	1.435434000	-0.000211000
6	-7.342623000	-0.732373000	-0.000244000
6	-7.342622000	0.732557000	-0.000245000
6	-8.560405000	-1.415449000	-0.000266000
6	-8.560412000	1.415631000	-0.000268000
6	-9.784845000	-0.733114000	-0.000288000
6	-9.784848000	0.733303000	-0.000290000
6	-11.009331000	-1.409302000	-0.000300000
6	-11.009347000	1.409483000	-0.000303000
6	-12.235436000	-0.732126000	-0.000308000
6	-12.235443000	0.732306000	-0.000310000
6	-13.459667000	-1.409457000	-0.000305000
6	-13.459693000	1.409621000	-0.000309000
6	-14.686035000	-0.733384000	-0.000299000
6	-14.686046000	0.733539000	-0.000301000
6	-15.908128000	-1.416273000	-0.000279000
6	-15.908164000	1.416401000	-0.000283000
6	-17.127993000	-0.733101000	-0.000257000
6	-17.128010000	0.733208000	-0.000259000
1	-8.537832000	-2.500961000	-0.000260000
1	-8.537840000	2.501142000	-0.000264000
1	-11.008981000	-2.496136000	-0.000294000
1	-11.009003000	2.496316000	-0.000299000
1	-13.460093000	-2.496273000	-0.000299000
1	-13.460133000	2.496436000	-0.000305000

1	-15.930579000	-2.501737000	-0.000272000
1	-15.930639000	2.501864000	-0.000279000
7	-18.274109000	-1.435179000	-0.000220000
7	-18.274158000	1.435252000	-0.000224000
6	-19.415269000	-0.732977000	-0.000180000
6	-19.415292000	0.733015000	-0.000182000
6	-20.640494000	-1.415713000	-0.000119000
6	-20.640547000	1.415704000	-0.000123000
6	-21.856620000	-0.732135000	-0.000054000
6	-21.856646000	0.732081000	-0.000056000
6	-23.090722000	-1.407904000	0.000022000
6	-23.090778000	1.407800000	0.000017000
6	-24.305072000	-0.729550000	0.000101000
6	-24.305101000	0.729397000	0.000098000
6	-25.545744000	-1.405992000	0.000190000
6	-25.545802000	1.405787000	0.000185000
6	-26.750554000	-0.727260000	0.000280000
6	-26.750584000	0.727004000	0.000277000
6	-28.008922000	-1.406465000	0.000379000
6	-28.008980000	1.406156000	0.000374000
6	-29.181440000	-0.714184000	0.000471000
6	-29.181470000	0.713826000	0.000469000
1	-20.618539000	-2.501223000	-0.000114000
1	-20.618634000	2.501215000	-0.000123000
1	-23.090605000	-2.494822000	0.000026000
1	-23.090706000	2.494717000	0.000018000
1	-25.546651000	-2.493300000	0.000194000
1	-25.546755000	2.493094000	0.000185000
1	-28.006477000	-2.492805000	0.000381000
1	-28.006582000	2.492496000	0.000372000
1	-30.128144000	-1.244870000	0.000547000
1	-30.128196000	1.244473000	0.000542000
7	18.165329000	1.356817000	0.000245000
7	18.165326000	-1.356850000	0.000241000
6	19.393334000	0.719768000	0.000166000
6	19.393332000	-0.719804000	0.000164000
6	20.579108000	1.402340000	0.000086000
6	20.579103000	-1.402380000	0.000081000
6	21.830166000	0.724663000	-0.000008000
6	21.830163000	-0.724708000	-0.000010000
6	23.041333000	1.401486000	-0.000104000
6	23.041328000	-1.401536000	-0.000110000
6	24.275366000	0.724256000	-0.000210000
6	24.275363000	-0.724311000	-0.000213000
6	25.503899000	1.401247000	-0.000319000
6	25.503894000	-1.401308000	-0.000324000
6	26.719202000	0.723006000	-0.000431000

6	26.719199000	-0.723071000	-0.000434000
6	27.972122000	1.402623000	-0.000545000
6	27.972116000	-1.402694000	-0.000551000
6	29.149604000	0.710977000	-0.000656000
6	29.149601000	-0.711053000	-0.000659000
1	27.969285000	2.489262000	-0.000543000
1	30.095062000	1.244129000	-0.000742000
1	30.095057000	-1.244209000	-0.000748000
1	27.969275000	-2.489332000	-0.000553000
1	25.504771000	-2.489025000	-0.000327000
1	25.504781000	2.488965000	-0.000318000
1	23.042042000	2.488974000	-0.000104000
1	23.042032000	-2.489024000	-0.000113000
1	20.570880000	2.489199000	0.000085000
1	20.570872000	-2.489240000	0.000077000
1	18.165291000	2.365468000	0.000238000
1	18.165286000	-2.365501000	0.000232000

Table S106: Coordinates of pT₄_3 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.000197000	-7.107452000	0.730269000
7	0.000174000	-5.957224000	1.434591000
6	0.000150000	-4.821318000	0.731446000
6	0.000150000	-4.821318000	-0.731446000
7	0.000174000	-5.957224000	-1.434591000
6	0.000197000	-7.107452000	-0.730269000
6	0.000091000	-2.375857000	-0.731043000
6	0.000091000	-2.375857000	0.731043000
6	0.000059000	-1.140354000	1.405024000
1	0.000059000	-1.140630000	2.492160000
6	0.000027000	0.077375000	0.730128000
6	0.000027000	0.077375000	-0.730128000
6	0.000059000	-1.140354000	-1.405024000
1	0.000059000	-1.140630000	-2.492160000
6	-0.000035000	2.531273000	-0.731012000
6	-0.000035000	2.531273000	0.731012000
6	-0.000064000	3.758616000	1.408910000
6	-0.000064000	3.758616000	-1.408910000
6	-0.000094000	4.979985000	-0.731750000
6	-0.000094000	4.979985000	0.731750000
1	-0.000062000	3.780659000	2.494912000
1	-0.000062000	3.780659000	-2.494912000
6	0.000225000	-9.549736000	0.729678000
6	0.000225000	-9.549736000	-0.729678000
6	0.000231000	-10.778416000	-1.404840000
6	0.000231000	-10.778416000	1.404840000

6	0.000234000	-11.998532000	-0.727484000
6	0.000234000	-11.998532000	0.727484000
1	0.000226000	-10.777961000	2.491985000
1	0.000226000	-10.777961000	-2.491985000
6	-0.000004000	1.310033000	1.404442000
6	-0.000004000	1.310033000	-1.404442000
6	0.000121000	-3.589726000	1.411739000
6	0.000121000	-3.589726000	-1.411739000
6	0.000212000	-8.325655000	1.411591000
6	0.000212000	-8.325655000	-1.411591000
6	0.000228000	-13.235275000	1.403381000
6	0.000228000	-13.235275000	-1.403381000
6	0.000219000	-14.445015000	0.726429000
6	0.000219000	-14.445015000	-0.726429000
6	0.000199000	-15.694618000	1.403682000
6	0.000199000	-15.694618000	-1.403682000
6	0.000176000	-16.881185000	0.720939000
6	0.000176000	-16.881185000	-0.720939000
1	0.000222000	-13.234797000	-2.490615000
1	0.000222000	-13.234797000	2.490615000
1	0.000207000	-8.303232000	-2.497352000
1	0.000207000	-8.303232000	2.497352000
1	0.000120000	-3.611379000	2.497547000
1	0.000120000	-3.611379000	-2.497547000
1	-0.000003000	1.310523000	2.491641000
1	-0.000003000	1.310523000	-2.491641000
1	0.000194000	-15.702861000	-2.490349000
1	0.000194000	-15.702861000	2.490349000
7	-0.000116000	6.123910000	-1.436687000
7	-0.000116000	6.123910000	1.436687000
6	-0.000139000	7.266310000	-0.731964000
6	-0.000139000	7.266310000	0.731964000
6	-0.000152000	8.489150000	-1.408880000
6	-0.000152000	8.489150000	1.408880000
6	-0.000167000	9.715312000	-0.731119000
6	-0.000167000	9.715312000	0.731119000
6	-0.000175000	10.937489000	-1.404303000
6	-0.000175000	10.937489000	1.404303000
6	-0.000182000	12.169591000	-0.730301000
6	-0.000182000	12.169591000	0.730301000
6	-0.000182000	13.387536000	-1.404923000
6	-0.000182000	13.387536000	1.404923000
6	-0.000181000	14.623355000	-0.731310000
6	-0.000181000	14.623355000	0.731310000
6	-0.000173000	15.836477000	-1.411809000
6	-0.000173000	15.836477000	1.411809000
6	-0.000164000	17.069626000	-0.732069000

6	-0.000164000	17.069626000	0.732069000
1	-0.000147000	8.467240000	-2.494887000
1	-0.000147000	8.467240000	2.494887000
1	-0.000170000	10.937005000	-2.491505000
1	-0.000170000	10.937005000	2.491505000
1	-0.000177000	13.387818000	-2.492054000
1	-0.000177000	13.387818000	2.492054000
1	-0.000167000	15.858008000	-2.497607000
1	-0.000167000	15.858008000	2.497607000
7	-0.000145000	18.203497000	-1.435088000
7	-0.000145000	18.203497000	1.435088000
6	-0.000126000	19.356108000	-0.730192000
6	-0.000126000	19.356108000	0.730192000
6	-0.000100000	20.571457000	-1.411800000
6	-0.000100000	20.571457000	1.411800000
6	-0.000072000	21.798567000	-0.729698000
6	-0.000072000	21.798567000	0.729698000
6	-0.000042000	23.023769000	-1.405498000
6	-0.000042000	23.023769000	1.405498000
6	-0.000008000	24.246861000	-0.727202000
6	-0.000008000	24.246861000	0.727202000
6	0.000029000	25.480750000	-1.403922000
6	0.000029000	25.480750000	1.403922000
6	0.000067000	26.691529000	-0.724876000
6	0.000067000	26.691529000	0.724876000
6	0.000110000	27.945931000	-1.404605000
6	0.000110000	27.945931000	1.404605000
6	0.000150000	29.121346000	-0.712059000
6	0.000150000	29.121346000	0.712059000
1	-0.000100000	20.548970000	-2.497509000
1	-0.000100000	20.548970000	2.497509000
1	-0.000043000	23.023612000	-2.492561000
1	-0.000043000	23.023612000	2.492561000
1	0.000026000	25.481598000	-2.491301000
1	0.000026000	25.481598000	2.491301000
1	0.000108000	27.943389000	-2.490963000
1	0.000108000	27.943389000	2.490963000
1	0.000182000	30.067311000	-1.244018000
1	0.000182000	30.067311000	1.244018000
7	0.000142000	-18.106531000	1.356588000
7	0.000142000	-18.106531000	-1.356588000
6	0.000108000	-19.335266000	0.719335000
6	0.000108000	-19.335266000	-0.719335000
6	0.000070000	-20.520421000	1.402875000
6	0.000070000	-20.520421000	-1.402875000
6	0.000025000	-21.770759000	0.724683000
6	0.000025000	-21.770759000	-0.724683000

6	-0.000022000	-22.982022000	1.401878000
6	-0.000022000	-22.982022000	-1.401878000
6	-0.000072000	-24.215388000	0.724341000
6	-0.000072000	-24.215388000	-0.724341000
6	-0.000124000	-25.443988000	1.401614000
6	-0.000124000	-25.443988000	-1.401614000
6	-0.000178000	-26.658820000	0.723140000
6	-0.000178000	-26.658820000	-0.723140000
6	-0.000235000	-27.911727000	1.403013000
6	-0.000235000	-27.911727000	-1.403013000
6	-0.000291000	-29.088785000	0.711094000
6	-0.000291000	-29.088785000	-0.711094000
1	-0.000237000	-27.908976000	2.489562000
1	-0.000334000	-30.034321000	1.243992000
1	-0.000334000	-30.034321000	-1.243992000
1	-0.000237000	-27.908976000	-2.489562000
1	-0.000127000	-25.444851000	-2.489238000
1	-0.000127000	-25.444851000	2.489238000
1	-0.000023000	-22.982687000	2.489275000
1	-0.000023000	-22.982687000	-2.489275000
1	0.000069000	-20.512035000	2.489652000
1	0.000069000	-20.512035000	-2.489652000
1	0.000139000	-18.106775000	2.365556000
1	0.000139000	-18.106775000	-2.365556000

Table S107: Coordinates of pT₄_4 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	7.182723000	0.730637000	0.000002000
7	6.047711000	1.435104000	0.000019000
6	4.897012000	0.728709000	-0.000006000
6	4.897012000	-0.728709000	-0.000039000
7	6.047711000	-1.435103000	-0.000064000
6	7.182723000	-0.730636000	-0.000049000
6	2.451388000	-0.728389000	-0.000028000
6	2.451388000	0.728390000	-0.000012000
6	1.226892000	1.403436000	-0.000010000
1	1.227266000	2.490615000	-0.000004000
6	0.000000000	0.727391000	-0.000016000
6	0.000000000	-0.727391000	-0.000017000
6	1.226892000	-1.403436000	-0.000026000
1	1.227266000	-2.490614000	-0.000032000
6	-2.451388000	-0.728389000	-0.000006000
6	-2.451388000	0.728390000	-0.000020000
6	-3.679128000	1.408280000	-0.000033000
6	-3.679128000	-1.408280000	0.000011000
6	-4.897012000	-0.728709000	0.000007000

6	-4.897012000	0.728709000	-0.000024000
1	-3.701532000	2.494191000	-0.000050000
1	-3.701532000	-2.494190000	0.000029000
6	9.632463000	0.729884000	0.000010000
6	9.632463000	-0.729883000	-0.000058000
6	10.864389000	-1.402493000	-0.000097000
6	10.864389000	1.402493000	0.000049000
6	12.088787000	-0.729342000	-0.000065000
6	12.088787000	0.729342000	0.000018000
1	10.863910000	2.489760000	0.000106000
1	10.863910000	-2.489759000	-0.000152000
6	-1.226892000	1.403436000	-0.000021000
6	-1.226892000	-1.403436000	-0.000008000
6	3.679128000	1.408281000	0.000002000
6	3.679128000	-1.408280000	-0.000044000
6	8.415279000	1.408079000	0.000035000
6	8.415279000	-1.408079000	-0.000082000
6	13.314130000	1.402587000	0.000062000
6	13.314130000	-1.402587000	-0.000108000
6	14.545641000	0.730387000	0.000025000
6	14.545641000	-0.730387000	-0.000069000
6	15.762289000	1.408441000	0.000076000
6	15.762289000	-1.408441000	-0.000117000
6	16.997158000	0.731805000	0.000035000
6	16.997158000	-0.731805000	-0.000070000
1	13.314433000	-2.489858000	-0.000173000
1	13.314434000	2.489858000	0.000128000
1	8.393679000	-2.494079000	-0.000126000
1	8.393679000	2.494079000	0.000080000
1	3.701532000	2.494191000	0.000021000
1	3.701532000	-2.494190000	-0.000062000
1	-1.227266000	2.490615000	-0.000026000
1	-1.227266000	-2.490614000	-0.000002000
1	15.783592000	-2.494474000	-0.000192000
1	15.783593000	2.494474000	0.000150000
7	-6.047711000	-1.435103000	0.000034000
7	-6.047711000	1.435104000	-0.000046000
6	-7.182723000	-0.730636000	0.000021000
6	-7.182723000	0.730637000	-0.000029000
6	-8.415279000	-1.408079000	0.000057000
6	-8.415279000	1.408079000	-0.000058000
6	-9.632463000	-0.729883000	0.000036000
6	-9.632463000	0.729884000	-0.000032000
6	-10.864389000	-1.402493000	0.000077000
6	-10.864389000	1.402493000	-0.000067000
6	-12.088787000	-0.729342000	0.000049000
6	-12.088787000	0.729342000	-0.000032000

6	-13.314130000	-1.402587000	0.000096000
6	-13.314130000	1.402587000	-0.000073000
6	-14.545641000	-0.730387000	0.000062000
6	-14.545641000	0.730387000	-0.000032000
6	-15.762289000	-1.408441000	0.000114000
6	-15.762289000	1.408441000	-0.000077000
6	-16.997158000	-0.731805000	0.000077000
6	-16.997158000	0.731805000	-0.000029000
1	-8.393679000	-2.494079000	0.000101000
1	-8.393679000	2.494079000	-0.000102000
1	-10.863910000	-2.489759000	0.000133000
1	-10.863910000	2.489759000	-0.000122000
1	-13.314433000	-2.489858000	0.000161000
1	-13.314434000	2.489858000	-0.000138000
1	-15.783592000	-2.494474000	0.000188000
1	-15.783593000	2.494474000	-0.000151000
7	-18.128518000	-1.436141000	0.000135000
7	-18.128518000	1.436141000	-0.000082000
6	-19.283908000	-0.729173000	0.000088000
6	-19.283908000	0.729173000	-0.000028000
6	-20.496129000	-1.408863000	0.000151000
6	-20.496129000	1.408862000	-0.000084000
6	-21.730119000	-0.728310000	0.000100000
6	-21.730119000	0.728310000	-0.000025000
6	-22.949040000	-1.403787000	0.000165000
6	-22.949040000	1.403787000	-0.000084000
6	-24.179783000	-0.725511000	0.000110000
6	-24.179783000	0.725510000	-0.000022000
6	-25.407214000	-1.402322000	0.000175000
6	-25.407214000	1.402321000	-0.000084000
6	-26.624299000	-0.722741000	0.000114000
6	-26.624299000	0.722741000	-0.000022000
6	-27.874221000	-1.403027000	0.000179000
6	-27.874221000	1.403027000	-0.000088000
6	-29.052859000	-0.709941000	0.000112000
6	-29.052859000	0.709941000	-0.000026000
1	-20.473549000	-2.494758000	0.000241000
1	-20.473549000	2.494758000	-0.000173000
1	-22.948903000	-2.490942000	0.000261000
1	-22.948903000	2.490941000	-0.000179000
1	-25.408108000	-2.489719000	0.000275000
1	-25.408108000	2.489719000	-0.000184000
1	-27.871666000	-2.489350000	0.000283000
1	-27.871667000	2.489349000	-0.000191000
1	-29.998010000	-1.243196000	0.000162000
1	-29.998010000	1.243195000	-0.000079000
7	18.128518000	1.436141000	0.000092000
7	18.128518000	-1.436141000	-0.000126000

6	19.283908000	0.729173000	0.000043000
6	19.283908000	-0.729173000	-0.000073000
6	20.496129000	1.408862000	0.000105000
6	20.496129000	-1.408863000	-0.000130000
6	21.730119000	0.728310000	0.000053000
6	21.730119000	-0.728310000	-0.000073000
6	22.949040000	1.403787000	0.000116000
6	22.949040000	-1.403787000	-0.000133000
6	24.179783000	0.725510000	0.000059000
6	24.179783000	-0.725511000	-0.000073000
6	25.407214000	1.402321000	0.000124000
6	25.407214000	-1.402322000	-0.000136000
6	26.624299000	0.722741000	0.000062000
6	26.624299000	-0.722741000	-0.000074000
6	27.874221000	1.403027000	0.000126000
6	27.874221000	-1.403027000	-0.000141000
6	29.052859000	0.709941000	0.000058000
6	29.052859000	-0.709941000	-0.000079000
1	27.871667000	2.489349000	0.000230000
1	29.998010000	1.243195000	0.000108000
1	29.998010000	-1.243196000	-0.000133000
1	27.871666000	-2.489350000	-0.000244000
1	25.408108000	-2.489719000	-0.000236000
1	25.408108000	2.489719000	0.000224000
1	22.948903000	2.490941000	0.000212000
1	22.948903000	-2.490942000	-0.000229000
1	20.473549000	2.494758000	0.000195000
1	20.473549000	-2.494758000	-0.000220000

Table S108: Coordinates of pT₅_1 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.719615000	1.315669000
7	0.000000000	1.356900000	0.088516000
6	0.000000000	0.718738000	-1.140349000
6	0.000000000	-0.718738000	-1.140349000
7	0.000000000	-1.356900000	0.088516000
6	0.000000000	-0.719615000	1.315669000
6	0.000000000	-0.723794000	-3.577146000
6	0.000000000	0.723794000	-3.577146000
6	0.000000000	1.400383000	-4.790996000
1	0.000000000	2.488067000	-4.791412000
6	0.000000000	0.723755000	-6.022715000
6	0.000000000	-0.723755000	-6.022715000
6	0.000000000	-1.400383000	-4.790996000
1	0.000000000	2.365451000	0.088330000
1	0.000000000	-2.365451000	0.088330000

1	0.000000000	-2.488067000	-4.791412000
6	0.000000000	-0.723903000	-8.468396000
6	0.000000000	0.723903000	-8.468396000
6	0.000000000	1.401387000	-9.718704000
6	0.000000000	-1.401387000	-9.718704000
6	0.000000000	-0.719113000	-10.905646000
6	0.000000000	0.719113000	-10.905646000
1	0.000000000	2.488397000	-9.727073000
1	0.000000000	-2.488397000	-9.727073000
6	0.000000000	0.724262000	3.752971000
6	0.000000000	-0.724262000	3.752971000
6	0.000000000	-1.400730000	4.966032000
6	0.000000000	1.400730000	4.966032000
6	0.000000000	-0.724022000	6.198565000
6	0.000000000	0.724022000	6.198565000
1	0.000000000	2.488345000	4.966526000
1	0.000000000	-2.488345000	4.966526000
6	0.000000000	1.400385000	-7.254750000
6	0.000000000	-1.400385000	-7.254750000
6	0.000000000	1.401391000	-2.326937000
6	0.000000000	-1.401391000	-2.326937000
6	0.000000000	1.401737000	2.502751000
6	0.000000000	-1.401737000	2.502751000
6	0.000000000	1.400787000	7.429123000
6	0.000000000	-1.400787000	7.429123000
6	0.000000000	0.723967000	8.643745000
6	0.000000000	-0.723967000	8.643745000
6	0.000000000	1.402032000	9.892496000
6	0.000000000	-1.402032000	9.892496000
6	0.000000000	0.718266000	11.079082000
6	0.000000000	-0.718266000	11.079082000
1	0.000000000	-2.488380000	7.428762000
1	0.000000000	2.488380000	7.428762000
1	0.000000000	-2.488666000	2.494487000
1	0.000000000	2.488666000	2.494487000
1	0.000000000	2.488411000	-2.318475000
1	0.000000000	-2.488411000	-2.318475000
1	0.000000000	2.488064000	-7.254304000
1	0.000000000	-2.488064000	-7.254304000
1	0.000000000	-2.488962000	9.901147000
1	0.000000000	2.488962000	9.901147000
7	0.000000000	-1.356953000	-12.133689000
7	0.000000000	1.356953000	-12.133689000
6	0.000000000	-0.719068000	-13.361887000
6	0.000000000	0.719068000	-13.361887000
6	0.000000000	-1.401383000	-14.548746000
6	0.000000000	1.401383000	-14.548746000

6	0.000000000	-0.723893000	-15.799090000
6	0.000000000	0.723893000	-15.799090000
6	0.000000000	-1.400388000	-17.012704000
6	0.000000000	1.400388000	-17.012704000
6	0.000000000	-0.723751000	-18.244747000
6	0.000000000	0.723751000	-18.244747000
6	0.000000000	-1.400396000	-19.476436000
6	0.000000000	1.400396000	-19.476436000
6	0.000000000	-0.723794000	-20.690280000
6	0.000000000	0.723794000	-20.690280000
6	0.000000000	-1.401408000	-21.940451000
6	0.000000000	1.401408000	-21.940451000
6	0.000000000	-0.718714000	-23.126996000
6	0.000000000	0.718714000	-23.126996000
1	0.000000000	-2.365458000	-12.133706000
1	0.000000000	2.365458000	-12.133706000
1	0.000000000	-2.488396000	-14.540370000
1	0.000000000	2.488396000	-14.540370000
1	0.000000000	-2.488067000	-17.013154000
1	0.000000000	2.488067000	-17.013154000
1	0.000000000	-2.488074000	-19.476030000
1	0.000000000	2.488074000	-19.476030000
1	0.000000000	-2.488416000	-21.948924000
1	0.000000000	2.488416000	-21.948924000
7	0.000000000	-1.356881000	-24.355807000
7	0.000000000	1.356881000	-24.355807000
6	0.000000000	-0.720100000	-25.583103000
6	0.000000000	0.720100000	-25.583103000
6	0.000000000	-1.402195000	-26.769401000
6	0.000000000	1.402195000	-26.769401000
6	0.000000000	-0.724744000	-28.020595000
6	0.000000000	0.724744000	-28.020595000
6	0.000000000	-1.401359000	-29.231808000
6	0.000000000	1.401359000	-29.231808000
6	0.000000000	-0.724283000	-30.466142000
6	0.000000000	0.724283000	-30.466142000
6	0.000000000	-1.401128000	-31.694633000
6	0.000000000	1.401128000	-31.694633000
6	0.000000000	-0.722996000	-32.910207000
6	0.000000000	0.722996000	-32.910207000
6	0.000000000	-1.402480000	-34.163109000
6	0.000000000	1.402480000	-34.163109000
6	0.000000000	-0.710980000	-35.340839000
6	0.000000000	0.710980000	-35.340839000
1	0.000000000	-2.365451000	-24.355563000
1	0.000000000	2.365451000	-24.355563000
1	0.000000000	-2.489091000	-26.761261000

1	0.000000000	2.489091000	-26.761261000
1	0.000000000	-2.488891000	-29.232542000
1	0.000000000	2.488891000	-29.232542000
1	0.000000000	-2.488894000	-31.695498000
1	0.000000000	2.488894000	-31.695498000
1	0.000000000	-2.489170000	-34.160163000
1	0.000000000	2.489170000	-34.160163000
1	0.000000000	-1.244242000	-36.286273000
1	0.000000000	1.244242000	-36.286273000
7	0.000000000	1.356246000	12.307974000
7	0.000000000	-1.356246000	12.307974000
6	0.000000000	0.722693000	13.533990000
6	0.000000000	-0.722693000	13.533990000
6	0.000000000	1.404857000	14.718972000
6	0.000000000	-1.404857000	14.718972000
6	0.000000000	0.728547000	15.971525000
6	0.000000000	-0.728547000	15.971525000
6	0.000000000	1.404764000	17.176961000
6	0.000000000	-1.404764000	17.176961000
6	0.000000000	0.729645000	18.419280000
6	0.000000000	-0.729645000	18.419280000
6	0.000000000	1.406586000	19.632713000
6	0.000000000	-1.406586000	19.632713000
6	0.000000000	0.731889000	20.868720000
6	0.000000000	-0.731889000	20.868720000
6	0.000000000	1.414426000	22.084428000
6	0.000000000	-1.414426000	22.084428000
6	0.000000000	0.732696000	23.310590000
6	0.000000000	-0.732696000	23.310590000
1	0.000000000	2.500062000	22.106323000
1	0.000000000	-2.500062000	22.106323000
1	0.000000000	-2.493674000	19.633182000
1	0.000000000	2.493674000	19.633182000
1	0.000000000	2.492023000	17.177461000
1	0.000000000	-2.492023000	17.177461000
1	0.000000000	2.491592000	14.710562000
1	0.000000000	-2.491592000	14.710562000
1	0.000000000	2.365197000	12.307086000
1	0.000000000	-2.365197000	12.307086000
7	0.000000000	1.434467000	24.452321000
7	0.000000000	-1.434467000	24.452321000
6	0.000000000	0.731528000	25.597882000
6	0.000000000	-0.731528000	25.597882000
6	0.000000000	1.414205000	26.820156000
6	0.000000000	-1.414205000	26.820156000
6	0.000000000	0.731320000	28.039236000
6	0.000000000	-0.731320000	28.039236000

6	0.000000000	1.407049000	29.271715000
6	0.000000000	-1.407049000	29.271715000
6	0.000000000	0.728956000	30.487731000
6	0.000000000	-0.728956000	30.487731000
6	0.000000000	1.405274000	31.727641000
6	0.000000000	-1.405274000	31.727641000
6	0.000000000	0.726743000	32.933375000
6	0.000000000	-0.726743000	32.933375000
6	0.000000000	1.405780000	34.191475000
6	0.000000000	-1.405780000	34.191475000
6	0.000000000	0.713759000	35.364571000
6	0.000000000	-0.713759000	35.364571000
1	0.000000000	2.499827000	26.797995000
1	0.000000000	-2.499827000	26.797995000
1	0.000000000	2.494082000	29.271590000
1	0.000000000	-2.494082000	29.271590000
1	0.000000000	2.492684000	31.728510000
1	0.000000000	-2.492684000	31.728510000
1	0.000000000	2.492212000	34.188883000
1	0.000000000	1.244713000	36.311182000
1	0.000000000	-1.244713000	36.311182000
1	0.000000000	-2.492212000	34.188883000

Table S109: Coordinates of pT₅_2 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.722882000	1.392383000
7	0.000000000	1.356122000	0.166621000
6	0.000000000	0.718285000	-1.062116000
6	0.000000000	-0.718285000	-1.062116000
7	0.000000000	-1.356122000	0.166621000
6	0.000000000	-0.722882000	1.392383000
6	0.000000000	-0.724061000	-3.497144000
6	0.000000000	0.724061000	-3.497144000
6	0.000000000	1.400929000	-4.711836000
1	0.000000000	2.488500000	-4.712194000
6	0.000000000	0.724115000	-5.942181000
6	0.000000000	-0.724115000	-5.942181000
6	0.000000000	-1.400929000	-4.711836000
1	0.000000000	2.365163000	0.165701000
1	0.000000000	-2.365163000	0.165701000
1	0.000000000	-2.488500000	-4.712194000
6	0.000000000	-0.724347000	-8.387650000
6	0.000000000	0.724347000	-8.387650000
6	0.000000000	1.401876000	-9.637725000
6	0.000000000	-1.401876000	-9.637725000
6	0.000000000	-0.719666000	-10.824749000

6	0.000000000	0.719666000	-10.824749000
1	0.000000000	2.488791000	-9.645984000
1	0.000000000	-2.488791000	-9.645984000
6	0.000000000	0.728836000	3.829621000
6	0.000000000	-0.728836000	3.829621000
6	0.000000000	-1.405069000	5.034902000
6	0.000000000	1.405069000	5.034902000
6	0.000000000	-0.730020000	6.277288000
6	0.000000000	0.730020000	6.277288000
1	0.000000000	2.492280000	5.035390000
1	0.000000000	-2.492280000	5.035390000
6	0.000000000	1.400870000	-7.174680000
6	0.000000000	-1.400870000	-7.174680000
6	0.000000000	1.402234000	-2.248735000
6	0.000000000	-1.402234000	-2.248735000
6	0.000000000	1.405175000	2.577358000
6	0.000000000	-1.405175000	2.577358000
6	0.000000000	1.406985000	7.490153000
6	0.000000000	-1.406985000	7.490153000
6	0.000000000	0.732437000	8.726766000
6	0.000000000	-0.732437000	8.726766000
6	0.000000000	1.415112000	9.941189000
6	0.000000000	-1.415112000	9.941189000
6	0.000000000	0.733775000	11.168997000
6	0.000000000	-0.733775000	11.168997000
1	0.000000000	-2.494033000	7.490607000
1	0.000000000	2.494033000	7.490607000
1	0.000000000	-2.491883000	2.568933000
1	0.000000000	2.491883000	2.568933000
1	0.000000000	2.489145000	-2.240081000
1	0.000000000	-2.489145000	-2.240081000
1	0.000000000	2.488439000	-7.174179000
1	0.000000000	-2.488439000	-7.174179000
1	0.000000000	-2.500711000	9.962931000
1	0.000000000	2.500711000	9.962931000
7	0.000000000	-1.356853000	-12.051802000
7	0.000000000	1.356853000	-12.051802000
6	0.000000000	-0.718814000	-13.280541000
6	0.000000000	0.718814000	-13.280541000
6	0.000000000	-1.401552000	-14.467053000
6	0.000000000	1.401552000	-14.467053000
6	0.000000000	-0.723876000	-15.717158000
6	0.000000000	0.723876000	-15.717158000
6	0.000000000	-1.400526000	-16.930845000
6	0.000000000	1.400526000	-16.930845000
6	0.000000000	-0.723798000	-18.162568000
6	0.000000000	0.723798000	-18.162568000

6	0.000000000	-1.400528000	-19.394348000
6	0.000000000	1.400528000	-19.394348000
6	0.000000000	-0.723895000	-20.607992000
6	0.000000000	0.723895000	-20.607992000
6	0.000000000	-1.401549000	-21.858089000
6	0.000000000	1.401549000	-21.858089000
6	0.000000000	-0.718900000	-23.044680000
6	0.000000000	0.718900000	-23.044680000
1	0.000000000	-2.365449000	-12.051984000
1	0.000000000	2.365449000	-12.051984000
1	0.000000000	-2.488539000	-14.458611000
1	0.000000000	2.488539000	-14.458611000
1	0.000000000	-2.488172000	-16.931278000
1	0.000000000	2.488172000	-16.931278000
1	0.000000000	-2.488169000	-19.393923000
1	0.000000000	2.488169000	-19.393923000
1	0.000000000	-2.488520000	-21.866511000
1	0.000000000	2.488520000	-21.866511000
7	0.000000000	-1.356863000	-24.273096000
7	0.000000000	1.356863000	-24.273096000
6	0.000000000	-0.719995000	-25.500653000
6	0.000000000	0.719995000	-25.500653000
6	0.000000000	-1.402234000	-26.686765000
6	0.000000000	1.402234000	-26.686765000
6	0.000000000	-0.724715000	-27.937936000
6	0.000000000	0.724715000	-27.937936000
6	0.000000000	-1.401397000	-29.149120000
6	0.000000000	1.401397000	-29.149120000
6	0.000000000	-0.724272000	-30.383366000
6	0.000000000	0.724272000	-30.383366000
6	0.000000000	-1.401166000	-31.611866000
6	0.000000000	1.401166000	-31.611866000
6	0.000000000	-0.723000000	-32.827352000
6	0.000000000	0.723000000	-32.827352000
6	0.000000000	-1.402527000	-34.080262000
6	0.000000000	1.402527000	-34.080262000
6	0.000000000	-0.710985000	-35.257906000
6	0.000000000	0.710985000	-35.257906000
1	0.000000000	-2.365458000	-24.272921000
1	0.000000000	2.365458000	-24.272921000
1	0.000000000	-2.489123000	-26.678604000
1	0.000000000	2.489123000	-26.678604000
1	0.000000000	-2.488916000	-29.149855000
1	0.000000000	2.488916000	-29.149855000
1	0.000000000	-2.488917000	-31.612735000
1	0.000000000	2.488917000	-31.612735000
1	0.000000000	-2.489202000	-34.077335000

1	0.000000000	2.489202000	-34.077335000
1	0.000000000	-1.244190000	-36.203358000
1	0.000000000	1.244190000	-36.203358000
7	0.000000000	1.435358000	12.308140000
7	0.000000000	-1.435358000	12.308140000
6	0.000000000	0.732438000	13.456723000
6	0.000000000	-0.732438000	13.456723000
6	0.000000000	1.415470000	14.674502000
6	0.000000000	-1.415470000	14.674502000
6	0.000000000	0.733204000	15.899017000
6	0.000000000	-0.733204000	15.899017000
6	0.000000000	1.409365000	17.123496000
6	0.000000000	-1.409365000	17.123496000
6	0.000000000	0.732219000	18.349642000
6	0.000000000	-0.732219000	18.349642000
6	0.000000000	1.409520000	19.573895000
6	0.000000000	-1.409520000	19.573895000
6	0.000000000	0.733467000	20.800273000
6	0.000000000	-0.733467000	20.800273000
6	0.000000000	1.416297000	22.022410000
6	0.000000000	-1.416297000	22.022410000
6	0.000000000	0.733145000	23.242279000
6	0.000000000	-0.733145000	23.242279000
1	0.000000000	2.501767000	22.044839000
1	0.000000000	-2.501767000	22.044839000
1	0.000000000	-2.496342000	19.574295000
1	0.000000000	2.496342000	19.574295000
1	0.000000000	2.496206000	17.123157000
1	0.000000000	-2.496206000	17.123157000
1	0.000000000	2.500991000	14.651937000
1	0.000000000	-2.500991000	14.651937000
7	0.000000000	1.435211000	24.388464000
7	0.000000000	-1.435211000	24.388464000
6	0.000000000	0.732980000	25.529573000
6	0.000000000	-0.732980000	25.529573000
6	0.000000000	1.415669000	26.754900000
6	0.000000000	-1.415669000	26.754900000
6	0.000000000	0.732111000	27.970993000
6	0.000000000	-0.732111000	27.970993000
6	0.000000000	1.407855000	29.205159000
6	0.000000000	-1.407855000	29.205159000
6	0.000000000	0.729483000	30.419467000
6	0.000000000	-0.729483000	30.419467000
6	0.000000000	1.405884000	31.660207000
6	0.000000000	-1.405884000	31.660207000
6	0.000000000	0.727146000	32.864980000
6	0.000000000	-0.727146000	32.864980000

6	0.000000000	1.406314000	34.123402000
6	0.000000000	-1.406314000	34.123402000
6	0.000000000	0.714033000	35.295898000
6	0.000000000	-0.714033000	35.295898000
1	0.000000000	2.501189000	26.732913000
1	0.000000000	-2.501189000	26.732913000
1	0.000000000	2.494779000	29.205023000
1	0.000000000	-2.494779000	29.205023000
1	0.000000000	2.493199000	31.661083000
1	0.000000000	-2.493199000	31.661083000
1	0.000000000	2.492663000	34.120895000
1	0.000000000	1.244652000	36.242643000
1	0.000000000	-1.244652000	36.242643000
1	0.000000000	-2.492663000	34.120895000

Table S110: Coordinates of pT₅_3 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.732491000	1.309664000
7	0.000000000	1.435413000	0.160954000
6	0.000000000	0.733859000	-0.978003000
6	0.000000000	-0.733859000	-0.978003000
7	0.000000000	-1.435413000	0.160954000
6	0.000000000	-0.732491000	1.309664000
6	0.000000000	-0.732508000	-3.420142000
6	0.000000000	0.732508000	-3.420142000
6	0.000000000	1.407067000	-4.656749000
1	0.000000000	2.494091000	-4.656295000
6	0.000000000	0.730043000	-5.869531000
6	0.000000000	-0.730043000	-5.869531000
6	0.000000000	-1.407067000	-4.656749000
1	0.000000000	-2.494091000	-4.656295000
6	0.000000000	-0.728877000	-8.317088000
6	0.000000000	0.728877000	-8.317088000
6	0.000000000	1.405256000	-9.569294000
6	0.000000000	-1.405256000	-9.569294000
6	0.000000000	-0.722894000	-10.754164000
6	0.000000000	0.722894000	-10.754164000
1	0.000000000	2.491942000	-9.577719000
1	0.000000000	-2.491942000	-9.577719000
6	0.000000000	0.733335000	3.751893000
6	0.000000000	-0.733335000	3.751893000
6	0.000000000	-1.409607000	4.975871000
6	0.000000000	1.409607000	4.975871000
6	0.000000000	-0.732466000	6.202526000
6	0.000000000	0.732466000	6.202526000
1	0.000000000	2.496392000	4.975529000

1	0.000000000	-2.496392000	4.975529000
6	0.000000000	1.405145000	-7.111872000
6	0.000000000	-1.405145000	-7.111872000
6	0.000000000	1.415236000	-2.205860000
6	0.000000000	-1.415236000	-2.205860000
6	0.000000000	1.415624000	2.527129000
6	0.000000000	-1.415624000	2.527129000
6	0.000000000	1.409850000	7.425901000
6	0.000000000	-1.409850000	7.425901000
6	0.000000000	0.733880000	8.653271000
6	0.000000000	-0.733880000	8.653271000
6	0.000000000	1.416966000	9.873822000
6	0.000000000	-1.416966000	9.873822000
6	0.000000000	0.734093000	11.095655000
6	0.000000000	-0.734093000	11.095655000
1	0.000000000	-2.496654000	7.426300000
1	0.000000000	2.496654000	7.426300000
1	0.000000000	-2.501152000	2.504540000
1	0.000000000	2.501152000	2.504540000
1	0.000000000	2.500814000	-2.184117000
1	0.000000000	-2.500814000	-2.184117000
1	0.000000000	2.492342000	-7.111384000
1	0.000000000	-2.492342000	-7.111384000
1	0.000000000	-2.502418000	9.896099000
1	0.000000000	2.502418000	9.896099000
7	0.000000000	-1.356153000	-11.979972000
7	0.000000000	1.356153000	-11.979972000
6	0.000000000	-0.718413000	-13.208515000
6	0.000000000	0.718413000	-13.208515000
6	0.000000000	-1.402374000	-14.395083000
6	0.000000000	1.402374000	-14.395083000
6	0.000000000	-0.724128000	-15.643458000
6	0.000000000	0.724128000	-15.643458000
6	0.000000000	-1.401061000	-16.857953000
6	0.000000000	1.401061000	-16.857953000
6	0.000000000	-0.724135000	-18.088350000
6	0.000000000	0.724135000	-18.088350000
6	0.000000000	-1.400997000	-19.320595000
6	0.000000000	1.400997000	-19.320595000
6	0.000000000	-0.724297000	-20.533551000
6	0.000000000	0.724297000	-20.533551000
6	0.000000000	-1.402003000	-21.783487000
6	0.000000000	1.402003000	-21.783487000
6	0.000000000	-0.719408000	-22.970099000
6	0.000000000	0.719408000	-22.970099000
1	0.000000000	-2.365222000	-11.980869000
1	0.000000000	2.365222000	-11.980869000

1	0.000000000	-2.489258000	-14.386461000
1	0.000000000	2.489258000	-14.386461000
1	0.000000000	-2.488599000	-16.858336000
1	0.000000000	2.488599000	-16.858336000
1	0.000000000	-2.488535000	-19.320116000
1	0.000000000	2.488535000	-19.320116000
1	0.000000000	-2.488888000	-21.791820000
1	0.000000000	2.488888000	-21.791820000
7	0.000000000	-1.356798000	-24.197632000
7	0.000000000	1.356798000	-24.197632000
6	0.000000000	-0.719781000	-25.425672000
6	0.000000000	0.719781000	-25.425672000
6	0.000000000	-1.402390000	-26.611418000
6	0.000000000	1.402390000	-26.611418000
6	0.000000000	-0.724680000	-27.862428000
6	0.000000000	0.724680000	-27.862428000
6	0.000000000	-1.401529000	-29.073598000
6	0.000000000	1.401529000	-29.073598000
6	0.000000000	-0.724275000	-30.307585000
6	0.000000000	0.724275000	-30.307585000
6	0.000000000	-1.401292000	-31.536131000
6	0.000000000	1.401292000	-31.536131000
6	0.000000000	-0.723035000	-32.751386000
6	0.000000000	0.723035000	-32.751386000
6	0.000000000	-1.402674000	-34.004324000
6	0.000000000	1.402674000	-34.004324000
6	0.000000000	-0.711019000	-35.181760000
6	0.000000000	0.711019000	-35.181760000
1	0.000000000	-2.365476000	-24.197604000
1	0.000000000	2.365476000	-24.197604000
1	0.000000000	-2.489251000	-26.603207000
1	0.000000000	2.489251000	-26.603207000
1	0.000000000	-2.489014000	-29.074325000
1	0.000000000	2.489014000	-29.074325000
1	0.000000000	-2.489006000	-31.536996000
1	0.000000000	2.489006000	-31.536996000
1	0.000000000	-2.489312000	-34.001434000
1	0.000000000	2.489312000	-34.001434000
1	0.000000000	-1.244107000	-36.127250000
1	0.000000000	1.244107000	-36.127250000
7	0.000000000	1.435915000	12.239061000
7	0.000000000	-1.435915000	12.239061000
6	0.000000000	0.733623000	13.383334000
6	0.000000000	-0.733623000	13.383334000
6	0.000000000	1.416840000	14.604142000
6	0.000000000	-1.416840000	14.604142000
6	0.000000000	0.733767000	15.825650000

6	0.000000000	-0.733767000	15.825650000
6	0.000000000	1.410044000	17.051935000
6	0.000000000	-1.410044000	17.051935000
6	0.000000000	0.732495000	18.276258000
6	0.000000000	-0.732495000	18.276258000
6	0.000000000	1.409983000	19.501560000
6	0.000000000	-1.409983000	19.501560000
6	0.000000000	0.733599000	20.726761000
6	0.000000000	-0.733599000	20.726761000
6	0.000000000	1.416596000	21.949559000
6	0.000000000	-1.416596000	21.949559000
6	0.000000000	0.733066000	23.168560000
6	0.000000000	-0.733066000	23.168560000
1	0.000000000	2.502023000	21.972105000
1	0.000000000	-2.502023000	21.972105000
1	0.000000000	-2.496734000	19.501953000
1	0.000000000	2.496734000	19.501953000
1	0.000000000	2.496792000	17.051574000
1	0.000000000	-2.496792000	17.051574000
1	0.000000000	2.502267000	14.581707000
1	0.000000000	-2.502267000	14.581707000
7	0.000000000	1.435317000	24.315220000
7	0.000000000	-1.435317000	24.315220000
6	0.000000000	0.733293000	25.455716000
6	0.000000000	-0.733293000	25.455716000
6	0.000000000	1.416039000	26.681402000
6	0.000000000	-1.416039000	26.681402000
6	0.000000000	0.732278000	27.896970000
6	0.000000000	-0.732278000	27.896970000
6	0.000000000	1.408067000	29.131340000
6	0.000000000	-1.408067000	29.131340000
6	0.000000000	0.729593000	30.345334000
6	0.000000000	-0.729593000	30.345334000
6	0.000000000	1.406056000	31.586150000
6	0.000000000	-1.406056000	31.586150000
6	0.000000000	0.727235000	32.790729000
6	0.000000000	-0.727235000	32.790729000
6	0.000000000	1.406484000	34.049159000
6	0.000000000	-1.406484000	34.049159000
6	0.000000000	0.714093000	35.221485000
6	0.000000000	-0.714093000	35.221485000
1	0.000000000	2.501522000	26.659454000
1	0.000000000	-2.501522000	26.659454000
1	0.000000000	2.494951000	29.131198000
1	0.000000000	-2.494951000	29.131198000
1	0.000000000	2.493334000	31.587025000
1	0.000000000	-2.493334000	31.587025000

1	0.000000000	2.492798000	34.046686000
1	0.000000000	1.244599000	36.168268000
1	0.000000000	-1.244599000	36.168268000
1	0.000000000	-2.492798000	34.046686000

Table S111: Coordinates of pT₅_4 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.733681000	1.230293000
7	0.000000000	1.435969000	0.085924000
6	0.000000000	0.734159000	-1.057311000
6	0.000000000	-0.734159000	-1.057311000
7	0.000000000	-1.435969000	0.085924000
6	0.000000000	-0.733681000	1.230293000
6	0.000000000	-0.733924000	-3.499588000
6	0.000000000	0.733924000	-3.499588000
6	0.000000000	1.409987000	-4.726912000
1	0.000000000	2.496744000	-4.726512000
6	0.000000000	0.732475000	-5.950237000
6	0.000000000	-0.732475000	-5.950237000
6	0.000000000	-1.409987000	-4.726912000
1	0.000000000	-2.496744000	-4.726512000
6	0.000000000	-0.733372000	-8.400765000
6	0.000000000	0.733372000	-8.400765000
6	0.000000000	1.415824000	-9.625330000
6	0.000000000	-1.415824000	-9.625330000
6	0.000000000	-0.732517000	-10.842816000
6	0.000000000	0.732517000	-10.842816000
1	0.000000000	2.501303000	-9.647946000
1	0.000000000	-2.501303000	-9.647946000
6	0.000000000	0.733895000	3.672532000
6	0.000000000	-0.733895000	3.672532000
6	0.000000000	-1.410289000	4.898339000
6	0.000000000	1.410289000	4.898339000
6	0.000000000	-0.732706000	6.123149000
6	0.000000000	0.732706000	6.123149000
1	0.000000000	2.496997000	4.897975000
1	0.000000000	-2.496997000	4.897975000
6	0.000000000	1.409723000	-7.176772000
6	0.000000000	-1.409723000	-7.176772000
6	0.000000000	1.417139000	-2.279166000
6	0.000000000	-1.417139000	-2.279166000
6	0.000000000	1.417042000	2.450819000
6	0.000000000	-1.417042000	2.450819000
6	0.000000000	1.410328000	7.347583000
6	0.000000000	-1.410328000	7.347583000
6	0.000000000	0.733985000	8.573764000

6	0.000000000	-0.733985000	8.573764000
6	0.000000000	1.417267000	9.794982000
6	0.000000000	-1.417267000	9.794982000
6	0.000000000	0.733957000	11.015935000
6	0.000000000	-0.733957000	11.015935000
1	0.000000000	-2.497045000	7.347962000
1	0.000000000	2.497045000	7.347962000
1	0.000000000	-2.502452000	2.428349000
1	0.000000000	2.502452000	2.428349000
1	0.000000000	2.502552000	-2.256880000
1	0.000000000	-2.502552000	-2.256880000
1	0.000000000	2.496509000	-7.177115000
1	0.000000000	-2.496509000	-7.177115000
1	0.000000000	-2.502663000	9.817385000
1	0.000000000	2.502663000	9.817385000
7	0.000000000	-1.435389000	-11.991388000
7	0.000000000	1.435389000	-11.991388000
6	0.000000000	-0.733823000	-13.130325000
6	0.000000000	0.733823000	-13.130325000
6	0.000000000	-1.415418000	-14.358096000
6	0.000000000	1.415418000	-14.358096000
6	0.000000000	-0.732468000	-15.572243000
6	0.000000000	0.732468000	-15.572243000
6	0.000000000	-1.407210000	-16.808826000
6	0.000000000	1.407210000	-16.808826000
6	0.000000000	-0.729999000	-18.021447000
6	0.000000000	0.729999000	-18.021447000
6	0.000000000	-1.405281000	-19.263804000
6	0.000000000	1.405281000	-19.263804000
6	0.000000000	-0.728773000	-20.468757000
6	0.000000000	0.728773000	-20.468757000
6	0.000000000	-1.405340000	-21.721131000
6	0.000000000	1.405340000	-21.721131000
6	0.000000000	-0.722687000	-22.905475000
6	0.000000000	0.722687000	-22.905475000
1	0.000000000	-2.500973000	-14.336332000
1	0.000000000	2.500973000	-14.336332000
1	0.000000000	-2.494206000	-16.808389000
1	0.000000000	2.494206000	-16.808389000
1	0.000000000	-2.492447000	-19.263332000
1	0.000000000	2.492447000	-19.263332000
1	0.000000000	-2.491992000	-21.729585000
1	0.000000000	2.491992000	-21.729585000
7	0.000000000	-1.356289000	-24.131765000
7	0.000000000	1.356289000	-24.131765000
6	0.000000000	-0.719361000	-25.359835000
6	0.000000000	0.719361000	-25.359835000
6	0.000000000	-1.403138000	-26.545409000

6	0.000000000	1.403138000	-26.545409000
6	0.000000000	-0.724821000	-27.795038000
6	0.000000000	0.724821000	-27.795038000
6	0.000000000	-1.402024000	-29.006800000
6	0.000000000	1.402024000	-29.006800000
6	0.000000000	-0.724467000	-30.239607000
6	0.000000000	0.724467000	-30.239607000
6	0.000000000	-1.401738000	-31.468616000
6	0.000000000	1.401738000	-31.468616000
6	0.000000000	-0.723283000	-32.683052000
6	0.000000000	0.723283000	-32.683052000
6	0.000000000	-1.403138000	-33.936216000
6	0.000000000	1.403138000	-33.936216000
6	0.000000000	-0.711238000	-35.113071000
6	0.000000000	0.711238000	-35.113071000
1	0.000000000	-2.365390000	-24.132460000
1	0.000000000	2.365390000	-24.132460000
1	0.000000000	-2.489901000	-26.537043000
1	0.000000000	2.489901000	-26.537043000
1	0.000000000	-2.489412000	-29.007496000
1	0.000000000	2.489412000	-29.007496000
1	0.000000000	-2.489360000	-31.469465000
1	0.000000000	2.489360000	-31.469465000
1	0.000000000	-2.489690000	-33.933390000
1	0.000000000	2.489690000	-33.933390000
1	0.000000000	-1.243996000	-36.058687000
1	0.000000000	1.243996000	-36.058687000
7	0.000000000	1.435982000	12.159833000
7	0.000000000	-1.435982000	12.159833000
6	0.000000000	0.733913000	13.303459000
6	0.000000000	-0.733913000	13.303459000
6	0.000000000	1.417213000	14.524691000
6	0.000000000	-1.417213000	14.524691000
6	0.000000000	0.733895000	15.745604000
6	0.000000000	-0.733895000	15.745604000
6	0.000000000	1.410228000	16.972174000
6	0.000000000	-1.410228000	16.972174000
6	0.000000000	0.732545000	18.196115000
6	0.000000000	-0.732545000	18.196115000
6	0.000000000	1.410110000	19.421586000
6	0.000000000	-1.410110000	19.421586000
6	0.000000000	0.733607000	20.646514000
6	0.000000000	-0.733607000	20.646514000
6	0.000000000	1.416671000	21.869433000
6	0.000000000	-1.416671000	21.869433000
6	0.000000000	0.733000000	23.088210000
6	0.000000000	-0.733000000	23.088210000

1	0.000000000	2.502081000	21.892020000
1	0.000000000	-2.502081000	21.892020000
1	0.000000000	-2.496839000	19.421965000
1	0.000000000	2.496839000	19.421965000
1	0.000000000	2.496942000	16.971801000
1	0.000000000	-2.496942000	16.971801000
1	0.000000000	2.502605000	14.502294000
1	0.000000000	-2.502605000	14.502294000
7	0.000000000	1.435344000	24.234951000
7	0.000000000	-1.435344000	24.234951000
6	0.000000000	0.733401000	25.375297000
6	0.000000000	-0.733401000	25.375297000
6	0.000000000	1.416169000	26.601052000
6	0.000000000	-1.416169000	26.601052000
6	0.000000000	0.732327000	27.816466000
6	0.000000000	-0.732327000	27.816466000
6	0.000000000	1.408137000	29.050872000
6	0.000000000	-1.408137000	29.050872000
6	0.000000000	0.729617000	30.264773000
6	0.000000000	-0.729617000	30.264773000
6	0.000000000	1.406112000	31.505590000
6	0.000000000	-1.406112000	31.505590000
6	0.000000000	0.727248000	32.710107000
6	0.000000000	-0.727248000	32.710107000
6	0.000000000	1.406539000	33.968524000
6	0.000000000	-1.406539000	33.968524000
6	0.000000000	0.714091000	35.140782000
6	0.000000000	-0.714091000	35.140782000
1	0.000000000	2.501635000	26.579127000
1	0.000000000	-2.501635000	26.579127000
1	0.000000000	2.495003000	29.050732000
1	0.000000000	-2.495003000	29.050732000
1	0.000000000	2.493372000	31.506468000
1	0.000000000	-2.493372000	31.506468000
1	0.000000000	2.492837000	33.966068000
1	0.000000000	1.244549000	36.087579000
1	0.000000000	-1.244549000	36.087579000
1	0.000000000	-2.492837000	33.966068000

Table S112: Coordinates of pT₅_5 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.730179000	-1.142594000
7	0.000000000	1.434485000	-0.000045000
6	0.000000000	0.730142000	1.142714000
6	0.000000000	-0.730142000	1.142714000
7	0.000000000	-1.434485000	-0.000045000

6	0.000000000	-0.730179000	-1.142594000
6	0.000000000	-0.729963000	3.586874000
6	0.000000000	0.729963000	3.586874000
6	0.000000000	1.404686000	4.818467000
1	0.000000000	2.491769000	4.818140000
6	0.000000000	0.729139000	6.038752000
6	0.000000000	-0.729139000	6.038752000
6	0.000000000	-1.404686000	4.818467000
1	0.000000000	-2.491769000	4.818140000
6	0.000000000	-0.730201000	8.491408000
6	0.000000000	0.730201000	8.491408000
6	0.000000000	1.408971000	9.719477000
6	0.000000000	-1.408971000	9.719477000
6	0.000000000	-0.730830000	10.938853000
6	0.000000000	0.730830000	10.938853000
1	0.000000000	2.494910000	9.741798000
1	0.000000000	-2.494910000	9.741798000
6	0.000000000	0.729972000	-3.586807000
6	0.000000000	-0.729972000	-3.586807000
6	0.000000000	-1.404698000	-4.818525000
6	0.000000000	1.404698000	-4.818525000
6	0.000000000	-0.729162000	-6.038720000
6	0.000000000	0.729162000	-6.038720000
1	0.000000000	2.491773000	-4.818081000
1	0.000000000	-2.491773000	-4.818081000
6	0.000000000	1.404368000	7.269949000
6	0.000000000	-1.404368000	7.269949000
6	0.000000000	1.410794000	2.367999000
6	0.000000000	-1.410794000	2.367999000
6	0.000000000	1.410802000	-2.368072000
6	0.000000000	-1.410802000	-2.368072000
6	0.000000000	1.404370000	-7.269997000
6	0.000000000	-1.404370000	-7.269997000
6	0.000000000	0.730214000	-8.491405000
6	0.000000000	-0.730214000	-8.491405000
6	0.000000000	1.408971000	-9.719513000
6	0.000000000	-1.408971000	-9.719513000
6	0.000000000	0.730837000	-10.938869000
6	0.000000000	-0.730837000	-10.938869000
1	0.000000000	-2.491515000	-7.270358000
1	0.000000000	2.491515000	-7.270358000
1	0.000000000	-2.496568000	-2.345905000
1	0.000000000	2.496568000	-2.345905000
1	0.000000000	2.496553000	2.345966000
1	0.000000000	-2.496553000	2.345966000
1	0.000000000	2.491504000	7.270406000
1	0.000000000	-2.491504000	7.270406000

1	0.000000000	-2.494919000	-9.741746000
1	0.000000000	2.494919000	-9.741746000
7	0.000000000	-1.436293000	12.085479000
7	0.000000000	1.436293000	12.085479000
6	0.000000000	-0.731599000	13.224759000
6	0.000000000	0.731599000	13.224759000
6	0.000000000	-1.408790000	14.451042000
6	0.000000000	1.408790000	14.451042000
6	0.000000000	-0.730780000	15.673935000
6	0.000000000	0.730780000	15.673935000
6	0.000000000	-1.403846000	16.899157000
6	0.000000000	1.403846000	16.899157000
6	0.000000000	-0.730026000	18.128765000
6	0.000000000	0.730026000	18.128765000
6	0.000000000	-1.404326000	19.348718000
6	0.000000000	1.404326000	19.348718000
6	0.000000000	-0.731033000	20.583356000
6	0.000000000	0.731033000	20.583356000
6	0.000000000	-1.410968000	21.797116000
6	0.000000000	1.410968000	21.797116000
6	0.000000000	-0.731948000	23.031017000
6	0.000000000	0.731948000	23.031017000
1	0.000000000	-2.494768000	14.429271000
1	0.000000000	2.494768000	14.429271000
1	0.000000000	-2.491033000	16.898708000
1	0.000000000	2.491033000	16.898708000
1	0.000000000	-2.491464000	19.349039000
1	0.000000000	2.491464000	19.349039000
1	0.000000000	-2.496812000	21.818632000
1	0.000000000	2.496812000	21.818632000
7	0.000000000	-1.435428000	24.163721000
7	0.000000000	1.435428000	24.163721000
6	0.000000000	-0.729836000	25.317310000
6	0.000000000	0.729836000	25.317310000
6	0.000000000	-1.411067000	26.531449000
6	0.000000000	1.411067000	26.531449000
6	0.000000000	-0.729247000	27.760626000
6	0.000000000	0.729247000	27.760626000
6	0.000000000	-1.405071000	28.983716000
6	0.000000000	1.405071000	28.983716000
6	0.000000000	-0.726643000	30.209158000
6	0.000000000	0.726643000	30.209158000
6	0.000000000	-1.403504000	31.440866000
6	0.000000000	1.403504000	31.440866000
6	0.000000000	-0.724184000	32.653608000
6	0.000000000	0.724184000	32.653608000
6	0.000000000	-1.404221000	33.906461000

6	0.000000000	1.404221000	33.906461000
6	0.000000000	-0.711367000	35.082804000
6	0.000000000	0.711367000	35.082804000
1	0.000000000	-2.496811000	26.508891000
1	0.000000000	2.496811000	26.508891000
1	0.000000000	-2.492126000	28.983598000
1	0.000000000	2.492126000	28.983598000
1	0.000000000	-2.490849000	31.441761000
1	0.000000000	2.490849000	31.441761000
1	0.000000000	-2.490528000	33.903955000
1	0.000000000	2.490528000	33.903955000
1	0.000000000	-1.243652000	36.028530000
1	0.000000000	1.243652000	36.028530000
7	0.000000000	1.436301000	-12.085505000
7	0.000000000	-1.436301000	-12.085505000
6	0.000000000	0.731618000	-13.224776000
6	0.000000000	-0.731618000	-13.224776000
6	0.000000000	1.408786000	-14.451051000
6	0.000000000	-1.408786000	-14.451051000
6	0.000000000	0.730786000	-15.673970000
6	0.000000000	-0.730786000	-15.673970000
6	0.000000000	1.403851000	-16.899155000
6	0.000000000	-1.403851000	-16.899155000
6	0.000000000	0.730026000	-18.128798000
6	0.000000000	-0.730026000	-18.128798000
6	0.000000000	1.404331000	-19.348718000
6	0.000000000	-1.404331000	-19.348718000
6	0.000000000	0.731029000	-20.583375000
6	0.000000000	-0.731029000	-20.583375000
6	0.000000000	1.410982000	-21.797127000
6	0.000000000	-1.410982000	-21.797127000
6	0.000000000	0.731936000	-23.031000000
6	0.000000000	-0.731936000	-23.031000000
1	0.000000000	2.496824000	-21.818622000
1	0.000000000	-2.496824000	-21.818622000
1	0.000000000	-2.491471000	-19.349038000
1	0.000000000	2.491471000	-19.349038000
1	0.000000000	2.491036000	-16.898697000
1	0.000000000	-2.491036000	-16.898697000
1	0.000000000	2.494767000	-14.429238000
1	0.000000000	-2.494767000	-14.429238000
7	0.000000000	1.435416000	-24.163741000
7	0.000000000	-1.435416000	-24.163741000
6	0.000000000	0.729853000	-25.317281000
6	0.000000000	-0.729853000	-25.317281000
6	0.000000000	1.411082000	-26.531465000
6	0.000000000	-1.411082000	-26.531465000

6	0.000000000	0.729259000	-27.760588000
6	0.000000000	-0.729259000	-27.760588000
6	0.000000000	1.405082000	-28.983724000
6	0.000000000	-1.405082000	-28.983724000
6	0.000000000	0.726657000	-30.209118000
6	0.000000000	-0.726657000	-30.209118000
6	0.000000000	1.403517000	-31.440866000
6	0.000000000	-1.403517000	-31.440866000
6	0.000000000	0.724203000	-32.653571000
6	0.000000000	-0.724203000	-32.653571000
6	0.000000000	1.404237000	-33.906450000
6	0.000000000	-1.404237000	-33.906450000
6	0.000000000	0.711388000	-35.082774000
6	0.000000000	-0.711388000	-35.082774000
1	0.000000000	2.496827000	-26.508883000
1	0.000000000	-2.496827000	-26.508883000
1	0.000000000	2.492138000	-28.983584000
1	0.000000000	-2.492138000	-28.983584000
1	0.000000000	2.490862000	-31.441746000
1	0.000000000	-2.490862000	-31.441746000
1	0.000000000	2.490544000	-33.903934000
1	0.000000000	1.243655000	-36.028509000
1	0.000000000	-1.243655000	-36.028509000
1	0.000000000	-2.490544000	-33.903934000

Table S113: Coordinates of pT₆_1 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.719630000	7.427564000
7	0.000000000	1.356878000	6.200479000
6	0.000000000	0.718685000	4.971523000
6	0.000000000	-0.718685000	4.971523000
7	0.000000000	-1.356878000	6.200479000
6	0.000000000	-0.719630000	7.427564000
6	0.000000000	-0.723777000	2.534731000
6	0.000000000	0.723777000	2.534731000
6	0.000000000	1.400346000	1.320837000
1	0.000000000	2.488035000	1.320430000
6	0.000000000	0.723744000	0.089139000
6	0.000000000	-0.723744000	0.089139000
6	0.000000000	-1.400346000	1.320837000
1	0.000000000	2.365427000	6.200276000

1	0.000000000	-2.365427000	6.200276000
1	0.000000000	-2.488035000	1.320430000
6	0.000000000	-0.723923000	-2.356604000
6	0.000000000	0.723923000	-2.356604000
6	0.000000000	1.401361000	-3.606924000
6	0.000000000	-1.401361000	-3.606924000
6	0.000000000	-0.719194000	-4.793977000
6	0.000000000	0.719194000	-4.793977000
1	0.000000000	2.488370000	-3.615272000
1	0.000000000	-2.488370000	-3.615272000
6	0.000000000	0.724264000	9.864909000
6	0.000000000	-0.724264000	9.864909000
6	0.000000000	-1.400725000	11.077975000
6	0.000000000	1.400725000	11.077975000
6	0.000000000	-0.724027000	12.310531000
6	0.000000000	0.724027000	12.310531000
1	0.000000000	2.488320000	11.078477000
1	0.000000000	-2.488320000	11.078477000
6	0.000000000	1.400348000	-1.142955000
6	0.000000000	-1.400348000	-1.142955000
6	0.000000000	1.401351000	3.784948000
6	0.000000000	-1.401351000	3.784948000
6	0.000000000	1.401719000	8.614687000
6	0.000000000	-1.401719000	8.614687000
6	0.000000000	1.400774000	13.541076000
6	0.000000000	-1.400774000	13.541076000
6	0.000000000	0.723955000	14.755712000
6	0.000000000	-0.723955000	14.755712000
6	0.000000000	1.402013000	16.004463000
6	0.000000000	-1.402013000	16.004463000
6	0.000000000	0.718244000	17.191050000
6	0.000000000	-0.718244000	17.191050000
1	0.000000000	-2.488388000	13.540713000
1	0.000000000	2.488388000	13.540713000
1	0.000000000	-2.488676000	8.606423000
1	0.000000000	2.488676000	8.606423000
1	0.000000000	2.488375000	3.793417000
1	0.000000000	-2.488375000	3.793417000
1	0.000000000	2.488032000	-1.142507000
1	0.000000000	-2.488032000	-1.142507000
1	0.000000000	-2.488963000	16.013119000
1	0.000000000	2.488963000	16.013119000
7	0.000000000	-1.356974000	-6.021848000
7	0.000000000	1.356974000	-6.021848000
6	0.000000000	-0.718942000	-7.250297000
6	0.000000000	0.718942000	-7.250297000
6	0.000000000	-1.401295000	-8.437147000

6	0.000000000	1.401295000	-8.437147000
6	0.000000000	-0.723825000	-9.687505000
6	0.000000000	0.723825000	-9.687505000
6	0.000000000	-1.400300000	-10.901306000
6	0.000000000	1.400300000	-10.901306000
6	0.000000000	-0.723730000	-12.133243000
6	0.000000000	0.723730000	-12.133243000
6	0.000000000	-1.400302000	-13.365210000
6	0.000000000	1.400302000	-13.365210000
6	0.000000000	-0.723841000	-14.578992000
6	0.000000000	0.723841000	-14.578992000
6	0.000000000	-1.401300000	-15.829347000
6	0.000000000	1.401300000	-15.829347000
6	0.000000000	-0.718991000	-17.016248000
6	0.000000000	0.718991000	-17.016248000
1	0.000000000	-2.365464000	-6.021906000
1	0.000000000	2.365464000	-6.021906000
1	0.000000000	-2.488331000	-8.428733000
1	0.000000000	2.488331000	-8.428733000
1	0.000000000	-2.488005000	-10.901735000
1	0.000000000	2.488005000	-10.901735000
1	0.000000000	-2.488006000	-13.364782000
1	0.000000000	2.488006000	-13.364782000
1	0.000000000	-2.488332000	-15.837751000
1	0.000000000	2.488332000	-15.837751000
7	0.000000000	-1.356974000	-18.244567000
7	0.000000000	1.356974000	-18.244567000
6	0.000000000	-0.719153000	-19.472575000
6	0.000000000	0.719153000	-19.472575000
6	0.000000000	-1.401364000	-20.659554000
6	0.000000000	1.401364000	-20.659554000
6	0.000000000	-0.723914000	-21.909920000
6	0.000000000	0.723914000	-21.909920000
6	0.000000000	-1.400363000	-23.123534000
6	0.000000000	1.400363000	-23.123534000
6	0.000000000	-0.723747000	-24.355641000
6	0.000000000	0.723747000	-24.355641000
6	0.000000000	-1.400365000	-25.587312000
6	0.000000000	1.400365000	-25.587312000
6	0.000000000	-0.723770000	-26.801202000
6	0.000000000	0.723770000	-26.801202000
6	0.000000000	-1.401371000	-28.051390000
6	0.000000000	1.401371000	-28.051390000
6	0.000000000	-0.718663000	-29.237919000
6	0.000000000	0.718663000	-29.237919000
1	0.000000000	-2.365463000	-18.244538000
1	0.000000000	2.365463000	-18.244538000

1	0.000000000	-2.488380000	-20.651194000
1	0.000000000	2.488380000	-20.651194000
1	0.000000000	-2.488049000	-23.123990000
1	0.000000000	2.488049000	-23.123990000
1	0.000000000	-2.488052000	-25.586911000
1	0.000000000	2.488052000	-25.586911000
1	0.000000000	-2.488387000	-28.059876000
1	0.000000000	2.488387000	-28.059876000
7	0.000000000	1.356230000	18.419969000
7	0.000000000	-1.356230000	18.419969000
6	0.000000000	0.722694000	19.645961000
6	0.000000000	-0.722694000	19.645961000
6	0.000000000	1.404849000	20.830962000
6	0.000000000	-1.404849000	20.830962000
6	0.000000000	0.728548000	22.083508000
6	0.000000000	-0.728548000	22.083508000
6	0.000000000	1.404757000	23.288953000
6	0.000000000	-1.404757000	23.288953000
6	0.000000000	0.729646000	24.531272000
6	0.000000000	-0.729646000	24.531272000
6	0.000000000	1.406582000	25.744708000
6	0.000000000	-1.406582000	25.744708000
6	0.000000000	0.731892000	26.980720000
6	0.000000000	-0.731892000	26.980720000
6	0.000000000	1.414426000	28.196429000
6	0.000000000	-1.414426000	28.196429000
6	0.000000000	0.732704000	29.422599000
6	0.000000000	-0.732704000	29.422599000
1	0.000000000	2.500062000	28.218321000
1	0.000000000	-2.500062000	28.218321000
1	0.000000000	-2.493670000	25.745179000
1	0.000000000	2.493670000	25.745179000
1	0.000000000	2.492016000	23.289454000
1	0.000000000	-2.492016000	23.289454000
1	0.000000000	2.491584000	20.822550000
1	0.000000000	-2.491584000	20.822550000
1	0.000000000	2.365182000	18.419076000
1	0.000000000	-2.365182000	18.419076000
7	0.000000000	1.434472000	30.564329000
7	0.000000000	-1.434472000	30.564329000
6	0.000000000	0.731531000	31.709905000
6	0.000000000	-0.731531000	31.709905000
6	0.000000000	1.414212000	32.932172000
6	0.000000000	-1.414212000	32.932172000
6	0.000000000	0.731329000	34.151265000
6	0.000000000	-0.731329000	34.151265000
6	0.000000000	1.407065000	35.383736000

6	0.000000000	-1.407065000	35.383736000
6	0.000000000	0.728970000	36.599762000
6	0.000000000	-0.728970000	36.599762000
6	0.000000000	1.405296000	37.839665000
6	0.000000000	-1.405296000	37.839665000
6	0.000000000	0.726761000	39.045405000
6	0.000000000	-0.726761000	39.045405000
6	0.000000000	1.405808000	40.303500000
6	0.000000000	-1.405808000	40.303500000
6	0.000000000	0.713780000	41.476601000
6	0.000000000	-0.713780000	41.476601000
1	0.000000000	2.499834000	32.910006000
1	0.000000000	-2.499834000	32.910006000
1	0.000000000	2.494098000	35.383608000
1	0.000000000	-2.494098000	35.383608000
1	0.000000000	2.492707000	37.840530000
1	0.000000000	-2.492707000	37.840530000
1	0.000000000	2.492240000	40.300904000
1	0.000000000	1.244750000	42.423205000
1	0.000000000	-1.244750000	42.423205000
1	0.000000000	-2.492240000	40.300904000
7	0.000000000	1.356879000	-30.466832000
7	0.000000000	-1.356879000	-30.466832000
6	0.000000000	0.720129000	-31.694055000
6	0.000000000	-0.720129000	-31.694055000
6	0.000000000	1.402189000	-32.880405000
6	0.000000000	-1.402189000	-32.880405000
6	0.000000000	0.724755000	-34.131600000
6	0.000000000	-0.724755000	-34.131600000
6	0.000000000	1.401351000	-35.342824000
6	0.000000000	-1.401351000	-35.342824000
6	0.000000000	0.724289000	-36.577178000
6	0.000000000	-0.724289000	-36.577178000
6	0.000000000	1.401122000	-37.805669000
6	0.000000000	-1.401122000	-37.805669000
6	0.000000000	0.722998000	-39.021265000
6	0.000000000	-0.722998000	-39.021265000
6	0.000000000	1.402468000	-40.274166000
6	0.000000000	-1.402468000	-40.274166000
6	0.000000000	0.710982000	-41.451919000
6	0.000000000	-0.710982000	-41.451919000
1	0.000000000	2.365445000	-30.466570000
1	0.000000000	-2.365445000	-30.466570000
1	0.000000000	2.489088000	-32.872265000
1	0.000000000	-2.489088000	-32.872265000
1	0.000000000	-2.488867000	-35.343561000
1	0.000000000	2.488867000	-35.343561000

1	0.000000000	2.488892000	-37.806532000
1	0.000000000	-2.488892000	-37.806532000
1	0.000000000	-2.489136000	-40.271217000
1	0.000000000	2.489136000	-40.271217000
1	0.000000000	1.244262000	-42.397347000
1	0.000000000	-1.244262000	-42.397347000

Table S114: Coordinates of pT₆_2 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.722884000	7.505609000
7	0.000000000	1.356100000	6.279886000
6	0.000000000	0.718252000	5.051108000
6	0.000000000	-0.718252000	5.051108000
7	0.000000000	-1.356100000	6.279886000
6	0.000000000	-0.722884000	7.505609000
6	0.000000000	-0.724063000	2.616086000
6	0.000000000	0.724063000	2.616086000
6	0.000000000	1.400908000	1.401344000
1	0.000000000	2.488483000	1.400988000
6	0.000000000	0.724120000	0.171021000
6	0.000000000	-0.724120000	0.171021000
6	0.000000000	-1.400908000	1.401344000
1	0.000000000	2.365141000	6.278956000
1	0.000000000	-2.365141000	6.278956000
1	0.000000000	-2.488483000	1.400988000
6	0.000000000	-0.724381000	-2.274504000
6	0.000000000	0.724381000	-2.274504000
6	0.000000000	1.401862000	-3.524564000
6	0.000000000	-1.401862000	-3.524564000
6	0.000000000	-0.719748000	-4.711711000
6	0.000000000	0.719748000	-4.711711000
1	0.000000000	2.488778000	-3.532810000
1	0.000000000	-2.488778000	-3.532810000
6	0.000000000	0.728837000	9.942865000
6	0.000000000	-0.728837000	9.942865000
6	0.000000000	-1.405058000	11.148178000
6	0.000000000	1.405058000	11.148178000
6	0.000000000	-0.730025000	12.390551000
6	0.000000000	0.730025000	12.390551000
1	0.000000000	2.492264000	11.148664000
1	0.000000000	-2.492264000	11.148664000
6	0.000000000	1.400848000	-1.061521000
6	0.000000000	-1.400848000	-1.061521000
6	0.000000000	1.402213000	3.864475000
6	0.000000000	-1.402213000	3.864475000
6	0.000000000	1.405164000	8.690625000

6	0.000000000	-1.405164000	8.690625000
6	0.000000000	1.406965000	13.603442000
6	0.000000000	-1.406965000	13.603442000
6	0.000000000	0.732434000	14.840044000
6	0.000000000	-0.732434000	14.840044000
6	0.000000000	1.415088000	16.054495000
6	0.000000000	-1.415088000	16.054495000
6	0.000000000	0.733777000	17.282301000
6	0.000000000	-0.733777000	17.282301000
1	0.000000000	-2.494024000	13.603898000
1	0.000000000	2.494024000	13.603898000
1	0.000000000	-2.491885000	8.682203000
1	0.000000000	2.491885000	8.682203000
1	0.000000000	2.489128000	3.873143000
1	0.000000000	-2.489128000	3.873143000
1	0.000000000	2.488421000	-1.061012000
1	0.000000000	-2.488421000	-1.061012000
1	0.000000000	-2.500695000	16.076239000
1	0.000000000	2.500695000	16.076239000
7	0.000000000	-1.356858000	-5.938577000
7	0.000000000	1.356858000	-5.938577000
6	0.000000000	-0.718689000	-7.167548000
6	0.000000000	0.718689000	-7.167548000
6	0.000000000	-1.401473000	-8.354068000
6	0.000000000	1.401473000	-8.354068000
6	0.000000000	-0.723821000	-9.604153000
6	0.000000000	0.723821000	-9.604153000
6	0.000000000	-1.400447000	-10.818041000
6	0.000000000	1.400447000	-10.818041000
6	0.000000000	-0.723795000	-12.049644000
6	0.000000000	0.723795000	-12.049644000
6	0.000000000	-1.400445000	-13.281698000
6	0.000000000	1.400445000	-13.281698000
6	0.000000000	-0.723961000	-14.495290000
6	0.000000000	0.723961000	-14.495290000
6	0.000000000	-1.401458000	-15.745539000
6	0.000000000	1.401458000	-15.745539000
6	0.000000000	-0.719196000	-16.932514000
6	0.000000000	0.719196000	-16.932514000
1	0.000000000	-2.365446000	-5.938802000
1	0.000000000	2.365446000	-5.938802000
1	0.000000000	-2.488483000	-8.345588000
1	0.000000000	2.488483000	-8.345588000
1	0.000000000	-2.488118000	-10.818451000
1	0.000000000	2.488118000	-10.818451000
1	0.000000000	-2.488110000	-13.281249000
1	0.000000000	2.488110000	-13.281249000

1	0.000000000	-2.488453000	-15.753892000
1	0.000000000	2.488453000	-15.753892000
7	0.000000000	-1.356949000	-18.160394000
7	0.000000000	1.356949000	-18.160394000
6	0.000000000	-0.719034000	-19.388688000
6	0.000000000	0.719034000	-19.388688000
6	0.000000000	-1.401414000	-20.575488000
6	0.000000000	1.401414000	-20.575488000
6	0.000000000	-0.723893000	-21.825797000
6	0.000000000	0.723893000	-21.825797000
6	0.000000000	-1.400411000	-23.039422000
6	0.000000000	1.400411000	-23.039422000
6	0.000000000	-0.723758000	-24.271413000
6	0.000000000	0.723758000	-24.271413000
6	0.000000000	-1.400415000	-25.503117000
6	0.000000000	1.400415000	-25.503117000
6	0.000000000	-0.723808000	-26.716928000
6	0.000000000	0.723808000	-26.716928000
6	0.000000000	-1.401427000	-27.967084000
6	0.000000000	1.401427000	-27.967084000
6	0.000000000	-0.718743000	-29.153640000
6	0.000000000	0.718743000	-29.153640000
1	0.000000000	-2.365467000	-18.160439000
1	0.000000000	2.365467000	-18.160439000
1	0.000000000	-2.488423000	-20.567102000
1	0.000000000	2.488423000	-20.567102000
1	0.000000000	-2.488085000	-23.039872000
1	0.000000000	2.488085000	-23.039872000
1	0.000000000	-2.488087000	-25.502711000
1	0.000000000	2.488087000	-25.502711000
1	0.000000000	-2.488428000	-27.975551000
1	0.000000000	2.488428000	-27.975551000
7	0.000000000	1.435360000	18.421460000
7	0.000000000	-1.435360000	18.421460000
6	0.000000000	0.732438000	19.570052000
6	0.000000000	-0.732438000	19.570052000
6	0.000000000	1.415445000	20.787835000
6	0.000000000	-1.415445000	20.787835000
6	0.000000000	0.733203000	22.012372000
6	0.000000000	-0.733203000	22.012372000
6	0.000000000	1.409352000	23.236848000
6	0.000000000	-1.409352000	23.236848000
6	0.000000000	0.732220000	24.463012000
6	0.000000000	-0.732220000	24.463012000
6	0.000000000	1.409507000	25.687264000
6	0.000000000	-1.409507000	25.687264000
6	0.000000000	0.733470000	26.913660000

6	0.000000000	-0.733470000	26.913660000
6	0.000000000	1.416289000	28.135795000
6	0.000000000	-1.416289000	28.135795000
6	0.000000000	0.733157000	29.355685000
6	0.000000000	-0.733157000	29.355685000
1	0.000000000	2.501761000	28.158218000
1	0.000000000	-2.501761000	28.158218000
1	0.000000000	-2.496327000	25.687664000
1	0.000000000	2.496327000	25.687664000
1	0.000000000	2.496195000	23.236507000
1	0.000000000	-2.496195000	23.236507000
1	0.000000000	2.500968000	20.765272000
1	0.000000000	-2.500968000	20.765272000
7	0.000000000	1.435217000	30.501863000
7	0.000000000	-1.435217000	30.501863000
6	0.000000000	0.732975000	31.642995000
6	0.000000000	-0.732975000	31.642995000
6	0.000000000	1.415658000	32.868310000
6	0.000000000	-1.415658000	32.868310000
6	0.000000000	0.732111000	34.084430000
6	0.000000000	-0.732111000	34.084430000
6	0.000000000	1.407855000	35.318587000
6	0.000000000	-1.407855000	35.318587000
6	0.000000000	0.729487000	36.532911000
6	0.000000000	-0.729487000	36.532911000
6	0.000000000	1.405887000	37.773645000
6	0.000000000	-1.405887000	37.773645000
6	0.000000000	0.727152000	38.978429000
6	0.000000000	-0.727152000	38.978429000
6	0.000000000	1.406320000	40.236850000
6	0.000000000	-1.406320000	40.236850000
6	0.000000000	0.714041000	41.409355000
6	0.000000000	-0.714041000	41.409355000
1	0.000000000	2.501179000	32.846316000
1	0.000000000	-2.501179000	32.846316000
1	0.000000000	2.494781000	35.318451000
1	0.000000000	-2.494781000	35.318451000
1	0.000000000	2.493205000	37.774518000
1	0.000000000	-2.493205000	37.774518000
1	0.000000000	2.492671000	40.234343000
1	0.000000000	1.244677000	42.356093000
1	0.000000000	-1.244677000	42.356093000
1	0.000000000	-2.492671000	40.234343000
7	0.000000000	1.356880000	-30.382373000
7	0.000000000	-1.356880000	-30.382373000
6	0.000000000	0.720086000	-31.609720000
6	0.000000000	-0.720086000	-31.609720000

6	0.000000000	1.402211000	-32.795981000
6	0.000000000	-1.402211000	-32.795981000
6	0.000000000	0.724747000	-34.047171000
6	0.000000000	-0.724747000	-34.047171000
6	0.000000000	1.401377000	-35.258377000
6	0.000000000	-1.401377000	-35.258377000
6	0.000000000	0.724292000	-36.492695000
6	0.000000000	-0.724292000	-36.492695000
6	0.000000000	1.401150000	-37.721185000
6	0.000000000	-1.401150000	-37.721185000
6	0.000000000	0.723010000	-38.936742000
6	0.000000000	-0.723010000	-38.936742000
6	0.000000000	1.402505000	-40.189643000
6	0.000000000	-1.402505000	-40.189643000
6	0.000000000	0.710995000	-41.367357000
6	0.000000000	-0.710995000	-41.367357000
1	0.000000000	2.365456000	-30.382140000
1	0.000000000	-2.365456000	-30.382140000
1	0.000000000	2.489107000	-32.787832000
1	0.000000000	-2.489107000	-32.787832000
1	0.000000000	-2.488883000	-35.259118000
1	0.000000000	2.488883000	-35.259118000
1	0.000000000	2.488914000	-37.722050000
1	0.000000000	-2.488914000	-37.722050000
1	0.000000000	-2.489155000	-40.186707000
1	0.000000000	2.489155000	-40.186707000
1	0.000000000	1.244249000	-42.312793000
1	0.000000000	-1.244249000	-42.312793000

Table S115: Coordinates of pT₆_3 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.731357000	-7.414605000
7	0.000000000	1.434591000	-6.278500000
6	0.000000000	0.730239000	-5.128499000
6	0.000000000	-0.730239000	-5.128499000
7	0.000000000	-1.434591000	-6.278500000
6	0.000000000	-0.731357000	-7.414605000
6	0.000000000	-0.729675000	-2.686119000
6	0.000000000	0.729675000	-2.686119000
6	0.000000000	1.404739000	-1.457103000
1	0.000000000	2.491904000	-1.457663000
6	0.000000000	0.727555000	-0.237137000
6	0.000000000	-0.727555000	-0.237137000
6	0.000000000	-1.404739000	-1.457103000
1	0.000000000	-2.491904000	-1.457663000
6	0.000000000	-0.726568000	2.209682000

6	0.000000000	0.726568000	2.209682000
6	0.000000000	1.403617000	3.459111000
6	0.000000000	-1.403617000	3.459111000
6	0.000000000	-0.721311000	4.646381000
6	0.000000000	0.721311000	4.646381000
1	0.000000000	2.490308000	3.467122000
1	0.000000000	-2.490308000	3.467122000
6	0.000000000	0.730989000	-9.860099000
6	0.000000000	-0.730989000	-9.860099000
6	0.000000000	-1.404973000	-11.095642000
6	0.000000000	1.404973000	-11.095642000
6	0.000000000	-0.730105000	-12.313340000
6	0.000000000	0.730105000	-12.313340000
1	0.000000000	2.492122000	-11.095152000
1	0.000000000	-2.492122000	-11.095152000
6	0.000000000	1.403267000	0.999812000
6	0.000000000	-1.403267000	0.999812000
6	0.000000000	1.411481000	-3.909955000
6	0.000000000	-1.411481000	-3.909955000
6	0.000000000	1.411623000	-8.646108000
6	0.000000000	-1.411623000	-8.646108000
6	0.000000000	1.404411000	-13.546179000
6	0.000000000	-1.404411000	-13.546179000
6	0.000000000	0.731012000	-14.767273000
6	0.000000000	-0.731012000	-14.767273000
6	0.000000000	1.408817000	-15.994881000
6	0.000000000	-1.408817000	-15.994881000
6	0.000000000	0.731730000	-17.216099000
6	0.000000000	-0.731730000	-17.216099000
1	0.000000000	-2.491622000	-13.546431000
1	0.000000000	2.491622000	-13.546431000
1	0.000000000	-2.497445000	-8.624269000
1	0.000000000	2.497445000	-8.624269000
1	0.000000000	2.497255000	-3.932333000
1	0.000000000	-2.497255000	-3.932333000
1	0.000000000	2.490525000	0.999157000
1	0.000000000	-2.490525000	0.999157000
1	0.000000000	-2.494835000	-16.016740000
1	0.000000000	2.494835000	-16.016740000
7	0.000000000	-1.356460000	5.870822000
7	0.000000000	1.356460000	5.870822000
6	0.000000000	-0.718145000	7.100420000
6	0.000000000	0.718145000	7.100420000
6	0.000000000	-1.401984000	8.286494000
6	0.000000000	1.401984000	8.286494000
6	0.000000000	-0.723836000	9.535556000
6	0.000000000	0.723836000	9.535556000

6	0.000000000	-1.400793000	10.749766000
6	0.000000000	1.400793000	10.749766000
6	0.000000000	-0.723927000	11.980561000
6	0.000000000	0.723927000	11.980561000
6	0.000000000	-1.400753000	13.212712000
6	0.000000000	1.400753000	13.212712000
6	0.000000000	-0.724174000	14.425978000
6	0.000000000	0.724174000	14.425978000
6	0.000000000	-1.401767000	15.675842000
6	0.000000000	1.401767000	15.675842000
6	0.000000000	-0.719579000	16.863064000
6	0.000000000	0.719579000	16.863064000
1	0.000000000	-2.365393000	5.871339000
1	0.000000000	2.365393000	5.871339000
1	0.000000000	-2.488908000	8.277885000
1	0.000000000	2.488908000	8.277885000
1	0.000000000	-2.488370000	10.750116000
1	0.000000000	2.488370000	10.750116000
1	0.000000000	-2.488319000	13.212190000
1	0.000000000	2.488319000	13.212190000
1	0.000000000	-2.488672000	15.684034000
1	0.000000000	2.488672000	15.684034000
7	0.000000000	-1.356887000	18.089888000
7	0.000000000	1.356887000	18.089888000
6	0.000000000	-0.718749000	19.318804000
6	0.000000000	0.718749000	19.318804000
6	0.000000000	-1.401515000	20.505193000
6	0.000000000	1.401515000	20.505193000
6	0.000000000	-0.723830000	21.755376000
6	0.000000000	0.723830000	21.755376000
6	0.000000000	-1.400511000	22.968995000
6	0.000000000	1.400511000	22.968995000
6	0.000000000	-0.723764000	24.200747000
6	0.000000000	0.723764000	24.200747000
6	0.000000000	-1.400518000	25.432489000
6	0.000000000	1.400518000	25.432489000
6	0.000000000	-0.723873000	26.646141000
6	0.000000000	0.723873000	26.646141000
6	0.000000000	-1.401545000	27.896208000
6	0.000000000	1.401545000	27.896208000
6	0.000000000	-0.718904000	29.082814000
6	0.000000000	0.718904000	29.082814000
1	0.000000000	-2.365470000	18.090065000
1	0.000000000	2.365470000	18.090065000
1	0.000000000	-2.488502000	20.496771000
1	0.000000000	2.488502000	20.496771000
1	0.000000000	-2.488154000	22.969431000

1	0.000000000	2.488154000	22.969431000
1	0.000000000	-2.488154000	25.432054000
1	0.000000000	2.488154000	25.432054000
1	0.000000000	-2.488509000	27.904597000
1	0.000000000	2.488509000	27.904597000
7	0.000000000	1.436762000	-18.360208000
7	0.000000000	-1.436762000	-18.360208000
6	0.000000000	0.732021000	-19.502470000
6	0.000000000	-0.732021000	-19.502470000
6	0.000000000	1.408783000	-20.725457000
6	0.000000000	-1.408783000	-20.725457000
6	0.000000000	0.731163000	-21.951683000
6	0.000000000	-0.731163000	-21.951683000
6	0.000000000	1.404253000	-23.173847000
6	0.000000000	-1.404253000	-23.173847000
6	0.000000000	0.730342000	-24.406105000
6	0.000000000	-0.730342000	-24.406105000
6	0.000000000	1.404878000	-25.623976000
6	0.000000000	-1.404878000	-25.623976000
6	0.000000000	0.731323000	-26.859996000
6	0.000000000	-0.731323000	-26.859996000
6	0.000000000	1.411725000	-28.073012000
6	0.000000000	-1.411725000	-28.073012000
6	0.000000000	0.732103000	-29.306443000
6	0.000000000	-0.732103000	-29.306443000
1	0.000000000	2.497534000	-28.094704000
1	0.000000000	-2.497534000	-28.094704000
1	0.000000000	-2.492020000	-25.624469000
1	0.000000000	2.492020000	-25.624469000
1	0.000000000	2.491470000	-23.173554000
1	0.000000000	-2.491470000	-23.173554000
1	0.000000000	2.494810000	-20.703671000
1	0.000000000	-2.494810000	-20.703671000
7	0.000000000	1.435154000	-30.440111000
7	0.000000000	-1.435154000	-30.440111000
6	0.000000000	0.730096000	-31.592982000
6	0.000000000	-0.730096000	-31.592982000
6	0.000000000	1.411712000	-32.808185000
6	0.000000000	-1.411712000	-32.808185000
6	0.000000000	0.729651000	-34.035458000
6	0.000000000	-0.729651000	-34.035458000
6	0.000000000	1.405451000	-35.260657000
6	0.000000000	-1.405451000	-35.260657000
6	0.000000000	0.727181000	-36.483757000
6	0.000000000	-0.727181000	-36.483757000
6	0.000000000	1.403874000	-37.717761000
6	0.000000000	-1.403874000	-37.717761000

6	0.000000000	0.724884000	-38.928476000
6	0.000000000	-0.724884000	-38.928476000
6	0.000000000	1.404568000	-40.183004000
6	0.000000000	-1.404568000	-40.183004000
6	0.000000000	0.712112000	-41.358401000
6	0.000000000	-0.712112000	-41.358401000
1	0.000000000	2.497426000	-32.785749000
1	0.000000000	-2.497426000	-32.785749000
1	0.000000000	2.492524000	-35.260444000
1	0.000000000	-2.492524000	-35.260444000
1	0.000000000	2.491268000	-37.718494000
1	0.000000000	-2.491268000	-37.718494000
1	0.000000000	2.490947000	-40.180294000
1	0.000000000	1.243985000	-42.304426000
1	0.000000000	-1.243985000	-42.304426000
1	0.000000000	-2.490947000	-40.180294000
7	0.000000000	1.356872000	30.311157000
7	0.000000000	-1.356872000	30.311157000
6	0.000000000	0.719973000	31.538767000
6	0.000000000	-0.719973000	31.538767000
6	0.000000000	1.402242000	32.724819000
6	0.000000000	-1.402242000	32.724819000
6	0.000000000	0.724704000	33.976003000
6	0.000000000	-0.724704000	33.976003000
6	0.000000000	1.401410000	35.187155000
6	0.000000000	-1.401410000	35.187155000
6	0.000000000	0.724264000	36.421393000
6	0.000000000	-0.724264000	36.421393000
6	0.000000000	1.401181000	37.649877000
6	0.000000000	-1.401181000	37.649877000
6	0.000000000	0.722997000	38.865342000
6	0.000000000	-0.722997000	38.865342000
6	0.000000000	1.402548000	40.118243000
6	0.000000000	-1.402548000	40.118243000
6	0.000000000	0.710991000	41.295861000
6	0.000000000	-0.710991000	41.295861000
1	0.000000000	2.365463000	30.310988000
1	0.000000000	-2.365463000	30.310988000
1	0.000000000	2.489127000	32.716675000
1	0.000000000	-2.489127000	32.716675000
1	0.000000000	-2.488925000	35.187897000
1	0.000000000	2.488925000	35.187897000
1	0.000000000	2.488928000	37.650741000
1	0.000000000	-2.488928000	37.650741000
1	0.000000000	-2.489217000	40.115309000
1	0.000000000	2.489217000	40.115309000
1	0.000000000	1.244179000	42.241319000

1	0.000000000	-1.244179000	42.241319000
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Table S116: Coordinates of pT₆_4 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.732652000	7.343968000
7	0.000000000	1.436316000	6.206133000
6	0.000000000	0.731663000	5.057610000
6	0.000000000	-0.731663000	5.057610000
7	0.000000000	-1.436316000	6.206133000
6	0.000000000	-0.732652000	7.343968000
6	0.000000000	-0.731582000	2.612095000
6	0.000000000	0.731582000	2.612095000
6	0.000000000	1.406369000	1.391578000
1	0.000000000	2.493417000	1.392077000
6	0.000000000	0.730630000	0.160155000
6	0.000000000	-0.730630000	0.160155000
6	0.000000000	-1.406369000	1.391578000
1	0.000000000	-2.493417000	1.392077000
6	0.000000000	-0.731625000	-2.291344000
6	0.000000000	0.731625000	-2.291344000
6	0.000000000	1.413357000	-3.508293000
6	0.000000000	-1.413357000	-3.508293000
6	0.000000000	-0.731523000	-4.734701000
6	0.000000000	0.731523000	-4.734701000
1	0.000000000	2.499026000	-3.530384000
1	0.000000000	-2.499026000	-3.530384000
6	0.000000000	0.731628000	9.790834000
6	0.000000000	-0.731628000	9.790834000
6	0.000000000	-1.404989000	11.019836000
6	0.000000000	1.404989000	11.019836000
6	0.000000000	-0.730646000	12.244099000
6	0.000000000	0.730646000	12.244099000
1	0.000000000	2.492123000	11.019517000
1	0.000000000	-2.492123000	11.019517000
6	0.000000000	1.406760000	-1.058989000
6	0.000000000	-1.406760000	-1.058989000
6	0.000000000	1.411353000	3.840446000
6	0.000000000	-1.411353000	3.840446000
6	0.000000000	1.410955000	8.571666000
6	0.000000000	-1.410955000	8.571666000
6	0.000000000	1.404931000	13.469466000
6	0.000000000	-1.404931000	13.469466000
6	0.000000000	0.731592000	14.697402000
6	0.000000000	-0.731592000	14.697402000
6	0.000000000	1.410696000	15.917606000
6	0.000000000	-1.410696000	15.917606000

6	0.000000000	0.732568000	17.144465000
6	0.000000000	-0.732568000	17.144465000
1	0.000000000	-2.492084000	13.469914000
1	0.000000000	2.492084000	13.469914000
1	0.000000000	-2.496830000	8.550069000
1	0.000000000	2.496830000	8.550069000
1	0.000000000	2.497153000	3.862917000
1	0.000000000	-2.497153000	3.862917000
1	0.000000000	2.493763000	-1.059294000
1	0.000000000	-2.493763000	-1.059294000
1	0.000000000	-2.496583000	15.939402000
1	0.000000000	2.496583000	15.939402000
7	0.000000000	-1.434647000	-5.875391000
7	0.000000000	1.434647000	-5.875391000
6	0.000000000	-0.731644000	-7.021029000
6	0.000000000	0.731644000	-7.021029000
6	0.000000000	-1.413242000	-8.243152000
6	0.000000000	1.413242000	-8.243152000
6	0.000000000	-0.730863000	-9.462816000
6	0.000000000	0.730863000	-9.462816000
6	0.000000000	-1.405831000	-10.694966000
6	0.000000000	1.405831000	-10.694966000
6	0.000000000	-0.728641000	-11.911767000
6	0.000000000	0.728641000	-11.911767000
6	0.000000000	-1.404185000	-13.150913000
6	0.000000000	1.404185000	-13.150913000
6	0.000000000	-0.727588000	-14.358750000
6	0.000000000	0.727588000	-14.358750000
6	0.000000000	-1.404418000	-15.609226000
6	0.000000000	1.404418000	-15.609226000
6	0.000000000	-0.722032000	-16.795505000
6	0.000000000	0.722032000	-16.795505000
1	0.000000000	-2.498903000	-8.221042000
1	0.000000000	2.498903000	-8.221042000
1	0.000000000	-2.492905000	-10.694516000
1	0.000000000	2.492905000	-10.694516000
1	0.000000000	-2.491381000	-13.150420000
1	0.000000000	2.491381000	-13.150420000
1	0.000000000	-2.491073000	-15.617441000
1	0.000000000	2.491073000	-15.617441000
7	0.000000000	-1.356348000	-18.020293000
7	0.000000000	1.356348000	-18.020293000
6	0.000000000	-0.718226000	-19.249558000
6	0.000000000	0.718226000	-19.249558000
6	0.000000000	-1.402225000	-20.435691000
6	0.000000000	1.402225000	-20.435691000
6	0.000000000	-0.723974000	-21.684479000

6	0.000000000	0.723974000	-21.684479000
6	0.000000000	-1.400997000	-22.898689000
6	0.000000000	1.400997000	-22.898689000
6	0.000000000	-0.724021000	-24.129310000
6	0.000000000	0.724021000	-24.129310000
6	0.000000000	-1.400945000	-25.361387000
6	0.000000000	1.400945000	-25.361387000
6	0.000000000	-0.724206000	-26.574470000
6	0.000000000	0.724206000	-26.574470000
6	0.000000000	-1.401943000	-27.824321000
6	0.000000000	1.401943000	-27.824321000
6	0.000000000	-0.719374000	-29.011043000
6	0.000000000	0.719374000	-29.011043000
1	0.000000000	-2.365348000	-18.020991000
1	0.000000000	2.365348000	-18.020991000
1	0.000000000	-2.489112000	-20.427068000
1	0.000000000	2.489112000	-20.427068000
1	0.000000000	-2.488529000	-22.899043000
1	0.000000000	2.488529000	-22.899043000
1	0.000000000	-2.488470000	-25.360898000
1	0.000000000	2.488470000	-25.360898000
1	0.000000000	-2.488815000	-27.832613000
1	0.000000000	2.488815000	-27.832613000
7	0.000000000	1.436413000	18.283015000
7	0.000000000	-1.436413000	18.283015000
6	0.000000000	0.731846000	19.430825000
6	0.000000000	-0.731846000	19.430825000
6	0.000000000	1.411159000	20.648518000
6	0.000000000	-1.411159000	20.648518000
6	0.000000000	0.731715000	21.876797000
6	0.000000000	-0.731715000	21.876797000
6	0.000000000	1.406283000	23.097132000
6	0.000000000	-1.406283000	23.097132000
6	0.000000000	0.730870000	24.329133000
6	0.000000000	-0.730870000	24.329133000
6	0.000000000	1.406821000	25.547376000
6	0.000000000	-1.406821000	25.547376000
6	0.000000000	0.731971000	26.781060000
6	0.000000000	-0.731971000	26.781060000
6	0.000000000	1.413766000	27.996246000
6	0.000000000	-1.413766000	27.996246000
6	0.000000000	0.732281000	29.224909000
6	0.000000000	-0.732281000	29.224909000
1	0.000000000	2.499402000	28.018080000
1	0.000000000	-2.499402000	28.018080000
1	0.000000000	-2.493801000	25.547685000
1	0.000000000	2.493801000	25.547685000

1	0.000000000	2.493330000	23.096625000
1	0.000000000	-2.493330000	23.096625000
1	0.000000000	2.496969000	20.626169000
1	0.000000000	-2.496969000	20.626169000
7	0.000000000	1.434948000	30.362943000
7	0.000000000	-1.434948000	30.362943000
6	0.000000000	0.731226000	31.511420000
6	0.000000000	-0.731226000	31.511420000
6	0.000000000	1.413550000	32.730334000
6	0.000000000	-1.413550000	32.730334000
6	0.000000000	0.730671000	33.952870000
6	0.000000000	-0.730671000	33.952870000
6	0.000000000	1.406548000	35.181760000
6	0.000000000	-1.406548000	35.181760000
6	0.000000000	0.728167000	36.400970000
6	0.000000000	-0.728167000	36.400970000
6	0.000000000	1.404836000	37.637853000
6	0.000000000	-1.404836000	37.637853000
6	0.000000000	0.725892000	38.845863000
6	0.000000000	-0.725892000	38.845863000
6	0.000000000	1.405418000	40.102082000
6	0.000000000	-1.405418000	40.102082000
6	0.000000000	0.712960000	41.276116000
6	0.000000000	-0.712960000	41.276116000
1	0.000000000	2.499150000	32.708044000
1	0.000000000	-2.499150000	32.708044000
1	0.000000000	2.493534000	35.181629000
1	0.000000000	-2.493534000	35.181629000
1	0.000000000	2.492169000	37.638740000
1	0.000000000	-2.492169000	37.638740000
1	0.000000000	2.491758000	40.099613000
1	0.000000000	1.244338000	42.222411000
1	0.000000000	-1.244338000	42.222411000
1	0.000000000	-2.491758000	40.099613000
7	0.000000000	1.356861000	-30.238401000
7	0.000000000	-1.356861000	-30.238401000
6	0.000000000	0.719725000	-31.466611000
6	0.000000000	-0.719725000	-31.466611000
6	0.000000000	1.402389000	-32.652233000
6	0.000000000	-1.402389000	-32.652233000
6	0.000000000	0.724666000	-33.903336000
6	0.000000000	-0.724666000	-33.903336000
6	0.000000000	1.401556000	-35.114438000
6	0.000000000	-1.401556000	-35.114438000
6	0.000000000	0.724269000	-36.348456000
6	0.000000000	-0.724269000	-36.348456000
6	0.000000000	1.401325000	-37.576966000

6	0.000000000	-1.401325000	-37.576966000
6	0.000000000	0.723041000	-38.792227000
6	0.000000000	-0.723041000	-38.792227000
6	0.000000000	1.402705000	-40.045148000
6	0.000000000	-1.402705000	-40.045148000
6	0.000000000	0.711032000	-41.222582000
6	0.000000000	-0.711032000	-41.222582000
1	0.000000000	2.365517000	-30.238386000
1	0.000000000	-2.365517000	-30.238386000
1	0.000000000	2.489244000	-32.644028000
1	0.000000000	-2.489244000	-32.644028000
1	0.000000000	-2.489022000	-35.115167000
1	0.000000000	2.489022000	-35.115167000
1	0.000000000	2.489029000	-37.577839000
1	0.000000000	-2.489029000	-37.577839000
1	0.000000000	-2.489317000	-40.042319000
1	0.000000000	2.489317000	-40.042319000
1	0.000000000	1.244173000	-42.168038000
1	0.000000000	-1.244173000	-42.168038000

Table S117: Coordinates of pT₆_5 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.732443000	7.267407000
7	0.000000000	1.436453000	6.124812000
6	0.000000000	0.732336000	4.981406000
6	0.000000000	-0.732336000	4.981406000
7	0.000000000	-1.436453000	6.124812000
6	0.000000000	-0.732443000	7.267407000
6	0.000000000	-0.731900000	2.535784000
6	0.000000000	0.731900000	2.535784000
6	0.000000000	1.406093000	1.311520000
1	0.000000000	2.493152000	1.312134000
6	0.000000000	0.731016000	0.083547000
6	0.000000000	-0.731016000	0.083547000
6	0.000000000	-1.406093000	1.311520000
1	0.000000000	-2.493152000	1.312134000
6	0.000000000	-0.732177000	-2.368607000
6	0.000000000	0.732177000	-2.368607000
6	0.000000000	1.412960000	-3.586139000
6	0.000000000	-1.412960000	-3.586139000
6	0.000000000	-0.733017000	-4.813607000
6	0.000000000	0.733017000	-4.813607000
1	0.000000000	2.498685000	-3.607748000
1	0.000000000	-2.498685000	-3.607748000
6	0.000000000	0.731926000	9.713192000
6	0.000000000	-0.731926000	9.713192000

6	0.000000000	-1.406004000	10.937991000
6	0.000000000	1.406004000	10.937991000
6	0.000000000	-0.731031000	12.165557000
6	0.000000000	0.731031000	12.165557000
1	0.000000000	2.493076000	10.937739000
1	0.000000000	-2.493076000	10.937739000
6	0.000000000	1.406383000	-1.138097000
6	0.000000000	-1.406383000	-1.138097000
6	0.000000000	1.411527000	3.759623000
6	0.000000000	-1.411527000	3.759623000
6	0.000000000	1.411500000	8.489977000
6	0.000000000	-1.411500000	8.489977000
6	0.000000000	1.406261000	13.387523000
6	0.000000000	-1.406261000	13.387523000
6	0.000000000	0.732167000	14.617862000
6	0.000000000	-0.732167000	14.617862000
6	0.000000000	1.412763000	15.835499000
6	0.000000000	-1.412763000	15.835499000
6	0.000000000	0.733034000	17.063122000
6	0.000000000	-0.733034000	17.063122000
1	0.000000000	-2.493306000	13.388098000
1	0.000000000	2.493306000	13.388098000
1	0.000000000	-2.497327000	8.468070000
1	0.000000000	2.497327000	8.468070000
1	0.000000000	2.497343000	3.781929000
1	0.000000000	-2.497343000	3.781929000
1	0.000000000	2.493410000	-1.138251000
1	0.000000000	-2.493410000	-1.138251000
1	0.000000000	-2.498513000	15.857632000
1	0.000000000	2.498513000	15.857632000
7	0.000000000	-1.436135000	-5.951601000
7	0.000000000	1.436135000	-5.951601000
6	0.000000000	-0.732109000	-7.100073000
6	0.000000000	0.732109000	-7.100073000
6	0.000000000	-1.413277000	-8.317169000
6	0.000000000	1.413277000	-8.317169000
6	0.000000000	-0.732204000	-9.543953000
6	0.000000000	0.732204000	-9.543953000
6	0.000000000	-1.407671000	-10.765710000
6	0.000000000	1.407671000	-10.765710000
6	0.000000000	-0.731139000	-11.995088000
6	0.000000000	0.731139000	-11.995088000
6	0.000000000	-1.407893000	-13.215986000
6	0.000000000	1.407893000	-13.215986000
6	0.000000000	-0.732159000	-14.445922000
6	0.000000000	0.732159000	-14.445922000
6	0.000000000	-1.414432000	-15.664921000

6	0.000000000	1.414432000	-15.664921000
6	0.000000000	-0.731781000	-16.888363000
6	0.000000000	0.731781000	-16.888363000
1	0.000000000	-2.498946000	-8.294691000
1	0.000000000	2.498946000	-8.294691000
1	0.000000000	-2.494613000	-10.765381000
1	0.000000000	2.494613000	-10.765381000
1	0.000000000	-2.494810000	-13.216455000
1	0.000000000	2.494810000	-13.216455000
1	0.000000000	-2.500028000	-15.687400000
1	0.000000000	2.500028000	-15.687400000
7	0.000000000	-1.434910000	-18.031514000
7	0.000000000	1.434910000	-18.031514000
6	0.000000000	-0.732410000	-19.174762000
6	0.000000000	0.732410000	-19.174762000
6	0.000000000	-1.414249000	-20.398701000
6	0.000000000	1.414249000	-20.398701000
6	0.000000000	-0.731468000	-21.616255000
6	0.000000000	0.731468000	-21.616255000
6	0.000000000	-1.406485000	-22.849912000
6	0.000000000	1.406485000	-22.849912000
6	0.000000000	-0.729136000	-24.065094000
6	0.000000000	0.729136000	-24.065094000
6	0.000000000	-1.404720000	-25.305344000
6	0.000000000	1.404720000	-25.305344000
6	0.000000000	-0.727992000	-26.511980000
6	0.000000000	0.727992000	-26.511980000
6	0.000000000	-1.404875000	-27.763174000
6	0.000000000	1.404875000	-27.763174000
6	0.000000000	-0.722181000	-28.948424000
6	0.000000000	0.722181000	-28.948424000
1	0.000000000	-2.499862000	-20.376814000
1	0.000000000	2.499862000	-20.376814000
1	0.000000000	-2.493506000	-22.849619000
1	0.000000000	2.493506000	-22.849619000
1	0.000000000	-2.491876000	-25.305033000
1	0.000000000	2.491876000	-25.305033000
1	0.000000000	-2.491500000	-27.771624000
1	0.000000000	2.491500000	-27.771624000
7	0.000000000	1.436353000	18.200815000
7	0.000000000	-1.436353000	18.200815000
6	0.000000000	0.732136000	19.349535000
6	0.000000000	-0.732136000	19.349535000
6	0.000000000	1.413175000	20.566222000
6	0.000000000	-1.413175000	20.566222000
6	0.000000000	0.732273000	21.793583000
6	0.000000000	-0.732273000	21.793583000

6	0.000000000	1.407706000	23.014619000
6	0.000000000	-1.407706000	23.014619000
6	0.000000000	0.731309000	24.244862000
6	0.000000000	-0.731309000	24.244862000
6	0.000000000	1.408046000	25.464667000
6	0.000000000	-1.408046000	25.464667000
6	0.000000000	0.732474000	26.695897000
6	0.000000000	-0.732474000	26.695897000
6	0.000000000	1.414929000	27.913203000
6	0.000000000	-1.414929000	27.913203000
6	0.000000000	0.732497000	29.138613000
6	0.000000000	-0.732497000	29.138613000
1	0.000000000	2.500485000	27.935185000
1	0.000000000	-2.500485000	27.935185000
1	0.000000000	-2.494931000	25.464910000
1	0.000000000	2.494931000	25.464910000
1	0.000000000	2.494635000	23.014239000
1	0.000000000	-2.494635000	23.014239000
1	0.000000000	2.498844000	20.543966000
1	0.000000000	-2.498844000	20.543966000
7	0.000000000	1.435046000	30.279444000
7	0.000000000	-1.435046000	30.279444000
6	0.000000000	0.731971000	31.425128000
6	0.000000000	-0.731971000	31.425128000
6	0.000000000	1.414609000	32.646297000
6	0.000000000	-1.414609000	32.646297000
6	0.000000000	0.731315000	33.866205000
6	0.000000000	-0.731315000	33.866205000
6	0.000000000	1.407172000	35.097038000
6	0.000000000	-1.407172000	35.097038000
6	0.000000000	0.728721000	36.314293000
6	0.000000000	-0.728721000	36.314293000
6	0.000000000	1.405361000	37.552539000
6	0.000000000	-1.405361000	37.552539000
6	0.000000000	0.726393000	38.759274000
6	0.000000000	-0.726393000	38.759274000
6	0.000000000	1.405848000	40.016240000
6	0.000000000	-1.405848000	40.016240000
6	0.000000000	0.713329000	41.189639000
6	0.000000000	-0.713329000	41.189639000
1	0.000000000	2.500161000	32.624118000
1	0.000000000	-2.500161000	32.624118000
1	0.000000000	2.494112000	35.097091000
1	0.000000000	-2.494112000	35.097091000
1	0.000000000	2.492657000	37.553680000
1	0.000000000	-2.492657000	37.553680000
1	0.000000000	2.492160000	40.014032000

1	0.000000000	1.244585000	42.135993000
1	0.000000000	-1.244585000	42.135993000
1	0.000000000	-2.492160000	40.014032000
7	0.000000000	1.356447000	-30.174014000
7	0.000000000	-1.356447000	-30.174014000
6	0.000000000	0.719267000	-31.402569000
6	0.000000000	-0.719267000	-31.402569000
6	0.000000000	1.403126000	-32.587835000
6	0.000000000	-1.403126000	-32.587835000
6	0.000000000	0.724760000	-33.837683000
6	0.000000000	-0.724760000	-33.837683000
6	0.000000000	1.402020000	-35.049259000
6	0.000000000	-1.402020000	-35.049259000
6	0.000000000	0.724443000	-36.282191000
6	0.000000000	-0.724443000	-36.282191000
6	0.000000000	1.401747000	-37.511056000
6	0.000000000	-1.401747000	-37.511056000
6	0.000000000	0.723255000	-38.725579000
6	0.000000000	-0.723255000	-38.725579000
6	0.000000000	1.403137000	-39.978641000
6	0.000000000	-1.403137000	-39.978641000
6	0.000000000	0.711176000	-41.155541000
6	0.000000000	-0.711176000	-41.155541000
1	0.000000000	2.365524000	-30.174590000
1	0.000000000	-2.365524000	-30.174590000
1	0.000000000	2.489885000	-32.579337000
1	0.000000000	-2.489885000	-32.579337000
1	0.000000000	-2.489399000	-35.049844000
1	0.000000000	2.489399000	-35.049844000
1	0.000000000	2.489357000	-37.511956000
1	0.000000000	-2.489357000	-37.511956000
1	0.000000000	-2.489667000	-39.976005000
1	0.000000000	2.489667000	-39.976005000
1	0.000000000	1.244122000	-42.101039000
1	0.000000000	-1.244122000	-42.101039000

Table S118: Coordinates of pT₆_6 optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	7.190414000	0.729067000
7	0.000000000	6.041905000	1.435293000
6	0.000000000	4.904711000	0.730494000
6	0.000000000	4.904711000	-0.730494000
7	0.000000000	6.041905000	-1.435293000
6	0.000000000	7.190414000	-0.729067000
6	0.000000000	2.455461000	-0.729701000
6	0.000000000	2.455461000	0.729701000

6	0.000000000	1.225206000	1.402747000
1	0.000000000	1.225626000	2.489981000
6	0.000000000	0.000000000	0.728929000
6	0.000000000	0.000000000	-0.728929000
6	0.000000000	1.225206000	-1.402747000
1	0.000000000	1.225626000	-2.489981000
6	0.000000000	-2.455461000	-0.729701000
6	0.000000000	-2.455461000	0.729701000
6	0.000000000	-3.674626000	1.408214000
6	0.000000000	-3.674626000	-1.408214000
6	0.000000000	-4.904711000	-0.730494000
6	0.000000000	-4.904711000	0.730494000
1	0.000000000	-3.696440000	2.494198000
1	0.000000000	-3.696440000	-2.494198000
6	0.000000000	9.636685000	0.728638000
6	0.000000000	9.636685000	-0.728638000
6	0.000000000	10.861693000	-1.403398000
6	0.000000000	10.861693000	1.403398000
6	0.000000000	12.088582000	-0.727536000
6	0.000000000	12.088582000	0.727536000
1	0.000000000	10.861269000	2.490632000
1	0.000000000	10.861269000	-2.490632000
6	0.000000000	-1.225206000	1.402747000
6	0.000000000	-1.225206000	-1.402747000
6	0.000000000	3.674626000	1.408214000
6	0.000000000	3.674626000	-1.408214000
6	0.000000000	8.410018000	1.408366000
6	0.000000000	8.410018000	-1.408366000
6	0.000000000	13.315051000	1.403400000
6	0.000000000	13.315051000	-1.403400000
6	0.000000000	14.540303000	0.728469000
6	0.000000000	14.540303000	-0.728469000
6	0.000000000	15.767059000	1.408272000
6	0.000000000	15.767059000	-1.408272000
6	0.000000000	16.986008000	0.728718000
6	0.000000000	16.986008000	-0.728718000
1	0.000000000	13.315510000	-2.490527000
1	0.000000000	13.315510000	2.490527000
1	0.000000000	8.387499000	-2.494242000
1	0.000000000	8.387499000	2.494242000
1	0.000000000	3.696440000	2.494198000
1	0.000000000	3.696440000	-2.494198000
1	0.000000000	-1.225626000	2.489981000
1	0.000000000	-1.225626000	-2.489981000
1	0.000000000	15.789640000	-2.494139000
1	0.000000000	15.789640000	2.494139000
7	0.000000000	-6.041905000	-1.435293000

7	0.000000000	-6.041905000	1.435293000
6	0.000000000	-7.190414000	-0.729067000
6	0.000000000	-7.190414000	0.729067000
6	0.000000000	-8.410018000	-1.408366000
6	0.000000000	-8.410018000	1.408366000
6	0.000000000	-9.636685000	-0.728638000
6	0.000000000	-9.636685000	0.728638000
6	0.000000000	-10.861693000	-1.403398000
6	0.000000000	-10.861693000	1.403398000
6	0.000000000	-12.088582000	-0.727536000
6	0.000000000	-12.088582000	0.727536000
6	0.000000000	-13.315051000	-1.403400000
6	0.000000000	-13.315051000	1.403400000
6	0.000000000	-14.540303000	-0.728469000
6	0.000000000	-14.540303000	0.728469000
6	0.000000000	-15.767059000	-1.408272000
6	0.000000000	-15.767059000	1.408272000
6	0.000000000	-16.986008000	-0.728718000
6	0.000000000	-16.986008000	0.728718000
1	0.000000000	-8.387499000	-2.494242000
1	0.000000000	-8.387499000	2.494242000
1	0.000000000	-10.861269000	-2.490632000
1	0.000000000	-10.861269000	2.490632000
1	0.000000000	-13.315510000	-2.490527000
1	0.000000000	-13.315510000	2.490527000
1	0.000000000	-15.789640000	-2.494139000
1	0.000000000	-15.789640000	2.494139000
7	0.000000000	-18.135662000	-1.435039000
7	0.000000000	-18.135662000	1.435039000
6	0.000000000	-19.271544000	-0.730406000
6	0.000000000	-19.271544000	0.730406000
6	0.000000000	-20.503341000	-1.408081000
6	0.000000000	-20.503341000	1.408081000
6	0.000000000	-21.720872000	-0.729778000
6	0.000000000	-21.720872000	0.729778000
6	0.000000000	-22.952613000	-1.402567000
6	0.000000000	-22.952613000	1.402567000
6	0.000000000	-24.176922000	-0.729262000
6	0.000000000	-24.176922000	0.729262000
6	0.000000000	-25.402443000	-1.402661000
6	0.000000000	-25.402443000	1.402661000
6	0.000000000	-26.633601000	-0.730353000
6	0.000000000	-26.633601000	0.730353000
6	0.000000000	-27.850625000	-1.408467000
6	0.000000000	-27.850625000	1.408467000
6	0.000000000	-29.085035000	-0.731750000
6	0.000000000	-29.085035000	0.731750000
1	0.000000000	-20.481561000	-2.494075000

1	0.000000000	-20.481561000	2.494075000
1	0.000000000	-22.952122000	-2.489820000
1	0.000000000	-22.952122000	2.489820000
1	0.000000000	-25.402767000	-2.489921000
1	0.000000000	-25.402767000	2.489921000
1	0.000000000	-27.872068000	-2.494498000
1	0.000000000	-27.872068000	2.494498000
7	0.000000000	18.135662000	1.435039000
7	0.000000000	18.135662000	-1.435039000
6	0.000000000	19.271544000	0.730406000
6	0.000000000	19.271544000	-0.730406000
6	0.000000000	20.503341000	1.408081000
6	0.000000000	20.503341000	-1.408081000
6	0.000000000	21.720872000	0.729778000
6	0.000000000	21.720872000	-0.729778000
6	0.000000000	22.952613000	1.402567000
6	0.000000000	22.952613000	-1.402567000
6	0.000000000	24.176922000	0.729262000
6	0.000000000	24.176922000	-0.729262000
6	0.000000000	25.402443000	1.402661000
6	0.000000000	25.402443000	-1.402661000
6	0.000000000	26.633601000	0.730353000
6	0.000000000	26.633601000	-0.730353000
6	0.000000000	27.850625000	1.408467000
6	0.000000000	27.850625000	-1.408467000
6	0.000000000	29.085035000	0.731750000
6	0.000000000	29.085035000	-0.731750000
1	0.000000000	27.872068000	2.494498000
1	0.000000000	27.872068000	-2.494498000
1	0.000000000	25.402767000	-2.489921000
1	0.000000000	25.402767000	2.489921000
1	0.000000000	22.952122000	2.489820000
1	0.000000000	22.952122000	-2.489820000
1	0.000000000	20.481561000	2.494075000
1	0.000000000	20.481561000	-2.494075000
7	0.000000000	30.216822000	1.436147000
7	0.000000000	30.216822000	-1.436147000
6	0.000000000	31.371814000	0.729206000
6	0.000000000	31.371814000	-0.729206000
6	0.000000000	32.584366000	1.408851000
6	0.000000000	32.584366000	-1.408851000
6	0.000000000	33.818180000	0.728344000
6	0.000000000	33.818180000	-0.728344000
6	0.000000000	35.037146000	1.403791000
6	0.000000000	35.037146000	-1.403791000
6	0.000000000	36.267937000	0.725495000
6	0.000000000	36.267937000	-0.725495000

6	0.000000000	37.495209000	1.402288000
6	0.000000000	37.495209000	-1.402288000
6	0.000000000	38.712474000	0.722662000
6	0.000000000	38.712474000	-0.722662000
6	0.000000000	39.962195000	1.402987000
6	0.000000000	39.962195000	-1.402987000
6	0.000000000	41.140928000	0.709826000
6	0.000000000	41.140928000	-0.709826000
1	0.000000000	32.561584000	2.494750000
1	0.000000000	32.561584000	-2.494750000
1	0.000000000	35.037020000	2.490940000
1	0.000000000	35.037020000	-2.490940000
1	0.000000000	37.496172000	2.489681000
1	0.000000000	37.496172000	-2.489681000
1	0.000000000	39.959716000	2.489300000
1	0.000000000	42.086033000	1.243146000
1	0.000000000	42.086033000	-1.243146000
1	0.000000000	39.959716000	-2.489300000
7	0.000000000	-30.216822000	1.436147000
7	0.000000000	-30.216822000	-1.436147000
6	0.000000000	-31.371814000	0.729206000
6	0.000000000	-31.371814000	-0.729206000
6	0.000000000	-32.584366000	1.408851000
6	0.000000000	-32.584366000	-1.408851000
6	0.000000000	-33.818180000	0.728344000
6	0.000000000	-33.818180000	-0.728344000
6	0.000000000	-35.037146000	1.403791000
6	0.000000000	-35.037146000	-1.403791000
6	0.000000000	-36.267937000	0.725495000
6	0.000000000	-36.267937000	-0.725495000
6	0.000000000	-37.495209000	1.402288000
6	0.000000000	-37.495209000	-1.402288000
6	0.000000000	-38.712474000	0.722662000
6	0.000000000	-38.712474000	-0.722662000
6	0.000000000	-39.962195000	1.402987000
6	0.000000000	-39.962195000	-1.402987000
6	0.000000000	-41.140928000	0.709826000
6	0.000000000	-41.140928000	-0.709826000
1	0.000000000	-32.561584000	2.494750000
1	0.000000000	-32.561584000	-2.494750000
1	0.000000000	-35.037020000	-2.490940000
1	0.000000000	-35.037020000	2.490940000
1	0.000000000	-37.496172000	2.489681000
1	0.000000000	-37.496172000	-2.489681000
1	0.000000000	-39.959716000	-2.489300000
1	0.000000000	-39.959716000	2.489300000
1	0.000000000	-42.086033000	1.243146000

1	0.000000000	-42.086033000	-1.243146000
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Table S119-S172: Cartesian coordinates of all the optimized structures at M06/6-311++g(d,p) and M062X/6-311++g(d,p). Atomic number followed by X, Y, Z coordinates in Angstrom.

Table S119: Coordinates of pN₁ at M06/6-311++G(d,p) level

atom	x	y	z
6	6.075784000	0.702856000	-0.000012000
6	6.075783000	-0.702856000	-0.000012000
6	4.889559000	-1.392619000	-0.000007000
6	4.889559000	1.392619000	-0.000008000
6	3.655325000	0.710684000	-0.000003000
6	3.655325000	-0.710683000	-0.000003000
1	4.885309000	-2.480138000	-0.000007000
1	4.885310000	2.480138000	-0.000008000
6	1.226747000	-0.712942000	0.000010000
6	1.226747000	0.712941000	0.000010000
7	0.000000000	1.359706000	0.000019000
7	0.000000000	-1.359706000	0.000020000
6	-1.226747000	0.712942000	0.000010000
6	-1.226747000	-0.712941000	0.000010000
1	0.000000000	2.368816000	0.000064000
1	0.000000000	-2.368816000	0.000051000
6	2.414518000	-1.391708000	0.000001000
6	2.414518000	1.391708000	0.000000000
6	-2.414518000	-1.391708000	0.000001000
6	-2.414518000	1.391708000	0.000000000
6	-3.655325000	-0.710684000	-0.000003000
6	-3.655325000	0.710684000	-0.000003000
6	-4.889559000	-1.392619000	-0.000008000
6	-4.889559000	1.392619000	-0.000008000
6	-6.075783000	-0.702856000	-0.000012000
6	-6.075783000	0.702856000	-0.000012000
1	-4.885310000	-2.480138000	-0.000008000
1	-7.018110000	-1.242170000	-0.000015000
1	-7.018110000	1.242170000	-0.000015000
1	-4.885309000	2.480138000	-0.000008000
1	-2.409131000	2.480262000	-0.000002000
1	-2.409131000	-2.480262000	-0.000001000
1	2.409131000	2.480262000	-0.000003000
1	2.409131000	-2.480262000	0.000000000
1	7.018110000	-1.242170000	-0.000015000
1	7.018110000	1.242170000	-0.000016000

Table S121: Coordinates of pN₂ at M06/6-311++G(d,p) level

atom	x	y	z
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Table S120: Coordinates of pN₁ at M062X/6-311++G(d,p) level

atom	x	y	z
6	6.085399000	0.705407000	-0.000009000
6	6.085399000	-0.705407000	-0.000009000
6	4.897906000	-1.395649000	-0.000005000
6	4.897906000	1.395649000	-0.000005000
6	3.660973000	0.710005000	-0.000002000
6	3.660973000	-0.710005000	-0.000002000
1	4.894125000	-2.480481000	-0.000005000
1	4.894125000	2.480481000	-0.000006000
6	1.229074000	-0.716004000	0.000007000
6	1.229074000	0.716004000	0.000007000
7	0.000000000	1.363825000	0.000014000
7	0.000000000	-1.363825000	0.000015000
6	-1.229074000	0.716004000	0.000007000
6	-1.229074000	-0.716004000	0.000007000
1	0.000000000	2.371178000	0.000044000
1	0.000000000	-2.371178000	0.000035000
6	2.416971000	-1.395394000	0.000001000
6	2.416971000	1.395394000	0.000001000
6	-2.416971000	-1.395394000	0.000001000
6	-2.416971000	1.395394000	0.000001000
6	-3.660973000	-0.710005000	-0.000002000
6	-3.660973000	0.710005000	-0.000002000
6	-4.897906000	-1.395649000	-0.000006000
6	-4.897906000	1.395649000	-0.000006000
6	-6.085399000	-0.705407000	-0.000009000
6	-6.085399000	0.705407000	-0.000009000
1	-4.894125000	-2.480481000	-0.000006000
1	-7.025388000	-1.243875000	-0.000012000
1	-7.025388000	1.243875000	-0.000012000
1	-4.894125000	2.480481000	-0.000006000
1	-2.411924000	2.480849000	-0.000001000
1	-2.411924000	-2.480849000	0.000000000
1	2.411924000	2.480849000	-0.000001000
1	2.411924000	-2.480849000	0.000000000
1	7.025388000	-1.243875000	-0.000011000
1	7.025388000	1.243875000	-0.000012000

Table S122: Coordinates of pN₂ at M062X/6-311++G(d,p) level

atom	x	y	z
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6	9.731978000	-0.702672000	0.000211000	6	9.746739000	-0.705284000	0.000305000
6	9.731978000	0.702672000	0.000219000	6	9.746739000	0.705284000	0.000309000
6	7.311141000	0.710678000	0.000063000	6	7.322121000	0.709592000	0.000085000
6	7.311141000	-0.710678000	0.000055000	6	7.322121000	-0.709592000	0.000081000
6	6.069839000	-1.391474000	-0.000031000	6	6.077523000	-1.395242000	-0.000038000
1	6.064614000	-2.480096000	-0.000032000	1	6.073183000	-2.480770000	-0.000040000
6	4.881397000	-0.713506000	-0.000120000	6	4.889186000	-0.716694000	-0.000162000
6	4.881397000	0.713506000	-0.000118000	6	4.889186000	0.716694000	-0.000159000
6	6.069839000	1.391474000	-0.000020000	6	6.077523000	1.395242000	-0.000032000
1	6.064614000	2.480096000	-0.000021000	1	6.073183000	2.480770000	-0.000033000
6	2.428099000	0.710142000	-0.000157000	6	2.430861000	0.712994000	-0.000221000
6	2.428099000	-0.710142000	-0.000158000	6	2.430861000	-0.712994000	-0.000225000
6	1.237397000	-1.389819000	-0.000102000	6	1.240209000	-1.393157000	-0.000159000
6	1.237397000	1.389819000	-0.000098000	6	1.240209000	1.393157000	-0.000151000
6	0.000000000	0.709709000	-0.000051000	6	0.000000000	0.708174000	-0.000094000
6	0.000000000	-0.709709000	-0.000055000	6	0.000000000	-0.708174000	-0.000100000
1	1.244501000	-2.478492000	-0.000103000	1	1.246349000	-2.478699000	-0.000161000
1	1.244501000	2.478492000	-0.000102000	1	1.246349000	2.478699000	-0.000152000
6	-2.428099000	-0.710142000	0.000023000	6	-2.430861000	-0.712994000	0.000007000
6	-2.428099000	0.710142000	0.000021000	6	-2.430861000	0.712994000	0.000010000
7	-3.655587000	1.360318000	0.000046000	7	-3.660888000	1.364184000	0.000064000
7	-3.655587000	-1.360318000	0.000078000	7	-3.660888000	-1.364184000	0.000073000
6	-4.881397000	0.713506000	0.000050000	6	-4.889186000	0.716694000	0.000066000
6	-4.881397000	-0.713506000	0.000052000	6	-4.889186000	-0.716694000	0.000062000
1	-3.655375000	2.369218000	0.000104000	1	-3.660513000	2.371363000	0.000096000
1	-3.655375000	-2.369218000	0.000003000	1	-3.660513000	-2.371363000	0.000010000
6	-1.237397000	-1.389819000	-0.000014000	6	-1.240209000	-1.393157000	-0.000046000
6	-1.237397000	1.389819000	-0.000013000	6	-1.240209000	1.393157000	-0.000039000
7	3.655587000	-1.360318000	-0.000237000	7	3.660888000	-1.364184000	-0.000322000
7	3.655587000	1.360318000	-0.000252000	7	3.660888000	1.364184000	-0.000325000
6	8.545214000	-1.392317000	0.000131000	6	8.558871000	-1.395289000	0.000195000
6	8.545214000	1.392317000	0.000147000	6	8.558871000	1.395289000	0.000202000
6	-6.069839000	-1.391474000	0.000042000	6	-6.077523000	-1.395242000	0.000061000
6	-6.069839000	1.391474000	0.000047000	6	-6.077523000	1.395242000	0.000070000
6	-7.311141000	-0.710678000	0.000037000	6	-7.322121000	-0.709592000	0.000067000
6	-7.311141000	0.710678000	0.000043000	6	-7.322121000	0.709592000	0.000073000
6	-8.545214000	-1.392317000	0.000028000	6	-8.558871000	-1.395289000	0.000068000
6	-8.545214000	1.392317000	0.000041000	6	-8.558871000	1.395289000	0.000079000
6	-9.731978000	-0.702672000	0.000026000	6	-9.746739000	-0.705284000	0.000073000
6	-9.731978000	0.702672000	0.000033000	6	-9.746739000	0.705284000	0.000079000
1	-8.540998000	-2.479894000	0.000023000	1	-8.554842000	-2.480214000	0.000064000
1	-10.674169000	-1.242297000	0.000019000	1	-10.686870000	-1.243721000	0.000074000
1	-10.674168000	1.242298000	0.000031000	1	-10.686870000	1.243721000	0.000083000
1	-8.540998000	2.479894000	0.000045000	1	-8.554842000	2.480214000	0.000082000
1	-6.064614000	2.480096000	0.000042000	1	-6.073183000	2.480770000	0.000070000
1	-6.064614000	-2.480096000	0.000045000	1	-6.073183000	-2.480770000	0.000061000
1	-1.244501000	2.478492000	-0.000020000	1	-1.246349000	2.478699000	-0.000040000

1	-1.244501000	-2.478492000	-0.000010000
1	3.655375000	2.369218000	-0.000116000
1	3.655375000	-2.369218000	-0.000185000
1	8.540998000	-2.479894000	0.000124000
1	8.540998000	2.479894000	0.000152000
1	10.674169000	-1.242297000	0.000268000
1	10.674168000	1.242298000	0.000283000

1	-1.246349000	-2.478699000	-0.000046000
1	3.660513000	2.371363000	-0.000204000
1	3.660513000	-2.371363000	-0.000259000
1	8.554842000	-2.480214000	0.000191000
1	8.554842000	2.480214000	0.000203000
1	10.686870000	-1.243721000	0.000391000
1	10.686870000	1.243721000	0.000397000

TableS123: Coordinates of pN₃ at M06/6-311++G(d,p) level

atom	x	y	z
6	0.000000000	8.532580000	0.713757000
7	0.000000000	7.307367000	1.360592000
6	0.000000000	6.079651000	0.709949000
6	0.000000000	6.079651000	-0.709949000
7	0.000000000	7.307367000	-1.360592000
6	0.000000000	8.532580000	-0.713757000
6	0.000000000	3.652619000	-0.709384000
6	0.000000000	3.652619000	0.709384000
6	0.000000000	2.416007000	1.390263000
1	0.000000000	2.409511000	2.478925000
6	0.000000000	1.225806000	0.710869000
6	0.000000000	1.225806000	-0.710869000
6	0.000000000	2.416007000	-1.390263000
1	0.000000000	7.307007000	2.369405000
1	0.000000000	7.307007000	-2.369405000
1	0.000000000	2.409511000	-2.478925000
6	0.000000000	-1.225806000	-0.710869000
6	0.000000000	-1.225806000	0.710869000
6	0.000000000	-2.416007000	1.390263000
6	0.000000000	-2.416007000	-1.390263000
6	0.000000000	-3.652619000	-0.709384000
6	0.000000000	-3.652619000	0.709384000
1	0.000000000	-2.409511000	2.478925000
1	0.000000000	-2.409511000	-2.478925000
6	0.000000000	10.962804000	0.710533000
6	0.000000000	10.962804000	-0.710533000
6	0.000000000	12.197207000	-1.392362000
6	0.000000000	12.197207000	1.392362000
6	0.000000000	13.384047000	-0.702845000
6	0.000000000	13.384047000	0.702845000
1	0.000000000	12.192438000	2.479940000
1	0.000000000	12.192438000	-2.479940000
6	0.000000000	-6.079651000	0.709949000
6	0.000000000	-6.079651000	-0.709949000
7	0.000000000	-7.307367000	-1.360592000
7	0.000000000	-7.307367000	1.360592000

TableS124: Coordinates of pN₃ at M062X/6-311++G(d,p) level

atom	x	y	z
6	0.000000000	8.544610000	0.717047000
7	0.000000000	7.316884000	1.364021000
6	0.000000000	6.086773000	0.712853000
6	0.000000000	6.086773000	-0.712853000
7	0.000000000	7.316884000	-1.364021000
6	0.000000000	8.544610000	-0.717047000
6	0.000000000	3.657236000	-0.707991000
6	0.000000000	3.657236000	0.707991000
6	0.000000000	2.418038000	1.393680000
1	0.000000000	2.412273000	2.479293000
6	0.000000000	1.228108000	0.713899000
6	0.000000000	1.228108000	-0.713899000
6	0.000000000	2.418038000	-1.393680000
1	0.000000000	7.316356000	2.371283000
1	0.000000000	7.316356000	-2.371283000
1	0.000000000	2.412273000	-2.479293000
6	0.000000000	-1.228108000	-0.713899000
6	0.000000000	-1.228108000	0.713899000
6	0.000000000	-2.418038000	1.393680000
6	0.000000000	-2.418038000	-1.393680000
6	0.000000000	-3.657236000	-0.707991000
6	0.000000000	-3.657236000	0.707991000
1	0.000000000	-2.412273000	2.479293000
1	0.000000000	-2.412273000	-2.479293000
6	0.000000000	10.978178000	0.709672000
6	0.000000000	10.978178000	-0.709672000
6	0.000000000	12.215189000	-1.395120000
6	0.000000000	12.215189000	1.395120000
6	0.000000000	13.403495000	-0.705228000
6	0.000000000	13.403495000	0.705228000
1	0.000000000	12.210905000	2.480089000
1	0.000000000	12.210905000	-2.480089000
6	0.000000000	-6.086773000	0.712853000
6	0.000000000	-6.086773000	-0.712853000
7	0.000000000	-7.316884000	-1.364021000
7	0.000000000	-7.316884000	1.364021000

6	0.000000000	-8.532580000	-0.713757000	6	0.000000000	-8.544610000	-0.717047000
6	0.000000000	-8.532580000	0.713757000	6	0.000000000	-8.544610000	0.717047000
1	0.000000000	-7.307007000	-2.369405000	1	0.000000000	-7.316356000	-2.371283000
1	0.000000000	-7.307007000	2.369405000	1	0.000000000	-7.316356000	2.371283000
6	0.000000000	-4.889237000	1.389832000	6	0.000000000	-4.896377000	1.393163000
6	0.000000000	-4.889237000	-1.389832000	6	0.000000000	-4.896377000	-1.393163000
7	0.000000000	0.000000000	1.361363000	7	0.000000000	0.000000000	1.364991000
7	0.000000000	0.000000000	-1.361363000	7	0.000000000	0.000000000	-1.364991000
6	0.000000000	4.889237000	1.389832000	6	0.000000000	4.896377000	1.393163000
6	0.000000000	4.889237000	-1.389832000	6	0.000000000	4.896377000	-1.393163000
6	0.000000000	9.720949000	1.391465000	6	0.000000000	9.732882000	1.395259000
6	0.000000000	9.720949000	-1.391465000	6	0.000000000	9.732882000	-1.395259000
6	0.000000000	-9.720949000	1.391465000	6	0.000000000	-9.732882000	1.395259000
6	0.000000000	-9.720949000	-1.391465000	6	0.000000000	-9.732882000	-1.395259000
6	0.000000000	-10.962804000	0.710533000	6	0.000000000	-10.978178000	0.709672000
6	0.000000000	-10.962804000	-0.710533000	6	0.000000000	-10.978178000	-0.709672000
6	0.000000000	-12.197207000	1.392362000	6	0.000000000	-12.215189000	1.395120000
6	0.000000000	-12.197207000	-1.392362000	6	0.000000000	-12.215189000	-1.395120000
6	0.000000000	-13.384047000	0.702845000	6	0.000000000	-13.403495000	0.705228000
6	0.000000000	-13.384047000	-0.702845000	6	0.000000000	-13.403495000	-0.705228000
1	0.000000000	-12.192438000	2.479940000	1	0.000000000	-12.210905000	2.480089000
1	0.000000000	-14.326379000	1.242230000	1	0.000000000	-14.343596000	1.243809000
1	0.000000000	-14.326379000	-1.242230000	1	0.000000000	-14.343596000	-1.243809000
1	0.000000000	-12.192438000	-2.479940000	1	0.000000000	-12.210905000	-2.480089000
1	0.000000000	-9.716240000	-2.480102000	1	0.000000000	-9.728563000	-2.480840000
1	0.000000000	-9.716240000	2.480102000	1	0.000000000	-9.728563000	2.480840000
1	0.000000000	-4.895183000	-2.478503000	1	0.000000000	-4.901966000	-2.478777000
1	0.000000000	-4.895183000	2.478503000	1	0.000000000	-4.901966000	2.478777000
1	0.000000000	0.000000000	-2.369957000	1	0.000000000	0.000000000	-2.372041000
1	0.000000000	0.000000000	2.369957000	1	0.000000000	0.000000000	2.372041000
1	0.000000000	4.895183000	2.478503000	1	0.000000000	4.901966000	2.478777000
1	0.000000000	4.895183000	-2.478503000	1	0.000000000	4.901966000	-2.478777000
1	0.000000000	9.716240000	-2.480102000	1	0.000000000	9.728563000	-2.480840000
1	0.000000000	9.716240000	2.480102000	1	0.000000000	9.728563000	2.480840000
1	0.000000000	14.326379000	1.242230000	1	0.000000000	14.343596000	1.243809000
1	0.000000000	14.326379000	-1.242230000	1	0.000000000	14.343596000	-1.243809000

TableS125: Coordinates of pN₄ at M06/6-311++G(d,p) level

atom	x	y	z
6	0.000000000	4.880306000	0.711202000
7	0.000000000	3.654308000	1.360784000
6	0.000000000	2.427504000	0.710738000
6	0.000000000	2.427504000	-0.710738000
7	0.000000000	3.654308000	-1.360784000
6	0.000000000	4.880306000	-0.711202000
6	0.000000000	0.000000000	-0.709319000

TableS126: Coordinates of pN₄ at M062X/6-311++G(d,p) level

atom	x	y	z
6	0.000000000	4.887439000	0.713762000
7	0.000000000	3.659267000	1.365318000
6	0.000000000	2.430235000	0.713268000
6	0.000000000	2.430235000	-0.713268000
7	0.000000000	3.659267000	-1.365318000
6	0.000000000	4.887439000	-0.713762000
6	0.000000000	0.000000000	-0.707943000

6	0.000000000	0.000000000	0.709319000	6	0.000000000	0.000000000	0.707943000
6	0.000000000	-1.236941000	1.389952000	6	0.000000000	-1.239647000	1.392985000
1	0.000000000	-1.243002000	2.478699000	1	0.000000000	-1.245400000	2.478542000
6	0.000000000	-2.427504000	0.710738000	6	0.000000000	-2.430235000	0.713268000
6	0.000000000	-2.427504000	-0.710738000	6	0.000000000	-2.430235000	-0.713268000
6	0.000000000	-1.236941000	-1.389952000	6	0.000000000	-1.239647000	-1.392985000
1	0.000000000	3.654352000	2.369464000	1	0.000000000	3.659236000	2.372175000
1	0.000000000	3.654352000	-2.369464000	1	0.000000000	3.659236000	-2.372175000
1	0.000000000	-1.243002000	-2.478699000	1	0.000000000	-1.245400000	-2.478542000
6	0.000000000	-4.880306000	-0.711202000	6	0.000000000	-4.887439000	-0.713762000
6	0.000000000	-4.880306000	0.711202000	6	0.000000000	-4.887439000	0.713762000
6	0.000000000	-6.071218000	1.389878000	6	0.000000000	-6.078280000	1.392975000
6	0.000000000	-6.071218000	-1.389878000	6	0.000000000	-6.078280000	-1.392975000
6	0.000000000	-7.309021000	-0.709397000	6	0.000000000	-7.318834000	-0.708093000
6	0.000000000	-7.309021000	0.709397000	6	0.000000000	-7.318834000	0.708093000
1	0.000000000	-6.064756000	2.478594000	1	0.000000000	-6.071868000	2.478536000
1	0.000000000	-6.064756000	-2.478594000	1	0.000000000	-6.071868000	-2.478536000
6	0.000000000	7.309021000	0.709397000	6	0.000000000	7.318834000	0.708093000
6	0.000000000	7.309021000	-0.709397000	6	0.000000000	7.318834000	-0.708093000
6	0.000000000	8.545711000	-1.389871000	6	0.000000000	8.558246000	-1.392834000
6	0.000000000	8.545711000	1.389871000	6	0.000000000	8.558246000	1.392834000
6	0.000000000	9.736287000	-0.710022000	6	0.000000000	9.748976000	-0.712495000
6	0.000000000	9.736287000	0.710022000	6	0.000000000	9.748976000	0.712495000
1	0.000000000	8.552101000	2.478590000	1	0.000000000	8.564484000	2.478417000
1	0.000000000	8.552101000	-2.478590000	1	0.000000000	8.564484000	-2.478417000
6	0.000000000	-9.736287000	0.710022000	6	0.000000000	-9.748976000	0.712495000
6	0.000000000	-9.736287000	-0.710022000	6	0.000000000	-9.748976000	-0.712495000
7	0.000000000	-10.964078000	-1.360120000	7	0.000000000	-10.979059000	-1.364603000
7	0.000000000	-10.964078000	1.360120000	7	0.000000000	-10.979059000	1.364603000
6	0.000000000	-12.189277000	-0.713950000	6	0.000000000	-12.206511000	-0.716825000
6	0.000000000	-12.189277000	0.713950000	6	0.000000000	-12.206511000	0.716825000
1	0.000000000	-10.963657000	-2.369012000	1	0.000000000	-10.978379000	-2.371704000
1	0.000000000	-10.963657000	2.369012000	1	0.000000000	-10.978379000	2.371704000
6	0.000000000	-8.545711000	1.389871000	6	0.000000000	-8.558246000	1.392834000
6	0.000000000	-8.545711000	-1.389871000	6	0.000000000	-8.558246000	-1.392834000
7	0.000000000	-3.654308000	1.360784000	7	0.000000000	-3.659267000	1.365318000
7	0.000000000	-3.654308000	-1.360784000	7	0.000000000	-3.659267000	-1.365318000
6	0.000000000	1.236941000	1.389952000	6	0.000000000	1.239647000	1.392985000
6	0.000000000	1.236941000	-1.389952000	6	0.000000000	1.239647000	-1.392985000
6	0.000000000	6.071218000	1.389878000	6	0.000000000	6.078280000	1.392975000
6	0.000000000	6.071218000	-1.389878000	6	0.000000000	6.078280000	-1.392975000
7	0.000000000	10.964078000	1.360120000	7	0.000000000	10.979059000	1.364603000
7	0.000000000	10.964078000	-1.360120000	7	0.000000000	10.979059000	-1.364603000
6	0.000000000	12.189277000	0.713950000	6	0.000000000	12.206511000	0.716825000
6	0.000000000	12.189277000	-0.713950000	6	0.000000000	12.206511000	-0.716825000
6	0.000000000	13.377425000	1.391606000	6	0.000000000	13.394635000	1.395072000
6	0.000000000	13.377425000	-1.391606000	6	0.000000000	13.394635000	-1.395072000
6	0.000000000	14.619525000	0.710598000	6	0.000000000	14.639956000	0.709707000

6	0.000000000	14.619525000	-0.710598000	6	0.000000000	14.639956000	-0.709707000
6	0.000000000	-13.377425000	1.391606000	6	0.000000000	-13.394635000	1.395072000
6	0.000000000	-13.377425000	-1.391606000	6	0.000000000	-13.394635000	-1.395072000
6	0.000000000	-14.619525000	0.710598000	6	0.000000000	-14.639956000	0.709707000
6	0.000000000	-14.619525000	-0.710598000	6	0.000000000	-14.639956000	-0.709707000
6	0.000000000	-15.854133000	1.392318000	6	0.000000000	-15.877056000	1.395061000
6	0.000000000	-15.854133000	-1.392318000	6	0.000000000	-15.877056000	-1.395061000
6	0.000000000	-17.041117000	0.702816000	6	0.000000000	-17.065249000	0.705227000
6	0.000000000	-17.041117000	-0.702816000	6	0.000000000	-17.065249000	-0.705227000
1	0.000000000	-15.849145000	2.479898000	1	0.000000000	-15.873041000	2.479996000
1	0.000000000	-17.983573000	1.242016000	1	0.000000000	-18.005079000	1.244165000
1	0.000000000	-17.983573000	-1.242016000	1	0.000000000	-18.005079000	-1.244165000
1	0.000000000	-15.849145000	-2.479898000	1	0.000000000	-15.873041000	-2.479996000
1	0.000000000	-13.372483000	-2.480229000	1	0.000000000	-13.389807000	-2.480603000
1	0.000000000	-13.372483000	2.480229000	1	0.000000000	-13.389807000	2.480603000
1	0.000000000	-8.552101000	-2.478590000	1	0.000000000	-8.564484000	-2.478417000
1	0.000000000	-8.552101000	2.478590000	1	0.000000000	-8.564484000	2.478417000
1	0.000000000	-3.654352000	-2.369464000	1	0.000000000	-3.659236000	-2.372175000
1	0.000000000	-3.654352000	2.369464000	1	0.000000000	-3.659236000	2.372175000
1	0.000000000	1.243002000	2.478699000	1	0.000000000	1.245400000	2.478542000
1	0.000000000	1.243002000	-2.478699000	1	0.000000000	1.245400000	-2.478542000
1	0.000000000	6.064756000	-2.478594000	1	0.000000000	6.071868000	-2.478536000
1	0.000000000	6.064756000	2.478594000	1	0.000000000	6.071868000	2.478536000
1	0.000000000	10.963657000	-2.369012000	1	0.000000000	10.978379000	-2.371704000
1	0.000000000	10.963657000	2.369012000	1	0.000000000	10.978379000	2.371704000
1	0.000000000	13.372483000	-2.480229000	1	0.000000000	13.389807000	-2.480603000
1	0.000000000	13.372483000	2.480229000	1	0.000000000	13.389807000	2.480603000
6	0.000000000	15.854133000	1.392318000	6	0.000000000	15.877056000	1.395061000
6	0.000000000	15.854133000	-1.392318000	6	0.000000000	15.877056000	-1.395061000
6	0.000000000	17.041117000	0.702816000	6	0.000000000	17.065249000	0.705227000
6	0.000000000	17.041117000	-0.702816000	6	0.000000000	17.065249000	-0.705227000
1	0.000000000	15.849145000	2.479898000	1	0.000000000	15.873041000	2.479996000
1	0.000000000	15.849145000	-2.479898000	1	0.000000000	15.873041000	-2.479996000
1	0.000000000	17.983573000	-1.242016000	1	0.000000000	18.005079000	-1.244165000
1	0.000000000	17.983573000	1.242016000	1	0.000000000	18.005079000	1.244165000

Table S127. Coordinates of pN₅ at M06/6-311++G(d,p) level

atom	x	y	z
6	0.000000000	8.534656000	0.710936000
7	0.000000000	7.308912000	1.361081000
6	0.000000000	6.082017000	0.710251000
6	0.000000000	6.082017000	-0.710251000
7	0.000000000	7.308912000	-1.361081000
6	0.000000000	8.534656000	-0.710936000
6	0.000000000	3.654228000	-0.709570000
6	0.000000000	3.654228000	0.709570000
6	0.000000000	2.417040000	1.389639000

Table S128. Coordinates of pN₅ at M062X/6-311++G(d,p) level

atom	x	y	z
6	0.000000000	8.547803000	0.713833000
7	0.000000000	7.319588000	1.365302000
6	0.000000000	6.090313000	0.713157000
6	0.000000000	6.090313000	-0.713157000
7	0.000000000	7.319588000	-1.365302000
6	0.000000000	8.547803000	-0.713833000
6	0.000000000	3.659664000	-0.707960000
6	0.000000000	3.659664000	0.707960000
6	0.000000000	2.419537000	1.392875000

1	0.000000000	2.410308000	2.478358000	1	0.000000000	2.413684000	2.478456000
6	0.000000000	1.226253000	0.710499000	6	0.000000000	1.228802000	0.713428000
6	0.000000000	1.226253000	-0.710499000	6	0.000000000	1.228802000	-0.713428000
6	0.000000000	2.417040000	-1.389639000	6	0.000000000	2.419537000	-1.392875000
1	0.000000000	7.308650000	2.369665000	1	0.000000000	7.319248000	2.372166000
1	0.000000000	7.308650000	-2.369665000	1	0.000000000	7.319248000	-2.372166000
1	0.000000000	2.410308000	-2.478358000	1	0.000000000	2.413684000	-2.478456000
6	0.000000000	-1.226253000	-0.710499000	6	0.000000000	-1.228802000	-0.713428000
6	0.000000000	-1.226253000	0.710499000	6	0.000000000	-1.228802000	0.713428000
6	0.000000000	-2.417040000	1.389639000	6	0.000000000	-2.419537000	1.392875000
6	0.000000000	-2.417040000	-1.389639000	6	0.000000000	-2.419537000	-1.392875000
6	0.000000000	-3.654228000	-0.709570000	6	0.000000000	-3.659664000	-0.707960000
6	0.000000000	-3.654228000	0.709570000	6	0.000000000	-3.659664000	0.707960000
1	0.000000000	-2.410308000	2.478358000	1	0.000000000	-2.413684000	2.478456000
1	0.000000000	-2.410308000	-2.478358000	1	0.000000000	-2.413684000	-2.478456000
6	0.000000000	10.963487000	0.709702000	6	0.000000000	10.979382000	0.708112000
6	0.000000000	10.963487000	-0.709702000	6	0.000000000	10.979382000	-0.708112000
6	0.000000000	12.200668000	-1.389468000	6	0.000000000	12.219398000	-1.392631000
6	0.000000000	12.200668000	1.389468000	6	0.000000000	12.219398000	1.392631000
6	0.000000000	13.391714000	-0.709628000	6	0.000000000	13.410367000	-0.712476000
6	0.000000000	13.391714000	0.709628000	6	0.000000000	13.410367000	0.712476000
1	0.000000000	12.207622000	2.478184000	1	0.000000000	12.225559000	2.478232000
1	0.000000000	12.207622000	-2.478184000	1	0.000000000	12.225559000	-2.478232000
6	0.000000000	-6.082017000	0.710251000	6	0.000000000	-6.090313000	0.713157000
6	0.000000000	-6.082017000	-0.710251000	6	0.000000000	-6.090313000	-0.713157000
7	0.000000000	-7.308912000	-1.361081000	7	0.000000000	-7.319588000	-1.365302000
7	0.000000000	-7.308912000	1.361081000	7	0.000000000	-7.319588000	1.365302000
6	0.000000000	-8.534656000	-0.710936000	6	0.000000000	-8.547803000	-0.713833000
6	0.000000000	-8.534656000	0.710936000	6	0.000000000	-8.547803000	0.713833000
1	0.000000000	-7.308650000	-2.369665000	1	0.000000000	-7.319248000	-2.372166000
1	0.000000000	-7.308650000	2.369665000	1	0.000000000	-7.319248000	2.372166000
6	0.000000000	-4.891093000	1.389573000	6	0.000000000	-4.899449000	1.392783000
6	0.000000000	-4.891093000	-1.389573000	6	0.000000000	-4.899449000	-1.392783000
7	0.000000000	0.000000000	1.361102000	7	0.000000000	0.000000000	1.365285000
7	0.000000000	0.000000000	-1.361102000	7	0.000000000	0.000000000	-1.365285000
6	0.000000000	4.891093000	1.389573000	6	0.000000000	4.899449000	1.392783000
6	0.000000000	4.891093000	-1.389573000	6	0.000000000	4.899449000	-1.392783000
6	0.000000000	9.725650000	1.389753000	6	0.000000000	9.738643000	1.393015000
6	0.000000000	9.725650000	-1.389753000	6	0.000000000	9.738643000	-1.393015000
7	0.000000000	14.619753000	1.360333000	7	0.000000000	14.640757000	1.364509000
7	0.000000000	14.619753000	-1.360333000	7	0.000000000	14.640757000	-1.364509000
6	0.000000000	15.845066000	0.713699000	6	0.000000000	15.868452000	0.716885000
6	0.000000000	15.845066000	-0.713699000	6	0.000000000	15.868452000	-0.716885000
6	0.000000000	17.033630000	1.391487000	6	0.000000000	17.056791000	1.395133000
6	0.000000000	17.033630000	-1.391487000	6	0.000000000	17.056791000	-1.395133000
6	0.000000000	18.275336000	0.710796000	6	0.000000000	18.301900000	0.709678000
6	0.000000000	18.275336000	-0.710796000	6	0.000000000	18.301900000	-0.709678000
6	0.000000000	-9.725650000	1.389753000	6	0.000000000	-9.738643000	1.393015000

6	0.000000000	-9.725650000	-1.389753000	6	0.000000000	-9.738643000	-1.393015000
6	0.000000000	-10.963487000	0.709702000	6	0.000000000	-10.979382000	0.708112000
6	0.000000000	-10.963487000	-0.709702000	6	0.000000000	-10.979382000	-0.708112000
6	0.000000000	-12.200668000	1.389468000	6	0.000000000	-12.219398000	1.392631000
6	0.000000000	-12.200668000	-1.389468000	6	0.000000000	-12.219398000	-1.392631000
6	0.000000000	-13.391714000	0.709628000	6	0.000000000	-13.410367000	0.712476000
6	0.000000000	-13.391714000	-0.709628000	6	0.000000000	-13.410367000	-0.712476000
1	0.000000000	-12.207622000	2.478184000	1	0.000000000	-12.225559000	2.478232000
1	0.000000000	-12.207622000	-2.478184000	1	0.000000000	-12.225559000	-2.478232000
1	0.000000000	-9.718569000	-2.478467000	1	0.000000000	-9.732188000	-2.478584000
1	0.000000000	-9.718569000	2.478467000	1	0.000000000	-9.732188000	2.478584000
1	0.000000000	-4.897982000	-2.478303000	1	0.000000000	-4.905574000	-2.478378000
1	0.000000000	-4.897982000	2.478303000	1	0.000000000	-4.905574000	2.478378000
1	0.000000000	0.000000000	-2.369659000	1	0.000000000	0.000000000	-2.372132000
1	0.000000000	0.000000000	2.369659000	1	0.000000000	0.000000000	2.372132000
1	0.000000000	4.897982000	2.478303000	1	0.000000000	4.905574000	2.478378000
1	0.000000000	4.897982000	-2.478303000	1	0.000000000	4.905574000	-2.478378000
1	0.000000000	9.718569000	-2.478467000	1	0.000000000	9.732188000	-2.478584000
1	0.000000000	9.718569000	2.478467000	1	0.000000000	9.732188000	2.478584000
1	0.000000000	14.619209000	-2.369148000	1	0.000000000	14.639990000	-2.371617000
1	0.000000000	14.619209000	2.369148000	1	0.000000000	14.639990000	2.371617000
1	0.000000000	17.028265000	-2.480105000	1	0.000000000	17.052206000	-2.480668000
1	0.000000000	17.028265000	2.480105000	1	0.000000000	17.052206000	2.480668000
6	0.000000000	19.509856000	1.392111000	6	0.000000000	19.538960000	1.395062000
6	0.000000000	19.509856000	-1.392111000	6	0.000000000	19.538960000	-1.395062000
6	0.000000000	20.696990000	0.702643000	6	0.000000000	20.727135000	0.705227000
6	0.000000000	20.696990000	-0.702643000	6	0.000000000	20.727135000	-0.705227000
1	0.000000000	19.505472000	2.479702000	1	0.000000000	19.534972000	2.479999000
1	0.000000000	19.505472000	-2.479702000	1	0.000000000	19.534972000	-2.479999000
1	0.000000000	21.639088000	-1.242463000	1	0.000000000	21.667008000	-1.244110000
1	0.000000000	21.639088000	1.242463000	1	0.000000000	21.667008000	1.244110000
7	0.000000000	-14.619753000	-1.360333000	7	0.000000000	-14.640757000	-1.364509000
7	0.000000000	-14.619753000	1.360333000	7	0.000000000	-14.640757000	1.364509000
6	0.000000000	-15.845066000	-0.713699000	6	0.000000000	-15.868452000	-0.716885000
6	0.000000000	-15.845066000	0.713699000	6	0.000000000	-15.868452000	0.716885000
6	0.000000000	-17.033630000	-1.391487000	6	0.000000000	-17.056791000	-1.395133000
6	0.000000000	-17.033630000	1.391487000	6	0.000000000	-17.056791000	1.395133000
6	0.000000000	-18.275336000	-0.710796000	6	0.000000000	-18.301900000	-0.709678000
6	0.000000000	-18.275336000	0.710796000	6	0.000000000	-18.301900000	0.709678000
1	0.000000000	-17.028265000	-2.480105000	1	0.000000000	-17.052206000	-2.480668000
1	0.000000000	-17.028265000	2.480105000	1	0.000000000	-17.052206000	2.480668000
1	0.000000000	-14.619209000	-2.369148000	1	0.000000000	-14.639990000	-2.371617000
1	0.000000000	-14.619209000	2.369148000	1	0.000000000	-14.639990000	2.371617000
6	0.000000000	-20.696990000	-0.702643000	6	0.000000000	-20.727135000	-0.705227000
6	0.000000000	-20.696990000	0.702643000	6	0.000000000	-20.727135000	0.705227000
6	0.000000000	-19.509856000	1.392111000	6	0.000000000	-19.538960000	1.395062000
6	0.000000000	-19.509856000	-1.392111000	6	0.000000000	-19.538960000	-1.395062000
1	0.000000000	-19.505472000	2.479702000	1	0.000000000	-19.534972000	2.479999000

1	0.000000000	-19.505472000	-2.479702000	1	0.000000000	-19.534972000	-2.479999000
1	0.000000000	-21.639088000	1.242463000	1	0.000000000	-21.667008000	1.244110000
1	0.000000000	-21.639088000	-1.242463000	1	0.000000000	-21.667008000	-1.244110000
Table S129. Coordinates of pN ₆ at M06/6-311++G(d,p) level				Table S130. Coordinates of pN ₆ at M062X/6-311++G(d,p) level			
atom	x	y	z	atom	x	y	z
6	0.000000000	4.882880000	0.710617000	6	0.000000000	4.890621000	0.713530000
7	0.000000000	3.656350000	1.361172000	7	0.000000000	3.661545000	1.365095000
6	0.000000000	2.429530000	0.710444000	6	0.000000000	2.432209000	0.713373000
6	0.000000000	2.429530000	-0.710444000	6	0.000000000	2.432209000	-0.713373000
7	0.000000000	3.656350000	-1.361172000	7	0.000000000	3.661545000	-1.365095000
6	0.000000000	4.882880000	-0.710617000	6	0.000000000	4.890621000	-0.713530000
6	0.000000000	0.000000000	-0.709572000	6	0.000000000	0.000000000	-0.707968000
6	0.000000000	0.000000000	0.709572000	6	0.000000000	0.000000000	0.707968000
6	0.000000000	-1.237870000	1.389254000	6	0.000000000	-1.240682000	1.392593000
1	0.000000000	-1.244886000	2.478055000	1	0.000000000	-1.246649000	2.478225000
6	0.000000000	-2.429530000	0.710444000	6	0.000000000	-2.432209000	0.713373000
6	0.000000000	-2.429530000	-0.710444000	6	0.000000000	-2.432209000	-0.713373000
6	0.000000000	-1.237870000	-1.389254000	6	0.000000000	-1.240682000	-1.392593000
1	0.000000000	3.656294000	2.369784000	1	0.000000000	3.661491000	2.371976000
1	0.000000000	3.656294000	-2.369784000	1	0.000000000	3.661491000	-2.371976000
1	0.000000000	-1.244886000	-2.478055000	1	0.000000000	-1.246649000	-2.478225000
6	0.000000000	-4.882880000	-0.710617000	6	0.000000000	-4.890621000	-0.713530000
6	0.000000000	-4.882880000	0.710617000	6	0.000000000	-4.890621000	0.713530000
6	0.000000000	-6.074576000	1.389310000	6	0.000000000	-6.082175000	1.392660000
6	0.000000000	-6.074576000	-1.389310000	6	0.000000000	-6.082175000	-1.392660000
6	0.000000000	-7.312509000	-0.709581000	6	0.000000000	-7.322901000	-0.707978000
6	0.000000000	-7.312509000	0.709581000	6	0.000000000	-7.322901000	0.707978000
1	0.000000000	-6.067585000	2.478103000	1	0.000000000	-6.076230000	2.478281000
1	0.000000000	-6.067585000	-2.478103000	1	0.000000000	-6.076230000	-2.478281000
6	0.000000000	7.312509000	0.709581000	6	0.000000000	7.322901000	0.707978000
6	0.000000000	7.312509000	-0.709581000	6	0.000000000	7.322901000	-0.707978000
6	0.000000000	8.550253000	-1.389261000	6	0.000000000	8.563469000	-1.392590000
6	0.000000000	8.550253000	1.389261000	6	0.000000000	8.563469000	1.392590000
6	0.000000000	9.741768000	-0.710235000	6	0.000000000	9.754864000	-0.713173000
6	0.000000000	9.741768000	0.710235000	6	0.000000000	9.754864000	0.713173000
1	0.000000000	8.557327000	2.478059000	1	0.000000000	8.569501000	2.478221000
1	0.000000000	8.557327000	-2.478059000	1	0.000000000	8.569501000	-2.478221000
6	0.000000000	-9.741768000	0.710235000	6	0.000000000	-9.754864000	0.713173000
6	0.000000000	-9.741768000	-0.710235000	6	0.000000000	-9.754864000	-0.713173000
7	0.000000000	-10.968942000	-1.361116000	7	0.000000000	-10.984525000	-1.365039000
7	0.000000000	-10.968942000	1.361116000	7	0.000000000	-10.984525000	1.365039000
6	0.000000000	-12.195017000	-0.711003000	6	0.000000000	-12.213175000	-0.713912000
6	0.000000000	-12.195017000	0.711003000	6	0.000000000	-12.213175000	0.713912000
1	0.000000000	-10.968745000	-2.369756000	1	0.000000000	-10.984319000	-2.371947000
1	0.000000000	-10.968745000	2.369756000	1	0.000000000	-10.984319000	2.371947000
6	0.000000000	-8.550253000	1.389261000	6	0.000000000	-8.563469000	1.392590000

6	0.000000000	-8.550253000	-1.389261000	6	0.000000000	-8.563469000	-1.392590000
7	0.000000000	-3.656350000	1.361172000	7	0.000000000	-3.661545000	1.365095000
7	0.000000000	-3.656350000	-1.361172000	7	0.000000000	-3.661545000	-1.365095000
6	0.000000000	1.237870000	1.389254000	6	0.000000000	1.240682000	1.392593000
6	0.000000000	1.237870000	-1.389254000	6	0.000000000	1.240682000	-1.392593000
6	0.000000000	6.074576000	1.389310000	6	0.000000000	6.082175000	1.392660000
6	0.000000000	6.074576000	-1.389310000	6	0.000000000	6.082175000	-1.392660000
7	0.000000000	10.968942000	1.361116000	7	0.000000000	10.984525000	1.365039000
7	0.000000000	10.968942000	-1.361116000	7	0.000000000	10.984525000	-1.365039000
6	0.000000000	12.195017000	0.711003000	6	0.000000000	12.213175000	0.713912000
6	0.000000000	12.195017000	-0.711003000	6	0.000000000	12.213175000	-0.713912000
6	0.000000000	13.386522000	1.389564000	6	0.000000000	13.404533000	1.392949000
6	0.000000000	13.386522000	-1.389564000	6	0.000000000	13.404533000	-1.392949000
6	0.000000000	14.624633000	0.709656000	6	0.000000000	14.645457000	0.708076000
6	0.000000000	14.624633000	-0.709656000	6	0.000000000	14.645457000	-0.708076000
6	0.000000000	-13.386522000	1.389564000	6	0.000000000	-13.404533000	1.392949000
6	0.000000000	-13.386522000	-1.389564000	6	0.000000000	-13.404533000	-1.392949000
6	0.000000000	-14.624633000	0.709656000	6	0.000000000	-14.645457000	0.708076000
6	0.000000000	-14.624633000	-0.709656000	6	0.000000000	-14.645457000	-0.708076000
6	0.000000000	-15.861820000	1.389459000	6	0.000000000	-15.885446000	1.392764000
6	0.000000000	-15.861820000	-1.389459000	6	0.000000000	-15.885446000	-1.392764000
6	0.000000000	-17.052825000	0.709605000	6	0.000000000	-17.076367000	0.712488000
6	0.000000000	-17.052825000	-0.709605000	6	0.000000000	-17.076367000	-0.712488000
1	0.000000000	-15.869101000	2.478200000	1	0.000000000	-15.891727000	2.478365000
1	0.000000000	-15.869101000	-2.478200000	1	0.000000000	-15.891727000	-2.478365000
1	0.000000000	-13.379639000	-2.478310000	1	0.000000000	-13.398689000	-2.478529000
1	0.000000000	-13.379639000	2.478310000	1	0.000000000	-13.398689000	2.478529000
1	0.000000000	-8.557327000	-2.478059000	1	0.000000000	-8.569501000	-2.478221000
1	0.000000000	-8.557327000	2.478059000	1	0.000000000	-8.569501000	2.478221000
1	0.000000000	-3.656294000	-2.369784000	1	0.000000000	-3.661491000	-2.371976000
1	0.000000000	-3.656294000	2.369784000	1	0.000000000	-3.661491000	2.371976000
1	0.000000000	1.244886000	2.478055000	1	0.000000000	1.246649000	2.478225000
1	0.000000000	1.244886000	-2.478055000	1	0.000000000	1.246649000	-2.478225000
1	0.000000000	6.067585000	-2.478103000	1	0.000000000	6.076230000	-2.478281000
1	0.000000000	6.067585000	2.478103000	1	0.000000000	6.076230000	2.478281000
1	0.000000000	10.968745000	-2.369756000	1	0.000000000	10.984319000	-2.371947000
1	0.000000000	10.968745000	2.369756000	1	0.000000000	10.984319000	2.371947000
1	0.000000000	13.379639000	-2.478310000	1	0.000000000	13.398689000	-2.478529000
1	0.000000000	13.379639000	2.478310000	1	0.000000000	13.398689000	2.478529000
6	0.000000000	15.861820000	1.389459000	6	0.000000000	15.885446000	1.392764000
6	0.000000000	15.861820000	-1.389459000	6	0.000000000	15.885446000	-1.392764000
6	0.000000000	17.052825000	0.709605000	6	0.000000000	17.076367000	0.712488000
6	0.000000000	17.052825000	-0.709605000	6	0.000000000	17.076367000	-0.712488000
1	0.000000000	15.869101000	2.478200000	1	0.000000000	15.891727000	2.478365000
1	0.000000000	15.869101000	-2.478200000	1	0.000000000	15.891727000	-2.478365000
7	0.000000000	-18.280946000	-1.360379000	7	0.000000000	-18.306979000	-1.364247000
7	0.000000000	-18.280946000	1.360379000	7	0.000000000	-18.306979000	1.364247000
6	0.000000000	-19.506270000	-0.713713000	6	0.000000000	-19.534835000	-0.716906000

6	0.000000000	-19.506270000	0.713713000	6	0.000000000	-19.534835000	0.716906000
6	0.000000000	-20.695052000	-1.391405000	6	0.000000000	-20.723447000	-1.395195000
6	0.000000000	-20.695052000	1.391405000	6	0.000000000	-20.723447000	1.395195000
6	0.000000000	-21.936453000	-0.710699000	6	0.000000000	-21.968142000	-0.709603000
6	0.000000000	-21.936453000	0.710699000	6	0.000000000	-21.968142000	0.709603000
1	0.000000000	-20.689812000	-2.480047000	1	0.000000000	-20.719131000	-2.480732000
1	0.000000000	-20.689812000	2.480047000	1	0.000000000	-20.719131000	2.480732000
1	0.000000000	-18.280521000	-2.369226000	1	0.000000000	-18.306392000	-2.371379000
1	0.000000000	-18.280521000	2.369226000	1	0.000000000	-18.306392000	2.371379000
7	0.000000000	18.280946000	-1.360379000	7	0.000000000	18.306979000	-1.364247000
7	0.000000000	18.280946000	1.360379000	7	0.000000000	18.306979000	1.364247000
6	0.000000000	19.506270000	-0.713713000	6	0.000000000	19.534835000	-0.716906000
6	0.000000000	19.506270000	0.713713000	6	0.000000000	19.534835000	0.716906000
6	0.000000000	20.695052000	-1.391405000	6	0.000000000	20.723447000	-1.395195000
6	0.000000000	20.695052000	1.391405000	6	0.000000000	20.723447000	1.395195000
6	0.000000000	21.936453000	-0.710699000	6	0.000000000	21.968142000	-0.709603000
6	0.000000000	21.936453000	0.710699000	6	0.000000000	21.968142000	0.709603000
6	0.000000000	23.170545000	-1.392187000	6	0.000000000	23.204889000	-1.395165000
6	0.000000000	23.170545000	1.392187000	6	0.000000000	23.204889000	1.395165000
6	0.000000000	24.357497000	-0.702632000	6	0.000000000	24.392923000	-0.705241000
6	0.000000000	24.357497000	0.702632000	6	0.000000000	24.392923000	0.705241000
1	0.000000000	18.280521000	-2.369226000	1	0.000000000	18.306392000	-2.371379000
1	0.000000000	18.280521000	2.369226000	1	0.000000000	18.306392000	2.371379000
1	0.000000000	20.689812000	2.480047000	1	0.000000000	20.719131000	2.480732000
1	0.000000000	20.689812000	-2.480047000	1	0.000000000	20.719131000	-2.480732000
1	0.000000000	23.166290000	-2.479790000	1	0.000000000	23.200837000	-2.480107000
1	0.000000000	23.166290000	2.479790000	1	0.000000000	23.200837000	2.480107000
1	0.000000000	25.299677000	1.242321000	1	0.000000000	25.333018000	1.243766000
1	0.000000000	25.299677000	-1.242321000	1	0.000000000	25.333018000	-1.243766000
6	0.000000000	-23.170545000	1.392187000	6	0.000000000	-23.204889000	1.395165000
6	0.000000000	-23.170545000	-1.392187000	6	0.000000000	-23.204889000	-1.395165000
6	0.000000000	-24.357497000	0.702632000	6	0.000000000	-24.392923000	0.705241000
6	0.000000000	-24.357497000	-0.702632000	6	0.000000000	-24.392923000	-0.705241000
1	0.000000000	-23.166290000	2.479790000	1	0.000000000	-23.200837000	2.480107000
1	0.000000000	-23.166290000	-2.479790000	1	0.000000000	-23.200837000	-2.480107000
1	0.000000000	-25.299677000	1.242321000	1	0.000000000	-25.333018000	1.243766000
1	0.000000000	-25.299677000	-1.242321000	1	0.000000000	-25.333018000	-1.243766000

TableS131. Coordinates of pN₁_1 at M06/6-311++G(d,p) level

atom	x	y	z
6	0.000000000	0.713904000	5.993402000
6	0.000000000	-0.713904000	5.993402000
6	0.000000000	-1.404473000	4.826513000
6	0.000000000	1.404473000	4.826513000
6	0.000000000	0.723914000	3.568324000
6	0.000000000	-0.723914000	3.568324000
1	0.000000000	-2.491144000	4.822290000

TableS132. Coordinates of pN₁_1 at M062X/6-311++G(d,p) level

atom	x	y	z
6	0.000000000	0.718524000	6.001771000
6	0.000000000	-0.718524000	6.001771000
6	0.000000000	-1.410064000	4.836271000
6	0.000000000	1.410064000	4.836271000
6	0.000000000	0.725811000	3.570269000
6	0.000000000	-0.725811000	3.570269000
1	0.000000000	-2.494160000	4.832880000

1	0.000000000	2.491144000	4.822290000	1	0.000000000	2.494160000	4.832880000
6	0.000000000	-0.724271000	1.139508000	6	0.000000000	-0.725225000	1.139085000
6	0.000000000	0.724271000	1.139508000	6	0.000000000	0.725225000	1.139085000
7	0.000000000	1.419765000	0.000000000	7	0.000000000	1.422540000	0.000000000
7	0.000000000	-1.419765000	0.000000000	7	0.000000000	-1.422540000	0.000000000
6	0.000000000	0.724271000	-1.139508000	6	0.000000000	0.725225000	-1.139085000
6	0.000000000	-0.724271000	-1.139508000	6	0.000000000	-0.725225000	-1.139085000
6	0.000000000	-1.408007000	2.370308000	6	0.000000000	-1.412434000	2.374485000
6	0.000000000	1.408007000	2.370308000	6	0.000000000	1.412434000	2.374485000
6	0.000000000	-1.408007000	-2.370308000	6	0.000000000	-1.412434000	-2.374485000
6	0.000000000	1.408007000	-2.370308000	6	0.000000000	1.412434000	-2.374485000
6	0.000000000	-0.723914000	-3.568324000	6	0.000000000	-0.725811000	-3.570269000
6	0.000000000	0.723914000	-3.568324000	6	0.000000000	0.725811000	-3.570269000
6	0.000000000	-1.404473000	-4.826513000	6	0.000000000	-1.410064000	-4.836271000
6	0.000000000	1.404473000	-4.826513000	6	0.000000000	1.410064000	-4.836271000
6	0.000000000	-0.713904000	-5.993402000	6	0.000000000	-0.718524000	-6.001771000
6	0.000000000	0.713904000	-5.993402000	6	0.000000000	0.718524000	-6.001771000
1	0.000000000	-2.491144000	-4.822290000	1	0.000000000	-2.494160000	-4.832880000
1	0.000000000	-1.244406000	-6.940625000	1	0.000000000	-1.246757000	-6.947531000
1	0.000000000	1.244406000	-6.940625000	1	0.000000000	1.246757000	-6.947531000
1	0.000000000	2.491144000	-4.822290000	1	0.000000000	2.494160000	-4.832880000
1	0.000000000	2.494453000	-2.346840000	1	0.000000000	2.496198000	-2.350269000
1	0.000000000	-2.494453000	-2.346840000	1	0.000000000	-2.496198000	-2.350269000
1	0.000000000	2.494453000	2.346840000	1	0.000000000	2.496198000	2.350269000
1	0.000000000	-2.494453000	2.346840000	1	0.000000000	-2.496198000	2.350269000
1	0.000000000	-1.244406000	6.940625000	1	0.000000000	-1.246757000	6.947531000
1	0.000000000	1.244406000	6.940625000	1	0.000000000	1.246757000	6.947531000

TableS133. Coordinates of pN₂_1 at M06/6-311++g(d,p) level

atom	x	y	z
6	9.654233000	0.713256000	-0.000018000
6	9.654233000	-0.713256000	-0.000023000
6	7.228538000	-0.722609000	-0.000018000
6	7.228538000	0.722609000	-0.000013000
6	6.027047000	1.406327000	-0.000009000
1	6.003038000	2.492918000	-0.000005000
6	4.799778000	0.722689000	-0.000009000
6	4.799778000	-0.722689000	-0.000013000
6	6.027047000	-1.406327000	-0.000018000
1	6.003038000	-2.492918000	-0.000022000
6	2.520354000	-0.725603000	-0.000009000
6	2.520354000	0.725603000	-0.000004000
6	1.284133000	1.407715000	0.000000000
6	1.284133000	-1.407715000	-0.000009000
6	0.088807000	-0.725690000	-0.000005000
6	0.088807000	0.725690000	0.000000000
1	1.309016000	2.494170000	0.000004000

TableS134. Coordinates of pN₂_1 at M062X/6-311++g(d,p) level

atom	x	y	z
6	9.666757000	0.717621000	-0.000014000
6	9.666757000	-0.717621000	-0.000019000
6	7.235349000	-0.723967000	-0.000016000
6	7.235349000	0.723967000	-0.000011000
6	6.035831000	1.410039000	-0.000007000
1	6.011043000	2.494035000	-0.000004000
6	4.804857000	0.722950000	-0.000008000
6	4.804857000	-0.722950000	-0.000013000
6	6.035831000	-1.410039000	-0.000016000
1	6.011043000	-2.494035000	-0.000020000
6	2.526275000	-0.726400000	-0.000010000
6	2.526275000	0.726400000	-0.000006000
6	1.284686000	1.412108000	-0.000002000
6	1.284686000	-1.412108000	-0.000012000
6	0.092405000	-0.727687000	-0.000008000
6	0.092405000	0.727687000	-0.000003000
1	1.310195000	2.495836000	0.000001000

1	1.309016000	-2.494170000	-0.000012000	1	1.310195000	-2.495836000	-0.000015000
6	-2.345507000	0.723027000	0.000001000	6	-2.347061000	0.728069000	-0.000003000
6	-2.345507000	-0.723027000	-0.000002000	6	-2.347061000	-0.728069000	-0.000007000
7	-3.571199000	-1.357562000	-0.000003000	7	-3.575708000	-1.361433000	-0.000008000
7	-3.571199000	1.357562000	0.000000000	7	-3.575708000	1.361433000	-0.000005000
6	-4.798156000	-0.711675000	0.000006000	6	-4.805070000	-0.714246000	0.000003000
6	-4.798156000	0.711675000	0.000009000	6	-4.805070000	0.714246000	0.000006000
1	-3.573482000	-2.367509000	-0.000008000	1	-3.579096000	-2.369686000	-0.000014000
1	-3.573482000	2.367509000	0.000009000	1	-3.579096000	2.369686000	0.000007000
6	-1.167739000	1.401622000	0.000003000	6	-1.171403000	1.407616000	-0.000001000
6	-1.167739000	-1.401622000	-0.000005000	6	-1.171403000	-1.407616000	-0.000009000
7	3.654707000	1.419677000	-0.000004000	7	3.659412000	1.421851000	-0.000005000
7	3.654707000	-1.419677000	-0.000013000	7	3.659412000	-1.421851000	-0.000014000
6	8.485557000	1.403184000	-0.000013000	6	8.499582000	1.408340000	-0.000011000
6	8.485557000	-1.403184000	-0.000023000	6	8.499582000	-1.408340000	-0.000020000
6	-5.985886000	1.392987000	0.000017000	6	-5.992882000	1.396270000	0.000017000
6	-5.985886000	-1.392987000	0.000011000	6	-5.992882000	-1.396270000	0.000011000
6	-7.223540000	0.711120000	0.000022000	6	-7.233721000	0.710195000	0.000024000
6	-7.223540000	-0.711120000	0.000019000	6	-7.233721000	-0.710195000	0.000021000
6	-8.459365000	1.394067000	0.000030000	6	-8.472257000	1.396847000	0.000035000
6	-8.459365000	-1.394067000	0.000024000	6	-8.472257000	-1.396847000	0.000028000
6	-9.643242000	0.703964000	0.000035000	6	-9.657482000	0.706419000	0.000041000
6	-9.643242000	-0.703964000	0.000031000	6	-9.657482000	-0.706419000	0.000038000
1	-8.454850000	2.481387000	0.000033000	1	-8.468383000	2.481614000	0.000037000
1	-10.586257000	1.241818000	0.000041000	1	-10.598149000	1.243730000	0.000049000
1	-10.586257000	-1.241818000	0.000035000	1	-10.598149000	-1.243730000	0.000044000
1	-8.454850000	-2.481387000	0.000021000	1	-8.468383000	-2.481614000	0.000026000
1	-5.980764000	-2.481360000	0.000009000	1	-5.987820000	-2.481710000	0.000009000
1	-5.980764000	2.481360000	0.000019000	1	-5.987820000	2.481710000	0.000018000
1	-1.172990000	-2.489449000	-0.000007000	1	-1.176696000	-2.492426000	-0.000012000
1	-1.172990000	2.489449000	0.000005000	1	-1.176696000	2.492426000	0.000001000
1	8.480328000	2.490002000	-0.000010000	1	8.495381000	2.492698000	-0.000007000
1	8.480328000	-2.490002000	-0.000027000	1	8.495381000	-2.492698000	-0.000023000
1	10.601337000	1.244121000	-0.000018000	1	10.612394000	1.246444000	-0.000014000
1	10.601337000	-1.244121000	-0.000027000	1	10.612394000	-1.246444000	-0.000022000

Table S135. Coordinates of pN₂_2 at M06/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	9.570041000	0.715953000
6	0.000000000	9.570041000	-0.715953000
6	0.000000000	7.143444000	-0.726667000
6	0.000000000	7.143444000	0.726667000
6	0.000000000	5.951794000	1.411313000
1	0.000000000	5.928397000	2.497608000
6	0.000000000	4.712302000	0.728757000
6	0.000000000	4.712302000	-0.728757000

Table S136. Coordinates of pN₂_2 at M062X/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	9.581648000	0.721297000
6	0.000000000	9.581648000	-0.721297000
6	0.000000000	7.148240000	-0.729555000
6	0.000000000	7.148240000	0.729555000
6	0.000000000	5.961371000	1.416676000
1	0.000000000	5.937189000	2.500400000
6	0.000000000	4.713578000	0.731000000
6	0.000000000	4.713578000	-0.731000000

6	0.000000000	5.951794000	-1.411313000	6	0.000000000	5.961371000	-1.416676000
1	0.000000000	5.928397000	-2.497608000	1	0.000000000	5.937189000	-2.500400000
6	0.000000000	2.432092000	-0.726995000	6	0.000000000	2.433266000	-0.727491000
6	0.000000000	2.432092000	0.726995000	6	0.000000000	2.433266000	0.727491000
6	0.000000000	1.220989000	1.411925000	6	0.000000000	1.223203000	1.415233000
6	0.000000000	1.220989000	-1.411925000	6	0.000000000	1.223203000	-1.415233000
6	0.000000000	0.000000000	-0.729432000	6	0.000000000	0.000000000	-0.729770000
6	0.000000000	0.000000000	0.729432000	6	0.000000000	0.000000000	0.729770000
1	0.000000000	1.246149000	2.497864000	1	0.000000000	1.248738000	2.498688000
1	0.000000000	1.246149000	-2.497864000	1	0.000000000	1.248738000	-2.498688000
6	0.000000000	-2.432092000	0.726995000	6	0.000000000	-2.433266000	0.727491000
6	0.000000000	-2.432092000	-0.726995000	6	0.000000000	-2.433266000	-0.727491000
7	0.000000000	-3.585141000	-1.423029000	7	0.000000000	-3.591095000	-1.426404000
7	0.000000000	-3.585141000	1.423029000	7	0.000000000	-3.591095000	1.426404000
6	0.000000000	-4.712302000	-0.728757000	6	0.000000000	-4.713578000	-0.731000000
6	0.000000000	-4.712302000	0.728757000	6	0.000000000	-4.713578000	0.731000000
6	0.000000000	-1.220989000	1.411925000	6	0.000000000	-1.223203000	1.415233000
6	0.000000000	-1.220989000	-1.411925000	6	0.000000000	-1.223203000	-1.415233000
7	0.000000000	3.585141000	1.423029000	7	0.000000000	3.591095000	1.426404000
7	0.000000000	3.585141000	-1.423029000	7	0.000000000	3.591095000	-1.426404000
6	0.000000000	8.405778000	1.406591000	6	0.000000000	8.420064000	1.412903000
6	0.000000000	8.405778000	-1.406591000	6	0.000000000	8.420064000	-1.412903000
6	0.000000000	-5.951794000	1.411313000	6	0.000000000	-5.961371000	1.416676000
6	0.000000000	-5.951794000	-1.411313000	6	0.000000000	-5.961371000	-1.416676000
6	0.000000000	-7.143444000	0.726667000	6	0.000000000	-7.148240000	0.729555000
6	0.000000000	-7.143444000	-0.726667000	6	0.000000000	-7.148240000	-0.729555000
6	0.000000000	-8.405778000	1.406591000	6	0.000000000	-8.420064000	1.412903000
6	0.000000000	-8.405778000	-1.406591000	6	0.000000000	-8.420064000	-1.412903000
6	0.000000000	-9.570041000	0.715953000	6	0.000000000	-9.581648000	0.721297000
6	0.000000000	-9.570041000	-0.715953000	6	0.000000000	-9.581648000	-0.721297000
1	0.000000000	-8.400902000	2.493100000	1	0.000000000	-8.416106000	2.496998000
1	0.000000000	-10.518231000	1.244551000	1	0.000000000	-10.528905000	1.246954000
1	0.000000000	-10.518231000	-1.244551000	1	0.000000000	-10.528905000	-1.246954000
1	0.000000000	-8.400902000	-2.493100000	1	0.000000000	-8.416106000	-2.496998000
1	0.000000000	-5.928397000	-2.497608000	1	0.000000000	-5.937189000	-2.500400000
1	0.000000000	-5.928397000	2.497608000	1	0.000000000	-5.937189000	2.500400000
1	0.000000000	-1.246149000	-2.497864000	1	0.000000000	-1.248738000	-2.498688000
1	0.000000000	-1.246149000	2.497864000	1	0.000000000	-1.248738000	2.498688000
1	0.000000000	8.400902000	2.493100000	1	0.000000000	8.416106000	2.496998000
1	0.000000000	8.400902000	-2.493100000	1	0.000000000	8.416106000	-2.496998000
1	0.000000000	10.518231000	1.244551000	1	0.000000000	10.528905000	1.246954000
1	0.000000000	10.518231000	-1.244551000	1	0.000000000	10.528905000	-1.246954000

Table S137. Coordinates of pN₃_1 at M06/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.722511000	8.457313000
7	0.000000000	1.419765000	7.311499000

Table S138. Coordinates of pN₃_1 at M062X/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.716103000	-8.460391000
7	0.000000000	1.364200000	-7.231562000

6	0.000000000	0.726103000	6.177475000	6	0.000000000	0.714677000	-6.002939000
6	0.000000000	-0.726103000	6.177475000	6	0.000000000	-0.714677000	-6.002939000
7	0.000000000	-1.419765000	7.311499000	7	0.000000000	-1.364200000	-7.231562000
6	0.000000000	-0.722511000	8.457313000	6	0.000000000	-0.716103000	-8.460391000
6	0.000000000	-0.725948000	3.744419000	6	0.000000000	-0.709095000	-3.571444000
6	0.000000000	0.725948000	3.744419000	6	0.000000000	0.709095000	-3.571444000
6	0.000000000	1.401733000	2.488397000	6	0.000000000	1.394132000	-2.335074000
1	0.000000000	2.489551000	2.483369000	1	0.000000000	2.479612000	-2.327988000
6	0.000000000	0.723534000	1.309617000	6	0.000000000	0.710844000	-1.144231000
6	0.000000000	-0.723534000	1.309617000	6	0.000000000	-0.710844000	-1.144231000
6	0.000000000	-1.401733000	2.488397000	6	0.000000000	-1.394132000	-2.335074000
1	0.000000000	-2.489551000	2.483369000	1	0.000000000	2.371491000	-7.232091000
6	0.000000000	-0.708640000	-1.143013000	1	0.000000000	-2.371491000	-7.232091000
6	0.000000000	0.708640000	-1.143013000	1	0.000000000	-2.479612000	-2.327988000
6	0.000000000	1.391322000	-2.333862000	6	0.000000000	-0.728695000	1.313403000
6	0.000000000	-1.391322000	-2.333862000	6	0.000000000	0.728695000	1.313403000
6	0.000000000	-0.710578000	-3.567648000	6	0.000000000	1.407797000	2.489874000
6	0.000000000	0.710578000	-3.567648000	6	0.000000000	-1.407797000	2.489874000
1	0.000000000	2.479780000	-2.326625000	6	0.000000000	-0.727917000	3.753009000
1	0.000000000	-2.479780000	-2.326625000	6	0.000000000	0.727917000	3.753009000
6	0.000000000	0.722535000	10.886710000	1	0.000000000	2.492578000	2.484846000
6	0.000000000	-0.722535000	10.886710000	1	0.000000000	-2.492578000	2.484846000
6	0.000000000	-1.402823000	12.144133000	6	0.000000000	0.709622000	-10.893060000
6	0.000000000	1.402823000	12.144133000	6	0.000000000	-0.709622000	-10.893060000
6	0.000000000	-0.713088000	13.313215000	6	0.000000000	-1.395516000	-12.130186000
6	0.000000000	0.713088000	13.313215000	6	0.000000000	1.395516000	-12.130186000
1	0.000000000	2.489676000	12.139033000	6	0.000000000	-0.705455000	-13.317754000
1	0.000000000	-2.489676000	12.139033000	6	0.000000000	0.705455000	-13.317754000
6	0.000000000	0.711943000	-5.996300000	1	0.000000000	2.480401000	-12.126034000
6	0.000000000	-0.711943000	-5.996300000	1	0.000000000	-2.480401000	-12.126034000
7	0.000000000	-1.360090000	-7.222273000	6	0.000000000	0.726740000	6.187711000
7	0.000000000	1.360090000	-7.222273000	6	0.000000000	-0.726740000	6.187711000
6	0.000000000	-0.713028000	-8.448870000	7	0.000000000	-1.421868000	7.320362000
6	0.000000000	0.713028000	-8.448870000	7	0.000000000	1.421868000	7.320362000
1	0.000000000	-2.369089000	-7.222876000	6	0.000000000	-0.722604000	8.466623000
1	0.000000000	2.369089000	-7.222876000	6	0.000000000	0.722604000	8.466623000
6	0.000000000	1.391317000	-4.806980000	6	0.000000000	1.411827000	4.945370000
6	0.000000000	-1.391317000	-4.806980000	6	0.000000000	-1.411827000	4.945370000
7	0.000000000	1.356981000	0.084764000	7	0.000000000	1.361272000	0.085922000
7	0.000000000	-1.356981000	0.084764000	7	0.000000000	-1.361272000	0.085922000
6	0.000000000	1.407192000	4.940220000	6	0.000000000	1.394487000	-4.813694000
6	0.000000000	-1.407192000	4.940220000	6	0.000000000	-1.394487000	-4.813694000
6	0.000000000	1.405618000	9.684050000	6	0.000000000	1.395143000	-9.648103000
6	0.000000000	-1.405618000	9.684050000	6	0.000000000	-1.395143000	-9.648103000
6	0.000000000	1.391639000	-9.636487000	6	0.000000000	1.409474000	9.696560000
6	0.000000000	-1.391639000	-9.636487000	6	0.000000000	-1.409474000	9.696560000
6	0.000000000	0.710563000	-10.878086000	6	0.000000000	0.723778000	10.897202000
6	0.000000000	-0.710563000	-10.878086000	6	0.000000000	-0.723778000	10.897202000

6	0.000000000	1.392820000	-12.112668000	6	0.000000000	1.407989000	12.161692000
6	0.000000000	-1.392820000	-12.112668000	6	0.000000000	-1.407989000	12.161692000
6	0.000000000	0.703044000	-13.298837000	6	0.000000000	0.717460000	13.329265000
6	0.000000000	-0.703044000	-13.298837000	6	0.000000000	-0.717460000	13.329265000
1	0.000000000	2.480290000	-12.107732000	1	0.000000000	2.492374000	12.157517000
1	0.000000000	1.241793000	-14.241484000	1	0.000000000	1.246708000	14.274649000
1	0.000000000	-1.241793000	-14.241484000	1	0.000000000	-1.246708000	14.274649000
1	0.000000000	-2.480290000	-12.107732000	1	0.000000000	-2.492374000	12.157517000
1	0.000000000	-2.480182000	-9.631677000	1	0.000000000	-2.493473000	9.671242000
1	0.000000000	2.480182000	-9.631677000	1	0.000000000	2.493473000	9.671242000
1	0.000000000	-2.479756000	-4.812954000	1	0.000000000	-2.495571000	4.970441000
1	0.000000000	2.479756000	-4.812954000	1	0.000000000	2.495571000	4.970441000
1	0.000000000	-2.366783000	0.082074000	1	0.000000000	-2.369329000	0.082015000
1	0.000000000	2.366783000	0.082074000	1	0.000000000	2.369329000	0.082015000
1	0.000000000	2.493731000	4.964441000	1	0.000000000	2.479885000	-4.819281000
1	0.000000000	-2.493731000	4.964441000	1	0.000000000	-2.479885000	-4.819281000
1	0.000000000	-2.492264000	9.659656000	1	0.000000000	-2.480675000	-9.643464000
1	0.000000000	2.492264000	9.659656000	1	0.000000000	2.480675000	-9.643464000
1	0.000000000	1.244417000	14.260066000	1	0.000000000	1.243839000	-14.257902000
1	0.000000000	-1.244417000	14.260066000	1	0.000000000	-1.243839000	-14.257902000

Table S139. Coordinates of pN₃_2 at M06/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.727589000	8.375480000
7	0.000000000	1.422536000	7.245599000
6	0.000000000	0.727028000	6.094825000
6	0.000000000	-0.727028000	6.094825000
7	0.000000000	-1.422536000	7.245599000
6	0.000000000	-0.727589000	8.375480000
6	0.000000000	-0.729037000	3.661960000
6	0.000000000	0.729037000	3.661960000
6	0.000000000	1.410475000	2.436424000
1	0.000000000	2.496511000	2.410559000
6	0.000000000	0.726354000	1.229858000
6	0.000000000	-0.726354000	1.229858000
6	0.000000000	-1.410475000	2.436424000
1	0.000000000	-2.496511000	2.410559000
6	0.000000000	-0.730446000	-1.051946000
6	0.000000000	0.730446000	-1.051946000
6	0.000000000	1.410521000	-2.294553000
6	0.000000000	-1.410521000	-2.294553000
6	0.000000000	-0.728593000	-3.485471000
6	0.000000000	0.728593000	-3.485471000
1	0.000000000	2.496815000	-2.269355000
1	0.000000000	-2.496815000	-2.269355000
6	0.000000000	0.726029000	10.806254000
6	0.000000000	-0.726029000	10.806254000

Table S140. Coordinates of pN₃_2 at M062X/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.713743000	-8.384697000
7	0.000000000	1.360688000	-7.155292000
6	0.000000000	0.730531000	-5.927638000
6	0.000000000	-0.730531000	-5.927638000
7	0.000000000	-1.360688000	-7.155292000
6	0.000000000	-0.713743000	-8.384697000
6	0.000000000	-0.731823000	-3.486406000
6	0.000000000	0.731823000	-3.486406000
6	0.000000000	1.416358000	-2.300546000
1	0.000000000	2.499937000	-2.275044000
6	0.000000000	0.733301000	-1.048482000
6	0.000000000	-0.733301000	-1.048482000
6	0.000000000	-1.416358000	-2.300546000
1	0.000000000	2.369214000	-7.159638000
1	0.000000000	-2.369214000	-7.159638000
1	0.000000000	-2.499937000	-2.275044000
6	0.000000000	-0.726934000	1.233924000
6	0.000000000	0.726934000	1.233924000
6	0.000000000	1.413883000	2.438889000
6	0.000000000	-1.413883000	2.438889000
6	0.000000000	-0.729322000	3.667797000
6	0.000000000	0.729322000	3.667797000
1	0.000000000	2.497419000	2.412908000
1	0.000000000	-2.497419000	2.412908000

6	0.000000000	-1.405860000	12.068215000	6	0.000000000	0.710387000	-10.812497000
6	0.000000000	1.405860000	12.068215000	6	0.000000000	-0.710387000	-10.812497000
6	0.000000000	-0.715528000	13.233231000	6	0.000000000	-1.397193000	-12.051841000
6	0.000000000	0.715528000	13.233231000	6	0.000000000	1.397193000	-12.051841000
1	0.000000000	2.492486000	12.063108000	6	0.000000000	-0.706702000	-13.236514000
1	0.000000000	-2.492486000	12.063108000	6	0.000000000	0.706702000	-13.236514000
6	0.000000000	0.724847000	-5.920598000	1	0.000000000	2.481913000	-12.047659000
6	0.000000000	-0.724847000	-5.920598000	1	0.000000000	-2.481913000	-12.047659000
7	0.000000000	-1.356940000	-7.145127000	6	0.000000000	0.727254000	6.102382000
7	0.000000000	1.356940000	-7.145127000	6	0.000000000	-0.727254000	6.102382000
6	0.000000000	-0.711276000	-8.371998000	7	0.000000000	-1.425236000	7.257618000
6	0.000000000	0.711276000	-8.371998000	7	0.000000000	1.425236000	7.257618000
1	0.000000000	-2.367149000	-7.148047000	6	0.000000000	-0.729720000	8.383393000
1	0.000000000	2.367149000	-7.148047000	6	0.000000000	0.729720000	8.383393000
6	0.000000000	1.403417000	-4.743754000	6	0.000000000	1.414152000	4.887649000
6	0.000000000	-1.403417000	-4.743754000	6	0.000000000	-1.414152000	4.887649000
7	0.000000000	1.423726000	0.071366000	7	0.000000000	1.426995000	0.069545000
7	0.000000000	-1.423726000	0.071366000	7	0.000000000	-1.426995000	0.069545000
6	0.000000000	1.411012000	4.880045000	6	0.000000000	1.410046000	-4.753357000
6	0.000000000	-1.411012000	4.880045000	6	0.000000000	-1.410046000	-4.753357000
6	0.000000000	1.410286000	9.612816000	6	0.000000000	1.396607000	-9.572170000
6	0.000000000	-1.410286000	9.612816000	6	0.000000000	-1.396607000	-9.572170000
6	0.000000000	1.393451000	-9.559353000	6	0.000000000	1.415500000	9.629060000
6	0.000000000	-1.393451000	-9.559353000	6	0.000000000	-1.415500000	9.629060000
6	0.000000000	0.711391000	-10.796346000	6	0.000000000	0.728864000	10.818004000
6	0.000000000	-0.711391000	-10.796346000	6	0.000000000	-0.728864000	10.818004000
6	0.000000000	1.394393000	-12.032859000	6	0.000000000	1.412131000	12.089320000
6	0.000000000	-1.394393000	-12.032859000	6	0.000000000	-1.412131000	12.089320000
6	0.000000000	0.704214000	-13.216222000	6	0.000000000	0.720788000	13.251660000
6	0.000000000	-0.704214000	-13.216222000	6	0.000000000	-0.720788000	13.251660000
1	0.000000000	2.481629000	-12.028194000	1	0.000000000	2.496367000	12.085116000
1	0.000000000	1.241733000	-14.159390000	1	0.000000000	1.246854000	14.198762000
1	0.000000000	-1.241733000	-14.159390000	1	0.000000000	-1.246854000	14.198762000
1	0.000000000	-2.481629000	-12.028194000	1	0.000000000	-2.496367000	12.085116000
1	0.000000000	-2.481727000	-9.553878000	1	0.000000000	-2.499352000	9.604506000
1	0.000000000	2.481727000	-9.553878000	1	0.000000000	2.499352000	9.604506000
1	0.000000000	-2.491121000	-4.748804000	1	0.000000000	-2.497749000	4.912966000
1	0.000000000	2.491121000	-4.748804000	1	0.000000000	2.497749000	4.912966000
1	0.000000000	2.497078000	4.905144000	1	0.000000000	2.494753000	-4.758185000
1	0.000000000	-2.497078000	4.905144000	1	0.000000000	-2.494753000	-4.758185000
1	0.000000000	-2.496665000	9.588724000	1	0.000000000	-2.481996000	-9.566920000
1	0.000000000	2.496665000	9.588724000	1	0.000000000	2.481996000	-9.566920000
1	0.000000000	1.244561000	14.181220000	1	0.000000000	1.243488000	-14.177500000
1	0.000000000	-1.244561000	14.181220000	1	0.000000000	-1.243488000	-14.177500000

Table S141. Coordinates of pN₃_3 at M06/6-311++g(d,p) level

atom	x	y	z
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Table S142. Coordinates of pN₃_3 at M062X/6-311++g(d,p) level

atom	x	y	z
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6	0.000000000	8.325353000	0.720207000	6	0.000000000	8.338947000	0.719872000
7	0.000000000	7.164133000	1.421388000	7	0.000000000	7.172768000	1.423797000
6	0.000000000	6.046033000	0.726767000	6	0.000000000	6.060164000	0.728852000
6	0.000000000	6.046033000	-0.726767000	6	0.000000000	6.060164000	-0.728852000
7	0.000000000	7.164133000	-1.421388000	7	0.000000000	7.172768000	-1.423797000
6	0.000000000	8.325353000	-0.720207000	6	0.000000000	8.338947000	-0.719872000
6	0.000000000	3.598811000	-0.729190000	6	0.000000000	3.609558000	-0.732826000
6	0.000000000	3.598811000	0.729190000	6	0.000000000	3.609558000	0.732826000
6	0.000000000	2.355190000	1.402775000	6	0.000000000	2.354149000	1.408019000
1	0.000000000	2.330003000	2.489437000	1	0.000000000	2.329390000	2.492379000
6	0.000000000	1.142440000	0.731386000	6	0.000000000	1.144401000	0.736923000
6	0.000000000	1.142440000	-0.731386000	6	0.000000000	1.144401000	-0.736923000
6	0.000000000	2.355190000	-1.402775000	6	0.000000000	2.354149000	-1.408019000
1	0.000000000	2.330003000	-2.489437000	1	0.000000000	2.329390000	-2.492379000
6	0.000000000	-1.142440000	-0.731386000	6	0.000000000	-1.144401000	-0.736923000
6	0.000000000	-1.142440000	0.731386000	6	0.000000000	-1.144401000	0.736923000
6	0.000000000	-2.355190000	1.402775000	6	0.000000000	-2.354149000	1.408019000
6	0.000000000	-2.355190000	-1.402775000	6	0.000000000	-2.354149000	-1.408019000
6	0.000000000	-3.598811000	-0.729190000	6	0.000000000	-3.609558000	-0.732826000
6	0.000000000	-3.598811000	0.729190000	6	0.000000000	-3.609558000	0.732826000
1	0.000000000	-2.330003000	2.489437000	1	0.000000000	-2.329390000	2.492379000
1	0.000000000	-2.330003000	-2.489437000	1	0.000000000	-2.329390000	-2.492379000
6	0.000000000	10.752122000	0.718578000	6	0.000000000	10.765463000	0.719043000
6	0.000000000	10.752122000	-0.718578000	6	0.000000000	10.765463000	-0.719043000
6	0.000000000	11.999729000	-1.400338000	6	0.000000000	12.019589000	-1.404873000
6	0.000000000	11.999729000	1.400338000	6	0.000000000	12.019589000	1.404873000
6	0.000000000	13.174408000	-0.709091000	6	0.000000000	13.192809000	-0.713284000
6	0.000000000	13.174408000	0.709091000	6	0.000000000	13.192809000	0.713284000
1	0.000000000	11.994383000	2.487004000	1	0.000000000	12.014747000	2.489152000
1	0.000000000	11.994383000	-2.487004000	1	0.000000000	12.014747000	-2.489152000
6	0.000000000	-6.046033000	0.726767000	6	0.000000000	-6.060164000	0.728852000
6	0.000000000	-6.046033000	-0.726767000	6	0.000000000	-6.060164000	-0.728852000
7	0.000000000	-7.164133000	-1.421388000	7	0.000000000	-7.172768000	-1.423797000
7	0.000000000	-7.164133000	1.421388000	7	0.000000000	-7.172768000	1.423797000
6	0.000000000	-8.325353000	-0.720207000	6	0.000000000	-8.338947000	-0.719872000
6	0.000000000	-8.325353000	0.720207000	6	0.000000000	-8.338947000	0.719872000
6	0.000000000	-4.795102000	1.407059000	6	0.000000000	-4.797933000	1.413674000
6	0.000000000	-4.795102000	-1.407059000	6	0.000000000	-4.797933000	-1.413674000
7	0.000000000	0.000000000	1.431047000	7	0.000000000	0.000000000	1.436979000
7	0.000000000	0.000000000	-1.431047000	7	0.000000000	0.000000000	-1.436979000
6	0.000000000	4.795102000	1.407059000	6	0.000000000	4.797933000	1.413674000
6	0.000000000	4.795102000	-1.407059000	6	0.000000000	4.797933000	-1.413674000
6	0.000000000	9.537227000	1.403661000	6	0.000000000	9.551491000	1.407051000
6	0.000000000	9.537227000	-1.403661000	6	0.000000000	9.551491000	-1.407051000
6	0.000000000	-9.537227000	1.403661000	6	0.000000000	-9.551491000	1.407051000
6	0.000000000	-9.537227000	-1.403661000	6	0.000000000	-9.551491000	-1.407051000
6	0.000000000	-10.752122000	0.718578000	6	0.000000000	-10.765463000	0.719043000

6	0.000000000	-10.752122000	-0.718578000	6	0.000000000	-10.765463000	-0.719043000
6	0.000000000	-11.999729000	1.400338000	6	0.000000000	-12.019589000	1.404873000
6	0.000000000	-11.999729000	-1.400338000	6	0.000000000	-12.019589000	-1.404873000
6	0.000000000	-13.174408000	0.709091000	6	0.000000000	-13.192809000	0.713284000
6	0.000000000	-13.174408000	-0.709091000	6	0.000000000	-13.192809000	-0.713284000
1	0.000000000	-11.994383000	2.487004000	1	0.000000000	-12.014747000	2.489152000
1	0.000000000	-14.119972000	1.242244000	1	0.000000000	-14.137026000	1.244400000
1	0.000000000	-14.119972000	-1.242244000	1	0.000000000	-14.137026000	-1.244400000
1	0.000000000	-11.994383000	-2.487004000	1	0.000000000	-12.014747000	-2.489152000
1	0.000000000	-9.512492000	-2.490148000	1	0.000000000	-9.526152000	-2.490998000
1	0.000000000	-9.512492000	2.490148000	1	0.000000000	-9.526152000	2.490998000
1	0.000000000	-4.819022000	-2.493530000	1	0.000000000	-4.822757000	-2.497717000
1	0.000000000	-4.819022000	2.493530000	1	0.000000000	-4.822757000	2.497717000
1	0.000000000	4.819022000	2.493530000	1	0.000000000	4.822757000	2.497717000
1	0.000000000	4.819022000	-2.493530000	1	0.000000000	4.822757000	-2.497717000
1	0.000000000	9.512492000	-2.490148000	1	0.000000000	9.526152000	-2.490998000
1	0.000000000	9.512492000	2.490148000	1	0.000000000	9.526152000	2.490998000
1	0.000000000	14.119972000	1.242244000	1	0.000000000	14.137026000	1.244400000
1	0.000000000	14.119972000	-1.242244000	1	0.000000000	14.137026000	-1.244400000

Table S143. Coordinates of pN_a_1 at M06/6-311++g(d,p) level

atom	x	y	z
6	-4.793840000	0.710257000	-0.000005000
7	-3.566076000	1.360599000	0.000035000
6	-2.340999000	0.712621000	0.000012000
6	-2.340999000	-0.712621000	0.000015000
7	-3.566076000	-1.360599000	0.000041000
6	-4.793840000	-0.710257000	-0.000002000
6	0.088465000	-0.710568000	-0.000010000
6	0.088465000	0.710568000	-0.000014000
6	1.321969000	1.391102000	-0.000026000
1	1.329110000	2.479595000	-0.000028000
6	2.513384000	0.708359000	-0.000031000
6	2.513384000	-0.708359000	-0.000027000
6	1.321969000	-1.391102000	-0.000017000
1	-3.566652000	2.369408000	0.000016000
1	-3.566652000	-2.369408000	0.000033000
1	1.329110000	-2.479595000	-0.000013000
6	4.965548000	-0.723644000	-0.000026000
6	4.965548000	0.723644000	-0.000031000
6	6.144675000	1.401488000	-0.000026000
6	6.144675000	-1.401488000	-0.000016000
6	7.400991000	-0.726002000	-0.000010000
6	7.400991000	0.726002000	-0.000015000
1	6.139805000	2.489375000	-0.000028000
1	6.139805000	-2.489375000	-0.000011000
6	-7.221847000	0.709569000	-0.000072000

Table S144. Coordinates of pN_a_1 at M062X/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.712961000	-4.804745000
7	0.000000000	1.364528000	-3.574221000
6	0.000000000	0.715424000	-2.346017000
6	0.000000000	-0.715424000	-2.346017000
7	0.000000000	-1.364528000	-3.574221000
6	0.000000000	-0.712961000	-4.804745000
6	0.000000000	-0.709069000	0.087492000
6	0.000000000	0.709069000	0.087492000
6	0.000000000	1.393161000	1.325403000
1	0.000000000	2.478715000	1.332233000
6	0.000000000	0.710549000	2.517663000
6	0.000000000	-0.710549000	2.517663000
6	0.000000000	-1.393161000	1.325403000
1	0.000000000	2.371587000	-3.575108000
1	0.000000000	-2.371587000	-3.575108000
1	0.000000000	-2.478715000	1.332233000
6	0.000000000	-0.728801000	4.977178000
6	0.000000000	0.728801000	4.977178000
6	0.000000000	1.407293000	6.154719000
6	0.000000000	-1.407293000	6.154719000
6	0.000000000	-0.728099000	7.419150000
6	0.000000000	0.728099000	7.419150000
1	0.000000000	2.492102000	6.149348000
1	0.000000000	-2.492102000	6.149348000
6	0.000000000	0.708177000	-7.236021000

6	-7.221847000	-0.709569000	-0.000069000	6	0.000000000	-0.708177000	-7.236021000
6	-8.459271000	-1.390107000	-0.000104000	6	0.000000000	-1.393401000	-8.476079000
6	-8.459271000	1.390107000	-0.000112000	6	0.000000000	1.393401000	-8.476079000
6	-9.649918000	-0.710447000	-0.000154000	6	0.000000000	-0.713099000	-9.666400000
6	-9.649918000	0.710447000	-0.000158000	6	0.000000000	0.713099000	-9.666400000
1	-8.465817000	2.478716000	-0.000114000	1	0.000000000	2.478929000	-8.481936000
1	-8.465817000	-2.478716000	-0.000101000	1	0.000000000	-2.478929000	-8.481936000
6	9.833459000	0.725960000	0.000005000	6	0.000000000	0.726797000	9.854464000
6	9.833459000	-0.725960000	0.000010000	6	0.000000000	-0.726797000	9.854464000
7	10.967409000	-1.419877000	0.000024000	7	0.000000000	-1.421923000	10.986938000
7	10.967409000	1.419877000	0.000014000	7	0.000000000	1.421923000	10.986938000
6	12.113408000	-0.722381000	0.000034000	6	0.000000000	-0.722619000	12.133248000
6	12.113408000	0.722381000	0.000028000	6	0.000000000	0.722619000	12.133248000
6	8.596625000	1.407467000	-0.000008000	6	0.000000000	1.411858000	8.612044000
6	8.596625000	-1.407467000	0.000002000	6	0.000000000	-1.411858000	8.612044000
7	3.741311000	1.357202000	-0.000040000	7	0.000000000	1.360978000	3.749202000
7	3.741311000	-1.357202000	-0.000032000	7	0.000000000	-1.360978000	3.749202000
6	-1.150915000	1.391147000	-0.000005000	6	0.000000000	1.394255000	-1.155646000
6	-1.150915000	-1.391147000	0.000002000	6	0.000000000	-1.394255000	-1.155646000
6	-5.984420000	1.390023000	-0.000040000	6	0.000000000	1.392982000	-5.995452000
6	-5.984420000	-1.390023000	-0.000033000	6	0.000000000	-1.392982000	-5.995452000
7	-10.877148000	1.360307000	-0.000233000	7	0.000000000	1.364474000	-10.895852000
7	-10.877148000	-1.360307000	-0.000225000	7	0.000000000	-1.364474000	-10.895852000
6	-12.103275000	0.713548000	-0.000105000	6	0.000000000	0.716549000	-12.123803000
6	-12.103275000	-0.713548000	-0.000101000	6	0.000000000	-0.716549000	-12.123803000
6	-13.291487000	1.391655000	-0.000010000	6	0.000000000	1.395068000	-13.311532000
6	-13.291487000	-1.391655000	-0.000002000	6	0.000000000	-1.395068000	-13.311532000
6	-14.532806000	0.710476000	0.000078000	6	0.000000000	0.709602000	-14.556832000
6	-14.532806000	-0.710476000	0.000083000	6	0.000000000	-0.709602000	-14.556832000
6	13.340163000	1.405819000	0.000039000	6	0.000000000	1.409584000	13.363016000
6	13.340163000	-1.405819000	0.000050000	6	0.000000000	-1.409584000	13.363016000
6	14.542469000	0.722329000	0.000056000	6	0.000000000	0.723666000	14.563365000
6	14.542469000	-0.722329000	0.000062000	6	0.000000000	-0.723666000	14.563365000
6	15.799207000	1.402811000	0.000068000	6	0.000000000	1.407889000	15.827358000
6	15.799207000	-1.402811000	0.000079000	6	0.000000000	-1.407889000	15.827358000
6	16.968334000	0.713099000	0.000084000	6	0.000000000	0.717427000	16.995137000
6	16.968334000	-0.713099000	0.000090000	6	0.000000000	-0.717427000	16.995137000
1	15.793571000	2.489683000	0.000064000	1	0.000000000	2.492266000	15.823097000
1	17.915484000	1.243936000	0.000093000	1	0.000000000	1.246749000	17.940495000
1	17.915484000	-1.243936000	0.000103000	1	0.000000000	-1.246749000	17.940495000
1	15.793571000	-2.489683000	0.000083000	1	0.000000000	-2.492266000	15.823097000
1	13.315921000	-2.492436000	0.000054000	1	0.000000000	-2.493581000	13.337844000
1	13.315921000	2.492436000	0.000035000	1	0.000000000	2.493581000	13.337844000
1	8.621667000	-2.493940000	0.000007000	1	0.000000000	-2.495604000	8.637218000
1	8.621667000	2.493940000	-0.000011000	1	0.000000000	2.495604000	8.637218000
1	3.738682000	-2.367024000	-0.000023000	1	0.000000000	-2.369032000	3.745497000
1	3.738682000	2.367024000	-0.000037000	1	0.000000000	2.369032000	3.745497000
1	-1.157018000	2.479645000	-0.000007000	1	0.000000000	2.479691000	-1.161158000

1	-1.157018000	-2.479645000	0.000006000	1	0.000000000	-2.479691000	-1.161158000
1	-5.977979000	-2.478660000	-0.000031000	1	0.000000000	-2.478560000	-5.989043000
1	-5.977979000	2.478660000	-0.000043000	1	0.000000000	2.478560000	-5.989043000
1	-10.877021000	-2.369180000	-0.000165000	1	0.000000000	-2.371632000	-10.895781000
1	-10.877021000	2.369180000	-0.000177000	1	0.000000000	2.371632000	-10.895781000
1	-13.286925000	-2.480229000	0.000001000	1	0.000000000	-2.480610000	-13.306868000
1	-13.286925000	2.480229000	-0.000013000	1	0.000000000	2.480610000	-13.306868000
6	-15.766993000	1.392630000	0.000160000	6	0.000000000	1.395232000	-15.793741000
6	-15.766993000	-1.392630000	0.000169000	6	0.000000000	-1.395232000	-15.793741000
6	-16.953431000	0.702916000	0.000241000	6	0.000000000	0.705323000	-16.981804000
6	-16.953431000	-0.702916000	0.000246000	6	0.000000000	-0.705323000	-16.981804000
1	-15.762261000	2.480153000	0.000156000	1	0.000000000	2.480153000	-15.789468000
1	-15.762261000	-2.480153000	0.000171000	1	0.000000000	-2.480153000	-15.789468000
1	-17.896007000	-1.241800000	0.000310000	1	0.000000000	-1.243969000	-17.921826000
1	-17.896007000	1.241800000	0.000302000	1	0.000000000	1.243969000	-17.921826000

Table S145. Coordinates of pN_a_2 at M06/6-311++g(d,p) level

atom	x	y	z
6	-4.888119000	0.726405000	0.000006000
7	-3.728809000	1.423871000	0.000004000
6	-2.605539000	0.730913000	0.000005000
6	-2.605539000	-0.730913000	0.000009000
7	-3.728809000	-1.423871000	0.000011000
6	-4.888119000	-0.726405000	0.000010000
6	-0.170809000	-0.728778000	0.000008000
6	-0.170809000	0.728778000	0.000004000
6	1.086426000	1.403463000	0.000002000
1	1.091474000	2.491230000	0.000000000
6	2.264436000	0.725241000	0.000002000
6	2.264436000	-0.725241000	0.000006000
6	1.086426000	-1.403463000	0.000009000
1	1.091474000	-2.491230000	0.000012000
6	4.715580000	-0.708420000	0.000002000
6	4.715580000	0.708420000	-0.000001000
6	5.906897000	1.391832000	-0.000005000
6	5.906897000	-1.391832000	0.000001000
6	7.139494000	-0.710947000	-0.000004000
6	7.139494000	0.710947000	-0.000007000
1	5.899783000	2.480206000	-0.000007000
1	5.899783000	-2.480206000	0.000004000
6	-7.321428000	0.728876000	0.000005000
6	-7.321428000	-0.728876000	0.000009000
6	-8.538905000	-1.411085000	0.000010000
6	-8.538905000	1.411085000	0.000002000
6	-9.754188000	-0.727071000	0.000006000
6	-9.754188000	0.727071000	0.000002000
1	-8.563534000	2.497163000	-0.000001000

Table S146. Coordinates of pN_a_2 at M062X/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.710429000	-4.726236000
7	0.000000000	1.360107000	-3.495065000
6	0.000000000	0.731137000	-2.267867000
6	0.000000000	-0.731137000	-2.267867000
7	0.000000000	-1.360107000	-3.495065000
6	0.000000000	-0.710429000	-4.726236000
6	0.000000000	-0.732197000	0.175485000
6	0.000000000	0.732197000	0.175485000
6	0.000000000	1.415513000	1.363107000
1	0.000000000	2.499147000	1.388044000
6	0.000000000	0.733701000	2.616834000
6	0.000000000	-0.733701000	2.616834000
6	0.000000000	-1.415513000	1.363107000
1	0.000000000	2.368505000	-3.499786000
1	0.000000000	-2.368505000	-3.499786000
1	0.000000000	-2.499147000	1.388044000
6	0.000000000	-0.726971000	4.900940000
6	0.000000000	0.726971000	4.900940000
6	0.000000000	1.413262000	6.106462000
6	0.000000000	-1.413262000	6.106462000
6	0.000000000	-0.729396000	7.337082000
6	0.000000000	0.729396000	7.337082000
1	0.000000000	2.496840000	6.080414000
1	0.000000000	-2.496840000	6.080414000
6	0.000000000	0.709461000	-7.154047000
6	0.000000000	-0.709461000	-7.154047000
6	0.000000000	-1.395112000	-8.396511000
6	0.000000000	1.395112000	-8.396511000
6	0.000000000	-0.715223000	-9.585588000

1	-8.563534000	-2.497163000	0.000013000	6	0.000000000	0.715223000	-9.585588000
6	9.567821000	0.712520000	-0.000015000	1	0.000000000	2.480436000	-8.401855000
6	9.567821000	-0.712520000	-0.000012000	1	0.000000000	-2.480436000	-8.401855000
7	10.793273000	-1.359833000	-0.000016000	6	0.000000000	0.727289000	9.772362000
7	10.793273000	1.359833000	-0.000022000	6	0.000000000	-0.727289000	9.772362000
6	12.020649000	-0.712890000	-0.000012000	7	0.000000000	-1.425146000	10.927060000
6	12.020649000	0.712890000	-0.000015000	7	0.000000000	1.425146000	10.927060000
1	10.793784000	-2.368917000	-0.000011000	6	0.000000000	-0.729533000	12.053294000
1	10.793784000	2.368917000	-0.000020000	6	0.000000000	0.729533000	12.053294000
6	8.378605000	1.391804000	-0.000012000	6	0.000000000	1.414020000	8.556827000
6	8.378605000	-1.391804000	-0.000006000	6	0.000000000	-1.414020000	8.556827000
7	3.488098000	1.356429000	0.000001000	7	0.000000000	1.426941000	3.735221000
7	3.488098000	-1.356429000	0.000007000	7	0.000000000	-1.426941000	3.735221000
6	-1.362237000	1.410354000	0.000003000	6	0.000000000	1.409805000	-1.091745000
6	-1.362237000	-1.410354000	0.000011000	6	0.000000000	-1.409805000	-1.091745000
6	-6.094788000	1.410129000	0.000004000	6	0.000000000	1.394252000	-5.917771000
6	-6.094788000	-1.410129000	0.000012000	6	0.000000000	-1.394252000	-5.917771000
7	-10.904873000	1.422398000	-0.000001000	7	0.000000000	1.363682000	-10.813957000
7	-10.904873000	-1.422398000	0.000007000	7	0.000000000	-1.363682000	-10.813957000
6	-12.035082000	0.727513000	-0.000001000	6	0.000000000	0.715931000	-12.043569000
6	-12.035082000	-0.727513000	0.000004000	6	0.000000000	-0.715931000	-12.043569000
6	-13.272911000	1.410119000	-0.000004000	6	0.000000000	1.395368000	-13.230859000
6	-13.272911000	-1.410119000	0.000005000	6	0.000000000	-1.395368000	-13.230859000
6	-14.466351000	0.725825000	-0.000003000	6	0.000000000	0.709555000	-14.475571000
6	-14.466351000	-0.725825000	0.000002000	6	0.000000000	-0.709555000	-14.475571000
6	13.208059000	1.391988000	-0.000012000	6	0.000000000	1.415392000	13.298686000
6	13.208059000	-1.391988000	-0.000006000	6	0.000000000	-1.415392000	13.298686000
6	14.448755000	0.710498000	-0.000007000	6	0.000000000	0.728666000	14.487658000
6	14.448755000	-0.710498000	-0.000004000	6	0.000000000	-0.728666000	14.487658000
6	15.683068000	1.393076000	-0.000005000	6	0.000000000	1.411899000	15.758646000
6	15.683068000	-1.393076000	0.000001000	6	0.000000000	-1.411899000	15.758646000
6	16.868798000	0.703111000	0.000000000	6	0.000000000	0.720719000	16.921277000
6	16.868798000	-0.703111000	0.000003000	6	0.000000000	-0.720719000	16.921277000
1	15.678408000	2.480500000	-0.000007000	1	0.000000000	2.496125000	15.754310000
1	17.811519000	1.241612000	0.000001000	1	0.000000000	1.246924000	17.868309000
1	17.811519000	-1.241612000	0.000007000	1	0.000000000	-1.246924000	17.868309000
1	15.678408000	-2.480500000	0.000004000	1	0.000000000	-2.496125000	15.754310000
1	13.203424000	-2.480489000	-0.000004000	1	0.000000000	-2.499242000	13.274253000
1	13.203424000	2.480489000	-0.000014000	1	0.000000000	2.499242000	13.274253000
1	8.384852000	-2.480165000	-0.000003000	1	0.000000000	-2.497621000	8.582203000
1	8.384852000	2.480165000	-0.000014000	1	0.000000000	2.497621000	8.582203000
1	3.491042000	-2.366576000	0.000009000	1	0.000000000	2.494530000	-1.096515000
1	3.491042000	2.366576000	-0.000001000	1	0.000000000	-2.494530000	-1.096515000
1	-1.386724000	2.496716000	0.000001000	1	0.000000000	-2.479687000	-5.910558000
1	-1.386724000	-2.496716000	0.000014000	1	0.000000000	2.479687000	-5.910558000
1	-6.069873000	-2.496237000	0.000015000	1	0.000000000	-2.371057000	-10.814623000
1	-6.069873000	2.496237000	0.000001000	1	0.000000000	2.371057000	-10.814623000
1	-13.249203000	-2.496547000	0.000008000	1	0.000000000	-2.480871000	-13.226477000

1	-13.249203000	2.496547000	-0.000007000	1	0.000000000	2.480871000	-13.226477000
6	-15.727783000	1.405766000	-0.000005000	6	0.000000000	1.395667000	-15.712575000
6	-15.727783000	-1.405766000	0.000003000	6	0.000000000	-1.395667000	-15.712575000
6	-16.892983000	0.715473000	-0.000003000	6	0.000000000	0.705521000	-16.899984000
6	-16.892983000	-0.715473000	0.000001000	6	0.000000000	-0.705521000	-16.899984000
1	-15.722472000	2.492421000	-0.000008000	1	0.000000000	2.480526000	-15.708195000
1	-15.722472000	-2.492421000	0.000007000	1	0.000000000	-2.480526000	-15.708195000
1	-17.841089000	-1.244385000	0.000003000	1	0.000000000	-1.243512000	-17.840363000
1	-17.841089000	1.244385000	-0.000005000	1	0.000000000	1.243512000	-17.840363000

Table S147. Coordinates of pN_a_3 at M06/6-311++g(d,p) level

atom	x	y	z
6	-4.805516000	0.729245000	-0.000366000
7	-3.661562000	1.424629000	-0.000414000
6	-2.523085000	0.730497000	-0.000448000
6	-2.523085000	-0.730497000	-0.000443000
7	-3.661562000	-1.424629000	-0.000405000
6	-4.805516000	-0.729245000	-0.000361000
6	-0.088316000	-0.730688000	-0.000470000
6	-0.088316000	0.730688000	-0.000475000
6	1.142851000	1.411617000	-0.000467000
1	1.168047000	2.497615000	-0.000463000
6	2.345587000	0.727508000	-0.000443000
6	2.345587000	-0.727508000	-0.000439000
6	1.142851000	-1.411617000	-0.000458000
1	1.168047000	-2.497615000	-0.000448000
6	4.628358000	-0.731897000	-0.000355000
6	4.628358000	0.731897000	-0.000359000
6	5.872854000	1.411357000	-0.000291000
6	5.872854000	-1.411357000	-0.000284000
6	7.062891000	-0.729261000	-0.000209000
6	7.062891000	0.729261000	-0.000212000
1	5.848483000	2.497643000	-0.000290000
1	5.848483000	-2.497643000	-0.000276000
6	-7.239937000	0.730470000	-0.000220000
6	-7.239937000	-0.730470000	-0.000215000
6	-8.465026000	-1.412604000	-0.000118000
6	-8.465026000	1.412604000	-0.000127000
6	-9.673145000	-0.727742000	-0.000017000
6	-9.673145000	0.727742000	-0.000022000
1	-8.490162000	2.498542000	-0.000123000
1	-8.490162000	-2.498542000	-0.000108000
6	9.497328000	0.725328000	-0.000020000
6	9.497328000	-0.725328000	-0.000016000
7	10.721632000	-1.356642000	0.000095000
7	10.721632000	1.356642000	0.000088000
6	11.948784000	-0.711227000	0.000213000

Table S148. Coordinates of pN_a_3 at M062X/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.730021000	4.814767000
7	0.000000000	1.426580000	3.669076000
6	0.000000000	0.731419000	2.530813000
6	0.000000000	-0.731419000	2.530813000
7	0.000000000	-1.426580000	3.669076000
6	0.000000000	-0.730021000	4.814767000
6	0.000000000	-0.732043000	0.091313000
6	0.000000000	0.732043000	0.091313000
6	0.000000000	1.415155000	-1.147950000
1	0.000000000	2.498623000	-1.174606000
6	0.000000000	0.728719000	-2.347082000
6	0.000000000	-0.728719000	-2.347082000
6	0.000000000	-1.415155000	-1.147950000
1	0.000000000	-2.498623000	-1.174606000
6	0.000000000	-0.735531000	-4.632372000
6	0.000000000	0.735531000	-4.632372000
6	0.000000000	1.417564000	-5.887599000
6	0.000000000	-1.417564000	-5.887599000
6	0.000000000	-0.733064000	-7.072176000
6	0.000000000	0.733064000	-7.072176000
1	0.000000000	2.501094000	-5.862326000
1	0.000000000	-2.501094000	-5.862326000
6	0.000000000	0.731482000	7.252683000
6	0.000000000	-0.731482000	7.252683000
6	0.000000000	-1.415827000	8.483977000
6	0.000000000	1.415827000	8.483977000
6	0.000000000	-0.728519000	9.689168000
6	0.000000000	0.728519000	9.689168000
1	0.000000000	2.499315000	8.510290000
1	0.000000000	-2.499315000	8.510290000
6	0.000000000	0.731268000	-9.514104000
6	0.000000000	-0.731268000	-9.514104000
7	0.000000000	-1.360457000	-10.741389000
7	0.000000000	1.360457000	-10.741389000
6	0.000000000	-0.713566000	-11.971102000

6	11.948784000	0.711227000	0.000209000	6	0.000000000	0.713566000	-11.971102000
1	10.724508000	-2.366971000	0.000100000	1	0.000000000	-2.369067000	-10.745940000
1	10.724508000	2.366971000	0.000089000	1	0.000000000	2.369067000	-10.745940000
6	8.320607000	1.404110000	-0.000119000	6	0.000000000	1.410761000	-8.340022000
6	8.320607000	-1.404110000	-0.000112000	6	0.000000000	-1.410761000	-8.340022000
7	3.507278000	1.424759000	-0.000407000	7	0.000000000	1.428405000	-3.517516000
7	3.507278000	-1.424759000	-0.000399000	7	0.000000000	-1.428405000	-3.517516000
6	-1.298857000	1.413461000	-0.000469000	6	0.000000000	1.416659000	1.301111000
6	-1.298857000	-1.413461000	-0.000461000	6	0.000000000	-1.416659000	1.301111000
6	-6.023944000	1.413109000	-0.000301000	6	0.000000000	1.416248000	6.036364000
6	-6.023944000	-1.413109000	-0.000292000	6	0.000000000	-1.416248000	6.036364000
7	-10.828967000	1.423671000	0.000087000	7	0.000000000	1.427304000	10.851700000
7	-10.828967000	-1.423671000	0.000096000	7	0.000000000	-1.427304000	10.851700000
6	-11.954483000	0.729552000	0.000203000	6	0.000000000	0.732492000	11.970974000
6	-11.954483000	-0.729552000	0.000208000	6	0.000000000	-0.732492000	11.970974000
6	-13.195530000	1.411771000	0.000336000	6	0.000000000	1.417593000	13.221356000
6	-13.195530000	-1.411771000	0.000345000	6	0.000000000	-1.417593000	13.221356000
6	-14.386269000	0.727011000	0.000471000	6	0.000000000	0.730420000	14.406559000
6	-14.386269000	-0.727011000	0.000476000	6	0.000000000	-0.730420000	14.406559000
6	13.136500000	1.393623000	0.000329000	6	0.000000000	1.396695000	-13.158580000
6	13.136500000	-1.393623000	0.000335000	6	0.000000000	-1.396695000	-13.158580000
6	14.372788000	0.711399000	0.000460000	6	0.000000000	0.710408000	-14.398641000
6	14.372788000	-0.711399000	0.000463000	6	0.000000000	-0.710408000	-14.398641000
6	15.609118000	1.394660000	0.000590000	6	0.000000000	1.397347000	-15.638203000
6	15.609118000	-1.394660000	0.000597000	6	0.000000000	-1.397347000	-15.638203000
6	16.792078000	0.704303000	0.000719000	6	0.000000000	0.706813000	-16.822609000
6	16.792078000	-0.704303000	0.000722000	6	0.000000000	-0.706813000	-16.822609000
1	15.604596000	2.481864000	0.000587000	1	0.000000000	2.482031000	-15.634066000
1	17.735378000	1.241526000	0.000818000	1	0.000000000	1.243453000	-17.763638000
1	17.735378000	-1.241526000	0.000824000	1	0.000000000	-1.243453000	-17.763638000
1	15.604596000	-2.481864000	0.000599000	1	0.000000000	-2.482031000	-15.634066000
1	13.131374000	-2.481892000	0.000339000	1	0.000000000	-2.482053000	-13.153297000
1	13.131374000	2.481892000	0.000327000	1	0.000000000	2.482053000	-13.153297000
1	8.325782000	-2.491772000	-0.000105000	1	0.000000000	-2.495411000	-8.345121000
1	8.325782000	2.491772000	-0.000117000	1	0.000000000	2.495411000	-8.345121000
1	-1.322937000	2.499444000	-0.000465000	1	0.000000000	2.500173000	1.326066000
1	-1.322937000	-2.499444000	-0.000451000	1	0.000000000	-2.500173000	1.326066000
1	-5.999370000	-2.499066000	-0.000284000	1	0.000000000	-2.499754000	6.011010000
1	-5.999370000	2.499066000	-0.000299000	1	0.000000000	2.499754000	6.011010000
1	-13.172143000	-2.498102000	0.000347000	1	0.000000000	-2.501344000	13.197094000
1	-13.172143000	2.498102000	0.000332000	1	0.000000000	2.501344000	13.197094000
6	-15.648968000	1.406866000	0.000613000	6	0.000000000	1.413348000	15.680036000
6	-15.648968000	-1.406866000	0.000621000	6	0.000000000	-1.413348000	15.680036000
6	-16.812856000	0.716205000	0.000748000	6	0.000000000	0.721789000	16.840846000
6	-16.812856000	-0.716205000	0.000752000	6	0.000000000	-0.721789000	16.840846000
1	-15.643816000	2.493412000	0.000609000	1	0.000000000	2.497482000	15.675916000
1	-15.643816000	-2.493412000	0.000624000	1	0.000000000	-2.497482000	15.675916000
1	-17.761281000	-1.244403000	0.000862000	1	0.000000000	-1.247000000	17.788360000

1	-17.761281000	1.244403000	0.000854000	1	0.000000000	1.247000000	17.788360000
Table S149. Coordinates of pN ₄ _4 at M06/6-311++g(d,p) level				Table S150. Coordinates of pN ₄ _4 at M062X/6-311++g(d,p) level			
atom	x	y	z	atom	x	y	z
6	0.000000000	4.741643000	0.728305000	6	0.000000000	4.756375000	0.731025000
7	0.000000000	3.577596000	1.428408000	7	0.000000000	3.577851000	1.434497000
6	0.000000000	2.457265000	0.733003000	6	0.000000000	2.469678000	0.738539000
6	0.000000000	2.457265000	-0.733003000	6	0.000000000	2.469678000	-0.738539000
7	0.000000000	3.577596000	-1.428408000	7	0.000000000	3.577851000	-1.434497000
6	0.000000000	4.741643000	-0.728305000	6	0.000000000	4.756375000	-0.731025000
6	0.000000000	0.000000000	-0.731779000	6	0.000000000	0.000000000	-0.736754000
6	0.000000000	0.000000000	0.731779000	6	0.000000000	0.000000000	0.736754000
6	0.000000000	-1.218015000	1.404891000	6	0.000000000	-1.217021000	1.409750000
1	0.000000000	-1.242131000	2.491538000	1	0.000000000	-1.241219000	2.494236000
6	0.000000000	-2.457265000	0.733003000	6	0.000000000	-2.469678000	0.738539000
6	0.000000000	-2.457265000	-0.733003000	6	0.000000000	-2.469678000	-0.738539000
6	0.000000000	-1.218015000	-1.404891000	6	0.000000000	-1.217021000	-1.409750000
1	0.000000000	-1.242131000	-2.491538000	1	0.000000000	-1.241219000	-2.494236000
6	0.000000000	-4.741643000	-0.728305000	6	0.000000000	-4.756375000	-0.731025000
6	0.000000000	-4.741643000	0.728305000	6	0.000000000	-4.756375000	0.731025000
6	0.000000000	-5.939382000	1.406601000	6	0.000000000	-5.944053000	1.412513000
6	0.000000000	-5.939382000	-1.406601000	6	0.000000000	-5.944053000	-1.412513000
6	0.000000000	-7.184493000	-0.728198000	6	0.000000000	-7.200334000	-0.729729000
6	0.000000000	-7.184493000	0.728198000	6	0.000000000	-7.200334000	0.729729000
1	0.000000000	-5.913931000	2.492918000	1	0.000000000	-5.918652000	2.496383000
1	0.000000000	-5.913931000	-2.492918000	1	0.000000000	-5.918652000	-2.496383000
6	0.000000000	7.184493000	0.728198000	6	0.000000000	7.200334000	0.729729000
6	0.000000000	7.184493000	-0.728198000	6	0.000000000	7.200334000	-0.729729000
6	0.000000000	8.384115000	-1.409189000	6	0.000000000	8.395261000	-1.413993000
6	0.000000000	8.384115000	1.409189000	6	0.000000000	8.395261000	1.413993000
6	0.000000000	9.621690000	-0.725498000	6	0.000000000	9.637497000	-0.726003000
6	0.000000000	9.621690000	0.725498000	6	0.000000000	9.637497000	0.726003000
1	0.000000000	8.408709000	2.495390000	1	0.000000000	8.420801000	2.497743000
1	0.000000000	8.408709000	-2.495390000	1	0.000000000	8.420801000	-2.497743000
6	0.000000000	-9.621690000	0.725498000	6	0.000000000	-9.637497000	0.726003000
6	0.000000000	-9.621690000	-0.725498000	6	0.000000000	-9.637497000	-0.726003000
7	0.000000000	-10.752720000	-1.420373000	7	0.000000000	-10.768729000	-1.422445000
7	0.000000000	-10.752720000	1.420373000	7	0.000000000	-10.768729000	1.422445000
6	0.000000000	-11.899980000	-0.723021000	6	0.000000000	-11.915049000	-0.723511000
6	0.000000000	-11.899980000	0.723021000	6	0.000000000	-11.915049000	0.723511000
6	0.000000000	-8.384115000	1.409189000	6	0.000000000	-8.395261000	1.413993000
6	0.000000000	-8.384115000	-1.409189000	6	0.000000000	-8.395261000	-1.413993000
7	0.000000000	-3.577596000	1.428408000	7	0.000000000	-3.577851000	1.434497000
7	0.000000000	-3.577596000	-1.428408000	7	0.000000000	-3.577851000	-1.434497000
6	0.000000000	1.218015000	1.404891000	6	0.000000000	1.217021000	1.409750000
6	0.000000000	1.218015000	-1.404891000	6	0.000000000	1.217021000	-1.409750000
6	0.000000000	5.939382000	1.406601000	6	0.000000000	5.944053000	1.412513000

6	0.000000000	5.939382000	-1.406601000	6	0.000000000	5.944053000	-1.412513000
7	0.000000000	10.752720000	1.420373000	7	0.000000000	10.768729000	1.422445000
7	0.000000000	10.752720000	-1.420373000	7	0.000000000	10.768729000	-1.422445000
6	0.000000000	11.899980000	0.723021000	6	0.000000000	11.915049000	0.723511000
6	0.000000000	11.899980000	-0.723021000	6	0.000000000	11.915049000	-0.723511000
6	0.000000000	13.123346000	1.407002000	6	0.000000000	13.143639000	1.411133000
6	0.000000000	13.123346000	-1.407002000	6	0.000000000	13.143639000	-1.411133000
6	0.000000000	14.327158000	0.722105000	6	0.000000000	14.343918000	0.723988000
6	0.000000000	14.327158000	-0.722105000	6	0.000000000	14.343918000	-0.723988000
6	0.000000000	-13.123346000	1.407002000	6	0.000000000	-13.143639000	1.411133000
6	0.000000000	-13.123346000	-1.407002000	6	0.000000000	-13.143639000	-1.411133000
6	0.000000000	-14.327158000	0.722105000	6	0.000000000	-14.343918000	0.723988000
6	0.000000000	-14.327158000	-0.722105000	6	0.000000000	-14.343918000	-0.723988000
6	0.000000000	-15.582100000	1.403273000	6	0.000000000	-15.607307000	1.408899000
6	0.000000000	-15.582100000	-1.403273000	6	0.000000000	-15.607307000	-1.408899000
6	0.000000000	-16.751404000	0.712429000	6	0.000000000	-16.774223000	0.717373000
6	0.000000000	-16.751404000	-0.712429000	6	0.000000000	-16.774223000	-0.717373000
1	0.000000000	-15.576657000	2.489852000	1	0.000000000	-15.602671000	2.493113000
1	0.000000000	-17.698281000	1.243220000	1	0.000000000	-17.720079000	1.245570000
1	0.000000000	-17.698281000	-1.243220000	1	0.000000000	-17.720079000	-1.245570000
1	0.000000000	-15.576657000	-2.489852000	1	0.000000000	-15.602671000	-2.493113000
1	0.000000000	-13.098882000	-2.493341000	1	0.000000000	-13.118319000	-2.494968000
1	0.000000000	-13.098882000	2.493341000	1	0.000000000	-13.118319000	2.494968000
1	0.000000000	-8.408709000	-2.495390000	1	0.000000000	-8.420801000	-2.497743000
1	0.000000000	-8.408709000	2.495390000	1	0.000000000	-8.420801000	2.497743000
1	0.000000000	1.242131000	2.491538000	1	0.000000000	1.241219000	2.494236000
1	0.000000000	1.242131000	-2.491538000	1	0.000000000	1.241219000	-2.494236000
1	0.000000000	5.913931000	-2.492918000	1	0.000000000	5.918652000	-2.496383000
1	0.000000000	5.913931000	2.492918000	1	0.000000000	5.918652000	2.496383000
1	0.000000000	13.098882000	-2.493341000	1	0.000000000	13.118319000	-2.494968000
1	0.000000000	13.098882000	2.493341000	1	0.000000000	13.118319000	2.494968000
6	0.000000000	15.582100000	1.403273000	6	0.000000000	15.607307000	1.408899000
6	0.000000000	15.582100000	-1.403273000	6	0.000000000	15.607307000	-1.408899000
6	0.000000000	16.751404000	0.712429000	6	0.000000000	16.774223000	0.717373000
6	0.000000000	16.751404000	-0.712429000	6	0.000000000	16.774223000	-0.717373000
1	0.000000000	15.576657000	2.489852000	1	0.000000000	15.602671000	2.493113000
1	0.000000000	15.576657000	-2.489852000	1	0.000000000	15.602671000	-2.493113000
1	0.000000000	17.698281000	-1.243220000	1	0.000000000	17.720079000	-1.245570000
1	0.000000000	17.698281000	1.243220000	1	0.000000000	17.720079000	1.245570000

Table S151. Coordinates of pN₅_1 at M06/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.723678000	8.633744000
7	0.000000000	1.356509000	7.408329000
6	0.000000000	0.708315000	6.178905000
6	0.000000000	-0.708315000	6.178905000
7	0.000000000	-1.356509000	7.408329000

Table S152. Coordinates of pN₅_1 at M062X/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.713506000	-8.474526000
7	0.000000000	1.364327000	-7.244127000
6	0.000000000	0.713839000	-6.014255000
6	0.000000000	-0.713839000	-6.014255000
7	0.000000000	-1.364327000	-7.244127000

6	0.000000000	-0.723678000	8.633744000	6	0.000000000	-0.713506000	-8.474526000
6	0.000000000	-0.710707000	3.750863000	6	0.000000000	-0.708163000	-3.580126000
6	0.000000000	0.710707000	3.750863000	6	0.000000000	0.708163000	-3.580126000
6	0.000000000	1.390460000	2.508653000	6	0.000000000	1.391919000	-2.337219000
1	0.000000000	2.479049000	2.502830000	1	0.000000000	2.477613000	-2.331087000
6	0.000000000	0.712880000	1.316609000	6	0.000000000	0.712709000	-1.144425000
6	0.000000000	-0.712880000	1.316609000	6	0.000000000	-0.712709000	-1.144425000
6	0.000000000	-1.390460000	2.508653000	6	0.000000000	-1.391919000	-2.337219000
1	0.000000000	2.366323000	7.406035000	1	0.000000000	2.371306000	-7.244417000
1	0.000000000	-2.366323000	7.406035000	1	0.000000000	-2.371306000	-7.244417000
1	0.000000000	-2.479049000	2.502830000	1	0.000000000	-2.477613000	-2.331087000
6	0.000000000	-0.709950000	-1.141949000	6	0.000000000	-0.715590000	1.319207000
6	0.000000000	0.709950000	-1.141949000	6	0.000000000	0.715590000	1.319207000
6	0.000000000	1.388787000	-2.334695000	6	0.000000000	1.393410000	2.511462000
6	0.000000000	-1.388787000	-2.334695000	6	0.000000000	-1.393410000	2.511462000
6	0.000000000	-0.709603000	-3.574821000	6	0.000000000	-0.709248000	3.757179000
6	0.000000000	0.709603000	-3.574821000	6	0.000000000	0.709248000	3.757179000
1	0.000000000	2.477582000	-2.328427000	1	0.000000000	2.478919000	2.505915000
1	0.000000000	-2.477582000	-2.328427000	1	0.000000000	-2.478919000	2.505915000
6	0.000000000	0.726132000	11.070755000	6	0.000000000	0.708141000	-10.907004000
6	0.000000000	-0.726132000	11.070755000	6	0.000000000	-0.708141000	-10.907004000
6	0.000000000	-1.407152000	12.267109000	6	0.000000000	-1.393274000	-12.146964000
6	0.000000000	1.407152000	12.267109000	6	0.000000000	1.393274000	-12.146964000
6	0.000000000	-0.726234000	13.504560000	6	0.000000000	-0.712761000	-13.337371000
6	0.000000000	0.726234000	13.504560000	6	0.000000000	0.712761000	-13.337371000
1	0.000000000	2.493700000	12.291495000	1	0.000000000	2.478861000	-12.152881000
1	0.000000000	-2.493700000	12.291495000	1	0.000000000	-2.478861000	-12.152881000
6	0.000000000	0.711165000	-6.006108000	6	0.000000000	0.710494000	6.188375000
6	0.000000000	-0.711165000	-6.006108000	6	0.000000000	-0.710494000	6.188375000
7	0.000000000	-1.360404000	-7.233425000	7	0.000000000	-1.360546000	7.420394000
7	0.000000000	1.360404000	-7.233425000	7	0.000000000	1.360546000	7.420394000
6	0.000000000	-0.710738000	-8.461516000	6	0.000000000	-0.728825000	8.648637000
6	0.000000000	0.710738000	-8.461516000	6	0.000000000	0.728825000	8.648637000
1	0.000000000	-2.369075000	-7.233822000	1	0.000000000	-2.368632000	7.416652000
1	0.000000000	2.369075000	-7.233822000	1	0.000000000	2.368632000	7.416652000
6	0.000000000	1.389746000	-4.814199000	6	0.000000000	1.393292000	4.995942000
6	0.000000000	-1.389746000	-4.814199000	6	0.000000000	-1.393292000	4.995942000
7	0.000000000	1.359407000	0.089064000	7	0.000000000	1.363370000	0.088942000
7	0.000000000	-1.359407000	0.089064000	7	0.000000000	-1.363370000	0.088942000
6	0.000000000	1.390541000	4.986702000	6	0.000000000	1.392905000	-4.822307000
6	0.000000000	-1.390541000	4.986702000	6	0.000000000	-1.392905000	-4.822307000
6	0.000000000	1.401309000	9.813488000	6	0.000000000	1.392855000	-9.665628000
6	0.000000000	-1.401309000	9.813488000	6	0.000000000	-1.392855000	-9.665628000
7	0.000000000	1.419895000	14.638426000	7	0.000000000	1.364388000	-14.567167000
7	0.000000000	-1.419895000	14.638426000	7	0.000000000	-1.364388000	-14.567167000
6	0.000000000	0.722522000	15.784461000	6	0.000000000	0.716660000	-15.794652000
6	0.000000000	-0.722522000	15.784461000	6	0.000000000	-0.716660000	-15.794652000

6	0.000000000	1.405565000	17.010901000	6	0.000000000	1.394969000	-16.982703000
6	0.000000000	-1.405565000	17.010901000	6	0.000000000	-1.394969000	-16.982703000
6	0.000000000	0.722411000	18.213624000	6	0.000000000	0.709620000	-18.228116000
6	0.000000000	-0.722411000	18.213624000	6	0.000000000	-0.709620000	-18.228116000
6	0.000000000	1.389688000	-9.652490000	6	0.000000000	1.407212000	9.826281000
6	0.000000000	-1.389688000	-9.652490000	6	0.000000000	-1.407212000	9.826281000
6	0.000000000	0.709540000	-10.891151000	6	0.000000000	0.728151000	11.090983000
6	0.000000000	-0.709540000	-10.891151000	6	0.000000000	-0.728151000	11.090983000
6	0.000000000	1.390142000	-12.128422000	6	0.000000000	1.411796000	12.283994000
6	0.000000000	-1.390142000	-12.128422000	6	0.000000000	-1.411796000	12.283994000
6	0.000000000	0.710105000	-13.318650000	6	0.000000000	0.726807000	13.526678000
6	0.000000000	-0.710105000	-13.318650000	6	0.000000000	-0.726807000	13.526678000
1	0.000000000	2.478784000	-12.134497000	1	0.000000000	2.495559000	12.309545000
1	0.000000000	-2.478784000	-12.134497000	1	0.000000000	-2.495559000	12.309545000
1	0.000000000	-2.478394000	-9.645897000	1	0.000000000	-2.492057000	9.821413000
1	0.000000000	2.478394000	-9.645897000	1	0.000000000	2.492057000	9.821413000
1	0.000000000	-2.478455000	-4.820396000	1	0.000000000	-2.478872000	5.002800000
1	0.000000000	2.478455000	-4.820396000	1	0.000000000	2.478872000	5.002800000
1	0.000000000	-2.368237000	0.088205000	1	0.000000000	-2.370471000	0.088026000
1	0.000000000	2.368237000	0.088205000	1	0.000000000	2.370471000	0.088026000
1	0.000000000	2.479108000	4.993540000	1	0.000000000	2.478522000	-4.828082000
1	0.000000000	-2.479108000	4.993540000	1	0.000000000	-2.478522000	-4.828082000
1	0.000000000	-2.489186000	9.808229000	1	0.000000000	-2.478472000	-9.659400000
1	0.000000000	2.489186000	9.808229000	1	0.000000000	2.478472000	-9.659400000
1	0.000000000	-2.492214000	16.986452000	1	0.000000000	-2.371542000	-14.566956000
1	0.000000000	2.492214000	16.986452000	1	0.000000000	2.371542000	-14.566956000
6	0.000000000	1.402688000	19.470756000	1	0.000000000	-2.480537000	-16.978129000
6	0.000000000	-1.402688000	19.470756000	1	0.000000000	2.480537000	-16.978129000
6	0.000000000	0.713050000	20.640058000	6	0.000000000	1.395177000	-19.465049000
6	0.000000000	-0.713050000	20.640058000	6	0.000000000	-1.395177000	-19.465049000
1	0.000000000	2.489554000	19.465572000	6	0.000000000	0.705279000	-20.653199000
1	0.000000000	-2.489554000	19.465572000	6	0.000000000	-0.705279000	-20.653199000
1	0.000000000	-1.244521000	21.586842000	1	0.000000000	2.480132000	-19.460602000
1	0.000000000	1.244521000	21.586842000	1	0.000000000	-2.480132000	-19.460602000
7	0.000000000	-1.360630000	-14.545849000	1	0.000000000	-1.243794000	-21.593355000
7	0.000000000	1.360630000	-14.545849000	1	0.000000000	1.243794000	-21.593355000
6	0.000000000	-0.713612000	-15.770878000	7	0.000000000	-1.421914000	14.659245000
6	0.000000000	0.713612000	-15.770878000	7	0.000000000	1.421914000	14.659245000
6	0.000000000	-1.391373000	-16.958759000	6	0.000000000	-0.722480000	15.805917000
6	0.000000000	1.391373000	-16.958759000	6	0.000000000	0.722480000	15.805917000
6	0.000000000	-0.710507000	-18.200977000	6	0.000000000	-1.409438000	17.035568000
6	0.000000000	0.710507000	-18.200977000	6	0.000000000	1.409438000	17.035568000
1	0.000000000	-2.479975000	-16.953780000	6	0.000000000	-0.723670000	18.236267000
1	0.000000000	2.479975000	-16.953780000	6	0.000000000	0.723670000	18.236267000
1	0.000000000	-2.369440000	-14.545910000	1	0.000000000	-2.493443000	17.009993000
1	0.000000000	2.369440000	-14.545910000	1	0.000000000	2.493443000	17.009993000
6	0.000000000	-0.702887000	-20.622336000	6	0.000000000	-0.717447000	20.668217000
6	0.000000000	0.702887000	-20.622336000	6	0.000000000	0.717447000	20.668217000

6	0.000000000	1.392387000	-19.435433000	6	0.000000000	1.407842000	19.500501000
6	0.000000000	-1.392387000	-19.435433000	6	0.000000000	-1.407842000	19.500501000
1	0.000000000	2.479940000	-19.430330000	1	0.000000000	2.492263000	19.495795000
1	0.000000000	-2.479940000	-19.430330000	1	0.000000000	-2.492263000	19.495795000
1	0.000000000	1.242090000	-21.564791000	1	0.000000000	1.246440000	21.613778000
1	0.000000000	-1.242090000	-21.564791000	1	0.000000000	-1.246440000	21.613778000

Table S153. Coordinates of pN ₅ _2 at M06/6-311++g(d,p) level				Table S154. Coordinates of pN ₅ _2 at M062X/6-311++g(d,p) level			
atom	X	Y	Z	atom	X	Y	Z
6	0.000000000	0.726497000	8.545435000	6	0.000000000	0.712720000	-8.386083000
7	0.000000000	1.424014000	7.386114000	7	0.000000000	1.364004000	-7.154866000
6	0.000000000	0.730996000	6.262725000	6	0.000000000	0.716002000	-5.926996000
6	0.000000000	-0.730996000	6.262725000	6	0.000000000	-0.716002000	-5.926996000
7	0.000000000	-1.424014000	7.386114000	7	0.000000000	-1.364004000	-7.154866000
6	0.000000000	-0.726497000	8.545435000	6	0.000000000	-0.712720000	-8.386083000
6	0.000000000	-0.728858000	3.827823000	6	0.000000000	-0.709549000	-3.492951000
6	0.000000000	0.728858000	3.827823000	6	0.000000000	0.709549000	-3.492951000
6	0.000000000	1.403443000	2.570773000	6	0.000000000	1.393611000	-2.255621000
1	0.000000000	2.491224000	2.565778000	1	0.000000000	2.479119000	-2.248550000
6	0.000000000	0.725349000	1.392462000	6	0.000000000	0.710101000	-1.062971000
6	0.000000000	-0.725349000	1.392462000	6	0.000000000	-0.710101000	-1.062971000
6	0.000000000	-1.403443000	2.570773000	6	0.000000000	-1.393611000	-2.255621000
1	0.000000000	-2.491224000	2.565778000	1	0.000000000	2.371163000	-7.155991000
6	0.000000000	-0.708076000	-1.058599000	1	0.000000000	-2.371163000	-7.155991000
6	0.000000000	0.708076000	-1.058599000	1	0.000000000	-2.479119000	-2.248550000
6	0.000000000	1.391667000	-2.250240000	6	0.000000000	-0.731206000	1.397426000
6	0.000000000	-1.391667000	-2.250240000	6	0.000000000	0.731206000	1.397426000
6	0.000000000	-0.711030000	-3.482541000	6	0.000000000	1.409330000	2.574525000
6	0.000000000	0.711030000	-3.482541000	6	0.000000000	-1.409330000	2.574525000
1	0.000000000	2.480087000	-2.243023000	6	0.000000000	-0.732455000	3.843183000
1	0.000000000	-2.480087000	-2.243023000	6	0.000000000	0.732455000	3.843183000
6	0.000000000	0.729002000	10.978928000	1	0.000000000	2.494087000	2.569344000
6	0.000000000	-0.729002000	10.978928000	1	0.000000000	-2.494087000	2.569344000
6	0.000000000	-1.411011000	12.196269000	6	0.000000000	0.708234000	-10.817473000
6	0.000000000	1.411011000	12.196269000	6	0.000000000	-0.708234000	-10.817473000
6	0.000000000	-0.727213000	13.411851000	6	0.000000000	-1.393570000	-12.057775000
6	0.000000000	0.727213000	13.411851000	6	0.000000000	1.393570000	-12.057775000
1	0.000000000	2.497113000	12.221142000	6	0.000000000	-0.713284000	-13.248137000
1	0.000000000	-2.497113000	12.221142000	6	0.000000000	0.713284000	-13.248137000
6	0.000000000	0.713232000	-5.912042000	1	0.000000000	2.479074000	-12.063475000
6	0.000000000	-0.713232000	-5.912042000	1	0.000000000	-2.479074000	-12.063475000
7	0.000000000	-1.360387000	-7.136312000	6	0.000000000	0.733909000	6.284852000
7	0.000000000	1.360387000	-7.136312000	6	0.000000000	-0.733909000	6.284852000
6	0.000000000	-0.709976000	-8.364559000	7	0.000000000	-1.427145000	7.402959000
6	0.000000000	0.709976000	-8.364559000	7	0.000000000	1.427145000	7.402959000
1	0.000000000	-2.369278000	-7.137125000	6	0.000000000	-0.726930000	8.569118000
1	0.000000000	2.369278000	-7.137125000	6	0.000000000	0.726930000	8.569118000

6	0.000000000	1.391659000	-4.722133000	6	0.000000000	1.415655000	5.031001000
6	0.000000000	-1.391659000	-4.722133000	6	0.000000000	-1.415655000	5.031001000
7	0.000000000	1.356290000	0.169153000	7	0.000000000	1.359502000	0.169622000
7	0.000000000	-1.356290000	0.169153000	7	0.000000000	-1.359502000	0.169622000
6	0.000000000	1.410250000	5.019451000	6	0.000000000	1.394751000	-4.736688000
6	0.000000000	-1.410250000	5.019451000	6	0.000000000	-1.394751000	-4.736688000
6	0.000000000	1.410005000	9.752152000	6	0.000000000	1.392966000	-9.576829000
6	0.000000000	-1.410005000	9.752152000	6	0.000000000	-1.392966000	-9.576829000
7	0.000000000	1.422468000	14.562334000	7	0.000000000	1.364171000	-14.477364000
7	0.000000000	-1.422468000	14.562334000	7	0.000000000	-1.364171000	-14.477364000
6	0.000000000	0.727407000	15.692781000	6	0.000000000	0.716444000	-15.705569000
6	0.000000000	-0.727407000	15.692781000	6	0.000000000	-0.716444000	-15.705569000
6	0.000000000	1.409995000	16.930482000	6	0.000000000	1.395121000	-16.893219000
6	0.000000000	-1.409995000	16.930482000	6	0.000000000	-1.395121000	-16.893219000
6	0.000000000	0.725786000	18.124080000	6	0.000000000	0.709610000	-18.138482000
6	0.000000000	-0.725786000	18.124080000	6	0.000000000	-0.709610000	-18.138482000
6	0.000000000	1.390149000	-9.554914000	6	0.000000000	1.413282000	9.773992000
6	0.000000000	-1.390149000	-9.554914000	6	0.000000000	-1.413282000	9.773992000
6	0.000000000	0.709629000	-10.792045000	6	0.000000000	0.729343000	11.005064000
6	0.000000000	-0.709629000	-10.792045000	6	0.000000000	-0.729343000	11.005064000
6	0.000000000	1.390277000	-12.029513000	6	0.000000000	1.413947000	12.224496000
6	0.000000000	-1.390277000	-12.029513000	6	0.000000000	-1.413947000	12.224496000
6	0.000000000	0.710689000	-13.220102000	6	0.000000000	0.727241000	13.440407000
6	0.000000000	-0.710689000	-13.220102000	6	0.000000000	-0.727241000	13.440407000
1	0.000000000	2.478849000	-12.036006000	1	0.000000000	2.497568000	12.249776000
1	0.000000000	-2.478849000	-12.036006000	1	0.000000000	-2.497568000	12.249776000
1	0.000000000	-2.478757000	-9.548448000	1	0.000000000	-2.496855000	9.748211000
1	0.000000000	2.478757000	-9.548448000	1	0.000000000	2.496855000	9.748211000
1	0.000000000	-2.480078000	-4.728166000	1	0.000000000	-2.499306000	5.056342000
1	0.000000000	2.480078000	-4.728166000	1	0.000000000	2.499306000	5.056342000
1	0.000000000	-2.366441000	0.166079000	1	0.000000000	-2.367914000	0.165144000
1	0.000000000	2.366441000	0.166079000	1	0.000000000	2.367914000	0.165144000
1	0.000000000	2.496630000	5.044084000	1	0.000000000	2.480140000	-4.741885000
1	0.000000000	-2.496630000	5.044084000	1	0.000000000	-2.480140000	-4.741885000
1	0.000000000	-2.496138000	9.726847000	1	0.000000000	-2.478546000	-9.570539000
1	0.000000000	2.496138000	9.726847000	1	0.000000000	2.478546000	-9.570539000
1	0.000000000	-2.496431000	16.906611000	1	0.000000000	-2.371376000	-14.477390000
1	0.000000000	2.496431000	16.906611000	1	0.000000000	2.371376000	-14.477390000
6	0.000000000	1.405701000	19.385459000	1	0.000000000	-2.480661000	-16.888695000
6	0.000000000	-1.405701000	19.385459000	1	0.000000000	2.480661000	-16.888695000
6	0.000000000	0.715444000	20.550734000	6	0.000000000	1.395325000	-19.375428000
6	0.000000000	-0.715444000	20.550734000	6	0.000000000	-1.395325000	-19.375428000
1	0.000000000	2.492367000	19.380174000	6	0.000000000	0.705333000	-20.563364000
1	0.000000000	-2.492367000	19.380174000	6	0.000000000	-0.705333000	-20.563364000
1	0.000000000	-1.244462000	21.498776000	1	0.000000000	2.480247000	-19.370953000
1	0.000000000	1.244462000	21.498776000	1	0.000000000	-2.480247000	-19.370953000
7	0.000000000	-1.360279000	-14.446950000	1	0.000000000	-1.243621000	-21.503618000
7	0.000000000	1.360279000	-14.446950000	1	0.000000000	1.243621000	-21.503618000

6	0.000000000	-0.713433000	-15.673346000	7	0.000000000	-1.425219000	14.594730000
6	0.000000000	0.713433000	-15.673346000	7	0.000000000	1.425219000	14.594730000
6	0.000000000	-1.391699000	-16.861378000	6	0.000000000	-0.729407000	15.721171000
6	0.000000000	1.391699000	-16.861378000	6	0.000000000	0.729407000	15.721171000
6	0.000000000	-0.710462000	-18.102633000	6	0.000000000	-1.415294000	16.966103000
6	0.000000000	0.710462000	-18.102633000	6	0.000000000	1.415294000	16.966103000
1	0.000000000	-2.480259000	-16.856841000	6	0.000000000	-0.728599000	18.155308000
1	0.000000000	2.480259000	-16.856841000	6	0.000000000	0.728599000	18.155308000
1	0.000000000	-2.369175000	-14.446937000	1	0.000000000	-2.499155000	16.941423000
1	0.000000000	2.369175000	-14.446937000	1	0.000000000	2.499155000	16.941423000
6	0.000000000	-0.702944000	-20.523129000	6	0.000000000	-0.720644000	20.589099000
6	0.000000000	0.702944000	-20.523129000	6	0.000000000	0.720644000	20.589099000
6	0.000000000	1.392711000	-19.336812000	6	0.000000000	1.411776000	19.426376000
6	0.000000000	-1.392711000	-19.336812000	6	0.000000000	-1.411776000	19.426376000
1	0.000000000	2.480215000	-19.332102000	1	0.000000000	2.496019000	19.421927000
1	0.000000000	-2.480215000	-19.332102000	1	0.000000000	-2.496019000	19.421927000
1	0.000000000	1.241756000	-21.465728000	1	0.000000000	1.246831000	21.536150000
1	0.000000000	-1.241756000	-21.465728000	1	0.000000000	-1.246831000	21.536150000

Table S155. Coordinates of pN_s_3 at M06/6-311++g(d,p) level

atom	x	y	z
6	-8.290080000	0.708338000	-0.000083000
7	-7.062663000	1.356141000	-0.000105000
6	-5.839459000	0.725677000	-0.000123000
6	-5.839459000	-0.725677000	-0.000119000
7	-7.062663000	-1.356141000	-0.000099000
6	-8.290080000	-0.708338000	-0.000080000
6	-3.404393000	-0.729508000	-0.000149000
6	-3.404393000	0.729508000	-0.000153000
6	-2.213695000	1.411089000	-0.000165000
1	-2.189338000	2.497409000	-0.000166000
6	-0.969258000	0.732212000	-0.000170000
6	-0.969258000	-0.732212000	-0.000166000
6	-2.213695000	-1.411089000	-0.000157000
1	-7.065744000	2.366406000	-0.000106000
1	-7.065744000	-2.366406000	-0.000096000
1	-2.189338000	-2.497409000	-0.000153000
6	1.313886000	-0.727624000	-0.000167000
6	1.313886000	0.727624000	-0.000172000
6	2.516371000	1.411360000	-0.000168000
6	2.516371000	-1.411360000	-0.000159000
6	3.748164000	-0.730760000	-0.000151000
6	3.748164000	0.730760000	-0.000156000
1	2.491238000	2.497376000	-0.000169000
1	2.491238000	-2.497375000	-0.000154000
6	-10.713639000	0.711147000	-0.000036000
6	-10.713639000	-0.711147000	-0.000033000

Table S156. Coordinates of pN_s_3 at M062X/6-311++g(d,p) level

atom	X	Y	Z
6	0.000000000	0.710201000	-8.309922000
7	0.000000000	1.359744000	-7.078607000
6	0.000000000	0.731877000	-5.851870000
6	0.000000000	-0.731877000	-5.851870000
7	0.000000000	-1.359744000	-7.078607000
6	0.000000000	-0.710201000	-8.309922000
6	0.000000000	-0.733441000	-3.408268000
6	0.000000000	0.733441000	-3.408268000
6	0.000000000	1.416861000	-2.222116000
1	0.000000000	2.500463000	-2.197245000
6	0.000000000	0.736006000	-0.965264000
6	0.000000000	-0.736006000	-0.965264000
6	0.000000000	-1.416861000	-2.222116000
1	0.000000000	2.368243000	-7.083623000
1	0.000000000	-2.368243000	-7.083623000
1	0.000000000	-2.500463000	-2.197245000
6	0.000000000	-0.728846000	1.321602000
6	0.000000000	0.728846000	1.321602000
6	0.000000000	1.414724000	2.521013000
6	0.000000000	-1.414724000	2.521013000
6	0.000000000	-0.732179000	3.761807000
6	0.000000000	0.732179000	3.761807000
1	0.000000000	2.498231000	2.494336000
1	0.000000000	-2.498231000	2.494336000
6	0.000000000	0.709557000	-10.737294000
6	0.000000000	-0.709557000	-10.737294000

6	-11.952805000	-1.391995000	-0.000005000	6	0.000000000	-1.395304000	-11.979928000
6	-11.952805000	1.391995000	-0.000011000	6	0.000000000	1.395304000	-11.979928000
6	-13.141991000	-0.712768000	0.000020000	6	0.000000000	-0.715456000	-13.168862000
6	-13.141991000	0.712768000	0.000017000	6	0.000000000	0.715456000	-13.168862000
1	-11.959001000	2.480316000	-0.000013000	1	0.000000000	2.480590000	-11.985184000
1	-11.959001000	-2.480316000	-0.000002000	1	0.000000000	-2.480590000	-11.985184000
6	6.183179000	0.730708000	-0.000124000	6	0.000000000	0.731573000	6.202077000
6	6.183179000	-0.730708000	-0.000119000	6	0.000000000	-0.731573000	6.202077000
7	7.321183000	-1.424701000	-0.000096000	7	0.000000000	-1.426902000	7.339324000
7	7.321183000	1.424701000	-0.000105000	7	0.000000000	1.426902000	7.339324000
6	8.465736000	-0.729114000	-0.000074000	6	0.000000000	-0.729937000	8.485315000
6	8.465736000	0.729114000	-0.000079000	6	0.000000000	0.729937000	8.485315000
6	4.958313000	1.413352000	-0.000144000	6	0.000000000	1.416523000	4.971488000
6	4.958313000	-1.413352000	-0.000135000	6	0.000000000	-1.416523000	4.971488000
7	0.151865000	1.425028000	-0.000174000	7	0.000000000	1.428475000	0.149902000
7	0.151865000	-1.425028000	-0.000166000	7	0.000000000	-1.428475000	0.149902000
6	-4.661478000	1.403991000	-0.000140000	6	0.000000000	1.410626000	-4.676042000
6	-4.661478000	-1.403991000	-0.000133000	6	0.000000000	-1.410626000	-4.676042000
6	-9.481480000	1.392050000	-0.000062000	6	0.000000000	1.394416000	-9.501405000
6	-9.481480000	-1.392050000	-0.000056000	6	0.000000000	-1.394416000	-9.501405000
7	-14.367069000	1.359783000	0.000042000	7	0.000000000	1.363683000	-14.396850000
7	-14.367069000	-1.359783000	0.000047000	7	0.000000000	-1.363683000	-14.396850000
6	-15.594649000	0.712782000	0.000077000	6	0.000000000	0.715868000	-15.626524000
6	-15.594649000	-0.712782000	0.000080000	6	0.000000000	-0.715868000	-15.626524000
6	-16.781942000	1.392043000	0.000109000	6	0.000000000	1.395413000	-16.813620000
6	-16.781942000	-1.392043000	0.000115000	6	0.000000000	-1.395413000	-16.813620000
6	-18.022535000	0.710517000	0.000146000	6	0.000000000	0.709542000	-18.058376000
6	-18.022535000	-0.710517000	0.000149000	6	0.000000000	-0.709542000	-18.058376000
6	9.683686000	1.412872000	-0.000051000	6	0.000000000	1.416218000	9.706214000
6	9.683686000	-1.412872000	-0.000041000	6	0.000000000	-1.416218000	9.706214000
6	10.900268000	0.730406000	-0.000016000	6	0.000000000	0.731341000	10.922663000
6	10.900268000	-0.730406000	-0.000011000	6	0.000000000	-0.731341000	10.922663000
6	12.124971000	1.412478000	0.000017000	6	0.000000000	1.415845000	12.153035000
6	12.124971000	-1.412478000	0.000027000	6	0.000000000	-1.415845000	12.153035000
6	13.333563000	0.727765000	0.000056000	6	0.000000000	0.728508000	13.358429000
6	13.333563000	-0.727765000	0.000061000	6	0.000000000	-0.728508000	13.358429000
1	12.150024000	2.498423000	0.000015000	1	0.000000000	2.499330000	12.179207000
1	12.150024000	-2.498423000	0.000032000	1	0.000000000	-2.499330000	12.179207000
1	9.659108000	-2.498841000	-0.000037000	1	0.000000000	-2.499722000	9.680865000
1	9.659108000	2.498841000	-0.000053000	1	0.000000000	2.499722000	9.680865000
1	4.982257000	-2.499346000	-0.000129000	1	0.000000000	-2.500059000	4.996487000
1	4.982257000	2.499346000	-0.000145000	1	0.000000000	2.500059000	4.996487000
1	-4.666490000	2.491707000	-0.000142000	1	0.000000000	2.495309000	-4.681017000
1	-4.666490000	-2.491707000	-0.000130000	1	0.000000000	-2.495309000	-4.681017000
1	-9.474353000	-2.480388000	-0.000053000	1	0.000000000	-2.479817000	-9.494133000
1	-9.474353000	2.480388000	-0.000064000	1	0.000000000	2.479817000	-9.494133000
1	-14.367664000	-2.368901000	0.000051000	1	0.000000000	-2.371080000	-14.397628000
1	-14.367664000	2.368901000	0.000042000	1	0.000000000	2.371080000	-14.397628000

1	-16.777327000	-2.480520000	0.000118000	1	0.000000000	-2.480898000	-16.809222000
1	-16.777327000	2.480520000	0.000107000	1	0.000000000	2.480898000	-16.809222000
6	-19.256870000	1.393155000	0.000182000	6	0.000000000	1.395746000	-19.295507000
6	-19.256870000	-1.393155000	0.000188000	6	0.000000000	-1.395746000	-19.295507000
6	-20.442481000	0.703151000	0.000221000	6	0.000000000	0.705547000	-20.482758000
6	-20.442481000	-0.703151000	0.000224000	6	0.000000000	-0.705547000	-20.482758000
1	-19.252248000	2.480563000	0.000180000	1	0.000000000	2.480589000	-19.291141000
1	-19.252248000	-2.480563000	0.000191000	1	0.000000000	-2.480589000	-19.291141000
1	-21.385227000	-1.241566000	0.000255000	1	0.000000000	-1.243434000	-21.423177000
1	-21.385227000	1.241566000	0.000250000	1	0.000000000	1.243434000	-21.423177000
7	14.489090000	-1.423627000	0.000101000	7	0.000000000	-1.427356000	14.520460000
7	14.489090000	1.423627000	0.000091000	7	0.000000000	1.427356000	14.520460000
6	15.614913000	-0.729388000	0.000136000	6	0.000000000	-0.732379000	15.639780000
6	15.614913000	0.729388000	0.000131000	6	0.000000000	0.732379000	15.639780000
6	16.855783000	-1.411611000	0.000184000	6	0.000000000	-1.417615000	16.889888000
6	16.855783000	1.411611000	0.000174000	6	0.000000000	1.417615000	16.889888000
6	18.046740000	-0.726917000	0.000226000	6	0.000000000	-0.730277000	18.074929000
6	18.046740000	0.726917000	0.000221000	6	0.000000000	0.730277000	18.074929000
1	16.832379000	-2.497945000	0.000187000	1	0.000000000	-2.501380000	16.865675000
1	16.832379000	2.497945000	0.000171000	1	0.000000000	2.501380000	16.865675000
6	20.473399000	-0.716158000	0.000321000	6	0.000000000	-0.721768000	20.509091000
6	20.473399000	0.716158000	0.000316000	6	0.000000000	0.721768000	20.509091000
6	19.309378000	1.406741000	0.000267000	6	0.000000000	1.413183000	19.348068000
6	19.309378000	-1.406741000	0.000277000	6	0.000000000	-1.413183000	19.348068000
1	19.304175000	2.493299000	0.000264000	1	0.000000000	2.497339000	19.343758000
1	19.304175000	-2.493299000	0.000280000	1	0.000000000	-2.497339000	19.343758000
1	21.421801000	1.244407000	0.000352000	1	0.000000000	1.247032000	21.456598000
1	21.421801000	-1.244407000	0.000361000	1	0.000000000	-1.247032000	21.456598000

Table S157: Coordinates of pN_s_4 at M06/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.728996000	8.403875000
7	0.000000000	1.429631000	7.242482000
6	0.000000000	0.733081000	6.120462000
6	0.000000000	-0.733081000	6.120462000
7	0.000000000	-1.429631000	7.242482000
6	0.000000000	-0.728996000	8.403875000
6	0.000000000	-0.731391000	3.664693000
6	0.000000000	0.731391000	3.664693000
6	0.000000000	1.405589000	2.451679000
1	0.000000000	2.492255000	2.428348000
6	0.000000000	0.732635000	1.210603000
6	0.000000000	-0.732635000	1.210603000
6	0.000000000	-1.405589000	2.451679000
1	0.000000000	-2.492255000	2.428348000
6	0.000000000	-0.727096000	-1.071987000
6	0.000000000	0.727096000	-1.071987000

Table S158: Coordinates of pN_s_4 at M062X/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.725762000	-8.243375000
7	0.000000000	1.421774000	-7.104942000
6	0.000000000	0.723482000	-5.964194000
6	0.000000000	-0.723482000	-5.964194000
7	0.000000000	-1.421774000	-7.104942000
6	0.000000000	-0.725762000	-8.243375000
6	0.000000000	-0.727728000	-3.528168000
6	0.000000000	0.727728000	-3.528168000
6	0.000000000	1.410856000	-2.274208000
1	0.000000000	2.494825000	-2.248923000
6	0.000000000	0.729157000	-1.084048000
6	0.000000000	-0.729157000	-1.084048000
6	0.000000000	-1.410856000	-2.274208000
1	0.000000000	-2.494825000	-2.248923000
6	0.000000000	-0.737873000	1.203647000
6	0.000000000	0.737873000	1.203647000

6	0.000000000	1.406133000	-2.270605000	6	0.000000000	1.409986000	2.461231000
6	0.000000000	-1.406133000	-2.270605000	6	0.000000000	-1.409986000	2.461231000
6	0.000000000	-0.726726000	-3.512231000	6	0.000000000	-0.736599000	3.674013000
6	0.000000000	0.726726000	-3.512231000	6	0.000000000	0.736599000	3.674013000
1	0.000000000	2.492556000	-2.244939000	1	0.000000000	2.494501000	2.436932000
1	0.000000000	-2.492556000	-2.244939000	1	0.000000000	-2.494501000	2.436932000
6	0.000000000	0.728384000	10.847655000	6	0.000000000	0.726813000	-10.676415000
6	0.000000000	-0.728384000	10.847655000	6	0.000000000	-0.726813000	-10.676415000
6	0.000000000	-1.409188000	12.045726000	6	0.000000000	-1.407079000	-11.937725000
6	0.000000000	1.409188000	12.045726000	6	0.000000000	1.407079000	-11.937725000
6	0.000000000	-0.725967000	13.285046000	6	0.000000000	-0.727499000	-13.115126000
6	0.000000000	0.725967000	13.285046000	6	0.000000000	0.727499000	-13.115126000
1	0.000000000	2.495448000	12.069980000	1	0.000000000	2.491853000	-11.942165000
1	0.000000000	-2.495448000	12.069980000	1	0.000000000	-2.491853000	-11.942165000
6	0.000000000	0.723633000	-5.947315000	6	0.000000000	0.738668000	6.146128000
6	0.000000000	-0.723633000	-5.947315000	6	0.000000000	-0.738668000	6.146128000
7	0.000000000	-1.420294000	-7.085691000	7	0.000000000	-1.435371000	7.256448000
7	0.000000000	1.420294000	-7.085691000	7	0.000000000	1.435371000	7.256448000
6	0.000000000	-0.724826000	-8.225956000	6	0.000000000	-0.731829000	8.432898000
6	0.000000000	0.724826000	-8.225956000	6	0.000000000	0.731829000	8.432898000
6	0.000000000	1.407646000	-4.715709000	6	0.000000000	1.408310000	4.896919000
6	0.000000000	-1.407646000	-4.715709000	6	0.000000000	-1.408310000	4.896919000
7	0.000000000	1.428278000	0.092162000	7	0.000000000	1.433148000	0.096442000
7	0.000000000	-1.428278000	0.092162000	7	0.000000000	-1.433148000	0.096442000
6	0.000000000	1.404586000	4.885064000	6	0.000000000	1.411527000	-4.729165000
6	0.000000000	-1.404586000	4.885064000	6	0.000000000	-1.411527000	-4.729165000
6	0.000000000	1.406143000	9.602688000	6	0.000000000	1.411396000	-9.480502000
6	0.000000000	-1.406143000	9.602688000	6	0.000000000	-1.411396000	-9.480502000
7	0.000000000	1.420682000	14.414584000	7	0.000000000	1.361046000	-14.341768000
7	0.000000000	-1.420682000	14.414584000	7	0.000000000	-1.361046000	-14.341768000
6	0.000000000	0.722572000	15.563753000	6	0.000000000	0.713954000	-15.571743000
6	0.000000000	-0.722572000	15.563753000	6	0.000000000	-0.713954000	-15.571743000
6	0.000000000	1.406316000	16.786244000	6	0.000000000	1.396560000	-16.758558000
6	0.000000000	-1.406316000	16.786244000	6	0.000000000	-1.396560000	-16.758558000
6	0.000000000	0.721558000	17.991276000	6	0.000000000	0.710249000	-17.999561000
6	0.000000000	-0.721558000	17.991276000	6	0.000000000	-0.710249000	-17.999561000
6	0.000000000	1.406857000	-9.456258000	6	0.000000000	1.411967000	9.621466000
6	0.000000000	-1.406857000	-9.456258000	6	0.000000000	-1.411967000	9.621466000
6	0.000000000	0.724383000	-10.656083000	6	0.000000000	0.730046000	10.878920000
6	0.000000000	-0.724383000	-10.656083000	6	0.000000000	-0.730046000	10.878920000
6	0.000000000	1.400939000	-11.908738000	6	0.000000000	1.414152000	12.072075000
6	0.000000000	-1.400939000	-11.908738000	6	0.000000000	-1.414152000	12.072075000
6	0.000000000	0.722091000	-13.088908000	6	0.000000000	0.726416000	13.316562000
6	0.000000000	-0.722091000	-13.088908000	6	0.000000000	-0.726416000	13.316562000
1	0.000000000	2.488665000	-11.913574000	1	0.000000000	2.497921000	12.097585000
1	0.000000000	-2.488665000	-11.913574000	1	0.000000000	-2.497921000	12.097585000
1	0.000000000	-2.493227000	-9.430937000	1	0.000000000	-2.495884000	9.596292000
1	0.000000000	2.493227000	-9.430937000	1	0.000000000	2.495884000	9.596292000

1	0.000000000	-2.493969000	-4.740407000	1	0.000000000	-2.492869000	4.921049000
1	0.000000000	2.493969000	-4.740407000	1	0.000000000	2.492869000	4.921049000
1	0.000000000	2.491289000	4.908704000	1	0.000000000	2.495355000	-4.755168000
1	0.000000000	-2.491289000	4.908704000	1	0.000000000	-2.495355000	-4.755168000
1	0.000000000	-2.492566000	9.577203000	1	0.000000000	-2.495068000	-9.454106000
1	0.000000000	2.492566000	9.577203000	1	0.000000000	2.495068000	-9.454106000
1	0.000000000	-2.492750000	16.761849000	1	0.000000000	-2.369411000	-14.345147000
1	0.000000000	2.492750000	16.761849000	1	0.000000000	2.369411000	-14.345147000
6	0.000000000	1.402806000	19.244998000	1	0.000000000	-2.481957000	-16.753384000
6	0.000000000	-1.402806000	19.244998000	1	0.000000000	2.481957000	-16.753384000
6	0.000000000	0.712012000	20.415128000	6	0.000000000	1.396933000	-19.238353000
6	0.000000000	-0.712012000	20.415128000	6	0.000000000	-1.396933000	-19.238353000
1	0.000000000	2.489454000	19.239666000	6	0.000000000	0.706416000	-20.423505000
1	0.000000000	-2.489454000	19.239666000	6	0.000000000	-0.706416000	-20.423505000
1	0.000000000	-1.243159000	21.361913000	1	0.000000000	2.481673000	-19.234183000
1	0.000000000	1.243159000	21.361913000	1	0.000000000	-2.481673000	-19.234183000
7	0.000000000	-1.357354000	-14.312408000	1	0.000000000	-1.243384000	-21.364396000
7	0.000000000	1.357354000	-14.312408000	1	0.000000000	1.243384000	-21.364396000
6	0.000000000	-0.711460000	-15.540347000	7	0.000000000	-1.422588000	14.445511000
6	0.000000000	0.711460000	-15.540347000	7	0.000000000	1.422588000	14.445511000
6	0.000000000	-1.393285000	-16.727438000	6	0.000000000	-0.722886000	15.593956000
6	0.000000000	1.393285000	-16.727438000	6	0.000000000	0.722886000	15.593956000
6	0.000000000	-0.711104000	-17.964999000	6	0.000000000	-1.410664000	16.820640000
6	0.000000000	0.711104000	-17.964999000	6	0.000000000	1.410664000	16.820640000
1	0.000000000	-2.481575000	-16.722445000	6	0.000000000	-0.723268000	18.021931000
1	0.000000000	2.481575000	-16.722445000	6	0.000000000	0.723268000	18.021931000
1	0.000000000	-2.367421000	-14.314483000	1	0.000000000	-2.494522000	16.795343000
1	0.000000000	2.367421000	-14.314483000	1	0.000000000	2.494522000	16.795343000
6	0.000000000	-0.703951000	-20.384251000	6	0.000000000	-0.716948000	20.452009000
6	0.000000000	0.703951000	-20.384251000	6	0.000000000	0.716948000	20.452009000
6	0.000000000	1.394316000	-19.200612000	6	0.000000000	1.408189000	19.284164000
6	0.000000000	-1.394316000	-19.200612000	6	0.000000000	-1.408189000	19.284164000
1	0.000000000	2.481551000	-19.196147000	1	0.000000000	2.492455000	19.279248000
1	0.000000000	-2.481551000	-19.196147000	1	0.000000000	-2.492455000	19.279248000
1	0.000000000	1.241502000	-21.327374000	1	0.000000000	1.245537000	21.397698000
1	0.000000000	-1.241502000	-21.327374000	1	0.000000000	-1.245537000	21.397698000

Table S159: Coordinates of pT₅_5 at M06/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	8.317493000	0.727324000
7	0.000000000	7.153493000	1.426646000
6	0.000000000	6.035986000	0.732079000
6	0.000000000	6.035986000	-0.732079000
7	0.000000000	7.153493000	-1.426646000
6	0.000000000	8.317493000	-0.727324000
6	0.000000000	3.590631000	-0.731389000
6	0.000000000	3.590631000	0.731389000

Table S160: Coordinates of pT₅_5 at M062X/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	8.347496000	0.728090000
7	0.000000000	7.170300000	1.430164000
6	0.000000000	6.063070000	0.735798000
6	0.000000000	6.063070000	-0.735798000
7	0.000000000	7.170300000	-1.430164000
6	0.000000000	8.347496000	-0.728090000
6	0.000000000	3.608644000	-0.735796000
6	0.000000000	3.608644000	0.735796000

6	0.000000000	2.355653000	1.405959000	6	0.000000000	2.357251000	1.409745000
1	0.000000000	2.330671000	2.492487000	1	0.000000000	2.332283000	2.494080000
6	0.000000000	1.141102000	0.732249000	6	0.000000000	1.144709000	0.737743000
6	0.000000000	1.141102000	-0.732249000	6	0.000000000	1.144709000	-0.737743000
6	0.000000000	2.355653000	-1.405959000	6	0.000000000	2.357251000	-1.409745000
1	0.000000000	2.330671000	-2.492487000	1	0.000000000	2.332283000	-2.494080000
6	0.000000000	-1.141102000	-0.732249000	6	0.000000000	-1.144709000	-0.737743000
6	0.000000000	-1.141102000	0.732249000	6	0.000000000	-1.144709000	0.737743000
6	0.000000000	-2.355653000	1.405959000	6	0.000000000	-2.357251000	1.409745000
6	0.000000000	-2.355653000	-1.405959000	6	0.000000000	-2.357251000	-1.409745000
6	0.000000000	-3.590631000	-0.731389000	6	0.000000000	-3.608644000	-0.735796000
6	0.000000000	-3.590631000	0.731389000	6	0.000000000	-3.608644000	0.735796000
1	0.000000000	-2.330671000	2.492487000	1	0.000000000	-2.332283000	2.494080000
1	0.000000000	-2.330671000	-2.492487000	1	0.000000000	-2.332283000	-2.494080000
6	0.000000000	10.752975000	0.728335000	6	0.000000000	10.784348000	0.728965000
6	0.000000000	10.752975000	-0.728335000	6	0.000000000	10.784348000	-0.728965000
6	0.000000000	11.960008000	-1.410556000	6	0.000000000	11.992428000	-1.413689000
6	0.000000000	11.960008000	1.410556000	6	0.000000000	11.992428000	1.413689000
6	0.000000000	13.186071000	-0.725840000	6	0.000000000	13.219358000	-0.725878000
6	0.000000000	13.186071000	0.725840000	6	0.000000000	13.219358000	0.725878000
1	0.000000000	11.985012000	2.496636000	1	0.000000000	12.018188000	2.497328000
1	0.000000000	11.985012000	-2.496636000	1	0.000000000	12.018188000	-2.497328000
6	0.000000000	-6.035986000	0.732079000	6	0.000000000	-6.063070000	0.735798000
6	0.000000000	-6.035986000	-0.732079000	6	0.000000000	-6.063070000	-0.735798000
7	0.000000000	-7.153493000	-1.426646000	7	0.000000000	-7.170300000	-1.430164000
7	0.000000000	-7.153493000	1.426646000	7	0.000000000	-7.170300000	1.430164000
6	0.000000000	-8.317493000	-0.727324000	6	0.000000000	-8.347496000	-0.728090000
6	0.000000000	-8.317493000	0.727324000	6	0.000000000	-8.347496000	0.728090000
6	0.000000000	-4.791458000	1.409628000	6	0.000000000	-4.800829000	1.416070000
6	0.000000000	-4.791458000	-1.409628000	6	0.000000000	-4.800829000	-1.416070000
7	0.000000000	0.000000000	1.430319000	7	0.000000000	0.000000000	1.435601000
7	0.000000000	0.000000000	-1.430319000	7	0.000000000	0.000000000	-1.435601000
6	0.000000000	4.791458000	1.409628000	6	0.000000000	4.800829000	1.416070000
6	0.000000000	4.791458000	-1.409628000	6	0.000000000	4.800829000	-1.416070000
6	0.000000000	9.516856000	1.409431000	6	0.000000000	9.540925000	1.413746000
6	0.000000000	9.516856000	-1.409431000	6	0.000000000	9.540925000	-1.413746000
7	0.000000000	14.326886000	1.421458000	7	0.000000000	14.363825000	1.423698000
7	0.000000000	14.326886000	-1.421458000	7	0.000000000	14.363825000	-1.423698000
6	0.000000000	15.464935000	0.725616000	6	0.000000000	15.498202000	0.727083000
6	0.000000000	15.464935000	-0.725616000	6	0.000000000	15.498202000	-0.727083000
6	0.000000000	16.696031000	1.409114000	6	0.000000000	16.736309000	1.413981000
6	0.000000000	16.696031000	-1.409114000	6	0.000000000	16.736309000	-1.413981000
6	0.000000000	17.893691000	0.724239000	6	0.000000000	17.929594000	0.726944000
6	0.000000000	17.893691000	-0.724239000	6	0.000000000	17.929594000	-0.726944000
6	0.000000000	-9.516856000	1.409431000	6	0.000000000	-9.540925000	1.413746000
6	0.000000000	-9.516856000	-1.409431000	6	0.000000000	-9.540925000	-1.413746000
6	0.000000000	-10.752975000	0.728335000	6	0.000000000	-10.784348000	0.728965000
6	0.000000000	-10.752975000	-0.728335000	6	0.000000000	-10.784348000	-0.728965000

6	0.000000000	-11.960008000	1.410556000	6	0.000000000	-11.992428000	1.413689000
6	0.000000000	-11.960008000	-1.410556000	6	0.000000000	-11.992428000	-1.413689000
6	0.000000000	-13.186071000	0.725840000	6	0.000000000	-13.219358000	0.725878000
6	0.000000000	-13.186071000	-0.725840000	6	0.000000000	-13.219358000	-0.725878000
1	0.000000000	-11.985012000	2.496636000	1	0.000000000	-12.018188000	2.497328000
1	0.000000000	-11.985012000	-2.496636000	1	0.000000000	-12.018188000	-2.497328000
1	0.000000000	-9.491163000	-2.495565000	1	0.000000000	-9.515083000	-2.497399000
1	0.000000000	-9.491163000	2.495565000	1	0.000000000	-9.515083000	2.497399000
1	0.000000000	-4.814718000	-2.496023000	1	0.000000000	-4.825281000	-2.500153000
1	0.000000000	-4.814718000	2.496023000	1	0.000000000	-4.825281000	2.500153000
1	0.000000000	4.814718000	2.496023000	1	0.000000000	4.825281000	2.500153000
1	0.000000000	4.814718000	-2.496023000	1	0.000000000	4.825281000	-2.500153000
1	0.000000000	9.491163000	-2.495565000	1	0.000000000	9.515083000	-2.497399000
1	0.000000000	9.491163000	2.495565000	1	0.000000000	9.515083000	2.497399000
1	0.000000000	16.671974000	-2.495446000	1	0.000000000	16.711363000	-2.497774000
1	0.000000000	16.671974000	2.495446000	1	0.000000000	16.711363000	2.497774000
6	0.000000000	19.151848000	1.405018000	6	0.000000000	19.197473000	1.411023000
6	0.000000000	19.151848000	-1.405018000	6	0.000000000	19.197473000	-1.411023000
6	0.000000000	20.318565000	0.714143000	6	0.000000000	20.361451000	0.719376000
6	0.000000000	20.318565000	-0.714143000	6	0.000000000	20.361451000	-0.719376000
1	0.000000000	19.146691000	2.491565000	1	0.000000000	19.193096000	2.495204000
1	0.000000000	19.146691000	-2.491565000	1	0.000000000	19.193096000	-2.495204000
1	0.000000000	21.266180000	-1.243720000	1	0.000000000	21.308113000	-1.246148000
1	0.000000000	21.266180000	1.243720000	1	0.000000000	21.308113000	1.246148000
7	0.000000000	-14.326886000	-1.421458000	7	0.000000000	-14.363825000	-1.423698000
7	0.000000000	-14.326886000	1.421458000	7	0.000000000	-14.363825000	1.423698000
6	0.000000000	-15.464935000	-0.725616000	6	0.000000000	-15.498202000	-0.727083000
6	0.000000000	-15.464935000	0.725616000	6	0.000000000	-15.498202000	0.727083000
6	0.000000000	-16.696031000	-1.409114000	6	0.000000000	-16.736309000	-1.413981000
6	0.000000000	-16.696031000	1.409114000	6	0.000000000	-16.736309000	1.413981000
6	0.000000000	-17.893691000	-0.724239000	6	0.000000000	-17.929594000	-0.726944000
6	0.000000000	-17.893691000	0.724239000	6	0.000000000	-17.929594000	0.726944000
1	0.000000000	-16.671974000	-2.495446000	1	0.000000000	-16.711363000	-2.497774000
1	0.000000000	-16.671974000	2.495446000	1	0.000000000	-16.711363000	2.497774000
6	0.000000000	-20.318565000	-0.714143000	6	0.000000000	-20.361451000	-0.719376000
6	0.000000000	-20.318565000	0.714143000	6	0.000000000	-20.361451000	0.719376000
6	0.000000000	-19.151848000	1.405018000	6	0.000000000	-19.197473000	1.411023000
6	0.000000000	-19.151848000	-1.405018000	6	0.000000000	-19.197473000	-1.411023000
1	0.000000000	-19.146691000	2.491565000	1	0.000000000	-19.193096000	2.495204000
1	0.000000000	-19.146691000	-2.491565000	1	0.000000000	-19.193096000	-2.495204000
1	0.000000000	-21.266180000	1.243720000	1	0.000000000	-21.308113000	1.246148000
1	0.000000000	-21.266180000	-1.243720000	1	0.000000000	-21.308113000	-1.246148000

Table S161: Coordinates of pT₆-1 at M06/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.712835000	4.971126000
7	0.000000000	1.360627000	3.746529000

Table S162: Coordinates of pT₆-1 at M062X/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.715654000	4.988971000
7	0.000000000	1.363930000	3.759315000

6	0.000000000	0.709769000	2.518146000	6	0.000000000	0.712668000	2.526406000
6	0.000000000	-0.709769000	2.518146000	6	0.000000000	-0.712668000	2.526406000
7	0.000000000	-1.360627000	3.746529000	7	0.000000000	-1.363930000	3.759315000
6	0.000000000	-0.712835000	4.971126000	6	0.000000000	-0.715654000	4.98971000
6	0.000000000	-0.709514000	0.090060000	6	0.000000000	-0.708270000	0.090641000
6	0.000000000	0.709514000	0.090060000	6	0.000000000	0.708270000	0.090641000
6	0.000000000	1.389881000	-1.148027000	6	0.000000000	1.392120000	-1.153603000
1	0.000000000	2.478560000	-1.154340000	1	0.000000000	2.477801000	-1.159590000
6	0.000000000	0.711253000	-2.339425000	6	0.000000000	0.714044000	-2.346720000
6	0.000000000	-0.711253000	-2.339425000	6	0.000000000	-0.714044000	-2.346720000
6	0.000000000	-1.389881000	-1.148027000	6	0.000000000	-1.392120000	-1.153603000
1	0.000000000	2.369399000	3.745767000	1	0.000000000	2.370984000	3.758435000
1	0.000000000	-2.369399000	3.745767000	1	0.000000000	-2.370984000	3.758435000
1	0.000000000	-2.478560000	-1.154340000	1	0.000000000	-2.477801000	-1.159590000
6	0.000000000	-0.710426000	-4.792745000	6	0.000000000	-0.713276000	-4.810733000
6	0.000000000	0.710426000	-4.792745000	6	0.000000000	0.713276000	-4.810733000
6	0.000000000	1.389578000	-5.983955000	6	0.000000000	1.391814000	-6.003416000
6	0.000000000	-1.389578000	-5.983955000	6	0.000000000	-1.391814000	-6.003416000
6	0.000000000	-0.709416000	-7.221741000	6	0.000000000	-0.708068000	-7.246753000
6	0.000000000	0.709416000	-7.221741000	6	0.000000000	0.708068000	-7.246753000
1	0.000000000	2.478311000	-5.977518000	1	0.000000000	2.477525000	-5.997111000
1	0.000000000	-2.478311000	-5.977518000	1	0.000000000	-2.477525000	-5.997111000
6	0.000000000	0.710601000	7.400981000	6	0.000000000	0.709193000	7.425333000
6	0.000000000	-0.710601000	7.400981000	6	0.000000000	-0.709193000	7.425333000
6	0.000000000	-1.391012000	8.634493000	6	0.000000000	-1.393259000	8.663681000
6	0.000000000	1.391012000	8.634493000	6	0.000000000	1.393259000	8.663681000
6	0.000000000	-0.708227000	9.825956000	6	0.000000000	-0.710440000	9.855723000
6	0.000000000	0.708227000	9.825956000	6	0.000000000	0.710440000	9.855723000
1	0.000000000	2.479526000	8.641605000	1	0.000000000	2.478821000	8.670467000
1	0.000000000	-2.479526000	8.641605000	1	0.000000000	-2.478821000	8.670467000
6	0.000000000	0.710695000	-9.650948000	6	0.000000000	0.713517000	-9.680527000
6	0.000000000	-0.710695000	-9.650948000	6	0.000000000	-0.713517000	-9.680527000
7	0.000000000	-1.361066000	-10.877762000	7	0.000000000	-1.364778000	-10.910663000
7	0.000000000	1.361066000	-10.877762000	7	0.000000000	1.364778000	-10.910663000
6	0.000000000	-0.711001000	-12.104292000	6	0.000000000	-0.713650000	-12.140469000
6	0.000000000	0.711001000	-12.104292000	6	0.000000000	0.713650000	-12.140469000
1	0.000000000	-2.369691000	-10.877716000	1	0.000000000	-2.371677000	-10.910897000
1	0.000000000	2.369691000	-10.877716000	1	0.000000000	2.371677000	-10.910897000
6	0.000000000	1.389634000	-8.459602000	6	0.000000000	1.392679000	-8.488666000
6	0.000000000	-1.389634000	-8.459602000	6	0.000000000	-1.392679000	-8.488666000
7	0.000000000	1.361041000	-3.565378000	7	0.000000000	1.363948000	-3.578105000
7	0.000000000	-1.361041000	-3.565378000	7	0.000000000	-1.363948000	-3.578105000
6	0.000000000	1.389694000	1.327305000	6	0.000000000	1.392020000	1.333973000
6	0.000000000	-1.389694000	1.327305000	6	0.000000000	-1.392020000	1.333973000
6	0.000000000	1.391116000	6.161515000	6	0.000000000	1.393722000	6.180369000
6	0.000000000	-1.391116000	6.161515000	6	0.000000000	-1.393722000	6.180369000
7	0.000000000	1.357087000	11.054148000	7	0.000000000	1.360947000	11.087473000
7	0.000000000	-1.357087000	11.054148000	7	0.000000000	-1.360947000	11.087473000

6	0.000000000	0.723694000	12.278213000	6	0.000000000	0.728787000	12.315268000
6	0.000000000	-0.723694000	12.278213000	6	0.000000000	-0.728787000	12.315268000
6	0.000000000	1.401523000	13.457528000	6	0.000000000	1.407305000	13.492490000
6	0.000000000	-1.401523000	13.457528000	6	0.000000000	-1.407305000	13.492490000
6	0.000000000	0.726089000	14.713811000	6	0.000000000	0.728094000	14.757092000
6	0.000000000	-0.726089000	14.713811000	6	0.000000000	-0.728094000	14.757092000
6	0.000000000	1.389796000	-13.295486000	6	0.000000000	1.392790000	-13.331511000
6	0.000000000	-1.389796000	-13.295486000	6	0.000000000	-1.392790000	-13.331511000
6	0.000000000	0.709476000	-14.533575000	6	0.000000000	0.708065000	-14.572937000
6	0.000000000	-0.709476000	-14.533575000	6	0.000000000	-0.708065000	-14.572937000
6	0.000000000	1.389748000	-15.770850000	6	0.000000000	1.393044000	-15.813122000
6	0.000000000	-1.389748000	-15.770850000	6	0.000000000	-1.393044000	-15.813122000
6	0.000000000	0.709925000	-16.961683000	6	0.000000000	0.712597000	-17.003510000
6	0.000000000	-0.709925000	-16.961683000	6	0.000000000	-0.712597000	-17.003510000
1	0.000000000	2.478434000	-15.777514000	1	0.000000000	2.478593000	-15.819143000
1	0.000000000	-2.478434000	-15.777514000	1	0.000000000	-2.478593000	-15.819143000
1	0.000000000	-2.478494000	-13.289182000	1	0.000000000	-2.478377000	-13.325037000
1	0.000000000	2.478494000	-13.289182000	1	0.000000000	2.478377000	-13.325037000
1	0.000000000	-2.478358000	-8.466024000	1	0.000000000	-2.478303000	-8.494624000
1	0.000000000	2.478358000	-8.466024000	1	0.000000000	2.478303000	-8.494624000
1	0.000000000	-2.369672000	-3.565619000	1	0.000000000	-2.370901000	-3.578457000
1	0.000000000	2.369672000	-3.565619000	1	0.000000000	2.370901000	-3.578457000
1	0.000000000	2.478395000	1.333876000	1	0.000000000	2.477734000	1.340273000
1	0.000000000	-2.478395000	1.333876000	1	0.000000000	-2.477734000	1.340273000
1	0.000000000	-2.479622000	6.155370000	1	0.000000000	-2.479206000	6.174561000
1	0.000000000	2.479622000	6.155370000	1	0.000000000	2.479206000	6.174561000
1	0.000000000	-2.366910000	11.051436000	1	0.000000000	-2.368978000	11.083918000
1	0.000000000	2.366910000	11.051436000	1	0.000000000	2.368978000	11.083918000
1	0.000000000	-2.489400000	13.452308000	1	0.000000000	-2.492058000	13.486996000
1	0.000000000	2.489400000	13.452308000	1	0.000000000	2.492058000	13.486996000
6	0.000000000	1.407374000	15.909534000	6	0.000000000	1.411885000	15.949956000
6	0.000000000	-1.407374000	15.909534000	6	0.000000000	-1.411885000	15.949956000
6	0.000000000	0.726256000	17.146661000	6	0.000000000	0.726780000	17.192356000
6	0.000000000	-0.726256000	17.146661000	6	0.000000000	-0.726780000	17.192356000
1	0.000000000	2.493898000	15.934126000	1	0.000000000	2.495576000	15.975434000
1	0.000000000	-2.493898000	15.934126000	1	0.000000000	-2.495576000	15.975434000
7	0.000000000	-1.360372000	-18.189663000	7	0.000000000	-1.364737000	-18.233438000
7	0.000000000	1.360372000	-18.189663000	7	0.000000000	1.364737000	-18.233438000
6	0.000000000	-0.713790000	-19.415228000	6	0.000000000	-0.716696000	-19.460663000
6	0.000000000	0.713790000	-19.415228000	6	0.000000000	0.716696000	-19.460663000
6	0.000000000	-1.391570000	-20.603801000	6	0.000000000	-1.394819000	-20.648805000
6	0.000000000	1.391570000	-20.603801000	6	0.000000000	1.394819000	-20.648805000
6	0.000000000	-0.710496000	-21.845260000	6	0.000000000	-0.709575000	-21.894412000
6	0.000000000	0.710496000	-21.845260000	6	0.000000000	0.709575000	-21.894412000
1	0.000000000	-2.480170000	-20.599240000	1	0.000000000	-2.480346000	-20.643960000
1	0.000000000	2.480170000	-20.599240000	1	0.000000000	2.480346000	-20.643960000
1	0.000000000	-2.369194000	-18.189322000	1	0.000000000	-2.371816000	-18.233180000
1	0.000000000	2.369194000	-18.189322000	1	0.000000000	2.371816000	-18.233180000

7	0.000000000	-1.419924000	18.280550000	7	0.000000000	-1.421736000	18.324945000
7	0.000000000	1.419924000	18.280550000	7	0.000000000	1.421736000	18.324945000
6	0.000000000	-0.722610000	19.426397000	6	0.000000000	-0.722499000	19.471455000
6	0.000000000	0.722610000	19.426397000	6	0.000000000	0.722499000	19.471455000
6	0.000000000	-1.405666000	20.653509000	6	0.000000000	-1.409447000	20.701019000
6	0.000000000	1.405666000	20.653509000	6	0.000000000	1.409447000	20.701019000
6	0.000000000	-0.722400000	21.855865000	6	0.000000000	-0.723612000	21.901712000
6	0.000000000	0.722400000	21.855865000	6	0.000000000	0.723612000	21.901712000
6	0.000000000	-1.402766000	23.112648000	6	0.000000000	-1.407776000	23.165962000
6	0.000000000	1.402766000	23.112648000	6	0.000000000	1.407776000	23.165962000
6	0.000000000	-0.713031000	24.281865000	6	0.000000000	-0.717334000	24.333817000
6	0.000000000	0.713031000	24.281865000	6	0.000000000	0.717334000	24.333817000
1	0.000000000	2.492338000	20.629595000	1	0.000000000	2.493380000	20.675196000
1	0.000000000	-2.492338000	20.629595000	1	0.000000000	-2.493380000	20.675196000
1	0.000000000	-2.489634000	23.107520000	1	0.000000000	-2.492106000	23.161882000
1	0.000000000	2.489634000	23.107520000	1	0.000000000	2.492106000	23.161882000
1	0.000000000	1.244289000	25.228797000	1	0.000000000	1.246888000	25.279030000
1	0.000000000	-1.244289000	25.228797000	1	0.000000000	-1.246888000	25.279030000
6	0.000000000	1.392480000	-23.079455000	6	0.000000000	1.395066000	-23.131381000
6	0.000000000	-1.392480000	-23.079455000	6	0.000000000	-1.395066000	-23.131381000
6	0.000000000	0.702858000	-24.266131000	6	0.000000000	0.705256000	-24.319676000
6	0.000000000	-0.702858000	-24.266131000	6	0.000000000	-0.705256000	-24.319676000
1	0.000000000	2.480038000	-23.074693000	1	0.000000000	2.479982000	-23.127166000
1	0.000000000	-2.480038000	-23.074693000	1	0.000000000	-2.479982000	-23.127166000
1	0.000000000	1.241889000	-25.208657000	1	0.000000000	1.244105000	-25.259601000
1	0.000000000	-1.241889000	-25.208657000	1	0.000000000	-1.244105000	-25.259601000

Table S163: Coordinates of pT₆_2 at M06/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.725370000	5.049415000
7	0.000000000	1.356212000	3.826220000
6	0.000000000	0.707977000	2.598344000
6	0.000000000	-0.707977000	2.598344000
7	0.000000000	-1.356212000	3.826220000
6	0.000000000	-0.725370000	5.049415000
6	0.000000000	-0.711077000	0.174370000
6	0.000000000	0.711077000	0.174370000
6	0.000000000	1.391649000	-1.065310000
1	0.000000000	2.480078000	-1.071331000
6	0.000000000	0.713411000	-2.255431000
6	0.000000000	-0.713411000	-2.255431000
6	0.000000000	-1.391649000	-1.065310000
1	0.000000000	2.366367000	3.823108000
1	0.000000000	-2.366367000	3.823108000
1	0.000000000	-2.480078000	-1.071331000
6	0.000000000	-0.709583000	-4.708043000
6	0.000000000	0.709583000	-4.708043000

Table S164: Coordinates of pT₆_2 at M062X/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.731182000	5.067517000
7	0.000000000	1.359494000	3.839855000
6	0.000000000	0.710054000	2.607102000
6	0.000000000	-0.710054000	2.607102000
7	0.000000000	-1.359494000	3.839855000
6	0.000000000	-0.731182000	5.067517000
6	0.000000000	-0.709628000	0.176371000
6	0.000000000	0.709628000	0.176371000
6	0.000000000	1.394119000	-1.069491000
1	0.000000000	2.479560000	-1.074652000
6	0.000000000	0.716209000	-2.261229000
6	0.000000000	-0.716209000	-2.261229000
6	0.000000000	-1.394119000	-1.069491000
1	0.000000000	2.367881000	3.835259000
1	0.000000000	-2.367881000	3.835259000
1	0.000000000	-2.479560000	-1.074652000
6	0.000000000	-0.712470000	-4.724355000
6	0.000000000	0.712470000	-4.724355000

6	0.000000000	1.389896000	-5.898650000	6	0.000000000	1.391935000	-5.916914000
6	0.000000000	-1.389896000	-5.898650000	6	0.000000000	-1.391935000	-5.916914000
6	0.000000000	-0.709598000	-7.135575000	6	0.000000000	-0.708149000	-7.159615000
6	0.000000000	0.709598000	-7.135575000	6	0.000000000	0.708149000	-7.159615000
1	0.000000000	2.478555000	-5.892051000	1	0.000000000	2.477621000	-5.911020000
1	0.000000000	-2.478555000	-5.892051000	1	0.000000000	-2.477621000	-5.911020000
6	0.000000000	0.728894000	7.484821000	6	0.000000000	0.732354000	7.513328000
6	0.000000000	-0.728894000	7.484821000	6	0.000000000	-0.732354000	7.513328000
6	0.000000000	-1.410234000	8.676529000	6	0.000000000	-1.415615000	8.701294000
6	0.000000000	1.410234000	8.676529000	6	0.000000000	1.415615000	8.701294000
6	0.000000000	-0.731029000	9.919784000	6	0.000000000	-0.733772000	9.954750000
6	0.000000000	0.731029000	9.919784000	6	0.000000000	0.733772000	9.954750000
1	0.000000000	2.496617000	8.701162000	1	0.000000000	2.499271000	8.726464000
1	0.000000000	-2.496617000	8.701162000	1	0.000000000	-2.499271000	8.726464000
6	0.000000000	0.711349000	-9.564777000	6	0.000000000	0.714071000	-9.593490000
6	0.000000000	-0.711349000	-9.564777000	6	0.000000000	-0.714071000	-9.593490000
7	0.000000000	-1.360933000	-10.790613000	7	0.000000000	-1.364248000	-10.823056000
7	0.000000000	1.360933000	-10.790613000	7	0.000000000	1.364248000	-10.823056000
6	0.000000000	-0.710634000	-12.017853000	6	0.000000000	-0.713416000	-12.053582000
6	0.000000000	0.710634000	-12.017853000	6	0.000000000	0.713416000	-12.053582000
1	0.000000000	-2.369623000	-10.790853000	1	0.000000000	-2.371235000	-10.823500000
1	0.000000000	2.369623000	-10.790853000	1	0.000000000	2.371235000	-10.823500000
6	0.000000000	1.390092000	-8.373602000	6	0.000000000	1.393163000	-8.401667000
6	0.000000000	-1.390092000	-8.373602000	6	0.000000000	-1.393163000	-8.401667000
7	0.000000000	1.360381000	-3.479360000	7	0.000000000	1.363247000	-3.490741000
7	0.000000000	-1.360381000	-3.479360000	7	0.000000000	-1.363247000	-3.490741000
6	0.000000000	1.391623000	1.406626000	6	0.000000000	1.393684000	1.414383000
6	0.000000000	-1.391623000	1.406626000	6	0.000000000	-1.393684000	1.414383000
6	0.000000000	1.403440000	6.227842000	6	0.000000000	1.409196000	6.244745000
6	0.000000000	-1.403440000	6.227842000	6	0.000000000	-1.409196000	6.244745000
7	0.000000000	1.424021000	11.043204000	7	0.000000000	1.426904000	11.073273000
7	0.000000000	-1.424021000	11.043204000	7	0.000000000	-1.426904000	11.073273000
6	0.000000000	0.726497000	12.202559000	6	0.000000000	0.726984000	12.239173000
6	0.000000000	-0.726497000	12.202559000	6	0.000000000	-0.726984000	12.239173000
6	0.000000000	1.409981000	13.409251000	6	0.000000000	1.413321000	13.444070000
6	0.000000000	-1.409981000	13.409251000	6	0.000000000	-1.413321000	13.444070000
6	0.000000000	0.729031000	14.636105000	6	0.000000000	0.729482000	14.674989000
6	0.000000000	-0.729031000	14.636105000	6	0.000000000	-0.729482000	14.674989000
6	0.000000000	1.389870000	-13.208696000	6	0.000000000	1.392952000	-13.244430000
6	0.000000000	-1.389870000	-13.208696000	6	0.000000000	-1.392952000	-13.244430000
6	0.000000000	0.709495000	-14.446544000	6	0.000000000	0.708126000	-14.485759000
6	0.000000000	-0.709495000	-14.446544000	6	0.000000000	-0.708126000	-14.485759000
6	0.000000000	1.389911000	-15.683853000	6	0.000000000	1.393398000	-15.725773000
6	0.000000000	-1.389911000	-15.683853000	6	0.000000000	-1.393398000	-15.725773000
6	0.000000000	0.710184000	-16.874634000	6	0.000000000	0.712862000	-16.916078000
6	0.000000000	-0.710184000	-16.874634000	6	0.000000000	-0.712862000	-16.916078000
1	0.000000000	2.478559000	-15.690464000	1	0.000000000	2.478968000	-15.731424000
1	0.000000000	-2.478559000	-15.690464000	1	0.000000000	-2.478968000	-15.731424000

1	0.000000000	-2.478542000	-13.202343000	1	0.000000000	-2.478569000	-13.238291000
1	0.000000000	2.478542000	-13.202343000	1	0.000000000	2.478569000	-13.238291000
1	0.000000000	-2.478723000	-8.379892000	1	0.000000000	-2.478743000	-8.407135000
1	0.000000000	2.478723000	-8.379892000	1	0.000000000	2.478743000	-8.407135000
1	0.000000000	-2.369251000	-3.480311000	1	0.000000000	-2.370399000	-3.491883000
1	0.000000000	2.369251000	-3.480311000	1	0.000000000	2.370399000	-3.491883000
1	0.000000000	2.480057000	1.413888000	1	0.000000000	2.479211000	1.421347000
1	0.000000000	-2.480057000	1.413888000	1	0.000000000	-2.479211000	1.421347000
1	0.000000000	-2.491225000	6.222819000	1	0.000000000	-2.493977000	6.239741000
1	0.000000000	2.491225000	6.222819000	1	0.000000000	2.493977000	6.239741000
1	0.000000000	-2.496117000	13.383912000	1	0.000000000	-2.496909000	13.417850000
1	0.000000000	2.496117000	13.383912000	1	0.000000000	2.496909000	13.417850000
6	0.000000000	1.411006000	15.853409000	6	0.000000000	1.413966000	15.894591000
6	0.000000000	-1.411006000	15.853409000	6	0.000000000	-1.413966000	15.894591000
6	0.000000000	0.727224000	17.069065000	6	0.000000000	0.727365000	17.110504000
6	0.000000000	-0.727224000	17.069065000	6	0.000000000	-0.727365000	17.110504000
1	0.000000000	2.497111000	15.878300000	1	0.000000000	2.497609000	15.919987000
1	0.000000000	-2.497111000	15.878300000	1	0.000000000	-2.497609000	15.919987000
7	0.000000000	-1.360347000	-18.102188000	7	0.000000000	-1.364328000	-18.145708000
7	0.000000000	1.360347000	-18.102188000	7	0.000000000	1.364328000	-18.145708000
6	0.000000000	-0.713653000	-19.328076000	6	0.000000000	-0.716656000	-19.373245000
6	0.000000000	0.713653000	-19.328076000	6	0.000000000	0.716656000	-19.373245000
6	0.000000000	-1.391611000	-20.516442000	6	0.000000000	-1.395091000	-20.561070000
6	0.000000000	1.391611000	-20.516442000	6	0.000000000	1.395091000	-20.561070000
6	0.000000000	-0.710482000	-21.757836000	6	0.000000000	-0.709610000	-21.806476000
6	0.000000000	0.710482000	-21.757836000	6	0.000000000	0.709610000	-21.806476000
1	0.000000000	-2.480196000	-20.511883000	1	0.000000000	-2.480662000	-20.556610000
1	0.000000000	2.480196000	-20.511883000	1	0.000000000	2.480662000	-20.556610000
1	0.000000000	-2.369193000	-18.101973000	1	0.000000000	-2.371489000	-18.145581000
1	0.000000000	2.369193000	-18.101973000	1	0.000000000	2.371489000	-18.145581000
7	0.000000000	-1.422447000	18.219503000	7	0.000000000	-1.425248000	18.264721000
7	0.000000000	1.422447000	18.219503000	7	0.000000000	1.425248000	18.264721000
6	0.000000000	-0.727372000	19.350022000	6	0.000000000	-0.729388000	19.391196000
6	0.000000000	0.727372000	19.350022000	6	0.000000000	0.729388000	19.391196000
6	0.000000000	-1.409962000	20.587676000	6	0.000000000	-1.415309000	20.635926000
6	0.000000000	1.409962000	20.587676000	6	0.000000000	1.415309000	20.635926000
6	0.000000000	-0.725778000	21.781337000	6	0.000000000	-0.728570000	21.825135000
6	0.000000000	0.725778000	21.781337000	6	0.000000000	0.728570000	21.825135000
6	0.000000000	-1.405671000	23.042702000	6	0.000000000	-1.411707000	23.096238000
6	0.000000000	1.405671000	23.042702000	6	0.000000000	1.411707000	23.096238000
6	0.000000000	-0.715426000	24.208010000	6	0.000000000	-0.720591000	24.258986000
6	0.000000000	0.715426000	24.208010000	6	0.000000000	0.720591000	24.258986000
1	0.000000000	2.496402000	20.563778000	1	0.000000000	2.499194000	20.611321000
1	0.000000000	-2.496402000	20.563778000	1	0.000000000	-2.499194000	20.611321000
1	0.000000000	-2.492344000	23.037427000	1	0.000000000	-2.495986000	23.091872000
1	0.000000000	2.492344000	23.037427000	1	0.000000000	2.495986000	23.091872000
1	0.000000000	1.244475000	25.156039000	1	0.000000000	1.246979000	25.205949000
1	0.000000000	-1.244475000	25.156039000	1	0.000000000	-1.246979000	25.205949000

6	0.000000000	1.392564000	-22.992025000	6	0.000000000	1.395215000	-23.043452000
6	0.000000000	-1.392564000	-22.992025000	6	0.000000000	-1.395215000	-23.043452000
6	0.000000000	0.702889000	-24.178566000	6	0.000000000	0.705306000	-24.231573000
6	0.000000000	-0.702889000	-24.178566000	6	0.000000000	-0.705306000	-24.231573000
1	0.000000000	2.480102000	-22.987283000	1	0.000000000	2.480182000	-23.038911000
1	0.000000000	-2.480102000	-22.987283000	1	0.000000000	-2.480182000	-23.038911000
1	0.000000000	1.241833000	-25.121122000	1	0.000000000	1.243736000	-25.171788000
1	0.000000000	-1.241833000	-25.121122000	1	0.000000000	-1.243736000	-25.171788000

Table S165: Coordinates of pT₆_3 at M06/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.723667000	4.947218000
7	0.000000000	1.419575000	3.822073000
6	0.000000000	0.721227000	2.668728000
6	0.000000000	-0.721227000	2.668728000
7	0.000000000	-1.419575000	3.822073000
6	0.000000000	-0.723667000	4.947218000
6	0.000000000	-0.720921000	0.239478000
6	0.000000000	0.720921000	0.239478000
6	0.000000000	1.398138000	-1.008399000
1	0.000000000	2.486008000	-1.012863000
6	0.000000000	0.719863000	-2.193314000
6	0.000000000	-0.719863000	-2.193314000
6	0.000000000	-1.398138000	-1.008399000
1	0.000000000	-2.486008000	-1.012863000
6	0.000000000	-0.708343000	-4.644044000
6	0.000000000	0.708343000	-4.644044000
6	0.000000000	1.391034000	-5.834449000
6	0.000000000	-1.391034000	-5.834449000
6	0.000000000	-0.710306000	-7.068874000
6	0.000000000	0.710306000	-7.068874000
1	0.000000000	2.479497000	-5.827472000
1	0.000000000	-2.479497000	-5.827472000
6	0.000000000	0.727250000	7.390747000
6	0.000000000	-0.727250000	7.390747000
6	0.000000000	-1.402018000	8.636039000
6	0.000000000	1.402018000	8.636039000
6	0.000000000	-0.730021000	9.845371000
6	0.000000000	0.730021000	9.845371000
1	0.000000000	2.488813000	8.660796000
1	0.000000000	-2.488813000	8.660796000
6	0.000000000	0.712564000	-9.498168000
6	0.000000000	-0.712564000	-9.498168000
7	0.000000000	-1.360619000	-10.722555000
7	0.000000000	1.360619000	-10.722555000
6	0.000000000	-0.710105000	-11.950760000
6	0.000000000	0.710105000	-11.950760000

Table S166: Coordinates of pT₆_3 at M062X/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.728705000	4.989396000
7	0.000000000	1.428844000	3.816835000
6	0.000000000	0.736185000	2.702117000
6	0.000000000	-0.736185000	2.702117000
7	0.000000000	-1.428844000	3.816835000
6	0.000000000	-0.728705000	4.989396000
6	0.000000000	-0.733792000	0.258744000
6	0.000000000	0.733792000	0.258744000
6	0.000000000	1.410146000	-1.010182000
1	0.000000000	2.494861000	-1.015675000
6	0.000000000	0.731908000	-2.186957000
6	0.000000000	-0.731908000	-2.186957000
6	0.000000000	-1.410146000	-1.010182000
1	0.000000000	-2.494861000	-1.015675000
6	0.000000000	-0.709839000	-4.646482000
6	0.000000000	0.709839000	-4.646482000
6	0.000000000	1.393716000	-5.839172000
6	0.000000000	-1.393716000	-5.839172000
6	0.000000000	-0.709694000	-7.075735000
6	0.000000000	0.709694000	-7.075735000
1	0.000000000	2.479203000	-5.832056000
1	0.000000000	-2.479203000	-5.832056000
6	0.000000000	0.732254000	7.429529000
6	0.000000000	-0.732254000	7.429529000
6	0.000000000	-1.416557000	8.638495000
6	0.000000000	1.416557000	8.638495000
6	0.000000000	-0.731613000	9.869839000
6	0.000000000	0.731613000	9.869839000
1	0.000000000	2.500105000	8.663432000
1	0.000000000	-2.500105000	8.663432000
6	0.000000000	0.716257000	-9.509076000
6	0.000000000	-0.716257000	-9.509076000
7	0.000000000	-1.364091000	-10.736314000
7	0.000000000	1.364091000	-10.736314000
6	0.000000000	-0.712582000	-11.967345000
6	0.000000000	0.712582000	-11.967345000

1	0.000000000	-2.369439000	-10.723194000	1	0.000000000	-2.371256000	-10.737697000
1	0.000000000	2.369439000	-10.723194000	1	0.000000000	2.371256000	-10.737697000
6	0.000000000	1.391078000	-8.307543000	6	0.000000000	1.395106000	-8.319162000
6	0.000000000	-1.391078000	-8.307543000	6	0.000000000	-1.395106000	-8.319162000
7	0.000000000	1.357899000	-3.414563000	7	0.000000000	1.359327000	-3.414049000
7	0.000000000	-1.357899000	-3.414563000	7	0.000000000	-1.359327000	-3.414049000
6	0.000000000	1.403491000	1.448210000	6	0.000000000	1.416985000	1.445167000
6	0.000000000	-1.403491000	1.448210000	6	0.000000000	-1.416985000	1.445167000
6	0.000000000	1.405793000	6.193687000	6	0.000000000	1.414717000	6.187658000
6	0.000000000	-1.405793000	6.193687000	6	0.000000000	-1.414717000	6.187658000
7	0.000000000	1.431071000	10.992823000	7	0.000000000	1.426754000	11.006730000
7	0.000000000	-1.431071000	10.992823000	7	0.000000000	-1.426754000	11.006730000
6	0.000000000	0.732060000	12.130705000	6	0.000000000	0.729743000	12.153639000
6	0.000000000	-0.732060000	12.130705000	6	0.000000000	-0.729743000	12.153639000
6	0.000000000	1.402064000	13.348117000	6	0.000000000	1.416001000	13.374040000
6	0.000000000	-1.402064000	13.348117000	6	0.000000000	-1.416001000	13.374040000
6	0.000000000	0.729435000	14.589759000	6	0.000000000	0.731362000	14.591387000
6	0.000000000	-0.729435000	14.589759000	6	0.000000000	-0.731362000	14.591387000
6	0.000000000	1.390043000	-13.141120000	6	0.000000000	1.393137000	-13.157667000
6	0.000000000	-1.390043000	-13.141120000	6	0.000000000	-1.393137000	-13.157667000
6	0.000000000	0.709532000	-14.378530000	6	0.000000000	0.708257000	-14.397877000
6	0.000000000	-0.709532000	-14.378530000	6	0.000000000	-0.708257000	-14.397877000
6	0.000000000	1.390183000	-15.615926000	6	0.000000000	1.393596000	-15.637948000
6	0.000000000	-1.390183000	-15.615926000	6	0.000000000	-1.393596000	-15.637948000
6	0.000000000	0.710572000	-16.806585000	6	0.000000000	0.713350000	-16.828269000
6	0.000000000	-0.710572000	-16.806585000	6	0.000000000	-0.713350000	-16.828269000
1	0.000000000	2.478764000	-15.622370000	1	0.000000000	2.479087000	-15.643599000
1	0.000000000	-2.478764000	-15.622370000	1	0.000000000	-2.479087000	-15.643599000
1	0.000000000	-2.478662000	-13.134738000	1	0.000000000	-2.478697000	-13.151330000
1	0.000000000	2.478662000	-13.134738000	1	0.000000000	2.478697000	-13.151330000
1	0.000000000	-2.479533000	-8.313512000	1	0.000000000	-2.480451000	-8.324280000
1	0.000000000	2.479533000	-8.313512000	1	0.000000000	2.480451000	-8.324280000
1	0.000000000	-2.367601000	-3.416333000	1	0.000000000	-2.367836000	-3.418684000
1	0.000000000	2.367601000	-3.416333000	1	0.000000000	2.367836000	-3.418684000
1	0.000000000	2.490007000	1.473724000	1	0.000000000	2.500612000	1.470579000
1	0.000000000	-2.490007000	1.473724000	1	0.000000000	-2.500612000	1.470579000
1	0.000000000	-2.492343000	6.169532000	1	0.000000000	-2.498221000	6.161003000
1	0.000000000	2.492343000	6.169532000	1	0.000000000	2.498221000	6.161003000
1	0.000000000	-2.488853000	13.324293000	1	0.000000000	-2.499530000	13.348638000
1	0.000000000	2.488853000	13.324293000	1	0.000000000	2.499530000	13.348638000
6	0.000000000	1.406686000	15.786638000	6	0.000000000	1.415755000	15.821644000
6	0.000000000	-1.406686000	15.786638000	6	0.000000000	-1.415755000	15.821644000
6	0.000000000	0.727362000	17.038734000	6	0.000000000	0.728477000	17.027599000
6	0.000000000	-0.727362000	17.038734000	6	0.000000000	-0.728477000	17.027599000
1	0.000000000	2.493188000	15.810317000	1	0.000000000	2.499278000	15.847696000
1	0.000000000	-2.493188000	15.810317000	1	0.000000000	-2.499278000	15.847696000
7	0.000000000	-1.360307000	-18.033571000	7	0.000000000	-1.364241000	-18.057272000
7	0.000000000	1.360307000	-18.033571000	7	0.000000000	1.364241000	-18.057272000

6	0.000000000	-0.713487000	-19.259891000	6	0.000000000	-0.716407000	-19.285487000
6	0.000000000	0.713487000	-19.259891000	6	0.000000000	0.716407000	-19.285487000
6	0.000000000	-1.391660000	-20.447982000	6	0.000000000	-1.395137000	-20.472985000
6	0.000000000	1.391660000	-20.447982000	6	0.000000000	1.395137000	-20.472985000
6	0.000000000	-0.710437000	-21.689304000	6	0.000000000	-0.709639000	-21.718287000
6	0.000000000	0.710437000	-21.689304000	6	0.000000000	0.709639000	-21.718287000
1	0.000000000	-2.480224000	-20.443496000	1	0.000000000	-2.480671000	-20.468369000
1	0.000000000	2.480224000	-20.443496000	1	0.000000000	2.480671000	-20.468369000
1	0.000000000	-2.369184000	-18.033489000	1	0.000000000	-2.371444000	-18.057334000
1	0.000000000	2.369184000	-18.033489000	1	0.000000000	2.371444000	-18.057334000
7	0.000000000	-1.421793000	18.155465000	7	0.000000000	-1.427340000	18.189376000
7	0.000000000	1.421793000	18.155465000	7	0.000000000	1.427340000	18.189376000
6	0.000000000	-0.719864000	19.318931000	6	0.000000000	-0.732256000	19.309180000
6	0.000000000	0.719864000	19.318931000	6	0.000000000	0.732256000	19.309180000
6	0.000000000	-1.402711000	20.529750000	6	0.000000000	-1.417387000	20.558833000
6	0.000000000	1.402711000	20.529750000	6	0.000000000	1.417387000	20.558833000
6	0.000000000	-0.717800000	21.746658000	6	0.000000000	-0.730260000	21.744466000
6	0.000000000	0.717800000	21.746658000	6	0.000000000	0.730260000	21.744466000
6	0.000000000	-1.399504000	22.993052000	6	0.000000000	-1.413081000	23.017466000
6	0.000000000	1.399504000	22.993052000	6	0.000000000	1.413081000	23.017466000
6	0.000000000	-0.708567000	24.168979000	6	0.000000000	-0.721554000	24.178644000
6	0.000000000	0.708567000	24.168979000	6	0.000000000	0.721554000	24.178644000
1	0.000000000	2.489304000	20.504977000	1	0.000000000	2.501186000	20.534717000
1	0.000000000	-2.489304000	20.504977000	1	0.000000000	-2.501186000	20.534717000
1	0.000000000	-2.486283000	22.987251000	1	0.000000000	-2.497248000	23.013524000
1	0.000000000	2.486283000	22.987251000	1	0.000000000	2.497248000	23.013524000
1	0.000000000	1.241927000	25.114553000	1	0.000000000	1.247126000	25.125997000
1	0.000000000	-1.241927000	25.114553000	1	0.000000000	-1.247126000	25.125997000
6	0.000000000	1.392685000	-22.923489000	6	0.000000000	1.395333000	-22.955276000
6	0.000000000	-1.392685000	-22.923489000	6	0.000000000	-1.395333000	-22.955276000
6	0.000000000	0.702943000	-24.109842000	6	0.000000000	0.705329000	-24.143178000
6	0.000000000	-0.702943000	-24.109842000	6	0.000000000	-0.705329000	-24.143178000
1	0.000000000	2.480191000	-22.918743000	1	0.000000000	2.480251000	-22.950865000
1	0.000000000	-2.480191000	-22.918743000	1	0.000000000	-2.480251000	-22.950865000
1	0.000000000	1.241752000	-25.052447000	1	0.000000000	1.243671000	-25.083387000
1	0.000000000	-1.241752000	-25.052447000	1	0.000000000	-1.243671000	-25.083387000

Table S167: Coordinates of pT₆_4 at M06/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.732505000	4.873854000
7	0.000000000	1.427919000	3.755494000
6	0.000000000	0.726844000	2.591331000
6	0.000000000	-0.726844000	2.591331000
7	0.000000000	-1.427919000	3.755494000
6	0.000000000	-0.732505000	4.873854000
6	0.000000000	-0.726424000	0.151142000
6	0.000000000	0.726424000	0.151142000

Table S168: Coordinates of pT₆_4 at M062X/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.730693000	4.906039000
7	0.000000000	1.427788000	3.752392000
6	0.000000000	0.733554000	2.620178000
6	0.000000000	-0.733554000	2.620178000
7	0.000000000	-1.427788000	3.752392000
6	0.000000000	-0.730693000	4.906039000
6	0.000000000	-0.733263000	0.177992000
6	0.000000000	0.733263000	0.177992000

6	0.000000000	1.407348000	-1.052974000	6	0.000000000	1.415458000	-1.065992000
1	0.000000000	2.493671000	-1.077501000	1	0.000000000	2.498949000	-1.092766000
6	0.000000000	0.723243000	-2.283936000	6	0.000000000	0.729482000	-2.262851000
6	0.000000000	-0.723243000	-2.283936000	6	0.000000000	-0.729482000	-2.262851000
6	0.000000000	-1.407348000	-1.052974000	6	0.000000000	-1.415458000	-1.065992000
1	0.000000000	-2.493671000	-1.077501000	1	0.000000000	-2.498949000	-1.092766000
6	0.000000000	-0.725213000	-4.562868000	6	0.000000000	-0.736871000	-4.550281000
6	0.000000000	0.725213000	-4.562868000	6	0.000000000	0.736871000	-4.550281000
6	0.000000000	1.406838000	-5.793716000	6	0.000000000	1.417312000	-5.808099000
6	0.000000000	-1.406838000	-5.793716000	6	0.000000000	-1.417312000	-5.808099000
6	0.000000000	-0.724710000	-6.993644000	6	0.000000000	-0.733930000	-6.993884000
6	0.000000000	0.724710000	-6.993644000	6	0.000000000	0.733930000	-6.993884000
1	0.000000000	2.493218000	-5.768481000	1	0.000000000	2.500918000	-5.783125000
1	0.000000000	-2.493218000	-5.768481000	1	0.000000000	-2.500918000	-5.783125000
6	0.000000000	0.731338000	7.327984000	6	0.000000000	0.733072000	7.347359000
6	0.000000000	-0.731338000	7.327984000	6	0.000000000	-0.733072000	7.347359000
6	0.000000000	-1.404473000	8.548567000	6	0.000000000	-1.417232000	8.567487000
6	0.000000000	1.404473000	8.548567000	6	0.000000000	1.417232000	8.567487000
6	0.000000000	-0.733011000	9.784007000	6	0.000000000	-0.731492000	9.787999000
6	0.000000000	0.733011000	9.784007000	6	0.000000000	0.731492000	9.787999000
1	0.000000000	2.491181000	8.572077000	1	0.000000000	2.500730000	8.593275000
1	0.000000000	-2.491181000	8.572077000	1	0.000000000	-2.500730000	8.593275000
6	0.000000000	0.722652000	-9.427461000	6	0.000000000	0.732109000	-9.437672000
6	0.000000000	-0.722652000	-9.427461000	6	0.000000000	-0.732109000	-9.437672000
7	0.000000000	-1.357083000	-10.649615000	7	0.000000000	-1.359462000	-10.664239000
7	0.000000000	1.357083000	-10.649615000	7	0.000000000	1.359462000	-10.664239000
6	0.000000000	-0.708423000	-11.878232000	6	0.000000000	-0.710112000	-11.895636000
6	0.000000000	0.708423000	-11.878232000	6	0.000000000	0.710112000	-11.895636000
1	0.000000000	-2.367053000	-10.652025000	1	0.000000000	-2.368029000	-10.669417000
1	0.000000000	2.367053000	-10.652025000	1	0.000000000	2.368029000	-10.669417000
6	0.000000000	1.400850000	-8.246070000	6	0.000000000	1.410844000	-8.261752000
6	0.000000000	-1.400850000	-8.246070000	6	0.000000000	-1.410844000	-8.261752000
7	0.000000000	1.420096000	-3.423162000	7	0.000000000	1.429316000	-3.436466000
7	0.000000000	-1.420096000	-3.423162000	7	0.000000000	-1.429316000	-3.436466000
6	0.000000000	1.405982000	1.392517000	6	0.000000000	1.417803000	1.384032000
6	0.000000000	-1.405982000	1.392517000	6	0.000000000	-1.417803000	1.384032000
6	0.000000000	1.405564000	6.115098000	6	0.000000000	1.416638000	6.119855000
6	0.000000000	-1.405564000	6.115098000	6	0.000000000	-1.416638000	6.119855000
7	0.000000000	1.429449000	10.905965000	7	0.000000000	1.427746000	10.933716000
7	0.000000000	-1.429449000	10.905965000	7	0.000000000	-1.427746000	10.933716000
6	0.000000000	0.728971000	12.067595000	6	0.000000000	0.731802000	12.071900000
6	0.000000000	-0.728971000	12.067595000	6	0.000000000	-0.731802000	12.071900000
6	0.000000000	1.406109000	13.266214000	6	0.000000000	1.417600000	13.299626000
6	0.000000000	-1.406109000	13.266214000	6	0.000000000	-1.417600000	13.299626000
6	0.000000000	0.728285000	14.511442000	6	0.000000000	0.732400000	14.510626000
6	0.000000000	-0.728285000	14.511442000	6	0.000000000	-0.732400000	14.510626000
6	0.000000000	1.391608000	-13.068790000	6	0.000000000	1.394502000	-13.087216000
6	0.000000000	-1.391608000	-13.068790000	6	0.000000000	-1.394502000	-13.087216000

6	0.000000000	0.710641000	-14.302306000	6	0.000000000	0.709698000	-14.322988000
6	0.000000000	-0.710641000	-14.302306000	6	0.000000000	-0.709698000	-14.322988000
6	0.000000000	1.391582000	-15.540958000	6	0.000000000	1.395372000	-15.565756000
6	0.000000000	-1.391582000	-15.540958000	6	0.000000000	-1.395372000	-15.565756000
6	0.000000000	0.712323000	-16.730542000	6	0.000000000	0.715556000	-16.754753000
6	0.000000000	-0.712323000	-16.730542000	6	0.000000000	-0.715556000	-16.754753000
1	0.000000000	2.479944000	-15.547113000	1	0.000000000	2.480659000	-15.570944000
1	0.000000000	-2.479944000	-15.547113000	1	0.000000000	-2.480659000	-15.570944000
1	0.000000000	-2.479988000	-13.061810000	1	0.000000000	-2.479905000	-13.079921000
1	0.000000000	2.479988000	-13.061810000	1	0.000000000	2.479905000	-13.079921000
1	0.000000000	-2.488622000	-8.250643000	1	0.000000000	-2.495531000	-8.266631000
1	0.000000000	2.488622000	-8.250643000	1	0.000000000	2.495531000	-8.266631000
1	0.000000000	2.492424000	1.417980000	1	0.000000000	2.501353000	1.408452000
1	0.000000000	-2.492424000	1.417980000	1	0.000000000	-2.501353000	1.408452000
1	0.000000000	-2.492237000	6.092012000	1	0.000000000	-2.500158000	6.093832000
1	0.000000000	2.492237000	6.092012000	1	0.000000000	2.500158000	6.093832000
1	0.000000000	-2.492536000	13.241033000	1	0.000000000	-2.501086000	13.274740000
1	0.000000000	2.492536000	13.241033000	1	0.000000000	2.501086000	13.274740000
6	0.000000000	1.409175000	15.709503000	6	0.000000000	1.416627000	15.745663000
6	0.000000000	-1.409175000	15.709503000	6	0.000000000	-1.416627000	15.745663000
6	0.000000000	0.725778000	16.948602000	6	0.000000000	0.729091000	16.947247000
6	0.000000000	-0.725778000	16.948602000	6	0.000000000	-0.729091000	16.947247000
1	0.000000000	2.495415000	15.733451000	1	0.000000000	2.500086000	15.771959000
1	0.000000000	-2.495415000	15.733451000	1	0.000000000	-2.500086000	15.771959000
7	0.000000000	-1.359952000	-17.955793000	7	0.000000000	-1.363528000	-17.982589000
7	0.000000000	1.359952000	-17.955793000	7	0.000000000	1.363528000	-17.982589000
6	0.000000000	-0.712884000	-19.183291000	6	0.000000000	-0.715804000	-19.212394000
6	0.000000000	0.712884000	-19.183291000	6	0.000000000	0.715804000	-19.212394000
6	0.000000000	-1.391943000	-20.370616000	6	0.000000000	-1.395472000	-20.399406000
6	0.000000000	1.391943000	-20.370616000	6	0.000000000	1.395472000	-20.399406000
6	0.000000000	-0.710450000	-21.611421000	6	0.000000000	-0.709603000	-21.644112000
6	0.000000000	0.710450000	-21.611421000	6	0.000000000	0.709603000	-21.644112000
1	0.000000000	-2.480439000	-20.366074000	1	0.000000000	-2.480965000	-20.395007000
1	0.000000000	2.480439000	-20.366074000	1	0.000000000	2.480965000	-20.395007000
1	0.000000000	-2.369015000	-17.956275000	1	0.000000000	-2.370955000	-17.983402000
1	0.000000000	2.369015000	-17.956275000	1	0.000000000	2.370955000	-17.983402000
7	0.000000000	-1.420352000	18.078433000	7	0.000000000	-1.428255000	18.112572000
7	0.000000000	1.420352000	18.078433000	7	0.000000000	1.428255000	18.112572000
6	0.000000000	-0.722582000	19.227287000	6	0.000000000	-0.733629000	19.229574000
6	0.000000000	0.722582000	19.227287000	6	0.000000000	0.733629000	19.229574000
6	0.000000000	-1.406324000	20.450128000	6	0.000000000	-1.418404000	20.481654000
6	0.000000000	1.406324000	20.450128000	6	0.000000000	1.418404000	20.481654000
6	0.000000000	-0.721585000	21.654894000	6	0.000000000	-0.731004000	21.665589000
6	0.000000000	0.721585000	21.654894000	6	0.000000000	0.731004000	21.665589000
6	0.000000000	-1.402781000	22.908922000	6	0.000000000	-1.413752000	22.939440000
6	0.000000000	1.402781000	22.908922000	6	0.000000000	1.413752000	22.939440000
6	0.000000000	-0.712136000	24.078952000	6	0.000000000	-0.722135000	24.099818000
6	0.000000000	0.712136000	24.078952000	6	0.000000000	0.722135000	24.099818000

1	0.000000000	2.492765000	20.425568000	1	0.000000000	2.502154000	20.457421000
1	0.000000000	-2.492765000	20.425568000	1	0.000000000	-2.502154000	20.457421000
1	0.000000000	-2.489444000	22.903264000	1	0.000000000	-2.497893000	22.935010000
1	0.000000000	2.489444000	22.903264000	1	0.000000000	2.497893000	22.935010000
1	0.000000000	1.243028000	25.025895000	1	0.000000000	1.246873000	25.047615000
1	0.000000000	-1.243028000	25.025895000	1	0.000000000	-1.246873000	25.047615000
6	0.000000000	1.393074000	-22.845697000	6	0.000000000	1.395782000	-22.881289000
6	0.000000000	-1.393074000	-22.845697000	6	0.000000000	-1.395782000	-22.881289000
6	0.000000000	0.703115000	-24.031421000	6	0.000000000	0.705529000	-24.068479000
6	0.000000000	-0.703115000	-24.031421000	6	0.000000000	-0.705529000	-24.068479000
1	0.000000000	2.480497000	-22.841036000	1	0.000000000	2.480632000	-22.876941000
1	0.000000000	-2.480497000	-22.841036000	1	0.000000000	-2.480632000	-22.876941000
1	0.000000000	1.241587000	-24.974147000	1	0.000000000	1.243332000	-25.008965000
1	0.000000000	-1.241587000	-24.974147000	1	0.000000000	-1.243332000	-25.008965000

Table S169: Coordinates of pT₆_5 at M06/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.732652000	4.805590000
7	0.000000000	1.429973000	3.668226000
6	0.000000000	0.731546000	2.522852000
6	0.000000000	-0.731546000	2.522852000
7	0.000000000	-1.429973000	3.668226000
6	0.000000000	-0.732652000	4.805590000
6	0.000000000	-0.730780000	0.074008000
6	0.000000000	0.730780000	0.074008000
6	0.000000000	1.409699000	-1.125367000
1	0.000000000	2.496092000	-1.148511000
6	0.000000000	0.730832000	-2.369855000
6	0.000000000	-0.730832000	-2.369855000
6	0.000000000	-1.409699000	-1.125367000
1	0.000000000	-2.496092000	-1.148511000
6	0.000000000	-0.726458000	-4.650838000
6	0.000000000	0.726458000	-4.650838000
6	0.000000000	1.408883000	-5.853572000
6	0.000000000	-1.408883000	-5.853572000
6	0.000000000	-0.727252000	-7.085285000
6	0.000000000	0.727252000	-7.085285000
1	0.000000000	2.495080000	-5.828229000
1	0.000000000	-2.495080000	-5.828229000
6	0.000000000	0.731479000	7.256820000
6	0.000000000	-0.731479000	7.256820000
6	0.000000000	-1.408868000	8.459353000
6	0.000000000	1.408868000	8.459353000
6	0.000000000	-0.732282000	9.703974000
6	0.000000000	0.732282000	9.703974000
1	0.000000000	2.495311000	8.482411000
1	0.000000000	-2.495311000	8.482411000

Table S170: Coordinates of pT₆_5 at M062X/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	0.738954000	4.811124000
7	0.000000000	1.435641000	3.683699000
6	0.000000000	0.735380000	2.522460000
6	0.000000000	-0.735380000	2.522460000
7	0.000000000	-1.435641000	3.683699000
6	0.000000000	-0.738954000	4.811124000
6	0.000000000	-0.734163000	0.065516000
6	0.000000000	0.734163000	0.065516000
6	0.000000000	1.416146000	-1.124753000
1	0.000000000	2.500156000	-1.149153000
6	0.000000000	0.733194000	-2.384061000
6	0.000000000	-0.733194000	-2.384061000
6	0.000000000	-1.416146000	-1.124753000
1	0.000000000	-2.500156000	-1.149153000
6	0.000000000	-0.726732000	-4.668748000
6	0.000000000	0.726732000	-4.668748000
6	0.000000000	1.412460000	-5.871481000
6	0.000000000	-1.412460000	-5.871481000
6	0.000000000	-0.727977000	-7.106129000
6	0.000000000	0.727977000	-7.106129000
1	0.000000000	2.496166000	-5.845854000
1	0.000000000	-2.496166000	-5.845854000
6	0.000000000	0.736432000	7.280147000
6	0.000000000	-0.736432000	7.280147000
6	0.000000000	-1.413474000	8.479520000
6	0.000000000	1.413474000	8.479520000
6	0.000000000	-0.737008000	9.741163000
6	0.000000000	0.737008000	9.741163000
1	0.000000000	2.497725000	8.503704000
1	0.000000000	-2.497725000	8.503704000

6	0.000000000	0.724383000	-9.517990000	6	0.000000000	0.724924000	-9.541217000
6	0.000000000	-0.724383000	-9.517990000	6	0.000000000	-0.724924000	-9.541217000
7	0.000000000	-1.421422000	-10.666259000	7	0.000000000	-1.424633000	-10.698515000
7	0.000000000	1.421422000	-10.666259000	7	0.000000000	1.424633000	-10.698515000
6	0.000000000	-0.727782000	-11.797980000	6	0.000000000	-0.731019000	-11.823638000
6	0.000000000	0.727782000	-11.797980000	6	0.000000000	0.731019000	-11.823638000
6	0.000000000	1.408882000	-8.298303000	6	0.000000000	1.412158000	-8.325403000
6	0.000000000	-1.408882000	-8.298303000	6	0.000000000	-1.412158000	-8.325403000
7	0.000000000	1.425065000	-3.488783000	7	0.000000000	1.427146000	-3.497633000
7	0.000000000	-1.425065000	-3.488783000	7	0.000000000	-1.427146000	-3.497633000
6	0.000000000	1.405743000	1.311963000	6	0.000000000	1.411218000	1.323411000
6	0.000000000	-1.405743000	1.311963000	6	0.000000000	-1.411218000	1.323411000
6	0.000000000	1.405452000	6.023929000	6	0.000000000	1.408524000	6.040634000
6	0.000000000	-1.405452000	6.023929000	6	0.000000000	-1.408524000	6.040634000
7	0.000000000	1.426704000	10.821066000	7	0.000000000	1.432064000	10.846209000
7	0.000000000	-1.426704000	10.821066000	7	0.000000000	-1.432064000	10.846209000
6	0.000000000	0.727351000	11.985962000	6	0.000000000	0.728680000	12.026004000
6	0.000000000	-0.727351000	11.985962000	6	0.000000000	-0.728680000	12.026004000
6	0.000000000	1.408867000	13.184408000	6	0.000000000	1.413081000	13.215885000
6	0.000000000	-1.408867000	13.184408000	6	0.000000000	-1.413081000	13.215885000
6	0.000000000	0.728127000	14.422265000	6	0.000000000	0.728814000	14.464262000
6	0.000000000	-0.728127000	14.422265000	6	0.000000000	-0.728814000	14.464262000
6	0.000000000	1.408969000	-13.034677000	6	0.000000000	1.414515000	-13.071419000
6	0.000000000	-1.408969000	-13.034677000	6	0.000000000	-1.414515000	-13.071419000
6	0.000000000	0.726614000	-14.229749000	6	0.000000000	0.730493000	-14.261185000
6	0.000000000	-0.726614000	-14.229749000	6	0.000000000	-0.730493000	-14.261185000
6	0.000000000	1.402385000	-15.484856000	6	0.000000000	1.409150000	-15.526152000
6	0.000000000	-1.402385000	-15.484856000	6	0.000000000	-1.409150000	-15.526152000
6	0.000000000	0.723698000	-16.663436000	6	0.000000000	0.729583000	-16.701781000
6	0.000000000	-0.723698000	-16.663436000	6	0.000000000	-0.729583000	-16.701781000
1	0.000000000	2.490065000	-15.489648000	1	0.000000000	2.493873000	-15.531338000
1	0.000000000	-2.490065000	-15.489648000	1	0.000000000	-2.493873000	-15.531338000
1	0.000000000	-2.495270000	-13.009678000	1	0.000000000	-2.498160000	-13.045677000
1	0.000000000	2.495270000	-13.009678000	1	0.000000000	2.498160000	-13.045677000
1	0.000000000	-2.495036000	-8.323103000	1	0.000000000	-2.495817000	-8.351282000
1	0.000000000	2.495036000	-8.323103000	1	0.000000000	2.495817000	-8.351282000
1	0.000000000	2.492287000	1.336920000	1	0.000000000	2.495380000	1.349185000
1	0.000000000	-2.492287000	1.336920000	1	0.000000000	-2.495380000	1.349185000
1	0.000000000	-2.492037000	5.999678000	1	0.000000000	-2.492994000	6.016056000
1	0.000000000	2.492037000	5.999678000	1	0.000000000	2.492994000	6.016056000
1	0.000000000	-2.495050000	13.158901000	1	0.000000000	-2.496789000	13.190014000
1	0.000000000	2.495050000	13.158901000	1	0.000000000	2.496789000	13.190014000
6	0.000000000	1.410258000	15.628102000	6	0.000000000	1.413676000	15.667155000
6	0.000000000	-1.410258000	15.628102000	6	0.000000000	-1.413676000	15.667155000
6	0.000000000	0.725661000	16.855532000	6	0.000000000	0.725596000	16.898603000
6	0.000000000	-0.725661000	16.855532000	6	0.000000000	-0.725596000	16.898603000
1	0.000000000	2.496352000	15.652451000	1	0.000000000	2.497360000	15.692360000
1	0.000000000	-2.496352000	15.652451000	1	0.000000000	-2.497360000	15.692360000

7	0.000000000	-1.357018000	-17.887109000	7	0.000000000	-1.360733000	-17.928699000
7	0.000000000	1.357018000	-17.887109000	7	0.000000000	1.360733000	-17.928699000
6	0.000000000	-0.711289000	-19.114861000	6	0.000000000	-0.713633000	-19.158518000
6	0.000000000	0.711289000	-19.114861000	6	0.000000000	0.713633000	-19.158518000
6	0.000000000	-1.393448000	-20.302131000	6	0.000000000	-1.396528000	-20.345809000
6	0.000000000	1.393448000	-20.302131000	6	0.000000000	1.396528000	-20.345809000
6	0.000000000	-0.711192000	-21.539105000	6	0.000000000	-0.710517000	-21.586222000
6	0.000000000	0.711192000	-21.539105000	6	0.000000000	0.710517000	-21.586222000
1	0.000000000	-2.481719000	-20.297169000	1	0.000000000	-2.481956000	-20.340322000
1	0.000000000	2.481719000	-20.297169000	1	0.000000000	2.481956000	-20.340322000
1	0.000000000	-2.367214000	-17.889644000	1	0.000000000	-2.369242000	-17.932694000
1	0.000000000	2.367214000	-17.889644000	1	0.000000000	2.369242000	-17.932694000
7	0.000000000	-1.420856000	17.995480000	7	0.000000000	-1.423142000	18.039081000
7	0.000000000	1.420856000	17.995480000	7	0.000000000	1.423142000	18.039081000
6	0.000000000	-0.725183000	19.134542000	6	0.000000000	-0.725968000	19.176640000
6	0.000000000	0.725183000	19.134542000	6	0.000000000	0.725968000	19.176640000
6	0.000000000	-1.408702000	20.365084000	6	0.000000000	-1.413036000	20.412028000
6	0.000000000	1.408702000	20.365084000	6	0.000000000	1.413036000	20.412028000
6	0.000000000	-0.723921000	21.563341000	6	0.000000000	-0.726016000	21.607021000
6	0.000000000	0.723921000	21.563341000	6	0.000000000	0.726016000	21.607021000
6	0.000000000	-1.404675000	22.821352000	6	0.000000000	-1.410200000	22.873520000
6	0.000000000	1.404675000	22.821352000	6	0.000000000	1.410200000	22.873520000
6	0.000000000	-0.714020000	23.988400000	6	0.000000000	-0.718774000	24.038500000
6	0.000000000	0.714020000	23.988400000	6	0.000000000	0.718774000	24.038500000
1	0.000000000	2.495062000	20.340891000	1	0.000000000	2.496887000	20.386865000
1	0.000000000	-2.495062000	20.340891000	1	0.000000000	-2.496887000	20.386865000
1	0.000000000	-2.491261000	22.815854000	1	0.000000000	-2.494423000	22.868960000
1	0.000000000	2.491261000	22.815854000	1	0.000000000	2.494423000	22.868960000
1	0.000000000	1.243576000	24.936063000	1	0.000000000	1.245971000	24.984968000
1	0.000000000	-1.243576000	24.936063000	1	0.000000000	-1.245971000	24.984968000
6	0.000000000	1.394514000	-22.775073000	6	0.000000000	1.397176000	-22.825535000
6	0.000000000	-1.394514000	-22.775073000	6	0.000000000	-1.397176000	-22.825535000
6	0.000000000	0.704153000	-23.958308000	6	0.000000000	0.706620000	-24.010240000
6	0.000000000	-0.704153000	-23.958308000	6	0.000000000	-0.706620000	-24.010240000
1	0.000000000	2.481728000	-22.770529000	1	0.000000000	2.481920000	-22.821398000
1	0.000000000	-2.481728000	-22.770529000	1	0.000000000	-2.481920000	-22.821398000
1	0.000000000	1.241455000	-24.901560000	1	0.000000000	1.243437000	-24.951211000
1	0.000000000	-1.241455000	-24.901560000	1	0.000000000	-1.243437000	-24.951211000

Table S171: Coordinates of pT₆_6 at M06/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	4.731601000	0.730191000
7	0.000000000	3.574084000	1.428822000
6	0.000000000	2.449552000	0.733365000
6	0.000000000	2.449552000	-0.733365000
7	0.000000000	3.574084000	-1.428822000
6	0.000000000	4.731601000	-0.730191000

Table S172: Coordinates of pT₆_6 at M062X/6-311++g(d,p) level

atom	x	y	z
6	0.000000000	4.754680000	0.733284000
7	0.000000000	3.579114000	1.434386000
6	0.000000000	2.466653000	0.739148000
6	0.000000000	2.466653000	-0.739148000
7	0.000000000	3.579114000	-1.434386000
6	0.000000000	4.754680000	-0.733284000

6	0.000000000	0.000000000	-0.732020000	6	0.000000000	0.000000000	-0.737338000
6	0.000000000	0.000000000	0.732020000	6	0.000000000	0.000000000	0.737338000
6	0.000000000	-1.216661000	1.407270000	6	0.000000000	-1.218050000	1.411003000
1	0.000000000	-1.240162000	2.493773000	1	0.000000000	-1.242241000	2.495447000
6	0.000000000	-2.449552000	0.733365000	6	0.000000000	-2.466653000	0.739148000
6	0.000000000	-2.449552000	-0.733365000	6	0.000000000	-2.466653000	-0.739148000
6	0.000000000	-1.216661000	-1.407270000	6	0.000000000	-1.218050000	-1.411003000
1	0.000000000	-1.240162000	-2.493773000	1	0.000000000	-1.242241000	-2.495447000
6	0.000000000	-4.731601000	-0.730191000	6	0.000000000	-4.754680000	-0.733284000
6	0.000000000	-4.731601000	0.730191000	6	0.000000000	-4.754680000	0.733284000
6	0.000000000	-5.932799000	1.408566000	6	0.000000000	-5.944705000	1.413814000
6	0.000000000	-5.932799000	-1.408566000	6	0.000000000	-5.944705000	-1.413814000
6	0.000000000	-7.173453000	-0.730824000	6	0.000000000	-7.203724000	-0.733697000
6	0.000000000	-7.173453000	0.730824000	6	0.000000000	-7.203724000	0.733697000
1	0.000000000	-5.907485000	2.494835000	1	0.000000000	-5.918603000	2.497708000
1	0.000000000	-5.907485000	-2.494835000	1	0.000000000	-5.918603000	-2.497708000
6	0.000000000	7.173453000	0.730824000	6	0.000000000	7.203724000	0.733697000
6	0.000000000	7.173453000	-0.730824000	6	0.000000000	7.203724000	-0.733697000
6	0.000000000	8.371866000	-1.411994000	6	0.000000000	8.395219000	-1.417466000
6	0.000000000	8.371866000	1.411994000	6	0.000000000	8.395219000	1.417466000
6	0.000000000	9.612485000	-0.730864000	6	0.000000000	9.648325000	-0.732936000
6	0.000000000	9.612485000	0.730864000	6	0.000000000	9.648325000	0.732936000
1	0.000000000	8.395382000	2.498153000	1	0.000000000	8.420050000	2.501246000
1	0.000000000	8.395382000	-2.498153000	1	0.000000000	8.420050000	-2.501246000
6	0.000000000	-9.612485000	0.730864000	6	0.000000000	-9.648325000	0.732936000
6	0.000000000	-9.612485000	-0.730864000	6	0.000000000	-9.648325000	-0.732936000
7	0.000000000	-10.735203000	-1.424725000	7	0.000000000	-10.766081000	-1.427247000
7	0.000000000	-10.735203000	1.424725000	7	0.000000000	-10.766081000	1.427247000
6	0.000000000	-11.893599000	-0.727454000	6	0.000000000	-11.931616000	-0.727881000
6	0.000000000	-11.893599000	0.727454000	6	0.000000000	-11.931616000	0.727881000
6	0.000000000	-8.371866000	1.411994000	6	0.000000000	-8.395219000	1.417466000
6	0.000000000	-8.371866000	-1.411994000	6	0.000000000	-8.395219000	-1.417466000
7	0.000000000	-3.574084000	1.428822000	7	0.000000000	-3.579114000	1.434386000
7	0.000000000	-3.574084000	-1.428822000	7	0.000000000	-3.579114000	-1.434386000
6	0.000000000	1.216661000	1.407270000	6	0.000000000	1.218050000	1.411003000
6	0.000000000	1.216661000	-1.407270000	6	0.000000000	1.218050000	-1.411003000
6	0.000000000	5.932799000	1.408566000	6	0.000000000	5.944705000	1.413814000
6	0.000000000	5.932799000	-1.408566000	6	0.000000000	5.944705000	-1.413814000
7	0.000000000	10.735203000	1.424725000	7	0.000000000	10.766081000	1.427247000
7	0.000000000	10.735203000	-1.424725000	7	0.000000000	10.766081000	-1.427247000
6	0.000000000	11.893599000	0.727454000	6	0.000000000	11.931616000	0.727881000
6	0.000000000	11.893599000	-0.727454000	6	0.000000000	11.931616000	-0.727881000
6	0.000000000	13.098805000	1.411173000	6	0.000000000	13.136147000	1.414644000
6	0.000000000	13.098805000	-1.411173000	6	0.000000000	13.136147000	-1.414644000
6	0.000000000	14.326958000	0.728833000	6	0.000000000	14.367351000	0.729607000
6	0.000000000	14.326958000	-0.728833000	6	0.000000000	14.367351000	-0.729607000
6	0.000000000	-13.098805000	1.411173000	6	0.000000000	-13.136147000	1.414644000
6	0.000000000	-13.098805000	-1.411173000	6	0.000000000	-13.136147000	-1.414644000

6	0.000000000	-14.326958000	0.728833000	6	0.000000000	-14.367351000	0.729607000
6	0.000000000	-14.326958000	-0.728833000	6	0.000000000	-14.367351000	-0.729607000
6	0.000000000	-15.541248000	1.411369000	6	0.000000000	-15.586159000	1.414337000
6	0.000000000	-15.541248000	-1.411369000	6	0.000000000	-15.586159000	-1.414337000
6	0.000000000	-16.759255000	0.726298000	6	0.000000000	-16.802580000	0.726784000
6	0.000000000	-16.759255000	-0.726298000	6	0.000000000	-16.802580000	-0.726784000
1	0.000000000	-15.566298000	2.497337000	1	0.000000000	-15.612212000	2.497905000
1	0.000000000	-15.566298000	-2.497337000	1	0.000000000	-15.612212000	-2.497905000
1	0.000000000	-13.073807000	-2.497160000	1	0.000000000	-13.110412000	-2.498211000
1	0.000000000	-13.073807000	2.497160000	1	0.000000000	-13.110412000	2.498211000
1	0.000000000	-8.395382000	-2.498153000	1	0.000000000	-8.420050000	-2.501246000
1	0.000000000	-8.395382000	2.498153000	1	0.000000000	-8.420050000	2.501246000
1	0.000000000	1.240162000	2.493773000	1	0.000000000	1.242241000	2.495447000
1	0.000000000	1.240162000	-2.493773000	1	0.000000000	1.242241000	-2.495447000
1	0.000000000	5.907485000	-2.494835000	1	0.000000000	5.918603000	-2.497708000
1	0.000000000	5.907485000	2.494835000	1	0.000000000	5.918603000	2.497708000
1	0.000000000	13.073807000	-2.497160000	1	0.000000000	13.110412000	-2.498211000
1	0.000000000	13.073807000	2.497160000	1	0.000000000	13.110412000	2.498211000
6	0.000000000	15.541248000	1.411369000	6	0.000000000	15.586159000	1.414337000
6	0.000000000	15.541248000	-1.411369000	6	0.000000000	15.586159000	-1.414337000
6	0.000000000	16.759255000	0.726298000	6	0.000000000	16.802580000	0.726784000
6	0.000000000	16.759255000	-0.726298000	6	0.000000000	16.802580000	-0.726784000
1	0.000000000	15.566298000	2.497337000	1	0.000000000	15.612212000	2.497905000
1	0.000000000	15.566298000	-2.497337000	1	0.000000000	15.612212000	-2.497905000
7	0.000000000	-17.906788000	-1.421986000	7	0.000000000	-17.955691000	-1.425279000
7	0.000000000	-17.906788000	1.421986000	7	0.000000000	-17.955691000	1.425279000
6	0.000000000	-19.039074000	-0.727442000	6	0.000000000	-19.082609000	-0.729722000
6	0.000000000	-19.039074000	0.727442000	6	0.000000000	-19.082609000	0.729722000
6	0.000000000	-20.274784000	-1.410574000	6	0.000000000	-20.326759000	-1.415863000
6	0.000000000	-20.274784000	1.410574000	6	0.000000000	-20.326759000	1.415863000
6	0.000000000	-21.468926000	-0.725567000	6	0.000000000	-21.515986000	-0.728729000
6	0.000000000	-21.468926000	0.725567000	6	0.000000000	-21.515986000	0.728729000
1	0.000000000	-20.251140000	-2.496849000	1	0.000000000	-20.302273000	-2.499639000
1	0.000000000	-20.251140000	2.496849000	1	0.000000000	-20.302273000	2.499639000
7	0.000000000	17.906788000	-1.421986000	7	0.000000000	17.955691000	-1.425279000
7	0.000000000	17.906788000	1.421986000	7	0.000000000	17.955691000	1.425279000
6	0.000000000	19.039074000	-0.727442000	6	0.000000000	19.082609000	-0.729722000
6	0.000000000	19.039074000	0.727442000	6	0.000000000	19.082609000	0.729722000
6	0.000000000	20.274784000	-1.410574000	6	0.000000000	20.326759000	-1.415863000
6	0.000000000	20.274784000	1.410574000	6	0.000000000	20.326759000	1.415863000
6	0.000000000	21.468926000	-0.725567000	6	0.000000000	21.515986000	-0.728729000
6	0.000000000	21.468926000	0.725567000	6	0.000000000	21.515986000	0.728729000
6	0.000000000	22.729333000	-1.405999000	6	0.000000000	22.786505000	-1.412304000
6	0.000000000	22.729333000	1.405999000	6	0.000000000	22.786505000	1.412304000
6	0.000000000	23.894524000	-0.715201000	6	0.000000000	23.948803000	-0.720571000
6	0.000000000	23.894524000	0.715201000	6	0.000000000	23.948803000	0.720571000
1	0.000000000	20.251140000	2.496849000	1	0.000000000	20.302273000	2.499639000
1	0.000000000	20.251140000	-2.496849000	1	0.000000000	20.302273000	-2.499639000

1	0.000000000	22.724054000	-2.492509000	1	0.000000000	22.782319000	-2.496455000
1	0.000000000	22.724054000	2.492509000	1	0.000000000	22.782319000	2.496455000
1	0.000000000	24.842615000	1.243909000	1	0.000000000	24.895904000	1.246546000
1	0.000000000	24.842615000	-1.243909000	1	0.000000000	24.895904000	-1.246546000
6	0.000000000	-22.729333000	1.405999000	6	0.000000000	-22.786505000	1.412304000
6	0.000000000	-22.729333000	-1.405999000	6	0.000000000	-22.786505000	-1.412304000
6	0.000000000	-23.894524000	0.715201000	6	0.000000000	-23.948803000	0.720571000
6	0.000000000	-23.894524000	-0.715201000	6	0.000000000	-23.948803000	-0.720571000
1	0.000000000	-22.724054000	2.492509000	1	0.000000000	-22.782319000	2.496455000
1	0.000000000	-22.724054000	-2.492509000	1	0.000000000	-22.782319000	-2.496455000
1	0.000000000	-24.842615000	1.243909000	1	0.000000000	-24.895904000	1.246546000
1	0.000000000	-24.842615000	-1.243909000	1	0.000000000	-24.895904000	-1.246546000