Supporting Information

Self-Assembling Purine and Pteridine Quartets: How Do π-Conjugation Patterns Affect Resonance-Assisted Hydrogen Bonding?

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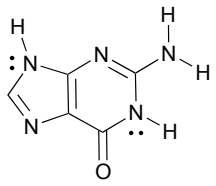
University of Houston, Houston, TX, 77004, USA

Structures of monomers used to form quartets



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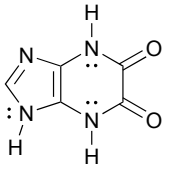

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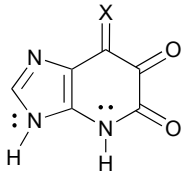
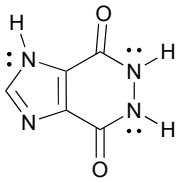


m 3 (X=S), m 4 (X=NH) and m 5 (X=O)



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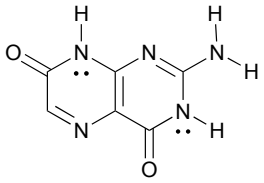

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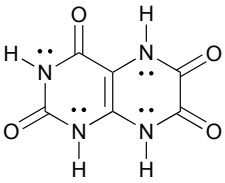

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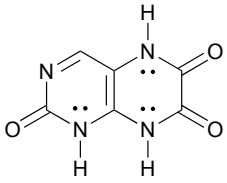

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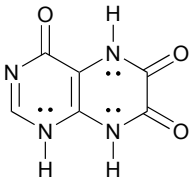

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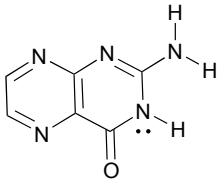

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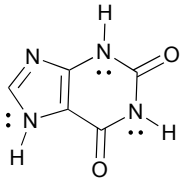

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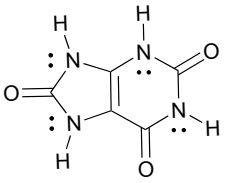

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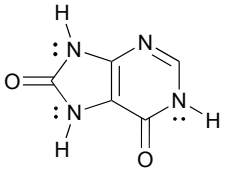

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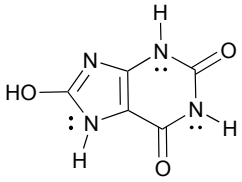

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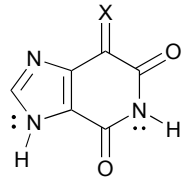
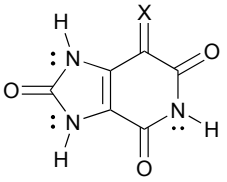


m 16 (X=O), m 17 (X=NH) and m 18 (X=S)



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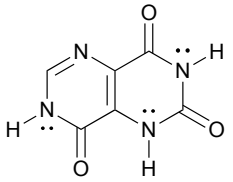

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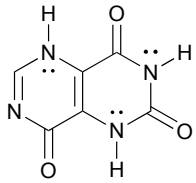

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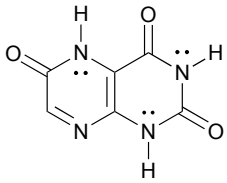

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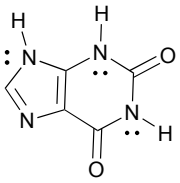

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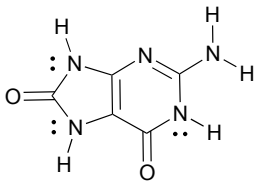

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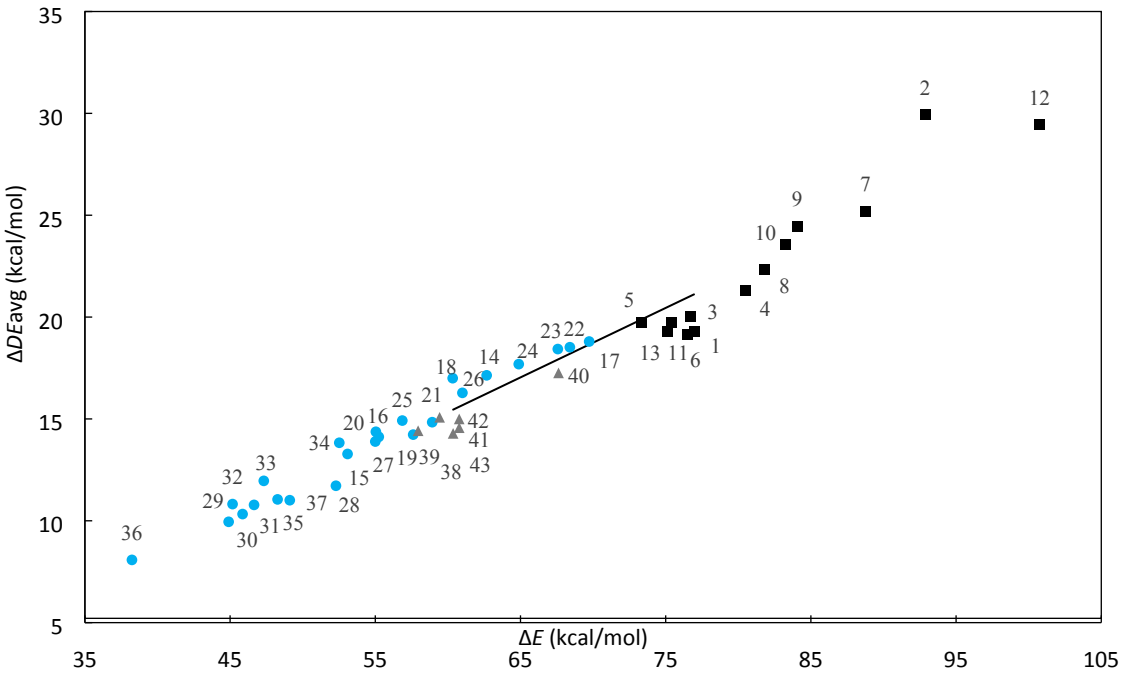


Figure S1. Plot of ΔE vs. ΔDE_{avg} for all 43 quartets. $[AA\text{-}DD]_4$ quartets are in black squares, quartets with mixed SEI patterns are in olive triangles, and $[AD\text{-}DA]_4$ quartets are in blue circles.

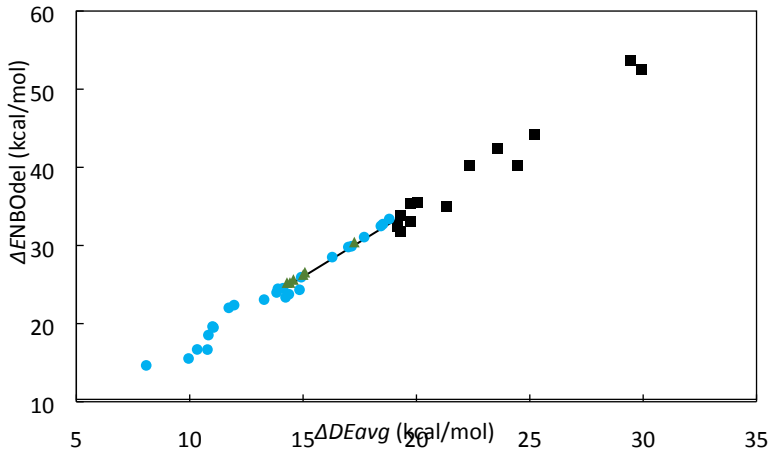


Figure S2. Correlation of ΔDE_{avg} and $\Delta E_{\mathrm{NBOdelavg}}$ for all 43 quartets. $[AA\text{-}DD]_4$ quartets are in black squares, mixed quartets are in olive triangles, and $[AD\text{-}DA]_4$ quartets are in blue circles.

Table S1.Computed gas-phase interaction energies (ΔE) including zero-point energy correction at ωB97XD/6-311+G (d,p) level, ΔDE_{avg} values at B3LYP/6-31G(d) level, and NBO deletion energy ($\Delta E_{\text{NBOdelavg}}$) at ωB97XD/Def2TZVPP level for $[AA\text{-}DD]_4$ type quartets. All monomers were optimized with C_s symmetry.

Quartets	ΔE (kcal/mol)	ΔDE_{avg} (kcal/mol)	$\Delta E_{\text{NBOdelavg}}$ (kcal/mol)	Name	Symm.	Monomers
1	76.95	19.28	33.79	G-quartet	C_{4h}	m1
2	92.87	29.94	52.50	-	C_{4h}	m2
3	76.74	20.04	35.51	G'_4	C_{4h}	m1
4	80.50	21.32	34.93	-	C_{4h}	m3
5	73.30	19.72	33.10	-	C_{4h}	m4
6	76.48	19.16	32.38	-	C_{4h}	m5
7	88.76	25.20	44.26	$G_2 2_2$	C_{2h}	m1, m2
8	81.83	22.34	40.19	-	C_{2h}	m1, m6
9	84.06	24.45	40.22	P_4	C_{4h}	m7
10	83.25	23.56	42.37	$[2467P]_4$	C_{4h}	m8
11	75.38	19.74	35.34	$[267P]_4$	C_{4h}	m9
12	100.74	29.44	53.72	$[467P]_4$	C_{4h}	m10
13	75.14	19.30	31.76	$[PT]_4$	C_{4h}	m11

single prime (') superscript over the quartet's name indicates quartet with different connectivity of that monomer.

Table S2. Computed gas-phase interaction energies (ΔE) including zero-point energy correction at ωB97XD/6-311+G (d,p) level, ΔDE_{avg} values at B3LYP/6-31G(d) level, and NBO deletion energy ($\Delta E_{\text{NBOdelavg}}$) at ωB97XD/Def2TZVPP level for $[AD\text{-}DA]_4$ type quartets. All monomers were optimized with C_s symmetry.

Quartets	ΔE (kcal/mol)	ΔDE_{avg} (kcal/mol)	$\Delta E_{\text{NBOdelavg}}$ (kcal/mol)	Name	Symm.	Monomers
14	62.67	17.14	29.91	X-quartet	C_{4h}	m12
15	53.09	13.28	23.07	U_4	C_{4h}	m13
16	55.00	13.89	24.46	U'_4	C_{4h}	m13
17	69.73	18.80	33.39	$[8H]_4$	C_{4h}	m14
18	60.33	17.00	29.80	U_{t4}	C_{4h}	m15
19	57.61	14.23	23.36	-	C_{4h}	m16
20	55.04	14.37	23.76	-	C_{4h}	m17
21	58.92	14.84	24.33	-	C_{4h}	m18
22	68.40	18.52	32.73	$[8H]_3X$	C_s	m14, m12
23	67.57	18.43	32.49	$[8H]_2X_2$	C_{2h}	m14, m12
24	64.88	17.69	31.07	$[8H]X_3$	C_s	m14, m12

25	56.86	14.92	25.94	U_2X_2	C_{2h}	m13, m12
26	61.00	16.28	28.51	U'_2X_2	C_{2h}	m13, m12
27	55.24	14.12	24.53	U_4	C_{2h}	m13
28	52.29	11.72	22.02	-	C_{4h}	m19
29	44.90	9.95	15.54	-	C_{4h}	m19
30	45.86	10.33	16.69	-	C_{4h}	m20
31	46.65	10.78	16.68	-	C_{4h}	m21
32	45.17	10.82	18.53	-	C_{4h}	m22
33	47.32	11.96	22.37	-	C_{4h}	m22
34	52.52	13.83	23.98	-	C_{4h}	m23
35	48.27	11.05	19.51	$[2467P']_4$	C_{4h}	m8
36	38.24	8.08	14.65	$[246P]_4$	C_{4h}	m24
37	49.11	11.01	19.63	$[246P']_4$	C_{4h}	m24

single prime (') superscript over the quartet's name indicates quartet with different connectivity of that monomer

Table S3. Computed gas-phase interaction energies (ΔE) including zero-point energy correction at ωB97XD/6-311+G (d,p) level, ΔDE_{avg} values at B3LYP/6-31G(d) level, and NBO deletion energy ($\Delta E_{\text{NBOdelavg}}$) at ωB97XD/Def2TZVPP level for mixed type quartets. All monomers were optimized with C_s symmetry.

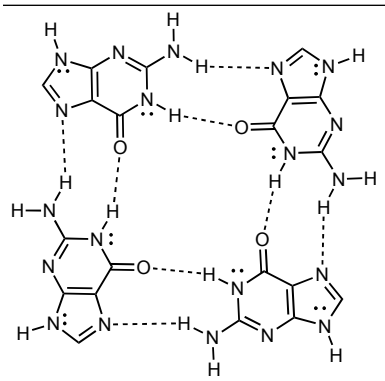
Quartets	**ΔE (kcal/mol)**	**ΔDE_{avg} (kcal/mol)**	**$\Delta E_{\text{NBOdelavg}}$ (kcal/mol)**	**Name**	**Symm.**	**Monomers**
38	59.43	15.08	26.58	X•O•X•O	C_{2h}	m25, m26
39	57.95	14.42	25.26	X•X•O•X	C_s	m12, m25, m26
40	67.62	17.26	30.44	G•G•X•O	C_s	m1, m25, m26
41	60.78	14.57	25.65	G•O•X•X	C_s	m1, m26, m12, m25
42	60.78	15.00	26.28	G•O•U'•X	C_s	m1, m26, m13, m25
43	60.36	14.29	25.25	G•O•U•X	C_s	m1, m26, m13, m25

single prime (') superscript over the quartet's name indicates quartet with different connectivity of that monomer

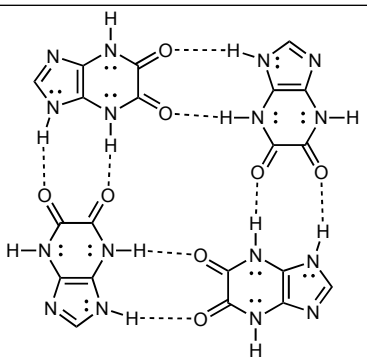
Table S4. Computed planarization energies (C_1 minima vs. planar C_s) for monomers at the ωB97XD/6-311+G (d,p) level (without zero-point energy correction).

Monomers	**Δ*E* (kcal/mol)**
m1	–0.42
m6	–0.81
m7	–0.07
m11	–0.26
m26	–0.34

Structures of $[AA\text{-}DD]_4$ quartets considered



1 G-quartet



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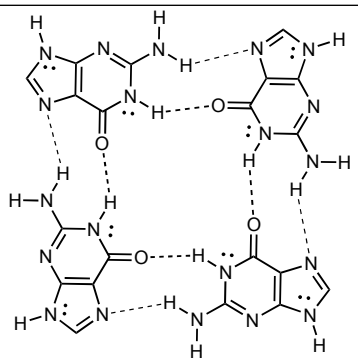
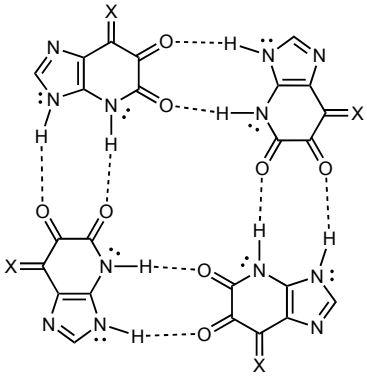


3 G'_4



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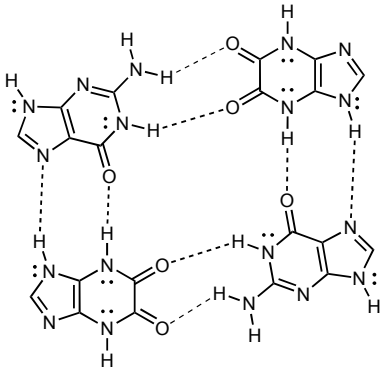
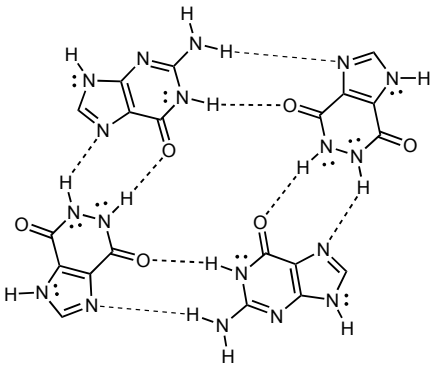


7 $G_2\,2_2$



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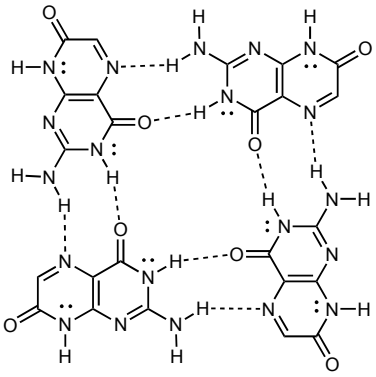
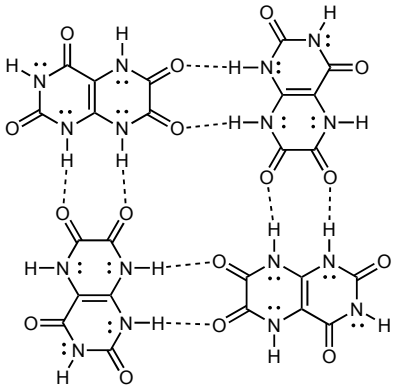


9 P_4



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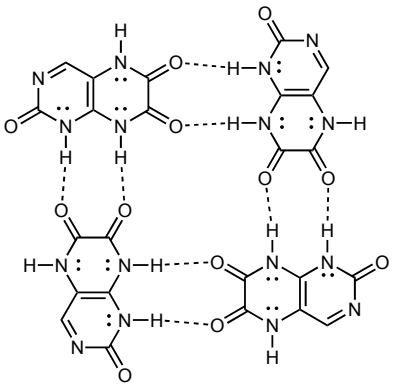

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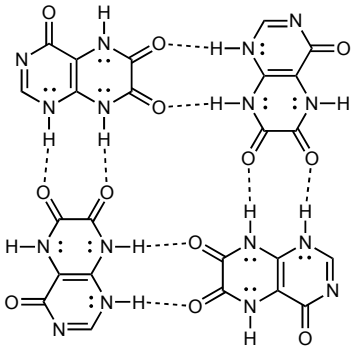

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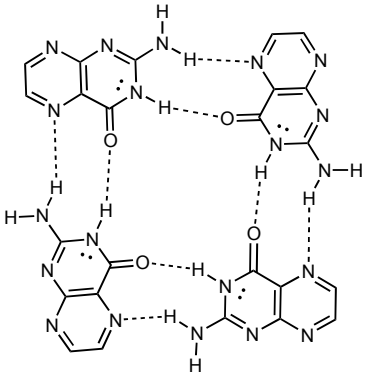
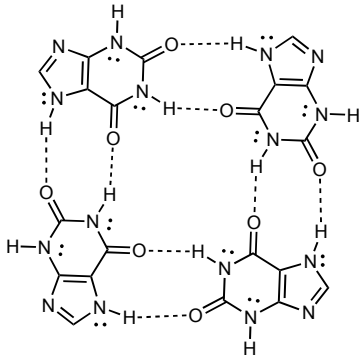
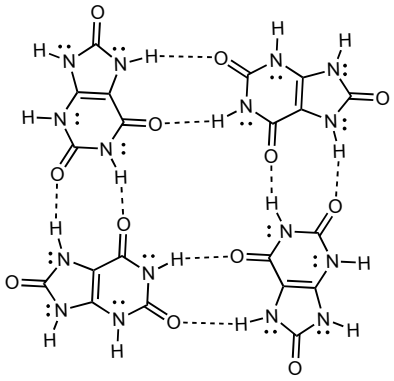


13 $[PT]_4$

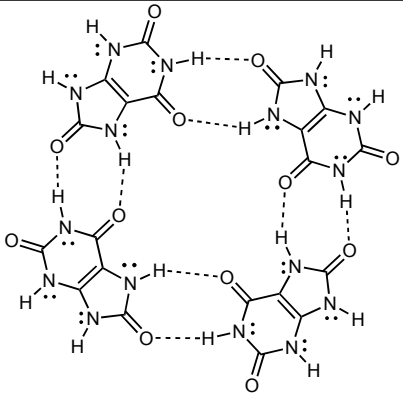
Structures of $[AD\text{-}DA]_4$ quartets considered



14 X-quartet



15 U_4



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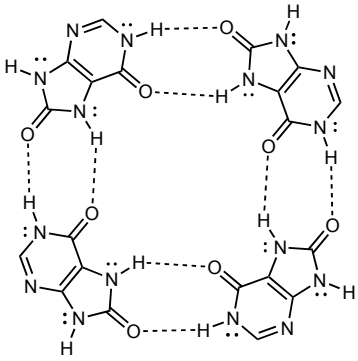
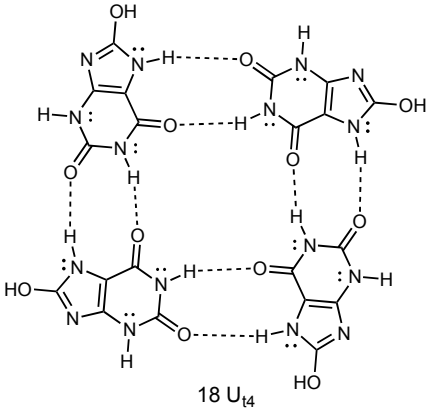


17 $[8H]_4$



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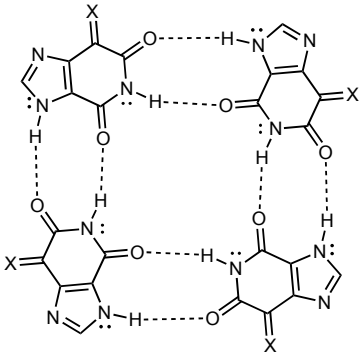
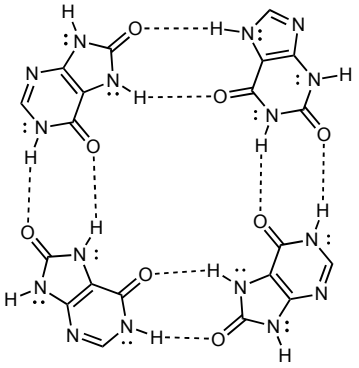
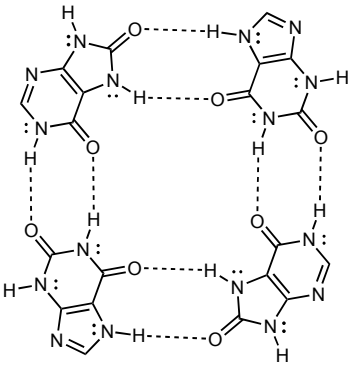


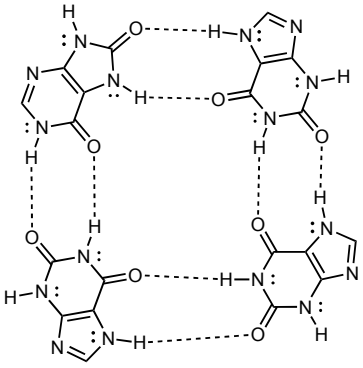
19 (X=O), 20 (X=NH), 21 (X=S)



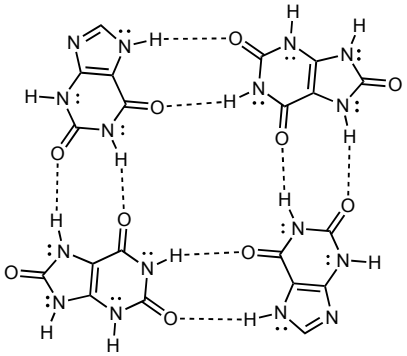
22 $[8H]_3X$



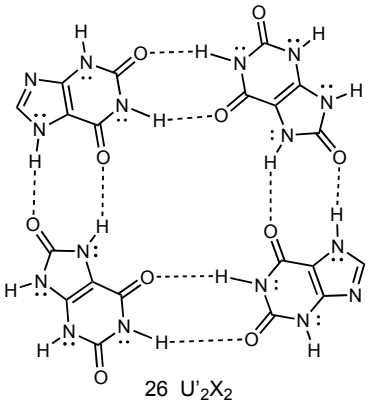
23 $[8H]_2X_2$



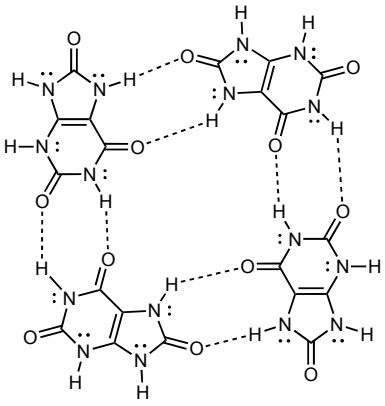
24 $[8H]X_3$



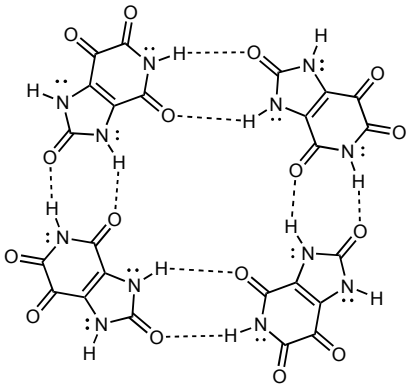
25 U_2X_2



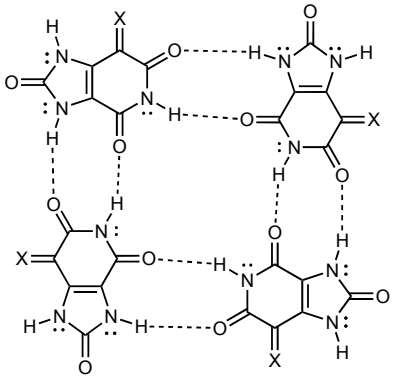
26 U'_2X_2



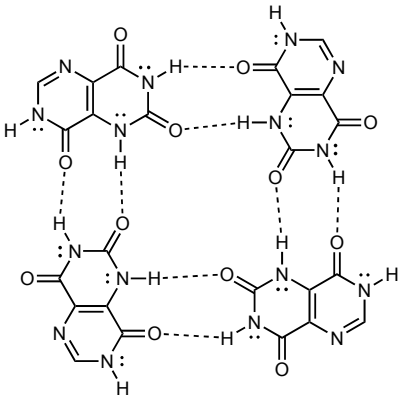
27 $U_4(c_{2h})$



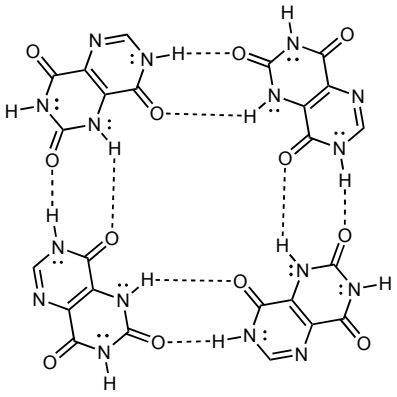
28



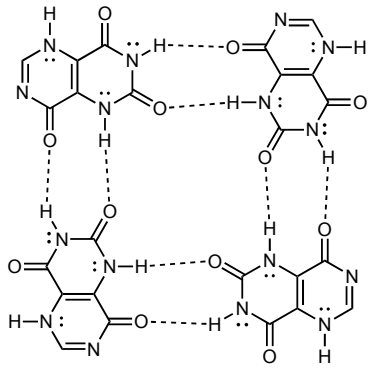
29 (X=O), 30 (X=NH), 31 (X=S)



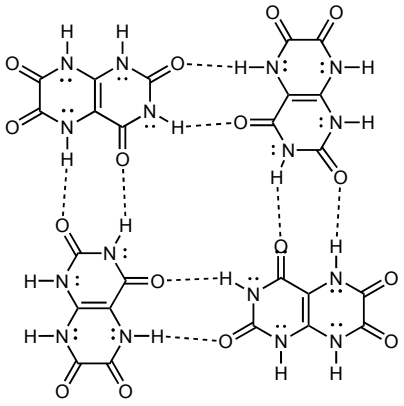
32



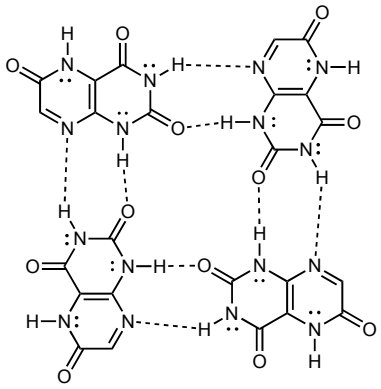
33



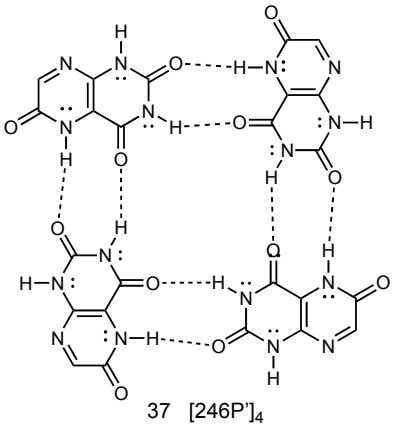
34



35 $[2467P']_4$

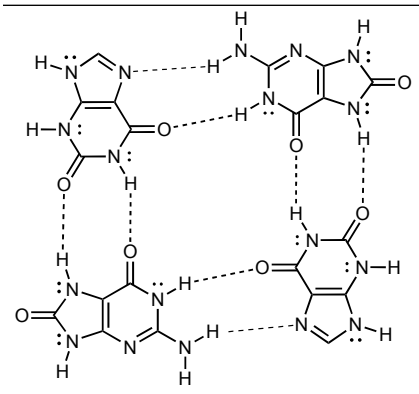


36 $[246P]_4$

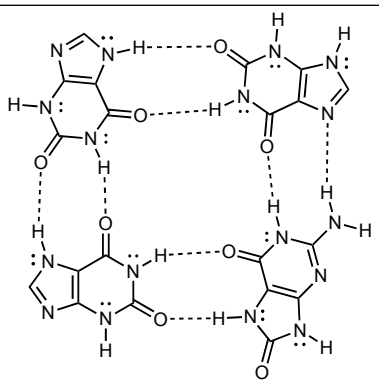


37 $[246P']_4$

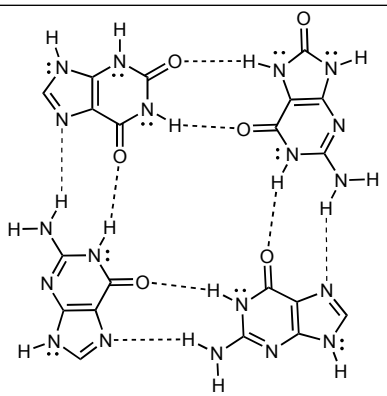
Structures of mixed quartets considered



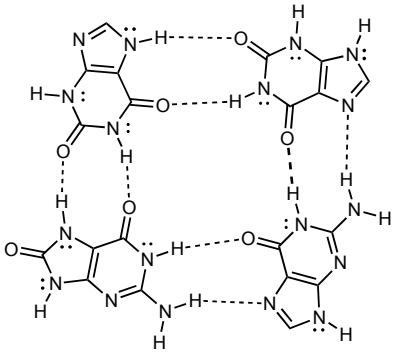
38 X•O•X•O



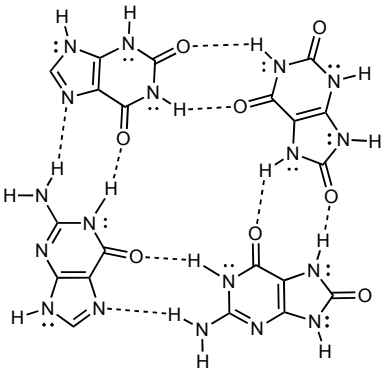
39 X•O•X•X



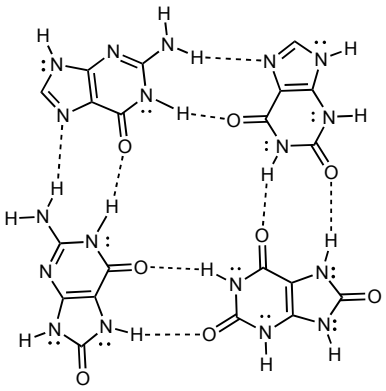
40 G•G•X•O



41 G•O•X•X



42 G•O•U'•X



43 G•O•U•X

Cartesian coordinates and sum of electronic and zero-point energies of monomers

Monomer m1
Sum of electronic and zero-point energy: -542.410714 a.u.
C_s, N_{im} = 1 (327*i* cm^{-1})

C	1.36678	0.00355	0.00000
C	-0.01794	0.01271	0.00000
C	-0.71456	-1.24345	0.00000
N	0.23118	-2.31493	0.00000
N	2.21763	-1.05083	0.00000
C	1.59365	-2.19656	0.00000
O	-1.89529	-1.49958	0.00000
H	-0.19949	-3.22852	0.00000
N	2.31481	-3.34737	0.00000
N	1.72865	1.31762	0.00000
H	2.67281	1.66566	0.00000
C	0.56026	2.05013	0.00000
N	-0.50164	1.30251	0.00000
H	3.31570	-3.26869	0.00000
H	1.89084	-4.25562	0.00000
H	0.56935	3.12992	0.00000

Monomer m2
Sum of electronic and zero-point energy: -562.267550 a.u.
C_s, N_{im} = 0

C	-2.96370	-1.34219	0.00000
N	-3.36093	-0.01670	0.00000
C	-4.70132	0.31524	0.00000
C	-5.69046	-0.61204	0.00000
N	-5.38371	-1.96480	0.00000
C	-4.08973	-2.42109	0.00000
N	-5.33290	1.53014	0.00000
C	-6.67766	1.25597	0.00000
N	-6.91991	-0.03167	0.00000
O	-1.80502	-1.66198	0.00000
H	-7.41951	2.03831	0.00000
O	-3.79738	-3.58896	0.00000
H	-6.12154	-2.65449	0.00000
H	-2.62179	0.67031	0.00000
H	-4.91005	2.44249	0.00000

Monomer m3
Sum of electronic and zero-point energy: -943.180306 a.u.
C_s, N_{im} = 0

C	1.48583	1.17494	0.00000
N	1.34768	-0.20176	0.00000
C	0.10188	-0.77822	0.00000
C	-1.11201	-0.12275	0.00000
C	-1.20666	1.30854	0.00000
C	0.15508	2.01354	0.00000
N	-0.17195	-2.10513	0.00000
C	-1.55622	-2.20914	0.00000
N	-2.13378	-1.05414	0.00000
O	2.55959	1.70650	0.00000

H	-2.04584	-3.17114	0.00000
O	0.27955	3.19963	0.00000
S	-2.57928	2.18242	0.00000
H	2.19806	-0.74588	0.00000
H	0.48763	-2.86570	0.00000

Monomer m4

Sum of electronic and zero-point energy: -600.325043 a.u.

C_s, $N_{im} = 0$

C	1.36398	1.19531	0.00000
N	1.21603	-0.17468	0.00000
C	-0.03689	-0.76173	0.00000
C	-1.24983	-0.12464	0.00000
C	-1.33123	1.32357	0.00000
C	0.03491	2.02305	0.00000
N	-0.29889	-2.09577	0.00000
C	-1.67726	-2.21102	0.00000
N	-2.26515	-1.05645	0.00000
O	2.43687	1.73329	0.00000
H	-2.16145	-3.17558	0.00000
O	0.12155	3.21603	0.00000
N	-2.40738	1.99555	0.00000
H	2.06479	-0.72079	0.00000
H	0.36637	-2.85081	0.00000
H	-2.18063	2.99351	0.00000

Monomer m5

Sum of electronic and zero-point energy: -620.211878 a.u.

C_s, $N_{im} = 0$

C	2.25530	0.88099	0.00000
N	1.01796	1.50208	0.00000
C	-0.14690	0.76757	0.00000
C	-0.27987	-0.60342	0.00000
C	0.87698	-1.47552	0.00000
C	2.23258	-0.68965	0.00000
N	-1.40506	1.27196	0.00000
C	-2.25995	0.17871	0.00000
N	-1.61845	-0.94271	0.00000
O	3.28191	1.49855	0.00000
H	-3.33193	0.30542	0.00000
O	3.27732	-1.26030	0.00000
O	0.89377	-2.67652	0.00000
H	1.01620	2.51158	0.00000
H	-1.67367	2.24230	0.00000

Monomer m6

Sum of electronic and zero-point energy: -562.246822 a.u.

C_s, $N_{im} = 1$ ($334i$ cm^{-1})

N	2.18934	-0.74167	0.00000
C	1.03353	-1.50153	0.00000
C	-0.16164	-0.64969	0.00000
C	-0.05381	0.71889	0.00000
C	1.18076	1.48388	0.00000
N	2.26126	0.64927	0.00000
O	1.08523	-2.71028	0.00000
N	-1.47173	-1.03118	0.00000
C	-2.14182	0.09430	0.00000
N	-1.33024	1.18982	0.00000
H	3.07097	-1.22851	0.00000
H	-3.21814	0.17944	0.00000

H	3.18507	1.05104	0.00000
O	1.27486	2.69898	0.00000
H	-1.59475	2.16264	0.00000

Monomer m7

Sum of electronic and zero-point energy: -655.734974 a.u.

C_s, N_{im} = 1 (201*i* cm^{-1})

N	-0.01217	0.00476	0.00000
C	0.04690	-1.38657	0.00000
O	1.10364	-1.97943	0.00000
C	-1.28724	-2.00959	0.00000
N	-2.39457	-1.35581	0.00000
C	-2.36313	0.01183	0.00000
C	-1.17005	0.72137	0.00000
N	-1.03686	2.06861	0.00000
C	-2.15426	2.74829	0.00000
N	-2.09826	4.09737	0.00000
N	-3.37910	2.16223	0.00000
C	-3.60627	0.75831	0.00000
O	-4.74050	0.34932	0.00000
H	-4.22400	2.71620	0.00000
H	0.86346	0.51217	0.00000
H	-1.31052	-3.09518	0.00000
H	-2.91717	4.67671	0.00000
H	-1.18929	4.52566	0.00000

Monomer m8

Sum of electronic and zero-point energy: -750.864475 a.u.

C_s, N_{im} = 0

H	-0.71562	2.68458	0.00000
C	0.94792	-1.50694	0.00000
N	2.22004	-0.93155	0.00000
C	2.54334	0.41134	0.00000
N	1.43477	1.24753	0.00000
C	0.13967	0.78388	0.00000
C	-0.12712	-0.53862	0.00000
N	-1.44373	-0.98825	0.00000
C	-2.54561	-0.18068	0.00000
C	-2.24222	1.33242	0.00000
N	-0.89271	1.68900	0.00000
O	-3.10475	2.16233	0.00000
O	3.67179	0.83375	0.00000
H	3.00356	-1.57037	0.00000
H	1.64391	2.23377	0.00000
O	-3.68031	-0.57862	0.00000
H	-1.58916	-1.99097	0.00000
O	0.78543	-2.70759	0.00000

Monomer m9

Sum of electronic and zero-point energy: -675.596542 a.u.

C_s, N_{im} = 0

H	2.00284	-1.02648	0.00000
C	-2.28621	0.12831	0.00000
N	-2.74135	-1.08971	0.00000
C	-1.85594	-2.14864	0.00000
N	-0.47646	-1.80509	0.00000
C	-0.01761	-0.53327	0.00000
C	-0.92103	0.49053	0.00000

N	-0.45252	1.80963	0.00000
C	0.86477	2.17744	0.00000
C	1.87342	1.01084	0.00000
N	1.32755	-0.27312	0.00000
O	3.05663	1.18664	0.00000
H	0.15647	-2.59259	0.00000
O	1.24426	3.31865	0.00000
H	-1.11718	2.57081	0.00000
H	-3.03257	0.92372	0.00000
O	-2.15827	-3.31541	0.00000

Monomer m10

Sum of electronic and zero-point energy: -675.595676 a.u.

C_s, $N_{im} = 0$

H	0.98680	-2.59947	0.00000
C	-1.23085	1.35650	0.00000
N	-2.45312	0.67084	0.00000
C	-2.45994	-0.61043	0.00000
N	-1.35017	-1.40945	0.00000
C	-0.11007	-0.81836	0.00000
C	-0.02808	0.52865	0.00000
N	1.21451	1.14061	0.00000
C	2.41532	0.48452	0.00000
C	2.31786	-1.05734	0.00000
N	1.03080	-1.58956	0.00000
O	3.28639	-1.76251	0.00000
H	-1.45167	-2.41153	0.00000
O	3.48681	1.02886	0.00000
H	1.21624	2.15506	0.00000
O	-1.15437	2.56727	0.00000
H	-3.40462	-1.14760	0.00000

Monomer m11

Sum of electronic and zero-point energy: -580.487953 a.u.

C_s, $N_{im} = 1$ ($289i$ cm^{-1})

N	0.49095	-1.84606	0.00000
C	1.36759	-0.75289	0.00000
C	0.64406	0.53387	0.00000
C	-0.76773	0.53036	0.00000
N	-1.51812	-0.61468	0.00000
C	-0.87852	-1.73999	0.00000
N	-1.57432	-2.90222	0.00000
O	2.55964	-0.92535	0.00000
H	0.94420	-2.74898	0.00000
N	1.36242	1.65707	0.00000
C	0.68452	2.78734	0.00000
N	-1.44146	1.69447	0.00000
C	-0.71788	2.79543	0.00000
H	1.24958	3.71365	0.00000
H	-1.13728	-3.80464	0.00000
H	-2.57698	-2.83574	0.00000
H	-1.25945	3.73770	0.00000

Monomer m12

Sum of electronic and zero-point energy: -562.312899 a.u.

C_s, $N_{im} = 0$

N	-1.50020	-0.94048	0.00000
C	-1.46226	0.46137	0.00000
C	-0.10027	0.91770	0.00000
C	0.97585	0.06966	0.00000

N	0.80874	-1.29229	0.00000
C	-0.44992	-1.86038	0.00000
O	-0.63840	-3.05338	0.00000
O	-2.46885	1.13628	0.00000
N	0.44872	2.17993	0.00000
C	1.78867	2.01353	0.00000
N	2.15056	0.74290	0.00000
H	-2.41996	-1.35930	0.00000
H	1.59973	-1.91684	0.00000
H	-0.06483	3.04603	0.00000
H	2.47432	2.84707	0.00000

Monomer m13

Sum of electronic and zero-point energy: -637.549731 a.u.

C_s, $N_{im} = 0$

N	-0.65773	-1.94018	0.00000
C	0.69678	-1.53819	0.00000
C	0.80662	-0.11209	0.00000
C	-0.28791	0.68718	0.00000
N	-1.56465	0.20475	0.00000
C	-1.80468	-1.16796	0.00000
O	-2.92200	-1.62344	0.00000
O	1.59587	-2.34936	0.00000
N	1.92362	0.72342	0.00000
C	1.54133	2.04202	0.00000
N	0.12658	1.98711	0.00000
H	-0.81798	-2.93818	0.00000
H	-2.37906	0.79741	0.00000
H	2.88325	0.42364	0.00000
O	2.21259	3.04305	0.00000
H	-0.43518	2.82136	0.00000

Monomer m14

Sum of electronic and zero-point energy: -562.306633 a.u.

C_s, $N_{im} = 0$

C	0.38794	0.08600	0.00000
C	-0.98009	-0.00756	0.00000
N	-1.85986	1.02155	0.00000
C	-1.28394	2.18303	0.00000
C	1.04022	1.35092	0.00000
N	0.06074	2.37395	0.00000
N	-1.29509	-1.34171	0.00000
O	2.22815	1.60640	0.00000
H	0.43000	3.31483	0.00000
N	0.89573	-1.20072	0.00000
C	-0.13464	-2.12569	0.00000
O	-0.06514	-3.32981	0.00000
H	1.86809	-1.45719	0.00000
H	-2.22113	-1.73486	0.00000
H	-1.89233	3.08081	0.00000

Monomer m15

Sum of electronic and zero-point energy: -637.542351 a.u.

C_s, $N_{im} = 0$

N	-1.59088	1.38249	0.00000
C	-1.53878	-0.02415	0.00000
C	-0.17897	-0.46538	0.00000
C	0.88778	0.39043	0.00000
N	0.71292	1.74828	0.00000

C	-0.55267	2.30880	0.00000
O	-0.74241	3.50211	0.00000
O	-2.54443	-0.70232	0.00000
N	0.38824	-1.73518	0.00000
C	1.71769	-1.53735	0.00000
N	2.07600	-0.26896	0.00000
H	-2.51580	1.78942	0.00000
H	1.49825	2.37967	0.00000
H	-0.09737	-2.61692	0.00000
O	2.54626	-2.57256	0.00000
H	3.44560	-2.23047	0.00000

Monomer m16
Sum of electronic and zero-point energy: -620.252080 a.u.
C_s, $N_{im} = 0$

N	1.94363	0.61043	0.00000
C	1.47411	-0.69478	0.00000
C	0.01517	-0.76224	0.00000
C	-0.86275	0.29178	0.00000
C	-0.36716	1.67075	0.00000
C	1.19676	1.79335	0.00000
O	1.73435	2.86240	0.00000
O	2.20373	-1.65764	0.00000
N	-0.75201	-1.88331	0.00000
C	-2.04954	-1.46089	0.00000
N	-2.15305	-0.15581	0.00000
H	2.94986	0.72495	0.00000
O	-1.02647	2.66870	0.00000
H	-0.40624	-2.83094	0.00000
H	-2.87699	-2.15446	0.00000

Monomer m17
Sum of electronic and zero-point energy: -600.369302 a.u.
C_s, $N_{im} = 0$

N	1.92602	0.28733	0.00000
C	1.46468	-1.02948	0.00000
C	0.01402	-1.10615	0.00000
C	-0.86012	-0.04942	0.00000
C	-0.35665	1.32129	0.00000
C	1.17351	1.45377	0.00000
O	1.70239	2.53636	0.00000
O	2.21624	-1.97586	0.00000
N	-0.75815	-2.23024	0.00000
C	-2.04934	-1.80239	0.00000
N	-2.14930	-0.49441	0.00000
H	2.93123	0.40710	0.00000
N	-1.08889	2.35172	0.00000
H	-0.41736	-3.17885	0.00000
H	-2.88114	-2.49079	0.00000
H	-0.49167	3.18410	0.00000

Monomer m18
Sum of electronic and zero-point energy: -943.219557 a.u.
C_s, $N_{im} = 0$

N	1.95772	0.49318	0.00000

C	1.48341	-0.80874	0.00000
C	0.02909	-0.85381	0.00000
C	-0.81687	0.22896	0.00000
C	-0.30433	1.58556	0.00000
C	1.23028	1.69060	0.00000
O	1.81389	2.73840	0.00000
O	2.20825	-1.77674	0.00000
N	-0.76650	-1.95482	0.00000
C	-2.05155	-1.49622	0.00000
N	-2.11967	-0.19004	0.00000
H	2.96386	0.60350	0.00000
S	-1.20646	2.92740	0.00000
H	-0.44621	-2.91110	0.00000
H	-2.89808	-2.16641	0.00000

Monomer m19

Sum of electronic and zero-point energy: -695.500649 a.u.

C_s, $N_{im} = 0$

N	0.05490	-2.38462	0.00000
C	-0.72739	-1.23520	0.00000
C	0.06107	-0.00118	0.00000
C	1.41572	0.04961	0.00000
C	2.24596	-1.13590	0.00000
C	1.44719	-2.47494	0.00000
O	2.00876	-3.53109	0.00000
O	-1.93276	-1.26429	0.00000
N	-0.41124	1.27851	0.00000
C	0.65160	2.19152	0.00000
N	1.77990	1.37442	0.00000
H	-0.44635	-3.26455	0.00000
O	3.44821	-1.14326	0.00000
H	-1.38050	1.55358	0.00000
O	0.59433	3.39209	0.00000
H	2.72120	1.73188	0.00000

Monomer m20

Sum of electronic and zero-point energy: -675.619692 a.u.

C_s, $N_{im} = 0$

N	-1.91984	-1.15364	0.00000
C	-3.31368	-1.30569	0.00000
C	-4.02747	-0.03880	0.00000
C	-3.42302	1.17215	0.00000
C	-1.98757	1.33148	0.00000
C	-1.19304	0.02299	0.00000
O	0.01111	0.03382	0.00000
O	-3.83352	-2.39421	0.00000
N	-5.38597	0.16692	0.00000
C	-5.66797	1.53161	0.00000
N	-4.40387	2.12707	0.00000
H	-1.38354	-2.01224	0.00000
N	-1.42226	2.46514	0.00000
H	-6.09597	-0.54651	0.00000
O	-6.74380	2.07188	0.00000
H	-4.25770	3.12333	0.00000
H	-0.40620	2.34223	0.00000

Monomer m21

Sum of electronic and zero-point energy: -1018.470785 a.u.

C_s, $N_{im} = 0$

N	2.01990	0.51030	0.00000
C	1.53340	-0.78937	0.00000
C	0.07384	-0.84124	0.00000
C	-0.72657	0.25943	0.00000
C	-0.22977	1.59750	0.00000
C	1.29956	1.70812	0.00000
O	1.87377	2.75999	0.00000
O	2.24891	-1.76126	0.00000
N	-0.71866	-1.94838	0.00000
C	-2.07131	-1.57825	0.00000
N	-2.02663	-0.18814	0.00000
H	3.02712	0.61050	0.00000
S	-1.17220	2.92370	0.00000
H	-0.40257	-2.90514	0.00000
O	-3.03189	-2.30063	0.00000
H	-2.84739	0.39632	0.00000

Monomer m22

Sum of electronic and zero-point energy: -675.636690 a.u.

C_s, $N_{im} = 0$

O	-1.32852	-2.66055	0.00000
C	1.03600	1.53668	0.00000
N	2.18555	0.74223	0.00000
C	2.29687	-0.64202	0.00000
N	1.07586	-1.28369	0.00000
C	-0.12074	-0.61949	0.00000
C	-0.21850	0.74086	0.00000
N	-1.41415	1.41133	0.00000
C	-2.47615	0.69345	0.00000
N	-2.47477	-0.67787	0.00000
C	-1.32535	-1.44685	0.00000
H	-3.34856	-1.18659	0.00000
O	3.35472	-1.21889	0.00000
H	3.06516	1.24094	0.00000
H	1.06895	-2.29514	0.00000
H	-3.45410	1.16301	0.00000
O	1.10324	2.73697	0.00000

Monomer m23

Sum of electronic and zero-point energy: -675.631792 a.u.

C_s, $N_{im} = 0$

O	0.59774	-2.83208	0.00000
C	-0.08089	1.90330	0.00000
N	1.29884	1.99130	0.00000
C	2.23633	0.95043	0.00000
N	1.66300	-0.30124	0.00000
C	0.31209	-0.51483	0.00000
C	-0.55502	0.52032	0.00000
N	-1.90469	0.26533	0.00000
C	-2.33046	-1.01571	0.00000
N	-1.56722	-2.06003	0.00000
C	-0.18815	-1.90870	0.00000
O	3.42216	1.15527	0.00000
H	1.69597	2.92145	0.00000
H	2.26775	-1.11363	0.00000
H	-3.40872	-1.14877	0.00000
O	-0.81533	2.86702	0.00000
H	-2.54074	1.05105	0.00000

Monomer m24
Sum of electronic and zero-point energy: -675.626871 a.u.
C_s, $N_{im} = 0$

C	-2.10770	-1.25293	0.00000
N	-1.29122	-2.37136	0.00000
C	0.10396	-2.42348	0.00000
N	0.69943	-1.18394	0.00000
C	-0.00081	0.00647	0.00000
C	-1.35733	0.00160	0.00000
N	-2.03724	1.19086	0.00000
C	-1.40021	2.41192	0.00000
C	0.07718	2.27467	0.00000
N	0.72962	1.16343	0.00000
O	0.71328	-3.46349	0.00000
H	-1.75328	-3.27085	0.00000
H	1.70809	-1.15350	0.00000
O	-1.97905	3.47703	0.00000
O	-3.31702	-1.31333	0.00000
H	-3.05099	1.16227	0.00000
H	0.63635	3.20592	0.00000

Monomer m25
Sum of electronic and zero-point energy: -562.299005 a.u.
C_s, $N_{im} = 0$

C	-0.79339	0.10903	0.00000
C	0.57493	0.19342	0.00000
C	1.37123	-1.01969	0.00000
N	0.54072	-2.17020	0.00000
N	-1.50488	-1.05958	0.00000
C	-0.83683	-2.27953	0.00000
O	2.56941	-1.13598	0.00000
H	1.03061	-3.05426	0.00000
O	-1.42722	-3.33327	0.00000
N	-1.25617	1.38532	0.00000
H	-2.21503	1.69060	0.00000
C	-0.13013	2.19593	0.00000
N	0.96971	1.51256	0.00000
H	-0.21447	3.27191	0.00000
H	-2.51063	-1.10576	0.00000

Monomer m26,
Sum of electronic and zero-point energy: -617.662717 a.u.
C_s, $N_{im} = 1$ ($312i$ cm^{-1})

C	0.49364	0.83184	0.00000
C	0.56769	-0.53825	0.00000
C	-0.60839	-1.32414	0.00000
N	-1.75059	-0.47329	0.00000
N	-0.62072	1.59089	0.00000
C	-1.72654	0.89106	0.00000
O	-0.74447	-2.53289	0.00000
H	-2.62882	-0.97234	0.00000
N	-2.91834	1.53851	0.00000
N	1.77905	1.30400	0.00000
H	2.05726	2.27049	0.00000

C	2.70150	0.24607	0.00000
N	1.91598	-0.88572	0.00000
H	-2.90136	2.54261	0.00000
H	-3.79912	1.05968	0.00000
O	3.90650	0.33489	0.00000
H	2.29122	-1.81790	0.00000

Cartesian coordinates and sum of electronic and zero-point energies of quartets

1, G-quartet

Sum of electronic and zero-point energy: -2169.765479 a.u.

C_{4h}, N_{im}= 1 (7*i* cm^{-1})

C	-4.20433	4.00302	0.00000
C	4.20433	-4.00302	0.00000
C	-4.00302	-4.20433	0.00000
C	4.00302	4.20433	0.00000
C	-4.03016	2.63266	0.00000
C	4.03016	-2.63266	0.00000
C	-2.63266	-4.03016	0.00000
C	2.63266	4.03016	0.00000
C	-2.70234	2.10909	0.00000
C	2.70234	-2.10909	0.00000
C	-2.10909	-2.70234	0.00000
C	2.10909	2.70234	0.00000
N	-1.75131	3.13468	0.00000
N	1.75131	-3.13468	0.00000
N	-3.13468	-1.75131	0.00000
N	3.13468	1.75131	0.00000
N	-3.26826	4.96344	0.00000
N	3.26826	-4.96344	0.00000
N	-4.96344	-3.26826	0.00000
N	4.96344	3.26826	0.00000
C	-2.03907	4.47458	0.00000
C	2.03907	-4.47458	0.00000
C	-4.47458	-2.03907	0.00000
C	4.47458	2.03907	0.00000
O	-2.35861	0.93543	0.00000
O	2.35861	-0.93543	0.00000
O	-0.93543	-2.35861	0.00000
O	0.93543	2.35861	0.00000
H	-0.76423	2.83687	0.00000
H	0.76423	-2.83687	0.00000
H	-2.83687	-0.76423	0.00000
H	2.83687	0.76423	0.00000
N	-1.00697	5.33193	0.00000
N	1.00697	-5.33193	0.00000
N	-5.33193	-1.00697	0.00000
N	5.33193	1.00697	0.00000

N	-5.56169	4.18179	0.00000
N	5.56169	-4.18179	0.00000
N	-4.18179	-5.56169	0.00000
N	4.18179	5.56169	0.00000
H	-6.03569	5.06933	0.00000
H	6.03569	-5.06933	0.00000
H	-5.06933	-6.03569	0.00000
H	5.06933	6.03569	0.00000
C	-6.13304	2.93051	0.00000
C	6.13304	-2.93051	0.00000
C	-2.93051	-6.13304	0.00000
C	2.93051	6.13304	0.00000
N	-5.24481	1.97902	0.00000
N	5.24481	-1.97902	0.00000
N	-1.97902	-5.24481	0.00000
N	1.97902	5.24481	0.00000
H	-1.24687	6.30726	0.00000
H	1.24687	-6.30726	0.00000
H	-6.30726	-1.24687	0.00000
H	6.30726	1.24687	0.00000
H	-0.01916	5.08111	0.00000
H	0.01916	-5.08111	0.00000
H	-5.08111	-0.01916	0.00000
H	5.08111	0.01916	0.00000
H	-2.79327	-7.20374	0.00000
H	7.20374	-2.79327	0.00000
H	2.79327	7.20374	0.00000
H	-7.20374	2.79327	0.00000

2

Sum of electronic and zero-point energy: -2249.218203 a.u.

C_{4h}, N_{im}= 4 (23*i* cm^{-1}, 10*i* cm^{-1},9*i* cm^{-1}, 9*i* cm^{-1})

C	0.76940	3.47149	0.00000
C	-0.76940	-3.47149	0.00000
C	-3.47149	0.76940	0.00000
C	3.47149	-0.76940	0.00000
N	1.92070	2.77565	0.00000
N	-1.92070	-2.77565	0.00000
N	-2.77565	1.92070	0.00000
N	2.77565	-1.92070	0.00000
C	3.13168	3.43016	0.00000
C	-3.13168	-3.43016	0.00000
C	-3.43016	3.13168	0.00000
C	3.43016	-3.13168	0.00000
C	3.23051	4.78520	0.00000
C	-3.23051	-4.78520	0.00000
C	-4.78520	3.23051	0.00000
C	4.78520	-3.23051	0.00000
N	2.07626	5.56239	0.00000

N	-2.07626	-5.56239	0.00000
N	-5.56239	2.07626	0.00000
N	5.56239	-2.07626	0.00000
C	0.83801	5.00555	0.00000
C	-0.83801	-5.00555	0.00000
C	-5.00555	0.83801	0.00000
C	5.00555	-0.83801	0.00000
N	4.40854	2.95284	0.00000
N	-4.40854	-2.95284	0.00000
N	-2.95284	4.40854	0.00000
N	2.95284	-4.40854	0.00000
C	5.20610	4.05952	0.00000
C	-5.20610	-4.05952	0.00000
C	-4.05952	5.20610	0.00000
C	4.05952	-5.20610	0.00000
N	4.52541	5.18826	0.00000
N	-4.52541	-5.18826	0.00000
N	-5.18826	4.52541	0.00000
N	5.18826	-4.52541	0.00000
O	-0.33448	2.94273	0.00000
O	0.33448	-2.94273	0.00000
O	-2.94273	-0.33448	0.00000
O	2.94273	0.33448	0.00000
H	6.28144	3.98182	0.00000
H	-6.28144	-3.98182	0.00000
H	-3.98182	6.28144	0.00000
H	3.98182	-6.28144	0.00000
O	-0.20229	5.64427	0.00000
O	0.20229	-5.64427	0.00000
O	-5.64427	-0.20229	0.00000
O	5.64427	0.20229	0.00000
H	2.14336	6.57125	0.00000
H	-2.14336	-6.57125	0.00000
H	-6.57125	2.14336	0.00000
H	6.57125	-2.14336	0.00000
H	1.90588	1.75359	0.00000
H	-1.90588	-1.75359	0.00000
H	-1.75359	1.90588	0.00000
H	1.75359	-1.90588	0.00000
H	4.70254	1.97119	0.00000
H	-4.70254	-1.97119	0.00000
H	-1.97119	4.70254	0.00000
H	1.97119	-4.70254	0.00000

3, G'$_4$

Sum of electronic and zero-point energy: -2169.765157 a.u.

C_{4h}, N_{im}= 1 (12*i* cm^{-1})

C	-5.16750	2.95814	0.00000
C	5.16750	-2.95814	0.00000

C	-2.95814	-5.16750	0.00000
C	2.95814	5.16750	0.00000
C	-4.79668	1.62494	0.00000
C	4.79668	-1.62494	0.00000
C	-1.62494	-4.79668	0.00000
C	1.62494	4.79668	0.00000
C	-3.40925	1.30389	0.00000
C	3.40925	-1.30389	0.00000
C	-1.30389	-3.40925	0.00000
C	1.30389	3.40925	0.00000
N	-2.61888	2.45080	0.00000
N	2.61888	-2.45080	0.00000
N	-2.45080	-2.61888	0.00000
N	2.45080	2.61888	0.00000
N	-4.38038	4.04518	0.00000
N	4.38038	-4.04518	0.00000
N	-4.04518	-4.38038	0.00000
N	4.04518	4.38038	0.00000
C	-3.09597	3.74154	0.00000
C	3.09597	-3.74154	0.00000
C	-3.74154	-3.09597	0.00000
C	3.74154	3.09597	0.00000
O	-2.90165	0.18463	0.00000
O	2.90165	-0.18463	0.00000
O	-0.18463	-2.90165	0.00000
O	0.18463	2.90165	0.00000
H	-1.60535	2.31919	0.00000
H	1.60535	-2.31919	0.00000
H	-2.31919	-1.60535	0.00000
H	2.31919	1.60535	0.00000
N	-2.17955	4.71715	0.00000
N	2.17955	-4.71715	0.00000
N	-4.71715	-2.17955	0.00000
N	4.71715	2.17955	0.00000
N	-6.53423	2.93671	0.00000
N	6.53423	-2.93671	0.00000
N	-2.93671	-6.53423	0.00000
N	2.93671	6.53423	0.00000
H	-7.13288	3.74549	0.00000
H	7.13288	-3.74549	0.00000
H	-3.74549	-7.13288	0.00000
H	3.74549	7.13288	0.00000
C	-6.91520	1.61165	0.00000
C	6.91520	-1.61165	0.00000
C	-1.61165	-6.91520	0.00000
C	1.61165	6.91520	0.00000
N	-5.90180	0.79770	0.00000
N	5.90180	-0.79770	0.00000
N	-0.79770	-5.90180	0.00000

N	0.79770	5.90180	0.00000
H	-2.49993	5.66802	0.00000
H	2.49993	-5.66802	0.00000
H	-5.66802	-2.49993	0.00000
H	5.66802	2.49993	0.00000
H	-1.18597	4.52515	0.00000
H	1.18597	-4.52515	0.00000
H	-4.52515	-1.18597	0.00000
H	4.52515	1.18597	0.00000
H	-7.95528	1.32184	0.00000
H	7.95528	-1.32184	0.00000
H	-1.32184	-7.95528	0.00000
H	1.32184	7.95528	0.00000

4

Sum of electronic and zero-point energy: -3772.849503 a.u.

C_{4h}, N_{im}=1 (11*i* cm^{-1})

C	-3.32708	1.33484	0.00000
C	3.32708	-1.33484	0.00000
C	-1.33484	-3.32708	0.00000
C	1.33484	3.32708	0.00000
N	-3.44662	-0.00418	0.00000
N	3.44662	0.00418	0.00000
N	0.00418	-3.44662	0.00000
N	-0.00418	3.44662	0.00000
C	-4.69767	-0.58623	0.00000
C	4.69767	0.58623	0.00000
C	0.58623	-4.69767	0.00000
C	-0.58623	4.69767	0.00000
C	-5.91359	0.07080	0.00000
C	5.91359	-0.07080	0.00000
C	-0.07080	-5.91359	0.00000
C	0.07080	5.91359	0.00000
C	-6.00361	1.49912	0.00000
C	6.00361	-1.49912	0.00000
C	-1.49912	-6.00361	0.00000
C	1.49912	6.00361	0.00000
C	-4.64263	2.18382	0.00000
C	4.64263	-2.18382	0.00000
C	-2.18382	-4.64263	0.00000
C	2.18382	4.64263	0.00000
N	-4.95430	-1.90791	0.00000
N	4.95430	1.90791	0.00000
N	1.90791	-4.95430	0.00000
N	-1.90791	4.95430	0.00000
C	-6.33264	-2.01650	0.00000
C	6.33264	2.01650	0.00000
C	2.01650	-6.33264	0.00000

C	-2.01650	6.33264	0.00000
N	-6.92843	-0.86483	0.00000
N	6.92843	0.86483	0.00000
N	0.86483	-6.92843	0.00000
N	-0.86483	6.92843	0.00000
O	-2.25764	1.91533	0.00000
O	2.25764	-1.91533	0.00000
O	-1.91533	-2.25764	0.00000
O	1.91533	2.25764	0.00000
H	-6.81444	-2.98227	0.00000
H	6.81444	2.98227	0.00000
H	2.98227	-6.81444	0.00000
H	-2.98227	6.81444	0.00000
O	-4.48614	3.37450	0.00000
O	4.48614	-3.37450	0.00000
O	-3.37450	-4.48614	0.00000
O	3.37450	4.48614	0.00000
S	-7.36179	2.40128	0.00000
S	7.36179	-2.40128	0.00000
S	-2.40128	-7.36179	0.00000
S	2.40128	7.36179	0.00000
H	-2.61640	-0.59732	0.00000
H	2.61640	0.59732	0.00000
H	0.59732	-2.61640	0.00000
H	-0.59732	2.61640	0.00000
H	-4.27290	-2.66815	0.00000
H	4.27290	2.66815	0.00000
H	2.66815	-4.27290	0.00000
H	-2.66815	4.27290	0.00000

5

Sum of electronic and zero-point energy: -2401.416991 a.u.

C_{4h}, N_{im}=1 (1*i* cm^{-1})

C	-3.33282	1.36392	0.00000
C	3.33282	-1.36392	0.00000
C	-1.36392	-3.33282	0.00000
C	1.36392	3.33282	0.00000
N	-3.45927	0.02876	0.00000
N	3.45927	-0.02876	0.00000
N	-0.02876	-3.45927	0.00000
N	0.02876	3.45927	0.00000
C	-4.71581	-0.56557	0.00000
C	4.71581	0.56557	0.00000
C	0.56557	-4.71581	0.00000
C	-0.56557	4.71581	0.00000
C	-5.93252	0.06763	0.00000
C	5.93252	-0.06763	0.00000
C	-0.06763	-5.93252	0.00000
C	0.06763	5.93252	0.00000

C	-6.01614	1.51406	0.00000
C	6.01614	-1.51406	0.00000
C	-1.51406	-6.01614	0.00000
C	1.51406	6.01614	0.00000
C	-4.64968	2.19811	0.00000
C	4.64968	-2.19811	0.00000
C	-2.19811	-4.64968	0.00000
C	2.19811	4.64968	0.00000
N	-4.95776	-1.89655	0.00000
N	4.95776	1.89655	0.00000
N	1.89655	-4.95776	0.00000
N	-1.89655	4.95776	0.00000
C	-6.32796	-2.02086	0.00000
C	6.32796	2.02086	0.00000
C	2.02086	-6.32796	0.00000
C	-2.02086	6.32796	0.00000
N	-6.93765	-0.87108	0.00000
N	6.93765	0.87108	0.00000
N	0.87108	-6.93765	0.00000
N	-0.87108	6.93765	0.00000
O	-2.26605	1.95428	0.00000
O	2.26605	-1.95428	0.00000
O	-1.95428	-2.26605	0.00000
O	1.95428	2.26605	0.00000
H	-6.80302	-2.98973	0.00000
H	6.80302	2.98973	0.00000
H	2.98973	-6.80302	0.00000
H	-2.98973	6.80302	0.00000
O	-4.53384	3.39577	0.00000
O	4.53384	-3.39577	0.00000
O	-3.39577	-4.53384	0.00000
O	3.39577	4.53384	0.00000
N	-7.08624	2.19903	0.00000
N	7.08624	-2.19903	0.00000
N	-2.19903	-7.08624	0.00000
N	2.19903	7.08624	0.00000
H	-2.62973	-0.56490	0.00000
H	2.62973	0.56490	0.00000
H	0.56490	-2.62973	0.00000
H	-0.56490	2.62973	0.00000
H	-4.26648	-2.64431	0.00000
H	4.26648	2.64431	0.00000
H	2.64431	-4.26648	0.00000
H	-2.64431	4.26648	0.00000
H	-6.85836	3.19601	0.00000
H	6.85836	-3.19601	0.00000
H	-3.19601	-6.85836	0.00000
H	3.19601	6.85836	0.00000

6

Sum of electronic and zero-point energy: -2480.969395 a.u.

C_{4h}, N_{im}=1 (10*i* cm^{-1})

C	-3.58407	0.00975	0.00000
C	3.58407	-0.00975	0.00000
C	-0.00975	-3.58407	0.00000
C	0.00975	3.58407	0.00000
N	-3.20987	1.30106	0.00000
N	3.20987	-1.30106	0.00000
N	-1.30106	-3.20987	0.00000
N	1.30106	3.20987	0.00000
C	-4.16052	2.30918	0.00000
C	4.16052	-2.30918	0.00000
C	-2.30918	-4.16052	0.00000
C	2.30918	4.16052	0.00000
C	-5.53445	2.17916	0.00000
C	5.53445	-2.17916	0.00000
C	-2.17916	-5.53445	0.00000
C	2.17916	5.53445	0.00000
C	-6.16687	0.88068	0.00000
C	6.16687	-0.88068	0.00000
C	-0.88068	-6.16687	0.00000
C	0.88068	6.16687	0.00000
C	-5.11966	-0.28374	0.00000
C	5.11966	0.28374	0.00000
C	0.28374	-5.11966	0.00000
C	-0.28374	5.11966	0.00000
N	-3.89093	3.62945	0.00000
N	3.89093	-3.62945	0.00000
N	-3.62945	-3.89093	0.00000
N	3.62945	3.89093	0.00000
C	-5.11874	4.26388	0.00000
C	5.11874	-4.26388	0.00000
C	-4.26388	-5.11874	0.00000
C	4.26388	5.11874	0.00000
N	-6.11279	3.43092	0.00000
N	6.11279	-3.43092	0.00000
N	-3.43092	-6.11279	0.00000
N	3.43092	6.11279	0.00000
O	-2.80498	-0.92459	0.00000
O	2.80498	0.92459	0.00000
O	0.92459	-2.80498	0.00000
O	-0.92459	2.80498	0.00000
H	-5.18940	5.34084	0.00000
H	5.18940	-5.34084	0.00000
H	-5.34084	-5.18940	0.00000
H	5.34084	5.18940	0.00000
O	-5.44987	-1.43451	0.00000
O	5.44987	1.43451	0.00000

O	1.43451	-5.44987	0.00000
O	-1.43451	5.44987	0.00000
O	-7.33598	0.60395	0.00000
O	7.33598	-0.60395	0.00000
O	-0.60395	-7.33598	0.00000
O	0.60395	7.33598	0.00000
H	-2.22035	1.54955	0.00000
H	2.22035	-1.54955	0.00000
H	-1.54955	-2.22035	0.00000
H	1.54955	2.22035	0.00000
H	-2.97068	4.06887	0.00000
H	2.97068	-4.06887	0.00000
H	-4.06887	-2.97068	0.00000
H	4.06887	2.97068	0.00000

7, $G_2 2_2$
Sum of electronic and zero-point energy: -2209.497979 a.u.
C_{2h}, N_{im}=1 ($8i$ cm^{-1})

C	3.54116	-1.23071	0.00000
C	-3.54116	1.23071	0.00000
N	2.77662	-2.34191	0.00000
N	-2.77662	2.34191	0.00000
C	3.37570	-3.58206	0.00000
C	-3.37570	3.58206	0.00000
C	4.72295	-3.76096	0.00000
C	-4.72295	3.76096	0.00000
N	5.56620	-2.65660	0.00000
N	-5.56620	2.65660	0.00000
C	5.07633	-1.38739	0.00000
C	-5.07633	1.38739	0.00000
N	2.82626	-4.82957	0.00000
N	-2.82626	4.82957	0.00000
C	3.88428	-5.69039	0.00000
C	-3.88428	5.69039	0.00000
N	5.05083	-5.07709	0.00000
N	-5.05083	5.07709	0.00000
O	3.08563	-0.09622	0.00000
O	-3.08563	0.09622	0.00000
H	3.74799	-6.76009	0.00000
H	-3.74799	6.76009	0.00000
O	5.77114	-0.38905	0.00000
O	-5.77114	0.38905	0.00000
H	6.56921	-2.77837	0.00000
H	-6.56921	2.77837	0.00000
H	1.74552	-2.26099	0.00000
H	-1.74552	2.26099	0.00000
H	1.82152	-5.07178	0.00000
H	-1.82152	5.07178	0.00000

C	2.25920	5.10760	0.00000
C	-2.25920	-5.10760	0.00000
C	1.00740	4.51454	0.00000
C	-1.00740	-4.51454	0.00000
C	0.93728	3.09038	0.00000
C	-0.93728	-3.09038	0.00000
N	2.20661	2.51962	0.00000
N	-2.20661	-2.51962	0.00000
N	3.46641	4.52656	0.00000
N	-3.46641	-4.52656	0.00000
C	3.39606	3.20576	0.00000
C	-3.39606	-3.20576	0.00000
O	-0.05555	2.36988	0.00000
O	0.05555	-2.36988	0.00000
H	2.24203	1.49788	0.00000
H	-2.24203	-1.49788	0.00000
N	4.51718	2.47556	0.00000
N	-4.51718	-2.47556	0.00000
N	2.00647	6.45342	0.00000
N	-2.00647	-6.45342	0.00000
H	2.70446	7.17873	0.00000
H	-2.70446	-7.17873	0.00000
C	0.64360	6.61173	0.00000
C	-0.64360	-6.61173	0.00000
N	0.01100	5.47285	0.00000
N	-0.01100	-5.47285	0.00000
H	5.39132	2.96969	0.00000
H	-5.39132	-2.96969	0.00000
H	4.51571	1.45851	0.00000
H	-4.51571	-1.45851	0.00000
H	0.18165	7.58724	0.00000
H	-0.18165	-7.58724	0.00000

8

Sum of electronic and zero-point energy: -2209.445481 a.u.

C_{2h}, N_{im}=0

N	-3.60151	-0.62069	0.00000
N	3.60151	0.62069	0.00000
C	-3.51199	-1.96422	0.00000
C	3.51199	1.96422	0.00000
C	-4.81101	-2.62113	0.00000
C	4.81101	2.62113	0.00000
C	-5.96218	-1.87772	0.00000
C	5.96218	1.87772	0.00000
C	-6.02591	-0.42479	0.00000
C	6.02591	0.42479	0.00000
N	-4.77658	0.10728	0.00000
N	4.77658	-0.10728	0.00000
O	-2.42130	-2.54856	0.00000

O	2.42130	2.54856	0.00000
N	-5.09301	-3.96019	0.00000
N	5.09301	3.96019	0.00000
C	-6.40173	-4.01515	0.00000
C	6.40173	4.01515	0.00000
N	-6.98082	-2.77942	0.00000
N	6.98082	2.77942	0.00000
H	-2.74839	-0.02990	0.00000
H	2.74839	0.02990	0.00000
H	-6.98868	-4.92139	0.00000
H	6.98868	4.92139	0.00000
H	-4.62940	1.13223	0.00000
H	4.62940	-1.13223	0.00000
O	-7.05508	0.23726	0.00000
O	7.05508	-0.23726	0.00000
C	2.44578	-4.53615	0.00000
C	-2.44578	4.53615	0.00000
C	2.64048	-3.16721	0.00000
C	-2.64048	3.16721	0.00000
C	1.49742	-2.31403	0.00000
C	-1.49742	2.31403	0.00000
N	0.31605	-3.05090	0.00000
N	-0.31605	3.05090	0.00000
N	1.28944	-5.21689	0.00000
N	-1.28944	5.21689	0.00000
C	0.23393	-4.42279	0.00000
C	-0.23393	4.42279	0.00000
O	1.46347	-1.08751	0.00000
O	-1.46347	1.08751	0.00000
H	-0.56134	-2.52050	0.00000
H	0.56134	2.52050	0.00000
N	-1.00028	-4.94571	0.00000
N	1.00028	4.94571	0.00000
N	3.70833	-5.06691	0.00000
N	-3.70833	5.06691	0.00000
H	3.93069	-6.04851	0.00000
H	-3.93069	6.04851	0.00000
C	4.59248	-4.01571	0.00000
C	-4.59248	4.01571	0.00000
N	3.98688	-2.86335	0.00000
N	-3.98688	2.86335	0.00000
H	-1.08171	-5.94597	0.00000
H	1.08171	5.94597	0.00000
H	-1.82022	-4.34345	0.00000
H	1.82022	4.34345	0.00000
H	5.66215	-4.15964	0.00000
H	-5.66215	4.15964	0.00000
H	-7.96225	-2.54961	0.00000
H	7.96225	2.54961	0.00000

9, P_4

Sum of electronic and zero-point energy: -2623.073860 a.u.

C_{4h}, N_{im}=3 (9*i* cm^{-1}, 5*i* cm^{-1}, 3*i* cm^{-1})

N	-3.59185	0.09458	0.00000
N	3.59185	-0.09458	0.00000
N	-0.09458	-3.59185	0.00000
N	0.09458	3.59185	0.00000
C	-3.28717	1.45222	0.00000
C	3.28717	-1.45222	0.00000
C	-1.45222	-3.28717	0.00000
C	1.45222	3.28717	0.00000
C	-4.45085	2.30163	0.00000
C	4.45085	-2.30163	0.00000
C	-2.30163	-4.45085	0.00000
C	2.30163	4.45085	0.00000
C	-5.70772	1.70123	0.00000
C	5.70772	-1.70123	0.00000
C	-1.70123	-5.70772	0.00000
C	1.70123	5.70772	0.00000
N	-5.94030	0.38642	0.00000
N	5.94030	-0.38642	0.00000
N	-0.38642	-5.94030	0.00000
N	0.38642	5.94030	0.00000
C	-4.86682	-0.39075	0.00000
C	4.86682	0.39075	0.00000
C	0.39075	-4.86682	0.00000
C	-0.39075	4.86682	0.00000
N	-5.03980	-1.70990	0.00000
N	5.03980	1.70990	0.00000
N	1.70990	-5.03980	0.00000
N	-1.70990	5.03980	0.00000
O	-2.12292	1.82917	0.00000
O	2.12292	-1.82917	0.00000
O	-1.82917	-2.12292	0.00000
O	1.82917	2.12292	0.00000
H	-2.81288	-0.57185	0.00000
H	2.81288	0.57185	0.00000
H	0.57185	-2.81288	0.00000
H	-0.57185	2.81288	0.00000
N	-4.29834	3.65785	0.00000
N	4.29834	-3.65785	0.00000
N	-3.65785	-4.29834	0.00000
N	3.65785	4.29834	0.00000
C	-5.33904	4.41729	0.00000
C	5.33904	-4.41729	0.00000
C	-4.41729	-5.33904	0.00000
C	4.41729	5.33904	0.00000
N	-6.79406	2.52681	0.00000
N	6.79406	-2.52681	0.00000

N	-2.52681	-6.79406	0.00000
N	2.52681	6.79406	0.00000
C	-6.72327	3.91563	0.00000
C	6.72327	-3.91563	0.00000
C	-3.91563	-6.72327	0.00000
C	3.91563	6.72327	0.00000
O	-7.71474	4.61104	0.00000
O	7.71474	-4.61104	0.00000
O	-4.61104	-7.71474	0.00000
O	4.61104	7.71474	0.00000
H	-7.71301	2.10210	0.00000
H	7.71301	-2.10210	0.00000
H	-2.10210	-7.71301	0.00000
H	2.10210	7.71301	0.00000
H	-5.21833	5.49600	0.00000
H	5.21833	-5.49600	0.00000
H	-5.49600	-5.21833	0.00000
H	5.49600	5.21833	0.00000
H	-4.29178	-2.40476	0.00000
H	4.29178	2.40476	0.00000
H	2.40476	-4.29178	0.00000
H	-2.40476	4.29178	0.00000
H	-5.99292	-2.03016	0.00000
H	5.99292	2.03016	0.00000
H	2.03016	-5.99292	0.00000
H	-2.03016	5.99292	0.00000

10, [2467P]$_4$

Sum of electronic and zero-point energy: -3003.590561 a.u.

C_{4h}, N_{im}=3 (8*i* cm^{-1}, 5*i* cm^{-1},5*i* cm^{-1})

H	-1.82384	-2.36979	0.00000
H	1.82384	2.36979	0.00000
H	2.36979	-1.82384	0.00000
H	-2.36979	1.82384	0.00000
C	-6.05053	-4.02053	0.00000
C	6.05053	4.02053	0.00000
C	4.02053	-6.05053	0.00000
C	-4.02053	6.05053	0.00000
N	-5.47774	-5.28350	0.00000
N	5.47774	5.28350	0.00000
N	5.28350	-5.47774	0.00000
N	-5.28350	5.47774	0.00000
C	-4.12447	-5.60480	0.00000
C	4.12447	5.60480	0.00000
C	5.60480	-4.12447	0.00000
C	-5.60480	4.12447	0.00000
N	-3.28101	-4.50410	0.00000
N	3.28101	4.50410	0.00000
N	4.50410	-3.28101	0.00000

N	-4.50410	3.28101	0.00000
C	-3.74610	-3.22092	0.00000
C	3.74610	3.22092	0.00000
C	3.22092	-3.74610	0.00000
C	-3.22092	3.74610	0.00000
C	-5.07391	-2.95536	0.00000
C	5.07391	2.95536	0.00000
C	2.95536	-5.07391	0.00000
C	-2.95536	5.07391	0.00000
N	-5.52452	-1.63951	0.00000
N	5.52452	1.63951	0.00000
N	1.63951	-5.52452	0.00000
N	-1.63951	5.52452	0.00000
C	-4.71547	-0.56758	0.00000
C	4.71547	0.56758	0.00000
C	0.56758	-4.71547	0.00000
C	-0.56758	4.71547	0.00000
C	-3.21720	-0.86934	0.00000
C	3.21720	0.86934	0.00000
C	0.86934	-3.21720	0.00000
C	-0.86934	3.21720	0.00000
N	-2.84036	-2.18429	0.00000
N	2.84036	2.18429	0.00000
N	2.18429	-2.84036	0.00000
N	-2.18429	2.84036	0.00000
O	-2.41399	0.03933	0.00000
O	2.41399	-0.03933	0.00000
O	-0.03933	-2.41399	0.00000
O	0.03933	2.41399	0.00000
O	-3.72777	-6.74088	0.00000
O	3.72777	6.74088	0.00000
O	6.74088	-3.72777	0.00000
O	-6.74088	3.72777	0.00000
H	-6.11029	-6.07195	0.00000
H	6.11029	6.07195	0.00000
H	6.07195	-6.11029	0.00000
H	-6.07195	6.11029	0.00000
H	-2.27162	-4.70220	0.00000
H	2.27162	4.70220	0.00000
H	4.70220	-2.27162	0.00000
H	-4.70220	2.27162	0.00000
O	-5.11008	0.58585	0.00000
O	5.11008	-0.58585	0.00000
O	-0.58585	-5.11008	0.00000
O	0.58585	5.11008	0.00000
H	-6.52958	-1.49582	0.00000
H	6.52958	1.49582	0.00000
H	1.49582	-6.52958	0.00000
H	-1.49582	6.52958	0.00000

O	-7.25112	-3.83907	0.00000
O	7.25112	3.83907	0.00000
O	3.83907	-7.25112	0.00000
O	-3.83907	7.25112	0.00000

11, $[267P]_4$
Sum of electronic and zero-point energy: -2702.506286 a.u.
C_{4h}, N_{im}=1 ($8i$ cm^{-1})

H	2.89663	0.79368	0.00000
H	-2.89663	-0.79368	0.00000
H	-0.79368	2.89663	0.00000
H	0.79368	-2.89663	0.00000
C	7.20934	-0.39362	0.00000
C	-7.20934	0.39362	0.00000
C	0.39362	7.20934	0.00000
C	-0.39362	-7.20934	0.00000
N	7.65869	0.82200	0.00000
N	-7.65869	-0.82200	0.00000
N	-0.82200	7.65869	0.00000
N	0.82200	-7.65869	0.00000
C	6.76264	1.88348	0.00000
C	-6.76264	-1.88348	0.00000
C	-1.88348	6.76264	0.00000
C	1.88348	-6.76264	0.00000
N	5.38585	1.54671	0.00000
N	-5.38585	-1.54671	0.00000
N	-1.54671	5.38585	0.00000
N	1.54671	-5.38585	0.00000
C	4.93544	0.27930	0.00000
C	-4.93544	-0.27930	0.00000
C	-0.27930	4.93544	0.00000
C	0.27930	-4.93544	0.00000
C	5.84115	-0.74656	0.00000
C	-5.84115	0.74656	0.00000
C	0.74656	5.84115	0.00000
C	-0.74656	-5.84115	0.00000
N	5.37196	-2.06511	0.00000
N	-5.37196	2.06511	0.00000
N	2.06511	5.37196	0.00000
N	-2.06511	-5.37196	0.00000
C	4.06879	-2.40535	0.00000
C	-4.06879	2.40535	0.00000
C	2.40535	4.06879	0.00000
C	-2.40535	-4.06879	0.00000
C	3.07273	-1.24561	0.00000
C	-3.07273	1.24561	0.00000
C	1.24561	3.07273	0.00000

C	-1.24561	-3.07273	0.00000
N	3.58395	0.02214	0.00000
N	-3.58395	-0.02214	0.00000
N	-0.02214	3.58395	0.00000
N	0.02214	-3.58395	0.00000
O	1.88231	-1.47183	0.00000
O	-1.88231	1.47183	0.00000
O	1.47183	1.88231	0.00000
O	-1.47183	-1.88231	0.00000
H	4.72612	2.33206	0.00000
H	-4.72612	-2.33206	0.00000
H	-2.33206	4.72612	0.00000
H	2.33206	-4.72612	0.00000
O	3.67075	-3.55547	0.00000
O	-3.67075	3.55547	0.00000
O	3.55547	3.67075	0.00000
O	-3.55547	-3.67075	0.00000
H	6.03272	-2.83156	0.00000
H	-6.03272	2.83156	0.00000
H	2.83156	6.03272	0.00000
H	-2.83156	-6.03272	0.00000
H	7.95365	-1.19176	0.00000
H	-7.95365	1.19176	0.00000
H	1.19176	7.95365	0.00000
H	-1.19176	-7.95365	0.00000
O	7.08607	3.04350	0.00000
O	-7.08607	-3.04350	0.00000
O	-3.04350	7.08607	0.00000
O	3.04350	-7.08607	0.00000

12, [467P]$_4$

Sum of electronic and zero-point energy: -2702.543249 a.u.

C_{4h}, N_{im}=0

H	-1.61675	-2.34964	0.00000
H	1.61675	2.34964	0.00000
H	2.34964	-1.61675	0.00000
H	-2.34964	1.61675	0.00000
C	-5.44107	-4.78089	0.00000
C	5.44107	4.78089	0.00000
C	4.78089	-5.44107	0.00000
C	-4.78089	5.44107	0.00000
N	-4.67682	-5.94621	0.00000
N	4.67682	5.94621	0.00000
N	5.94621	-4.67682	0.00000
N	-5.94621	4.67682	0.00000
C	-3.39109	-5.85908	0.00000
C	3.39109	5.85908	0.00000
C	5.85908	-3.39109	0.00000

C	-5.85908	3.39109	0.00000
N	-2.66176	-4.70904	0.00000
N	2.66176	4.70904	0.00000
N	4.70904	-2.66176	0.00000
N	-4.70904	2.66176	0.00000
C	-3.33674	-3.52417	0.00000
C	3.33674	3.52417	0.00000
C	3.52417	-3.33674	0.00000
C	-3.52417	3.33674	0.00000
C	-4.68839	-3.53113	0.00000
C	4.68839	3.53113	0.00000
C	3.53113	-4.68839	0.00000
C	-3.53113	4.68839	0.00000
N	-5.37686	-2.32524	0.00000
N	5.37686	2.32524	0.00000
N	2.32524	-5.37686	0.00000
N	-2.32524	5.37686	0.00000
C	-4.79006	-1.11446	0.00000
C	4.79006	1.11446	0.00000
C	1.11446	-4.79006	0.00000
C	-1.11446	4.79006	0.00000
C	-3.26212	-1.12546	0.00000
C	3.26212	1.12546	0.00000
C	1.12546	-3.26212	0.00000
C	-1.12546	3.26212	0.00000
N	-2.64536	-2.33382	0.00000
N	2.64536	2.33382	0.00000
N	2.33382	-2.64536	0.00000
N	-2.33382	2.64536	0.00000
O	-2.64381	-0.07764	0.00000
O	2.64381	0.07764	0.00000
O	0.07764	-2.64381	0.00000
O	-0.07764	2.64381	0.00000
H	-1.63291	-4.76479	0.00000
H	1.63291	4.76479	0.00000
H	4.76479	-1.63291	0.00000
H	-4.76479	1.63291	0.00000
O	-5.39206	-0.05093	0.00000
O	5.39206	0.05093	0.00000
O	0.05093	-5.39206	0.00000
O	-0.05093	5.39206	0.00000
H	-6.39134	-2.39475	0.00000
H	6.39134	2.39475	0.00000
H	2.39475	-6.39134	0.00000
H	-2.39475	6.39134	0.00000
O	-6.65694	-4.76733	0.00000
O	6.65694	4.76733	0.00000
O	4.76733	-6.65694	0.00000
O	-4.76733	6.65694	0.00000

H	-6.76440	2.79128	0.00000
H	-2.79128	-6.76440	0.00000
H	6.76440	-2.79128	0.00000
H	2.79128	6.76440	0.00000

13, $[PT]_4$

Sum of electronic and zero-point energy: -2322.071551 a.u.

C_{4h}, N_{im}=2 (10*i* cm^{-1}, 1*i* cm^{-1})

N	-2.79907	-2.27480	0.00000
N	2.79907	2.27480	0.00000
N	2.27480	-2.79907	0.00000
N	-2.27480	2.79907	0.00000
C	-3.43317	-1.05543	0.00000
C	3.43317	1.05543	0.00000
C	1.05543	-3.43317	0.00000
C	-1.05543	3.43317	0.00000
C	-4.89715	-1.16256	0.00000
C	4.89715	1.16256	0.00000
C	1.16256	-4.89715	0.00000
C	-1.16256	4.89715	0.00000
C	-5.49506	-2.44153	0.00000
C	5.49506	2.44153	0.00000
C	2.44153	-5.49506	0.00000
C	-2.44153	5.49506	0.00000
N	-4.77837	-3.58764	0.00000
N	4.77837	3.58764	0.00000
N	3.58764	-4.77837	0.00000
N	-3.58764	4.77837	0.00000
C	-3.47347	-3.47810	0.00000
C	3.47347	3.47810	0.00000
C	3.47810	-3.47347	0.00000
C	-3.47810	3.47347	0.00000
N	-2.72678	-4.58567	0.00000
N	2.72678	4.58567	0.00000
N	4.58567	-2.72678	0.00000
N	-4.58567	2.72678	0.00000
O	-2.81031	-0.00561	0.00000
O	2.81031	0.00561	0.00000
O	0.00561	-2.81031	0.00000
O	-0.00561	2.81031	0.00000
H	-1.77500	-2.28409	0.00000
H	1.77500	2.28409	0.00000
H	2.28409	-1.77500	0.00000
H	-2.28409	1.77500	0.00000
N	-5.61000	-0.03453	0.00000
N	5.61000	0.03453	0.00000
N	0.03453	-5.61000	0.00000
N	-0.03453	5.61000	0.00000
C	-6.92192	-0.15712	0.00000

C	6.92192	0.15712	0.00000
C	0.15712	-6.92192	0.00000
C	-0.15712	6.92192	0.00000
N	-6.84303	-2.54820	0.00000
N	6.84303	2.54820	0.00000
N	2.54820	-6.84303	0.00000
N	-2.54820	6.84303	0.00000
C	-7.52603	-1.42572	0.00000
C	7.52603	1.42572	0.00000
C	1.42572	-7.52603	0.00000
C	-1.42572	7.52603	0.00000
H	-7.51922	0.74838	0.00000
H	7.51922	-0.74838	0.00000
H	-0.74838	-7.51922	0.00000
H	0.74838	7.51922	0.00000
H	-1.70770	-4.61434	0.00000
H	1.70770	4.61434	0.00000
H	4.61434	-1.70770	0.00000
H	-4.61434	1.70770	0.00000
H	-3.23689	-5.45198	0.00000
H	3.23689	5.45198	0.00000
H	5.45198	-3.23689	0.00000
H	-5.45198	3.23689	0.00000
H	-8.60966	-1.50983	0.00000
H	8.60966	1.50983	0.00000
H	1.50983	-8.60966	0.00000
H	-1.50983	8.60966	0.00000

14, X-quartet

Sum of electronic and zero-point energy: -2249.351470 a.u.

C_{4h}, N_{im}= 1 (20*i* cm^{-1})

C	0.79897	4.58963	0.00000
C	-0.79897	-4.58963	0.00000
C	-4.58963	0.79897	0.00000
C	4.58963	-0.79897	0.00000
C	1.90519	5.40104	0.00000
C	-1.90519	-5.40104	0.00000
C	-5.40104	1.90519	0.00000
C	5.40104	-1.90519	0.00000
N	3.17423	4.86503	0.00000
N	-3.17423	-4.86503	0.00000
N	-4.86503	3.17423	0.00000
N	4.86503	-3.17423	0.00000
C	3.36782	3.50468	0.00000
C	-3.36782	-3.50468	0.00000
C	-3.50468	3.36782	0.00000
C	3.50468	-3.36782	0.00000
C	0.89920	3.16664	0.00000
C	-0.89920	-3.16664	0.00000

C	-3.16664	0.89920	0.00000
C	3.16664	-0.89920	0.00000
N	2.22492	2.74022	0.00000
N	-2.22492	-2.74022	0.00000
N	-2.74022	2.22492	0.00000
N	2.74022	-2.22492	0.00000
N	1.56715	6.70765	0.00000
N	-1.56715	-6.70765	0.00000
N	-6.70765	1.56715	0.00000
N	6.70765	-1.56715	0.00000
O	4.48900	3.00771	0.00000
O	-4.48900	-3.00771	0.00000
O	-3.00771	4.48900	0.00000
O	3.00771	-4.48900	0.00000
O	-0.01376	2.35905	0.00000
O	0.01376	-2.35905	0.00000
O	-2.35905	-0.01376	0.00000
O	2.35905	0.01376	0.00000
H	2.35754	1.71578	0.00000
H	-2.35754	-1.71578	0.00000
H	-1.71578	2.35754	0.00000
H	1.71578	-2.35754	0.00000
N	-0.27861	5.44326	0.00000
N	0.27861	-5.44326	0.00000
N	-5.44326	-0.27861	0.00000
N	5.44326	0.27861	0.00000
C	0.23914	6.68535	0.00000
C	-0.23914	-6.68535	0.00000
C	-6.68535	0.23914	0.00000
C	6.68535	-0.23914	0.00000
H	-0.38344	7.56682	0.00000
H	0.38344	-7.56682	0.00000
H	-7.56682	-0.38344	0.00000
H	7.56682	0.38344	0.00000
H	-1.26698	5.16278	0.00000
H	1.26698	-5.16278	0.00000
H	-5.16278	-1.26698	0.00000
H	5.16278	1.26698	0.00000
H	3.99080	5.45598	0.00000
H	-3.99080	-5.45598	0.00000
H	-5.45598	3.99080	0.00000
H	5.45598	-3.99080	0.00000

15, U_4

Sum of electronic and zero-point energy: -2550.283521a.u.

C_{4h}, N_{im}= 1 (13*i* cm^{-1})

N	-2.75440	-2.23495	0.00000
N	2.75440	2.23495	0.00000
N	2.23495	-2.75440	0.00000
N	-2.23495	2.75440	0.00000
C	-3.23447	-0.91996	0.00000

C	3.23447	0.91996	0.00000
C	0.91996	-3.23447	0.00000
C	-0.91996	3.23447	0.00000
C	-4.65607	-0.85473	0.00000
C	4.65607	0.85473	0.00000
C	0.85473	-4.65607	0.00000
C	-0.85473	4.65607	0.00000
C	-5.40268	-1.98908	0.00000
C	5.40268	1.98908	0.00000
C	1.98908	-5.40268	0.00000
C	-1.98908	5.40268	0.00000
N	-4.85220	-3.23892	0.00000
N	4.85220	3.23892	0.00000
N	3.23892	-4.85220	0.00000
N	-3.23892	4.85220	0.00000
C	-3.47232	-3.39847	0.00000
C	3.47232	3.39847	0.00000
C	3.39847	-3.47232	0.00000
C	-3.39847	3.47232	0.00000
O	-2.97113	-4.50990	0.00000
O	2.97113	4.50990	0.00000
O	4.50990	-2.97113	0.00000
O	-4.50990	2.97113	0.00000
O	-2.45314	0.01713	0.00000
O	2.45314	-0.01713	0.00000
O	-0.01713	-2.45314	0.00000
O	0.01713	2.45314	0.00000
N	-5.53243	0.22843	0.00000
N	5.53243	-0.22843	0.00000
N	-0.22843	-5.53243	0.00000
N	0.22843	5.53243	0.00000
C	-6.82878	-0.21455	0.00000
C	6.82878	0.21455	0.00000
C	0.21455	-6.82878	0.00000
C	-0.21455	6.82878	0.00000
N	-6.71594	-1.63308	0.00000
N	6.71594	1.63308	0.00000
N	1.63308	-6.71594	0.00000
N	-1.63308	6.71594	0.00000
H	-1.72706	-2.34094	0.00000
H	1.72706	2.34094	0.00000
H	2.34094	-1.72706	0.00000
H	-2.34094	1.72706	0.00000
H	-5.39980	-4.08462	0.00000
H	5.39980	4.08462	0.00000
H	4.08462	-5.39980	0.00000
H	-4.08462	5.39980	0.00000
H	-5.25756	1.21146	0.00000
H	5.25756	-1.21146	0.00000
H	-1.21146	-5.25756	0.00000
H	1.21146	5.25756	0.00000
O	-7.86640	0.39961	0.00000
O	7.86640	-0.39961	0.00000
O	-0.39961	-7.86640	0.00000
O	0.39961	7.86640	0.00000
H	-7.52647	-2.22837	0.00000
H	7.52647	2.22837	0.00000
H	2.22837	-7.52647	0.00000
H	-2.22837	7.52647	0.00000

16, U'$_4$

Sum of electronic and zero-point energy: -2550.286579 a.u.

C_{4h}, N_{im}= 0

C	-4.45218	-0.07301	0.00000
C	4.45218	0.07301	0.00000
C	0.07301	-4.45218	0.00000
C	-0.07301	4.45218	0.00000
C	-5.80194	-0.21378	0.00000
C	5.80194	0.21378	0.00000
C	0.21378	-5.80194	0.00000
C	-0.21378	5.80194	0.00000
N	-6.65791	0.84478	0.00000
N	6.65791	-0.84478	0.00000
N	-0.84478	-6.65791	0.00000
N	0.84478	6.65791	0.00000
C	-6.16986	2.15527	0.00000
C	6.16986	-2.15527	0.00000
C	-2.15527	-6.16986	0.00000
C	2.15527	6.16986	0.00000
C	-3.84813	1.22018	0.00000
C	3.84813	-1.22018	0.00000
C	-1.22018	-3.84813	0.00000
C	1.22018	3.84813	0.00000
N	-4.79073	2.25259	0.00000
N	4.79073	-2.25259	0.00000
N	-2.25259	-4.79073	0.00000
N	2.25259	4.79073	0.00000
N	-6.09024	-1.54824	0.00000
N	6.09024	1.54824	0.00000
N	1.54824	-6.09024	0.00000
N	-1.54824	6.09024	0.00000
O	-6.91690	3.10198	0.00000
O	6.91690	-3.10198	0.00000
O	-3.10198	-6.91690	0.00000
O	3.10198	6.91690	0.00000
O	-2.64634	1.44320	0.00000
O	2.64634	-1.44320	0.00000
O	-1.44320	-2.64634	0.00000
O	1.44320	2.64634	0.00000
H	-4.41497	3.21217	0.00000
H	4.41497	-3.21217	0.00000
H	-3.21217	-4.41497	0.00000
H	3.21217	4.41497	0.00000
N	-3.90105	-1.35176	0.00000
N	3.90105	1.35176	0.00000
N	1.35176	-3.90105	0.00000
N	-1.35176	3.90105	0.00000
C	-4.88876	-2.28220	0.00000
C	4.88876	2.28220	0.00000
C	2.28220	-4.88876	0.00000
C	-2.28220	4.88876	0.00000
O	-4.81325	-3.50034	0.00000
O	4.81325	3.50034	0.00000
O	3.50034	-4.81325	0.00000
O	-3.50034	4.81325	0.00000
H	-2.91242	-1.62327	0.00000
H	2.91242	1.62327	0.00000
H	1.62327	-2.91242	0.00000
H	-1.62327	2.91242	0.00000
H	-7.66034	0.74755	0.00000
H	7.66034	-0.74755	0.00000
H	-0.74755	-7.66034	0.00000
H	0.74755	7.66034	0.00000
H	-6.99116	-1.99541	0.00000

H	6.99116	1.99541	0.00000
H	1.99541	-6.99116	0.00000
H	-1.99541	6.99116	0.00000

17, $[8H]_4$

Sum of electronic and zero-point energy: -2249.337646 a.u.

C_{4h} , N_{im}= 1 (11*i* cm^{-1})

C	-4.37820	-0.01518	0.00000
C	4.37820	0.01518	0.00000
C	0.01518	-4.37820	0.00000
C	-0.01518	4.37820	0.00000
C	-5.74827	-0.08330	0.00000
C	5.74827	0.08330	0.00000
C	0.08330	-5.74827	0.00000
C	-0.08330	5.74827	0.00000
N	-6.60245	0.96194	0.00000
N	6.60245	-0.96194	0.00000
N	-0.96194	-6.60245	0.00000
N	0.96194	6.60245	0.00000
C	-5.99304	2.11292	0.00000
C	5.99304	-2.11292	0.00000
C	-2.11292	-5.99304	0.00000
C	2.11292	5.99304	0.00000
C	-3.71803	1.23917	0.00000
C	3.71803	-1.23917	0.00000
C	-1.23917	-3.71803	0.00000
C	1.23917	3.71803	0.00000
N	-4.64913	2.28442	0.00000
N	4.64913	-2.28442	0.00000
N	-2.28442	-4.64913	0.00000
N	2.28442	4.64913	0.00000
N	-6.07456	-1.42013	0.00000
N	6.07456	1.42013	0.00000
N	1.42013	-6.07456	0.00000
N	-1.42013	6.07456	0.00000
O	-2.50717	1.43586	0.00000
O	2.50717	-1.43586	0.00000
O	-1.43586	-2.50717	0.00000
O	1.43586	2.50717	0.00000
H	-4.25919	3.24239	0.00000
H	4.25919	-3.24239	0.00000
H	-3.24239	-4.25919	0.00000
H	3.24239	4.25919	0.00000
N	-3.88258	-1.30202	0.00000
N	3.88258	1.30202	0.00000
N	1.30202	-3.88258	0.00000
N	-1.30202	3.88258	0.00000
C	-4.91580	-2.19081	0.00000
C	4.91580	2.19081	0.00000
C	2.19081	-4.91580	0.00000
C	-2.19081	4.91580	0.00000
O	-4.85751	-3.41718	0.00000
O	4.85751	3.41718	0.00000
O	3.41718	-4.85751	0.00000
O	-3.41718	4.85751	0.00000
H	-2.89827	-1.60941	0.00000
H	2.89827	1.60941	0.00000
H	1.60941	-2.89827	0.00000
H	-1.60941	2.89827	0.00000
H	-7.00213	-1.80968	0.00000
H	7.00213	1.80968	0.00000
H	1.80968	-7.00213	0.00000

H	-1.80968	7.00213	0.00000
H	-6.58016	3.02418	0.00000
H	6.58016	-3.02418	0.00000
H	-3.02418	-6.58016	0.00000
H	3.02418	6.58016	0.00000

18, U_{t4}

Sum of electronic and zero-point energy: -2550.265540 a.u.

C_{4h}, N_{im}= 3 (18*i* cm^{-1}, 7*i* cm^{-1},7*i* cm^{-1})

N	-2.18121	2.77216	0.00000
N	2.18121	-2.77216	0.00000
N	-2.77216	-2.18121	0.00000
N	2.77216	2.18121	0.00000
C	-0.84805	3.18860	0.00000
C	0.84805	-3.18860	0.00000
C	-3.18860	-0.84805	0.00000
C	3.18860	0.84805	0.00000
C	-0.73468	4.60436	0.00000
C	0.73468	-4.60436	0.00000
C	-4.60436	-0.73468	0.00000
C	4.60436	0.73468	0.00000
C	-1.83092	5.42509	0.00000
C	1.83092	-5.42509	0.00000
C	-5.42509	-1.83092	0.00000
C	5.42509	1.83092	0.00000
N	-3.10315	4.90705	0.00000
N	3.10315	-4.90705	0.00000
N	-4.90705	-3.10315	0.00000
N	4.90705	3.10315	0.00000
C	-3.31350	3.54483	0.00000
C	3.31350	-3.54483	0.00000
C	-3.54483	-3.31350	0.00000
C	3.54483	3.31350	0.00000
O	-4.44312	3.06865	0.00000
O	4.44312	-3.06865	0.00000
O	-3.06865	-4.44312	0.00000
O	3.06865	4.44312	0.00000
O	0.05436	2.36712	0.00000
O	-0.05436	-2.36712	0.00000
O	-2.36712	0.05436	0.00000
O	2.36712	-0.05436	0.00000
N	0.36263	5.45558	0.00000
N	-0.36263	-5.45558	0.00000
N	-5.45558	0.36263	0.00000
N	5.45558	-0.36263	0.00000
C	-0.15822	6.69042	0.00000
C	0.15822	-6.69042	0.00000
C	-6.69042	-0.15822	0.00000
C	6.69042	0.15822	0.00000
N	-1.48348	6.73401	0.00000

N	1.48348	-6.73401	0.00000
N	-6.73401	-1.48348	0.00000
N	6.73401	1.48348	0.00000
H	-2.32323	1.74820	0.00000
H	2.32323	-1.74820	0.00000
H	-1.74820	-2.32323	0.00000
H	1.74820	2.32323	0.00000
H	-3.91416	5.50526	0.00000
H	3.91416	-5.50526	0.00000
H	-5.50526	-3.91416	0.00000
H	5.50526	3.91416	0.00000
H	1.35181	5.17705	0.00000
H	-1.35181	-5.17705	0.00000
H	-5.17705	1.35181	0.00000
H	5.17705	-1.35181	0.00000
O	0.62957	7.75706	0.00000
O	-0.62957	-7.75706	0.00000
O	-7.75706	0.62957	0.00000
O	7.75706	-0.62957	0.00000
H	0.06391	8.53501	0.00000
H	-0.06391	-8.53501	0.00000
H	-8.53501	0.06391	0.00000
H	8.53501	-0.06391	0.00000

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Sum of electronic and zero-point energy: -2481.100125 a.u.

C_{4h}, N_{im}= 1(11*i* cm^{-1})

N	-2.77841	2.24946	0.00000
N	2.77841	-2.24946	0.00000
N	-2.24946	-2.77841	0.00000
N	2.24946	2.77841	0.00000
C	-3.26111	0.95226	0.00000
C	3.26111	-0.95226	0.00000
C	-0.95226	-3.26111	0.00000
C	0.95226	3.26111	0.00000
C	-4.70957	0.86121	0.00000
C	4.70957	-0.86121	0.00000
C	-0.86121	-4.70957	0.00000
C	0.86121	4.70957	0.00000
C	-5.58479	1.92300	0.00000
C	5.58479	-1.92300	0.00000
C	-1.92300	-5.58479	0.00000
C	1.92300	5.58479	0.00000
C	-5.08510	3.29976	0.00000
C	5.08510	-3.29976	0.00000
C	-3.29976	-5.08510	0.00000
C	3.29976	5.08510	0.00000
C	-3.51907	3.41001	0.00000
C	3.51907	-3.41001	0.00000

C	-3.41001	-3.51907	0.00000
C	3.41001	3.51907	0.00000
O	-2.98495	4.49547	0.00000
O	2.98495	-4.49547	0.00000
O	-4.49547	-2.98495	0.00000
O	4.49547	2.98495	0.00000
O	-2.50086	0.00606	0.00000
O	2.50086	-0.00606	0.00000
O	-0.00606	-2.50086	0.00000
O	0.00606	2.50086	0.00000
N	-5.47549	-0.26057	0.00000
N	5.47549	0.26057	0.00000
N	0.26057	-5.47549	0.00000
N	-0.26057	5.47549	0.00000
C	-6.76536	0.16940	0.00000
C	6.76536	-0.16940	0.00000
C	-0.16940	-6.76536	0.00000
C	0.16940	6.76536	0.00000
N	-6.87151	1.47968	0.00000
N	6.87151	-1.47968	0.00000
N	-1.47968	-6.87151	0.00000
N	1.47968	6.87151	0.00000
H	-1.75563	2.35015	0.00000
H	1.75563	-2.35015	0.00000
H	-2.35015	-1.75563	0.00000
H	2.35015	1.75563	0.00000
O	-5.73196	4.30604	0.00000
O	5.73196	-4.30604	0.00000
O	-4.30604	-5.73196	0.00000
O	4.30604	5.73196	0.00000
H	-5.13949	-1.22963	0.00000
H	5.13949	1.22963	0.00000
H	1.22963	-5.13949	0.00000
H	-1.22963	5.13949	0.00000
H	-7.59442	-0.52207	0.00000
H	7.59442	0.52207	0.00000
H	0.52207	-7.59442	0.00000
H	-0.52207	7.59442	0.00000

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Sum of electronic and zero-point energy: -2401.564924 a.u.

C_{4h}, N_{im}= 1(6*i* cm^{-1})

N	-2.77800	2.25580	0.00000
N	2.77800	-2.25580	0.00000
N	-2.25580	-2.77800	0.00000
N	2.25580	2.77800	0.00000
C	-3.25658	0.94850	0.00000
C	3.25658	-0.94850	0.00000
C	-0.94850	-3.25658	0.00000

C	0.94850	3.25658	0.00000
C	-4.69668	0.85403	0.00000
C	4.69668	-0.85403	0.00000
C	-0.85403	-4.69668	0.00000
C	0.85403	4.69668	0.00000
C	-5.56586	1.91948	0.00000
C	5.56586	-1.91948	0.00000
C	-1.91948	-5.56586	0.00000
C	1.91948	5.56586	0.00000
C	-5.05345	3.28730	0.00000
C	5.05345	-3.28730	0.00000
C	-3.28730	-5.05345	0.00000
C	3.28730	5.05345	0.00000
C	-3.52320	3.40371	0.00000
C	3.52320	-3.40371	0.00000
C	-3.40371	-3.52320	0.00000
C	3.40371	3.52320	0.00000
O	-2.99549	4.50205	0.00000
O	2.99549	-4.50205	0.00000
O	-4.50205	-2.99549	0.00000
O	4.50205	2.99549	0.00000
O	-2.48226	0.01253	0.00000
O	2.48226	-0.01253	0.00000
O	-0.01253	-2.48226	0.00000
O	0.01253	2.48226	0.00000
N	-5.46979	-0.26943	0.00000
N	5.46979	0.26943	0.00000
N	0.26943	-5.46979	0.00000
N	-0.26943	5.46979	0.00000
C	-6.75215	0.16846	0.00000
C	6.75215	-0.16846	0.00000
C	-0.16846	-6.75215	0.00000
C	0.16846	6.75215	0.00000
N	-6.85251	1.48197	0.00000
N	6.85251	-1.48197	0.00000
N	-1.48197	-6.85251	0.00000
N	1.48197	6.85251	0.00000
H	-1.75453	2.35880	0.00000
H	1.75453	-2.35880	0.00000
H	-2.35880	-1.75453	0.00000
H	2.35880	1.75453	0.00000
N	-5.77670	4.32471	0.00000
N	5.77670	-4.32471	0.00000
N	-4.32471	-5.77670	0.00000
N	4.32471	5.77670	0.00000
H	-5.13737	-1.23840	0.00000
H	5.13737	1.23840	0.00000
H	1.23840	-5.13737	0.00000
H	-1.23840	5.13737	0.00000

H	-7.58775	-0.51515	0.00000
H	7.58775	0.51515	0.00000
H	0.51515	-7.58775	0.00000
H	-0.51515	7.58775	0.00000
H	-5.17463	5.15301	0.00000
H	5.17463	-5.15301	0.00000
H	-5.15301	-5.17463	0.00000
H	5.15301	5.17463	0.00000

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Sum of electronic and zero-point energy: -3772.972131 a.u.

C_{4h}, N_{im}= 1(10*i* cm^{-1})

N	-2.77077	2.26295	0.00000
N	2.77077	-2.26295	0.00000
N	-2.26295	-2.77077	0.00000
N	2.26295	2.77077	0.00000
C	-3.24204	0.96278	0.00000
C	3.24204	-0.96278	0.00000
C	-0.96278	-3.24204	0.00000
C	0.96278	3.24204	0.00000
C	-4.68567	0.87627	0.00000
C	4.68567	-0.87627	0.00000
C	-0.87627	-4.68567	0.00000
C	0.87627	4.68567	0.00000
C	-5.54218	1.95572	0.00000
C	5.54218	-1.95572	0.00000
C	-1.95572	-5.54218	0.00000
C	1.95572	5.54218	0.00000
C	-5.04091	3.31581	0.00000
C	5.04091	-3.31581	0.00000
C	-3.31581	-5.04091	0.00000
C	3.31581	5.04091	0.00000
C	-3.50851	3.42819	0.00000
C	3.50851	-3.42819	0.00000
C	-3.42819	-3.50851	0.00000
C	3.42819	3.50851	0.00000
O	-2.94314	4.50139	0.00000
O	2.94314	-4.50139	0.00000
O	-4.50139	-2.94314	0.00000
O	4.50139	2.94314	0.00000
O	-2.47685	0.01929	0.00000
O	2.47685	-0.01929	0.00000
O	-0.01929	-2.47685	0.00000
O	0.01929	2.47685	0.00000
N	-5.46472	-0.23538	0.00000
N	5.46472	0.23538	0.00000
N	0.23538	-5.46472	0.00000
N	-0.23538	5.46472	0.00000
C	-6.74806	0.21390	0.00000

C	6.74806	-0.21390	0.00000
C	-0.21390	-6.74806	0.00000
C	0.21390	6.74806	0.00000
N	-6.83635	1.52419	0.00000
N	6.83635	-1.52419	0.00000
N	-1.52419	-6.83635	0.00000
N	1.52419	6.83635	0.00000
H	-1.74838	2.36892	0.00000
H	1.74838	-2.36892	0.00000
H	-2.36892	-1.74838	0.00000
H	2.36892	1.74838	0.00000
S	-5.94875	4.65531	0.00000
S	5.94875	-4.65531	0.00000
S	-4.65531	-5.94875	0.00000
S	4.65531	5.94875	0.00000
H	-5.13807	-1.20815	0.00000
H	5.13807	1.20815	0.00000
H	1.20815	-5.13807	0.00000
H	-1.20815	5.13807	0.00000
H	-7.58715	-0.46536	0.00000
H	7.58715	0.46536	0.00000
H	0.46536	-7.58715	0.00000
H	-0.46536	7.58715	0.00000

22, $[8H]_3X$

Sum of electronic and zero-point energy: -2249.341806 a.u.

C_s, N_{im}=1 (17*i* cm^{-1})

C	-4.09285	-0.03078	0.00000
C	4.43018	0.26841	0.00000
C	1.30093	4.88673	0.00000
C	-5.46317	-0.05505	0.00000
C	5.79896	0.36946	0.00000
C	0.53927	6.03023	0.00000
N	-6.27827	1.02227	0.00000
N	6.68386	-0.64953	0.00000
N	-0.83506	5.96551	0.00000
C	-5.62868	2.15114	0.00000
C	6.10842	-1.81712	0.00000
C	-1.48302	4.75659	0.00000
C	-3.38701	1.19678	0.00000
C	3.80711	-1.00692	0.00000
C	0.71802	3.58181	0.00000
N	-4.27813	2.27499	0.00000
N	4.77063	-2.02472	0.00000
N	-0.67467	3.64236	0.00000
N	-5.82943	-1.38320	0.00000
N	6.09480	1.71134	0.00000
N	1.30031	7.14292	0.00000
O	-2.70776	4.68069	0.00000

O	-2.17058	1.34648	0.00000
O	2.60463	-1.24726	0.00000
O	1.29619	2.50610	0.00000
H	-3.83470	3.20473	0.00000
H	4.41572	-2.99592	0.00000
H	-1.18052	2.73961	0.00000
N	-3.63568	-1.32776	0.00000
N	3.90540	1.54826	0.00000
N	2.60407	5.32503	0.00000
C	-4.69087	-2.18817	0.00000
C	4.92251	2.45754	0.00000
C	2.54111	6.66714	0.00000
O	-4.65766	-3.41545	0.00000
O	4.85420	3.68238	0.00000
H	-2.65555	-1.65449	0.00000
H	2.91403	1.82097	0.00000
H	3.44838	4.73065	0.00000
H	-1.39800	6.80154	0.00000
H	-6.76798	-1.74546	0.00000
H	7.01347	2.12154	0.00000
H	3.42788	7.28222	0.00000
H	-6.18457	3.08174	0.00000
H	6.72043	-2.71192	0.00000
C	0.27634	-4.30828	0.00000
C	0.38494	-5.67424	0.00000
N	-0.63920	-6.55447	0.00000
C	-1.80649	-5.97697	0.00000
C	-0.99257	-3.68253	0.00000
N	-2.01638	-4.63673	0.00000
N	1.73199	-5.95835	0.00000
O	-1.20753	-2.47525	0.00000
H	-2.98347	-4.27335	0.00000
N	1.54433	-3.77003	0.00000
C	2.46565	-4.77435	0.00000
O	3.68882	-4.67324	0.00000
H	1.81076	-2.77285	0.00000
H	2.15189	-6.87265	0.00000
H	-2.70098	-6.58922	0.00000

23, $[8H]_2X_2$

Sum of electronic and zero-point energy: -2249.346742 a.u.

C_{2h}, N_{im}=1 (15*i* cm^{-1})

C	-4.16773	-0.12817	0.00000
C	4.16773	0.12817	0.00000
C	-1.23165	-4.76169	0.00000
C	1.23165	4.76169	0.00000
C	-5.53876	-0.12864	0.00000
C	5.53876	0.12864	0.00000
C	-0.48927	-5.91783	0.00000

C	0.48927	5.91783	0.00000
N	-6.34088	0.95806	0.00000
N	6.34088	-0.95806	0.00000
N	0.88662	-5.87727	0.00000
N	-0.88662	5.87727	0.00000
C	-5.67752	2.07826	0.00000
C	5.67752	-2.07826	0.00000
C	1.55683	-4.67989	0.00000
C	-1.55683	4.67989	0.00000
C	-3.44701	1.09268	0.00000
C	3.44701	-1.09268	0.00000
C	-0.62163	-3.47006	0.00000
C	0.62163	3.47006	0.00000
N	-4.32626	2.18261	0.00000
N	4.32626	-2.18261	0.00000
N	0.76758	-3.55332	0.00000
N	-0.76758	3.55332	0.00000
N	-5.92915	-1.44819	0.00000
N	5.92915	1.44819	0.00000
N	-1.26977	-7.01729	0.00000
N	1.26977	7.01729	0.00000
O	2.78239	-4.62130	0.00000
O	-2.78239	4.62130	0.00000
O	-2.23039	1.23500	0.00000
O	2.23039	-1.23500	0.00000
O	-1.17460	-2.38133	0.00000
O	1.17460	2.38133	0.00000
H	-3.87576	3.10915	0.00000
H	3.87576	-3.10915	0.00000
H	1.28029	-2.65351	0.00000
H	-1.28029	2.65351	0.00000
N	-3.73434	-1.43771	0.00000
N	3.73434	1.43771	0.00000
N	-2.54330	-5.17733	0.00000
N	2.54330	5.17733	0.00000
C	-4.80939	-2.27501	0.00000
C	4.80939	2.27501	0.00000
C	-2.50215	-6.52078	0.00000
C	2.50215	6.52078	0.00000
O	-4.81575	-3.50228	0.00000
O	4.81575	3.50228	0.00000
H	-2.75737	-1.76591	0.00000
H	2.75737	1.76591	0.00000
H	-3.38183	-4.57527	0.00000
H	3.38183	4.57527	0.00000
H	1.43386	-6.72376	0.00000
H	-1.43386	6.72376	0.00000
H	-6.87422	-1.79324	0.00000
H	6.87422	1.79324	0.00000

H	-3.39920	-7.12079	0.00000
H	3.39920	7.12079	0.00000
H	-6.22067	3.01640	0.00000
H	6.22067	-3.01640	0.00000

24, $[8H]X_3$

Sum of electronic and zero-point energy: -2249.348726 a.u.

C_s, N_{im}=1 (21*i* cm^{-1})

C	-1.71730	-3.86594	0.00000
C	0.83666	4.52334	0.00000
C	-4.66076	0.74449	0.00000
C	4.78960	-0.77805	0.00000
C	-2.28380	-5.11295	0.00000
C	1.93385	5.34758	0.00000
C	-5.41029	1.89536	0.00000
C	5.62157	-1.86979	0.00000
N	-1.62082	-6.29043	0.00000
N	3.20837	4.82659	0.00000
N	-4.80743	3.13161	0.00000
N	5.11097	-3.15012	0.00000
C	-0.32695	-6.14830	0.00000
C	3.41558	3.46896	0.00000
C	-3.44106	3.25351	0.00000
C	3.75332	-3.36714	0.00000
C	-0.31035	-3.71184	0.00000
C	0.94825	3.10012	0.00000
C	-3.23203	0.76812	0.00000
C	3.36912	-0.90670	0.00000
N	0.32663	-4.95899	0.00000
N	2.28119	2.69113	0.00000
N	-2.73361	2.07212	0.00000
N	2.97236	-2.23675	0.00000
N	-3.64655	-4.92101	0.00000
N	1.58194	6.65026	0.00000
N	-6.73340	1.63699	0.00000
N	6.92141	-1.50580	0.00000
O	-2.89560	4.35134	0.00000
O	3.26574	-4.49274	0.00000
O	0.30894	-2.65610	0.00000
O	0.04199	2.28416	0.00000
O	-2.47317	-0.18785	0.00000
O	2.53740	-0.01443	0.00000
H	1.35499	-4.93128	0.00000
H	2.43550	1.66991	0.00000
H	-1.70611	2.16591	0.00000
H	1.94825	-2.39687	0.00000
N	-2.72654	-2.92659	0.00000
N	-0.24855	5.36538	0.00000
N	-5.57991	-0.28034	0.00000

N	5.62182	0.31514	0.00000
C	-3.93457	-3.55818	0.00000
C	0.25394	6.61286	0.00000
C	-6.78754	0.30976	0.00000
C	6.87368	-0.17828	0.00000
O	-5.05282	-3.05407	0.00000
H	-2.61269	-1.90209	0.00000
H	-1.23127	5.06539	0.00000
H	-5.38405	-1.29362	0.00000
H	5.31466	1.29540	0.00000
H	-5.35365	3.97877	0.00000
H	5.71828	-3.95453	0.00000
H	-4.35344	-5.63703	0.00000
H	-7.70307	-0.26170	0.00000
H	7.74327	0.46076	0.00000
H	0.30349	-7.03007	0.00000
O	4.54355	2.98685	0.00000
H	4.01862	5.42604	0.00000
H	-0.37846	7.48730	0.00000

25, U_2X_2

Sum of electronic and zero-point energy: -2399.815874 a.u.

C_{2h}, N_{im}=1 (16*i* cm^{-1})

N	-2.76441	-2.16651	0.00000
N	2.76441	2.16651	0.00000
N	2.21426	-2.79554	0.00000
N	-2.21426	2.79554	0.00000
C	-3.18599	-0.84261	0.00000
C	3.18599	0.84261	0.00000
C	0.88497	-3.24426	0.00000
C	-0.88497	3.24426	0.00000
C	-4.60928	-0.73899	0.00000
C	4.60928	0.73899	0.00000
C	0.78436	-4.66378	0.00000
C	-0.78436	4.66378	0.00000
C	-5.42520	-1.84249	0.00000
C	5.42520	1.84249	0.00000
C	1.90085	-5.43601	0.00000
C	-1.90085	5.43601	0.00000
N	-4.89543	-3.11163	0.00000
N	4.89543	3.11163	0.00000
N	3.16504	-4.91365	0.00000
N	-3.16504	4.91365	0.00000
C	-3.53388	-3.31177	0.00000
C	3.53388	3.31177	0.00000
C	3.35580	-3.54016	0.00000
C	-3.35580	3.54016	0.00000
O	-3.04114	-4.42915	0.00000
O	3.04114	4.42915	0.00000

O	4.48411	-3.06509	0.00000
O	-4.48411	3.06509	0.00000
O	-2.37703	0.07219	0.00000
O	2.37703	-0.07219	0.00000
O	-0.02878	-2.43908	0.00000
O	0.02878	2.43908	0.00000
N	-5.46064	0.34103	0.00000
N	5.46064	-0.34103	0.00000
N	-0.32002	-5.51204	0.00000
N	0.32002	5.51204	0.00000
C	-6.70479	-0.17237	0.00000
C	6.70479	0.17237	0.00000
C	0.09200	-6.81908	0.00000
C	-0.09200	6.81908	0.00000
N	-6.73119	-1.49929	0.00000
N	6.73119	1.49929	0.00000
N	1.51435	-6.74023	0.00000
N	-1.51435	6.74023	0.00000
H	-1.74462	-2.31482	0.00000
H	1.74462	2.31482	0.00000
H	2.33346	-1.76684	0.00000
H	-2.33346	1.76684	0.00000
H	-5.48771	-3.92743	0.00000
H	5.48771	3.92743	0.00000
H	3.99605	-5.48288	0.00000
H	-3.99605	5.48288	0.00000
H	-5.17796	1.32628	0.00000
H	5.17796	-1.32628	0.00000
H	-1.29762	-5.21173	0.00000
H	1.29762	5.21173	0.00000
O	-0.54415	-7.84256	0.00000
O	0.54415	7.84256	0.00000
H	2.08896	-7.56549	0.00000
H	-2.08896	7.56549	0.00000
H	-7.58428	0.45311	0.00000
H	7.58428	-0.45311	0.00000

26, U'$_2$X$_2$

Sum of electronic and zero-point energy: -2399.822464 a.u.

C_{2h}, N_{im}=1 (5*i* cm^{-1})

C	-4.23273	-0.13154	0.00000
C	4.23273	0.13154	0.00000
C	-1.23949	-4.77039	0.00000
C	1.23949	4.77039	0.00000
C	-5.58715	-0.17893	0.00000
C	5.58715	0.17893	0.00000
C	-0.49193	-5.92383	0.00000
C	0.49193	5.92383	0.00000
N	-6.36715	0.93801	0.00000

N	6.36715	-0.93801	0.00000
N	0.88154	-5.87784	0.00000
N	-0.88154	5.87784	0.00000
C	-5.78786	2.21247	0.00000
C	5.78786	-2.21247	0.00000
C	1.54907	-4.67712	0.00000
C	-1.54907	4.67712	0.00000
C	-3.53799	1.11665	0.00000
C	3.53799	-1.11665	0.00000
C	-0.63776	-3.47451	0.00000
C	0.63776	3.47451	0.00000
N	-4.40506	2.21306	0.00000
N	4.40506	-2.21306	0.00000
N	0.75037	-3.55071	0.00000
N	-0.75037	3.55071	0.00000
N	-5.96155	-1.49425	0.00000
N	5.96155	1.49425	0.00000
N	-1.26776	-7.02703	0.00000
N	1.26776	7.02703	0.00000
O	-6.46697	3.20846	0.00000
O	6.46697	-3.20846	0.00000
O	2.76885	-4.61281	0.00000
O	-2.76885	4.61281	0.00000
O	-2.32612	1.25277	0.00000
O	2.32612	-1.25277	0.00000
O	-1.20070	-2.38885	0.00000
O	1.20070	2.38885	0.00000
H	-3.95244	3.13617	0.00000
H	3.95244	-3.13617	0.00000
H	1.26559	-2.65811	0.00000
H	-1.26559	2.65811	0.00000
N	-3.76581	-1.44254	0.00000
N	3.76581	1.44254	0.00000
N	-2.54906	-5.19354	0.00000
N	2.54906	5.19354	0.00000
C	-4.81080	-2.30146	0.00000
C	4.81080	2.30146	0.00000
C	-2.50190	-6.53666	0.00000
C	2.50190	6.53666	0.00000
O	-4.81752	-3.52750	0.00000
O	4.81752	3.52750	0.00000
H	-2.78098	-1.74984	0.00000
H	2.78098	1.74984	0.00000
H	-3.38872	-4.59641	0.00000
H	3.38872	4.59641	0.00000
H	-7.37395	0.91315	0.00000
H	7.37395	-0.91315	0.00000
H	1.43441	-6.72084	0.00000
H	-1.43441	6.72084	0.00000

H	-6.88974	-1.88154	0.00000
H	6.88974	1.88154	0.00000
H	-3.39615	-7.14091	0.00000
H	3.39615	7.14091	0.00000

27, U_4
Sum of electronic and zero-point energy: -2550.286955 a.u.
C_{2h}, N_{im}= 0

C	-3.66028	-2.08791	0.00000
C	3.66028	2.08791	0.00000
C	1.22600	-4.86228	0.00000
C	-1.22600	4.86228	0.00000
C	-4.82661	-2.78160	0.00000
C	4.82661	2.78160	0.00000
C	2.44008	-5.47469	0.00000
C	-2.44008	5.47469	0.00000
N	-6.04856	-2.17903	0.00000
N	6.04856	2.17903	0.00000
N	3.62040	-4.78939	0.00000
N	-3.62040	4.78939	0.00000
C	-6.15599	-0.78544	0.00000
C	6.15599	0.78544	0.00000
C	3.62487	-3.40265	0.00000
C	-3.62487	3.40265	0.00000
C	-3.65449	-0.66152	0.00000
C	3.65449	0.66152	0.00000
C	1.13261	-3.44046	0.00000
C	-1.13261	3.44046	0.00000
N	-4.94419	-0.12002	0.00000
N	4.94419	0.12002	0.00000
N	2.38786	-2.81836	0.00000
N	-2.38786	2.81836	0.00000
N	-4.52642	-4.11318	0.00000
N	4.52642	4.11318	0.00000
N	2.24063	-6.81888	0.00000
N	-2.24063	6.81888	0.00000
O	-7.23008	-0.23658	0.00000
O	7.23008	0.23658	0.00000
O	4.67361	-2.78035	0.00000
O	-4.67361	2.78035	0.00000
O	-2.66106	0.04870	0.00000
O	2.66106	-0.04870	0.00000
O	0.11752	-2.76117	0.00000
O	-0.11752	2.76117	0.00000
H	-4.99519	0.90470	0.00000
H	4.99519	-0.90470	0.00000
H	2.39591	-1.78596	0.00000
H	-2.39591	1.78596	0.00000
N	-2.62207	-3.01499	0.00000

N	2.62207	3.01499	0.00000
N	0.25312	-5.86068	0.00000
N	-0.25312	5.86068	0.00000
C	-3.12646	-4.27354	0.00000
C	3.12646	4.27354	0.00000
C	0.84427	-7.09552	0.00000
C	-0.84427	7.09552	0.00000
O	-2.54875	-5.34855	0.00000
O	2.54875	5.34855	0.00000
H	-1.61238	-2.82485	0.00000
H	1.61238	2.82485	0.00000
H	-0.76185	-5.71362	0.00000
H	0.76185	5.71362	0.00000
H	-6.91753	-2.68828	0.00000
H	6.91753	2.68828	0.00000
H	4.52162	-5.23975	0.00000
H	-4.52162	5.23975	0.00000
H	-5.15490	-4.89853	0.00000
H	5.15490	4.89853	0.00000
O	0.35803	-8.19892	0.00000
O	-0.35803	8.19892	0.00000
H	-2.92678	7.55403	0.00000
H	2.92678	-7.55403	0.00000

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Sum of electronic and zero-point energy: -2782.085929 a.u.

C_{4h}, N_{im}= 0

N	-3.12982	4.29767	0.00000
N	3.12982	-4.29767	0.00000
N	-4.29767	-3.12982	0.00000
N	4.29767	3.12982	0.00000
C	-2.85027	2.95175	0.00000
C	2.85027	-2.95175	0.00000
C	-2.95175	-2.85027	0.00000
C	2.95175	2.85027	0.00000
C	-4.03786	2.09003	0.00000
C	4.03786	-2.09003	0.00000
C	-2.09003	-4.03786	0.00000
C	2.09003	4.03786	0.00000
C	-5.30833	2.56409	0.00000
C	5.30833	-2.56409	0.00000
C	-2.56409	-5.30833	0.00000
C	2.56409	5.30833	0.00000
C	-5.63177	3.97530	0.00000
C	5.63177	-3.97530	0.00000
C	-3.97530	-5.63177	0.00000
C	3.97530	5.63177	0.00000
C	-4.38620	4.90664	0.00000
C	4.38620	-4.90664	0.00000

C	-4.90664	-4.38620	0.00000
C	4.90664	4.38620	0.00000
O	-4.51328	6.09532	0.00000
O	4.51328	-6.09532	0.00000
O	-6.09532	-4.51328	0.00000
O	6.09532	4.51328	0.00000
O	-1.71633	2.50949	0.00000
O	1.71633	-2.50949	0.00000
O	-2.50949	-1.71633	0.00000
O	2.50949	1.71633	0.00000
N	-4.09540	0.72345	0.00000
N	4.09540	-0.72345	0.00000
N	-0.72345	-4.09540	0.00000
N	0.72345	4.09540	0.00000
C	-5.41916	0.31316	0.00000
C	5.41916	-0.31316	0.00000
C	-0.31316	-5.41916	0.00000
C	0.31316	5.41916	0.00000
N	-6.15292	1.48172	0.00000
N	6.15292	-1.48172	0.00000
N	-1.48172	-6.15292	0.00000
N	1.48172	6.15292	0.00000
H	-2.31423	4.93303	0.00000
H	2.31423	-4.93303	0.00000
H	-4.93303	-2.31423	0.00000
H	4.93303	2.31423	0.00000
O	-6.74591	4.42708	0.00000
O	6.74591	-4.42708	0.00000
O	-4.42708	-6.74591	0.00000
O	4.42708	6.74591	0.00000
H	-3.32558	0.05269	0.00000
H	3.32558	-0.05269	0.00000
H	-0.05269	-3.32558	0.00000
H	0.05269	3.32558	0.00000
O	-5.85322	-0.82374	0.00000
O	5.85322	0.82374	0.00000
O	0.82374	-5.85322	0.00000
O	-0.82374	5.85322	0.00000
H	-7.15998	1.50936	0.00000
H	7.15998	-1.50936	0.00000
H	-1.50936	-7.15998	0.00000
H	1.50936	7.15998	0.00000

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Sum of electronic and zero-point energy: -2782.074153 a.u.

C_{4h}, N_{im}= 0

N	-2.76550	2.29673	0.00000
N	2.76550	-2.29673	0.00000
N	-2.29673	-2.76550	0.00000

N	2.29673	2.76550	0.00000
C	-3.30163	1.02099	0.00000
C	3.30163	-1.02099	0.00000
C	-1.02099	-3.30163	0.00000
C	1.02099	3.30163	0.00000
C	-4.75984	0.97285	0.00000
C	4.75984	-0.97285	0.00000
C	-0.97285	-4.75984	0.00000
C	0.97285	4.75984	0.00000
C	-5.54695	2.08102	0.00000
C	5.54695	-2.08102	0.00000
C	-2.08102	-5.54695	0.00000
C	2.08102	5.54695	0.00000
C	-5.01537	3.42615	0.00000
C	5.01537	-3.42615	0.00000
C	-3.42615	-5.01537	0.00000
C	3.42615	5.01537	0.00000
C	-3.45844	3.49044	0.00000
C	3.45844	-3.49044	0.00000
C	-3.49044	-3.45844	0.00000
C	3.49044	3.45844	0.00000
O	-2.89224	4.55405	0.00000
O	2.89224	-4.55405	0.00000
O	-4.55405	-2.89224	0.00000
O	4.55405	2.89224	0.00000
O	-2.58602	0.04188	0.00000
O	2.58602	-0.04188	0.00000
O	-0.04188	-2.58602	0.00000
O	0.04188	2.58602	0.00000
N	-5.56225	-0.12913	0.00000
N	5.56225	0.12913	0.00000
N	0.12913	-5.56225	0.00000
N	-0.12913	5.56225	0.00000
C	-6.90804	0.25945	0.00000
C	6.90804	-0.25945	0.00000
C	-0.25945	-6.90804	0.00000
C	0.25945	6.90804	0.00000
N	-6.84879	1.65677	0.00000
N	6.84879	-1.65677	0.00000
N	-1.65677	-6.84879	0.00000
N	1.65677	6.84879	0.00000
H	-1.74179	2.36344	0.00000
H	1.74179	-2.36344	0.00000
H	-2.36344	-1.74179	0.00000
H	2.36344	1.74179	0.00000
O	-5.66581	4.43712	0.00000
O	5.66581	-4.43712	0.00000
O	-4.43712	-5.66581	0.00000
O	4.43712	5.66581	0.00000

H	-5.25647	-1.10284	0.00000
H	5.25647	1.10284	0.00000
H	1.10284	-5.25647	0.00000
H	-1.10284	5.25647	0.00000
O	-7.88516	-0.43783	0.00000
O	7.88516	0.43783	0.00000
O	0.43783	-7.88516	0.00000
O	-0.43783	7.88516	0.00000
H	-7.66693	2.24383	0.00000
H	7.66693	-2.24383	0.00000
H	-2.24383	-7.66693	0.00000
H	2.24383	7.66693	0.00000

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Sum of electronic and zero-point energy: -2702.551848 a.u.

C_{4h}, N_{im}= 0

N	-2.79186	2.26470	0.00000
N	2.79186	-2.26470	0.00000
N	-2.26470	-2.79186	0.00000
N	2.26470	2.79186	0.00000
C	-3.30459	0.96770	0.00000
C	3.30459	-0.96770	0.00000
C	-0.96770	-3.30459	0.00000
C	0.96770	3.30459	0.00000
C	-4.75015	0.88976	0.00000
C	4.75015	-0.88976	0.00000
C	-0.88976	-4.75015	0.00000
C	0.88976	4.75015	0.00000
C	-5.55040	1.98500	0.00000
C	5.55040	-1.98500	0.00000
C	-1.98500	-5.55040	0.00000
C	1.98500	5.55040	0.00000
C	-5.03317	3.33378	0.00000
C	5.03317	-3.33378	0.00000
C	-3.33378	-5.03317	0.00000
C	3.33378	5.03317	0.00000
C	-3.50745	3.43255	0.00000
C	3.50745	-3.43255	0.00000
C	-3.43255	-3.50745	0.00000
C	3.43255	3.50745	0.00000
O	-2.97276	4.52155	0.00000
O	2.97276	-4.52155	0.00000
O	-4.52155	-2.97276	0.00000
O	4.52155	2.97276	0.00000
O	-2.55394	0.01348	0.00000
O	2.55394	-0.01348	0.00000
O	-0.01348	-2.55394	0.00000
O	0.01348	2.55394	0.00000
N	-5.54826	-0.22819	0.00000

N	5.54826	0.22819	0.00000
N	0.22819	-5.54826	0.00000
N	-0.22819	5.54826	0.00000
C	-6.88761	0.14697	0.00000
C	6.88761	-0.14697	0.00000
C	-0.14697	-6.88761	0.00000
C	0.14697	6.88761	0.00000
N	-6.84343	1.54907	0.00000
N	6.84343	-1.54907	0.00000
N	-1.54907	-6.84343	0.00000
N	1.54907	6.84343	0.00000
H	-1.76806	2.34843	0.00000
H	1.76806	-2.34843	0.00000
H	-2.34843	-1.76806	0.00000
H	2.34843	1.76806	0.00000
N	-5.77886	4.35790	0.00000
N	5.77886	-4.35790	0.00000
N	-4.35790	-5.77886	0.00000
N	4.35790	5.77886	0.00000
H	-5.23228	-1.19713	0.00000
H	5.23228	1.19713	0.00000
H	1.19713	-5.23228	0.00000
H	-1.19713	5.23228	0.00000
O	-7.86623	-0.55383	0.00000
O	7.86623	0.55383	0.00000
O	0.55383	-7.86623	0.00000
O	-0.55383	7.86623	0.00000
H	-7.66473	2.13175	0.00000
H	7.66473	-2.13175	0.00000
H	-2.13175	-7.66473	0.00000
H	2.13175	7.66473	0.00000
H	-5.20495	5.20537	0.00000
H	5.20495	-5.20537	0.00000
H	-5.20537	-5.20495	0.00000
H	5.20537	5.20495	0.00000

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Sum of electronic and zero-point energy: -4073.957480 a.u.

C_{4h}, $N_{im}= 0$

N	-2.80353	2.24757	0.00000
N	2.80353	-2.24757	0.00000
N	-2.24757	-2.80353	0.00000
N	2.24757	2.80353	0.00000
C	-3.30076	0.95920	0.00000
C	3.30076	-0.95920	0.00000
C	-0.95920	-3.30076	0.00000
C	0.95920	3.30076	0.00000
C	-4.75422	0.88439	0.00000
C	4.75422	-0.88439	0.00000

C	-0.88439	-4.75422	0.00000
C	0.88439	4.75422	0.00000
C	-5.55077	1.99235	0.00000
C	5.55077	-1.99235	0.00000
C	-1.99235	-5.55077	0.00000
C	1.99235	5.55077	0.00000
C	-5.05008	3.32808	0.00000
C	5.05008	-3.32808	0.00000
C	-3.32808	-5.05008	0.00000
C	3.32808	5.05008	0.00000
C	-3.52303	3.42828	0.00000
C	3.52303	-3.42828	0.00000
C	-3.42828	-3.52303	0.00000
C	3.42828	3.52303	0.00000
O	-2.95263	4.49294	0.00000
O	2.95263	-4.49294	0.00000
O	-4.49294	-2.95263	0.00000
O	4.49294	2.95263	0.00000
O	-2.56100	-0.00300	0.00000
O	2.56100	0.00300	0.00000
O	0.00300	-2.56100	0.00000
O	-0.00300	2.56100	0.00000
N	-5.54227	-0.22409	0.00000
N	5.54227	0.22409	0.00000
N	0.22409	-5.54227	0.00000
N	-0.22409	5.54227	0.00000
C	-6.89254	0.15291	0.00000
C	6.89254	-0.15291	0.00000
C	-0.15291	-6.89254	0.00000
C	0.15291	6.89254	0.00000
N	-6.84739	1.54813	0.00000
N	6.84739	-1.54813	0.00000
N	-1.54813	-6.84739	0.00000
N	1.54813	6.84739	0.00000
H	-1.78196	2.34328	0.00000
H	1.78196	-2.34328	0.00000
H	-2.34328	-1.78196	0.00000
H	2.34328	1.78196	0.00000
S	-5.98280	4.66195	0.00000
S	5.98280	-4.66195	0.00000
S	-4.66195	-5.98280	0.00000
S	4.66195	5.98280	0.00000
H	-5.22356	-1.19460	0.00000
H	5.22356	1.19460	0.00000
H	1.19460	-5.22356	0.00000
H	-1.19460	5.22356	0.00000
O	-7.86134	-0.55640	0.00000
O	7.86134	0.55640	0.00000
O	0.55640	-7.86134	0.00000

O	-0.55640	7.86134	0.00000
H	-7.66898	2.13128	0.00000
H	7.66898	-2.13128	0.00000
H	-2.13128	-7.66898	0.00000
H	2.13128	7.66898	0.00000

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Sum of electronic and zero-point energy: -2702.618746 a.u.

C_{4h}, N_{im}=1 (7*i* cm^{-1})

O	-4.73942	-2.56652	0.00000
O	4.73942	2.56652	0.00000
O	2.56652	-4.73942	0.00000
O	-2.56652	4.73942	0.00000
C	-5.40687	2.22615	0.00000
C	5.40687	-2.22615	0.00000
C	-2.22615	-5.40687	0.00000
C	2.22615	5.40687	0.00000
N	-4.02150	2.31877	0.00000
N	4.02150	-2.31877	0.00000
N	-2.31877	-4.02150	0.00000
N	2.31877	4.02150	0.00000
C	-3.09212	1.29890	0.00000
C	3.09212	-1.29890	0.00000
C	-1.29890	-3.09212	0.00000
C	1.29890	3.09212	0.00000
N	-3.62126	0.02963	0.00000
N	3.62126	-0.02963	0.00000
N	-0.02963	-3.62126	0.00000
N	0.02963	3.62126	0.00000
C	-4.97348	-0.19099	0.00000
C	4.97348	0.19099	0.00000
C	0.19099	-4.97348	0.00000
C	-0.19099	4.97348	0.00000
C	-5.89520	0.82327	0.00000
C	5.89520	-0.82327	0.00000
C	-0.82327	-5.89520	0.00000
C	0.82327	5.89520	0.00000
N	-7.25023	0.62830	0.00000
N	7.25023	-0.62830	0.00000
N	-0.62830	-7.25023	0.00000
N	0.62830	7.25023	0.00000
C	-7.66054	-0.58518	0.00000
C	7.66054	0.58518	0.00000
C	0.58518	-7.66054	0.00000
C	-0.58518	7.66054	0.00000
N	-6.81925	-1.66492	0.00000
N	6.81925	1.66492	0.00000
N	1.66492	-6.81925	0.00000
N	-1.66492	6.81925	0.00000

C	-5.44402	-1.57248	0.00000
C	5.44402	1.57248	0.00000
C	1.57248	-5.44402	0.00000
C	-1.57248	5.44402	0.00000
H	-7.19236	-2.60511	0.00000
H	7.19236	2.60511	0.00000
H	2.60511	-7.19236	0.00000
H	-2.60511	7.19236	0.00000
O	-1.89647	1.51299	0.00000
O	1.89647	-1.51299	0.00000
O	-1.51299	-1.89647	0.00000
O	1.51299	1.89647	0.00000
H	-3.61813	3.25657	0.00000
H	3.61813	-3.25657	0.00000
H	-3.25657	-3.61813	0.00000
H	3.25657	3.61813	0.00000
H	-2.95145	-0.75347	0.00000
H	2.95145	0.75347	0.00000
H	0.75347	-2.95145	0.00000
H	-0.75347	2.95145	0.00000
H	-8.72164	-0.81023	0.00000
H	8.72164	0.81023	0.00000
H	0.81023	-8.72164	0.00000
H	-0.81023	8.72164	0.00000
O	-6.11205	3.20235	0.00000
O	6.11205	-3.20235	0.00000
O	-3.20235	-6.11205	0.00000
O	3.20235	6.11205	0.00000

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Sum of electronic and zero-point energy: -2702.622173 a.u.

C_{4h}, N_{im}=2 (20*i* cm^{-1}, 10*i* cm^{-1})

O	-2.37642	2.02606	0.00000
O	2.37642	-2.02606	0.00000
O	-2.02606	-2.37642	0.00000
O	2.02606	2.37642	0.00000
C	-7.18035	1.59531	0.00000
C	7.18035	-1.59531	0.00000
C	-1.59531	-7.18035	0.00000
C	1.59531	7.18035	0.00000
N	-6.92943	0.21637	0.00000
N	6.92943	-0.21637	0.00000
N	-0.21637	-6.92943	0.00000
N	0.21637	6.92943	0.00000
C	-5.72059	-0.43827	0.00000
C	5.72059	0.43827	0.00000
C	0.43827	-5.72059	0.00000
C	-0.43827	5.72059	0.00000
N	-4.62867	0.37646	0.00000

N	4.62867	-0.37646	0.00000
N	-0.37646	-4.62867	0.00000
N	0.37646	4.62867	0.00000
C	-4.73569	1.75229	0.00000
C	4.73569	-1.75229	0.00000
C	-1.75229	-4.73569	0.00000
C	1.75229	4.73569	0.00000
C	-5.93649	2.40275	0.00000
C	5.93649	-2.40275	0.00000
C	-2.40275	-5.93649	0.00000
C	2.40275	5.93649	0.00000
N	-6.06433	3.76306	0.00000
N	6.06433	-3.76306	0.00000
N	-3.76306	-6.06433	0.00000
N	3.76306	6.06433	0.00000
C	-4.96298	4.43077	0.00000
C	4.96298	-4.43077	0.00000
C	-4.43077	-4.96298	0.00000
C	4.43077	4.96298	0.00000
N	-3.72287	3.87400	0.00000
N	3.72287	-3.87400	0.00000
N	-3.87400	-3.72287	0.00000
N	3.87400	3.72287	0.00000
C	-3.49099	2.51715	0.00000
C	3.49099	-2.51715	0.00000
C	-2.51715	-3.49099	0.00000
C	2.51715	3.49099	0.00000
H	-2.89446	4.48745	0.00000
H	2.89446	-4.48745	0.00000
H	-4.48745	-2.89446	0.00000
H	4.48745	2.89446	0.00000
O	-5.66810	-1.65926	0.00000
O	5.66810	1.65926	0.00000
O	1.65926	-5.66810	0.00000
O	-1.65926	5.66810	0.00000
H	-7.74454	-0.38199	0.00000
H	7.74454	0.38199	0.00000
H	0.38199	-7.74454	0.00000
H	-0.38199	7.74454	0.00000
H	-3.70258	-0.04259	0.00000
H	3.70258	0.04259	0.00000
H	0.04259	-3.70258	0.00000
H	-0.04259	3.70258	0.00000
H	-4.98632	5.51524	0.00000
H	4.98632	-5.51524	0.00000
H	-5.51524	-4.98632	0.00000
H	5.51524	4.98632	0.00000
O	-8.30349	2.01876	0.00000
O	8.30349	-2.01876	0.00000

O	-2.01876	-8.30349	0.00000
O	2.01876	8.30349	0.00000

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Sum of electronic and zero-point energy: -2702.610868 a.u.

C_{4h}, N_{im}=0

O	-4.72215	-2.52629	0.00000
O	4.72215	2.52629	0.00000
O	2.52629	-4.72215	0.00000
O	-2.52629	4.72215	0.00000
C	-5.36842	2.23873	0.00000
C	5.36842	-2.23873	0.00000
C	-2.23873	-5.36842	0.00000
C	2.23873	5.36842	0.00000
N	-3.99910	2.35151	0.00000
N	3.99910	-2.35151	0.00000
N	-2.35151	-3.99910	0.00000
N	2.35151	3.99910	0.00000
C	-3.07263	1.31416	0.00000
C	3.07263	-1.31416	0.00000
C	-1.31416	-3.07263	0.00000
C	1.31416	3.07263	0.00000
N	-3.60034	0.04569	0.00000
N	3.60034	-0.04569	0.00000
N	-0.04569	-3.60034	0.00000
N	0.04569	3.60034	0.00000
C	-4.94884	-0.18811	0.00000
C	4.94884	0.18811	0.00000
C	0.18811	-4.94884	0.00000
C	-0.18811	4.94884	0.00000
C	-5.82297	0.84679	0.00000
C	5.82297	-0.84679	0.00000
C	-0.84679	-5.82297	0.00000
C	0.84679	5.82297	0.00000
N	-7.17168	0.60551	0.00000
N	7.17168	-0.60551	0.00000
N	-0.60551	-7.17168	0.00000
N	0.60551	7.17168	0.00000
C	-7.61255	-0.66346	0.00000
C	7.61255	0.66346	0.00000
C	0.66346	-7.61255	0.00000
C	-0.66346	7.61255	0.00000
N	-6.84929	-1.71098	0.00000
N	6.84929	1.71098	0.00000
N	1.71098	-6.84929	0.00000
N	-1.71098	6.84929	0.00000
C	-5.47657	-1.56765	0.00000
C	5.47657	1.56765	0.00000
C	1.56765	-5.47657	0.00000

C	-1.56765	5.47657	0.00000
O	-1.87829	1.52728	0.00000
O	1.87829	-1.52728	0.00000
O	-1.52728	-1.87829	0.00000
O	1.52728	1.87829	0.00000
H	-3.58683	3.29137	0.00000
H	3.58683	-3.29137	0.00000
H	-3.29137	-3.58683	0.00000
H	3.29137	3.58683	0.00000
H	-2.93205	-0.73919	0.00000
H	2.93205	0.73919	0.00000
H	0.73919	-2.93205	0.00000
H	-0.73919	2.93205	0.00000
H	-8.69096	-0.79226	0.00000
H	8.69096	0.79226	0.00000
H	0.79226	-8.69096	0.00000
H	-0.79226	8.69096	0.00000
O	-6.13953	3.17524	0.00000
O	6.13953	-3.17524	0.00000
O	-3.17524	-6.13953	0.00000
O	3.17524	6.13953	0.00000
H	-7.78947	1.40760	0.00000
H	7.78947	-1.40760	0.00000
H	-1.40760	-7.78947	0.00000
H	1.40760	7.78947	0.00000

35, [2467P']$_4$

Sum of electronic and zero-point energy: -3003.534819 a.u.

C_{4h}, N_{im}=1 (3*i* cm^{-1})

H	-7.93352	1.02414	0.00000
H	7.93352	-1.02414	0.00000
H	-1.02414	-7.93352	0.00000
H	1.02414	7.93352	0.00000
C	-3.55205	0.01434	0.00000
C	3.55205	-0.01434	0.00000
C	-0.01434	-3.55205	0.00000
C	0.01434	3.55205	0.00000
N	-3.29831	1.37888	0.00000
N	3.29831	-1.37888	0.00000
N	-1.37888	-3.29831	0.00000
N	1.37888	3.29831	0.00000
C	-4.22389	2.38850	0.00000
C	4.22389	-2.38850	0.00000
C	-2.38850	-4.22389	0.00000
C	2.38850	4.22389	0.00000
N	-5.53622	1.95900	0.00000
N	5.53622	-1.95900	0.00000
N	-1.95900	-5.53622	0.00000
N	1.95900	5.53622	0.00000

C	-5.88904	0.63111	0.00000
C	5.88904	-0.63111	0.00000
C	-0.63111	-5.88904	0.00000
C	0.63111	5.88904	0.00000
C	-4.95142	-0.34585	0.00000
C	4.95142	0.34585	0.00000
C	0.34585	-4.95142	0.00000
C	-0.34585	4.95142	0.00000
N	-5.33420	-1.68402	0.00000
N	5.33420	1.68402	0.00000
N	1.68402	-5.33420	0.00000
N	-1.68402	5.33420	0.00000
C	-6.63121	-2.11496	0.00000
C	6.63121	2.11496	0.00000
C	2.11496	-6.63121	0.00000
C	-2.11496	6.63121	0.00000
C	-7.70015	-1.00337	0.00000
C	7.70015	1.00337	0.00000
C	1.00337	-7.70015	0.00000
C	-1.00337	7.70015	0.00000
N	-7.22040	0.30706	0.00000
N	7.22040	-0.30706	0.00000
N	-0.30706	-7.22040	0.00000
N	0.30706	7.22040	0.00000
O	-8.87543	-1.23190	0.00000
O	8.87543	1.23190	0.00000
O	1.23190	-8.87543	0.00000
O	-1.23190	8.87543	0.00000
O	-3.94949	3.57086	0.00000
O	3.94949	-3.57086	0.00000
O	-3.57086	-3.94949	0.00000
O	3.57086	3.94949	0.00000
H	-2.31987	1.68521	0.00000
H	2.31987	-1.68521	0.00000
H	-1.68521	-2.31987	0.00000
H	1.68521	2.31987	0.00000
H	-6.22786	2.69339	0.00000
H	6.22786	-2.69339	0.00000
H	-2.69339	-6.22786	0.00000
H	2.69339	6.22786	0.00000
O	-6.96891	-3.26964	0.00000
O	6.96891	3.26964	0.00000
O	3.26964	-6.96891	0.00000
O	-3.26964	6.96891	0.00000
H	-4.60723	-2.40862	0.00000
H	4.60723	2.40862	0.00000
H	2.40862	-4.60723	0.00000
H	-2.40862	4.60723	0.00000
O	-2.63362	-0.78811	0.00000

O	2.63362	0.78811	0.00000
O	0.78811	-2.63362	0.00000
O	-0.78811	2.63362	0.00000

36, [246P]$_4$

Sum of electronic and zero-point energy: -2702.568424 a.u.

C_{4h}, N_{im}=4 (24*i* cm^{-1}, 13*i* cm^{-1}, 6*i* cm^{-1}, 6*i* cm^{-1})

C	-5.37635	2.25378	0.00000
C	5.37635	-2.25378	0.00000
C	-2.25378	-5.37635	0.00000
C	2.25378	5.37635	0.00000
N	-3.99884	2.41086	0.00000
N	3.99884	-2.41086	0.00000
N	-2.41086	-3.99884	0.00000
N	2.41086	3.99884	0.00000
C	-3.03950	1.40692	0.00000
C	3.03950	-1.40692	0.00000
C	-1.40692	-3.03950	0.00000
C	1.40692	3.03950	0.00000
N	-3.52488	0.13833	0.00000
N	3.52488	-0.13833	0.00000
N	-0.13833	-3.52488	0.00000
N	0.13833	3.52488	0.00000
C	-4.86979	-0.14904	0.00000
C	4.86979	0.14904	0.00000
C	0.14904	-4.86979	0.00000
C	-0.14904	4.86979	0.00000
C	-5.78902	0.85169	0.00000
C	5.78902	-0.85169	0.00000
C	-0.85169	-5.78902	0.00000
C	0.85169	5.78902	0.00000
N	-7.12521	0.54721	0.00000
N	7.12521	-0.54721	0.00000
N	-0.54721	-7.12521	0.00000
N	0.54721	7.12521	0.00000
C	-7.59137	-0.74770	0.00000
C	7.59137	0.74770	0.00000
C	0.74770	-7.59137	0.00000
C	-0.74770	7.59137	0.00000
C	-6.49024	-1.74341	0.00000
C	6.49024	1.74341	0.00000
C	1.74341	-6.49024	0.00000
C	-1.74341	6.49024	0.00000
N	-5.22953	-1.47514	0.00000
N	5.22953	1.47514	0.00000
N	1.47514	-5.22953	0.00000
N	-1.47514	5.22953	0.00000
O	-1.84914	1.65895	0.00000
O	1.84914	-1.65895	0.00000
O	-1.65895	-1.84914	0.00000

O	1.65895	1.84914	0.00000
H	-3.63475	3.35770	0.00000
H	3.63475	-3.35770	0.00000
H	-3.35770	-3.63475	0.00000
H	3.35770	3.63475	0.00000
H	-2.84309	-0.63498	0.00000
H	2.84309	0.63498	0.00000
H	0.63498	-2.84309	0.00000
H	-0.63498	2.84309	0.00000
O	-8.76624	-1.04566	0.00000
O	8.76624	1.04566	0.00000
O	1.04566	-8.76624	0.00000
O	-1.04566	8.76624	0.00000
O	-6.15023	3.18556	0.00000
O	6.15023	-3.18556	0.00000
O	-3.18556	-6.15023	0.00000
O	3.18556	6.15023	0.00000
H	-7.79110	1.31204	0.00000
H	7.79110	-1.31204	0.00000
H	-1.31204	-7.79110	0.00000
H	1.31204	7.79110	0.00000
H	-6.80230	-2.78416	0.00000
H	6.80230	2.78416	0.00000
H	2.78416	-6.80230	0.00000
H	-2.78416	6.80230	0.00000

37, [246P']$_4$

Sum of electronic and zero-point energy: -2702.585750 a.u.

C_{4h}, N_{im}=0

C	-3.51962	0.18162	0.00000
C	3.51962	-0.18162	0.00000
C	-0.18162	-3.51962	0.00000
C	0.18162	3.51962	0.00000
N	-3.22974	1.52764	0.00000
N	3.22974	-1.52764	0.00000
N	-1.52764	-3.22974	0.00000
N	1.52764	3.22974	0.00000
C	-4.12515	2.58109	0.00000
C	4.12515	-2.58109	0.00000
C	-2.58109	-4.12515	0.00000
C	2.58109	4.12515	0.00000
N	-5.43806	2.20407	0.00000
N	5.43806	-2.20407	0.00000
N	-2.20407	-5.43806	0.00000
N	2.20407	5.43806	0.00000
C	-5.85515	0.88712	0.00000
C	5.85515	-0.88712	0.00000
C	-0.88712	-5.85515	0.00000
C	0.88712	5.85515	0.00000

C	-4.94711	-0.12632	0.00000
C	4.94711	0.12632	0.00000
C	0.12632	-4.94711	0.00000
C	-0.12632	4.94711	0.00000
N	-5.38088	-1.42679	0.00000
N	5.38088	1.42679	0.00000
N	1.42679	-5.38088	0.00000
N	-1.42679	5.38088	0.00000
C	-6.72168	-1.74689	0.00000
C	6.72168	1.74689	0.00000
C	1.74689	-6.72168	0.00000
C	-1.74689	6.72168	0.00000
C	-7.60109	-0.55177	0.00000
C	7.60109	0.55177	0.00000
C	0.55177	-7.60109	0.00000
C	-0.55177	7.60109	0.00000
N	-7.20532	0.67388	0.00000
N	7.20532	-0.67388	0.00000
N	-0.67388	-7.20532	0.00000
N	0.67388	7.20532	0.00000
O	-3.77314	3.74514	0.00000
O	3.77314	-3.74514	0.00000
O	-3.74514	-3.77314	0.00000
O	3.74514	3.77314	0.00000
H	-2.24227	1.80217	0.00000
H	2.24227	-1.80217	0.00000
H	-1.80217	-2.24227	0.00000
H	1.80217	2.24227	0.00000
H	-6.13592	2.93382	0.00000
H	6.13592	-2.93382	0.00000
H	-2.93382	-6.13592	0.00000
H	2.93382	6.13592	0.00000
O	-7.15403	-2.87939	0.00000
O	7.15403	2.87939	0.00000
O	2.87939	-7.15403	0.00000
O	-2.87939	7.15403	0.00000
O	-2.63912	-0.65968	0.00000
O	2.63912	0.65968	0.00000
O	0.65968	-2.63912	0.00000
O	-0.65968	2.63912	0.00000
H	-4.70016	-2.19960	0.00000
H	4.70016	2.19960	0.00000
H	2.19960	-4.70016	0.00000
H	-2.19960	4.70016	0.00000
H	-8.66866	-0.75316	0.00000
H	8.66866	0.75316	0.00000
H	0.75316	-8.66866	0.00000
H	-0.75316	8.66866	0.00000

38, X•O•X•O
Sum of electronic and zero-point energy: -2360.018154 a.u.
C_{2h}, N_{im}= 2(19*i* cm^{-1}, 19*i* cm^{-1})

C	-5.92550	2.08205	0.00000
C	5.92550	-2.08205	0.00000
C	-1.53948	-5.26614	0.00000
C	1.53948	5.26614	0.00000
C	-5.23130	0.90391	0.00000
C	5.23130	-0.90391	0.00000
C	-0.35868	-4.55401	0.00000
C	0.35868	4.55401	0.00000
C	-3.78708	0.91744	0.00000
C	3.78708	-0.91744	0.00000
C	-0.39347	-3.15005	0.00000
C	0.39347	3.15005	0.00000
N	-3.25583	2.20562	0.00000
N	3.25583	-2.20562	0.00000
N	-1.71200	-2.67216	0.00000
N	1.71200	2.67216	0.00000
N	-5.32865	3.30745	0.00000
N	5.32865	-3.30745	0.00000
N	-2.78592	-4.77607	0.00000
N	2.78592	4.77607	0.00000
C	-3.93923	3.39885	0.00000
C	3.93923	-3.39885	0.00000
C	-2.83072	-3.45730	0.00000
C	2.83072	3.45730	0.00000
O	-3.07397	-0.06922	0.00000
O	3.07397	0.06922	0.00000
O	0.54292	-2.34268	0.00000
O	-0.54292	2.34268	0.00000
H	-2.21427	2.29083	0.00000
H	2.21427	-2.29083	0.00000
H	-1.81998	-1.66001	0.00000
H	1.81998	1.66001	0.00000
O	-3.40562	4.48870	0.00000
O	3.40562	-4.48870	0.00000
N	-4.02037	-2.83248	0.00000
N	4.02037	2.83248	0.00000
N	-7.24216	1.74969	0.00000
N	7.24216	-1.74969	0.00000
N	-1.19990	-6.59108	0.00000
N	1.19990	6.59108	0.00000
H	-8.03375	2.37138	0.00000
H	8.03375	-2.37138	0.00000
H	-1.83911	-7.36708	0.00000
H	1.83911	7.36708	0.00000
C	-7.28343	0.36350	0.00000

C	7.28343	-0.36350	0.00000
C	0.19774	-6.75065	0.00000
C	-0.19774	6.75065	0.00000
N	-6.09961	-0.16520	0.00000
N	6.09961	0.16520	0.00000
N	0.69121	-5.47072	0.00000
N	-0.69121	5.47072	0.00000
H	-4.84794	-3.39942	0.00000
H	4.84794	3.39942	0.00000
H	-4.08873	-1.82371	0.00000
H	4.08873	1.82371	0.00000
O	0.79554	-7.80414	0.00000
O	-0.79554	7.80414	0.00000
H	-8.22198	-0.16902	0.00000
H	8.22198	0.16902	0.00000
H	-5.82602	4.18359	0.00000
H	5.82602	-4.18359	0.00000
H	1.67970	-5.23865	0.00000
H	-1.67970	5.23865	0.00000

39, X•X•O•X
Sum of electronic and zero-point energy: -2304.679876 a.u.
C_s, N_{im}=2 (34*i* cm^{-1}, 9*i* cm^{-1})

N	-2.26071	2.65517	0.00000
N	-2.74054	-2.31348	0.00000
N	2.74853	2.28475	0.00000
C	-0.95739	3.14171	0.00000
C	-3.18466	-1.00009	0.00000
C	3.30849	0.99631	0.00000
C	-0.92412	4.56991	0.00000
C	-4.61054	-0.91623	0.00000
C	4.75291	1.02618	0.00000
C	-2.06288	5.33439	0.00000
C	-5.41239	-2.02966	0.00000
C	5.41332	2.22246	0.00000
N	-3.30329	4.74397	0.00000
N	-4.86412	-3.28858	0.00000
N	4.78375	3.43572	0.00000
C	-3.43543	3.37560	0.00000
C	-3.49721	-3.46914	0.00000
C	3.39571	3.49020	0.00000
O	-4.53703	2.84225	0.00000
O	-2.99672	-4.58060	0.00000
O	2.82939	4.57140	0.00000
O	0.00065	2.38414	0.00000
O	-2.39456	-0.06577	0.00000
O	2.60856	0.01111	0.00000
N	0.11328	5.47163	0.00000
N	-5.47607	0.15223	0.00000

N	5.65053	-0.01692	0.00000
C	-0.45645	6.69107	0.00000
C	-6.71325	-0.37613	0.00000
C	6.82083	0.54400	0.00000
N	-1.78270	6.65519	0.00000
N	-6.72352	-1.70349	0.00000
N	6.73957	1.92625	0.00000
H	-2.36217	1.62238	0.00000
H	-1.71046	-2.44733	0.00000
H	1.71278	2.33386	0.00000
H	-4.14748	5.29476	0.00000
H	-5.44154	-4.11466	0.00000
H	5.26266	4.32183	0.00000
H	1.10717	5.22937	0.00000
H	-5.20245	1.14033	0.00000
H	0.12727	7.59882	0.00000
H	-7.60022	0.23875	0.00000
H	7.77340	0.03722	0.00000
C	2.00038	-5.43223	0.00000
C	0.83062	-4.70612	0.00000
C	0.88678	-3.30148	0.00000
N	2.21407	-2.84177	0.00000
N	3.25722	-4.95494	0.00000
C	3.31629	-3.63931	0.00000
O	-0.03155	-2.48206	0.00000
H	2.31961	-1.82689	0.00000
N	4.52521	-3.03261	0.00000
N	1.64113	-6.75174	0.00000
C	0.23907	-6.89040	0.00000
N	-0.23594	-5.60220	0.00000
H	5.32973	-3.63271	0.00000
H	4.65809	-2.03030	0.00000
O	-0.36979	-7.93657	0.00000
H	7.51520	2.56803	0.00000
H	-1.22351	-5.35222	0.00000
H	2.26608	-7.53910	0.00000

40, G•G•X•O
Sum of electronic and zero-point energy: -2264.890907 a.u.
C_s, N_{im}= 1(8*i* cm^{-1})

N	1.97448	6.19152	0.00000
C	0.60708	6.51639	0.00000
O	0.13809	7.63424	0.00000
N	-0.03593	5.30541	0.00000
C	0.89654	4.26799	0.00000
C	2.15442	4.83449	0.00000
N	3.33208	4.20162	0.00000
C	3.21938	2.88397	0.00000
N	4.32096	2.12138	0.00000

N	2.01332	2.23816	0.00000
C	0.76455	2.87037	0.00000
O	-0.26645	2.18276	0.00000
C	5.65488	-2.89914	0.00000
C	-2.19518	-5.23698	0.00000
C	5.10403	-1.63084	0.00000
C	-0.92388	-4.69378	0.00000
C	3.68428	-1.50601	0.00000
C	-0.78354	-3.27355	0.00000
N	3.05616	-2.75349	0.00000
N	-2.03478	-2.64592	0.00000
N	5.02255	-4.08404	0.00000
N	-3.37865	-4.60239	0.00000
C	3.70850	-3.96022	0.00000
C	-3.24956	-3.29000	0.00000
O	3.02893	-0.46831	0.00000
O	0.24235	-2.60918	0.00000
H	2.02693	-2.73652	0.00000
H	-2.02516	-1.62680	0.00000
N	2.95380	-5.07175	0.00000
N	-4.34147	-2.51287	0.00000
N	7.00565	-2.69111	0.00000
N	-1.99584	-6.59027	0.00000
H	7.71010	-3.40945	0.00000
H	-2.72021	-7.28891	0.00000
C	7.19991	-1.32549	0.00000
C	-0.63662	-6.79814	0.00000
N	6.08431	-0.65895	0.00000
N	0.03588	-5.68387	0.00000
H	3.45585	-5.94165	0.00000
H	-5.23924	-2.96089	0.00000
H	1.93484	-5.09973	0.00000
H	-4.27244	-1.50285	0.00000
H	-0.21179	-7.79042	0.00000
H	8.19016	-0.89502	0.00000
H	2.00970	1.21817	0.00000
H	2.70227	6.88502	0.00000
H	5.21420	2.57784	0.00000
H	4.26241	1.11005	0.00000
H	-1.04438	5.19497	0.00000
C	-5.63045	2.56350	0.00000
C	-5.07890	1.31252	0.00000
C	-3.64306	1.15660	0.00000
N	-2.96156	2.36918	0.00000
N	-4.89298	3.70854	0.00000
C	-3.50132	3.63487	0.00000
O	-3.05655	0.08812	0.00000
H	-1.91300	2.33226	0.00000
O	-2.84576	4.65485	0.00000

N	-6.97708	2.38761	0.00000
H	-7.69025	3.09791	0.00000
C	-7.18056	1.01608	0.00000
N	-6.06666	0.35213	0.00000
H	-8.17511	0.59739	0.00000
H	-5.28209	4.63787	0.00000

41, G•O•X•X

Sum of electronic and zero-point energy: -2284.782191 a.u.

C_s, N_{im}=2 (13*i* cm^{-1}, 4*i* cm^{-1})

N	-2.75169	-2.26288	0.00000
N	2.24218	-2.68619	0.00000
C	-3.30300	-0.97386	0.00000
C	0.93927	-3.15654	0.00000
C	-4.74818	-0.99132	0.00000
C	0.88450	-4.58566	0.00000
C	-5.42123	-2.17992	0.00000
C	2.01069	-5.36882	0.00000
N	-4.80233	-3.39634	0.00000
N	3.25638	-4.79833	0.00000
C	-3.41336	-3.46223	0.00000
C	3.41110	-3.42740	0.00000
O	-2.86277	-4.54955	0.00000
O	4.51539	-2.91612	0.00000
O	-2.60208	0.01282	0.00000
O	-0.01909	-2.39237	0.00000
N	-5.63589	0.06040	0.00000
N	-0.16697	-5.47226	0.00000
C	-6.81238	-0.48820	0.00000
C	0.38275	-6.70073	0.00000
N	-6.74448	-1.87056	0.00000
N	1.70861	-6.68648	0.00000
H	-1.71205	-2.32550	0.00000
H	2.37339	-1.65149	0.00000
H	-5.28658	-4.27959	0.00000
H	4.09474	-5.35786	0.00000
H	-1.15576	-5.21675	0.00000
H	-7.75970	0.02822	0.00000
H	-0.21609	-7.59868	0.00000
C	5.46940	2.01332	0.00000
C	4.72795	0.85299	0.00000
C	3.32425	0.92663	0.00000
N	2.87974	2.25678	0.00000
N	5.01031	3.27335	0.00000
C	3.69160	3.34935	0.00000
O	2.49680	0.01125	0.00000
H	1.86075	2.37947	0.00000

N	3.10884	4.56575	0.00000
N	6.78559	1.63657	0.00000
C	6.90592	0.23453	0.00000
N	5.61318	-0.22368	0.00000
H	3.73023	5.35422	0.00000
H	2.10706	4.73366	0.00000
O	7.94486	-0.38968	0.00000
H	5.34790	-1.20558	0.00000
N	-1.69629	6.76761	0.00000
C	-0.32109	6.82271	0.00000
N	0.22483	5.64143	0.00000
C	-0.84010	4.76588	0.00000
C	-2.04338	5.44492	0.00000
N	-3.29163	4.94092	0.00000
C	-3.30469	3.62393	0.00000
N	-4.48920	2.98118	0.00000
N	-2.17479	2.85177	0.00000
C	-0.85851	3.33845	0.00000
O	0.08238	2.56374	0.00000
H	-2.26586	1.83387	0.00000
H	-2.33769	7.54303	0.00000
H	-5.31180	3.55680	0.00000
H	-4.59926	1.97494	0.00000
H	0.21048	7.76222	0.00000
H	-7.52606	-2.50508	0.00000
H	7.57994	2.25240	0.00000

42, G•O•U'•X
Sum of electronic and zero-point energy: -2360.019025 a.u.
C_s, N_{im}=1 (16*i* cm^{-1})

N	-1.98814	-3.40661	0.00000
N	-4.71977	-0.64636	0.00000
C	-0.71184	-3.97225	0.00000
C	-3.47778	0.00454	0.00000
C	-0.74175	-5.41538	0.00000
C	-3.60774	1.42577	0.00000
C	-1.93814	-6.07727	0.00000
C	-4.84380	1.99781	0.00000
N	-3.14770	-5.44699	0.00000
N	-6.00712	1.28864	0.00000
C	-3.20073	-4.05802	0.00000
C	-5.98804	-0.10327	0.00000
O	-4.27391	-3.48990	0.00000
O	-7.00521	-0.75534	0.00000
O	0.29154	-3.28668	0.00000
O	-2.43754	-0.64100	0.00000
N	0.30333	-6.31175	0.00000
N	-2.67156	2.45975	0.00000
C	-0.25721	-7.48112	0.00000

C	-3.31042	3.65789	0.00000
N	-1.64133	-7.40208	0.00000
N	-4.68820	3.34800	0.00000
H	-2.06039	-2.37156	0.00000
H	-4.68128	-1.66867	0.00000
H	-4.03698	-5.92079	0.00000
H	-6.91612	1.72229	0.00000
H	-1.63531	2.39823	0.00000
H	0.24963	-8.43373	0.00000
O	-2.86807	4.79121	0.00000
C	2.08931	5.47850	0.00000
C	0.91438	4.75719	0.00000
C	0.96553	3.35157	0.00000
N	2.28958	2.88647	0.00000
N	3.34058	4.99990	0.00000
C	3.39577	3.68033	0.00000
O	0.03793	2.53492	0.00000
H	2.40153	1.86691	0.00000
N	4.60377	3.08266	0.00000
N	1.73931	6.80099	0.00000
C	0.34034	6.94844	0.00000
N	-0.14365	5.66571	0.00000
H	5.39889	3.69562	0.00000
H	4.76517	2.08024	0.00000
O	-0.26280	7.99991	0.00000
H	-1.13562	5.43058	0.00000
N	6.86685	-1.67092	0.00000
C	6.91555	-0.29547	0.00000
N	5.73177	0.24439	0.00000
C	4.86095	-0.82412	0.00000
C	5.54618	-2.02477	0.00000
N	5.05025	-3.27566	0.00000
C	3.73366	-3.29610	0.00000
N	3.08466	-4.47347	0.00000
N	2.95633	-2.16592	0.00000
C	3.43407	-0.84875	0.00000
O	2.65168	0.08749	0.00000
H	1.94336	-2.26979	0.00000
H	7.64504	-2.30900	0.00000
H	3.63551	-5.31209	0.00000
H	2.07666	-4.53320	0.00000
H	7.85243	0.24067	0.00000
H	-2.28367	-8.17725	0.00000
H	2.37176	7.58218	0.00000
H	-5.39549	4.06301	0.00000

43, G•O•U•X
Sum of electronic and zero-point energy: -2360.018362 a.u.
C_s, N_{im}=2 (13*i* cm^{-1}, 5*i* cm^{-1})

N	-2.74385	-2.23905	0.00000

N	2.26641	-2.70677	0.00000
C	-3.29167	-0.95185	0.00000
C	0.96281	-3.20723	0.00000
C	-4.73671	-0.96712	0.00000
C	0.91609	-4.63226	0.00000
C	-5.41193	-2.15522	0.00000
C	2.05555	-5.36898	0.00000
N	-4.79673	-3.37228	0.00000
N	3.29451	-4.80481	0.00000
C	-3.40614	-3.44205	0.00000
C	3.43691	-3.41948	0.00000
O	-2.85459	-4.52425	0.00000
O	4.54596	-2.92153	0.00000
O	-2.58850	0.03486	0.00000
O	0.00121	-2.45039	0.00000
N	-5.62304	0.08599	0.00000
N	-0.15603	-5.52356	0.00000
C	-6.80052	-0.46054	0.00000
C	0.29916	-6.81406	0.00000
N	-6.73456	-1.84280	0.00000
N	1.71339	-6.68744	0.00000
H	-1.70857	-2.30924	0.00000
H	2.37554	-1.66763	0.00000
H	-5.28162	-4.25544	0.00000
H	4.14958	-5.33741	0.00000
H	-1.13890	-5.25839	0.00000
H	-7.74695	0.05742	0.00000
O	-0.30858	-7.85785	0.00000
C	5.45795	2.01738	0.00000
C	4.72574	0.85111	0.00000
C	3.32170	0.91243	0.00000
N	2.86540	2.23811	0.00000
N	4.98858	3.27250	0.00000
C	3.66863	3.33768	0.00000
O	2.50318	-0.01203	0.00000
H	1.84544	2.35564	0.00000
N	3.07819	4.54920	0.00000
N	6.77768	1.65178	0.00000
C	6.90992	0.25159	0.00000
N	5.62103	-0.21748	0.00000
H	3.69488	5.34142	0.00000
H	2.07569	4.71349	0.00000
O	7.95314	-0.36576	0.00000
H	5.36618	-1.20094	0.00000
N	-1.70334	6.77873	0.00000
C	-0.32809	6.83196	0.00000
N	0.21604	5.64992	0.00000
C	-0.85001	4.77573	0.00000
C	-2.05247	5.45645	0.00000

N	-3.30076	4.95409	0.00000
C	-3.31508	3.63658	0.00000
N	-4.50002	2.99583	0.00000
N	-2.18582	2.86312	0.00000
C	-0.86993	3.34859	0.00000
O	0.07197	2.57392	0.00000
H	-2.27924	1.84461	0.00000
H	-2.34371	7.55500	0.00000
H	-5.32121	3.57354	0.00000
H	-4.61362	1.98932	0.00000
H	0.20472	7.77076	0.00000
H	-7.51674	-2.47659	0.00000
H	7.56646	2.27483	0.00000
H	2.31864	-7.49035	0.00000