

Electronic Supplementary Information

Benchmarking the inversion barriers in $\sigma^3\lambda^3$ -phosphorus compounds: a computational study

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Computational methods

Hard and soft acid and bases (HSAB) theory^[1] derived parameters such as chemical potential (μ)^[2], softness (S)^[3] and electrophilicity (ω)^[4] were obtained via eqs 1-3:

$$\mu = \left(\frac{\partial E}{\partial N} \right)_V = \frac{1}{2(I+A)} \quad (1)$$

$$\frac{1}{S} = \left(\frac{\partial^2 E}{\partial^2 N} \right)_V = \left(\frac{\partial \mu}{\partial N} \right)_V = I - A \quad (2)$$

$$\omega = \mu^2 S \quad (3)$$

By means of finite difference approximations, all aforementioned properties can be obtained from the vertical ionization potential (I) and the electron affinity (A) which, in turn, are easily accessible from the diabatic energy differences with the system having $N-1$ and $N+1$ electrons, respectively. Local variants of the above global properties are obtained by multiplying them by the Fukui function, $f(r)$,^[5] that can be approximated by the local variation of electric charges upon diabatic one-electron oxidation, in the case of nucleophiles.

Intrinsic group electronegativities were calculated following the procedure of De Proft and Geerlings^[6] with a different level of calculation: for every R group the corresponding hydrogen-linked species (R-H) was optimized at the working RIJCOSX/B3LYP-D3/def2-TZVP level. Thereafter, the H atom was removed and three single point (SP) calculations were carried out with the frozen geometry of the R group: the anion (R^-), the cation (R^+) and the radical ($R\cdot$). With these three energy values, the vertical ionization potential (I) and the electron affinity (A) were calculated using equations 4 and 5, and intrinsic group electronegativities (χ) were subsequently obtained by means of equation 6:

$$I = E_{R^+} - E_R. \quad (4)$$

$$A = E_{R^+} - E_{R^-} \quad (5)$$

$$\chi = \frac{I+A}{2} \quad (6)$$

Table S1. Computed $\Delta\epsilon_{\text{H-L}}$ and HSAB-related magnitudes (au) for compounds **1-43**.

Comp.	$\Delta\epsilon_{\text{H-L}}$	μ	S	ω	$f^{\text{M a)}$	$f^{\text{N b)}$
1	8.2	0.1406	2.0454	0.0404	-1.1617	-0.7406
2	5.4	0.1254	2.9897	0.0470	-0.2499	-0.4319
3	5.1	0.1258	3.4382	0.0544	-0.2082	-0.3455
4	8.5	0.1826	1.9289	0.0643	-0.4757	-0.5872
5	6.5	0.1766	2.5096	0.0783	-0.1896	-0.2711
6	5.3	0.1874	2.9614	0.1040	-0.1445	-0.1633
7	4.0	0.1891	3.6489	0.1305	-0.0955	-0.0563
8a	7.0	0.1100	2.5221	0.0305	-0.3409	-0.6090
8b	6.7	0.1061	2.5688	0.0289	-0.1775	-0.4405
8c	7.1	0.1297	2.3392	0.0394	-0.3717	-0.4768
8d	5.6	0.1375	2.8607	0.0541	-0.1108	-0.1320
9a	6.9	0.1062	2.6208	0.0296	-0.3464	-0.6053
9b	6.3	0.0969	2.8016	0.0263	-0.1971	-0.3048
9c	7.1	0.1149	3.6764	0.0486	-0.2912	-0.4059
9d	5.3	0.1228	3.1160	0.0470	-0.0899	-0.1170
10	6.5	0.1468	2.4147	0.0520	-0.4464	-0.6628
11	6.3	0.1197	2.7850	0.0399	-0.2871	-0.4963
12	6.0	0.1460	2.6794	0.0571	-0.3754	-0.6280
13	5.6	0.1385	2.8420	0.0545	-0.3306	-0.6254
14	5.9	0.1391	2.8071	0.0543	-0.2384	-0.2921
15	5.4	0.1225	3.0120	0.0452	-0.2442	-0.4134
16	5.3	0.1342	3.1897	0.0575	-0.2314	-0.3346
17	5.2	0.1269	3.2646	0.0526	-0.2172	-0.3569
18a	6.9	0.1192	2.4739	0.0352	-0.3865	-0.6099
18b	7.0	0.1168	2.4782	0.0338	-0.2541	-0.3375
18c	6.5	0.1221	2.4984	0.0372	-0.3141	-0.4765

Table S1. Cont.

Comp.	$\Delta\epsilon_{H-L}$	μ	S	ω	$f^{M\ a)}$	$f^{N\ b)}$
18d	6.2	0.1237	2.6574	0.0406	-0.1621	-0.1958
19a	6.9	0.1086	2.5584	0.0302	-0.3426	-0.6096
19b	6.9	0.1091	2.5881	0.0308	-0.2087	-0.3396
19c	6.7	0.1089	2.5215	0.0299	-0.2886	-0.5228
19d	6.2	0.1226	2.7053	0.0407	-0.1772	-0.2851
20	6.0	0.1358	2.5249	0.0466	-0.3724	-0.3917
21	5.8	0.1269	2.6571	0.0428	-0.3225	-0.4067
22a	7.4	0.1385	2.2900	0.0439	-0.4029	-0.5222
22b	6.4	0.1422	2.4563	0.0497	-0.2882	-0.3150
22c	6.3	0.1613	2.4163	0.0628	-0.3434	-0.3915
22d	5.3	0.1453	2.7411	0.0578	-0.2128	-0.2015
23a	7.3	0.1215	2.3591	0.0348	-0.3446	-0.5122
23b	6.7	0.1293	2.4729	0.0413	-0.2501	-0.3288
23c	6.4	0.1423	2.4855	0.0503	-0.2982	-0.4165
23d	5.5	0.1343	2.7555	0.0497	-0.1824	-0.2105
24a	6.5	0.1251	2.5284	0.0396	-0.3821	-0.5377
24b	5.7	0.1221	2.7363	0.0408	-0.2639	-0.2879
24c	6.0	0.1428	2.5865	0.0528	-0.3374	-0.4058
24d	5.3	0.1379	2.8347	0.0539	-0.2038	-0.1992
25a	6.6	0.1090	2.5577	0.0304	-0.3369	-0.5391
25b	5.7	0.1081	2.7942	0.0327	-0.2401	-0.3544
25c	5.9	0.1250	2.6625	0.0416	-0.3012	-0.4323
25d	5.1	0.1231	2.9710	0.0450	-0.1920	-0.2521
26b	6.3	0.1256	2.5859	0.0408	-0.2542	-0.2899
26c	6.4	0.1403	2.5190	0.0496	-0.3619	-0.4569
26d	5.2	0.1380	2.8681	0.0546	-0.2083	-0.2569
27b	6.3	0.1113	2.6283	0.0326	-0.2547	-0.3421

Table S1. Cont.

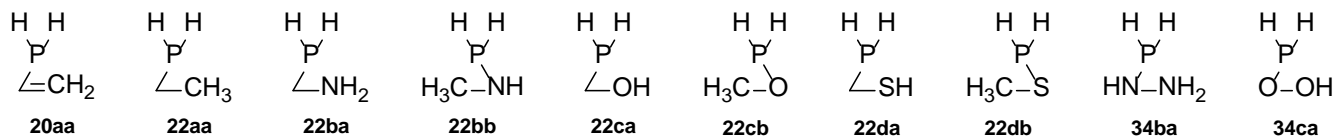
Comp.	$\Delta\epsilon_{\text{H-L}}$	μ	S	ω	$f^{M \text{ a)}}$	$f^{N \text{ b)}}$
27c	6.4	0.1257	2.5562	0.0404	-0.3480	-0.5036
27d	5.4	0.1276	2.8848	0.0470	-0.2067	-0.3065
28a	6.8	0.1238	2.5439	0.0390	-0.4019	-0.5829
28b	6.6	0.1228	2.5797	0.0389	-0.2855	-0.3376
28c	6.7	0.1329	2.4789	0.0438	-0.3758	-0.4934
28d	6.1	0.1256	2.6704	0.0421	-0.1984	-0.1909
29a	6.8	0.1084	2.5971	0.0305	-0.3586	-0.5820
29b	6.6	0.1082	2.6378	0.0309	-0.2739	-0.4038
29c	6.7	0.1135	2.5448	0.0328	-0.3245	-0.4886
29d	6.2	0.1131	2.7161	0.0348	-0.2066	-0.2620
30b	6.7	0.1201	2.5755	0.0372	-0.2360	-0.3045
30c	6.9	0.1285	2.4851	0.0410	-0.3376	-0.4593
30d	6.0	0.1181	2.7228	0.0380	-0.2053	-0.2657
31b	6.9	0.1116	2.5821	0.0322	-0.2659	-0.4224
31c	7.0	0.1145	2.5033	0.0328	-0.3299	-0.5179
31d	6.2	0.1111	2.7042	0.0334	-0.2071	-0.3276
32	5.2	0.1551	2.7550	0.0663	-0.3487	-0.5274
33	5.0	0.1459	2.9765	0.0633	-0.3099	-0.5296
34b	6.6	0.1340	2.4481	0.0440	-0.1179	-0.1147
34c	6.5	0.1254	2.5550	0.0402	-0.1102	-0.0624
35b	6.0	0.1055	2.7177	0.0303	-0.2060	-0.2683
35c	5.9	0.1040	2.7658	0.0299	-0.1938	-0.2608
36b	6.4	0.1062	2.7076	0.0305	-0.1906	-0.2603
36c	6.2	0.0980	2.7868	0.0267	-0.1816	-0.2686
37b	6.0	0.1967	2.3201	0.0898	-0.4071	-0.2017
37c	5.9	0.1824	2.4738	0.0823	-0.1408	-0.1302
38b	6.5	0.1486	2.4299	0.0537	-0.2984	-0.3790

Table S1. Cont.

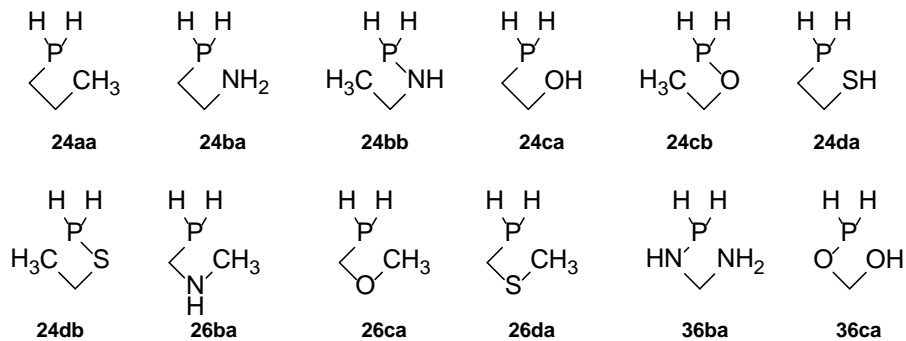
Comp.	$\Delta\epsilon_{H-L}$	μ	S	ω	f^M ^{a)}	f^N ^{b)}
38c	6.4	0.1448	2.4977	0.0524	-0.2733	-0.3657
39b	7.6	0.1350	2.3152	0.0422	-0.3121	-0.4269
39c	7.4	0.1289	2.3644	0.0393	-0.2638	-0.3832
40a	6.8	0.1264	2.4066	0.0384	-0.3411	-0.5662
40b	6.2	0.1369	2.5900	0.0485	-0.2768	-0.4482
40c	6.8	0.1156	2.5174	0.0336	-0.3420	-0.6175
40d	5.8	0.1014	2.8473	0.0293	-0.2119	-0.3474
40e	6.5	0.1169	2.5866	0.0353	-0.3340	-0.5613
41a	5.1	0.1217	3.1854	0.0471	-0.3164	-0.5728
41b	5.1	0.1161	3.2875	0.0443	-0.2753	-0.4483
41c	5.1	0.1154	3.3177	0.0442	-0.2660	-0.4179
41d	4.9	0.1157	3.4399	0.0460	-0.2616	-0.3765
42	5.3	0.1222	3.1179	0.0465	-0.2663	-0.4511
43	5.2	0.1187	3.3663	0.0474	-0.2024	-0.3090

^{a)} Fukui function obtained from Mulliken charges. ^{b)} *Idem* from natural charges.

From 3-membered heterocycles



From 4-membered heterocycles



From 5-membered heterocycles

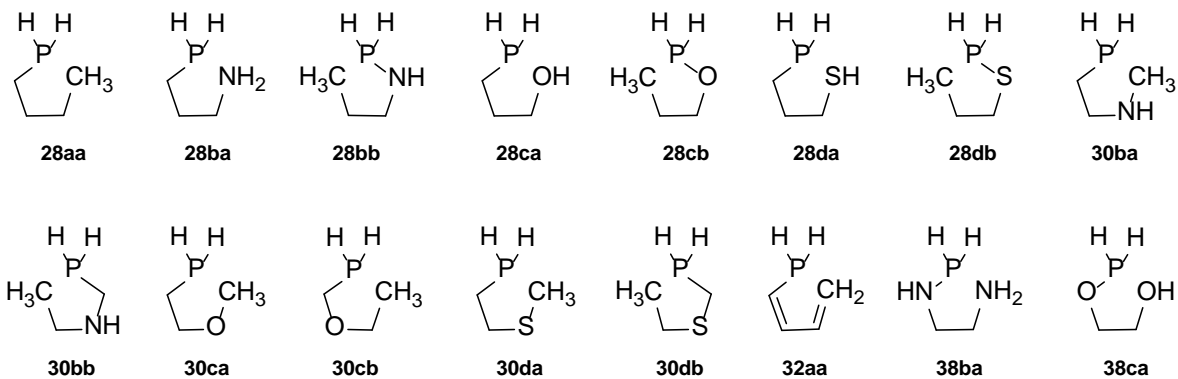


Figure S1. Selected structures for the intrinsic group electronegativity calculation in cyclic compounds.

Table S2. Computed intrinsic group electronegativities χ (eV).

Group	χ	Group	χ	Group	χ
H	6.85	24ca	6.57	38ca	6.75
CH₃	5.19	24cb	4.89		
CH₂=CH	5.23	24da	5.93		
NH₂	6.12	24db	4.92		
OH	8.28	26ba	3.55		
SH	6.78	26ca	4.24		
CH₃-CH₂	4.49	26da	4.28		
CH₃-NH	5.17	28aa	4.60		
CH₃-O	6.75	28ba	5.16		
CH₃-S	5.96	28bb	4.66		
C₆H₅	5.11	28ca	6.31		
F	11.46	28cb	4.76		
Cl	8.64	28da	6.06		
Br	7.99	28db	4.76		
I	7.15	30ba	3.45		
20aa	5.20	30bb	4.64		
22aa	4.73	30ca	4.12		
22ba	5.16	30cb	4.80		
22bb	3.57	30da	4.18		
22ca	6.52	30db	4.88		
22cb	4.44	32aa	5.45		
22da	5.99	34ba	4.72		
22db	4.38	34ca	5.23		
24aa	4.68	36ba	5.30		
24ba	5.29	36ca	5.93		
24bb	4.68	38ba	6.78		

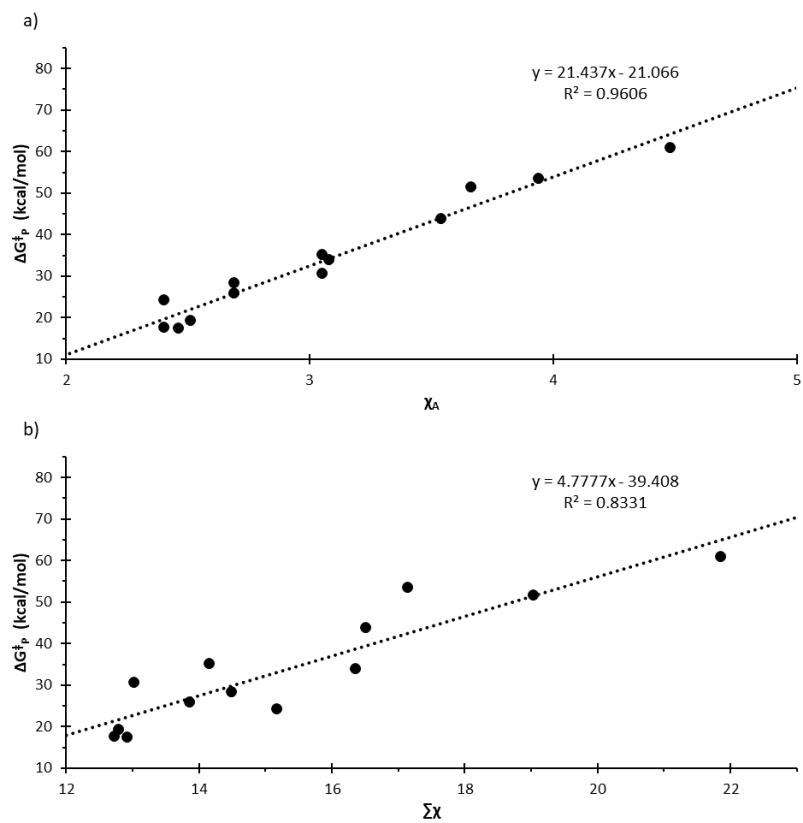


Figure S2. Plot of the P-inversion barrier versus a) Allred heteroatom electronegativity (χ_A) and b) sum of P-substituents intrinsic electronegativity ($\Sigma\chi$) in compounds **19c-d** and **40-43**.

Calculated structures

Cartesian coordinates (in Å), G correction (G-E) and ZPE (in hartrees) for minima and transition states were computed at B3LYP-D3/def2-TZVP(ecp). Electronic energies (in hartrees) are quoted at the (gas-phase) DLPNO-CCSD(T)/def2-TZVPP level unless otherwise stated. Imaginary frequencies are obtained upon frequency calculation (at the optimization level).

1: E = -342.689254623292 au
ZPE = 0.02386624 au
G_{corr} = 0.00386797 au

P	-2.177588	0.290092	-0.000000	H	-1.407939	0.886756	1.032314
H	-1.407363	-0.901797	0.000000	H	-1.407939	0.886756	-1.032313

TS(1^{P-inv}): E = -342.634895414806 au
ZPE = 0.02270566 au
G_{corr} = 0.00282722 au
 $\nu = -1109.09 \text{ cm}^{-1}$

P	-0.788833	-0.622407	0.000000	H	-1.478239	0.573536	-0.000000
H	0.591785	-0.622407	-0.000000	H	-1.478240	-1.818350	-0.000000

2: E = -574.442623436394 au
ZPE = 0.12861493 au
G_{corr} = 0.09554538 au

P	-2.745742	0.296104	-0.027450	H	-0.975248	-1.262098	1.880573
C	-1.802558	-1.260089	-0.064700	H	-0.636731	-2.756404	0.853717
H	-1.916750	-1.827692	-0.985189	C	-2.389514	1.838279	2.239774
C	-1.806953	1.265478	1.192242	H	-3.456571	1.751632	2.410738
H	-0.735008	1.363589	1.037714	H	-1.822855	2.413197	2.964030
C	-2.166799	1.023032	-1.592313	C	-1.780393	2.282088	-1.776715
H	-2.235884	0.357036	-2.449003	H	-1.523900	2.655041	-2.761157
C	-1.103191	-1.782124	0.938403	H	-1.711921	2.987521	-0.956782

TS(2^{P-inv}): E = -574.401649309991 au
ZPE = 0.12743477 au
G_{corr} = 0.09479511 au
 $\nu = -255.03 \text{ cm}^{-1}$

P	0.152265	-0.177267	-0.014996	C	-0.164812	1.538126	-0.070638
C	-1.083123	-1.410197	0.013910	H	0.744773	2.108654	-0.234597
H	-0.644947	-2.404077	0.048696	C	1.811843	-0.735661	-0.027062

H	1.878047	-1.814500	-0.134810	H	-2.272240	1.682565	0.211142
C	-2.417978	-1.284196	-0.000404	H	-1.365594	3.263914	-0.049647
H	-2.920353	-0.329396	-0.033903	C	2.936296	-0.014066	0.063423
H	-3.044329	-2.165466	0.013854	H	3.902095	-0.497337	0.013135
C	-1.333608	2.186296	0.036150	H	2.934649	1.061079	0.185780

3:

E = -1034.5409118531 au

ZPE = 0.27305441 au

G_{corr} = 0.23204781 au

P	0.009264	-0.077873	-0.212586	C	-0.486212	2.590707	0.349800
C	1.831831	-0.007374	0.012799	H	-0.503982	1.377837	-2.812739
C	2.630545	1.072024	-0.368414	H	-1.047300	3.728159	-3.291733
C	4.004621	1.043571	-0.156009	H	-1.214805	5.371554	-1.445841
C	4.600327	-0.066155	0.431792	H	-0.849171	4.632002	0.892064
C	3.813747	-1.148043	0.814310	H	-0.343459	2.270562	1.375477
C	2.440366	-1.112899	0.615330	C	-0.131735	-0.941627	-1.828005
H	2.178402	1.937974	-0.832730	C	-1.381442	-1.472235	-2.160628
H	4.610547	1.890278	-0.453938	C	-1.582688	-2.107306	-3.379316
H	5.670290	-0.087282	0.595534	C	-0.528966	-2.237324	-4.277747
H	4.269234	-2.014386	1.277309	C	0.722613	-1.727900	-3.950121
H	1.829614	-1.951329	0.929632	C	0.920079	-1.081925	-2.735163
C	-0.374324	1.656193	-0.685415	H	-2.201189	-1.384262	-1.457182
C	-0.581383	2.083810	-1.997474	H	-2.558431	-2.508113	-3.623603
C	-0.886461	3.413829	-2.267958	H	-0.680997	-2.738914	-5.225049
C	-0.979020	4.336497	-1.233521	H	1.547955	-1.829329	-4.643893
C	-0.774078	3.920977	0.078893	H	1.895932	-0.683425	-2.492420

TS(3^{P-inv}):

E = -1034.49271774559 au

ZPE = 0.2719313 au

G_{corr} = 0.22840845 au

$\nu = -289.32 \text{ cm}^{-1}$

P	-0.002120	-0.011687	0.003320	C	-2.167758	1.703808	-0.136002
C	1.770690	-0.004485	0.015595	H	0.630620	1.952505	-2.049235
C	2.482486	1.203929	0.091668	H	-0.591107	3.909677	-2.885449
C	3.868665	1.203514	0.084041	H	-2.850965	4.446541	-2.014337
C	4.578454	0.007474	0.035249	H	-3.852553	3.011618	-0.255846
C	3.879648	-1.194541	-0.023524	H	-2.602274	1.106257	0.654159
C	2.493747	-1.206788	-0.050496	C	-0.890691	-1.414982	0.625011
H	1.946392	2.140554	0.165311	C	-2.158539	-1.740361	0.115567
H	4.398246	2.146636	0.136555	C	-0.344779	-2.222602	1.636173
H	5.660323	0.012078	0.042941	C	-2.857864	-2.827759	0.615644
H	4.417934	-2.133107	-0.068645	H	-2.587833	-1.143862	-0.678232
H	1.966797	-2.147956	-0.131669	C	-1.040182	-3.327448	2.103189
C	-0.892526	1.384928	-0.630850	H	0.619941	-1.976537	2.059218
C	-0.340158	2.193828	-1.637439	C	-2.302721	-3.634430	1.604566
C	-1.036616	3.293870	-2.114111	H	-3.836965	-3.058006	0.214436
C	-2.306335	3.594372	-1.629963	H	-0.599653	-3.942056	2.878338
C	-2.867779	2.786257	-0.645792	H	-2.846615	-4.490411	1.981433

4: E = -640.238654083942 au
ZPE = 0.00842149 au
G_{corr} = -0.01769521 au

P	-0.379686	-1.853730	-1.007807	F	-0.677938	-0.844842	-2.188130
F	-1.743681	-1.676924	-0.228561	F	-0.748628	-3.186227	-1.775533

TS(4^{P-inv}): E = -640.151299744596 au
ZPE = 0.00688877 au
G_{corr} = -0.01907162 au
 $\nu = -318.98 \text{ cm}^{-1}$

P	-0.000429	-0.422478	-0.000002	F	-1.649684	-0.363610	0.000001
F	0.001179	1.153113	0.000000	F	1.648935	-0.367025	0.000001

5: E = -1720.14911011365 au
ZPE = 0.00470122 au
G_{corr} = -0.02475261 au

P	0.000000	0.001242	0.732937	Cl	1.591636	-0.921012	-0.215898
Cl	-0.000000	1.840782	-0.215250	Cl	-1.591636	-0.921012	-0.215898

TS(5^{P-inv}): E = -1720.06499490399 au
ZPE = 0.00352513 au
G_{corr} = -0.02594065 au
 $\nu = -264.19 \text{ cm}^{-1}$

P	0.382432	0.213724	-0.000000	Cl	-1.388877	-0.772329	-0.000000
Cl	-0.576384	2.222385	0.000000	Cl	1.582829	-1.663779	0.000000

6: E = -8058.76621292407 au
ZPE = 0.00343623 au
G_{corr} = -0.02948094 au

P	-2.774383	0.160976	0.000007	Br	-1.767036	-1.850167	0.000017
Br	-1.767988	1.162026	1.744270	Br	-1.768053	1.162057	-1.744294

TS(6^{P-inv}): E = -8058.68901815619 au
ZPE = 0.00247336 au
G_{corr} = -0.03055203 au
 $\nu = -242.09 \text{ cm}^{-1}$

P	-0.362707	0.208480	-0.000003	Br	0.588276	2.425926	0.000001
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Br	-1.776597	-1.753770	0.000001	Br	1.551028	-0.880636	0.000002
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7: E = -1228.29484988819 au
ZPE = 0.00275518 au
G_{corr} = -0.03267986 au

P	-2.774817	0.160111	0.000000	I	-1.704417	1.275468	1.939433
I	-1.703809	-2.076157	0.000000	I	-1.704417	1.275468	-1.939433

TS(7^{P-inv}): E = -1228.21918723923 au
ZPE = 0.00192013 au
G_{corr} = -0.03385136 au
 $\nu = -249.43 \text{ cm}^{-1}$

P	0.319218	0.186324	0.000001	I	-1.781911	-1.033141	-0.000000
I	-0.570422	2.681243	-0.000000	I	2.033115	-1.834427	-0.000000

8a: E = -460.426209151875 au
ZPE = 0.11213395 au
G_{corr} = 0.08393501 au

P	-0.000942	0.001311	-0.602216	H	-0.814857	-2.225501	-0.014477
C	-0.503602	1.548845	0.279574	H	-1.009155	-1.122796	1.364953
H	0.156250	2.366594	-0.014668	C	1.590357	-0.337346	0.279852
H	-1.520279	1.820144	-0.009591	H	1.965671	-1.320691	-0.008601
H	-0.463522	1.436235	1.366487	H	2.336140	0.402944	-0.014434
C	-1.088503	-1.210247	0.277774	H	1.473832	-0.308562	1.366715
H	-2.127558	-1.048583	-0.013899				

TS(8a^{P-inv}): E = -460.357083107978 au
ZPE = 0.11069545 au
G_{corr} = 0.08091510 au
 $\nu = -426.79 \text{ cm}^{-1}$

P	0.020268	-0.051181	-0.656035	H	-1.637879	-1.904811	-0.625626
C	-0.031092	1.156721	-2.025526	H	-1.506511	-1.054041	0.925997
H	0.233530	0.746557	-3.001692	C	1.558376	-0.283648	0.301506
H	-1.038866	1.572172	-2.083633	H	2.265828	-0.985170	-0.144068
H	0.647075	1.981251	-1.797481	H	2.057106	0.676328	0.447314
C	-1.504157	-0.927872	-0.158139	H	1.278062	-0.657572	1.288180
H	-2.359742	-0.299435	-0.412549				

8b: E = -508.569838239098 au
ZPE = 0.08010340 au

$$G_{\text{corr}} = 0.05289647 \text{ au}$$

P	0.048193	0.083907	-0.163782	H	1.404650	-1.708264	-0.780973
N	0.152472	0.414277	1.502015	H	0.057945	-2.272209	0.062869
H	1.020031	0.814375	1.824572	N	-1.658073	-0.224038	-0.117563
H	-0.252175	-0.240173	2.161567	H	-2.180259	0.595079	0.168140
N	0.449523	-1.533028	-0.509306	H	-2.005880	-0.548550	-1.011428

TS(8b^{P-inv}):

$$E = -508.490049227564 \text{ au}$$

$$ZPE = 0.07778616 \text{ au}$$

$$G_{\text{corr}} = 0.05071750 \text{ au}$$

$$\nu = -592.34 \text{ cm}^{-1}$$

P	-0.484912	-0.041687	-0.165088	H	0.057692	-2.583016	0.231098
N	-0.326516	1.735905	-0.287078	H	-1.493061	-2.173794	-0.247181
H	-1.191422	2.172697	-0.576225	N	1.119348	-0.117646	0.300941
H	0.403404	2.432773	-0.141522	H	1.572644	-0.985171	0.520448
N	-0.572315	-1.822509	-0.021579	H	1.690758	0.702538	0.386186

TS(8b^{N-inv}):

$$E = -508.562280899815 \text{ au}$$

$$ZPE = 0.07789630 \text{ au}$$

$$G_{\text{corr}} = 0.04995000 \text{ au}$$

$$\nu = -333.72 \text{ cm}^{-1}$$

P	-0.058816	0.003709	0.038917	H	-0.200391	-2.327914	0.333187
N	-0.054055	0.007872	1.729649	H	0.198216	-1.916454	-1.226558
H	0.604144	0.583191	2.223093	N	-1.715193	0.074837	-0.410701
H	-0.672720	-0.532887	2.315040	H	-2.357021	-0.577584	0.028485
N	0.278253	-1.652249	-0.252831	H	-2.104931	1.008813	-0.409023

8c:

$$E = -568.183496538448 \text{ au}$$

$$ZPE = 0.04249893 \text{ au}$$

$$G_{\text{corr}} = 0.01471066 \text{ au}$$

P	-0.000962	0.000355	-0.000380	H	-0.202411	-1.874596	-1.103609
O	1.632140	0.067269	0.081562	O	-0.303019	0.073901	1.606409
H	1.956433	0.970170	-0.017340	H	-1.233980	0.251314	1.785460
O	-0.144117	-1.620511	-0.175049				

TS(8c^{P-inv}):

$$E = -568.114168550005 \text{ au}$$

$$ZPE = 0.04322930 \text{ au}$$

$$G_{\text{corr}} = 0.01714725 \text{ au}$$

$$\nu = -308.69 \text{ cm}^{-1}$$

P	-0.558575	-0.141258	-0.006723	O	-0.526002	-1.817742	-0.013401
O	1.069640	-0.143527	0.011027	H	0.333055	-2.271734	-0.005780
H	1.402359	0.765867	0.018686	O	-0.418171	1.609706	0.002075

H -1.301499 1.998413 -0.005884

8d:

E = -1535.94322574905 au

ZPE = 0.02957488 au

G_{corr} = -0.00154547 au

P	-0.017198	-0.020966	-0.043783	H	-0.891600	2.072416	-1.341715
S	-0.001059	-0.361289	2.073628	S	-1.582652	-1.392338	-0.561687
H	1.154307	0.302462	2.271058	H	-0.739943	-2.414242	-0.806092
S	-1.171496	1.786262	-0.055581				

TS(8d^{P-inv}):

E = -1535.89203752858 au

ZPE = 0.03032583 au

G_{corr} = 0.00060239 au

$\nu = -318.84 \text{ cm}^{-1}$

P	-0.071773	0.159362	-0.034724	H	2.028346	-0.116536	-1.628925
S	0.268201	0.470717	1.961381	S	-1.854587	-0.640931	-0.648164
H	0.937855	-0.663532	2.274633	H	-1.517046	-1.949201	-0.735955
S	1.217199	0.946608	-1.418507				

9a:

E = -578.139658401438 au

ZPE = 0.19817248 au

G_{corr} = 0.16306280 au

P	-0.013499	0.036190	0.013386	H	-0.628566	-1.357937	3.498794
C	-0.077162	-0.024898	1.871241	H	-1.700511	-1.462195	2.107086
H	0.949910	0.090283	2.226325	H	-0.098567	-2.192583	2.034833
H	-0.643422	0.833410	2.248686	C	2.164697	1.846476	0.052994
C	0.662674	1.753366	-0.217048	H	2.538355	2.852736	-0.148318
H	0.458481	2.036628	-1.252656	H	2.401429	1.612266	1.092688
H	0.111216	2.453696	0.419502	H	2.719948	1.148828	-0.577034
C	-1.809137	0.357401	-0.347186	C	-2.106280	0.478981	-1.841907
H	-2.368677	-0.483941	0.068967	H	-3.176705	0.601094	-2.020653
H	-2.138719	1.254278	0.188247	H	-1.600210	1.339200	-2.284401
C	-0.659016	-1.332846	2.407389	H	-1.774555	-0.411104	-2.380112

TS(9a^{P-inv}):

E = -578.077393517289 au

ZPE = 0.19644629 au

G_{corr} = 0.16507027 au

$\nu = -350.23 \text{ cm}^{-1}$

P	0.615622	-0.315312	-0.013374	H	2.317264	1.334383	0.347249
C	0.346083	-0.829619	1.724331	H	1.987809	1.087786	-1.347297
H	0.507976	-1.910158	1.768598	C	0.077511	-1.407412	-1.383672
H	1.163676	-0.382286	2.296870	H	0.808600	-1.277748	-2.186434
C	1.504596	1.245519	-0.378836	H	0.205407	-2.434479	-1.030333

C	-1.002334	-0.471346	2.355380	H	-0.116256	2.471230	-1.150490
H	-1.050345	-0.817456	3.393427	H	0.198783	2.704181	0.565179
H	-1.162433	0.607425	2.343364	C	-1.342157	-1.204197	-1.920639
H	-1.823377	-0.931686	1.804066	H	-1.555382	-1.906932	-2.733366
C	0.674250	2.532164	-0.401449	H	-2.080812	-1.357045	-1.132734
H	1.304283	3.398409	-0.630530	H	-1.472410	-0.189862	-2.299898

9b:

E = -626.246275486443 au

ZPE = 0.16434646 au

G_{corr} = 0.12956744 au

P	-0.001555	-0.044115	0.035720	H	-1.848921	-1.037012	2.148892
N	-0.072708	-0.014840	1.741956	C	0.451582	-2.102902	-1.679809
H	0.810797	0.243261	2.157239	H	0.869502	-3.111251	-1.713881
N	0.213520	-1.707613	-0.295256	H	-0.447418	-2.074322	-2.307250
H	-0.408378	-2.346928	0.185335	H	1.182893	-1.422483	-2.119614
N	-1.636173	0.159361	-0.431661	C	-2.235158	1.481781	-0.301767
H	-2.272268	-0.589657	-0.185224	H	-3.138968	1.547467	-0.911134
C	-0.833525	-0.960089	2.544039	H	-2.487514	1.750215	0.731399
H	-0.399185	-1.968216	2.570724	H	-1.527537	2.226435	-0.671591
H	-0.915791	-0.600933	3.571495				

TS(9b^{P-inv}):

E = -626.173641166476 au

ZPE = 0.16307243 au

G_{corr} = 0.12940043 au

$\nu = -190.68 \text{ cm}^{-1}$

P	0.187259	0.400282	0.598819	H	3.184540	0.311520	-1.084581
N	1.992967	0.364020	0.673064	C	-2.295623	1.112980	1.572854
H	2.260718	0.875307	1.502715	H	-2.959531	0.448727	2.136546
N	-1.599262	0.419539	0.506766	H	-1.550938	1.512449	2.267668
H	-2.242217	0.027807	-0.172325	H	-2.892178	1.953031	1.200990
N	0.272276	-0.482455	-0.830947	C	-0.772767	-0.979755	-1.697447
H	1.195946	-0.717807	-1.141736	H	-0.317483	-1.512976	-2.531762
C	3.129085	-0.142209	-0.086137	H	-1.439276	-1.676225	-1.178849
H	4.075323	0.066834	0.416382	H	-1.380839	-0.169488	-2.111969
H	3.069029	-1.230465	-0.217850				

TS(9b^{N-inv}):

E = -626.243164102705 au

ZPE = 0.16362071 au

G_{corr} = 0.12905579 au

$\nu = -283.97 \text{ cm}^{-1}$

P	-0.379694	-0.209204	0.145750	C	-0.372492	-0.566660	2.944226
N	-0.080423	0.244333	1.767540	H	-0.325920	0.048667	3.845383
H	0.785041	0.756713	1.847814	H	-1.382367	-0.969707	2.873405
N	-0.086157	-1.870350	-0.068122	H	0.315448	-1.411291	3.069269
H	0.714794	-2.079934	-0.642103	C	-0.680221	-3.002257	0.622719
N	-2.079158	-0.234261	0.279100	H	-0.913218	-3.809841	-0.077066
H	-2.508280	0.152613	1.100069	H	-0.040951	-3.407452	1.415086

H	-1.615475	-2.680474	1.079607	H	-2.492252	-0.653357	-1.726510
C	-2.941352	-0.789207	-0.738945	H	-3.132285	-1.863239	-0.614890
H	-3.902897	-0.272064	-0.744453				

9c: E = -685.84629038455 au
 ZPE = 0.12793135 au
 G_{corr} = 0.09232323 au

P	-0.017560	0.026151	-0.021919	H	-0.850980	-3.034926	-1.515703
O	1.613872	-0.002414	-0.054346	H	-0.784808	-1.411459	-2.240701
C	2.315104	1.239393	-0.000529	H	0.723083	-2.291672	-1.887716
H	3.307156	1.070336	-0.415918	O	-0.214682	0.095853	1.596667
H	1.806704	2.010990	-0.587508	C	-1.539321	0.220271	2.113036
H	2.407226	1.579125	1.033078	H	-1.458637	0.630408	3.118283
O	-0.280034	-1.572934	-0.217183	H	-2.146104	0.892826	1.498336
C	-0.295208	-2.099185	-1.543783	H	-2.023155	-0.757571	2.157439

TS(9c^{P-inv}): E = -685.774135770341 au
 ZPE = 0.12708242 au
 G_{corr} = 0.09430647 au
 $\nu = -210.05 \text{ cm}^{-1}$

P	-0.700891	-0.299493	-0.186151	H	1.300399	-2.724288	-0.588848
O	0.868654	-0.217872	0.215506	H	0.877000	-2.689813	1.130040
C	1.675639	0.938651	0.434850	H	0.113370	-3.889479	0.053281
H	1.742353	1.539826	-0.470428	O	-0.741097	1.448403	-0.202233
H	1.261184	1.554877	1.230656	C	-1.987183	2.034981	-0.518351
H	2.659818	0.566368	0.716090	H	-1.886755	2.653879	-1.412915
O	-0.592745	-1.981709	-0.158261	H	-2.751318	1.267679	-0.705010
C	0.487661	-2.868038	0.125829	H	-2.319019	2.665095	0.309870

9d: E = -1653.65679810353 au
 ZPE = 0.11814453 au
 G_{corr} = 0.07886299 au

P	-0.023050	-0.027313	-0.034023	C	-2.135643	2.091652	-0.385445
S	2.106852	-0.049114	-0.044336	H	-2.684174	1.712458	0.474477
S	-0.338462	2.078952	-0.058590	H	-2.410949	3.131055	-0.558976
S	-0.353972	-0.395521	2.037760	H	-2.371991	1.504261	-1.271295
C	2.380307	-0.060131	-1.850460	C	-0.413146	-2.220787	1.993675
H	2.081743	0.890037	-2.288858	H	0.568058	-2.630529	1.762364
H	3.449141	-0.206329	-2.000340	H	-0.713323	-2.544385	2.989375
H	1.836056	-0.878384	-2.319387	H	-1.146283	-2.566735	1.266745

TS(9d^{P-inv}): E = -1653.61050103149 au
 ZPE = 0.11759543 au
 G_{corr} = 0.07989004 au

$$\nu = -210.05 \text{ cm}^{-1}$$

P	-0.001973	0.007891	1.401945	C	-2.351525	1.149094	-0.243905
S	1.697725	1.139961	1.497174	H	-2.449943	0.189859	-0.746264
S	-1.832886	0.911924	1.500398	H	-3.324757	1.641839	-0.204617
S	0.130664	-2.029826	1.505418	H	-1.643188	1.785322	-0.769021
C	2.173260	1.438663	-0.249810	C	0.180903	-2.592309	-0.240207
H	1.388162	1.982139	-0.769925	H	1.058115	-2.193190	-0.743852
H	3.078674	2.047469	-0.217231	H	0.243262	-3.681483	-0.205311
H	2.384992	0.498279	-0.752805	H	-0.725856	-2.295743	-0.761986

10:

$$E = -419.937895700482 \text{ au}$$

$$ZPE = 0.05964257 \text{ au}$$

$$G_{\text{corr}} = 0.03421296 \text{ au}$$

P	-0.064097	-0.180410	-0.000002	H	2.086105	-2.145487	0.000002
C	1.763950	-0.060664	-0.000001	H	3.604468	-1.094953	0.000001
H	2.233440	0.918154	-0.000003	H	-0.309972	0.772346	1.025701
C	2.521642	-1.152178	0.000001	H	-0.309972	0.772353	-1.025699

TS(10^{P-inv}):

$$E = -419.887822859823 \text{ au}$$

$$ZPE = 0.05812489 \text{ au}$$

$$G_{\text{corr}} = 0.03300229 \text{ au}$$

$$\nu = -907.59 \text{ cm}^{-1}$$

P	-0.080804	0.139203	0.176849	H	2.051723	-1.991135	-0.298302
C	1.667587	0.017252	0.282994	H	3.519756	-0.961200	0.139012
H	2.112265	0.954367	0.605476	H	-0.701543	1.333788	0.487767
C	2.447217	-1.037100	0.026369	H	-0.873969	-0.926746	-0.211181

11:

$$E = -498.431561274933 \text{ au}$$

$$ZPE = 0.11784141 \text{ au}$$

$$G_{\text{corr}} = 0.08822015 \text{ au}$$

P	-2.898302	0.108188	0.006464	H	-2.882260	-2.147405	-0.920167
C	-1.830701	0.738630	-1.360155	H	-1.367797	-1.844966	-0.034661
H	-2.195007	0.326010	-2.302160	C	-1.962066	0.614827	1.477704
H	-1.908342	1.824518	-1.423526	H	-2.286324	0.120177	2.391200
H	-0.782347	0.460763	-1.229940	C	-1.028328	1.559729	1.562762
C	-2.448430	-1.689639	-0.029719	H	-0.669418	2.099782	0.694993
H	-2.874837	-2.187159	0.842517	H	-0.588394	1.835991	2.514019

TS(11^{P-inv}):

$$E = -498.375587343184 \text{ au}$$

$$ZPE = 0.11637599 \text{ au}$$

$$G_{\text{corr}} = 0.08534031 \text{ au}$$

$$\nu = -378.27 \text{ cm}^{-1}$$

P	-1.963067	-0.162536	-0.003055	H	-3.599648	-1.928089	-0.505580
C	-1.683779	0.806718	-1.514666	H	-1.930200	-2.516043	-0.692806
H	-1.830120	0.139160	-2.364913	C	-1.604004	0.540969	1.550016
H	-2.377878	1.643410	-1.608465	H	-1.771696	-0.153554	2.369034
H	-0.661111	1.185932	-1.552323	C	-1.161757	1.781666	1.819748
C	-2.586110	-1.870593	-0.107694	H	-0.984081	2.517106	1.045405
H	-2.602907	-2.248812	0.915771	H	-0.966197	2.084112	2.838856

12: E = -497.188960283891 au
ZPE = 0.09433408 au
G_{corr} = 0.06431865 au

P	-0.087364	-0.276327	0.016265	C	-0.558147	0.746728	1.460168
C	1.730818	-0.065363	0.068826	H	-0.128191	1.739957	1.564344
H	2.140818	0.931242	0.213480	C	-1.397572	0.294864	2.385386
C	2.552918	-1.102232	-0.049761	H	-1.675144	0.893077	3.246320
H	2.176741	-2.109826	-0.188930	H	-1.839863	-0.692718	2.314064
H	3.630330	-0.984451	-0.013506	H	-0.329880	0.724554	-0.965856

TS(12^{P-inv}): E = -497.143167516595 au
ZPE = 0.09261803 au
G_{corr} = 0.06275950 au
ν = -640.56 cm⁻¹

P	0.053235	-0.137704	0.254609	C	-0.843036	0.948404	1.295200
C	1.782490	-0.376252	0.391217	H	-1.900560	0.948461	1.046919
H	2.213405	0.212655	1.195502	C	-0.397232	1.723858	2.291090
C	2.572513	-1.162319	-0.349508	H	-1.085327	2.345921	2.846172
H	2.193992	-1.768192	-1.163083	H	0.644167	1.765617	2.581928
H	3.633913	-1.214525	-0.150812	H	-0.662691	-0.829007	-0.708909

13: E = -536.437454378251 au
ZPE = 0.12295183 au
G_{corr} = 0.06088575 au

P	0.012315	-0.005396	-0.061620	H	-0.207486	0.853505	1.050295
C	1.838774	-0.005161	0.028766	C	-0.244956	1.289737	-1.370057
H	2.358914	0.949452	0.073746	H	-0.018363	0.855574	-2.344372
C	2.542053	-1.132750	0.024226	H	-1.293642	1.590945	-1.368968
H	2.056147	-2.101079	-0.024906	H	0.377662	2.173325	-1.223739
H	3.625445	-1.132198	0.072404				

TS(13^{P-inv}): E = -536.389891120953 au
ZPE = 0.12179219 au
G_{corr} = 0.05897641 au
ν = -317.85 cm⁻¹

P	0.000029	0.032073	-0.000810	H	-0.734534	-1.142192	0.000468
C	1.751166	-0.003959	-0.000332	C	-0.893985	1.619211	-0.003155
H	2.162846	1.002715	-0.002004	H	-0.684329	2.209212	-0.894868
C	2.586425	-1.050740	0.001674	H	-1.955962	1.370170	-0.003557
H	2.237111	-2.075487	0.003432	H	-0.685450	2.211296	0.887436
H	3.656333	-0.895969	0.001548				

14: E = -573.302230013588 au
ZPE = 0.10781413 au
G_{corr} = 0.07748978 au

P	0.092956	-0.059767	-0.014814	H	2.217490	0.054706	1.924030
C	0.071207	-0.028790	1.825044	H	2.305667	0.102746	4.384719
C	1.296211	0.030322	2.494149	H	0.208663	0.098234	5.704256
C	1.347202	0.063920	3.882650	H	-1.975247	0.022426	4.538102
C	0.171187	0.061922	4.622988	H	-2.064253	-0.071066	2.081492
C	-1.054727	0.020387	3.967838	H	-0.035965	-1.464381	-0.189949
C	-1.104312	-0.028945	2.580337	H	-1.290784	0.172426	-0.218541

TS(14^{P-inv}): E = -573.250714303145 au
ZPE = 0.10623861 au
G_{corr} = 0.07641575 au
ν = -929.18 cm⁻¹

P	-0.032481	-0.001743	0.049117	H	2.203500	0.002814	1.908063
C	0.045678	0.019180	1.820642	H	2.302857	0.032456	4.354854
C	1.283218	0.017353	2.478787	H	0.219400	0.065993	5.702944
C	1.337374	0.034139	3.864454	H	-1.976067	0.068462	4.546005
C	0.171116	0.052779	4.622354	H	-2.095673	0.039767	2.100146
C	-1.058198	0.054252	3.971567	H	1.126726	-0.017023	-0.703808
C	-1.128086	0.037883	2.586552	H	-1.253234	-0.002774	-0.599477

15: E = -651.796320059568 au
ZPE = 0.16596293 au
G_{corr} = 0.13372516 au

P	0.009575	0.003607	-0.009069	H	-1.953976	0.004815	4.606554
C	0.007903	0.004893	1.829442	H	-2.120148	-0.046506	2.164229
C	1.251873	0.059792	2.469184	C	-1.788802	-0.095797	-0.414059
C	1.345884	0.071252	3.853361	H	-2.286406	0.837867	-0.149549
C	0.191931	0.051351	4.630972	H	-1.879745	-0.225222	-1.493651
C	-1.049765	0.015510	4.010499	H	-2.296203	-0.927269	0.080105
C	-1.141122	-0.011293	2.622159	C	0.477325	-1.766812	-0.304986
H	2.156899	0.101324	1.873220	H	0.435769	-1.972956	-1.376178
H	2.319234	0.107117	4.326582	H	1.501416	-1.930852	0.030728
H	0.261702	0.070544	5.711062	H	-0.183330	-2.457813	0.222406

TS(15^{P-inv}): E = -651.738602922878 au

ZPE = 0.16465573 au

G_{corr} = 0.13021749 au

$\nu = -384.02 \text{ cm}^{-1}$

P	0.005678	-0.047647	0.029578	H	-2.001257	0.078601	4.491814
C	0.057374	0.039926	1.784209	H	-2.088068	-0.042870	2.052941
C	1.285105	0.127471	2.468332	C	-1.600908	-0.143418	-0.821459
C	1.317710	0.194652	3.851941	H	-2.155809	-1.045212	-0.559059
C	0.142481	0.178814	4.598007	H	-2.222713	0.731523	-0.627212
C	-1.075474	0.092992	3.929394	H	-1.387534	-0.175962	-1.890594
C	-1.126668	0.024181	2.546381	C	1.560861	-0.043339	-0.916916
H	2.214764	0.143639	1.913568	H	2.123889	0.881677	-0.785673
H	2.275721	0.261041	4.353332	H	2.197906	-0.891981	-0.664098
H	0.175123	0.232594	5.677842	H	1.287819	-0.127941	-1.969493

16:

E = -803.919800535643 au

ZPE = 0.19062615 au

G_{corr} = 0.15642575 au

P	0.053828	-0.101491	0.500955	H	2.283803	1.624903	1.131596
H	0.399673	-0.436600	1.835162	C	-0.490773	-1.770942	-0.024179
C	1.778088	-0.033708	-0.147096	C	-0.011769	-2.946453	0.562330
C	2.242909	-0.866900	-1.164492	C	-0.449680	-4.187285	0.119807
C	3.533364	-0.721059	-1.663656	C	-1.368408	-4.272383	-0.922555
C	4.378657	0.254137	-1.150571	C	-1.849662	-3.111965	-1.515614
C	3.922418	1.093100	-0.138230	C	-1.417534	-1.869368	-1.063870
C	2.631196	0.956378	0.351560	H	0.714214	-2.887526	1.363498
H	1.601179	-1.640169	-1.564830	H	-0.072812	-5.088957	0.586216
H	3.878069	-1.378654	-2.452063	H	-1.709004	-5.240244	-1.268191
H	5.384282	0.363021	-1.536065	H	-2.566262	-3.172066	-2.324902
H	4.572697	1.858096	0.267436	H	-1.804225	-0.965995	-1.520129

TS(16^{P-inv}):

E = -803.870058911565 au

ZPE = 0.18919994 au

G_{corr} = 0.15186482 au

$\nu = -681.56 \text{ cm}^{-1}$

P	0.000672	0.164854	-0.026791	H	2.617569	-0.603489	0.924899
H	-0.019859	0.322725	1.348642	C	-1.550582	0.060081	-0.876837
C	1.574723	0.079999	-0.836550	C	-1.658131	-0.552713	-2.134877
C	1.719688	0.418461	-2.190824	C	-2.887072	-0.623476	-2.774520
C	2.962865	0.341412	-2.801303	C	-4.033880	-0.118380	-2.170774
C	4.088237	-0.040105	-2.078029	C	-3.935879	0.472299	-0.914476
C	3.953706	-0.356229	-0.729365	C	-2.709303	0.579240	-0.278096
C	2.711744	-0.316589	-0.114969	H	-0.785677	-0.989476	-2.601672
H	0.864332	0.758307	-2.758842	H	-2.949766	-1.095073	-3.747366
H	3.053897	0.600842	-3.848760	H	-4.990601	-0.183711	-2.671509
H	5.056447	-0.090889	-2.557994	H	-4.819187	0.872337	-0.432380
H	4.820013	-0.657623	-0.153762	H	-2.644551	1.073945	0.682902

17:

E = -843.168458870203 au

ZPE = 0.21953736 au

G_{corr} = 0.18372351 au

P	-0.334038	0.080460	0.149851	C	-3.930078	-1.352345	1.637253
C	0.176142	0.367797	1.889516	C	-4.332079	-2.227753	0.633121
C	0.650873	-0.735234	2.609456	C	-3.527397	-2.410013	-0.484883
C	1.073678	-0.601654	3.923160	C	-2.323970	-1.721393	-0.594906
C	1.047605	0.645640	4.541845	H	-2.425092	0.014520	2.310974
C	0.595014	1.751040	3.834597	H	-4.551567	-1.209965	2.512750
C	0.161131	1.613119	2.519018	H	-5.265479	-2.768531	0.725784
H	0.681708	-1.708644	2.133480	H	-3.830691	-3.094572	-1.267151
H	1.430433	-1.468881	4.464743	H	-1.690130	-1.877707	-1.460001
H	1.382363	0.752781	5.565710	C	-1.013336	1.728903	-0.342287
H	0.572635	2.725674	4.306158	H	-0.200748	2.449436	-0.445796
H	-0.195573	2.487145	1.991712	H	-1.486640	1.611195	-1.317498
C	-1.915369	-0.832585	0.401323	H	-1.755233	2.110461	0.360934
C	-2.732587	-0.658948	1.521263				

TS(17P^{-inv}):

E = -843.114872109449 au

ZPE = 0.21835180 au

G_{corr} = 0.17924689 auv = -332.36 cm⁻¹

P	-0.497015	0.410559	-0.028956	C	-3.477299	-2.252189	0.653618
C	1.267976	0.453521	-0.066418	C	-2.953138	-3.454275	0.188984
C	2.057348	-0.661889	0.267513	C	-1.663534	-3.471593	-0.333950
C	3.440079	-0.580888	0.229837	C	-0.911903	-2.309528	-0.409938
C	4.078897	0.605127	-0.120878	H	-3.136047	-0.176790	1.027246
C	3.305876	1.718463	-0.434290	H	-4.476648	-2.221522	1.069886
C	1.921656	1.649809	-0.416182	H	-3.539561	-4.362253	0.233179
H	1.587674	-1.584685	0.577186	H	-1.243566	-4.396544	-0.709616
H	4.025413	-1.454145	0.490389	H	0.065260	-2.337063	-0.870953
H	5.158854	0.661863	-0.144423	C	-1.390159	1.991034	-0.105462
H	3.783996	2.651901	-0.704631	H	-1.261584	2.594333	0.793282
H	1.345486	2.528088	-0.676329	H	-1.084881	2.572092	-0.976255
C	-1.426602	-1.092908	0.072320	H	-2.447053	1.751986	-0.222155
C	-2.723268	-1.089242	0.616949				

18a:

E = -460.415674569846 au

ZPE = 0.11216420 au

G_{corr} = 0.08357466 au

P	1.802488	-0.224846	-0.924510	H	-1.662606	-1.702648	-0.457325
C	2.040432	1.526774	-1.489811	H	-0.133203	-2.169657	0.291465
C	-0.578395	-1.698927	-0.587401	H	-0.345932	-2.325498	-1.451390
H	1.886507	-0.837154	-2.204947	C	-0.053441	-0.276531	-0.780237
H	1.860291	2.197237	-0.647811	H	-0.315658	0.339598	0.084646
H	3.074065	1.666751	-1.808978	H	-0.514229	0.189043	-1.655176
H	1.375042	1.804236	-2.308746				

TS(18a^{P-inv}):

E = -460.356446674048 au

ZPE = 0.11101137 au

G_{corr} = 0.08318089 au

$\nu = -838.36 \text{ cm}^{-1}$

P	1.539095	-0.026295	-1.056356	H	-1.591102	-1.942994	-0.347280
C	2.212157	1.615594	-1.482412	H	0.021550	-2.155440	0.340645
C	-0.526481	-1.782604	-0.526508	H	-0.233320	-2.375268	-1.394330
H	2.396581	-1.107730	-0.962031	C	-0.250564	-0.296224	-0.756074
H	2.058825	2.349588	-0.690609	H	-0.577335	0.278279	0.113222
H	3.286897	1.478495	-1.611947	H	-0.819952	0.055936	-1.618934
H	1.806674	2.001645	-2.418456				

18b:

E = -476.448252541379 au

ZPE = 0.10102256 au

G_{corr} = 0.07262814 au

P	1.856527	0.134244	-0.190061	H	1.207411	0.719983	-2.529132
C	1.755175	1.184128	-1.708538	H	-1.512574	-1.322173	-0.604128
C	-0.469545	-1.215972	-0.908282	H	-0.024404	-2.217284	-0.982113
H	2.400931	-1.012200	-0.854202	H	-0.463068	-0.773380	-1.904836
H	1.279276	2.131440	-1.453504	N	0.233671	-0.346644	0.024277
H	2.773279	1.391009	-2.046601	H	0.013494	-0.534961	0.989841

TS(18b^{P-inv}):

E = -476.385972984312 au

ZPE = 0.10002708 au

G_{corr} = 0.07191787 au

$\nu = -833.86 \text{ cm}^{-1}$

P	1.538461	0.828829	-0.025807	H	1.755880	-0.085669	-2.293717
C	1.848136	0.890939	-1.818903	H	-1.299166	-1.187448	0.996870
C	-0.228376	-0.982502	1.082710	H	0.061043	-1.089516	2.134123
H	2.559841	1.195852	0.836241	H	0.316192	-1.726601	0.503060
H	1.207156	1.608531	-2.330947	N	0.064069	0.346135	0.551163
H	2.884220	1.222927	-1.919210	H	-0.596868	1.054316	0.828228

TS(18b^{N-inv}):

E = -476.446768147092 au

ZPE = 0.1001952 au

G_{corr} = 0.07138525 au

$\nu = -241.75 \text{ cm}^{-1}$

P	1.804696	0.229568	-0.127951	H	1.323950	0.556015	-2.557874
C	1.793693	1.122516	-1.752845	H	-1.396878	-1.566827	-0.465519
C	-0.513555	-1.131455	-0.934690	H	0.102590	-1.953330	-1.314509
H	2.436813	-0.946205	-0.636992	H	-0.848984	-0.538708	-1.792703
H	1.273783	2.074678	-1.637042	N	0.224280	-0.343662	0.033697
H	2.828761	1.330637	-2.034902	H	-0.232528	-0.159368	0.907745

18c:

E = -496.306996957407 au

ZPE = 0.08848289 au

G_{corr} = 0.05961932 au

P	-1.531010	0.549702	0.041609	O	-0.737877	-0.904834	0.150717
H	-0.765769	1.311064	0.982758	C	-1.317349	-1.906926	0.978075
C	-0.662955	1.186370	-1.447442	H	-0.837281	-2.851556	0.724577
H	-1.047963	0.685907	-2.336244	H	-1.142067	-1.694383	2.037667
H	-0.867248	2.255868	-1.537565	H	-2.395325	-1.991511	0.808576
H	0.414023	1.029922	-1.381765				

TS(18c^{P-inv}):

E = -496.231804574267 au

ZPE = 0.08756054 au

G_{corr} = 0.05902152 au $\nu = -975.88 \text{ cm}^{-1}$

O	0.159718	0.178581	-0.227022	H	3.675243	0.555942	1.152499
P	1.744934	0.547068	-0.169876	H	2.266966	0.689166	2.216826
C	2.670449	0.172173	1.345976	H	-1.317721	-1.159576	-0.645751
C	-0.230326	-1.115817	-0.713538	H	0.209427	-1.907995	-0.103478
H	2.280211	1.172843	-1.277679	H	0.084008	-1.245492	-1.750872
H	2.746350	-0.896032	1.550066				

18d:

E = -818.921398599159 au

ZPE = 0.08555515 au

G_{corr} = 0.05531079 au

S	-0.212428	-0.088077	-0.821052	H	3.334339	1.732629	0.086537
P	1.905009	-0.110331	-0.610498	H	1.726906	2.359309	-0.354556
C	2.258246	1.548411	0.141272	H	-1.740956	-1.500354	0.323352
C	-0.666606	-1.347850	0.420618	H	-0.446596	-1.005590	1.430111
H	2.164753	0.251896	-1.956380	H	-0.150168	-2.284963	0.223572
H	1.969724	1.523595	1.192482				

TS(18d^{P-inv}):

E = -818.870584325725 au

ZPE = 0.08442622 au

G_{corr} = 0.05462024 au $\nu = -714.37 \text{ cm}^{-1}$

S	-0.164359	-0.418295	-0.992107	H	3.406522	1.551082	0.128289
P	1.770465	0.027794	-0.668875	H	1.933475	2.440588	-0.290214
C	2.316583	1.544423	0.194819	H	-1.774247	-1.654729	0.274117
C	-0.725724	-1.410218	0.455939	H	-0.638231	-0.827008	1.369859
H	2.770598	-0.789382	-1.178140	H	-0.139357	-2.322879	0.530853
H	2.033433	1.543048	1.246186				

19a:

E = -499.664121334572 au

ZPE = 0.14081475 au

G_{corr} = 0.11031995 au

P	-3.133107	1.001751	0.042790	H	-1.113080	1.686151	1.309680
C	-2.249990	1.754972	-1.398692	C	-2.320110	-0.669447	0.041835
H	-2.585245	1.278987	-2.321656	H	-2.598530	-1.150738	-0.900142
H	-2.496833	2.815942	-1.462606	H	-1.231629	-0.547256	0.028439
H	-1.164313	1.650094	-1.321598	C	-2.749959	-1.545292	1.218409
C	-2.194133	1.811815	1.417796	H	-2.294943	-2.536124	1.157699
H	-2.424761	2.878367	1.430623	H	-2.452565	-1.106613	2.172998
H	-2.504392	1.396370	2.377178	H	-3.834056	-1.673975	1.236909

TS(19a^{P-inv}):

E = -499.597371919578 au

ZPE = 0.13949783 au

G_{corr} = 0.10899207 auν = -408.02 cm⁻¹

C	-2.694681	-1.620631	1.222413	C	-4.466251	1.449778	-0.769336
H	-2.296507	-2.633861	1.099136	H	-5.262443	1.732341	-0.078902
H	-2.299569	-1.208571	2.152108	H	-4.322164	2.251402	-1.496341
H	-3.778600	-1.686325	1.325927	H	-4.793633	0.563075	-1.315732
C	-2.314935	-0.737516	0.031018	C	-1.891245	2.295412	0.855197
H	-1.228570	-0.703393	-0.085677	H	-1.703767	3.130622	0.177678
H	-2.696526	-1.168313	-0.898516	H	-2.317019	2.678510	1.783947
P	-2.902212	0.998156	0.060261	H	-0.927642	1.838023	1.089022

19b:

E = -515.69637152279 au

ZPE = 0.12932316 au

G_{corr} = 0.09870861 au

P	-3.051150	0.969687	0.182562	H	-1.056151	1.978941	1.268568
C	-2.271616	1.659512	-1.338002	C	-2.777074	-1.592555	1.097946
H	-2.631789	1.113747	-2.209935	H	-2.384193	-2.563350	0.787715
H	-2.554254	2.708644	-1.444119	H	-2.532838	-1.450058	2.159208
H	-1.179761	1.596624	-1.305538	H	-3.863522	-1.626121	1.008185
C	-2.137616	1.993411	1.434300	N	-2.262212	-0.545954	0.224630
H	-2.484593	3.028598	1.390326	H	-1.249223	-0.522498	0.198639
H	-2.347036	1.614576	2.436134				

TS(19b^{P-inv}):

E = -515.626142352209 au

ZPE = 0.12864665 au

G_{corr} = 0.09677008 auν = -450.27 cm⁻¹

P	-0.424427	-0.006374	-0.125094	H	-2.385415	-1.176936	0.531134
C	-1.422894	-1.513735	0.141252	H	-1.604773	-2.076695	-0.775103
H	-0.972855	-2.172503	0.884275	C	-1.198204	1.639194	0.090486

H	-2.199438	1.455983	0.485600	H	2.592599	1.035055	0.536597
H	-0.662563	2.250678	0.817392	H	2.004206	-0.409857	1.373065
H	-1.298069	2.195161	-0.842954	N	1.176438	-0.165591	-0.527616
C	2.292646	-0.010987	0.401162	H	1.442049	-0.084060	-1.496876
H	3.159799	-0.570390	0.037877				

TS(19b^{N-inv}):

E = -515.695554708298 au

ZPE = 0.12875688 au

G_{corr} = 0.09840284 au

$\nu = -248.9 \text{ cm}^{-1}$

P	1.854664	0.096713	-0.215033	H	-0.752200	-0.449361	-1.858616
C	1.742399	1.133717	-1.746292	N	0.264014	-0.443976	0.003647
C	-0.604703	-1.075405	-0.972866	H	-0.135762	-0.271663	0.907374
H	1.149421	2.024639	-1.535351	C	2.685874	-1.375591	-0.969140
H	2.747774	1.453772	-2.028257	H	3.701827	-1.097277	-1.257161
H	1.300839	0.604389	-2.594058	H	2.748856	-2.173722	-0.228196
H	-1.584840	-1.250551	-0.528208	H	2.169853	-1.752290	-1.855577
H	-0.216684	-2.043446	-1.306129				

19c:

E = -535.559138471535 au

ZPE = 0.11698316 au

G_{corr} = 0.08592250 au

P	-3.071891	0.982380	0.228210	H	-2.357286	1.631247	2.471165
C	-2.284175	1.625780	-1.300147	H	-1.063906	1.943959	1.289334
H	-2.649207	1.069397	-2.163633	C	-2.773048	-1.506118	1.072159
H	-2.557402	2.675592	-1.426709	H	-2.237768	-2.416260	0.802853
H	-1.196589	1.539656	-1.249941	H	-2.640907	-1.325217	2.144009
C	-2.141146	1.990867	1.463848	H	-3.839517	-1.639427	0.866635
H	-2.473164	3.030263	1.403441	O	-2.223618	-0.448149	0.297278

TS(19c^{P-inv}):

E = -535.473209131621 au

ZPE = 0.11638864 au

G_{corr} = 0.08531671 au

$\nu = -518.18 \text{ cm}^{-1}$

P	-0.359561	0.032495	-0.140030	H	-0.927203	2.272272	-0.972497
C	-1.334869	-1.487165	0.100122	H	-2.078329	1.603964	0.191138
H	-1.351281	-2.116240	-0.790884	C	2.195891	-0.166939	0.512701
H	-1.014599	-2.078221	0.959219	H	3.162072	-0.345935	0.038796
H	-2.352830	-1.139582	0.289527	H	2.219496	0.788440	1.042144
C	-1.016248	1.728358	-0.031048	H	1.981423	-0.965400	1.226588
H	-0.570226	2.315293	0.773134	O	1.217732	-0.142680	-0.536233

19d:

E = -858.170385831107 au

ZPE = 0.11418663 au

$G_{\text{corr}} = 0.08350501 \text{ au}$

P	-2.901240	1.093886	0.397175	H	-1.982962	1.978202	2.474488
C	-2.400801	1.690559	-1.281213	H	-0.862316	2.300635	1.135267
H	-2.811425	1.021795	-2.037157	C	-2.943132	-1.868847	1.105157
H	-2.819946	2.687707	-1.435606	H	-2.420714	-2.818711	1.215338
H	-1.317129	1.739871	-1.400425	H	-3.364295	-1.577844	2.065146
C	-1.913308	2.271730	1.427497	H	-3.736838	-1.978027	0.369138
H	-2.339904	3.272009	1.319532	S	-1.695614	-0.658991	0.544164

TS(19d^{P-inv}):

$E = -858.114049855059 \text{ au}$

$ZPE = 0.11340783 \text{ au}$

$G_{\text{corr}} = 0.08138366 \text{ au}$

$\nu = -364.92 \text{ cm}^{-1}$

P	-0.693116	0.000006	-0.048416	H	-0.968877	2.364328	-0.144385
C	-1.623372	-1.557933	0.185533	H	-2.523777	1.571545	-0.430723
H	-2.523784	-1.571522	-0.430738	C	2.296661	-0.000007	0.814571
H	-0.968891	-2.364314	-0.144390	H	2.113449	-0.893027	1.407980
H	-1.895181	-1.731753	1.227463	H	3.327681	-0.000008	0.453521
C	-1.623361	1.557950	0.185542	H	2.113452	0.893008	1.407988
H	-1.895162	1.731771	1.227474	S	1.213584	0.000002	-0.682489

20:

$E = -418.685068180746 \text{ au}$

$ZPE = 0.03844898 \text{ au}$

$G_{\text{corr}} = 0.01435821 \text{ au}$

C	-0.828969	0.227712	-0.501296	H	1.305526	-0.330832	-0.983949
C	0.461181	0.186684	-0.559662	P	-0.091953	1.528256	0.571773
H	-1.739617	-0.233228	-0.846235	H	-0.097300	2.637389	-0.342951

TS(20^{P-inv}):

$E = -418.594875158836 \text{ au}$

$ZPE = 0.03526348 \text{ au}$

$G_{\text{corr}} = 0.01089367 \text{ au}$

$\nu = -841.20 \text{ cm}^{-1}$

C	0.904627	0.636821	0.325845	H	-0.102388	0.194267	-1.438490
C	0.397928	-0.321785	-0.598940	P	1.660534	-0.179651	1.595263
H	0.837428	1.726178	0.261052	H	2.083567	0.952100	2.382989

21:

$E = -457.933236817693 \text{ au}$

$ZPE = 0.06708706 \text{ au}$

$G_{\text{corr}} = 0.04022599 \text{ au}$

P	-0.180051	0.246753	-0.157621	H	2.468900	-0.631277	-0.335839
C	1.636975	0.035878	-0.176684	H	1.724944	2.232622	0.340324
C	1.318496	1.260185	0.112485	C	-0.688494	-0.288439	1.557875

H	-1.103845	-1.298283	1.511864	H	-1.474448	0.376797	1.924429
H	0.147533	-0.275619	2.257937				

TS(21^{P-inv}): E = -457.846362006959 au
 ZPE = 0.06383380 au
 G_{corr} = 0.03638915 au
 ν = -548.69 cm⁻¹

C	0.953490	0.526097	0.261704	C	2.178193	0.738095	2.774905
C	0.128692	-0.196393	-0.634735	H	3.092550	0.173903	2.988315
H	1.449741	1.487911	0.088263	H	2.438974	1.695143	2.325046
H	0.039471	0.357605	-1.587109	H	1.689769	0.900487	3.740158
P	1.087780	-0.314944	1.723523				

22a: E = -419.944463098234 au
 ZPE = 0.06308674 au
 G_{corr} = 0.03864479 au

H	0.000397	0.002538	-0.001271	H	0.752532	2.447062	0.301323
P	1.421103	-0.000127	0.000023	H	2.550149	2.219860	0.391683
C	1.607617	1.857491	0.000251	H	0.752384	1.436218	-2.003912
C	1.607492	1.258254	-1.366360	H	2.550092	1.215832	-1.897903

TS(22a^{P-inv}): E = -419.841210687582 au
 ZPE = 0.06126937 au
 G_{corr} = 0.03688613 au
 ν = -1197.22 cm⁻¹

H	-0.000000	-0.000000	-2.171423	H	-1.257636	0.907286	1.178275
P	0.000000	0.000001	-0.786914	H	-1.257636	-0.907286	1.178275
C	-0.794216	0.000000	0.804306	H	1.257636	0.907286	1.178275
C	0.794215	0.000000	0.804307	H	1.257636	-0.907286	1.178275

22b: E = -435.969492633839 au
 ZPE = 0.05188620 au
 G_{corr} = 0.02758925 au

N	1.388867	1.909772	-0.030162	C	1.596060	1.289963	-1.333065
H	2.250154	2.292588	0.348060	H	0.770495	1.412697	-2.023854
P	1.425568	0.129503	0.074311	H	2.579046	1.345679	-1.790216
H	0.014816	-0.050302	0.012447				

TS(22b^{P-inv}): E = -435.848816106165 au
 ZPE = 0.04970703 au

$$G_{\text{corr}} = 0.02530889 \text{ au}$$

$$\nu = -1434.71 \text{ cm}^{-1}$$

N	1.373436	1.811006	0.038630	C	1.606094	1.265950	-1.371212
H	2.259518	2.196207	0.363246	H	0.768311	1.420929	-2.040442
P	1.435961	0.070922	-0.070678	H	2.581412	1.448513	-1.809970
H	1.362856	-0.997718	0.801332				

TS(22b^{N-inv}):

$$E = -435.949744434543 \text{ au}$$

$$ZPE = 0.05008436 \text{ au}$$

$$G_{\text{corr}} = 0.02585760 \text{ au}$$

$$\nu = -707.79 \text{ cm}^{-1}$$

N	1.389394	1.862287	-0.018537	C	1.579565	1.335105	-1.316692
H	1.375185	2.764080	0.412945	H	0.752201	1.392613	-2.024241
P	1.397546	0.190172	0.149852	H	2.568287	1.393542	-1.768743
H	0.001883	-0.119048	-0.043737				

22c:

$$E = -455.829721367961 \text{ au}$$

$$ZPE = 0.03930906 \text{ au}$$

$$G_{\text{corr}} = 0.01512696 \text{ au}$$

O	0.004156	0.003639	-0.000495	H	1.928442	-0.019318	1.413944
P	1.700745	-0.004182	-0.000945	H	0.301458	1.896772	0.911990
C	0.496093	1.343762	-0.001889	H	0.328011	1.888437	-0.926094

TS(22c^{P-inv}):

$$E = -455.705378461827 \text{ au}$$

$$ZPE = 0.03512969 \text{ au}$$

$$G_{\text{corr}} = 0.01082562 \text{ au}$$

$$\nu = -2278.43 \text{ cm}^{-1}$$

O	-0.056039	-0.073814	0.008452	H	3.083746	0.561745	-0.007370
P	1.676596	-0.131587	0.002241	H	0.425926	1.854112	0.899743
C	0.600017	1.269897	-0.002322	H	0.419028	1.842954	-0.910165

22d:

$$E = -778.460115328478 \text{ au}$$

$$ZPE = 0.03743870 \text{ au}$$

$$G_{\text{corr}} = 0.01208172 \text{ au}$$

C	-4.346697	-0.246120	0.044444	P	-3.222678	1.162620	0.420992
H	-4.862712	-0.246550	-0.908070	H	-3.175657	1.676626	-0.908186
H	-4.934240	-0.619605	0.874628	S	-2.627705	-0.833944	-0.000281

TS(22d^{P-inv}):

$$E = -778.346603048698 \text{ au}$$

ZPE = 0.03569532 au

G_{corr} = 0.01033709 au

$\nu = -1361.33 \text{ cm}^{-1}$

C	0.086455	0.000721	-0.040854	H	3.093723	-0.006469	0.535270
S	0.051663	-0.001957	1.875624	H	-0.319611	-0.913685	-0.457258
P	1.715996	-0.003726	0.655815	H	-0.315758	0.918015	-0.454637

23a:

E = -459.190427121632 au

ZPE = 0.09176243 au

G_{corr} = 0.06491312 au

C	-0.541230	1.293896	0.035563	P	0.595663	2.679432	0.507650
C	0.915269	0.928043	-0.008223	C	0.765402	3.550403	-1.125807
H	-1.069968	1.381464	-0.905320	H	0.059640	4.382170	-1.167006
H	-1.141028	0.875583	0.834337	H	1.773427	3.959054	-1.216430
H	1.368306	0.769475	-0.978879	H	0.578030	2.887448	-1.971644
H	1.291349	0.264763	0.760747				

TS(23a^{P-inv}):

E = -459.083210807552 au

ZPE = 0.09065538 au

G_{corr} = 0.06345956 au

$\nu = -548.25 \text{ cm}^{-1}$

C	-1.675267	-0.343345	-0.000344	P	-0.904378	1.258045	-0.000010
C	-0.079625	-0.316444	0.000375	C	-0.905145	3.100673	-0.000033
H	-2.125774	-0.741669	-0.905651	H	-1.372349	3.502751	-0.896962
H	-2.126589	-0.741654	0.904562	H	-1.373048	3.502782	0.896518
H	0.384979	-0.699049	-0.904533	H	0.151950	3.368486	0.000370
H	0.384164	-0.699034	0.905708				

23b:

E = -475.219763568833 au

ZPE = 0.08047218 au

G_{corr} = 0.05366361 au

C	-0.404164	1.240106	-0.169380	H	-0.049961	4.521751	-0.995305
H	-0.884895	1.309165	-1.139203	H	1.690311	4.209566	-1.026177
H	-0.949327	0.646241	0.557469	H	0.595080	3.157932	-1.947933
P	0.544327	2.661845	0.464172	N	1.056715	1.113038	-0.229381
C	0.707233	3.734956	-1.030514	H	1.415158	0.490542	0.487593

TS(23b^{P-inv}):

E = -475.09163692977 au

ZPE = 0.07921697 au

G_{corr} = 0.05214405 au

$\nu = -712.20 \text{ cm}^{-1}$

C	-1.577817	-0.417169	-0.109351	H	-1.738474	-0.886001	-1.073537
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H	-2.170567	-0.838489	0.697198	H	-0.655490	3.487689	0.976993
P	-1.070719	1.284015	-0.053426	H	-0.008603	3.384628	-0.698487
C	-0.821817	3.107015	-0.029189	N	-0.100915	-0.147935	0.204191
H	-1.756147	3.508925	-0.420988	H	0.030541	-0.344014	1.196523

TS(23b^{N-inv}):

E = -475.200071352538 au

ZPE = 0.07872961 au

G_{corr} = 0.05207554 au

$\nu = -678.85 \text{ cm}^{-1}$

C	-0.353931	1.205985	-0.200369	H	-0.059370	4.547685	-0.937494
H	-0.830984	1.320389	-1.174313	H	1.673227	4.246496	-1.092618
H	-0.932757	0.623371	0.514806	H	0.522354	3.216679	-1.974936
P	0.637004	2.645880	0.441165	N	1.063991	1.132523	-0.146114
C	0.694666	3.763194	-1.047172	H	1.766056	0.457940	-0.375150

23c:

E = -495.081164626568 au

ZPE = 0.06790793 au

G_{corr} = 0.04121240 au

C	-0.413669	1.286348	-0.186033	H	-0.046331	4.546568	-0.958302
H	-0.856626	1.350027	-1.176122	H	1.682474	4.206066	-1.077783
H	-0.930676	0.634190	0.511616	H	0.523410	3.194245	-1.971358
P	0.574252	2.654373	0.440810	O	1.016816	1.143492	-0.184257
C	0.693202	3.745578	-1.046527				

TS(23c^{P-inv}):

E = -494.961841925034 au

ZPE = 0.06359361 au

G_{corr} = 0.03668374 au

$\nu = -1031.34 \text{ cm}^{-1}$

O	-0.021715	-0.015368	0.192387	C	3.497435	0.518613	-0.035932
P	1.717508	-0.175694	0.090855	H	4.246437	-0.254705	-0.224133
C	0.685978	1.260318	-0.066182	H	3.655639	1.392329	-0.673946
H	0.594544	1.990273	0.737639	H	3.642510	0.861284	1.009256
H	0.469421	1.700190	-1.039365				

23d:

E = -817.710065218876 au

ZPE = 0.06614380 au

G_{corr} = 0.03852635 au

C	-0.446629	1.301282	-0.184405	H	-0.117746	4.520636	-0.996427
H	-0.917998	1.422386	-1.153530	H	1.633845	4.285000	-1.045719
H	-1.040461	0.749705	0.534723	H	0.578994	3.195419	-1.971194
P	0.562188	2.689736	0.454550	S	1.317059	0.829143	-0.237139
C	0.673600	3.767579	-1.048813				

TS(23d^{P-inv}):

E = -817.590841917512 au

ZPE = 0.06516888 au

G_{corr} = 0.03729118 au

$\nu = -613.02 \text{ cm}^{-1}$

C	-0.612303	1.082318	-0.034447	H	-0.141624	4.541096	-1.120853
H	-1.294988	0.591035	-0.719470	H	1.531551	4.563266	-0.519671
H	-0.927737	1.077477	1.003408	H	1.181084	4.080029	-2.215195
P	0.489476	2.339848	-0.624716	S	1.183361	0.429378	-0.233104
C	0.834031	4.056442	-1.183907				

24a:

E = -459.186487484337 au

ZPE = 0.09220867 au

G_{corr} = 0.06611381 au

C	-3.213426	0.544208	-0.521213	H	-1.995913	0.068167	1.248746
C	-1.861729	0.385107	0.215286	H	-3.948509	2.645675	-0.890057
C	-3.462344	2.023503	-0.141099	H	-3.996577	2.116517	0.803643
H	-3.068447	0.451878	-1.599320	P	-1.598972	2.250460	0.073969
H	-3.997038	-0.158433	-0.231947	H	-1.532600	2.614123	1.446839
H	-1.117259	-0.250455	-0.260386				

TS(24a^{P-inv}):

E = -459.120490354024 au

ZPE = 0.09116747 au

G_{corr} = 0.06476506 au

$\nu = -884.70 \text{ cm}^{-1}$

P	-0.131761	0.992755	0.000000	H	0.863339	-0.375745	-1.859567
C	-0.028724	-0.353351	-1.235256	H	-0.790631	-2.018205	0.000000
C	0.044117	-1.319227	-0.000000	H	0.973556	-1.886222	-0.000000
C	-0.028724	-0.353351	1.235256	H	-0.906825	-0.510444	1.860030
H	-0.238542	2.381537	0.000001	H	0.863339	-0.375745	1.859567
H	-0.906825	-0.510445	-1.860030				

24b:

E = -475.214048365739 au

ZPE = 0.08067290 au

G_{corr} = 0.05386135 au

N	-0.029854	-0.003139	-0.115522	H	2.109402	-0.192492	-1.236466
P	1.705138	0.022509	0.116976	H	1.482316	2.396366	0.883459
C	1.317331	1.856250	-0.048265	H	1.801514	2.391723	-0.861572
C	-0.164513	1.464916	-0.285598	H	-0.858924	1.919698	0.424324
H	-0.570286	-0.410292	0.633686	H	-0.506904	1.710629	-1.295070

TS(24b^{P-inv}):

E = -475.131336527127 au

ZPE = 0.07991774 au

G_{corr} = 0.05396402 au

$\nu = -1055.22 \text{ cm}^{-1}$

N	-0.071887	-0.078550	-0.050071	H	2.667129	-0.875657	0.083468
P	1.669545	0.088330	0.053136	H	1.414053	2.404330	0.981321
C	1.327010	1.889150	0.022956	H	1.797781	2.476677	-0.760832
C	-0.121501	1.405544	-0.322442	H	-0.889639	1.893170	0.277732
H	-0.466116	-0.252749	0.870191	H	-0.324710	1.558526	-1.381756

TS(24b^{N-inv}):

E = -475.211258265379 au

ZPE = 0.07986343 au

G_{corr} = 0.05390882 au

$\nu = -392.31 \text{ cm}^{-1}$

N	-0.000886	0.026066	-0.101050	H	2.113229	-0.136448	-1.331015
P	1.703471	-0.016495	0.046562	H	1.431550	2.303384	0.938401
C	1.303411	1.825105	-0.031613	H	1.812276	2.406822	-0.795821
C	-0.175473	1.454545	-0.330048	H	-0.897628	1.928804	0.341479
H	-0.712757	-0.633932	0.149447	H	-0.460829	1.694632	-1.363178

24c:

E = -495.08130687215 au

ZPE = 0.06867512 au

G_{corr} = 0.04277667 au

P	-0.594289	0.040636	-0.644633	H	-1.697035	-2.039410	0.167559
H	-0.916432	1.265051	0.036439	C	-0.143201	-1.020535	1.360432
O	0.693472	-0.480695	0.305621	H	0.249763	-1.981401	1.697153
C	-1.475660	-1.059699	0.589058	H	-0.173255	-0.323321	2.204020
H	-2.349922	-0.670097	1.104174				

TS(24c^{P-inv}):

E = -494.983767071967 au

ZPE = 0.06699104 au

G_{corr} = 0.04156762 au

$\nu = -1200.08 \text{ cm}^{-1}$

O	0.265741	-0.253356	0.151626	H	1.972156	2.290845	0.708884
P	1.901080	-0.047811	-0.198483	H	1.597489	2.297700	-1.037364
C	1.518655	1.735869	-0.109321	H	-0.261463	1.480792	1.189136
C	0.084242	1.191757	0.196608	H	-0.638483	1.488375	-0.563446
H	2.808825	-1.072823	-0.396973				

24d:

E = -817.69880979382 au

ZPE = 0.06635142 au

G_{corr} = 0.03938544 au

P	-0.825343	0.147701	-0.729040	H	-0.962738	1.311067	0.088956
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S	1.039157	-0.555946	0.121771	C	-0.165607	-1.060024	1.436938
C	-1.440368	-1.045447	0.586152	H	0.094402	-2.018144	1.886464
H	-2.349519	-0.744403	1.107351	H	-0.189866	-0.291757	2.210687
H	-1.606677	-2.012516	0.110545				

TS(24d^{P-inv}):

E = -817.616427994735 au

ZPE = 0.06502537 au

G_{corr} = 0.03791472 au

$\nu = -1052.02 \text{ cm}^{-1}$

P	-0.748517	0.084954	-0.688415	H	-1.718304	-2.031719	0.159757
H	-1.153518	0.939747	-1.704875	C	-0.167396	-1.035204	1.383329
S	1.117017	-0.410178	0.180865	H	0.122406	-2.021498	1.740212
C	-1.483786	-1.044525	0.559310	H	-0.234926	-0.331446	2.209916
H	-2.333945	-0.662826	1.120260				

25a:

E = -498.432972439673 au

ZPE = 0.12073936 au

G_{corr} = 0.09228958 au

C	0.036397	1.224183	-0.136734	H	-0.222744	3.309578	-0.963390
C	1.485005	0.707329	0.038769	H	0.430432	3.226442	0.686209
C	0.391646	2.723683	-0.281968	P	2.110725	2.232194	-0.869128
H	-0.391719	0.844752	-1.066139	C	3.239778	3.040358	0.352663
H	-0.655662	0.977000	0.670191	H	3.384654	4.085734	0.072359
H	1.714606	-0.264786	-0.393946	H	2.850523	2.995618	1.372254
H	1.792803	0.714142	1.086184	H	4.215317	2.550932	0.322102

TS(25a^{P-inv}):

E = -498.362996189542 au

ZPE = 0.12017669 au

G_{corr} = 0.09118353 au

$\nu = -429.35 \text{ cm}^{-1}$

C	-1.204445	0.548600	-0.577935	H	-1.882002	2.488728	-1.464625
C	0.349013	0.334416	-0.576505	H	-1.883350	2.488070	0.309030
C	-1.374688	2.108145	-0.577553	P	0.455710	2.161397	-0.576051
H	-1.659477	0.106397	-1.463136	C	1.749237	3.460419	-0.576352
H	-1.661247	0.105686	0.306000	H	2.367212	3.446666	0.321913
H	0.716897	-0.183644	-1.462955	H	2.380741	3.429399	-1.464723
H	0.715212	-0.184119	0.310362	H	1.193604	4.401526	-0.590436

25b:

E = -514.466683950073 au

ZPE = 0.10946861 au

G_{corr} = 0.08086949 au

C	0.159516	1.231956	-0.104971	H	-0.473090	0.824642	-0.899474
C	0.417002	2.743594	-0.315440	H	-0.294875	0.969690	0.854329

H	-0.245783	3.237882	-1.021661	H	2.803291	2.851814	1.356214
H	0.443387	3.311789	0.613387	H	4.199160	2.513837	0.306184
P	2.124837	2.293881	-0.948842	N	1.573668	0.798848	-0.207232
C	3.220916	2.995863	0.358389	H	1.736414	-0.064089	-0.708060
H	3.363085	4.062827	0.165199				

TS(25b^{P-inv}):

E = -514.374784957639 au

ZPE = 0.10889969 au

G_{corr} = 0.08054818 au

v = -510.79 cm⁻¹

C	-1.080455	0.572235	-0.713244	C	1.774880	3.459075	-0.694366
C	-1.413097	2.075263	-0.436764	H	2.414023	3.519919	0.187591
H	-1.323555	0.320047	-1.745036	H	2.376334	3.273029	-1.584966
H	-1.592740	-0.109452	-0.033179	H	1.270758	4.420227	-0.824037
H	-2.014749	2.542389	-1.213209	N	0.415207	0.496883	-0.538739
H	-1.862318	2.264390	0.541918	H	0.612145	0.140503	0.393461
P	0.411580	2.254827	-0.542160				

TS(25b^{N-inv}):

E = -514.462366114808 au

ZPE = 0.10838034 au

G_{corr} = 0.08030642 au

v = -357.58 cm⁻¹

C	0.305703	1.278417	0.040383	C	3.152701	2.979984	0.486475
C	0.458649	2.747038	-0.441711	H	3.291160	4.060320	0.381836
H	-0.555862	0.762982	-0.395920	H	2.641598	2.770207	1.428266
H	0.228399	1.197328	1.132278	H	4.142659	2.519615	0.505834
H	-0.196599	2.994556	-1.274931	N	1.585975	0.841014	-0.497058
H	0.365355	3.507879	0.330622	H	1.913608	-0.103102	-0.584598
P	2.216715	2.355100	-0.995282				

25c:

E = -534.332820609037 au

ZPE = 0.09713048 au

G_{corr} = 0.06890728 au

C	0.338655	1.335009	-0.161372	P	2.071124	2.561973	-1.119199
C	0.373996	2.859724	-0.387473	C	3.107249	2.858070	0.382446
H	-0.521890	0.822615	-0.594771	H	3.282536	3.934440	0.468845
H	0.426772	1.049213	0.890113	H	2.644195	2.494263	1.301329
H	-0.352006	3.211623	-1.118349	H	4.074964	2.371243	0.249957
H	0.322294	3.477128	0.507195	O	1.542925	0.974887	-0.882812

TS(25c^{P-inv}):

E = -534.228267136372 au

ZPE = 0.09605264 au

G_{corr} = 0.06850089 au

$$\nu = -510.79 \text{ cm}^{-1}$$

C	-1.153235	0.574090	-0.575980	P	0.299299	2.275677	-0.577105
C	-1.522408	2.093380	-0.580324	C	1.781406	3.328616	-0.576506
H	-1.510482	0.064262	-1.471282	H	2.388939	3.206448	0.321731
H	-1.513759	0.068636	0.320493	H	2.392962	3.201642	-1.471339
H	-2.051120	2.421411	-1.474020	H	1.373446	4.343120	-0.580194
H	-2.054741	2.425617	0.309656	O	0.300257	0.582294	-0.573353

25d:

$$E = -856.945407377745 \text{ au}$$

$$ZPE = 0.09483893 \text{ au}$$

$$G_{\text{corr}} = 0.06519963 \text{ au}$$

C	0.009137	1.238374	-0.218432	P	2.184835	2.361375	-0.999708
C	0.464478	2.701801	-0.323269	C	3.259921	3.091266	0.313437
H	-0.543285	0.913456	-1.098281	H	3.321277	4.170692	0.145947
H	-0.573266	1.000935	0.670065	H	2.880165	2.893074	1.316112
H	-0.160595	3.325335	-0.962721	H	4.267656	2.682482	0.222158
H	0.533710	3.165111	0.661021	S	1.666781	0.406286	-0.190422

TS(25d^{P-inv}):

$$E = -856.860326169307 \text{ au}$$

$$ZPE = 0.09413462 \text{ au}$$

$$G_{\text{corr}} = 0.06463208 \text{ au}$$

$$\nu = -482.34 \text{ cm}^{-1}$$

C	-1.309960	0.525656	-0.653679	P	0.458674	2.171920	-0.437724
C	-1.377043	2.060136	-0.430788	C	1.760204	3.437632	-0.654082
H	-1.462326	0.282543	-1.702835	H	2.374193	3.578305	0.235509
H	-2.006054	-0.027446	-0.025420	H	2.387919	3.237939	-1.522633
H	-1.903745	2.574497	-1.232729	H	1.202196	4.359407	-0.839631
H	-1.830614	2.321113	0.527619	S	0.437120	0.063492	-0.191831

26b:

$$E = -475.200904532896 \text{ au}$$

$$ZPE = 0.08085909 \text{ au}$$

$$G_{\text{corr}} = 0.05485227 \text{ au}$$

P	-0.064614	-0.101003	-0.089166	N	-0.934669	1.590755	1.398144
H	1.217716	0.358591	0.315761	H	-1.760414	2.033938	1.787967
C	-0.857854	1.612806	-0.071485	C	-0.857816	0.136073	1.608419
H	-1.831099	1.570233	-0.577470	H	-1.831145	-0.371006	1.631665
H	-0.277804	2.437937	-0.484847	H	-0.277631	-0.167990	2.479789

TS(26b^{P-inv}):

$$E = -475.129948023196 \text{ au}$$

$$ZPE = 0.07978992 \text{ au}$$

$$G_{\text{corr}} = 0.05357223 \text{ au}$$

$$\nu = -910.02 \text{ cm}^{-1}$$

P	-0.228988	-0.078986	-0.077369	N	-1.205324	1.507369	1.324855
H	0.237617	-1.064245	-0.951586	H	-2.217265	1.525788	1.342427
C	-0.767223	1.694399	-0.087644	C	-0.764393	0.130078	1.684783
H	-1.585974	1.984125	-0.746781	H	-1.581551	-0.489500	2.054803
H	0.045636	2.413624	-0.181055	H	0.050316	0.127691	2.407765

TS(26b^{N-inv}):

E = -475.190620744332 au

ZPE = 0.07947349 au

G_{corr} = 0.05334951 au

$\nu = -482.34 \text{ cm}^{-1}$

P	-0.245460	-0.130961	-0.116958	N	-1.153019	1.508401	1.343615
H	1.134118	0.122545	0.105556	H	-1.502669	2.211670	1.969835
C	-0.811251	1.681783	-0.048054	C	-0.808330	0.146941	1.676646
H	-1.658928	1.888080	-0.712474	H	-1.654682	-0.490341	1.959567
H	-0.017521	2.405829	-0.262849	H	-0.013103	0.018776	2.419186

26c:

E = -495.051034494673 au

ZPE = 0.06820997 au

G_{corr} = 0.04210116 au

P	-0.185411	-0.179447	-0.157491	O	-0.951407	1.569058	1.379351
H	1.158466	0.168219	0.147098	C	-0.837293	0.150756	1.583917
C	-0.837436	1.589851	-0.053548	H	-1.818763	-0.308010	1.745204
H	-1.818612	1.691572	-0.529789	H	-0.181386	-0.088219	2.420484
H	-0.181211	2.388667	-0.397973				

TS(26c^{P-inv}):

E = -494.978171574372 au

ZPE = 0.06692204 au

G_{corr} = 0.04091214 au

$\nu = -943.73 \text{ cm}^{-1}$

P	-0.259521	-0.147121	-0.132485	O	-1.176997	1.439355	1.265634
H	0.297437	-1.103020	-0.977765	C	-0.834664	0.081234	1.608958
C	-0.835620	1.608739	-0.125624	H	-1.718420	-0.479911	1.916415
H	-1.719560	1.843216	-0.720855	H	-0.073619	0.053306	2.390162
H	-0.075217	2.380939	-0.252531				

26d:

E = -817.682820133505 au

ZPE = 0.06542726 au

G_{corr} = 0.03815902 au

P	-0.254132	-0.067386	-0.061490	S	-0.505332	1.940662	1.767107
H	1.157833	0.038716	0.035708	C	-0.562180	0.104731	1.785597
C	-0.562152	1.787803	-0.062624	H	-1.544428	-0.268886	2.073097
H	-1.544467	2.038724	-0.461623	H	0.195850	-0.345335	2.422219
H	0.195672	2.379527	-0.570574				

TS(26d^{P-inv}):

E = -817.618464496917 au

ZPE = 0.06438373 au

G_{corr} = 0.03751796 au

$\nu = -890.81 \text{ cm}^{-1}$

P	-0.342420	-0.005673	-0.008730	S	-0.758217	1.864705	1.698089
H	-0.120073	-1.019494	-0.933938	C	-0.544291	0.022052	1.803286
C	-0.544848	1.801185	-0.146594	H	-1.436244	-0.456587	2.202524
H	-1.437004	2.154887	-0.659443	H	0.329834	-0.240821	2.395678
H	0.329096	2.367249	-0.462678				

27b:

E = -514.448918315656 au

ZPE = 0.10952400 au

G_{corr} = 0.08032800 au

P	0.576801	-0.000020	-0.752905	H	-0.455454	-1.962620	0.550799
C	1.723461	0.000010	0.701723	C	-0.776417	1.120803	-0.065989
H	2.365482	-0.880972	0.648665	H	-1.406176	1.496912	-0.881332
H	2.365481	0.880989	0.648617	H	-0.455405	1.962628	0.550746
H	1.182356	0.000033	1.647590	N	-1.356758	0.000017	0.690744
C	-0.776437	-1.120797	-0.065954	H	-2.368438	0.000026	0.755904
H	-1.406197	-1.496905	-0.881299				

TS(27b^{P-inv}):

E = -514.372648075405 au

ZPE = 0.10894444 au

G_{corr} = 0.08009903 au

$\nu = -435.46 \text{ cm}^{-1}$

C	-1.993113	0.865710	0.059654	H	-3.752113	0.781356	-0.975879
C	-3.631724	2.574587	-0.004622	P	-1.782751	2.706874	0.037622
H	-1.593828	0.283765	-0.773676	C	-0.480924	4.003708	-0.022547
H	-1.720252	0.379504	0.996815	H	0.156955	4.001059	0.861298
H	-4.164837	2.963663	-0.874480	H	0.124806	3.960222	-0.927634
H	-4.140479	2.902813	0.902093	H	-1.039981	4.943185	-0.032107
N	-3.461247	1.094600	-0.058278				

TS(27b^{N-inv}):

E = -514.439703068125 au

ZPE = 0.10814530 au

G_{corr} = 0.07988926 au

$\nu = -482.61 \text{ cm}^{-1}$

C	1.790322	-0.091152	0.162147	H	-0.285866	2.166053	0.541382
C	0.191542	1.528052	-0.213016	P	2.074757	1.728591	-0.284071
H	2.154705	-0.790545	-0.599936	C	2.363870	2.408260	1.412868
H	2.222974	-0.375050	1.129767	H	3.405645	2.244250	1.695208
H	-0.303970	1.698867	-1.176333	H	2.185821	3.485319	1.404580

H	1.712847	1.941167	2.154256	H	-0.354299	-0.508391	0.412615
N	0.365233	0.141184	0.149478				

27c: E = -534.299775711853 au
 ZPE = 0.09690551 au
 G_{corr} = 0.06866110 au

C	-0.118385	0.448204	-0.011043	P	-0.062970	2.079580	0.930008
C	1.695616	1.541701	0.518564	O	1.270283	0.506312	-0.386969
H	-0.771859	0.405592	-0.884433	C	-0.338855	3.229547	-0.496399
H	-0.319140	-0.410658	0.637685	H	-1.411512	3.342280	-0.664212
H	2.332557	2.275866	0.021440	H	0.062656	4.213313	-0.246149
H	2.225279	1.122952	1.380424	H	0.134094	2.869415	-1.411030

TS(27c^{P-inv}): E = -534.221205767967 au
 ZPE = 0.09607448 au
 G_{corr} = 0.06748141 au
 $\nu = -446.21 \text{ cm}^{-1}$

C	-1.988888	0.893645	0.026468	P	-1.749711	2.728095	0.003645
C	-3.592332	2.557325	-0.029745	C	-0.456530	4.028053	0.006092
H	-1.665680	0.333628	-0.854057	H	0.132486	4.041435	0.922658
H	-1.700947	0.360071	0.935183	H	0.194530	3.975699	-0.866079
H	-4.110080	2.868848	-0.939670	H	-1.020446	4.962932	-0.049915
H	-4.144933	2.895218	0.849753	O	-3.411154	1.127251	-0.004906

27d: E = -856.931853548935 au
 ZPE = 0.09394895 au
 G_{corr} = 0.06566269 au

C	1.798848	-0.188657	0.356076	P	1.919063	1.589453	-0.233457
C	0.049791	1.591093	-0.057743	C	2.396185	2.422887	1.343619
H	2.220672	-0.912864	-0.337901	H	3.458161	2.253263	1.531214
H	2.211903	-0.354503	1.350726	H	2.242189	3.498831	1.241789
H	-0.479122	1.834307	-0.977091	H	1.818235	2.056076	2.194503
H	-0.319740	2.220258	0.751570	S	-0.038355	-0.198506	0.348809

TS(27d^{P-inv}): E = -856.861906156289 au
 ZPE = 0.09335720 au
 G_{corr} = 0.06391529 au
 $\nu = -440.43 \text{ cm}^{-1}$

C	-1.812604	0.836510	0.025269	H	-4.144406	3.137608	0.852720
C	-3.649002	2.731021	-0.028121	P	-1.824549	2.661653	0.003624
H	-1.414630	0.334692	-0.856133	C	-0.532632	3.957456	0.006087
H	-1.444737	0.355286	0.930897	H	0.058197	3.969366	0.921996
H	-4.114011	3.116604	-0.934640	H	0.121355	3.900740	-0.864126

H	-1.089546	4.896190	-0.051939	S	-3.667120	0.875073	-0.006209
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28a:

E = -498.452838578353 au

ZPE = 0.12176431 au

G_{corr} = 0.09394151 au

C	-1.481038	0.585195	0.603213	H	0.212411	0.532812	-0.774279
C	-0.770165	1.004160	-0.685633	H	0.099232	2.852212	0.048651
C	-0.675932	2.531229	-0.651896	H	-0.444686	2.976089	-1.620183
C	-2.713669	1.490764	0.790911	H	-2.950263	1.635706	1.844564
H	-1.759161	-0.470953	0.591314	H	-3.597050	1.065079	0.314757
H	-0.797049	0.724811	1.445391	P	-2.324333	3.152537	-0.018444
H	-1.361388	0.694180	-1.552683	H	-3.034831	2.911684	-1.225570

TS(28a^{P-inv}):

E = -498.390303998560 au

ZPE = 0.12092220 au

G_{corr} = 0.09349695 au $\nu = -859.01 \text{ cm}^{-1}$

C	-1.486437	0.603406	0.641902	H	0.273347	0.533323	-0.642668
C	-0.719109	0.988582	-0.638212	H	0.241056	2.898757	-0.169863
C	-0.610177	2.524221	-0.740036	H	-0.506040	2.844310	-1.775062
C	-2.793997	1.417203	0.731784	H	-3.121297	1.524527	1.764339
H	-1.700471	-0.467293	0.654164	H	-3.593347	0.945719	0.158609
H	-0.867474	0.831052	1.512842	P	-2.225254	3.000834	-0.006004
H	-1.262704	0.614257	-1.508707	H	-2.851914	4.236266	-0.009945

28b:

E = -514.486209939983 au

ZPE = 0.11067844 au

G_{corr} = 0.08308037 au

C	-1.509486	0.533964	0.587628	H	-2.868027	1.686483	1.862929
C	-0.780089	0.975525	-0.690642	H	-3.616462	1.110512	0.376174
C	-2.692228	1.498922	0.804377	P	-2.195434	3.097488	-0.079068
H	-1.841257	-0.504874	0.524899	H	-2.993842	2.859570	-1.232303
H	-0.817380	0.606629	1.430412	N	-0.724672	2.440416	-0.701284
H	-1.342032	0.648604	-1.571615	H	0.087317	2.803851	-0.221391
H	0.224204	0.554104	-0.763168				

TS(28b^{P-inv}):

E = -514.408382731157 au

ZPE = 0.10974596 au

G_{corr} = 0.08245420 au $\nu = -978.33 \text{ cm}^{-1}$

C	-1.490891	0.528156	0.583992	H	-1.795723	-0.517965	0.521358
C	-0.745281	0.968884	-0.704123	H	-0.808105	0.627506	1.430469
C	-2.723120	1.440527	0.823155	H	-1.308025	0.657415	-1.586525

H	0.252292	0.527122	-0.744601	H	0.095392	2.725133	-0.092196
H	-2.862707	1.637678	1.884573	P	-2.193646	2.911884	-0.159945
H	-3.634714	1.002164	0.421113	H	-2.761232	4.131942	-0.470042
N	-0.640127	2.438383	-0.730724				

TS(28b^{N-inv}):

E = -514.482246219524 au

ZPE = 0.10961048 au

G_{corr} = 0.08200085 au

$\nu = -388.72 \text{ cm}^{-1}$

C	-1.516927	0.543713	0.548257	H	-2.775321	1.747125	1.874313
C	-0.762424	1.003264	-0.709419	H	-3.634538	1.143313	0.462135
C	-2.678024	1.532079	0.810901	P	-2.263761	3.109590	-0.135529
H	-1.879432	-0.480749	0.444455	H	-3.113933	2.789144	-1.247597
H	-0.827061	0.568353	1.393299	N	-0.794289	2.452700	-0.662884
H	-1.265754	0.624409	-1.610751	H	0.019786	3.000109	-0.866035
H	0.265555	0.636002	-0.722585				

28c:

E = -534.34955327319 au

ZPE = 0.09825905 au

G_{corr} = 0.07068442 au

C	-1.524436	0.546854	0.562838	H	0.249879	0.698153	-0.724642
C	-0.783486	1.042152	-0.679549	H	-2.781446	1.762317	1.884012
C	-2.692705	1.524425	0.825197	H	-3.650294	1.128552	0.488360
H	-1.874190	-0.477839	0.427442	P	-2.244191	3.065679	-0.156920
H	-0.839956	0.555468	1.412059	H	-2.999010	2.678963	-1.313565
H	-1.302490	0.735167	-1.596081	O	-0.764195	2.473173	-0.609185

TS(28c^{P-inv}):

E = -534.25704289138 au

ZPE = 0.09690114 au

G_{corr} = 0.06949223 au

$\nu = -1109.35 \text{ cm}^{-1}$

C	-1.478846	0.541038	0.600754	H	0.260967	0.625137	-0.728589
C	-0.763441	0.993597	-0.685502	H	-2.931441	1.594135	1.859370
C	-2.747859	1.407588	0.803541	H	-3.628511	0.948448	0.358984
H	-1.741404	-0.516447	0.547673	O	-0.699966	2.422190	-0.671142
H	-0.806116	0.689518	1.445871	P	-2.202749	2.900127	-0.126000
H	-1.318637	0.659606	-1.570737	H	-2.641468	4.165214	-0.454399

28d:

E = -856.961470813006 au

ZPE = 0.09548636 au

G_{corr} = 0.06681235 au

C	-1.514690	0.558449	0.569700	C	-2.691781	1.525016	0.807044
C	-0.765829	0.904449	-0.712921	H	-1.871413	-0.474923	0.529937

H	-0.816958	0.630268	1.404973	H	-3.627022	1.121980	0.415929
H	-1.352834	0.664767	-1.601793	P	-2.408546	3.181074	-0.048518
H	0.193835	0.390746	-0.777639	H	-3.079786	2.821410	-1.252140
H	-2.832676	1.702857	1.872727	S	-0.438819	2.706969	-0.687333

TS(28d^{P-inv}):

E = -856.886771044779 au

ZPE = 0.09424802 au

G_{corr} = 0.06581031 au

$\nu = -945.20 \text{ cm}^{-1}$

C	-1.491196	0.530524	0.580312	H	0.223472	0.338282	-0.747846
C	-0.722407	0.879537	-0.706327	H	-2.865492	1.595361	1.894316
C	-2.721957	1.440226	0.826220	H	-3.628446	1.007046	0.406489
H	-1.815082	-0.512574	0.538832	S	-0.320306	2.671457	-0.671808
H	-0.805460	0.633605	1.421419	P	-2.297651	2.984367	-0.089869
H	-1.311594	0.667776	-1.598939	H	-3.061175	4.107429	-0.357940

29a:

E = -537.699959095287 au

ZPE = 0.15036906 au

G_{corr} = 0.12057576 au

C	-1.527312	0.603126	0.557159	H	-0.569516	3.114285	-1.559570
C	-0.889444	1.087849	-0.746155	H	-2.931376	1.562114	1.940288
C	-0.721399	2.604217	-0.606906	H	-3.616226	1.201907	0.361342
C	-2.710592	1.534076	0.873489	P	-2.258002	3.253115	0.245572
H	-1.842706	-0.441021	0.496515	C	-3.394662	3.370559	-1.218031
H	-0.787744	0.666111	1.360884	H	-4.419234	3.502399	-0.865979
H	-1.551061	0.860561	-1.587077	H	-3.130788	4.251065	-1.806289
H	0.061822	0.586846	-0.942670	H	-3.356993	2.489119	-1.861723
H	0.139460	2.833950	0.025422				

TS(29a^{P-inv}):

E = -537.631068296169 au

ZPE = 0.14980342 au

G_{corr} = 0.11961341 au

$\nu = -419.22 \text{ cm}^{-1}$

C	-1.503512	0.605868	0.631914	H	-0.495008	2.882341	-1.738808
C	-0.711679	1.016760	-0.625809	H	-3.164736	1.494535	1.736613
C	-0.616096	2.553669	-0.707105	H	-3.605305	0.933520	0.118187
C	-2.817478	1.409184	0.706969	P	-2.249092	3.008490	0.004972
H	-1.706547	-0.467392	0.622869	C	-3.076530	4.638853	-0.002138
H	-0.904623	0.825313	1.518903	H	-4.031574	4.625095	-0.528604
H	-1.232447	0.648000	-1.512513	H	-3.216338	5.051236	0.997856
H	0.284772	0.569451	-0.613203	H	-2.404120	5.303485	-0.548547
H	0.229247	2.926585	-0.124651				

29b:

E = -553.735839232306 au

ZPE = 0.13918954 au

G_{corr} = 0.10961683 au

C	-1.556661	0.563993	0.535598	H	-3.635990	1.230523	0.407844
C	-0.902583	1.075689	-0.755034	P	-2.156333	3.207918	0.181159
C	-2.698618	1.537273	0.876102	C	-3.373652	3.351046	-1.203478
H	-1.915260	-0.462948	0.431488	H	-4.361902	3.555634	-0.784723
H	-0.813267	0.572042	1.337077	H	-3.092642	4.190955	-1.839464
H	-1.526590	0.818882	-1.616408	H	-3.430062	2.446462	-1.812291
H	0.081749	0.637039	-0.926381	N	-0.798622	2.537201	-0.660564
H	-2.869720	1.600675	1.950212	H	0.076127	2.832208	-0.250438

TS(29b^{P-inv}):

E = -553.650461458097 au

ZPE = 0.13862989 au

G_{corr} = 0.10889867 au

$\nu = -477.20 \text{ cm}^{-1}$

C	-1.525389	0.497847	0.521737	H	-3.649521	1.067737	0.422972
C	-0.747321	1.063051	-0.697126	N	-0.588741	2.518543	-0.546759
C	-2.720829	1.423857	0.867862	H	0.156010	2.696403	0.121371
H	-1.870019	-0.519601	0.326981	P	-2.132871	2.982620	0.066803
H	-0.848109	0.461853	1.377933	C	-2.857697	4.635389	-0.173091
H	-1.310733	0.881096	-1.614652	H	-3.903334	4.538091	0.127123
H	0.233450	0.588955	-0.780670	H	-2.397432	5.418529	0.430746
H	-2.854918	1.489520	1.947447	H	-2.835089	4.919662	-1.225606

TS(29b^{N-inv}):

E = -553.731650090146 au

ZPE = 0.13806585 au

G_{corr} = 0.10849447 au

$\nu = -335.05 \text{ cm}^{-1}$

C	-1.577721	0.575487	0.484662	H	-3.649116	1.302457	0.480463
C	-0.872546	1.109762	-0.768495	P	-2.176032	3.252047	0.161783
C	-2.675287	1.585455	0.882897	C	-3.430737	3.324933	-1.212849
H	-1.989648	-0.422586	0.321979	H	-4.415066	3.535281	-0.785834
H	-0.843692	0.506263	1.289302	H	-3.175424	4.145435	-1.885649
H	-1.438749	0.838980	-1.670995	H	-3.487465	2.397501	-1.787015
H	0.131191	0.693558	-0.875014	N	-0.811767	2.546459	-0.566411
H	-2.775111	1.652403	1.965617	H	-0.013740	3.073824	-0.866504

29c:

E = -573.599455009953 au

ZPE = 0.12667952 au

G_{corr} = 0.09710839 au

C	-1.574661	0.612455	0.511444	H	0.123031	0.873506	-0.853962
C	-0.900271	1.222436	-0.714689	H	-2.861333	1.600135	1.983076
C	-2.731161	1.553126	0.902905	H	-3.679038	1.238001	0.464180
H	-1.922801	-0.402418	0.310528	P	-2.229664	3.231497	0.215383
H	-0.849112	0.560936	1.324992	C	-3.395018	3.304566	-1.222787
H	-1.467146	1.007984	-1.627807	H	-4.392049	3.544694	-0.844240

H	-3.086464	4.109755	-1.891051	O	-0.846298	2.636923	-0.492761
H	-3.450999	2.371155	-1.786246				

TS(29c^{P-inv}):

E = -573.500238705991 au

ZPE = 0.12588042 au

G_{corr} = 0.09623579 au

$\nu = -553.16 \text{ cm}^{-1}$

C	-1.507380	0.523048	0.570056	H	-3.648266	0.920689	0.269679
C	-0.750795	1.115596	-0.633243	P	-2.230692	2.945586	0.086155
C	-2.798766	1.344056	0.804139	C	-2.807219	4.649858	-0.159889
H	-1.744243	-0.528518	0.400106	H	-3.810881	4.660026	0.271349
H	-0.871724	0.596982	1.453206	H	-2.199915	5.385862	0.369371
H	-1.273431	0.870603	-1.566908	H	-2.883432	4.917000	-1.214848
H	0.277227	0.756045	-0.679005	O	-0.703552	2.532021	-0.469441
H	-3.036605	1.396568	1.865363				

29d:

E = -896.20996668341 au

ZPE = 0.12412863 au

G_{corr} = 0.09352388 au

C	-1.546881	0.627198	0.543484	H	-3.629550	1.258266	0.400480
C	-0.871934	1.040455	-0.758062	P	-2.353978	3.334804	0.277538
C	-2.702951	1.581442	0.879058	C	-3.478605	3.367970	-1.199866
H	-1.910174	-0.402838	0.474260	H	-4.512607	3.427001	-0.849601
H	-0.804917	0.659147	1.342878	H	-3.265186	4.264331	-1.782195
H	-1.515507	0.866444	-1.621941	H	-3.370207	2.492468	-1.841515
H	0.069072	0.514313	-0.918690	S	-0.487113	2.827793	-0.620817
H	-2.882445	1.605957	1.953956				

TS(29d^{P-inv}):

E = -896.129643292361 au

ZPE = 0.12324113 au

G_{corr} = 0.09214873 au

$\nu = -434.31 \text{ cm}^{-1}$

C	-1.536530	0.501237	0.520353	H	-3.608180	1.240742	0.491353
C	-0.722749	0.907235	-0.722228	P	-2.075287	3.093773	0.122941
C	-2.639722	1.522462	0.905228	C	-2.976466	4.662414	-0.126661
H	-1.990245	-0.478799	0.350425	H	-4.037856	4.422791	-0.032478
H	-0.844637	0.405828	1.357642	H	-2.724331	5.441262	0.592524
H	-1.324432	0.864221	-1.630231	H	-2.801618	5.024682	-1.139987
H	0.158042	0.271645	-0.825870	S	-0.136422	2.631863	-0.487449
H	-2.729243	1.574066	1.990528				

30b:

E = -514.469812710394 au

ZPE = 0.11045883 au

G_{corr} = 0.08284713 au

C	-0.430157	-0.430872	0.549744	H	-1.927913	0.501145	1.835236
C	0.310291	1.503944	-0.585104	H	-2.560522	-0.032926	0.277578
C	-1.697821	0.407337	0.774945	P	-1.355013	2.102141	0.021248
H	-0.656677	-1.494606	0.454657	H	-2.032238	1.865834	-1.202975
H	0.235479	-0.307189	1.419986	N	0.180668	0.054931	-0.684741
H	1.068245	1.826488	0.146188	H	1.074401	-0.393001	-0.856415
H	0.556244	1.950024	-1.549182				

TS(30b^{P-inv}):

E = -514.401524325786 au

ZPE = 0.10939834 au

G_{corr} = 0.08206095 au

$\nu = -903.85 \text{ cm}^{-1}$

C	-0.423443	-0.411732	0.614903	H	-2.130083	0.361997	1.719684
C	0.381103	1.483080	-0.686257	H	-2.522351	-0.168489	0.065964
C	-1.774962	0.317836	0.692110	N	0.257410	0.019158	-0.616665
H	-0.571430	-1.492081	0.566527	H	1.171775	-0.411481	-0.684016
H	0.152403	-0.177557	1.522437	P	-1.247493	1.947492	0.040467
H	1.223219	1.880407	-0.106144	H	-1.860171	3.187009	0.079794
H	0.482463	1.795920	-1.724804				

TS(30b^{N-inv}):

E = -514.459922244029 au

ZPE = 0.10900571 au

G_{corr} = 0.08086061 au

$\nu = -607.40 \text{ cm}^{-1}$

C	-0.457950	-0.465599	0.474141	H	-1.770874	0.592186	1.880802
C	0.303521	1.562516	-0.594721	H	-2.611045	0.015835	0.447487
C	-1.675430	0.444011	0.805640	P	-1.415528	2.103560	-0.037422
H	-0.770740	-1.475493	0.201648	H	-2.045961	1.750872	-1.260465
H	0.157769	-0.552433	1.383045	N	0.263827	0.133397	-0.613934
H	1.030364	1.973295	0.123279	H	0.679971	-0.408071	-1.344522
H	0.536663	1.976484	-1.575932				

30c:

E = -534.323621862898 au

ZPE = 0.09793534 au

G_{corr} = 0.07027977 au

C	-0.423306	-0.395291	0.527282	H	0.588220	1.914469	-1.504408
C	0.293099	1.515147	-0.535668	H	-1.890584	0.539604	1.850166
C	-1.701686	0.428375	0.783096	H	-2.578542	-0.031834	0.330554
H	-0.631589	-1.447843	0.339375	P	-1.408581	2.109107	-0.006814
H	0.241538	-0.321198	1.398187	H	-2.031244	1.808380	-1.246276
H	1.026828	1.831782	0.217750	O	0.242380	0.102714	-0.623796

TS(30c^{P-inv}):

E = -534.253741834501 au

ZPE = 0.09674148 au

G_{corr} = 0.06938275 au

$\nu = -909.39 \text{ cm}^{-1}$

C	-0.406591	-0.366626	0.634786	H	0.545103	1.721906	-1.670750
C	0.396059	1.468130	-0.623776	H	-2.140089	0.372926	1.713190
C	-1.777589	0.329755	0.687593	H	-2.509011	-0.180060	0.061265
H	-0.506097	-1.447146	0.542700	P	-1.270906	1.964808	0.036437
H	0.164934	-0.128274	1.538815	H	-1.935394	3.179669	0.041190
H	1.221176	1.860334	-0.022079	O	0.318391	0.056299	-0.527091

30d:

E = -856.944694304469 au

ZPE = 0.09448430 au

G_{corr} = 0.06579339 au

C	-0.473297	-0.508326	0.658734	H	0.504784	2.148789	-1.577930
C	0.333380	1.639516	-0.630437	H	-1.980747	0.512252	1.832264
C	-1.701888	0.401659	0.783098	H	-2.553235	-0.024124	0.253957
H	-0.744401	-1.564420	0.653388	P	-1.343611	2.099895	0.051764
H	0.210456	-0.341125	1.493346	H	-2.040409	1.896775	-1.166064
H	1.109388	1.949463	0.071317	S	0.406114	-0.156942	-0.893992

TS(30d^{P-inv}):

E = -856.881098946221 au

ZPE = 0.09340911 au

G_{corr} = 0.06497392 au

$\nu = -863.60 \text{ cm}^{-1}$

C	-0.478108	-0.496998	0.769053	H	0.444978	1.939122	-1.778090
C	0.426389	1.640727	-0.731539	H	-2.219777	0.408489	1.679659
C	-1.774576	0.308826	0.689575	H	-2.488549	-0.169642	0.019669
H	-0.671202	-1.570062	0.763093	P	-1.199098	1.935023	0.065253
H	0.081228	-0.237491	1.667091	H	-1.842786	3.156447	0.181279
H	1.258421	2.099253	-0.200049	S	0.563067	-0.181975	-0.712713

31b:

E = -553.718175605291 au

ZPE = 0.13911582 au

G_{corr} = 0.10956263 au

C	-0.523448	-0.399595	0.454713	H	-2.629649	0.171417	0.453327
C	0.250865	1.608909	-0.512069	P	-1.301879	2.236760	0.321748
C	-1.690819	0.489395	0.908042	N	-0.003600	0.195893	-0.773317
H	-0.842281	-1.425717	0.261355	H	0.825644	-0.286470	-1.101265
H	0.234045	-0.430707	1.255201	C	-2.408813	2.314103	-1.163904
H	1.097335	1.781723	0.170716	H	-3.448566	2.363238	-0.835814
H	0.441663	2.155897	-1.436743	H	-2.194218	3.225149	-1.725180
H	-1.813994	0.463306	1.989929	H	-2.273609	1.446239	-1.810437

TS(31b^{P-inv}):

E = -553.642422586599 au

ZPE = 0.13832047 au

G_{corr} = 0.10825013 auν = -429.09 cm⁻¹

C	-0.442172	-0.411918	0.599694	H	-2.529355	-0.194257	-0.001839
C	0.372732	1.524486	-0.632903	N	0.277176	0.057351	-0.596833
C	-1.805060	0.296764	0.650137	H	1.203485	-0.351768	-0.629186
H	-0.569506	-1.493504	0.520710	P	-1.286701	1.949176	0.050936
H	0.098878	-0.190937	1.531762	C	-2.105702	3.580967	0.102212
H	1.196745	1.921621	-0.024564	H	-3.041618	3.600786	-0.456895
H	0.503720	1.857566	-1.662968	H	-2.274270	3.944000	1.116472
H	-2.189343	0.307704	1.669529	H	-1.409601	4.264743	-0.388376

TS(31b^{N-inv}):

E = -553.708273666155 au

ZPE = 0.13771423 au

G_{corr} = 0.10774905 auν = -595.54 cm⁻¹

C	-0.582779	-0.409861	0.362904	H	-2.665112	0.258000	0.633904
C	0.267205	1.678127	-0.497351	P	-1.321214	2.279398	0.323294
C	-1.660882	0.542474	0.950481	N	0.074892	0.276363	-0.715629
H	-1.019674	-1.342118	0.000266	H	0.329293	-0.181117	-1.567400
H	0.117708	-0.674909	1.170085	C	-2.409040	2.258792	-1.178980
H	1.106344	1.904574	0.177878	H	-3.455770	2.254454	-0.871004
H	0.438305	2.214350	-1.431718	H	-2.236995	3.163097	-1.765249
H	-1.644274	0.529885	2.039829	H	-2.216467	1.380985	-1.799270

31c:

E = -573.571873190563 au

ZPE = 0.12658282 au

G_{corr} = 0.09693875 au

C	-0.554906	-0.357895	0.371162	H	-2.665200	0.214421	0.551551
C	0.219126	1.634635	-0.477849	P	-1.345092	2.273509	0.335179
C	-1.689583	0.524900	0.926408	C	-2.432631	2.302080	-1.167218
H	-0.900430	-1.342183	0.057043	H	-3.477436	2.347146	-0.855831
H	0.219880	-0.489127	1.138224	H	-2.219785	3.201836	-1.746968
H	1.063023	1.759347	0.213762	H	-2.282765	1.423489	-1.796229
H	0.443813	2.157739	-1.406754	O	0.012589	0.262520	-0.774463
H	-1.720663	0.487941	2.014781				

TS(31c^{P-inv}):

E = -573.494860518477 au

ZPE = 0.12575791 au

G_{corr} = 0.09571023 auν = -429.02 cm⁻¹

C	-0.421742	-0.368709	0.620512	C	-1.794580	0.321255	0.654541
C	0.404848	1.506478	-0.564907	H	-0.511272	-1.446755	0.491409

H	0.121122	-0.156964	1.548662	C	-2.142724	3.591984	0.094351
H	1.220501	1.887055	0.059087	H	-3.054721	3.590066	-0.502887
H	0.579671	1.782930	-1.603320	H	-2.360694	3.939142	1.104423
H	-2.183649	0.327905	1.672584	H	-1.445113	4.297949	-0.361083
H	-2.509349	-0.179836	-0.000312	O	0.339299	0.091418	-0.504680
P	-1.280644	1.979025	0.067787				

31d:

E = -896.19348390939 au

ZPE = 0.12312644 au

G_{corr} = 0.09259621 au

C	-0.568521	-0.484955	0.552737	H	-2.626527	0.183515	0.402709
C	0.264905	1.726807	-0.603490	P	-1.288244	2.230748	0.305536
C	-1.700769	0.490776	0.890777	C	-2.443203	2.353059	-1.136436
H	-0.922487	-1.513437	0.476016	H	-3.470714	2.381451	-0.770290
H	0.209447	-0.453798	1.317854	H	-2.254461	3.285579	-1.670648
H	1.134323	1.904021	0.031058	H	-2.329407	1.510221	-1.820559
H	0.376703	2.320480	-1.510598	S	0.168409	-0.034586	-1.049287
H	-1.879514	0.500479	1.967417				

TS(31d^{P-inv}):

E = -896.122624873788 au

ZPE = 0.12234360 au

G_{corr} = 0.09109539 au

$\nu = -422.77 \text{ cm}^{-1}$

C	-0.468441	-0.442061	0.809280	H	-2.491981	-0.181226	0.076430
C	0.377967	1.625026	-0.827606	P	-1.225630	1.948936	-0.000474
C	-1.772753	0.344654	0.706006	C	-2.067200	3.566628	0.135343
H	-0.646400	-1.517107	0.856790	H	-2.501979	3.912173	-0.802994
H	0.098198	-0.131180	1.686092	H	-2.874422	3.423636	0.856310
H	1.220913	2.132835	-0.358065	H	-1.400471	4.331790	0.534287
H	0.365555	1.851958	-1.893380	S	0.553481	-0.189577	-0.699256
H	-2.205885	0.486458	1.697403				

32:

E = -496.005500069283 au

ZPE = 0.07443442 au

G_{corr} = 0.04792119 au

P	-0.059701	-0.055188	0.058805	H	-0.428671	-0.446167	-1.253015
C	1.738675	-0.011400	-0.075432	H	2.372552	-0.885634	-0.075854
C	2.176660	1.264875	0.006867	H	3.222272	1.540542	0.071888
C	1.116569	2.260049	0.008671	H	1.325853	3.320856	0.075130
C	-0.129681	1.742584	-0.072352	H	-1.042192	2.319994	-0.070180

TS(32^{P-inv}):

E = -495.977486656091 au

ZPE = 0.07352106 au

G_{corr} = 0.04726291 au

$$\nu = -596.41 \text{ cm}^{-1}$$

P	0.015978	0.017169	-0.000006	H	-0.931767	-0.996673	0.000220
C	1.728916	-0.060893	0.000066	H	2.350309	-0.939225	0.000305
C	2.150492	1.263142	-0.000255	H	3.197799	1.530555	-0.000291
C	1.116524	2.230297	-0.000529	H	1.313496	3.293105	-0.000794
C	-0.176515	1.721086	-0.000435	H	-1.094509	2.282251	-0.000601

33:

$$E = -535.252217882949 \text{ au}$$

$$ZPE = 0.10358459 \text{ au}$$

$$G_{\text{corr}} = 0.07474929 \text{ au}$$

P	0.030691	0.018209	-0.078509	H	1.476573	3.367094	-0.098807
C	1.829307	0.025319	-0.017993	H	-0.883471	2.393704	-0.442833
C	2.286205	1.297343	0.037437	C	-0.399847	-0.699321	-1.732474
C	1.252639	2.307542	-0.131733	H	-0.209966	-1.772727	-1.709423
C	0.011435	1.802073	-0.315572	H	-1.464217	-0.548042	-1.914259
H	2.441914	-0.856470	0.101297	H	0.177800	-0.241770	-2.534013
H	3.323711	1.561743	0.203435				

TS(33^{P-inv}):

$$E = -535.226785292322 \text{ au}$$

$$ZPE = 0.10257976 \text{ au}$$

$$G_{\text{corr}} = 0.07339533 \text{ au}$$

$$\nu = -239.74 \text{ cm}^{-1}$$

P	0.062847	0.044969	0.056495	H	1.429455	3.272564	-0.360202
C	1.766500	-0.049932	0.165087	H	-0.995242	2.294218	-0.347274
C	2.221788	1.258736	-0.008145	C	-1.219226	-1.231652	0.174322
C	1.213933	2.223632	-0.212382	H	-1.231784	-1.694651	1.159808
C	-0.090554	1.727046	-0.210331	H	-2.174669	-0.733183	0.008402
H	2.372264	-0.923762	0.332829	H	-1.087533	-1.995341	-0.590868
H	3.273622	1.507444	0.014464				

34b:

$$E = -507.284088975184 \text{ au}$$

$$ZPE = 0.05773401 \text{ au}$$

$$G_{\text{corr}} = 0.03130860 \text{ au}$$

P	1.037329	0.394113	-0.431499	H	1.777337	2.149830	0.875579
N	0.285887	1.952127	-0.500515	N	0.436109	-0.180677	1.034483
H	0.247992	2.333332	-1.442907	H	-0.201065	0.381536	1.581767
N	1.762719	1.935031	-0.119787	H	0.288101	-1.173407	1.117724

TS(34b^{P-inv}):

$$E = -507.239821499 \text{ au}$$

$$ZPE = 0.05674696 \text{ au}$$

$$G_{\text{corr}} = 0.03005648 \text{ au}$$

$$\nu = -338.81 \text{ cm}^{-1}$$

P	0.187686	-0.043101	-0.434170	H	1.925864	1.450233	-0.236300
N	0.368084	2.602017	-0.771884	N	1.567504	-1.040171	-0.114098
H	1.087434	3.316176	-0.678724	H	1.308417	-1.869769	0.405091
N	0.927473	1.451975	-0.462970	H	2.379286	-0.622796	0.326361

TS(34b^{N-endo-inv}): E = -507.257693937179 au
 ZPE = 0.05615621 au
 G_{corr} = 0.02989198 au
 ν = -779.07 cm⁻¹

P	1.088319	0.392670	-0.308099	H	2.084191	2.649603	0.532386
N	0.220170	1.953670	-0.499669	N	0.381270	-0.324795	1.030545
H	0.372084	2.291861	-1.457994	H	-0.143254	0.224842	1.697771
N	1.545835	1.889359	0.169858	H	0.085795	-1.285323	0.950046

TS(34b^{N-exo-inv}): E = -507.283609066054 au
 ZPE = 0.05723205 au
 G_{corr} = 0.03119597 au
 ν = -183.89 cm⁻¹

P	1.011058	0.395794	-0.450899	H	1.785352	2.130934	0.878275
N	0.296844	1.966453	-0.501212	N	0.316445	-0.192407	0.956859
H	0.264242	2.356606	-1.439684	H	-0.221256	0.375822	1.593679
N	1.772402	1.922805	-0.118423	H	0.409323	-1.164119	1.196250

34c: E = -566.846115044736 au
 ZPE = 0.02069231 au
 G_{corr} = -0.00524670 au

P	0.410145	-0.760405	0.172103	O	0.410098	-0.042507	-1.281121
O	1.180723	-2.175830	-0.109555	H	0.410073	0.920097	-1.203506
O	-0.360377	-2.175865	-0.109524				

TS(34c^{P-inv}): E = -566.795091838353 au
 ZPE = 0.01953442 au
 G_{corr} = -0.00600267 au
 ν = -286.94 cm⁻¹

P	0.091855	0.662287	0.103245	O	1.031831	-0.564545	0.678280
O	-0.195423	2.307798	-0.314807	H	1.942488	-0.397323	0.970357
O	1.167890	1.827440	0.266714				

35b: E = -546.512152369485 au
 ZPE = 0.08655168 au

$$G_{\text{corr}} = 0.05781672 \text{ au}$$

P	1.111546	0.404878	-0.406271	H	0.205533	-1.307822	0.794389
N	0.427739	1.980680	-0.574288	C	-0.814540	0.314566	1.657167
H	0.680088	2.424158	-1.453562	H	-0.363529	0.336575	2.654872
N	1.712470	1.903547	0.242590	H	-1.017693	1.334855	1.336060
H	1.415934	2.063556	1.203634	H	-1.767986	-0.213091	1.720907
N	0.047703	-0.319899	0.670112				

TS(35b^{P-inv}):

$$E = -546.466062041745 \text{ au}$$

$$ZPE = 0.08507743 \text{ au}$$

$$G_{\text{corr}} = 0.05621155 \text{ au}$$

$$\nu = -182.19 \text{ cm}^{-1}$$

P	-0.075835	0.305508	-0.393683	H	2.065711	-0.678880	-0.643567
N	0.513560	2.903888	-0.175815	C	0.756540	-2.267003	-0.449626
H	1.355179	3.476489	-0.160470	H	0.841680	-2.473264	0.624717
N	0.903607	1.656005	-0.344035	H	-0.270961	-2.479574	-0.750349
H	1.903255	1.482022	-0.478396	H	1.404498	-2.954503	-0.994233
N	1.090913	-0.891496	-0.814502				

TS(35b^{N-endo-inv}):

$$E = -546.487020208206 \text{ au}$$

$$ZPE = 0.08476879 \text{ au}$$

$$G_{\text{corr}} = 0.05595430 \text{ au}$$

$$\nu = -760.71 \text{ cm}^{-1}$$

P	1.168973	0.413036	-0.243055	H	0.132838	-1.370991	0.730895
N	0.307469	1.933717	-0.657735	C	-0.824982	0.222555	1.724776
H	0.681358	2.277880	-1.550028	H	-0.788366	-0.245577	2.711088
N	1.421690	1.930321	0.326248	H	-0.597817	1.281305	1.834439
H	1.807754	2.718196	0.805534	H	-1.838014	0.130414	1.324628
N	0.166359	-0.368851	0.838820				

TS(35b^{N-exo-inv}):

$$E = -546.510726671102 \text{ au}$$

$$ZPE = 0.08579799 \text{ au}$$

$$G_{\text{corr}} = 0.05715785 \text{ au}$$

$$\nu = -179.02 \text{ cm}^{-1}$$

P	0.006084	0.013529	0.006301	H	-1.593395	1.026281	-1.272565
N	-0.009524	-0.021856	1.735963	C	-2.676508	0.748997	0.514834
H	0.926089	-0.022014	2.134385	H	-2.970024	-0.230405	0.901482
N	-0.165461	-1.370089	1.039106	H	-2.498697	1.407130	1.366037
H	-1.135285	-1.633919	1.199045	H	-3.512576	1.138543	-0.064944
N	-1.500736	0.657381	-0.341307				

35c:

$$E = -606.066755765905 \text{ au}$$

$$ZPE = 0.04898514 \text{ au}$$

$$G_{\text{corr}} = 0.01996731 \text{ au}$$

P	0.766922	-0.896993	0.134014	C	0.354922	1.469755	-0.952273
O	1.047478	-2.313149	-0.641904	H	0.955254	1.751028	-0.082983
O	-0.252918	-2.178606	0.173266	H	0.870216	1.773938	-1.861892
O	0.141842	0.051852	-1.007449	H	-0.615475	1.960407	-0.897127

TS(35c^{P-inv}):

$$E = -606.017366947454 \text{ au}$$

$$ZPE = 0.04803175 \text{ au}$$

$$G_{\text{corr}} = 0.02013185 \text{ au}$$

$$\nu = -274.27 \text{ cm}^{-1}$$

P	-0.307968	0.380759	-0.000044	C	2.340010	0.168908	0.000024
O	-1.243417	-0.905331	0.000078	H	2.894739	-0.127574	-0.889358
O	-2.016926	0.449006	-0.000078	H	2.202571	1.255448	-0.000119
O	1.083038	-0.509755	0.000067	H	2.894680	-0.127346	0.889518

36b:

$$E = -546.558563605451 \text{ au}$$

$$ZPE = 0.08707089 \text{ au}$$

$$G_{\text{corr}} = 0.05911015 \text{ au}$$

C	2.102160	-2.944341	0.389696	N	2.039719	-1.486468	0.267436
H	1.203939	-3.440632	0.006846	N	4.663864	-0.840991	0.145246
H	2.281020	-3.300427	1.412906	H	4.947058	-1.332969	0.983337
P	3.396548	-1.397220	-0.819909	H	5.422471	-0.366832	-0.319639
N	3.272998	-3.113577	-0.491836	H	1.991915	-0.924246	1.104248
H	3.171395	-3.753142	-1.268231				

TS(36b^{P-inv}):

$$E = -546.503972420116 \text{ au}$$

$$ZPE = 0.08530158 \text{ au}$$

$$G_{\text{corr}} = 0.05795122 \text{ au}$$

$$\nu = -228.15 \text{ cm}^{-1}$$

C	1.869284	-3.034526	0.325178	N	2.135415	-1.640430	0.007861
H	1.035208	-3.445298	-0.258696	N	3.847536	-0.009942	-0.663237
H	1.649086	-3.174335	1.393231	H	4.739976	0.333973	-0.986451
P	3.733791	-1.752264	-0.544662	H	3.186549	0.742131	-0.494288
N	3.161873	-3.472931	-0.093221	H	1.722995	-0.874459	0.516228
H	3.333167	-4.427499	-0.376242				

TS(36b^{N-endo-inv}):

$$E = -546.556406882725 \text{ au}$$

$$ZPE = 0.08636085 \text{ au}$$

$$G_{\text{corr}} = 0.05868208 \text{ au}$$

$$\nu = -367.50 \text{ cm}^{-1}$$

C	2.105062	-2.969518	0.420729	H	2.240195	-3.435285	1.407010
H	1.190288	-3.375707	-0.030218	P	3.403504	-1.378184	-0.753621

N	3.287215	-3.113189	-0.457514	H	5.053389	-1.295197	0.956838
H	3.157512	-3.708854	-1.264691	H	5.476662	-0.376422	-0.407484
N	2.170340	-1.522724	0.425345	H	1.663509	-0.883013	1.007977
N	4.745410	-0.842753	0.105728				

TS(36b^{N-exo-inv}):

E = -546.557773578082 au

ZPE = 0.08636754 au

G_{corr} = 0.05867576 au

$\nu = -90.72 \text{ cm}^{-1}$

C	2.080920	-2.922553	0.407834	N	2.061112	-1.466622	0.262274
H	1.200345	-3.404015	-0.030890	N	4.764096	-0.955258	0.269152
H	2.181460	-3.270156	1.444692	H	4.940476	-1.323782	1.193110
P	3.499131	-1.425564	-0.729052	H	5.411840	-0.255127	-0.050035
N	3.307022	-3.128791	-0.385302	H	1.962991	-0.893377	1.087147
H	3.255261	-3.782536	-1.154481				

36c:

E = -606.174279206985 au

ZPE = 0.05108218 au

G_{corr} = 0.02363533 au

C	2.030244	-2.812283	0.050182	O	2.084496	-1.396611	-0.150468
H	1.208723	-3.263835	-0.508565	P	3.600476	-1.525032	-0.831206
H	1.987216	-3.073585	1.111027	O	4.560296	-1.134606	0.431634
O	3.298141	-3.135854	-0.527795	H	5.289062	-0.564579	0.157305

TS(36c^{P-inv}):

E = -606.12469345206 au

ZPE = 0.05018826 au

G_{corr} = 0.02341759 au

$\nu = -200.57 \text{ cm}^{-1}$

C	1.501176	0.437674	-0.125043	O	0.162590	0.890897	0.163307
H	2.173503	0.754963	0.678292	P	-0.514507	-0.610119	0.218546
H	1.825545	0.849923	-1.085658	O	-2.001670	0.051075	0.543677
O	1.254930	-0.912193	-0.148826	H	-2.077843	1.015711	0.610076

37b:

E = -585.78482971657 au

ZPE = 0.08459294 au

G_{corr} = 0.11534102 au

C	2.181209	-3.123666	0.436523	N	4.263074	-0.539401	0.140953
H	1.293876	-3.700693	0.154273	H	4.739331	-1.119185	0.820555
H	2.674523	-3.639565	1.271458	H	1.961943	-1.358504	1.639234
P	2.876547	-1.128587	-0.606483	C	5.062666	0.536290	-0.424758
N	3.087142	-2.868539	-0.698263	H	4.467061	1.056136	-1.176314
H	2.876789	-3.341964	-1.566549	H	5.345157	1.262118	0.342110
N	1.882054	-1.715297	0.698707	H	5.974329	0.171968	-0.909511

TS(37b^{P-inv}):

E = -585.733118830228 au

ZPE = 0.11378971 au

G_{corr} = 0.08428358 au

v = -148.53 cm⁻¹

C	1.889679	-3.161319	0.300579	N	3.755876	-0.214161	-1.084555
H	1.279622	-3.838836	-0.311283	H	4.696686	0.111186	-1.256159
H	1.410336	-3.057255	1.284878	H	1.476993	-1.083724	-0.174392
P	3.779391	-1.853298	-0.476529	C	2.726675	0.777610	-1.359130
N	3.281835	-3.471523	0.327997	H	2.274098	1.163988	-0.437135
H	3.609353	-4.426918	0.351589	H	3.134733	1.629915	-1.904895
N	2.086548	-1.868543	-0.337205	H	1.930194	0.338794	-1.967231

TS(37b^{N-endo-inv}):

E = -585.782961139331 au

ZPE = 0.11476107 au

G_{corr} = 0.08449546 au

v = -362.70 cm⁻¹

C	2.198132	-3.162372	0.443376	N	4.294996	-0.493604	0.164369
H	1.270670	-3.645035	0.108712	H	4.772318	-1.042061	0.868953
H	2.655173	-3.793229	1.218991	H	1.623288	-1.401782	1.653328
P	2.887896	-1.107729	-0.512270	C	5.090067	0.544596	-0.470053
N	3.115872	-2.853398	-0.673838	H	4.479434	1.039643	-1.226698
H	2.871410	-3.268817	-1.563263	H	5.404527	1.298594	0.256184
N	2.038989	-1.772071	0.819143	H	5.982931	0.148377	-0.965000

TS(37b^{N-exo-inv}):

E = -585.782238045302 au

ZPE = 0.11481399 au

G_{corr} = 0.08452611 au

v = -180.72 cm⁻¹

C	-0.000623	-0.031895	0.003489	N	-1.505646	0.047098	-2.970230
H	-0.013462	-0.057596	1.098526	H	-0.552733	-0.164433	-3.232063
H	1.046186	-0.050097	-0.327777	H	-0.300587	1.812690	-1.041180
P	-1.931016	0.033614	-1.344476	C	-2.488313	-0.025535	-4.049215
N	-0.815127	-1.100380	-0.606498	H	-3.035833	0.913213	-4.159939
H	-1.178975	-1.809416	0.016007	H	-1.972695	-0.221461	-4.988967
N	-0.782017	1.078377	-0.543492	H	-3.214791	-0.827228	-3.894503

37c:

E = -645.394476253134 au

ZPE = 0.07931292 au

G_{corr} = 0.04871411 au

C	2.019411	-2.817709	0.161768	O	3.332749	-3.239972	-0.210757
H	1.263785	-3.541957	-0.147498	O	1.964920	-1.630920	-0.634004
H	1.948423	-2.595197	1.230340	P	3.522262	-1.889347	-1.176907

O	4.367180	-0.892834	-0.213606	H	5.641389	-0.369776	-1.790176
C	5.489449	-0.166923	-0.726735	H	5.308489	0.898014	-0.584274
H	6.379328	-0.463006	-0.171819				

TS(37c^{P-inv}):

E = -645.344907536781 au

ZPE = 0.07843866 au

G_{corr} = 0.04936033 au

$\nu = -199.58 \text{ cm}^{-1}$

C	2.120606	-0.242043	-0.028710	O	-1.369179	-0.534782	-0.544991
H	2.566108	-0.686416	0.867027	C	-2.646200	0.089129	-0.576893
H	2.800448	-0.330532	-0.881963	H	-2.575437	1.156867	-0.338070
O	0.881982	-0.907262	-0.329488	H	-3.073033	-0.027527	-1.573656
O	1.629766	1.028220	0.163240	H	-3.295864	-0.398467	0.150737
P	-0.055432	0.426876	-0.183010				

38b:

E = -585.82297753984 au

ZPE = 0.11633855 au

G_{corr} = 0.08690221 au

C	0.012816	0.027745	0.018947	N	-1.267811	3.190910	1.270330
C	0.021578	0.049588	1.542415	H	-0.277920	3.325231	1.426104
H	1.026284	0.084495	-0.386609	N	-1.343281	0.455438	1.866296
H	-0.450674	-0.902641	-0.330647	H	-1.555986	0.557357	2.847813
H	0.781315	0.757502	1.905211	N	-0.766446	1.208800	-0.355788
H	0.248630	-0.934363	1.956609	H	-1.095199	1.214077	-1.308792
P	-1.933755	1.692811	0.820255	H	-1.858380	3.825376	1.784417

TS(38b^{P-inv}):

E = -585.754394739586 au

ZPE = 0.11508367 au

G_{corr} = 0.08636510 au

$\nu = -263.37 \text{ cm}^{-1}$

P	-2.352282	0.660462	0.421178	H	-2.234931	1.668306	-1.696289
N	-2.475009	2.449590	0.497202	C	-2.176722	-1.605965	-1.215568
H	-2.479093	3.225847	-0.164242	H	-1.454517	-2.406112	-1.401553
H	-2.593149	2.780271	1.445991	H	-3.175988	-1.994202	-1.455895
N	-2.125712	-1.074382	0.129133	C	-1.857819	-0.368602	-2.059751
H	-2.228154	-1.709500	0.907739	H	-2.362903	-0.397239	-3.026914
N	-2.313702	0.762642	-1.267892	H	-0.776768	-0.304642	-2.241024

TS(38b^{N-endo-inv}):

E = -585.821123429781 au

ZPE = 0.11585535 au

G_{corr} = 0.08683721 au

$\nu = -316.02 \text{ cm}^{-1}$

C	-1.153975	0.887948	-0.057422	C	0.358572	0.704471	-0.172611
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H	-1.682163	0.403234	-0.882608	H	0.381012	3.864801	-1.596634
H	-1.505521	0.449293	0.886256	N	0.890234	1.811545	0.604638
H	0.664791	0.749402	-1.226591	H	1.724862	1.700919	1.148844
H	0.680231	-0.256060	0.231919	N	-1.339227	2.336400	-0.110043
P	-0.056598	3.226094	0.652241	H	-2.268248	2.652351	0.123418
N	0.304695	4.241472	-0.660282	H	0.938132	5.005606	-0.478647

TS(38b^{N-exo-inv}):

E = -585.822732494839 au

ZPE = 0.11582861 au

G_{corr} = 0.08671067 au

$\nu = -212.38 \text{ cm}^{-1}$

C	0.013279	0.027188	0.016964	N	-1.267043	3.162587	1.344048
C	0.022383	0.035235	1.540308	H	-0.279449	3.356862	1.418079
H	1.027012	0.085187	-0.387844	N	-1.342404	0.437917	1.869910
H	-0.452638	-0.898693	-0.341235	H	-1.542774	0.550920	2.853110
H	0.781335	0.741102	1.908895	N	-0.764121	1.213318	-0.345865
H	0.250838	-0.952133	1.945508	H	-1.096983	1.224798	-1.297546
P	-1.929486	1.688378	0.838106	H	-1.878777	3.879659	1.694122

38c:

E = -645.435047533215 au

ZPE = 0.08022193 au

G_{corr} = 0.05104574 au

C	-1.046616	0.988302	0.015996	O	0.883171	2.169232	0.682568
C	0.484277	0.971825	-0.008946	O	-1.434955	2.371404	0.111876
H	-1.476106	0.562941	-0.890758	P	-0.175848	3.383307	0.377345
H	-1.444012	0.464889	0.887636	O	0.173230	3.740945	-1.196622
H	0.871872	0.997690	-1.029428	H	0.521069	4.635663	-1.281820
H	0.904594	0.119304	0.521422				

TS(38c^{P-inv}):

E = -645.363703867552 au

ZPE = 0.07917962 au

G_{corr} = 0.05068201 au

$\nu = -247.89 \text{ cm}^{-1}$

C	-0.969326	1.089140	0.270946	O	1.123160	2.107321	0.107781
C	0.479154	0.880305	-0.182498	O	-1.172015	2.501503	0.350873
H	-1.698157	0.682235	-0.428923	P	0.148080	3.498893	0.418064
H	-1.154008	0.668262	1.262015	O	-0.907468	4.755900	0.786813
H	0.549545	0.683415	-1.256270	H	-1.853421	4.556521	0.880613
H	0.961222	0.059575	0.351583				

39b:

E = -625.050539952441 au

ZPE = 0.14504734 au

G_{corr} = 0.11315191 au

C	-1.104159	0.907583	-0.061660	N	1.004155	1.867016	0.583297
C	0.412282	0.800255	-0.233255	H	1.281689	1.552932	1.502946
H	-1.636462	0.432542	-0.890494	N	-1.350214	2.348480	-0.048264
H	-1.412470	0.413977	0.870967	H	-2.272239	2.617539	0.259897
H	0.674233	0.962468	-1.282691	C	1.331003	5.245783	-0.587276
H	0.797192	-0.176349	0.059079	H	1.319323	5.674775	0.416816
P	-0.042894	3.246779	0.665074	H	2.342778	4.867869	-0.775407
N	0.304730	4.219287	-0.671961	H	1.124445	6.049962	-1.297022
H	0.194249	3.794216	-1.583571				

TS(39b^{P-inv}):

E = -624.982964692889 au

ZPE = 0.14334909 au

G_{corr} = 0.11254586 au

$\nu = -251.36 \text{ cm}^{-1}$

C	-0.923465	0.614688	-0.523781	N	0.487144	1.980934	0.809703
C	0.388133	0.635761	0.266012	H	1.279426	2.155328	1.402625
H	-0.863330	-0.079528	-1.367055	N	-1.059130	2.000120	-0.916753
H	-1.757895	0.294424	0.115177	H	-1.817507	2.260907	-1.530740
H	1.232620	0.422215	-0.403052	C	0.563668	5.831992	0.765337
H	0.391170	-0.108447	1.064613	H	1.461996	6.351802	0.414806
P	-0.230830	3.282319	-0.013144	H	-0.215174	5.960025	0.007078
N	0.782687	4.411856	0.946524	H	0.221705	6.324257	1.682644
H	1.502236	4.217941	1.640092				

TS(39b^{N-endo-inv}):

E = -625.047901954914 au

ZPE = 0.14416253 au

G_{corr} = 0.11257678 au

$\nu = -316.43 \text{ cm}^{-1}$

C	-1.155353	0.901060	-0.063635	N	0.898593	1.778619	0.625579
C	0.354245	0.684478	-0.160044	H	1.724197	1.651216	1.179863
H	-1.684390	0.424275	-0.892901	N	-1.311040	2.353453	-0.123252
H	-1.526653	0.474401	0.877764	H	-2.233208	2.686056	0.114662
H	0.674346	0.724222	-1.210186	C	1.300914	5.317968	-0.545621
H	0.648998	-0.283826	0.246499	H	1.269829	5.681784	0.483704
P	-0.013332	3.219403	0.644735	H	2.340543	5.050851	-0.771909
N	0.375110	4.207656	-0.675982	H	1.011408	6.143930	-1.200241
H	0.293434	3.809567	-1.602560				

TS(39b^{N-exo-inv}):

E = -625.049137368388 au

ZPE = 0.14457463 au

G_{corr} = 0.11365051 au

$\nu = -48.43 \text{ cm}^{-1}$

C	0.041903	0.084643	-0.007473	H	0.724566	0.594451	1.981456
C	-0.014669	-0.067966	1.507169	H	0.200227	-1.092722	1.815184
H	1.072167	0.180741	-0.360084	P	-1.933516	1.659888	0.908926
H	-0.407871	-0.796379	-0.480608	N	-1.287836	3.045957	1.640722

H	-0.289367	3.198561	1.617686	C	-2.095717	4.204064	1.974746
N	-1.394383	0.298350	1.819780	H	-1.866659	5.069742	1.343657
H	-1.625564	0.321542	2.802771	H	-3.147214	3.952939	1.823874
N	-0.721900	1.304895	-0.276805	H	-1.971923	4.502054	3.020760
H	-1.026734	1.405364	-1.232946				

39c:

E = -684.655408416869 au

ZPE = 0.10857060 au

G_{corr} = 0.07653099 au

C	-0.985431	0.919606	-0.136935	O	-1.656098	2.184728	0.005579
C	0.500256	1.190118	0.110180	P	-0.690076	3.366142	0.595488
H	-1.172208	0.533120	-1.138569	O	-0.195879	3.977747	-0.848328
H	-1.400282	0.232085	0.602709	C	0.450045	5.251082	-0.860235
H	1.024164	1.428123	-0.817873	H	0.165110	5.760700	-1.779731
H	1.001219	0.364897	0.612944	H	0.145768	5.861657	-0.004303
O	0.530414	2.332978	0.983506	H	1.534402	5.124434	-0.836953

TS(39c^{P-inv}):

E = -684.584627141942 au

ZPE = 0.10719696 au

G_{corr} = 0.07641037 au

$\nu = -172.55 \text{ cm}^{-1}$

C	-0.960741	1.056357	0.264202	O	-1.181839	2.464923	0.343662
C	0.491127	0.865410	-0.185841	P	0.118610	3.479154	0.413785
H	-1.683849	0.639449	-0.435941	O	-0.925273	4.741656	0.783418
H	-1.141879	0.633782	1.255328	C	-2.335411	4.806619	0.995155
H	0.565375	0.673128	-1.260619	H	-2.585924	5.829822	1.275132
H	0.979886	0.046112	0.345057	H	-2.870800	4.534203	0.083955
O	1.118993	2.097753	0.112128	H	-2.637390	4.122334	1.789848

40a:

E = -520.354372851307 au

ZPE = 0.07711363 au

G_{corr} = 0.04945096 au

P	2.877073	0.605136	0.000159	C	3.724699	1.448019	-1.395739
C	3.726843	1.446520	1.395648	H	3.467291	0.954137	-2.333372
H	3.366214	2.476998	1.448844	H	3.364112	2.478610	-1.447099
H	3.471024	0.951449	2.333088	H	4.809663	1.452124	-1.272921
H	4.811604	1.450885	1.271064	F	3.731514	-0.782251	-0.001155

TS(40a^{P-inv}):

E = -520.2564338092 au

ZPE = 0.07665637 au

G_{corr} = 0.04883486 au

$\nu = -576.57 \text{ cm}^{-1}$

P	3.544402	0.716007	0.057436	C	3.629196	1.502588	1.690324
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H	3.713441	2.568291	1.463578	H	2.661928	1.254791	-2.169099
H	2.727287	1.348921	2.284157	H	3.678381	2.503790	-1.433945
H	4.508437	1.203208	2.262135	H	4.442092	1.099621	-2.194344
C	3.582140	1.429658	-1.610189	F	3.413849	-0.891681	0.093584

40b:

E = -880.338516927652 au

ZPE = 0.0764154 au

G_{corr} = 0.0478062 au

P	2.858929	0.626759	0.000181	C	3.723059	1.451834	-1.402142
C	3.725246	1.450282	1.402071	H	3.448040	0.962756	-2.336309
H	3.381405	2.487317	1.445221	H	3.379198	2.488935	-1.443552
H	3.451747	0.960112	2.336111	H	4.807489	1.433528	-1.287590
H	4.809492	1.432157	1.285766	Cl	3.902706	-1.198390	-0.001615

TS(40b^{P-inv}):

E = -880.255063194884 au

ZPE = 0.07575703 au

G_{corr} = 0.04658142 au

$\nu = -490.64 \text{ cm}^{-1}$

P	3.458402	0.675382	-0.077480	C	3.655534	1.539193	-1.670420
C	3.572609	1.426677	1.579339	H	2.752514	1.493876	-2.278672
H	3.787588	2.481194	1.391864	H	3.840529	2.581675	-1.401566
H	2.635827	1.356798	2.131654	H	4.508774	1.171334	-2.239771
H	4.387049	1.007030	2.169238	Cl	3.074142	-1.319805	-0.159397

40c:

E = -476.470408428643 au

ZPE = 0.10110076 au

G_{corr} = 0.07314554 au

P	3.774263	0.261310	-0.474475	H	3.213804	1.679039	-2.368999
C	3.930272	0.908720	1.255829	H	2.606526	2.404119	-0.865044
H	3.074083	1.528460	1.539898	H	4.333102	2.496840	-1.266744
H	4.008514	0.072672	1.952444	N	2.199741	-0.407433	-0.521636
H	4.838563	1.509299	1.345410	H	2.155239	-1.409459	-0.422519
C	3.443356	1.866153	-1.320040	H	1.455014	0.048279	-0.008416

TS(40c^{P-inv}):

E = -476.398438434292 au

ZPE = 0.10048605 au

G_{corr} = 0.07118866 au

$\nu = -473.98 \text{ cm}^{-1}$

P	3.147878	0.723455	-0.104468	C	3.681046	1.552164	-1.643575
C	3.467401	1.515086	1.511413	H	2.845658	1.833428	-2.286182
H	4.004738	2.440001	1.292606	H	4.190081	2.466453	-1.331739
H	2.552225	1.775026	2.045010	H	4.389349	0.952534	-2.216664
H	4.099329	0.904798	2.157942	N	2.384976	-0.746550	-0.170652

H	2.883758	-1.620463	-0.157298	H	1.386038	-0.837932	-0.250684
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40d:

E = -841.134487354019 au

ZPE = 0.15078677 au

G_{corr} = 0.11673333 au

P	2.883526	0.568845	0.002798	P	4.069196	-1.320300	-0.004091
C	3.743966	1.413305	1.414825	C	3.218073	-2.169116	1.410948
H	3.424677	2.456784	1.445261	H	3.537254	-3.212779	1.435818
H	3.449173	0.948865	2.356450	H	3.519379	-1.707828	2.352062
H	4.831321	1.376400	1.323827	H	2.130138	-2.131614	1.327435
C	3.734678	1.417674	-1.412215	C	3.208728	-2.164776	-1.416092
H	3.433355	0.956425	-2.353343	H	3.503517	-1.700362	-2.357730
H	3.415532	2.461349	-1.437053	H	3.528002	-3.208261	-1.446508
H	4.822612	1.380134	-1.328705	H	2.121375	-2.127853	-1.325081

TS(40d^{P-inv}):

E = -841.180203219837 au

ZPE = 0.15128442 au

G_{corr} = 0.11710550 au

$\nu = -303.42 \text{ cm}^{-1}$

P	3.110312	0.721057	0.372415	P	1.867980	-0.863699	0.977865
C	4.497829	1.201616	1.460870	C	0.136323	-0.200593	0.849781
H	4.403579	2.230493	1.811093	H	-0.568570	-1.010978	1.053498
H	4.462722	0.538565	2.325564	H	0.000807	0.579886	1.597092
H	5.464075	1.076397	0.970099	H	-0.084243	0.210185	-0.137205
C	2.962035	1.716599	-1.162436	C	1.814616	-2.030711	-0.467898
H	2.095947	1.344520	-1.711486	H	2.798276	-2.479861	-0.596797
H	2.797229	2.772961	-0.944704	H	1.090199	-2.821680	-0.256185
H	3.839929	1.612669	-1.801801	H	1.525675	-1.535718	-1.396855

40e:

E = -711.436695074355 au

ZPE = 0.10031733 au

G_{corr} = 0.07025199 au

P	2.830921	0.648147	0.003092	H	3.492329	2.473972	-1.477054
C	3.756869	1.409509	1.428712	H	4.831589	1.318628	-1.340899
H	3.501674	2.469226	1.484979	Si	3.827529	-1.376880	-0.003286
H	3.439204	0.940126	2.360582	H	3.412084	-2.132462	1.204277
H	4.840549	1.315117	1.335323	H	3.404847	-2.128448	-1.210849
C	3.747330	1.413926	-1.426300	H	5.311896	-1.266124	-0.007533
H	3.422802	0.947979	-2.357530				

TS(40e^{P-inv}):

E = -711.397152311737 au

ZPE = 0.10000741 au

G_{corr} = 0.06945094 au

$\nu = -285.96 \text{ cm}^{-1}$

P	3.183841	0.668311	0.240126	H	3.293727	2.324843	-1.563451
C	3.885734	1.641968	1.622103	H	4.711219	1.249926	-1.591456
H	3.539449	2.676412	1.603561	Si	1.914847	-1.073699	0.479160
H	3.547773	1.188058	2.554427	H	0.644849	-0.814649	1.206876
H	4.976643	1.628859	1.614149	H	1.621256	-1.448391	-0.925025
C	3.635353	1.299061	-1.418117	H	2.558892	-2.217995	1.176294
H	3.140230	0.666381	-2.155037				

41a:

E = -847.987902690636 au

ZPE = 0.30774111 au

G_{corr} = 0.26783731 au

P	-0.686705	0.043257	-0.104617	C	1.575453	-1.897056	0.216124
C	0.005089	0.904571	-1.577741	H	1.778165	-2.972387	0.225910
C	-0.895849	1.695324	-2.299535	H	2.231783	-1.456850	-0.533310
C	1.325011	0.834617	-2.038337	H	1.861985	-1.505544	1.190000
C	-0.496827	2.398660	-3.430641	C	-0.211779	0.200772	2.616225
H	-1.925721	1.749999	-1.968294	H	0.407802	-0.695678	2.655037
C	1.724217	1.520834	-3.178055	H	0.021578	0.802878	3.499149
H	2.055118	0.248446	-1.502648	H	-1.257519	-0.106508	2.689236
C	0.815485	2.308598	-3.876715	C	1.518262	1.409556	1.241850
H	-1.213536	3.007271	-3.967795	H	1.702481	2.040319	0.372643
H	2.749775	1.445080	-3.518041	H	1.808915	1.979011	2.130752
H	1.129195	2.845648	-4.762923	H	2.175712	0.545401	1.176747
C	0.095333	-1.666958	-0.096164	C	-0.793995	2.312965	1.413145
H	-0.479251	-2.152857	0.700262	H	-1.855777	2.094780	1.536506
C	-0.291816	-2.350852	-1.413428	H	-0.467132	2.920510	2.262293
H	0.262489	-1.926692	-2.252547	H	-0.673385	2.912579	0.508965
H	-0.065159	-3.418917	-1.366988	C	0.040427	1.023181	1.345347
H	-1.356178	-2.237738	-1.626843				

TS(41a^{P-inv}):

E = -847.938360573235 au

ZPE = 0.30666843 au

G_{corr} = 0.26727600 au

$\nu = -297.32 \text{ cm}^{-1}$

P	-0.315461	0.134538	0.156959	H	-2.273922	-3.104681	-0.167326
C	0.168724	0.733968	-1.438961	H	-2.874143	-1.437193	-0.080928
C	0.557913	2.071552	-1.651972	C	0.411941	-2.603889	0.067353
C	0.177657	-0.125410	-2.556944	H	0.108642	-3.637197	0.260227
C	0.930086	2.517163	-2.910863	H	0.731014	-2.542523	-0.973099
H	0.574164	2.772015	-0.830874	H	1.273393	-2.370608	0.691777
C	0.557721	0.332092	-3.808055	C	-0.882987	0.501021	2.827418
H	-0.116849	-1.158880	-2.449345	H	-0.203894	-0.312402	3.086855
C	0.937069	1.656824	-4.003301	H	-0.941150	1.172732	3.687457
H	1.220853	3.553434	-3.034733	H	-1.878557	0.088323	2.658569
H	0.553617	-0.358500	-4.642787	C	1.015051	1.854452	1.935485
H	1.230369	2.009263	-4.982918	H	1.444541	2.390135	1.090120
C	-0.753656	-1.650375	0.361512	H	0.954401	2.551370	2.777924
H	-0.961812	-1.707037	1.431760	H	1.699056	1.047924	2.198362
C	-2.032205	-2.059300	-0.382066	C	-1.364752	2.449585	1.345050
H	-1.918541	-1.961004	-1.461828	H	-2.374183	2.067536	1.194955

H	-1.372583	3.136384	2.197672	C	-0.382570	1.298933	1.617140
H	-1.092000	3.021523	0.459677				

41b:

E = -1099.05017911428 au

ZPE = 0.29735510 au

G_{corr} = 0.25408212 au

P	-0.818473	-0.189684	-0.342399	C	1.487986	-1.945098	0.262022
C	-0.077016	0.778047	-1.721564	H	1.801913	-2.992341	0.308610
C	-0.873513	1.807005	-2.240916	H	2.196389	-1.422065	-0.379062
C	1.198462	0.602004	-2.268675	H	1.582039	-1.531939	1.265013
C	-0.405747	2.644420	-3.245271	Si	0.000601	1.050798	1.374717
H	-1.874649	1.946021	-1.850935	C	-0.325107	0.114969	2.975056
C	1.659773	1.424201	-3.289575	H	0.243004	-0.815257	3.030687
H	1.847941	-0.174122	-1.894334	H	-0.046476	0.726806	3.837248
C	0.864141	2.454402	-3.777665	H	-1.384644	-0.132485	3.068579
H	-1.039995	3.437587	-3.621266	C	1.820045	1.502545	1.216589
H	2.650485	1.264643	-3.697257	H	2.013273	1.971877	0.250324
H	1.228125	3.099006	-4.567420	H	2.093220	2.217722	1.997846
C	0.051309	-1.858804	-0.257265	H	2.477121	0.637807	1.307833
H	-0.583050	-2.373487	0.473133	C	-1.003830	2.639634	1.360668
C	-0.108634	-2.592192	-1.592807	H	-2.071570	2.435281	1.458456
H	0.497858	-2.132991	-2.374705	H	-0.702513	3.285354	2.189971
H	0.209519	-3.633214	-1.492511	H	-0.848256	3.193229	0.432767
H	-1.146086	-2.583457	-1.930320				

TS(41b^{P-inv}):

E = -1099.02132899457 au

ZPE = 0.29648293 au

G_{corr} = 0.25346433 au

$\nu = -185.21 \text{ cm}^{-1}$

P	-0.344282	0.024123	0.016124	C	0.262164	-2.749498	-0.055509
C	0.145733	0.615147	-1.595563	H	-0.094854	-3.767015	0.129221
C	0.447841	1.978293	-1.765668	H	0.644851	-2.714243	-1.075919
C	0.256653	-0.222025	-2.716888	H	1.094768	-2.546836	0.617325
C	0.850222	2.473751	-2.994686	Si	-0.328399	1.359002	1.773066
H	0.362380	2.658589	-0.928199	C	-0.889792	0.268446	3.194989
C	0.653938	0.284561	-3.947177	H	-0.222883	-0.583304	3.338130
H	0.037487	-1.276341	-2.632177	H	-0.888366	0.852773	4.119114
C	0.957020	1.632328	-4.099044	H	-1.902808	-0.106605	3.039849
H	1.077434	3.528394	-3.091907	C	1.400007	2.023605	2.085269
H	0.730134	-0.386293	-4.794253	H	1.781804	2.554794	1.211334
H	1.269070	2.021854	-5.058853	H	1.401672	2.720766	2.928369
C	-0.875323	-1.743558	0.157799	H	2.091508	1.208821	2.304986
H	-1.168656	-1.792473	1.210685	C	-1.501267	2.812630	1.564525
C	-2.109504	-2.079892	-0.687128	H	-2.524289	2.467403	1.407642
H	-1.904680	-1.984258	-1.753775	H	-1.481565	3.450081	2.453567
H	-2.422395	-3.111504	-0.501441	H	-1.225249	3.429629	0.707485
H	-2.939597	-1.415756	-0.448691				

41c:

E = -2885.45671515146 au

ZPE = 0.29602594 au

G_{corr} = 0.25108416 au

P	-0.853128	-0.232462	-0.418428	C	1.486939	-1.912311	0.243449
C	-0.072259	0.749625	-1.764278	H	1.836885	-2.947469	0.300388
C	-0.811897	1.857380	-2.201937	H	2.180237	-1.367657	-0.395638
C	1.168769	0.517207	-2.366124	H	1.559979	-1.488871	1.244025
C	-0.318568	2.716662	-3.173732	C	-0.352556	0.071883	3.052243
H	-1.789504	2.041687	-1.772508	H	0.237483	-0.843285	3.097043
C	1.654889	1.365005	-3.354948	H	-0.079736	0.700547	3.901507
H	1.772643	-0.324351	-2.064256	H	-1.407391	-0.189702	3.139504
C	0.919654	2.473264	-3.757736	C	1.866554	1.547473	1.185319
H	-0.908477	3.570064	-3.484371	H	2.055235	1.919501	0.178512
H	2.618593	1.161313	-3.805414	H	2.104349	2.337162	1.900274
H	1.303690	3.136134	-4.522371	H	2.520839	0.697736	1.372467
C	0.049939	-1.878359	-0.281480	C	-1.105826	2.705464	1.380264
H	-0.574054	-2.381152	0.466283	H	-2.168197	2.473048	1.453524
C	-0.096947	-2.663302	-1.589942	H	-0.820292	3.320868	2.235098
H	0.499628	-2.224664	-2.390558	H	-0.933282	3.277223	0.468700
H	0.239239	-3.694238	-1.451504	Ge	-0.034891	1.050709	1.367555
H	-1.134895	-2.685909	-1.925361				

TS(41c^{P-inv}):

E = -2885.42498695535 au

ZPE = 0.29504900 au

G_{corr} = 0.25010051 auν = -205.08 cm⁻¹

P	-0.339961	-0.005446	-0.016173	C	0.275764	-2.775398	-0.120837
C	0.143434	0.607111	-1.619971	H	-0.073122	-3.796557	0.059815
C	0.465044	1.968668	-1.767669	H	0.639292	-2.727641	-1.147787
C	0.229491	-0.210703	-2.758249	H	1.119357	-2.574754	0.538638
C	0.859910	2.481464	-2.991721	C	-0.963509	0.229482	3.279133
H	0.401584	2.633251	-0.915279	H	-0.305228	-0.627778	3.417162
C	0.621903	0.313598	-3.982553	H	-0.971871	0.812542	4.201348
H	-0.006148	-1.262882	-2.691224	H	-1.974966	-0.125485	3.083659
C	0.942552	1.659679	-4.113080	C	1.498420	2.016696	2.159021
H	1.101648	3.534390	-3.071461	H	1.891431	2.536475	1.285699
H	0.679465	-0.342290	-4.842775	H	1.496284	2.705896	3.005804
H	1.249815	2.062725	-5.068790	H	2.152153	1.174344	2.382178
C	-0.862231	-1.776908	0.121861	C	-1.528059	2.909350	1.554838
H	-1.135906	-1.833789	1.180141	H	-2.536182	2.563762	1.329658
C	-2.109664	-2.112824	-0.703374	H	-1.549274	3.512186	2.464954
H	-1.922431	-2.010242	-1.772673	H	-1.185010	3.535400	0.731733
H	-2.416012	-3.146725	-0.518668	Ge	-0.327117	1.367012	1.805354
H	-2.937509	-1.452589	-0.447281				

41d:

E = -1022.50287397304 au

ZPE = 0.29372107 au

G_{corr} = 0.24623609 au

P	-0.921552	-0.310433	-0.537183	C	-0.089224	0.708710	-1.825198
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C	-0.796525	1.850841	-2.230003	H	1.829249	-2.940735	0.250712
C	1.155366	0.471753	-2.418485	H	2.123823	-1.326752	-0.389961
C	-0.270325	2.734113	-3.161293	H	1.444604	-1.523379	1.218614
H	-1.775454	2.042710	-1.806050	C	-0.404578	0.007957	3.273743
C	1.675043	1.346551	-3.366380	H	0.213863	-0.887609	3.321931
H	1.735515	-0.395178	-2.143176	H	-0.156411	0.653666	4.116393
C	0.971465	2.485732	-3.736931	H	-1.452682	-0.280493	3.346649
H	-0.836742	3.611815	-3.447023	C	2.032172	1.570490	1.175947
H	2.640566	1.137807	-3.810661	H	2.247427	1.711982	0.117608
H	1.381493	3.168356	-4.469933	H	2.252895	2.493813	1.711491
C	0.015763	-1.936091	-0.375036	H	2.660118	0.770981	1.565845
H	-0.619980	-2.457304	0.349875	C	-1.228554	2.895570	1.415767
C	-0.062326	-2.725736	-1.687272	H	-2.285979	2.664078	1.538311
H	0.543680	-2.269831	-2.470510	H	-0.905752	3.536431	2.236479
H	0.302483	-3.745245	-1.536307	H	-1.085427	3.425896	0.475252
H	-1.087951	-2.782574	-2.054742	Sn	-0.064786	1.070426	1.412877
C	1.432368	-1.922096	0.204221				

TS(41d^{P-inv}):

E = -1022.47448272323 au

ZPE = 0.29304405 au

G_{corr} = 0.24559252 au

$\nu = -197.53 \text{ cm}^{-1}$

P	-0.163007	-0.124644	-0.526475	C	0.795518	-2.598828	0.264490
C	-0.768726	0.817724	-1.923214	H	1.114708	-3.609128	-0.001490
C	-0.742420	2.221651	-1.903965	H	1.639606	-2.103190	0.750298
C	-1.300406	0.187704	-3.059968	H	-0.017714	-2.677592	0.986081
C	-1.253056	2.960160	-2.960287	C	-1.878071	2.194344	1.772608
H	-0.297755	2.738174	-1.062269	H	-2.766576	1.588101	1.941237
C	-1.782756	0.933111	-4.126789	H	-1.772856	2.918931	2.580205
H	-1.350392	-0.892294	-3.105976	H	-1.985110	2.721105	0.826610
C	-1.772770	2.323149	-4.083605	C	-0.256660	-0.650235	3.204900
H	-1.225111	4.042052	-2.914854	H	0.639655	-1.267015	3.183556
H	-2.182699	0.420994	-4.993579	H	-0.347529	-0.188895	4.188539
H	-2.156983	2.901071	-4.913757	H	-1.129245	-1.273756	3.019165
C	0.367494	-1.842006	-0.991999	C	1.661856	2.074395	2.001289
H	-0.509621	-2.347308	-1.406471	H	1.708169	2.863637	1.251931
C	1.476352	-1.830121	-2.045245	H	1.669441	2.521461	2.996080
H	2.385096	-1.384889	-1.636492	H	2.532047	1.429351	1.887731
H	1.703232	-2.852337	-2.365336	Sn	-0.141178	0.909354	1.712481
H	1.190311	-1.256100	-2.926572				

42:

E = -769.517063348533 au

ZPE = 0.25084687 au

G_{corr} = 0.21240708 au

P	3.043978	0.664012	0.207824	C	2.981958	-2.032220	-0.438244
C	4.150313	1.504182	1.427313	C	5.035784	-1.369409	0.607387
H	3.812365	2.532907	1.550927	C	3.457412	-3.331340	-0.560841
H	4.042714	1.004034	2.390610	H	1.982837	-1.793101	-0.782295
H	5.206118	1.516074	1.154991	C	5.508140	-2.672705	0.502633
C	3.622361	1.408693	-1.442326	H	5.668821	-0.619737	1.061932
C	3.768349	-1.024042	0.130898	C	4.724635	-3.656148	-0.089672

H	2.833776	-4.092586	-1.012778	H	3.792112	3.449280	-0.665908
H	6.492916	-2.918455	0.880613	H	3.444210	3.347630	-2.390056
H	5.094566	-4.669946	-0.175159	H	2.166063	3.020830	-1.214434
C	2.844112	0.701975	-2.558609	C	5.122681	1.266976	-1.700618
H	3.067924	1.172405	-3.520411	H	5.429515	0.220977	-1.718134
H	3.117221	-0.351089	-2.632868	H	5.374401	1.705350	-2.671391
H	1.766290	0.764748	-2.394938	H	5.718725	1.784831	-0.947802
C	3.231152	2.892625	-1.418441				

TS(42^{P-inv}):

E = -769.459888617417 au

ZPE = 0.24970759 au

G_{corr} = 0.21129663 au

$\nu = -345.68 \text{ cm}^{-1}$

P	3.598760	0.673079	-0.082449	H	4.547316	-3.370105	2.482573
C	3.345601	1.569543	1.487244	H	4.859365	-4.827295	0.493524
H	3.044587	2.587323	1.245219	C	2.299596	0.900467	-2.557306
H	2.550246	1.115533	2.079924	H	2.239015	1.389708	-3.534933
H	4.255971	1.617250	2.086369	H	2.450589	-0.165056	-2.726461
C	3.443772	1.517977	-1.737042	H	1.345792	1.024396	-2.045350
C	3.993134	-1.041556	0.060496	C	3.129868	2.994933	-1.470596
C	4.171093	-1.881835	-1.055962	H	3.921428	3.480346	-0.898125
C	4.138452	-1.616171	1.339946	H	3.045106	3.511820	-2.429535
C	4.478817	-3.223394	-0.893663	H	2.184745	3.119499	-0.940193
H	4.065593	-1.488449	-2.056539	C	4.765612	1.419194	-2.515473
C	4.443587	-2.959911	1.485293	H	5.069458	0.384748	-2.672367
H	4.013947	-1.006044	2.224916	H	4.650622	1.887249	-3.498473
C	4.618969	-3.779469	0.374088	H	5.568444	1.924630	-1.979382
H	4.608618	-3.842226	-1.773380				

43:

E = -1302.40774471418 au

ZPE = 0.31470838 au

G_{corr} = 0.27227031 au

P	0.178247	0.379280	-0.002327	C	0.040371	-6.120902	1.228761
P	1.276626	-1.563684	0.017462	H	-1.227980	-4.442990	0.803002
C	0.347858	-2.357206	-1.380442	C	2.215956	-5.595293	2.101091
H	0.690385	-1.934777	-2.325441	H	2.653030	-3.509101	2.337173
H	0.582202	-3.422430	-1.385573	C	1.279306	-6.541367	1.696731
H	-0.733489	-2.229732	-1.302456	H	-0.696162	-6.849108	0.912949
C	1.061801	1.157086	-1.434630	H	3.184162	-5.912982	2.467363
H	0.733986	0.667650	-2.352348	H	1.513783	-7.596878	1.747550
H	0.775516	2.208512	-1.499841	C	2.475306	1.267417	1.535099
H	2.146949	1.086008	-1.358958	C	3.156472	0.276281	2.244752
C	0.362450	-2.341151	1.464293	C	3.228347	2.241951	0.877362
H	0.692601	-1.817755	2.363616	C	4.543712	0.248630	2.283998
H	-0.711268	-2.175565	1.359189	H	2.592929	-0.479092	2.778094
C	0.979747	1.265549	1.454828	C	4.617186	2.217649	0.912520
H	0.593546	2.286621	1.402331	H	2.720064	3.030998	0.336473
H	0.542767	0.814390	2.347728	C	5.281256	1.217088	1.612581
C	0.670729	-3.806616	1.570296	H	5.050024	-0.530191	2.840203
C	-0.259295	-4.764523	1.166597	H	5.181043	2.984354	0.396018
C	1.914493	-4.241785	2.034166	H	6.363034	1.196374	1.640849

TS(43^{P-inv}):

E = -1302.36273396949 au

ZPE = 0.31380103 au

G_{corr} = 0.26857818 au

v = -292.59 cm⁻¹

P	0.231210	0.421523	0.277570	C	0.540686	-6.258783	0.525844
P	1.224575	-1.436706	0.211716	H	-0.932143	-4.736334	0.187426
C	0.714979	-2.153867	-1.422618	C	2.491646	-5.575474	1.749247
H	1.181258	-1.570506	-2.215123	H	2.547539	-3.518353	2.354834
H	1.073983	-3.182923	-1.478209	C	1.775441	-6.566186	1.085087
H	-0.366404	-2.155944	-1.571097	H	-0.026742	-7.022760	0.008969
C	-1.524743	0.751836	-0.147741	H	3.453938	-5.805231	2.189510
H	-2.080756	1.148746	0.702940	H	2.175816	-7.568736	1.005563
H	-1.617082	1.437503	-0.991129	C	2.545282	1.531218	1.280986
H	-1.974166	-0.200131	-0.433727	C	2.745443	1.153440	2.607956
C	0.220700	-2.559589	1.347591	C	3.621812	1.482339	0.398379
H	0.333240	-2.132289	2.344666	C	3.995689	0.736393	3.044930
H	-0.837351	-2.523406	1.083188	H	1.909644	1.176743	3.297141
C	1.178683	1.924746	0.797052	C	4.873668	1.062445	0.830749
H	1.257609	2.617862	-0.042325	H	3.471569	1.760694	-0.637798
H	0.621641	2.422450	1.593447	C	5.063692	0.686048	2.155128
C	0.738565	-3.966553	1.289956	H	4.136712	0.449345	4.079416
C	0.029842	-4.970150	0.628338	H	5.699998	1.025342	0.132163
C	1.978852	-4.288883	1.847917	H	6.038155	0.357006	2.492824

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