

Supporting Information

Unmasking the elusive 1,4-diazabutatrienes: the stabilizing role of the *N*-substituents

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1. Computational Methods

The geometries of the molecules were fully optimized by using the wB97X-D hybrid functional¹ in combination with the def2-TZVPD basis set.^{2,3} The nature of minimum of all computed structures was confirmed by performing a frequency analysis at the same level of theory. Thermochemical corrections at 298.15 K were calculated for all stationary points from unscaled vibrational frequencies. The stability of the wave functions was checked for all the optimized structures.⁴ Single point calculations of the optimized geometries were performed at the DLPNO-CSSD(T)⁵/ma-def2-TZVPP⁶ theoretical level and were combined with the previous computed thermochemical corrections to yield free energies G_{298} at 298.15 K. All calculations were performed by using both the Gaussian 09⁷ and the ORCA 4.0.1 programs.⁸ Natural Bond Orbital analyses⁹ were performed at the wB97XD/def2-TZVPD level with the NBO 7.0 software.¹⁰

2. Relative Energies of the 1,4-Diazabutatrienes

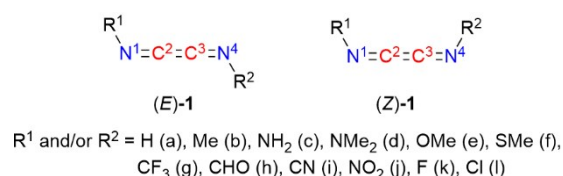


Table S1. Gibbs free energy difference between the (*E*)- and (*Z*)-diazabutatrienes **1** (kcal mol⁻¹). Values are obtained as $G_E - G_Z$

R ¹	R ²											
	H	Me	NH ₂	NMe ₂	OMe	SMe	CF ₃	CHO	CN	NO ₂	F	Cl
H	-1.49	-0.81	-0.94	-1.00	-0.62	-1.00	-0.93	-0.86	-1.06	-0.56	-0.55	-0.38
Me		-0.37	-0.13	-0.27	0.04	-0.52	-0.26	-0.35	-0.26	0.11	0.09	-0.07
NH ₂			-0.37	-0.56	-0.07	-0.52	-0.13	0.01	-0.61	0.30	-0.01	-0.10
NMe ₂				-0.59	0.01	-0.82	-0.09	0.30	0.05	0.80	0.14	0.10
OMe					-0.35	0.32	-0.50	-0.17	-0.58	1.59	-0.21	-0.23
SMe						-0.34	0.13	0.30	0.12	1.47	0.23	0.52
CF ₃							-0.51	-0.65	-0.76	-0.41	-0.33	-0.33
CHO								-0.49	-0.70	-0.34	-0.21	-0.30
CN									-0.92	-0.55	-0.48	-0.41
NO ₂										-0.15	-0.17	-0.14
F											-0.29	-0.16
Cl												-0.18

Table S2. Enthalpy energy difference between the (*E*)- and (*Z*)-diazabutatrienes **1** (kcal mol⁻¹). Values are obtained as $H_E - H_Z$

R ¹	R ²											
	H	Me	NH ₂	NMe ₂	OMe	SMe	CF ₃	CHO	CN	NO ₂	F	Cl
H	-1.63	-0.97	-1.06	-1.09	-0.78	-1.00	-1.09	-0.45	-1.25	-0.99	-0.82	-0.45
Me		-0.50	-0.17	-0.34	-0.01	-0.60	-0.44	-0.53	-0.38	-0.23	-0.05	-0.10
NH ₂			-0.41	-0.61	-0.07	-0.50	-0.30	0.15	-0.31	0.41	-0.04	-0.11

NMe ₂	-0.56	0.03	-0.59	0.08	0.38	0.12	1.50	0.10	0.06
OMe		-0.29	0.65	-0.47	-0.32	-0.57	1.00	-0.21	-0.21
SMe			-0.73	0.21	0.31	0.10	1.84	0.19	0.83
CF ₃				-0.76	-0.79	-0.87	-0.57	-0.45	-0.33
CHO					-0.75	-0.85	-0.60	-0.36	-0.32
CN						-1.04	-0.74	-0.58	-0.44
NO ₂							-0.39	-0.27	-0.23
F								-0.31	-0.17
Cl									-0.17

3. Geometry of the 1,4-diazabutatrienes 1

Table S3. Representative distances (Å), bond angles (°) and dihedral angles (°) of the 1,4-diazabutatrienes 1.

R ¹	R ²		R ¹ -N ¹	N ¹ -C ²	C ² -C ³	C ³ -N ⁴	N ⁴ -R ²	C ² -N ¹ -R ¹	C ³ -N ⁴ -R ²	N ¹ -C ² -C ³	C ² -C ³ -N ⁴	R ¹ -N ¹ -N ⁴ -R ²
H	H	E	1.021	1.237	1.290	1.237	1.021	112.8	112.8	161.0	161.0	-180.0
		Z	1.022	1.237	1.276	1.237	1.022	113.0	113.0	174.4	174.4	0.0
H	Me	E	1.021	1.237	1.284	1.233	1.453	112.8	119.9	164.0	164.2	180.0
		Z	1.021	1.238	1.277	1.232	1.453	112.9	120.2	169.3	179.1	0.0
H	NH ₂	E	1.018	1.234	1.274	1.253	1.340	113.9	119.4	167.0	161.1	-177.2
		Z	1.018	1.235	1.268	1.253	1.340	114.2	119.6	177.9	168.1	2.9
H	NMe ₂	E	1.018	1.238	1.269	1.264	1.323	113.6	119.9	167.8	162.0	177.3
		Z	1.018	1.238	1.265	1.263	1.323	114.0	120.3	178.1	166.9	2.5
H	OMe	E	1.018	1.228	1.277	1.248	1.371	114.7	113.5	167.3	158.8	-180.0
		Z	1.018	1.229	1.271	1.247	1.373	114.6	113.6	177.6	167.4	0.0
H	SMe	E	1.020	1.237	1.273	1.244	1.663	113.3	123.2	168.5	168.0	180.0
		Z	1.020	1.238	1.270	1.243	1.664	113.5	124.0	172.0	178.3	0.0
H	CF ₃	E	1.021	1.230	1.285	1.237	1.436	113.7	118.9	163.9	161.8	176.0
		Z	1.021	1.232	1.274	1.236	1.437	113.6	119.1	174.2	175.9	0.0
H	CHO	E	1.021	1.233	1.284	1.242	1.437	113.5	115.8	164.7	164.2	180.0
		Z	1.022	1.235	1.282	1.240	1.441	113.4	124.2	171.2	179.2	3.0
H	CN	E	1.021	1.230	1.284	1.246	1.340	113.9	121.9	162.9	159.2	-180.0
		Z	1.021	1.232	1.271	1.246	1.341	113.9	121.6	176.8	171.5	0.0
H	NO ₂	E	1.019	1.223	1.286	1.238	1.479	115.2	113.3	165.4	159.7	-180.0
		Z	1.020	1.225	1.276	1.237	1.484	114.9	113.3	175.2	173.7	0.0
H	F	E	1.017	1.216	1.286	1.239	1.415	116.9	110.4	167.2	154.4	180.0
		Z	1.018	1.218	1.277	1.236	1.421	116.5	110.2	176.8	167.5	0.0
H	Cl	E	1.019	1.225	1.280	1.235	1.762	115.0	114.3	169.2	164.5	180.0
		Z	1.020	1.225	1.277	1.233	1.768	115.0	114.3	172.5	176.7	0.0
Me	Me	E	1.454	1.233	1.280	1.233	1.454	119.8	119.8	167.3	167.3	-176.8
		Z	1.453	1.233	1.275	1.233	1.453	120.0	120.0	175.4	175.4	0.0
Me	NH ₂	E	1.453	1.229	1.272	1.250	1.349	119.6	119.6	169.6	164.8	-176.8
		Z	1.452	1.227	1.273	1.251	1.348	121.4	119.4	177.5	163.8	3.2
Me	NMe ₂	E	1.453	1.232	1.268	1.259	1.333	120.5	120.1	170.3	165.6	-176.8
		Z	1.452	1.230	1.269	1.261	1.331	120.9	120.4	177.7	163.4	2.9
Me	OMe	E	1.452	1.223	1.276	1.247	1.377	121.9	113.4	169.6	161.8	180.0

		<i>Z</i>	1.452	1.222	1.274	1.247	1.377	122.0	113.4	178.2	162.9	0.0
Me	SMe	<i>E</i>	1.453	1.232	1.271	1.243	1.669	120.3	123.1	171.8	171.4	179.8
		<i>Z</i>	1.452	1.232	1.270	1.242	1.669	120.4	123.7	176.3	174.7	0.0
Me	CF₃	<i>E</i>	1.452	1.228	1.279	1.238	1.433	120.9	119.0	166.8	165.0	-180.0
		<i>Z</i>	1.452	1.227	1.274	1.238	1.433	120.8	119.0	179.7	170.9	0.0
Me	CHO	<i>E</i>	1.452	1.230	1.281	1.232	1.406	120.5	125.1	165.3	165.6	-177.7
		<i>Z</i>	1.453	1.230	1.274	1.233	1.407	120.5	124.0	177.8	174.0	-3.5
Me	CN	<i>E</i>	1.450	1.228	1.278	1.247	1.341	121.2	121.7	165.4	162.0	180.0
		<i>Z</i>	1.451	1.227	1.272	1.248	1.341	121.2	121.4	177.6	166.4	0.0
Me	NO₂	<i>E</i>	1.451	1.220	1.281	1.239	1.477	122.6	113.3	168.0	162.9	180.0
		<i>Z</i>	1.452	1.219	1.277	1.239	1.477	122.5	113.2	179.4	167.3	0.0
Me	F	<i>E</i>	1.450	1.212	1.284	1.238	1.424	124.9	110.2	169.4	157.8	-180.0
		<i>Z</i>	1.451	1.211	1.282	1.237	1.425	124.6	110.1	179.0	160.9	0.0
Me	Cl	<i>E</i>	1.452	1.220	1.278	1.234	1.772	122.6	114.0	172.7	168.9	180.0
		<i>Z</i>	1.452	1.220	1.277	1.233	1.775	122.6	114.0	175.5	173.8	0.0
NH₂	NH₂	<i>E</i>	1.366	1.244	1.265	1.243	1.366	119.6	119.6	171.1	171.1	180.0
		<i>Z</i>	1.366	1.243	1.264	1.243	1.366	119.8	119.8	174.7	174.7	6.8
NH₂	NMe₂	<i>E</i>	1.373	1.244	1.264	1.250	1.349	119.3	120.9	170.7	169.9	-179.9
		<i>Z</i>	1.374	1.243	1.263	1.250	1.349	119.4	121.3	176.6	171.9	6.6
NH₂	OMe	<i>E</i>	1.356	1.240	1.264	1.244	1.384	120.6	113.4	171.4	169.2	-176.8
		<i>Z</i>	1.355	1.240	1.263	1.244	1.386	120.7	113.4	175.7	173.2	3.6
NH₂	SMe	<i>E</i>	1.354	1.248	1.265	1.238	1.673	119.6	123.7	170.2	172.7	-176.7
		<i>Z</i>	1.355	1.248	1.266	1.237	1.674	119.7	124.5	169.9	179.2	3.1
NH₂	CF₃	<i>E</i>	1.320	1.254	1.262	1.238	1.419	120.4	120.0	165.9	169.3	178.1
		<i>Z</i>	1.318	1.254	1.258	1.239	1.419	120.4	120.2	171.9	177.7	1.9
NH₂	CHO	<i>E</i>	1.323	1.256	1.265	1.233	1.402	120.1	124.8	163.7	169.5	-172.3
		<i>Z</i>	1.321	1.256	1.260	1.239	1.407	119.9	121.2	169.2	178.1	8.9
NH₂	CN	<i>E</i>	1.308	1.260	1.256	1.247	1.334	120.5	122.7	165.5	168.5	-180.0
		<i>Z</i>	1.307	1.259	1.252	1.249	1.334	120.5	122.2	172.7	176.5	0.0
NH₂	NO₂	<i>E</i>	1.314	1.249	1.259	1.246	1.475	121.7	112.7	170.6	170.9	-178.7
		<i>Z</i>	1.311	1.250	1.256	1.246	1.481	121.2	112.5	174.1	177.7	-1.4
NH₂	F	<i>E</i>	1.339	1.235	1.267	1.241	1.421	122.6	109.9	171.9	168.5	-177.0
		<i>Z</i>	1.338	1.235	1.266	1.240	1.425	122.6	109.7	174.8	173.5	3.3
NH₂	Cl	<i>E</i>	1.336	1.243	1.265	1.238	1.753	121.4	113.9	171.4	170.5	-177.2
		<i>Z</i>	1.335	1.243	1.265	1.237	1.756	121.5	113.9	172.4	176.2	3.1
NMe₂	NMe₂	<i>E</i>	1.357	1.250	1.263	1.250	1.357	120.8	120.8	169.5	169.5	-172.6
		<i>Z</i>	1.358	1.249	1.262	1.249	1.358	120.9	120.9	174.2	174.2	6.4
NMe₂	OMe	<i>E</i>	1.339	1.248	1.263	1.245	1.391	121.6	113.2	170.7	169.3	-176.6
		<i>Z</i>	1.337	1.248	1.261	1.245	1.394	121.6	112.9	174.0	174.9	3.3
NMe₂	SMe	<i>E</i>	1.333	1.258	1.262	1.240	1.693	120.5	120.3	168.4	171.3	176.9
		<i>Z</i>	1.338	1.256	1.264	1.238	1.678	120.8	124.1	168.3	179.5	2.8
NMe₂	CF₃	<i>E</i>	1.303	1.268	1.256	1.243	1.412	120.2	120.1	167.1	170.4	-180.0
		<i>Z</i>	1.303	1.268	1.252	1.244	1.411	120.0	119.6	173.8	177.7	0.0
NMe₂	CHO	<i>E</i>	1.302	1.271	1.255	1.250	1.409	119.9	117.0	169.2	172.4	-180.0
		<i>Z</i>	1.299	1.275	1.246	1.256	1.406	118.6	116.1	178.6	179.4	0.0
NMe₂	CN	<i>E</i>	1.297	1.272	1.250	1.252	1.332	120.1	122.5	166.8	169.6	-180.0

		Z	1.297	1.273	1.247	1.254	1.332	120.0	121.3	173.4	176.9	0.0
NMe ₂	NO ₂	E	1.298	1.264	1.252	1.253	1.460	121.0	112.8	171.0	170.9	-180.0
		Z	1.297	1.266	1.248	1.255	1.457	119.8	112.0	177.1	178.3	0.0
NMe ₂	F	E	1.322	1.245	1.264	1.243	1.427	122.8	109.6	171.7	169.1	-177.0
		Z	1.320	1.246	1.263	1.242	1.433	122.7	109.1	173.8	175.2	3.0
NMe ₂	Cl	E	1.317	1.254	1.262	1.241	1.758	121.7	113.6	171.3	170.8	-177.4
		Z	1.316	1.255	1.261	1.241	1.762	121.4	113.1	172.3	177.0	2.4
OMe	OMe	E	1.375	1.242	1.264	1.242	1.375	114.1	114.1	169.3	169.3	180.0
		Z	1.375	1.242	1.263	1.242	1.375	114.2	114.2	173.3	173.3	0.0
OMe	SMe	E	1.378	1.247	1.267	1.233	1.681	113.5	122.2	166.6	171.2	180.0
		Z	1.381	1.246	1.266	1.233	1.668	113.2	124.8	169.5	179.4	0.0
OMe	CF ₃	E	1.357	1.248	1.268	1.231	1.426	114.2	120.5	163.4	169.4	180.0
		Z	1.357	1.248	1.265	1.231	1.427	114.2	120.8	167.0	179.6	0.0
OMe	CHO	E	1.362	1.249	1.272	1.224	1.405	113.9	127.0	160.7	169.5	180.0
		Z	1.362	1.248	1.268	1.225	1.407	113.9	126.3	165.6	178.7	4.0
OMe	CN	E	1.350	1.251	1.263	1.240	1.335	122.8	122.8	162.8	168.2	-180.0
		Z	1.351	1.251	1.258	1.240	1.335	114.2	123.5	170.6	176.2	0.0
OMe	NO ₂	E	1.342	1.248	1.267	1.235	1.469	119.5	114.1	166.1	169.5	180.0
		Z	1.354	1.243	1.264	1.236	1.470	114.9	114.0	171.0	176.8	0.0
OMe	F	E	1.360	1.237	1.267	1.239	1.409	115.5	110.3	169.7	168.6	-180.0
		Z	1.360	1.237	1.266	1.239	1.410	115.6	110.3	172.7	173.0	0.0
OMe	Cl	E	1.363	1.242	1.267	1.234	1.741	114.7	114.6	168.9	170.3	180.0
		Z	1.363	1.242	1.272	1.234	1.741	114.7	114.8	170.3	175.7	0.0
SMe	SMe	E	1.669	1.242	1.265	1.242	1.669	123.6	123.6	174.1	174.1	180.0
		Z	1.686	1.242	1.265	1.241	1.667	120.1	123.6	177.1	175.0	0.0
SMe	CF ₃	E	1.650	1.243	1.266	1.239	1.427	124.2	119.5	170.9	170.1	180.0
		Z	1.651	1.242	1.264	1.240	1.425	124.1	119.1	179.1	174.1	0.0
SMe	CHO	E	1.650	1.245	1.265	1.245	1.426	124.0	116.3	173.5	173.4	-180.0
		Z	1.653	1.245	1.263	1.241	1.412	123.5	119.7	177.6	176.8	4.9
SMe	CN	E	1.643	1.246	1.261	1.249	1.337	124.5	122.3	170.2	168.6	-179.9
		Z	1.643	1.246	1.259	1.250	1.337	124.5	121.1	179.5	172.7	0.0
SMe	NO ₂	E	1.649	1.236	1.267	1.241	1.470	125.4	113.6	172.6	170.2	-180.0
		Z	1.646	1.237	1.264	1.244	1.502	124.6	111.6	177.6	177.7	0.0
SMe	F	E	1.656	1.226	1.271	1.240	1.421	126.7	110.1	173.7	167.2	180.0
		Z	1.657	1.226	1.271	1.239	1.426	126.6	109.6	179.4	169.0	-0.1
SMe	Cl	E	1.671	1.232	1.270	1.237	1.761	123.3	114.1	172.8	170.4	-180.0
		Z	1.657	1.233	1.269	1.236	1.741	125.0	113.5	174.0	179.8	0.0
CF ₃	CF ₃	E	1.441	1.231	1.279	1.231	1.441	119.3	119.3	165.5	165.5	180.0
		Z	1.442	1.231	1.272	1.231	1.442	119.4	119.5	175.5	175.5	0.1
CF ₃	CHO	E	1.439	1.234	1.282	1.226	1.415	119.1	125.3	163.5	165.8	178.4
		Z	1.440	1.234	1.273	1.226	1.416	119.2	124.8	172.8	178.4	-2.5
CF ₃	CN	E	1.442	1.231	1.277	1.241	1.339	119.5	122.6	164.8	163.1	180.0
		Z	1.443	1.231	1.269	1.241	1.340	119.7	122.6	177.9	171.5	0.0
CF ₃	NO ₂	E	1.441	1.225	1.278	1.234	1.485	120.4	113.5	168.1	165.5	180.0
		Z	1.442	1.226	1.273	1.234	1.488	120.4	113.5	176.3	173.8	0.0
CF ₃	F	E	1.436	1.220	1.275	1.239	1.400	121.7	110.7	169.7	161.3	-180.0

		Z	1.437	1.221	1.272	1.238	1.402	121.8	110.7	177.8	167.3	0.0
CF ₃	Cl	E	1.437	1.227	1.274	1.234	1.740	120.4	114.9	170.6	167.4	180.0
		Z	1.437	1.227	1.272	1.234	1.741	120.5	115.0	174.6	174.1	0.0
CHO	CHO	E	1.412	1.228	1.285	1.228	1.412	125.1	125.1	163.9	163.9	180.0
		Z	1.414	1.229	1.274	1.229	1.414	124.3	124.3	176.3	176.3	5.7
CHO	CN	E	1.416	1.225	1.281	1.243	1.340	125.3	122.2	164.6	160.5	178.3
		Z	1.418	1.226	1.272	1.244	1.340	124.8	122.1	178.0	167.7	-3.0
CHO	NO ₂	E	1.418	1.218	1.282	1.236	1.482	126.7	113.4	167.7	161.9	178.6
		Z	1.419	1.220	1.276	1.236	1.486	126.2	113.4	179.1	170.3	-2.3
CHO	F	E	1.415	1.212	1.282	1.240	1.407	129.0	110.5	169.5	157.1	178.7
		Z	1.417	1.213	1.277	1.239	1.409	128.5	110.5	178.8	162.2	-2.3
CHO	Cl	E	1.414	1.220	1.276	1.235	1.751	126.9	114.6	171.6	166.4	178.2
		Z	1.414	1.221	1.274	1.234	1.753	126.7	114.7	176.1	173.5	-2.6
CN	CN	E	1.338	1.241	1.273	1.241	1.338	122.8	122.8	163.1	163.1	180.0
		Z	1.337	1.241	1.264	1.242	1.338	122.9	122.8	174.3	174.2	0.0
CN	NO ₂	E	1.337	1.234	1.274	1.235	1.485	124.1	113.5	166.3	165.1	-180.0
		Z	1.337	1.235	1.269	1.235	1.487	124.0	113.6	173.2	176.1	0.0
CN	F	E	1.334	1.228	1.271	1.242	1.393	125.8	110.8	168.3	160.9	-180.0
		Z	1.335	1.229	1.266	1.241	1.395	125.7	110.7	175.7	169.8	0.0
CN	Cl	E	1.337	1.236	1.270	1.237	1.730	124.0	115.1	168.6	166.2	-180.0
		Z	1.337	1.236	1.267	1.236	1.732	123.9	115.3	172.6	175.4	0.0
NO ₂	NO ₂	E	1.488	1.230	1.275	1.230	1.488	113.9	113.9	169.2	169.2	180.0
		Z	1.490	1.230	1.273	1.230	1.490	114.0	114.0	174.9	174.9	0.0
NO ₂	F	E	1.484	1.227	1.272	1.238	1.392	114.5	111.0	171.0	165.9	-180.0
		Z	1.485	1.227	1.271	1.237	1.394	114.5	111.0	176.8	169.8	0.0
NO ₂	Cl	E	1.483	1.232	1.273	1.231	1.728	114.0	115.6	170.7	169.2	180.0
		Z	1.484	1.232	1.272	1.231	1.729	114.0	115.7	174.2	174.2	0.0
F	F	E	1.390	1.237	1.268	1.237	1.390	111.2	111.2	168.6	168.6	180.0
		Z	1.391	1.236	1.267	1.236	1.391	111.1	111.2	172.3	172.3	0.0
F	Cl	E	1.400	1.238	1.271	1.228	1.721	110.8	116.1	167.4	170.4	-180.0
		Z	1.401	1.238	1.271	1.228	1.721	110.8	116.3	170.0	175.0	0.0
Cl	Cl	E	1.735	1.232	1.272	1.232	1.735	115.3	115.3	170.9	170.9	-180.0
		Z	1.735	1.231	1.272	1.231	1.736	115.4	115.4	173.4	173.4	0.0

3. NBO charges of the 1,4-diazabutatrienes

Table S4. NBO charges at the N¹, C², C³, N⁴ atoms of the 1,4-diazabutatrienes **1**, sum of those charges (Σq) and charge difference.

R ¹	R ²		N ¹	C ²	C ³	N ⁴	Σq	$\Sigma q (E) - \Sigma q (Z)$
H	H	E	-0.5356	0.1766	0.1765	-0.5356	-0.7182	-0.0069
		Z	-0.5309	0.1753	0.1753	-0.5309	-0.7113	
H	Me	E	-0.5517	0.1955	0.1467	-0.3288	-0.5384	-0.0032
		Z	-0.5493	0.1792	0.1602	-0.3254	-0.5353	
H	NH ₂	E	-0.6047	0.2700	-0.0210	-0.1618	-0.5175	-0.0027
		Z	-0.6038	0.2655	-0.0183	-0.1582	-0.5148	

H	NMe ₂	E	-0.6357	0.2822	-0.0629	-0.1580	-0.5744	-0.0032
		Z	-0.6349	0.2828	-0.0628	-0.1563	-0.5712	
H	OMe	E	-0.5736	0.2902	0.0326	-0.0786	-0.3295	-0.0023
		Z	-0.5788	0.2986	0.0269	-0.0739	-0.3272	
H	SMe	E	-0.5762	0.2255	0.0759	-0.5013	-0.7761	-0.0093
		Z	-0.5717	0.2154	0.0891	-0.4997	-0.7669	
H	CF ₃	E	-0.5045	0.2132	0.2062	-0.4133	-0.4983	-0.0045
		Z	-0.5026	0.2065	0.2114	-0.4091	-0.4938	
H	CHO	E	-0.5056	0.1991	0.1988	-0.4165	-0.5243	-0.0190
		Z	-0.5117	0.1871	0.2151	-0.3958	-0.5053	
H	CN	E	-0.4944	0.2116	0.2348	-0.4032	-0.4512	-0.0042
		Z	-0.4913	0.2054	0.2373	-0.3984	-0.4470	
H	NO ₂	E	-0.5064	0.2707	0.1280	-0.2289	-0.3366	-0.0028
		Z	-0.5045	0.2600	0.1345	-0.2238	-0.3337	
H	F	E	-0.5360	0.3359	0.0181	0.0434	-0.1386	-0.0071
		Z	-0.5343	0.3273	0.0236	0.0520	-0.1315	
H	Cl	E	-0.5274	0.2766	0.0979	-0.2997	-0.4527	-0.0105
		Z	-0.5267	0.2746	0.1022	-0.2922	-0.4421	
Me	Me	E	-0.3472	0.1705	0.1705	-0.3472	-0.3534	-0.0022
		Z	-0.3417	0.1596	0.1781	-0.3471	-0.3512	
Me	NH ₂	E	-0.3863	0.2366	0.0196	-0.1798	-0.3099	0.0012
		Z	-0.3923	0.2724	-0.0158	-0.1754	-0.3111	
Me	NMe ₂	E	-0.4128	0.2521	-0.0229	-0.1726	-0.3561	-0.0009
		Z	-0.4131	0.2742	-0.0430	-0.1734	-0.3553	
Me	OMe	E	-0.3648	0.2742	0.0500	-0.0923	-0.1328	0.0015
		Z	-0.3665	0.2894	0.0351	-0.0924	-0.1344	
Me	SMe	E	-0.3571	0.2052	0.1218	-0.5172	-0.5473	0.0183
		Z	-0.3646	0.2114	0.0978	-0.5102	-0.5656	
Me	CF ₃	E	-0.3019	0.1903	0.2211	-0.4299	-0.3203	-0.0018
		Z	-0.3018	0.1994	0.2128	-0.4289	-0.3185	
Me	CHO	E	-0.3118	0.1742	0.2208	-0.4101	-0.3269	0.0004
		Z	-0.3102	0.1823	0.2151	-0.4144	-0.3273	
Me	CN	E	-0.2910	0.1877	0.2509	-0.4197	-0.2722	-0.0003
		Z	-0.2901	0.2008	0.2357	-0.4184	-0.2719	
Me	NO ₂	E	-0.3033	0.2508	0.1415	-0.2434	-0.1543	-0.0017
		Z	-0.3038	0.2598	0.1323	-0.2409	-0.1526	
Me	F	E	-0.3255	0.3149	0.0326	0.0285	0.0506	0.0006
		Z	-0.3269	0.3222	0.0228	0.0318	0.0499	
Me	Cl	E	-0.3174	0.2556	0.1117	-0.3080	-0.2581	-0.0045
		Z	-0.3186	0.2583	0.1114	-0.3047	-0.2536	
NH ₂	NH ₂	E	-0.2148	0.1031	0.1031	-0.2148	-0.2234	-0.0020
		Z	-0.2146	0.1040	0.1039	-0.2146	-0.2214	
NH ₂	NMe ₂	E	-0.2363	0.1231	0.0732	-0.2108	-0.2508	-0.0044
		Z	-0.2366	0.1321	0.0693	-0.2112	-0.2463	
NH ₂	OMe	E	-0.1979	0.1340	0.1282	-0.1326	-0.0684	-0.0001
		Z	-0.1991	0.1389	0.1250	-0.1332	-0.0684	

NH ₂	SMe	E	-0.1865	0.0576	0.1991	-0.5566	-0.4865	0.0089
		Z	-0.1948	0.0612	0.1847	-0.5465	-0.4954	
NH ₂	CF ₃	E	-0.1305	0.0072	0.2979	-0.4909	-0.3163	0.0002
		Z	-0.1318	0.0114	0.2959	-0.4919	-0.3165	
NH ₂	CHO	E	-0.1378	-0.0069	0.3046	-0.4773	-0.3174	0.0055
		Z	-0.1353	-0.0043	0.3136	-0.4969	-0.3229	
NH ₂	CN	E	-0.1167	-0.0094	0.3285	-0.4798	-0.2775	0.0015
		Z	-0.1121	-0.0196	0.3373	-0.4846	-0.2790	
NH ₂	NO ₂	E	-0.1237	0.0668	0.2468	-0.3294	-0.1395	0.0018
		Z	-0.1243	0.0699	0.2497	-0.3367	-0.1414	
NH ₂	F	E	-0.1640	0.1557	0.1119	-0.0150	0.0886	-0.0010
		Z	-0.1652	0.1577	0.1103	-0.0132	0.0896	
NH ₂	Cl	E	-0.1547	0.0932	0.1863	-0.3692	-0.2443	-0.0034
		Z	-0.1559	0.0930	0.1884	-0.3663	-0.2408	
NMe ₂	NMe ₂	E	-0.2299	0.0960	0.0960	-0.2299	-0.2677	-0.0099
		Z	-0.2312	0.1023	0.1022	-0.2311	-0.2578	
NMe ₂	OMe	E	-0.1908	0.0917	0.1523	-0.1579	-0.1047	0.0001
		Z	-0.1919	0.0922	0.1530	-0.1580	-0.1048	
NMe ₂	SMe	E	-0.1814	0.0246	0.2075	-0.5745	-0.5238	0.0006
		Z	-0.1861	0.0181	0.2066	-0.5631	-0.5245	
NMe ₂	CF ₃	E	-0.1245	-0.0512	0.3132	-0.5262	-0.3887	-0.0015
		Z	-0.1308	-0.0325	0.2995	-0.5235	-0.3872	
NMe ₂	CHO	E	-0.1237	-0.0662	0.3092	-0.5200	-0.4007	0.0058
		Z	-0.1251	-0.0509	0.3315	-0.5620	-0.4065	
NMe ₂	CN	E	-0.1156	-0.0591	0.3395	-0.5107	-0.3459	0.0016
		Z	-0.1175	-0.0540	0.3349	-0.5109	-0.3474	
NMe ₂	NO ₂	E	-0.1177	0.0040	0.2745	-0.3681	-0.2073	0.0007
		Z	-0.1213	0.0081	0.2724	-0.3673	-0.2081	
NMe ₂	F	E	-0.1622	0.1100	0.1305	-0.0427	0.0356	-0.0019
		Z	-0.1634	0.1107	0.1309	-0.0406	0.0376	
NMe ₂	Cl	E	-0.1519	0.0466	0.2025	-0.3962	-0.2990	-0.0048
		Z	-0.1534	0.0457	0.2058	-0.3923	-0.2942	
OMe	OMe	E	-0.1179	0.1633	0.1633	-0.1179	0.0908	0.0002
		Z	-0.1203	0.1656	0.1656	-0.1203	0.0906	
OMe	SMe	E	-0.1072	0.0984	0.2210	-0.5388	-0.3266	0.0180
		Z	-0.1091	0.0830	0.2146	-0.5331	-0.3446	
OMe	CF ₃	E	-0.0530	0.0721	0.3149	-0.4552	-0.1213	0.0027
		Z	-0.0485	0.0531	0.3319	-0.4604	-0.1240	
OMe	CHO	E	-0.0635	0.0573	0.3165	-0.4347	-0.1245	0.0041
		Z	-0.0578	0.0388	0.3324	-0.4420	-0.1286	
OMe	CN	E	-0.0411	0.0652	0.3434	-0.4415	-0.0740	0.0028
		Z	-0.0346	0.0495	0.3547	-0.4463	-0.0768	
OMe	NO ₂	E	-0.0011	0.0410	0.2578	-0.2831	0.0145	-0.0207
		Z	-0.0527	0.1111	0.2519	-0.2751	0.0352	
OMe	F	E	-0.0816	0.1835	0.1462	0.0035	0.2515	0.0006
		Z	-0.0835	0.1836	0.1480	0.0029	0.2509	

OMe	Cl	E	-0.0732	0.1275	0.2202	-0.3566	-0.0822	0.0005
		Z	-0.0756	0.1258	0.2253	-0.3582	-0.0827	
SMe	SMe	E	-0.5321	0.1379	0.1379	-0.5321	-0.7884	-0.0282
		Z	-0.5249	0.1443	0.1554	-0.5350	-0.7602	
SMe	CF ₃	E	-0.4884	0.1082	0.2546	-0.4596	-0.5852	-0.0040
		Z	-0.4888	0.1161	0.2502	-0.4587	-0.5812	
SMe	CHO	E	-0.4892	0.0899	0.2495	-0.4594	-0.6092	-0.0170
		Z	-0.4899	0.0990	0.2677	-0.4690	-0.5922	
SMe	CN	E	-0.4863	0.0992	0.2832	-0.4493	-0.5533	-0.0018
		Z	-0.4870	0.1079	0.2754	-0.4478	-0.5515	
SMe	NO ₂	E	-0.4926	0.1647	0.1787	-0.2712	-0.4204	-0.0026
		Z	-0.4836	0.1591	0.2146	-0.3078	-0.4178	
SMe	F	E	-0.5085	0.2345	0.0730	0.0077	-0.1933	-0.0044
		Z	-0.5096	0.2418	0.0668	0.0121	-0.1889	
SMe	Cl	E	-0.5095	0.2021	0.1533	-0.3351	-0.4893	0.0158
		Z	-0.5011	0.1814	0.1484	-0.3338	-0.5051	
CF ₃	CF ₃	E	-0.3897	0.2445	0.2445	-0.3897	-0.2904	-0.0008
		Z	-0.3902	0.2455	0.2452	-0.3901	-0.2896	
CF ₃	CHO	E	-0.3951	0.2191	0.2476	-0.3728	-0.3012	0.0003
		Z	-0.3937	0.2164	0.2497	-0.3739	-0.3015	
CF ₃	CN	E	-0.3762	0.2334	0.2763	-0.3807	-0.2473	0.0002
		Z	-0.3746	0.2328	0.2747	-0.3803	-0.2475	
CF ₃	NO ₂	E	-0.3876	0.2888	0.1700	-0.2123	-0.1411	0.0013
		Z	-0.3873	0.2859	0.1716	-0.2125	-0.1423	
CF ₃	F	E	-0.4153	0.3514	0.0642	0.0667	0.0670	0.0002
		Z	-0.4158	0.3510	0.0649	0.0667	0.0668	
CF ₃	Cl	E	-0.4093	0.2960	0.1411	-0.2947	-0.2669	-0.0012
		Z	-0.4102	0.2951	0.1445	-0.2951	-0.2657	
CHO	CHO	E	-0.3820	0.2279	0.2279	-0.3820	-0.3081	0.0025
		Z	-0.3782	0.2179	0.2326	-0.3828	-0.3106	
CHO	CN	E	-0.3650	0.2468	0.2464	-0.3866	-0.2584	0.0020
		Z	-0.3660	0.2512	0.2396	-0.3852	-0.2604	
CHO	NO ₂	E	-0.3755	0.3036	0.1394	-0.2157	-0.1482	0.0013
		Z	-0.3765	0.3031	0.1387	-0.2149	-0.1496	
CHO	F	E	-0.3977	0.3615	0.0328	0.0601	0.0567	0.0011
		Z	-0.3994	0.3633	0.0294	0.0622	0.0556	
CHO	Cl	E	-0.3906	0.2968	0.1245	-0.2965	-0.2657	-0.0019
		Z	-0.3925	0.3037	0.1143	-0.2893	-0.2638	
CN	CN	E	-0.3726	0.2694	0.2694	-0.3726	-0.2064	0.0011
		Z	-0.3716	0.2679	0.2679	-0.3717	-0.2075	
CN	NO ₂	E	-0.3813	0.3292	0.1548	-0.2006	-0.0980	0.0023
		Z	-0.3813	0.3250	0.1562	-0.2002	-0.1003	
CN	F	E	-0.4008	0.3788	0.0618	0.0775	0.1175	0.0004
		Z	-0.4014	0.3821	0.0516	0.0847	0.1170	
CN	Cl	E	-0.3984	0.3229	0.1377	-0.2919	-0.2297	-0.0011
		Z	-0.3990	0.3262	0.1294	-0.2853	-0.2286	

NO ₂	NO ₂	E	-0.2203	0.2175	0.2175	-0.2203	-0.0055	0.0021
		Z	-0.2216	0.2178	0.2177	-0.2216	-0.0076	
NO ₂	F	E	-0.2438	0.2754	0.1072	0.0668	0.2057	0.0012
		Z	-0.2450	0.2770	0.1055	0.0670	0.2045	
NO ₂	Cl	E	-0.2344	0.2213	0.1838	-0.3024	-0.1317	-0.0001
		Z	-0.2351	0.2214	0.1847	-0.3025	-0.1316	
F	F	E	0.0396	0.1725	0.1725	0.0396	0.4241	0.0002
		Z	0.0389	0.1731	0.1730	0.0389	0.4239	
F	Cl	E	0.0462	0.1147	0.2500	-0.3342	0.0767	0.0004
		Z	0.0457	0.1136	0.2526	-0.3355	0.0764	
Cl	Cl	E	-0.3176	0.1934	0.1934	-0.3176	-0.2484	0.0005
		Z	-0.3186	0.1942	0.1943	-0.3188	-0.2489	

3.1. Statistical Analysis involving NBO charges.

Table S5. Group electronegativities (χ)¹¹ and substituent constants: Hammett constant (σ_p) and inductive (σ_I) and resonance (σ_R) contributions.¹²

Substituent	χ	σ_p	σ_I	σ_R
H	2.2	0	0	0
Me	2.56	-0.17	0.01	-0.18
NH ₂	3.1	-0.66	0.08	-0.74
NMe ₂	3.13	-0.83	0.15	-0.98
OMe	3.53	-0.27	0.29	-0.56
SMe	2.65	0	0.23	-0.23
CF ₃	2.68	0.54	0.38	0.04
CHO	2.6	0.42	0.33	0.09
CN	2.69	0.66	0.51	0.15
NO ₂	3.22	0.78	0.65	0.13
F	4	0.06	0.45	-0.39
Cl	3.05	0.23	0.42	-0.19

Table S6. Linear correlations between NBO charge at N¹ atom of 1,4-diazabutatrienes **1** and the group electronegativity (χ) of R¹

$$qN^1 (a.u.) = A + B * \chi (R^1)$$

R ²		A	B	r ²	Std Err	Points
H	E	-1.296	0.341	0.882	0.061	12
	Z	-1.289	0.341	0.883	0.060	12
Me	E	-1.306	0.340	0.884	0.060	12
	Z	-1.303	0.340	0.886	0.059	12
NH ₂	E	-1.371	0.344	0.859	0.068	12

	Z	-1.381	0.347	0.866	0.067	12
NMe₂	E	-1.409	0.347	0.852	0.071	12
	Z	-1.425	0.352	0.856	0.070	12
OMe	E	-1.318	0.335	0.864	0.065	12
	Z	-1.328	0.338	0.871	0.063	12
SMe	E	-1.346	0.346	0.868	0.066	12
	Z	-1.341	0.343	0.869	0.065	12
CF₃	E	-1.259	0.337	0.854	0.068	12
	Z	-1.260	0.337	0.857	0.067	12
CHO	E	-1.260	0.335	0.858	0.066	12
	Z	-1.268	0.339	0.862	0.066	12
CN	E	-1.255	0.338	0.846	0.070	12
	Z	-1.263	0.342	0.850	0.070	12
NO₂	E	-1.293	0.349	0.842	0.074	12
	Z	-1.258	0.336	0.849	0.069	12
F	E	-1.277	0.333	0.858	0.066	12
	Z	-1.276	0.332	0.857	0.066	12
Cl	E	-1.276	0.335	0.854	0.067	12
	Z	-1.271	0.334	0.860	0.066	12

Table S7. Linear correlations between NBO charge at N¹ atom of 1,4-diazabutatrienes **1** and the Hammett constant (σ_p) of R²

$$qN^1 (a.u.) = A + B * \sigma_p (R^2)$$

R ¹		A	B	r ²	Std Err	Points
H	E	-0.551	0.084	0.900	0.014	12
	Z	-0.550	0.085	0.904	0.014	12
Me	E	-0.342	0.071	0.918	0.011	12
	Z	-0.343	0.073	0.892	0.013	12
NH₂	E	-0.172	0.073	0.959	0.008	12
	Z	-0.172	0.074	0.922	0.011	12
NMe₂	E	-0.166	0.073	0.957	0.008	12
	Z	-0.168	0.071	0.939	0.009	12
OMe	E	-0.089	0.082	0.918	0.012	12
	Z	-0.091	0.071	0.904	0.012	12
SMe	E	-0.520	0.054	0.865	0.011	12
	Z	-0.515	0.049	0.895	0.008	12
CF₃	E	-0.434	0.086	0.879	0.016	12
	Z	-0.434	0.086	0.877	0.016	12
CHO	E	-0.422	0.088	0.829	0.020	12
	Z	-0.429	0.107	0.784	0.028	12
CN	E	-0.424	0.081	0.860	0.016	12
	Z	-0.424	0.083	0.857	0.017	12
NO₂	E	-0.260	0.093	0.828	0.021	12
	Z	-0.263	0.094	0.747	0.027	12
F	E	0.027	0.070	0.902	0.012	12
	Z	0.030	0.070	0.882	0.013	12

Cl	<i>E</i>	-0.329	0.059	0.749	0.017	12
	<i>Z</i>	-0.327	0.059	0.700	0.019	12

Table S8. Linear correlations between NBO charge at C² atom of 1,4-diazabutatrienes **1** and the group electronegativity (χ) of R²

$$qC^2 (a.u.) = A + B * \chi(R^2)$$

R¹		A	B	r²	Std Err	Points
H	<i>E</i>	-0.036	0.095	0.927	0.013	12
	<i>Z</i>	-0.053	0.099	0.895	0.017	12
Me	<i>E</i>	-0.071	0.099	0.941	0.012	12
	<i>Z</i>	-0.074	0.104	0.890	0.018	12
NH₂	<i>E</i>	-0.274	0.113	0.789	0.028	12
	<i>Z</i>	-0.296	0.120	0.763	0.032	12
NMe₂	<i>E</i>	-0.323	0.115	0.666	0.039	12
	<i>Z</i>	-0.322	0.115	0.712	0.035	12
OMe	<i>E</i>	-0.156	0.086	0.625	0.032	12
	<i>Z</i>	-0.213	0.105	0.850	0.021	12
SMe	<i>E</i>	-0.149	0.103	0.785	0.026	12
	<i>Z</i>	-0.137	0.099	0.843	0.021	12
CF₃	<i>E</i>	0.006	0.090	0.889	0.015	12
	<i>Z</i>	-0.004	0.092	0.902	0.015	12
CHO	<i>E</i>	-0.008	0.096	0.933	0.012	12
	<i>Z</i>	-0.005	0.097	0.848	0.020	12
CN	<i>E</i>	0.037	0.089	0.898	0.015	12
	<i>Z</i>	0.015	0.096	0.879	0.017	12
NO₂	<i>E</i>	-0.094	0.100	0.775	0.026	12
	<i>Z</i>	-0.076	0.095	0.699	0.030	12
F	<i>E</i>	-0.193	0.096	0.904	0.015	12
	<i>Z</i>	-0.202	0.098	0.886	0.017	12
Cl	<i>E</i>	-0.103	0.091	0.924	0.013	12
	<i>Z</i>	-0.114	0.095	0.909	0.015	12

Table S9. Linear correlations between NBO charge at C² atom of 1,4-diazabutatrienes **1** and the resonant contribution (σ_R) of R¹

$$qC^2 (a.u.) = A + B * \sigma_R(R^1)$$

R²		A	B	r²	Std Err	Points
H	<i>E</i>	0.161	0.247	0.871	0.034	12
	<i>Z</i>	0.168	0.254	0.879	0.034	12
Me	<i>E</i>	0.180	0.227	0.836	0.036	12
	<i>Z</i>	0.170	0.242	0.861	0.035	12
NH₂	<i>E</i>	0.260	0.223	0.858	0.033	12
	<i>Z</i>	0.265	0.231	0.830	0.038	12
NMe₂	<i>E</i>	0.275	0.214	0.866	0.031	12

	Z	0.277	0.210	0.837	0.033	12
OMe	E	0.281	0.210	0.863	0.030	12
	Z	0.289	0.218	0.822	0.037	12
SMe	E	0.213	0.214	0.827	0.035	12
	Z	0.218	0.229	0.873	0.032	12
CF₃	E	0.204	0.267	0.893	0.034	12
	Z	0.204	0.260	0.887	0.034	12
CHO	E	0.181	0.257	0.866	0.037	12
	Z	0.176	0.246	0.860	0.036	12
CN	E	0.198	0.270	0.882	0.036	12
	Z	0.197	0.275	0.876	0.037	12
NO₂	E	0.253	0.281	0.863	0.041	12
	Z	0.253	0.260	0.865	0.037	12
F	E	0.315	0.227	0.830	0.037	12
	Z	0.316	0.227	0.830	0.037	12
Cl	E	0.259	0.232	0.855	0.035	12
	Z	0.259	0.235	0.846	0.036	12

5. Stabilization Energies

The stabilization energy values are calculated as the variation of the reaction enthalpy of the reaction shown in the schemes. Thus, the SE values shown in Table S10 are obtained as follow:

$$SE = [\Delta H \mathbf{2a(a-l)} + \Delta H \mathbf{1(a-l)b}] - [\Delta H \mathbf{1(a-l)(a-l)} + \Delta H \mathbf{2ab}]$$

Table S10. Computed stabilization energies (SE, kcal mol⁻¹) following the homodesmotic reaction shown below.

		$\begin{array}{c} \text{R}^1 \\ \text{N}=\text{C}=\text{C}=\text{N}\sim\text{R}^2 + \text{H} \\ \text{N}=\text{C}=\text{N} \\ \text{Me} \end{array} \xrightarrow{\text{SE}} \begin{array}{c} \text{R}^1 \\ \text{N}=\text{C}=\text{C}=\text{N}\sim\text{Me} + \text{H} \\ \text{N}=\text{C}=\text{N} \\ \text{R}^2 \end{array}$											
		R²											
R¹		H	Me	NH₂	NMe₂	OMe	SMe	CF₃	CHO	CN	NO₂	F	Cl
H	E	-3.3	0.0	11.7	12.9	14.3	5.5	-2.9	-4.4	-3.1	3.8	16.3	7.9
	Z	-4.0	0.0	11.6	12.8	14.5	5.5	-3.0	-3.9	-3.4	3.8	16.4	8.4
Me	E	-3.2	0.0	11.1	12.0	14.0	4.5	-2.1	-3.3	-2.1	4.7	16.7	8.5
	Z	-3.7	0.0	11.4	12.2	14.5	5.3	-2.0	-3.3	-2.0	5.0	17.2	9.0
NH₂	E	-2.5	0.0	8.6	9.5	11.1	3.6	-1.2	-2.5	-0.7	4.0	13.3	6.8
	Z	-3.4	0.0	8.3	9.0	11.2	3.9	-1.3	-2.2	-0.8	4.6	13.4	6.9
NMe₂	E	-2.3	0.0	8.5	9.3	11.2	3.9	0.3	-0.7	1.8	6.3	14.3	7.8
	Z	-3.0	0.0	8.2	9.0	11.6	4.2	0.7	0.0	2.3	8.1	14.7	8.2
OMe	E	-3.7	0.0	8.2	9.3	10.0	3.4	-3.0	-3.5	-3.0	1.4	10.8	5.1
	Z	-3.7	0.0	8.1	9.3	9.7	4.1	-3.4	-3.8	-3.6	1.1	10.6	4.8
SMe	E	-2.2	0.0	10.2	11.4	12.9	6.0	-1.9	-3.0	-1.5	4.2	15.1	7.9
	Z	-3.5	0.0	9.9	11.1	13.2	5.0	-1.0	-2.1	-0.8	6.5	15.5	8.4
CF₃	E	-4.0	0.0	12.0	14.4	13.1	4.7	-5.4	-5.4	-6.2	0.2	12.3	5.2
	Z	-4.7	0.0	12.1	14.9	13.1	6.4	-5.7	-5.8	-6.7	0.0	12.3	5.3

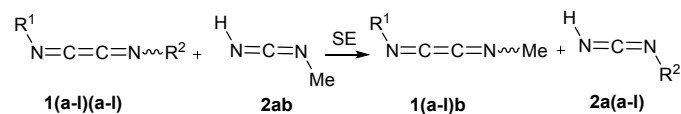
CHO	E	-4.4	0.0	11.8	14.6	13.8	4.8	-4.3	-4.6	-4.7	1.9	14.3	6.5
	Z	-4.3	0.0	12.5	15.5	14.0	6.5	-4.5	-4.8	-5.1	1.9	14.5	6.7
CN	E	-4.2	0.0	12.5	15.9	13.1	5.1	-6.2	-5.9	-7.1	-1.0	11.1	4.4
	Z	-5.1	0.0	12.6	16.4	12.9	6.5	-6.7	-6.4	-7.8	-1.4	10.9	4.3
NO ₂	E	-4.1	0.0	10.4	13.6	10.7	4.0	-6.6	-6.0	-7.8	-2.2	8.6	2.9
	Z	-4.8	0.0	11.0	15.3	10.6	6.9	-7.0	-6.4	-8.3	-2.4	8.6	3.0
F	E	-3.6	0.0	7.6	9.5	8.1	2.9	-6.5	-5.7	-7.8	-3.4	5.9	1.5
	Z	-4.4	0.0	7.6	9.7	7.9	3.6	-6.9	-6.0	-8.3	-3.7	5.6	1.4
Cl	E	-3.8	0.0	9.3	11.3	10.5	3.8	-5.4	-5.3	-6.3	-0.9	9.7	3.9
	Z	-4.2	0.0	9.3	11.4	10.4	4.8	-5.7	-5.5	-6.6	-1.0	9.6	3.8

Table S11. Computed stabilization energies (SE, kcal mol⁻¹) following the homodesmotic reaction shown below.

$$\begin{array}{c}
 \text{R}^1 \\
 \diagdown \\
 \text{N}=\text{C}=\text{C}=\text{N}\sim\text{R}^2 \\
 \text{1(a-l)(a-l)}
 \end{array}
 +
 \begin{array}{c}
 \text{H} \\
 | \\
 \text{N}=\text{C}=\text{N} \\
 | \\
 \text{H} \\
 \text{2aa}
 \end{array}
 \xrightarrow{\text{SE}}
 \begin{array}{c}
 \text{R}^1 \\
 \diagdown \\
 \text{N}=\text{C}=\text{C}=\text{N}\sim\text{H} \\
 \text{1(a-l)a}
 \end{array}
 +
 \begin{array}{c}
 \text{H} \\
 | \\
 \text{N}=\text{C}=\text{N} \\
 | \\
 \text{R}^2 \\
 \text{2a(a-l)}
 \end{array}$$

		R²											
R¹		H	Me	NH₂	NMe₂	OMe	SMe	CF₃	CHO	CN	NO₂	F	Cl
H	E	0.0	3.3	15.0	16.2	17.6	8.8	0.4	-1.1	0.2	7.1	19.6	11.2
	Z	0.0	4.0	15.6	16.8	18.4	9.4	0.9	0.1	0.6	7.7	20.4	12.4
Me	E	0.0	3.2	14.2	15.2	17.2	8.6	1.1	-0.1	1.1	7.9	19.9	11.7
	Z	0.0	3.7	15.0	15.8	18.1	9.0	1.6	0.4	1.7	8.6	20.8	12.6
NH₂	E	0.0	2.5	11.1	12.0	13.6	6.7	1.4	0.1	1.9	6.6	15.9	9.3
	Z	0.0	3.4	11.8	12.5	14.6	7.3	2.1	1.3	2.6	8.0	16.9	10.3
NMe₂	E	0.0	2.3	10.8	11.6	13.5	6.8	2.6	1.6	4.1	8.5	16.5	10.1
	Z	0.0	3.0	11.3	12.1	14.6	7.3	3.8	3.1	5.3	11.1	17.7	11.2
OMe	E	0.0	2.9	11.1	12.2	12.9	6.3	-0.1	-0.6	-0.1	3.0	13.7	7.9
	Z	0.0	3.7	11.8	13.0	13.4	7.8	0.2	-0.1	0.1	4.8	14.3	8.5
SMe	E	0.0	3.1	13.0	14.2	15.1	8.2	1.3	0.1	1.6	7.2	17.8	10.1
	Z	0.0	3.5	13.5	14.6	16.8	8.5	2.5	1.4	2.7	10.0	19.0	11.9
CF₃	E	0.0	4.0	16.0	18.4	17.1	9.7	-1.4	-1.4	-2.2	4.2	16.3	9.2
	Z	0.0	4.7	16.7	19.6	17.7	11.0	-1.1	-1.1	-2.0	4.7	17.0	10.0
CHO	E	0.0	4.4	16.2	19.0	18.1	10.0	0.1	-0.2	-0.4	6.3	18.7	10.9
	Z	0.0	4.3	16.8	19.8	18.2	10.8	-0.2	-0.5	-0.8	6.2	18.8	11.0
CN	E	0.0	4.2	16.7	20.1	17.3	10.2	-2.0	-1.7	-2.9	3.2	15.3	8.6
	Z	0.0	5.1	17.6	21.5	17.9	11.6	-1.7	-1.3	-2.7	3.7	15.9	9.4
NO₂	E	0.0	4.1	14.5	17.7	13.5	8.9	-2.5	-1.9	-3.7	1.9	12.7	7.0
	Z	0.0	4.8	15.9	20.2	15.4	11.7	-2.1	-1.5	-3.5	2.5	13.4	7.8
F	E	0.0	3.6	11.3	13.2	11.7	7.0	-2.9	-2.0	-4.1	0.2	9.5	5.1
	Z	0.0	4.4	12.0	14.1	12.3	8.0	-2.5	-1.6	-3.9	0.7	10.0	5.8
Cl	E	0.0	3.8	13.1	15.1	14.3	7.7	-1.6	-1.4	-2.4	2.9	13.5	7.8
	Z	0.0	4.2	13.5	15.6	14.6	9.0	-1.5	-1.3	-2.4	3.2	13.8	8.0

Table S12. Computed stabilization energies (SE, kcal mol⁻¹) in different solvents following the homodesmotic reaction shown below at the PCM(solvent)/DLPNO-CSSD(T)/ma-def2-TZVPP//wB97X-D/def2-TZVPD.



R ¹	R ²	Gas	Acetone	MeCN	Ammonia	CCl ₄	DCM	CHCl ₃	DMF	DMSO	EtOH	C6	MeOH	Pyridine	THF	Toluene	Water
CF₃	OMe	13.1	12.5	12.5	12.5	12.8	12.6	12.6	12.5	12.5	12.5	12.9	12.5	12.5	12.6	12.8	12.5
CHO	OMe	13.8	13.3	13.3	13.3	13.5	13.4	13.4	13.3	13.3	13.3	13.6	13.3	13.3	13.4	13.5	13.3
Me	OMe	14.0	14.0	14.0	14.0	13.9	14.0	14.0	14.0	14.0	14.0	14.0	14.0	14.0	14.0	13.9	14.0
NMe₂	F	14.3	15.5	15.5	15.5	14.8	15.3	15.1	15.5	15.5	15.5	14.7	15.5	15.4	15.3	14.8	15.5
H	OMe	14.3	14.4	14.4	14.4	14.3	14.4	14.4	14.4	14.4	14.4	14.3	14.4	14.4	14.4	14.3	14.4
CHO	F	14.3	13.8	13.8	13.8	14.0	13.8	13.9	13.8	13.8	13.8	14.1	13.8	13.8	13.8	14.0	13.8
SMe	F	14.7	15.0	15.0	15.0	14.8	15.0	14.9	15.0	15.0	15.0	14.8	15.0	15.0	14.9	14.8	15.0
CN	NMe₂	15.9	20.5	20.7	20.5	18.0	20.0	19.4	20.7	20.7	20.6	17.6	20.6	20.3	19.8	18.1	20.9
H	F	16.3	16.8	16.8	16.8	16.5	16.8	16.7	16.8	16.9	16.8	16.5	16.8	16.8	16.7	16.5	16.9
Me	F	16.7	17.2	17.2	17.2	16.9	17.1	17.1	17.2	17.2	17.2	16.9	17.2	17.2	17.1	16.9	17.2

5. Computational Data

Table S13. Electronic ($E_{\text{SCF},298}$), Gibbs free (G_{298}), and enthalpic (H_{298}) energies for systems shown in Table S10 (in Hartree) computed at the DLPNO-CSSD(T)/ma-def2-TZVPP//wB97X-D/def2-TZVPD level. The wB97X-D/def2-TZVPD level of theory was used to optimize the geometries and calculate the thermal corrections.

	R ¹	R ²	E_{tot} wB97X-D/def2- TZVPD	G_{298} wB97X- D/def2- TZVPD	H_{298} wB97X- D/def2- TZVPD	E_{tot} DLPNO- CSSD(T)/ma- def2-TZVPP// wB97X- D/def2- TZVPD	G_{298} DLPNO- CSSD(T)/ma- def2-TZVPP// wB97X- D/def2- TZVPD	H_{298} DLPNO- CSSD(T)/ma- def2-TZVPP// wB97X- D/def2- TZVPD
(E)-1,4-Duazabutatrienes 1								
<i>E-1aa</i>	H	H	-186.80982	-186.79729	-186.76650	-186.49807	-186.48554	-186.45475
<i>E-1ab</i>	H	Me	-226.12086	-226.08274	-226.04756	-225.73122	-225.69310	-225.65792
<i>E-1ac</i>	H	NH ₂	-242.15018	-242.12231	-242.08799	-241.74683	-241.71895	-241.68464
<i>E-1ad</i>	H	NMe ₂	-320.77394	-320.69475	-320.65281	-320.21620	-320.13701	-320.09507
<i>E-1ae</i>	H	OMe	-301.30276	-301.26230	-301.22416	-300.81084	-300.77038	-300.73224
<i>E-1af</i>	H	SMe	-624.32338	-624.28721	-624.24782	-623.46217	-623.42600	-623.38661
<i>E-1ag</i>	H	CF ₃	-523.90976	-523.89879	-523.85771	-523.16697	-523.15600	-523.11492
<i>E-1ah</i>	H	CHO	-300.13549	-300.11892	-300.08076	-299.65064	-299.63406	-299.59591
<i>E-1ai</i>	H	CN	-279.02883	-279.02074	-278.98508	-278.56847	-278.56038	-278.52472
<i>E-1aj</i>	H	NO ₂	-391.30362	-391.29441	-391.25516	-390.70062	-390.69141	-390.65217
<i>E-1ak</i>	H	F	-286.00330	-286.00145	-285.96764	-285.57004	-285.56819	-285.53438
<i>E-1al</i>	H	Cl	-646.38742	-646.38753	-646.35243	-645.59117	-645.59128	-645.55618
<i>E-1ab</i>	Me	Me	-265.43131	-265.36766	-265.32813	-264.96408	-264.90043	-264.86090
<i>E-1bc</i>	Me	NH ₂	-281.45888	-281.40549	-281.36675	-280.97872	-280.92533	-280.88659
<i>E-1bd</i>	Me	NMe ₂	-360.08195	-359.97710	-359.93099	-359.44759	-359.34273	-359.29663
<i>E-1be</i>	Me	OMe	-340.61245	-340.54658	-340.50391	-340.04330	-339.97743	-339.93475
<i>E-1bf</i>	Me	SMe	-663.63329	-663.57168	-663.52786	-662.69494	-662.63333	-662.58951
<i>E-1bg</i>	Me	CF ₃	-563.22202	-563.18553	-563.14005	-562.40117	-562.36467	-562.31920
<i>E-1bh</i>	Me	CHO	-339.44964	-339.40645	-339.36484	-338.88556	-338.84236	-338.80075
<i>E-1bi</i>	Me	CN	-318.34158	-318.30790	-318.26784	-317.80305	-317.76936	-317.72931
<i>E-1bj</i>	Me	NO ₂	-430.61601	-430.58143	-430.53755	-429.93504	-429.90045	-429.85658
<i>E-1bk</i>	Me	F	-325.31483	-325.28758	-325.24909	-324.80382	-324.77657	-324.73808
<i>E-1bl</i>	Me	Cl	-685.69912	-685.67371	-685.63414	-684.82519	-684.79978	-684.76021
<i>E-1cc</i>	NH ₂	NH ₂	-297.48112	-297.43757	-297.40003	-296.98944	-296.94589	-296.90836
<i>E-1cd</i>	NH ₂	NMe ₂	-376.10308	-376.00784	-375.96332	-375.45806	-375.36282	-375.31829
<i>E-1ce</i>	NH ₂	OMe	-356.63485	-356.57892	-356.53749	-356.05322	-355.99729	-355.95585
<i>E-1cf</i>	NH ₂	SMe	-679.65841	-679.60687	-679.56406	-678.70759	-678.65605	-678.61323
<i>E-1cg</i>	NH ₂	CF ₃	-579.25287	-579.22714	-579.18207	-578.41712	-578.39139	-578.34632
<i>E-1ch</i>	NH ₂	CHO	-355.48010	-355.44743	-355.40628	-354.90148	-354.86881	-354.82766
<i>E-1ci</i>	NH ₂	CN	-334.37444	-334.35260	-334.31173	-333.82001	-333.79816	-333.75730
<i>E-1cj</i>	NH ₂	NO ₂	-446.64410	-446.62062	-446.57689	-445.94842	-445.92493	-445.88121
<i>E-1ck</i>	NH ₂	F	-341.33717	-341.31967	-341.28259	-340.81289	-340.79539	-340.75832
<i>E-1cl</i>	NH ₂	Cl	-701.72458	-701.70904	-701.67072	-700.83697	-700.82144	-700.78312
<i>E-1dd</i>	NMe ₂	NMe ₂	-454.72454	-454.57745	-454.52617	-453.92633	-453.77924	-453.72796
<i>E-1de</i>	NMe ₂	OMe	-435.25765	-435.15017	-435.10155	-434.52220	-434.41472	-434.36610
<i>E-1df</i>	NMe ₂	SMe	-758.28137	-758.17828	-758.12821	-757.17691	-757.07382	-757.02376

E-1dg	NMe ₂	CF ₃	-657.87929	-657.80296	-657.74939	-656.88867	-656.81233	-656.75877
E-1dh	NMe ₂	CHO	-434.10672	-434.02253	-433.97387	-433.37346	-433.28926	-433.24060
E-1di	NMe ₂	CN	-413.00225	-412.92730	-412.88022	-412.29331	-412.21836	-412.17128
E-1dj	NMe ₂	NO ₂	-525.27167	-525.19617	-525.14524	-524.42122	-524.34571	-524.29479
E-1dk	NMe ₂	F	-419.96162	-419.89269	-419.84819	-419.28329	-419.21436	-419.16986
E-1dl	NMe ₂	Cl	-780.34935	-780.28251	-780.23657	-779.30751	-779.24067	-779.19473
E-1ee	OMe	OMe	-415.78700	-415.71853	-415.67325	-415.11606	-415.04758	-415.00230
E-1ef	OMe	SMe	-738.81067	-738.74693	-738.69979	-737.77103	-737.70730	-737.66015
E-1eg	OMe	CF ₃	-638.40244	-638.36369	-638.31507	-637.47905	-637.44030	-637.39167
E-1eh	OMe	CHO	-414.63092	-414.58527	-414.54064	-413.96454	-413.91888	-413.87425
E-1ei	OMe	CN	-393.52244	-393.48615	-393.44315	-392.88101	-392.84472	-392.80172
E-1ej	OMe	NO ₂	-505.79067	-505.75284	-505.70694	-505.00681	-504.96899	-504.92308
E-1ek	OMe	F	-400.48621	-400.45604	-400.41520	-399.87351	-399.84335	-399.80251
E-1el	OMe	Cl	-760.87466	-760.84643	-760.80437	-759.89879	-759.87056	-759.82850
E-1ff	SMe	SMe	-1061.83441	-1061.77442	-1061.72670	-1060.42529	-1060.36529	-1060.31758
E-1fg	SMe	CF ₃	-961.42504	-961.39049	-961.34086	-960.13245	-960.09789	-960.04826
E-1fh	SMe	CHO	-737.65175	-737.61049	-737.56475	-736.61670	-736.57544	-736.52970
E-1fi	SMe	CN	-716.54559	-716.51355	-716.46951	-715.53492	-715.50288	-715.45884
E-1fj	SMe	NO ₂	-828.81734	-828.78514	-828.73666	-827.66484	-827.63263	-827.58415
E-1fk	SMe	F	-723.51339	-723.48779	-723.44551	-722.53129	-722.50569	-722.46341
E-1fl	SMe	Cl	-1083.89808	-1083.87466	-1083.83075	-1082.55361	-1082.53020	-1082.48628
E-1gg	CF ₃	CF ₃	-861.00676	-860.99713	-860.94597	-859.83303	-859.82340	-859.77224
E-1gh	CF ₃	CHO	-637.23601	-637.21993	-637.17243	-636.31917	-636.30309	-636.25559
E-1gi	CF ₃	CN	-616.12475	-616.11818	-616.07222	-615.23355	-615.22698	-615.18102
E-1gj	CF ₃	NO ₂	-728.39867	-728.39090	-728.34148	-727.36486	-727.35710	-727.30767
E-1gk	CF ₃	F	-623.09809	-623.09768	-623.05356	-622.23387	-622.23345	-622.18933
E-1gl	CF ₃	Cl	-983.48406	-983.48559	-983.44030	-982.25695	-982.25848	-982.21320
E-1hh	CHO	CHO	-413.46495	-413.44207	-413.39856	-412.80486	-412.78198	-412.73847
E-1hi	CHO	CN	-392.35444	-392.34119	-392.29915	-391.72024	-391.70699	-391.66496
E-1hj	CHO	NO ₂	-504.62886	-504.61445	-504.56886	-503.85206	-503.83765	-503.79205
E-1hk	CHO	F	-399.32871	-399.32162	-399.28134	-398.72143	-398.71434	-398.67407
E-1hl	CHO	Cl	-759.71366	-759.70853	-759.66707	-758.74342	-758.73829	-758.69683
E-1ii	CN	CN	-371.24274	-371.23905	-371.19851	-370.63395	-370.63026	-370.58972
E-1ij	CN	NO ₂	-483.51601	-483.51101	-483.46708	-482.76483	-482.75984	-482.71590
E-1ik	CN	F	-378.21567	-378.21792	-378.17931	-377.63380	-377.63605	-377.59744
E-1il	CN	Cl	-738.60223	-738.60644	-738.56668	-737.65754	-737.66175	-737.62198
E-1jj	NO ₂	NO ₂	-595.78837	-595.78218	-595.73484	-594.89478	-594.88858	-594.84124
E-1jk	NO ₂	F	-490.48572	-490.48673	-490.44480	-489.76170	-489.76271	-489.72078
E-1jl	NO ₂	Cl	-850.87414	-850.87720	-850.83398	-849.78713	-849.79019	-849.74697
E-1kk	F	F	-385.17964	-385.18776	-385.15139	-384.62622	-384.63435	-384.59797
E-1kl	F	Cl	-745.57046	-745.58072	-745.54300	-744.65363	-744.66388	-744.62616
E-1ll	Cl	Cl	-1105.95871	-1105.97095	-1105.93201	-1104.67882	-1104.69107	-1104.65213
(Z)-1,4-Diazabutatrienes 1								
Z-1aa	H	H	-186.80817	-186.79584	-186.76483	-186.49550	-186.48317	-186.45216
Z-1ab	H	Me	-226.11987	-226.08197	-226.04654	-225.72971	-225.69181	-225.65638
Z-1ac	H	NH ₂	-242.14892	-242.12124	-242.08673	-241.74513	-241.71746	-241.68294
Z-1ad	H	NMe ₂	-320.77257	-320.69356	-320.65148	-320.21443	-320.13542	-320.09334
Z-1ae	H	OMe	-301.30210	-301.26188	-301.22348	-300.80961	-300.76939	-300.73100

Z-1af	H	SMe	-624.32206	-624.28590	-624.24651	-623.46058	-623.42442	-623.38502
Z-1ag	H	CF ₃	-523.90896	-523.89816	-523.85684	-523.16531	-523.15451	-523.11319
Z-1ah	H	CHO	-300.13695	-300.11947	-300.08197	-299.65017	-299.63269	-299.59519
Z-1ai	H	CN	-279.02774	-279.01988	-278.98392	-278.56655	-278.55870	-278.52273
Z-1aj	H	NO ₂	-391.30284	-391.29427	-391.25435	-390.69909	-390.69051	-390.65059
Z-1ak	H	F	-286.00261	-286.00116	-285.96693	-285.56877	-285.56731	-285.53308
Z-1al	H	Cl	-646.38708	-646.38730	-646.35209	-645.59045	-645.59067	-645.55546
Z-1ab	Me	Me	-265.43090	-265.36748	-265.32773	-264.96327	-264.89985	-264.86010
Z-1bc	Me	NH ₂	-281.45861	-281.40533	-281.36653	-280.97840	-280.92513	-280.88633
Z-1bd	Me	NMe ₂	-360.08152	-359.97686	-359.93064	-359.44697	-359.34231	-359.29609
Z-1be	Me	OMe	-340.61260	-340.54681	-340.50406	-340.04327	-339.97748	-339.93474
Z-1bf	Me	SMe	-663.63254	-663.57114	-663.52718	-662.69391	-662.63251	-662.58855
Z-1bg	Me	CF ₃	-563.22186	-563.18564	-563.13988	-562.40048	-562.36426	-562.31850
Z-1bh	Me	CHO	-339.44938	-339.40638	-339.36449	-338.88479	-338.84180	-338.79991
Z-1bi	Me	CN	-318.34135	-318.30785	-318.26760	-317.80245	-317.76895	-317.72870
Z-1bj	Me	NO ₂	-430.61594	-430.58192	-430.53750	-429.93465	-429.90062	-429.85620
Z-1bk	Me	F	-325.31478	-325.28780	-325.24909	-324.80370	-324.77672	-324.73800
Z-1bl	Me	Cl	-685.69909	-685.67375	-685.63413	-684.82502	-684.79967	-684.76006
Z-1cc	NH ₂	NH ₂	-297.48050	-297.43706	-297.39946	-296.98875	-296.94530	-296.90771
Z-1cd	NH ₂	NMe ₂	-376.10227	-376.00716	-375.96257	-375.45702	-375.36192	-375.31732
Z-1ce	NH ₂	OMe	-356.63491	-356.57899	-356.53755	-356.05310	-355.99718	-355.95574
Z-1cf	NH ₂	SMe	-679.65754	-679.60607	-679.56329	-678.70670	-678.65523	-678.61244
Z-1cg	NH ₂	CF ₃	-579.25285	-579.22741	-579.18207	-578.41662	-578.39118	-578.34584
Z-1ch	NH ₂	CHO	-355.48065	-355.44767	-355.40673	-354.90181	-354.86883	-354.82790
Z-1ci	NH ₂	CN	-334.37442	-334.35206	-334.31168	-333.81954	-333.79719	-333.75681
Z-1cj	NH ₂	NO ₂	-446.64521	-446.62158	-446.57804	-445.94904	-445.92541	-445.88186
Z-1ck	NH ₂	F	-341.33720	-341.31980	-341.28267	-340.81278	-340.79538	-340.75825
Z-1cl	NH ₂	Cl	-701.72458	-701.70909	-701.67075	-700.83677	-700.82129	-700.78294
Z-1dd	NMe ₂	NMe ₂	-454.72403	-454.57695	-454.52572	-453.92538	-453.77830	-453.72707
Z-1de	NMe ₂	OMe	-435.25785	-435.15037	-435.10178	-434.52222	-434.41473	-434.36615
Z-1df	NMe ₂	SMe	-758.28068	-758.17727	-758.12756	-757.17593	-757.07252	-757.02281
Z-1dg	NMe ₂	CF ₃	-657.87989	-657.80329	-657.75000	-656.88879	-656.81218	-656.75890
Z-1dh	NMe ₂	CHO	-434.10825	-434.02360	-433.97506	-433.37439	-433.28974	-433.24120
Z-1di	NMe ₂	CN	-413.00268	-412.92760	-412.88064	-412.29352	-412.21844	-412.17147
Z-1dj	NMe ₂	NO ₂	-525.27425	-525.19762	-525.14782	-524.42362	-524.34699	-524.29718
Z-1dk	NMe ₂	F	-419.96190	-419.89308	-419.84852	-419.28340	-419.21457	-419.17001
Z-1dl	NMe ₂	Cl	-780.34975	-780.28298	-780.23697	-779.30760	-779.24083	-779.19483
Z-1ee	OMe	OMe	-415.78681	-415.71825	-415.67306	-415.11559	-415.04703	-415.00184
Z-1ef	OMe	SMe	-738.81204	-738.74797	-738.70135	-737.77188	-737.70782	-737.66120
Z-1eg	OMe	CF ₃	-638.40206	-638.36326	-638.31469	-637.47829	-637.43949	-637.39092
Z-1eh	OMe	CHO	-414.63065	-414.58522	-414.54035	-413.96404	-413.91861	-413.87374
Z-1ei	OMe	CN	-393.52198	-393.48565	-393.44267	-392.88012	-392.84379	-392.80081
Z-1ej	OMe	NO ₂	-505.79232	-505.75532	-505.70848	-505.00852	-504.97152	-504.92468
Z-1ek	OMe	F	-400.48598	-400.45582	-400.41499	-399.87317	-399.84302	-399.80218
Z-1el	OMe	Cl	-760.87447	-760.84622	-760.80419	-759.89844	-759.87019	-759.82815
Z-1ff	SMe	SMe	-1061.83298	-1061.77349	-1061.72514	-1060.42425	-1060.36475	-1060.31641
Z-1fg	SMe	CF ₃	-961.42576	-961.39110	-961.34160	-960.13276	-960.09810	-960.04860
Z-1fh	SMe	CHO	-737.65317	-737.61164	-737.56592	-736.61744	-736.57591	-736.53019

Z-1fi	SMe	CN	-716.54606	-716.51404	-716.46998	-715.53508	-715.50306	-715.45900
Z-1fj	SMe	NO ₂	-828.81949	-828.78695	-828.73906	-827.66751	-827.63497	-827.58708
Z-1fk	SMe	F	-723.51370	-723.48823	-723.44588	-722.53153	-722.50606	-722.46371
Z-1fl	SMe	Cl	-1083.89978	-1083.87608	-1083.83265	-1082.55474	-1082.53103	-1082.48761
Z-1gg	CF ₃	CF ₃	-861.00635	-860.99705	-860.94549	-859.83190	-859.82260	-859.77103
Z-1gh	CF ₃	CHO	-637.23549	-637.21955	-637.17184	-636.31799	-636.30205	-636.25434
Z-1gi	CF ₃	CN	-616.12408	-616.11764	-616.07149	-615.23222	-615.22577	-615.17962
Z-1gj	CF ₃	NO ₂	-728.39837	-728.39084	-728.34115	-727.36398	-727.35645	-727.30676
Z-1gk	CF ₃	F	-623.09772	-623.09751	-623.05320	-622.23314	-622.23292	-622.18862
Z-1gl	CF ₃	Cl	-983.48385	-983.48537	-983.44009	-982.25643	-982.25795	-982.21267
Z-1hh	CHO	CHO	-413.46449	-413.44191	-413.39798	-412.80378	-412.78119	-412.73727
Z-1hi	CHO	CN	-392.35372	-392.34062	-392.29835	-391.71898	-391.70588	-391.66361
Z-1hj	CHO	NO ₂	-504.62844	-504.61442	-504.56842	-503.85112	-503.83710	-503.79110
Z-1hk	CHO	F	-399.32838	-399.32155	-399.28103	-398.72084	-398.71401	-398.67349
Z-1hl	CHO	Cl	-759.71348	-759.70837	-759.66687	-758.74293	-758.73782	-758.69632
Z-1ii	CN	CN	-371.24181	-371.23822	-371.19750	-370.63238	-370.62879	-370.58807
Z-1ij	CN	NO ₂	-483.51543	-483.51073	-483.46648	-482.76366	-482.75896	-482.71471
Z-1ik	CN	F	-378.21514	-378.21754	-378.17878	-377.63288	-377.63528	-377.59652
Z-1il	CN	Cl	-738.60190	-738.60615	-738.56633	-737.65685	-737.66110	-737.62128
Z-1jj	NO ₂	NO ₂	-595.78813	-595.78233	-595.73460	-594.89415	-594.88835	-594.84062
Z-1jk	NO ₂	F	-490.48557	-490.48675	-490.44467	-489.76125	-489.76244	-489.72035
Z-1jl	NO ₂	Cl	-850.87404	-850.87725	-850.83390	-849.78675	-849.78997	-849.74661
Z-1kk	F	F	-385.17939	-385.18756	-385.15115	-384.62571	-384.63388	-384.59748
Z-1kl	F	Cl	-745.57026	-745.58055	-745.54281	-744.65334	-744.66363	-744.62590
Z-1ll	Cl	Cl	-1105.95853	-1105.97077	-1105.93183	-1104.67854	-1104.69078	-1104.65185
Carbodiimides 2								
2aa	H	H	-148.792222	-148.782503	-148.754778	-148.547762	-148.538043	-148.510318
2ab	H	Me	-188.097980	-188.062977	-188.030019	-187.776178	-187.741174	-187.708216
2ac	H	NH ₂	-204.104955	-204.079798	-204.048124	-203.773128	-203.747971	-203.716297
2ad	H	NMe ₂	-282.724668	-282.647620	-282.609424	-282.240037	-282.162989	-282.124793
2ae	H	OMe	-263.254928	-263.217439	-263.182050	-262.832676	-262.795187	-262.759798
2af	H	SMe	-586.290170	-586.257227	-586.219996	-585.498336	-585.465393	-585.428162
2ag	H	CF ₃	-485.891868	-485.885107	-485.845498	-485.216220	-485.209460	-485.169851
2ah	H	CHO	-262.121040	-262.106286	-262.071866	-261.702436	-261.687682	-261.653262
2ai	H	CN	-241.011956	-241.006434	-240.973665	-240.618273	-240.612751	-240.579982
2aj	H	NO ₂	-353.274705	-353.267706	-353.231955	-352.739162	-352.732163	-352.696412
2ak	H	F	-247.952153	-247.952756	-247.922006	-247.588877	-247.589479	-247.558729
2al	H	Cl	-608.351160	-608.353636	-608.321662	-607.623409	-607.625885	-607.593911

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7. Cartesian Coordinates

(E)-1,4-Duazabutatrienes 1

E-1aa

SCF = -186.809821135
 Num. Imaginary Freq = 0

C	-0.639071	0.086712	0.000007
N	-1.851788	-0.154883	0.000030
C	0.639075	-0.086779	-0.000024
N	1.851775	0.154927	-0.000038
H	2.423596	-0.691219	0.000031
H	-2.423528	0.691316	0.000130

E-1ab

SCF = -226.120856287
 Num. Imaginary Freq = 0

C	0.041890	-0.174538	0.000012
N	-1.119523	-0.588838	0.000055
C	1.323330	-0.089148	-0.000007
N	2.487481	0.329185	-0.000053
C	-2.225651	0.353230	-0.000001
H	-1.908489	1.398880	-0.000079
H	-2.841374	0.152037	-0.878018
H	-2.841356	0.152162	0.878058
H	3.178096	-0.422773	0.000007

E-1ac

SCF = -242.150179115
 Num. Imaginary Freq = 0

C	0.020037	-0.096646	0.000057
N	-1.150829	-0.543981	0.008536
C	1.292779	-0.051857	0.001499
N	2.484419	0.268383	-0.001050
N	-2.181358	0.308776	-0.069467

H	-2.016001	1.277481	0.170997
H	-3.050220	-0.095101	0.232031
H	3.123710	-0.523606	0.021496

E-1ad

SCF = -320.773942248
 Num. Imaginary Freq = 0

C	-2.161951	-0.176574	0.011861
N	-3.341222	0.197006	0.050462
C	-0.899545	-0.296240	-0.024610
N	0.259342	-0.797428	-0.078465
N	1.317093	-0.007251	-0.159200
C	1.173212	1.418015	0.008316
H	2.136940	1.893590	-0.161715
H	0.446781	1.803548	-0.709140
H	0.816218	1.665196	1.016007
C	2.590357	-0.634248	0.104181
H	2.507317	-1.690089	-0.140927
H	3.362832	-0.179286	-0.517060
H	2.881867	-0.535955	1.156490
H	-4.010881	-0.569006	0.068281

E-1ae

SCF = -301.302755852
 Num. Imaginary Freq = 0

C	-0.654504	0.034549	0.000016
N	0.514133	0.473589	0.000022
C	-1.931497	0.048828	0.000006
N	-3.132216	-0.207046	0.000134
H	-3.740805	0.609048	-0.000290
O	1.468582	-0.510311	-0.000053
C	2.760520	0.080244	-0.000056
H	3.459299	-0.753412	-0.000119
H	2.906134	0.689711	-0.893505

H 2.906180 0.689615 0.893451

E-1af

SCF = -624.323382904

Num. Imaginary Freq = 0

C -0.800369 -0.492631 0.000004
N 0.279770 -1.109972 -0.000213
C -2.012663 -0.105212 0.000178
N -3.092067 0.498864 0.000166
H -3.901340 -0.121545 0.000150
S 1.761423 -0.354251 -0.000105
C 1.383721 1.398755 0.000073
H 2.342068 1.918225 0.000148
H 0.819250 1.671907 -0.891594
H 0.819215 1.671714 0.891776

E-1ag

SCF = -523.909763854

Num. Imaginary Freq = 0

C -1.102646 -0.318642 -0.000149
N 0.017919 -0.841739 -0.001372
C -2.378391 -0.166308 0.000950
N -3.511477 0.313275 -0.000248
C 1.178819 0.003799 -0.000095
H -4.253547 -0.387842 -0.002053
F 0.918790 1.312255 0.000950
F 1.902389 -0.269647 1.079928
F 1.903461 -0.267721 -1.079860

E-1ah

SCF = -300.135488140

Num. Imaginary Freq = 0

C 0.526849 -0.191164 0.000009
N -0.636162 -0.628246 -0.000006
C 1.806463 -0.083628 0.000028
N 2.964071 0.339663 0.000042
C -1.675803 0.363512 -0.000027
O -2.823644 0.059774 -0.000044
H -1.318850 1.410200 -0.000027
H 3.667593 -0.400620 0.000064

E-1ai

SCF = -279.028827517

Num. Imaginary Freq = 0

C -0.417081 0.162627 0.000014
N 0.701964 0.709930 0.000049
C -1.695435 0.043994 0.000011
N -2.832420 -0.425687 -0.000017
H -3.571535 0.278297 0.000037
C 1.838127 -0.001239 -0.000009
N 2.875866 -0.500042 -0.000051

E-1aj

SCF = -391.303616591

Num. Imaginary Freq = 0

C 0.777456 0.000914 0.253467
N -0.298576 0.002437 0.866008
C 2.045951 0.000473 0.043720
N 3.163460 -0.001040 -0.452725
H 3.934187 0.000902 0.214619
N -1.479331 -0.000235 -0.024372
O -1.909626 -1.082013 -0.293566
O -1.912062 1.079845 -0.296449

E-1ak

SCF = -286.003303997

Num. Imaginary Freq = 0

C 0.030228 0.046547 -0.000004
N 1.141003 0.596356 -0.000055
C -1.255991 0.030058 -0.000011
N -2.438246 -0.255515 -0.000133
F 2.170456 -0.373736 0.000130
H -3.098823 0.518103 0.000227

E-1al

SCF = -646.387419669

Num. Imaginary Freq = 0

C 0.506129 0.275693 0.000016
N -0.600115 0.824214 0.000005
C 1.762804 0.034034 -0.000023
N 2.900644 -0.419153 0.000016
H 3.643248 0.279154 -0.000053
Cl -1.962385 -0.292526 -0.000003

E-1bb

SCF = -265.431309122

Num. Imaginary Freq = 0

C 0.628510 -0.120871 0.000131
N 1.758445 -0.614866 0.000125
C -0.628511 0.120875 0.000121
N -1.758447 0.614868 0.000065
C -2.926145 -0.251497 -0.000180
H -3.527226 -0.011995 -0.878804
H -2.678491 -1.316076 0.000034
H -3.527792 -0.011744 0.877981
C 2.926147 0.251494 -0.000083
H 3.527792 0.011703 0.878069
H 3.527225 0.012023 -0.878718
H 2.678496 1.316074 0.000173

E-1bc

SCF = -281.458879151

Num. Imaginary Freq = 0

C -0.606542 -0.179217 -0.004190
N -1.757718 -0.610215 -0.007616
C 0.645638 0.044759 -0.000943
N 1.776015 0.579272 0.003363
C -2.892042 0.297612 0.008728
N 2.875438 -0.199445 -0.072135

H	3.697298	0.272846	0.262537
H	2.774797	-1.165434	0.213276
H	-2.604074	1.352079	0.025971
H	-3.503938	0.101880	-0.873208
H	-3.502548	0.072416	0.884570

E-1bd

SCF = -360.081953564
Num. Imaginary Freq = 0

C	1.540906	0.080213	-0.014828
N	2.680518	0.546553	0.024807
C	0.303624	-0.196300	-0.050817
N	-0.817181	-0.767464	-0.111692
C	3.836445	-0.333054	0.050370
N	-1.932694	-0.043554	-0.197957
C	-1.876532	1.380044	0.028378
H	-1.161064	1.835645	-0.657508
H	-2.862881	1.805020	-0.147139
H	-1.557583	1.610499	1.053617
C	-3.142939	-0.755671	0.139275
H	-3.985164	-0.324334	-0.402538
H	-3.021896	-1.795493	-0.154573
H	-3.357269	-0.714360	1.214513
H	4.469957	-0.102348	-0.807932
H	3.574725	-1.394803	0.031890
H	4.417645	-0.119954	0.949292

E-1be

SCF = -340.612452170
Num. Imaginary Freq = 0

C	0.010789	-0.073684	-0.000014
N	1.144265	0.445845	0.000016
C	-1.256583	-0.217492	-0.000022
N	-2.427065	-0.572182	-0.000032
O	2.168380	-0.475029	-0.000021
C	3.413100	0.205323	0.000025
H	4.170598	-0.575682	-0.000013
H	3.516736	0.824516	-0.893073
H	3.516724	0.824418	0.893191
C	-3.519391	0.384524	0.000023
H	-3.184483	1.424438	0.000071
H	-4.137261	0.197480	-0.879042
H	-4.137247	0.197394	0.879081

E-1bf

SCF = -663.633291931
Num. Imaginary Freq = 0

C	0.216902	-0.475346	-0.004546
N	-0.850281	-1.112016	-0.000830
C	1.394063	0.004799	-0.002713
N	2.456881	0.628235	0.000809
S	-2.349792	-0.379014	0.002004
C	-2.000715	1.380063	-0.000610
H	-2.967994	1.882798	0.001365
H	-1.439013	1.664916	0.889090
H	-1.443700	1.663046	-0.893852

C	3.724188	-0.083438	0.001996
H	3.611050	-1.170624	0.002693
H	4.292187	0.226344	-0.876660
H	4.291322	0.227743	0.880676

E-1bg

SCF = -563.222020688
Num. Imaginary Freq = 0

C	-1.797927	-0.031153	0.000266
N	-2.904997	-0.562420	-0.000112
C	-0.548833	0.244420	0.000454
N	0.549316	0.815180	0.000231
C	1.743250	0.022614	-0.000038
C	-4.116066	0.238218	-0.000194
H	-3.928179	1.313808	-0.003276
H	-4.701955	-0.042740	-0.876259
H	-4.698681	-0.038023	0.879594
F	1.542271	-1.297494	0.000136
F	2.458273	0.323842	-1.079914
F	2.459017	0.323989	1.079354

E-1bh

SCF = -339.449644768
Num. Imaginary Freq = 0

C	1.064790	0.027888	0.099640
N	2.166465	0.504682	0.368805
C	-0.187389	-0.232148	0.019389
N	-1.291527	-0.716576	-0.232223
C	3.374733	-0.057836	-0.207823
H	3.188951	-0.908707	-0.866945
H	3.884318	0.735251	-0.756791
H	4.030623	-0.355507	0.611465
C	-2.518853	-0.218341	0.238655
O	-3.085564	0.719050	-0.234187
H	-2.943624	-0.857555	1.030520

E-1bi

SCF = -318.341580804
Num. Imaginary Freq = 0

C	0.268057	0.117296	-0.000007
N	1.366329	0.707661	-0.000023
C	-0.989567	-0.110361	-0.000002
N	-2.103469	-0.627460	0.000010
C	2.527154	0.037188	0.000003
N	3.581936	-0.425130	0.000021
C	-3.307711	0.180948	-0.000001
H	-3.893664	-0.095573	-0.877573
H	-3.893660	-0.095542	0.877583
H	-3.113845	1.255188	-0.000021

E-1bj

SCF = -430.616012514
Num. Imaginary Freq = 0

C	-0.162918	0.000006	0.222128
N	0.898780	0.000003	0.860333

C -1.406578 0.000005 -0.086424
N -2.503703 0.000005 -0.619524
N 2.098787 -0.000002 -0.001201
O 2.539323 1.080434 -0.263267
O 2.539316 -1.080441 -0.263266
C -3.741819 -0.000006 0.137448
H -4.314422 -0.878515 -0.160992
H -3.589408 -0.000002 1.218072
H -4.314439 0.878491 -0.160995

E-1bk

SCF = -325.314827229
Num. Imaginary Freq = 0

C -0.699847 0.004661 0.000022
N -1.765408 0.634735 -0.000007
C 0.570688 -0.182724 0.000025
N 1.716035 -0.577813 -0.000024
F -2.868106 -0.266146 -0.000009
C 2.887567 0.277014 -0.000009
H 3.482639 0.031691 0.879517
H 3.483052 0.031258 -0.879127
H 2.642429 1.340204 -0.000326

E-1bl

SCF = -685.699121462
Num. Imaginary Freq = 0

C 0.128620 0.252449 0.000053
N 1.216204 0.835058 0.000119
C -1.092916 -0.122288 0.000007
N -2.204542 -0.625348 -0.000071
Cl 2.616035 -0.251491 -0.000053
C -3.421240 0.167491 0.000017
H -4.003216 -0.110755 -0.879013
H -4.003244 -0.111000 0.878951
H -3.234551 1.243227 0.000171

E-1cc

SCF = -297.481118718
Num. Imaginary Freq = 0

C -0.617400 0.137143 -0.003865
N -1.775140 0.590805 -0.014230
C 0.617303 -0.136551 0.003025
N 1.774876 -0.590717 0.014010
N -2.835569 -0.262641 0.095252
H -2.666590 -1.205693 -0.233209
H -3.664257 0.157043 -0.292265
N 2.835875 0.262282 -0.094649
H 3.663912 -0.158196 0.293446
H 2.667213 1.205185 0.234387

E-1cd

SCF = -376.103083419
Num. Imaginary Freq = 0

C 1.539715 0.030325 -0.018270
N 2.678758 0.527748 0.025102

C 0.315946 -0.282338 -0.062111
N -0.821314 -0.797432 -0.130018
N -1.923241 -0.029479 -0.259721
C -1.807267 1.381697 0.024303
H -1.048122 1.827730 -0.618709
H -2.764372 1.860646 -0.174421
H -1.521850 1.563076 1.070281
C -3.128847 -0.694643 0.181646
H -3.994006 -0.208961 -0.269815
H -3.091313 -1.731759 -0.143625
H -3.239672 -0.670599 1.273955
N 3.768090 -0.297959 0.156038
H 4.587792 0.159012 -0.209615
H 3.638204 -1.229530 -0.221255

E-1ce

SCF = -356.634852398
Num. Imaginary Freq = 0

C 0.015094 0.060924 0.005536
N -1.147196 0.505505 0.009972
C 1.259625 -0.162445 0.001965
N 2.433805 -0.561756 -0.005568
O -2.115399 -0.483853 -0.013797
C -3.396016 0.120671 -0.000750
H -4.106254 -0.703673 -0.021404
H -3.538885 0.711480 0.906551
H -3.536854 0.754579 -0.878847
N 3.462861 0.316560 0.079327
H 4.312588 -0.085608 -0.278566
H 3.274091 1.256981 -0.243981

E-1cf

SCF = -679.658412321
Num. Imaginary Freq = 0

C 0.230927 -0.520515 -0.005488
N -0.851399 -1.121826 -0.004178
C 1.405970 -0.051878 -0.003647
N 2.469502 0.600779 -0.002328
S -2.339246 -0.356176 0.003216
C -1.949260 1.395421 0.004195
H -2.906318 1.917694 0.007146
H -1.383940 1.669116 0.894999
H -1.388662 1.670468 -0.889198
N 3.654948 -0.050635 -0.072667
H 4.409069 0.517040 0.274440
H 3.660602 -1.011899 0.245012

E-1cg

SCF = -579.252868505
Num. Imaginary Freq = 0

C -0.565517 0.342705 0.006083
N 0.564885 0.847939 0.010530
C -1.792916 0.049703 0.001248
N -2.905765 -0.529286 -0.003872
C 1.714941 0.016036 -0.000389
F 1.458047 -1.298785 -0.012740

F 2.455978 0.266885 1.078545
F 2.450514 0.288000 -1.078253
N -4.023423 0.170700 0.040764
H -4.859999 -0.349877 -0.146584
H -4.009787 1.168840 -0.114984

E-1ch

SCF = -355.480098802
Num. Imaginary Freq = 0

C -0.183150 -0.340184 -0.013392
N -1.309812 -0.821463 -0.154080
C 1.046670 -0.049458 0.050544
N 2.139439 0.522083 0.286406
N 3.268227 0.013914 -0.181759
H 4.102595 0.407358 0.212285
H 3.288135 -0.930469 -0.540765
C -2.502754 -0.188436 0.221560
O -2.893643 0.849387 -0.224617
H -3.091167 -0.805258 0.919169

E-1ci

SCF = -334.374442581
Num. Imaginary Freq = 0

C -0.234817 0.237142 -0.000311
N -1.374462 0.744458 0.000049
C 0.991463 -0.033861 -0.000624
N 2.114042 -0.605342 -0.000110
C -2.489900 0.012795 0.000116
N -3.511607 -0.520560 0.000223
N 3.216867 0.097706 0.000432
H 4.076430 -0.417690 0.000486
H 3.209215 1.107390 0.000276

E-1cj

SCF = -446.644102503
Num. Imaginary Freq = 0

C -0.178782 -0.355545 -0.097449
N 0.941905 -0.878950 -0.247468
C -1.383604 -0.010184 0.017426
N -2.504756 0.515710 0.181867
N 2.048168 0.066270 -0.007042
O 3.074894 -0.467573 0.295820
O 1.845366 1.240997 -0.166026
N -3.616301 -0.169705 0.037839
H -4.461476 0.369709 0.049347
H -3.609387 -1.096007 -0.363936

E-1ck

SCF = -341.337168625
Num. Imaginary Freq = 0

C 0.660718 0.148026 -0.005589
N 1.793064 0.654764 -0.007719
C -0.575167 -0.129064 -0.002350
N -1.730460 -0.566112 0.004295
N -2.804168 0.230252 -0.067796

F 2.779457 -0.367987 0.010724
H -2.693159 1.195017 0.213029
H -3.644307 -0.229231 0.236628

E-1cl

SCF = -701.724575896
Num. Imaginary Freq = 0

C 0.113426 0.297057 -0.005975
N 1.223543 0.844689 -0.006812
C -1.097943 -0.068080 -0.002705
N -2.221114 -0.600341 0.001316
N -3.337888 0.129582 -0.060447
Cl 2.570573 -0.277563 0.005378
H -3.287745 1.105484 0.199020
H -4.156687 -0.378297 0.223253

E-1dd

SCF = -454.724535881
Num. Imaginary Freq = 0

C 0.606760 0.175880 -0.149151
N 1.723688 0.736107 -0.170857
C -0.606760 -0.175741 -0.149176
N -1.723640 -0.736061 -0.170841
N 2.865232 0.005532 -0.243316
N -2.865237 -0.005576 -0.243310
C -2.784067 1.400235 0.077496
H -2.464898 1.563783 1.117228
H -2.066106 1.889539 -0.580934
H -3.763413 1.852098 -0.071233
C -4.008799 -0.721709 0.276386
H -4.035546 -0.723211 1.374881
H -4.922617 -0.258363 -0.095949
H -3.962711 -1.750666 -0.073281
C 4.008862 0.721625 0.276286
H 4.035634 0.723225 1.374781
H 4.922636 0.258175 -0.096027
H 3.962845 1.750554 -0.073472
C 2.783972 -1.400245 0.077617
H 2.464852 -1.563679 1.117382
H 2.065935 -1.889551 -0.580729
H 3.763275 -1.852195 -0.071130

E-1de

SCF = -435.257645218
Num. Imaginary Freq = 0

C 0.945976 -0.058536 -0.040104
N 2.088940 0.435312 -0.010655
C -0.285495 -0.335912 -0.069117
N -1.442182 -0.802203 -0.119196
O 3.097400 -0.521409 0.031576
C 4.350072 0.133908 0.059049
H 5.094172 -0.659921 0.093136
H 4.495210 0.739271 -0.838819
H 4.441961 0.766078 0.945390
N -2.514570 -0.008137 -0.227092
C -3.750386 -0.637279 0.182777

H	-4.588301	-0.133388	-0.298842
H	-3.729416	-1.677751	-0.132361
H	-3.891470	-0.598820	1.270352
C	-2.356551	1.404832	0.025728
H	-1.598231	1.816938	-0.640930
H	-3.304282	1.905033	-0.163723
H	-2.045856	1.596950	1.061798

E-1df

SCF = -758.281365435
 Num. Imaginary Freq = 0

C	0.677130	0.466207	-0.030558
N	1.751800	1.082679	0.010319
C	-0.490780	-0.013129	-0.065988
N	-1.545130	-0.693756	-0.126310
S	3.248991	0.327076	0.042339
C	2.874500	-1.427776	0.003087
H	3.835744	-1.942064	0.023874
H	2.287244	-1.722031	0.872957
H	2.340963	-1.693558	-0.909515
N	-2.737435	-0.095184	-0.215691
C	-3.851654	-0.936148	0.157207
H	-4.754576	-0.586896	-0.343934
H	-3.636452	-1.953662	-0.160219
H	-4.025272	-0.932479	1.240802
C	-2.833020	1.322067	0.039290
H	-2.165498	1.864639	-0.631120
H	-3.856958	1.644380	-0.139477
H	-2.550753	1.564959	1.072749

E-1dg

SCF = -657.879292636
 Num. Imaginary Freq = 0

C	0.317132	0.250321	0.000213
N	1.436082	0.791837	0.000160
C	-0.888756	-0.099565	0.000353
N	-1.997050	-0.715634	0.000293
C	2.605233	-0.000017	-0.000014
F	2.393698	-1.325703	0.003642
F	3.345202	0.282272	1.075956
F	3.341449	0.276905	-1.080047
N	-3.116453	-0.049370	0.000346
C	-3.126130	1.393680	-0.000056
H	-2.609445	1.776112	-0.885285
H	-4.156069	1.741920	0.001171
H	-2.607244	1.776480	0.883701
C	-4.346828	-0.805941	-0.000392
H	-4.939688	-0.575576	-0.888886
H	-4.092581	-1.862159	-0.001022
H	-4.940074	-0.576738	0.888152

E-1dh

SCF = -434.106724790
 Num. Imaginary Freq = 0

C	1.073895	0.080975	0.000100
N	2.229863	0.557066	0.000081

C	-0.139089	-0.239117	0.000102
N	-1.285950	-0.787243	0.000087
N	-2.357280	-0.048126	0.000151
C	-2.272582	1.393096	-0.000057
H	-1.730000	1.740100	-0.884146
H	-3.277669	1.807363	-0.000284
H	-1.730288	1.740387	0.884092
C	-3.635792	-0.720689	-0.000144
H	-4.211110	-0.450961	-0.888959
H	-3.453057	-1.791549	0.000403
H	-4.211867	-0.450173	0.887930
C	3.299506	-0.359591	-0.000025
H	3.000215	-1.426478	-0.000005
O	4.443963	-0.018577	-0.000140

E-1di

SCF = -413.002248044
 Num. Imaginary Freq = 0

C	1.201159	0.145594	-0.000004
N	2.333892	0.679899	0.000026
C	-0.007262	-0.174175	0.000020
N	-1.130856	-0.771472	0.000001
C	3.460370	-0.030895	0.000020
N	4.491424	-0.547710	-0.000035
N	-2.231771	-0.084907	-0.000004
C	-3.478794	-0.816356	0.000001
H	-4.065057	-0.570638	-0.888269
H	-3.247198	-1.877587	-0.000693
H	-4.064544	-0.571674	0.888905
C	-2.215718	1.359569	-0.000014
H	-1.691602	1.730531	-0.885307
H	-3.239104	1.725888	0.001026
H	-1.689839	1.730386	0.884284

E-1dj

SCF = -525.271668443
 Num. Imaginary Freq = 0

C	-0.737425	0.260066	0.000045
N	-1.847736	0.841803	0.000126
C	0.448815	-0.138837	-0.000019
N	1.569215	-0.725052	-0.000046
N	-2.973971	-0.087214	-0.000008
O	-2.760974	-1.274319	0.000234
O	-4.043420	0.454881	-0.000302
N	2.676923	-0.049108	0.000133
C	3.917752	-0.791378	-0.000165
H	3.677584	-1.850704	-0.000728
H	4.505772	-0.551071	-0.888728
H	4.505699	-0.552001	0.888700
C	2.668812	1.395260	0.000083
H	3.694043	1.756266	0.000035
H	2.146620	1.769622	-0.885110
H	2.146708	1.769719	0.885279

E-1dk

SCF = -419.961621618
 Num. Imaginary Freq = 0

C	1.573820	0.048459	-0.012200
N	2.690530	0.592353	0.021960
C	0.353935	-0.279848	-0.044183
N	-0.788716	-0.772259	-0.095607
N	-1.882958	-0.036387	-0.183053
C	-1.793314	1.390286	0.023869
H	-1.068798	1.818579	-0.670618
H	-2.768419	1.835918	-0.159402
H	-1.472703	1.624912	1.046627
C	-3.117604	-0.724010	0.125192
H	-3.933871	-0.271163	-0.437235
H	-3.013944	-1.765476	-0.168219
H	-3.353166	-0.675931	1.194333
F	3.708653	-0.406901	0.048372

E-1dl

SCF = -780.349353077

Num. Imaginary Freq = 0

C	1.048279	0.215211	-0.016891
N	2.147316	0.790393	0.013795
C	-0.148124	-0.184071	-0.042835
N	-1.263502	-0.755613	-0.086379
N	-2.388238	-0.073039	-0.147789
C	-2.373660	1.359693	0.025659
H	-1.697549	1.813491	-0.701342
H	-3.378733	1.745356	-0.129245
H	-2.028979	1.632928	1.030427
C	-3.598486	-0.821075	0.105802
H	-4.407614	-0.430269	-0.511711
H	-3.417965	-1.861048	-0.153360
H	-3.896048	-0.761993	1.158501
Cl	3.517048	-0.311129	0.024643

E-1ee

SCF = -415.787002817

Num. Imaginary Freq = 0

C	0.625194	0.093709	-0.000048
N	1.797598	0.502936	-0.000031
C	-0.625194	-0.093737	-0.000046
N	-1.797605	-0.502945	-0.000009
O	-2.742099	0.496503	-0.000002
O	2.742106	-0.496500	0.000023
C	-4.037868	-0.082765	0.000036
H	-4.728328	0.757968	0.000046
H	-4.189783	-0.690958	-0.893454
H	-4.189737	-0.690941	0.893545
C	4.037867	0.082787	0.000035
H	4.189729	0.691006	0.893516
H	4.728339	-0.757937	0.000083
H	4.189775	0.690940	-0.893484

E-1ef

SCF = -738.810664985

Num. Imaginary Freq = 0

C	1.079238	-0.013714	0.000014
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N	2.243417	-0.459779	0.000061
C	-0.176654	0.153753	-0.000026
N	-1.359672	0.502431	-0.000067
O	3.208772	0.522992	0.000081
C	4.492515	-0.080203	0.000115
H	5.200662	0.745824	0.000119
H	4.633374	-0.691894	0.893253
H	4.633411	-0.691916	-0.893003
S	-2.620486	-0.609471	-0.000025
C	-3.988768	0.546449	-0.000125
H	-4.894100	-0.061644	-0.000112
H	-3.970000	1.165533	0.894498
H	-3.969957	1.165430	-0.894818

E-1eg

SCF = -638.402441490

Num. Imaginary Freq = 0

C	-1.237451	-0.194004	0.000096
N	-2.348999	0.373408	0.000066
C	0.008929	-0.424478	0.000165
N	1.157523	-0.867851	0.000248
O	-3.406369	-0.476387	-0.000074
C	-4.623915	0.264258	-0.000097
H	-5.412659	-0.484008	-0.000222
H	-4.692703	0.884334	0.894243
H	-4.692573	0.884496	-0.894334
C	2.274694	0.018746	-0.000012
F	1.952517	1.316566	-0.001009
F	3.015392	-0.213082	1.079151
F	3.016056	-0.214570	-1.078388

E-1eh

SCF = -414.630923143

Num. Imaginary Freq = 0

C	-0.445891	-0.184978	0.002102
N	-1.553233	0.331218	-0.255702
C	0.811226	-0.376193	0.034406
N	1.968189	-0.750937	0.170570
O	-2.612504	-0.343109	0.271016
C	-3.824052	0.322613	-0.067885
H	-4.614327	-0.273471	0.382178
H	-3.834298	1.332328	0.344402
H	-3.951169	0.358935	-1.150587
C	3.126926	-0.098674	-0.284595
H	3.597202	-0.638478	-1.121785
O	3.598586	0.865872	0.233678

E-1ei

SCF = -393.522436925

Num. Imaginary Freq = 0

C	0.357522	-0.104254	0.000148
N	1.483154	0.441937	0.000202
C	-0.890674	-0.295505	0.000111
N	-2.051589	-0.730225	0.000027
O	2.519037	-0.423873	-0.000081
C	3.755159	0.289801	-0.000064

H 4.525669 -0.476838 -0.000200
H 3.835557 0.907518 -0.894605
H 3.835653 0.907299 0.894619
C -3.133230 0.052249 -0.000106
N -4.128971 0.631039 -0.000187

E-1ej

SCF = -505.790671097
Num. Imaginary Freq = 0

C -0.957248 -0.319146 0.001383
N -1.958014 -1.064678 0.003995
C 0.211248 0.171097 -0.000343
N 1.244446 0.848503 -0.002806
O -3.185698 -0.522788 0.002032
C -3.249679 0.900314 -0.003322
H -4.310106 1.135498 -0.004782
H -2.768322 1.307433 0.889449
H -2.767516 1.300664 -0.898742
N 2.481314 0.055675 -0.000348
O 2.932137 -0.189585 -1.079750
O 2.934285 -0.179337 1.080452

E-1ek

SCF = -400.486207682
Num. Imaginary Freq = 0

C -0.049592 -0.044815 -0.000006
N 1.111797 -0.471838 -0.000014
C -1.297595 0.171598 -0.000001
N -2.452152 0.621349 0.000001
O 2.085395 0.477698 0.000008
C 3.366001 -0.147306 -0.000006
H 4.080038 0.672663 0.000012
H 3.493029 -0.757793 0.894629
H 3.493028 -0.757754 -0.894668
F -3.386627 -0.433571 0.000015

E-1el

SCF = -760.874663417
Num. Imaginary Freq = 0

C 0.000000 0.492684 0.000000
N 0.646908 1.552947 0.000000
C -0.439134 -0.695845 0.000000
N -1.055550 -1.765177 0.000000
O -0.112604 2.684484 0.000000
C 0.733088 3.830045 0.000000
H 1.357329 3.844878 -0.894299
H 0.057610 4.682269 0.000000
H 1.357329 3.844878 0.894299
Cl -0.045568 -3.183741 0.000000

E-1ff

SCF = -1061.83441433
Num. Imaginary Freq = 0

C 0.543763 0.323310 0.000117
N 1.539835 1.064462 0.000036

C -0.543798 -0.323683 0.000117
N -1.540023 -1.064631 0.000027
S -3.110693 -0.500075 -0.000127
S 3.110616 0.500223 -0.000118
C -2.955170 1.286799 0.000097
H -3.972290 1.679171 -0.000029
H -2.432198 1.631595 0.892163
H -2.431902 1.631791 -0.891720
C 2.955452 -1.286682 0.000105
H 2.432247 -1.631779 -0.891707
H 3.972651 -1.678848 -0.000028
H 2.432557 -1.631587 0.892174

E-1fg

SCF = -961.425042163
Num. Imaginary Freq = 0

C 0.953937 -0.408189 0.000749
N 2.012216 -1.059402 0.000161
C -0.215804 0.076021 0.000187
N -1.261835 0.740007 0.000279
S 3.517896 -0.383596 -0.000283
C 3.229490 1.385920 0.000061
H 4.212993 1.855646 -0.001754
H 2.678745 1.685457 -0.891680
H 2.681879 1.685714 0.893641
C -2.521127 0.068914 -0.000057
F -2.445971 -1.265910 -0.000711
F -3.209875 0.433025 1.079093
F -3.209889 0.434051 -1.078872

E-1fh

SCF = -737.651752208
Num. Imaginary Freq = 0

C -0.226969 -0.508929 0.000325
N -1.319664 -1.105887 -0.000257
C 0.945018 -0.032345 -0.000079
N 2.036716 0.566601 0.000031
S -2.784559 -0.346849 -0.000464
C -2.400029 1.403349 -0.000023
H -3.356390 1.926164 -0.000110
H -1.834942 1.672644 0.892445
H -1.834569 1.673018 -0.892138
C 3.205811 -0.249911 0.000178
H 3.009952 -1.339356 0.000026
O 4.300817 0.214891 0.000797

E-1fi

SCF = -716.545589566
Num. Imaginary Freq = 0

C 0.095834 -0.449106 -0.001025
N 1.162087 -1.093184 -0.000229
C -1.078967 0.009097 -0.000707
N -2.129915 0.683370 -0.000128
S 2.657958 -0.414819 0.000463
C 2.368751 1.353945 0.000012
H 3.351687 1.824734 0.000363

H	1.819655	1.651923	-0.893324
H	1.818858	1.652277	0.892738
C	-3.340914	0.117269	0.000248
N	-4.430136	-0.258624	0.000592

E-1fj

SCF = -828.817343774
 Num. Imaginary Freq = 0

C	0.522980	-0.413474	-0.001816
N	1.567238	-1.073901	-0.005148
C	-0.625882	0.121219	0.000649
N	-1.644842	0.829540	0.003844
S	3.093767	-0.449484	-0.002584
C	2.857774	1.327648	0.006206
H	3.855705	1.766077	0.009406
H	2.321037	1.649240	-0.886326
H	2.319413	1.640067	0.901024
N	-2.896746	0.058821	0.000469
O	-3.353858	-0.183302	1.079432
O	-3.359293	-0.163850	-1.080326

E-1fk

SCF = -723.513386891
 Num. Imaginary Freq = 0

C	-0.270889	-0.504991	-0.000053
N	0.808828	-1.086493	-0.000012
C	-1.449210	-0.028775	-0.000050
N	-2.466861	0.679279	0.000016
F	-3.630128	-0.137605	0.000029
S	2.309596	-0.385539	0.000025
C	1.974938	1.376754	-0.000011
H	2.948718	1.866911	0.000121
H	1.423158	1.666408	-0.894094
H	1.422943	1.666322	0.893970

E-1fl

SCF = -1083.89807724
 Num. Imaginary Freq = 0

C	0.050805	-0.019166	0.000098
N	1.201798	0.421083	0.000092
C	-1.182766	-0.320780	0.000117
N	-2.318405	-0.810213	0.000199
S	2.557161	-0.557059	-0.000024
C	3.814152	0.718956	0.000027
H	4.769839	0.193526	-0.000031
H	3.739078	1.332285	-0.895292
H	3.739124	1.332171	0.895428
Cl	-3.614089	0.382636	-0.000189

E-1gg

SCF = -861.006760060
 Num. Imaginary Freq = 0

C	-0.618267	-0.163504	-0.000487
N	-1.692476	-0.765675	-0.000528
C	0.618267	0.163503	-0.000467

N	1.692476	0.765675	-0.000495
C	2.922644	0.014801	0.000118
C	-2.922644	-0.014801	0.000004
F	-3.615920	-0.345949	-1.080147
F	-2.760463	1.307605	0.000597
F	-3.615651	-0.346971	1.080015
F	3.615964	0.345906	-1.080017
F	3.615607	0.347015	1.080144
F	2.760464	-1.307605	0.000759

E-1gh

SCF = -637.236006537
 Num. Imaginary Freq = 0

C	0.159740	-0.037570	-0.210185
N	-0.913314	-0.472839	-0.636507
C	1.406619	0.205836	-0.039132
N	2.494775	0.624333	0.338732
C	-2.138306	-0.054406	-0.007474
C	3.746979	0.244590	-0.198563
O	4.314126	-0.756406	0.103719
H	4.164603	1.029857	-0.848797
F	-2.896206	0.542705	-0.918175
F	-1.977791	0.788417	1.013059
F	-2.770230	-1.129985	0.442404

E-1gi

SCF = -616.124750066
 Num. Imaginary Freq = 0

C	-1.489569	0.040484	0.000014
N	-2.569353	0.651348	-0.000055
C	-0.243610	-0.238883	0.000057
N	0.845003	-0.814230	0.000124
C	-3.753357	0.025084	-0.000034
N	-4.823040	-0.400549	-0.000024
C	2.058825	-0.035871	0.000010
F	1.863625	1.281731	-0.000265
F	2.756926	-0.351807	1.080124
F	2.757004	-0.352243	-1.079925

E-1gj

SCF = -728.398670046
 Num. Imaginary Freq = 0

C	-1.029678	0.000165	0.184328
N	-2.080986	0.001330	0.831248
C	0.191475	-0.000327	-0.191161
N	1.263494	-0.001392	-0.784698
N	-3.298966	-0.000085	-0.018020
O	-3.732886	-1.082220	-0.269466
O	-3.734154	1.081228	-0.270801
C	2.503166	-0.000047	-0.049827
F	2.349241	0.001899	1.273027
F	3.189661	1.079297	-0.390197
F	3.190182	-1.080061	-0.387009

E-1gk

SCF = -623.098092086

Num. Imaginary Freq = 0

C	1.830694	-0.057027	0.000014
N	2.883461	0.596741	0.000009
C	0.588487	-0.346528	0.000019
N	-0.531473	-0.831492	0.000047
F	3.994905	-0.254994	-0.000016
C	-1.709075	-0.009766	-0.000001
F	-1.452676	1.297805	-0.000030
F	-2.422502	-0.292312	1.079083
F	-2.422455	-0.292368	-1.079101

E-1gl

SCF = -983.484058500

Num. Imaginary Freq = 0

C	1.323238	0.136938	0.000046
N	2.388444	0.760629	0.000060
C	0.109778	-0.250475	0.000042
N	-0.982841	-0.809379	-0.000114
Cl	3.818648	-0.231193	-0.000041
C	-2.195255	-0.037795	-0.000023
F	-2.003498	1.281603	-0.000850
F	-2.896833	-0.352450	1.079608
F	-2.897759	-0.353650	-1.078682

E-1hh

SCF = -413.464947850

Num. Imaginary Freq = 0

C	0.622891	0.150469	-0.043984
N	1.697100	0.642630	-0.378827
C	-0.622851	-0.150534	0.043762
N	-1.697063	-0.642632	0.378685
C	2.945437	0.340022	0.207158
O	3.583688	-0.627876	-0.064301
H	3.293791	1.152423	0.865271
C	-2.945451	-0.339951	-0.207136
O	-3.583736	0.627850	0.064592
H	-3.293818	-1.152228	-0.865398

E-1hi

SCF = -392.354435972

Num. Imaginary Freq = 0

C	-0.712161	0.008327	0.106201
N	-1.782617	0.569182	0.399151
C	0.543029	-0.240238	0.043467
N	1.638509	-0.738648	-0.186082
C	-2.968941	0.102316	-0.014020
N	-4.039748	-0.203588	-0.306227
C	2.883371	-0.209069	0.233602
O	3.439064	0.677877	-0.330079
H	3.302689	-0.779644	1.077246

E-1hj

SCF = -504.628861861

Num. Imaginary Freq = 0

C	-0.252192	-0.053036	0.195338
N	-1.290768	0.144112	0.836760
C	0.985613	-0.200814	-0.104817
N	2.068884	-0.395261	-0.627558
N	-2.517920	0.060610	0.009653
O	-3.016601	-1.023041	-0.045031
O	-2.901094	1.102228	-0.429035
C	3.337885	-0.328271	0.001058
O	3.918901	0.690653	0.188317
H	3.741141	-1.332215	0.204535

E-1hk

SCF = -399.328705566

Num. Imaginary Freq = 0

C	-1.131976	-0.048894	0.021082
N	-2.164519	0.546114	0.362052
C	0.123960	-0.297963	-0.033468
N	1.251227	-0.709027	-0.204853
F	-3.297176	-0.065449	-0.206236
C	2.473358	-0.183622	0.278772
H	2.846659	-0.756890	1.140654
O	3.053615	0.708649	-0.247905

E-1hl

SCF = -759.713663248

Num. Imaginary Freq = 0

C	-0.554612	0.119057	0.162622
N	-1.615993	0.699496	0.409348
C	0.663665	-0.246300	0.054880
N	1.763082	-0.745886	-0.120964
Cl	-3.048528	-0.122606	-0.171945
C	3.012573	-0.198696	0.251460
H	3.426519	-0.701040	1.139623
O	3.579886	0.633212	-0.381129

E-1ii

SCF = -371.242742022

Num. Imaginary Freq = 0

C	-0.623904	0.126350	-0.000038
N	-1.715743	0.715961	-0.000070
C	0.623904	-0.126347	-0.000014
N	1.715742	-0.715960	0.000001
C	-2.888111	0.071873	-0.000048
N	-3.950044	-0.373135	-0.000027
C	2.888111	-0.071873	0.000065
N	3.950045	0.373132	0.000125

E-1ij

SCF = -483.516007604

Num. Imaginary Freq = 0

C	0.162583	0.000457	0.252983
N	1.226031	0.001497	0.881847
C	-1.064100	-0.000127	-0.090876
N	-2.140088	-0.001229	-0.695197
N	2.428633	-0.000034	0.011450

O 2.856973 1.081561 -0.248685
O 2.856048 -1.082510 -0.246448
C -3.335627 -0.000109 -0.096451
N -4.411906 0.000662 0.311490

E-1ik

SCF = -378.215665547
Num. Imaginary Freq = 0

C -1.045518 0.034624 -0.000027
N -2.113007 0.669309 -0.000080
C 0.199258 -0.222115 -0.000005
N 1.327285 -0.708088 0.000025
F -3.203253 -0.197281 0.000051
C 2.471678 -0.022030 0.000012
N 3.510974 0.472015 0.000007

E-1il

SCF = -738.602233822
Num. Imaginary Freq = 0

C -0.474557 0.199047 0.000020
N -1.550321 0.809515 0.000037
C 0.747049 -0.146687 0.000023
N 1.846195 -0.712299 0.000027
Cl -2.962237 -0.190795 -0.000054
C 3.017680 -0.068514 0.000019
N 4.077983 0.379988 0.000014

E-1jj

SCF = -595.788372565
Num. Imaginary Freq = 0

C -0.596062 0.000179 0.226374
N -1.643526 0.000196 0.871903
C 0.596061 0.000182 -0.226364
N 1.643521 0.000207 -0.871899
N -2.870620 -0.000051 0.030790
O -3.303018 -1.082124 -0.216667
O -3.303223 1.081863 -0.216990
N 2.870620 -0.000052 -0.030791
O 3.303014 -1.082129 0.216656
O 3.303232 1.081858 0.216990

E-1jk

SCF = -490.485719996
Num. Imaginary Freq = 0

C 1.428941 -0.000145 -0.030257
N 2.481092 0.002833 -0.682470
C 0.217309 -0.001799 0.356662
N -0.878740 -0.003743 0.908826
F 3.590624 -0.000865 0.158715
N -2.035166 0.000268 -0.020720
O -2.448968 -1.080026 -0.304515
O -2.446459 1.083019 -0.298774

E-1jl

SCF = -850.874137022

Num. Imaginary Freq = 0

C 0.901949 -0.000241 -0.160094
N 1.956400 -0.001646 -0.796261
C -0.291466 0.000536 0.282309
N -1.362433 0.001836 0.890832
Cl 3.400348 0.000390 0.152645
N -2.555749 -0.000027 0.010612
O -2.982993 -1.081913 -0.252578
O -2.984050 1.080721 -0.255490

E-1kk

SCF = -385.179640748
Num. Imaginary Freq = 0

C -0.618967 -0.137990 -0.000188
N -1.748871 -0.640590 -0.000136
C 0.618966 0.138026 -0.000126
N 1.748887 0.640592 0.000094
F 2.734775 -0.339457 0.000161
F -2.734787 0.339431 0.000080

E-1kl

SCF = -745.570464925
Num. Imaginary Freq = 0

C 1.139344 -0.077942 0.000015
N 2.224713 -0.672684 0.000027
C -0.081680 0.275816 0.000017
N -1.187732 0.810209 0.000020
F 3.289470 0.236567 -0.000032
Cl -2.541770 -0.251707 -0.000014

E-1ll

SCF = -1105.95870893
Num. Imaginary Freq = 0

C -0.598160 -0.216336 0.000057
N -1.675035 -0.813974 0.000011
C 0.598169 0.216491 0.000082
N 1.675099 0.814028 0.000125
Cl -3.085533 0.196730 -0.000027
Cl 3.085504 -0.196807 -0.000078

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Z-1aa

SCF = -186.808172038
Num. Imaginary Freq = 0

C -0.637944 0.004568 -0.000017
N -1.869406 -0.115498 0.000000
C 0.637909 0.004042 -0.000022
N 1.869501 -0.115388 0.000029
H 2.357298 0.782489 -0.000061
H -2.357755 0.782057 0.000092

Z-1ab

SCF = -226.119871557
Num. Imaginary Freq = 0

C	-0.043821	-0.322850	-0.000113
N	1.151592	-0.619607	0.000076
C	-1.278406	0.003990	-0.000169
N	-2.513673	0.092611	0.000137
H	-2.841881	1.059462	-0.000009
C	2.163076	0.423706	0.000000
H	2.795597	0.283120	-0.877790
H	1.741619	1.432814	-0.001076
H	2.794135	0.284498	0.879077

Z-1ac

SCF = -242.148919007
Num. Imaginary Freq = 0

C	0.021418	-0.167259	0.004641
N	-1.171117	-0.550635	0.007690
C	1.282412	-0.037348	0.001955
N	2.514557	0.044472	0.003349
H	2.869128	0.998619	-0.019922
N	-2.157810	0.352946	-0.071526
H	-3.046358	-0.008856	0.226476
H	-1.945168	1.310401	0.177280

Z-1ad

SCF = -320.772570670
Num. Imaginary Freq = 0

C	0.898283	-0.352509	-0.024857
N	-0.275800	-0.816243	-0.075709
C	2.148652	-0.167508	0.011719
N	3.377914	-0.026036	0.051628
H	3.683380	0.944647	0.062079
N	-1.313051	0.000487	-0.156024
C	-2.602248	-0.595216	0.104311
H	-2.895900	-0.484675	1.154676
H	-3.361081	-0.126145	-0.523233
H	-2.541719	-1.653892	-0.134766
C	-1.135629	1.421905	0.004490
H	-2.091302	1.917776	-0.151883
H	-0.757974	1.664298	1.005953
H	-0.413185	1.790501	-0.726071

Z-1ae

SCF = -301.302097384
Num. Imaginary Freq = 0

C	-0.656009	-0.145753	0.000235
N	0.532587	-0.522858	0.000181
C	-1.921641	-0.033907	0.000092
N	-3.149133	0.023053	-0.000275
H	-3.530519	0.967379	-0.000296
O	1.436683	0.509803	0.000293
C	2.756681	-0.014876	-0.000328
H	2.932837	-0.615662	-0.894099
H	3.412781	0.852787	0.000273
H	2.933073	-0.617074	0.892438

Z-1af

SCF = -624.322063722
Num. Imaginary Freq = 0

C	-0.799694	-0.597751	-0.000058
N	0.316599	-1.144133	-0.000097
C	-1.956783	-0.073459	-0.000175
N	-3.144255	0.275455	0.000021
H	-3.270864	1.287278	0.000141
S	1.758452	-0.313179	0.000095
C	1.298244	1.419248	0.000035
H	0.723036	1.667386	0.892282
H	2.232207	1.981322	0.000213
H	0.723374	1.667392	-0.892430

Z-1ag

SCF = -523.908955747
Num. Imaginary Freq = 0

C	-1.093197	-0.479932	-0.000116
N	0.063683	-0.915563	0.000093
C	-2.314591	-0.117561	0.000044
N	-3.525110	0.111035	0.000031
H	-3.752651	1.106836	-0.000159
C	1.160296	0.012862	0.000025
F	1.901640	-0.203713	-1.080060
F	1.901856	-0.203887	1.079862
F	0.804015	1.300117	0.000152

Z-1ah

SCF = -300.136945591
Num. Imaginary Freq = 0

C	0.472861	-0.404839	-0.118595
N	-0.682082	-0.819731	-0.223252
C	1.670756	0.015449	0.004919
N	2.877968	0.273610	0.015750
H	3.105051	1.117630	0.544563
C	-1.812529	-0.157732	0.298306
O	-2.273916	0.839120	-0.165501
H	-2.271451	-0.725008	1.124186

Z-1ai

SCF = -279.027737676
Num. Imaginary Freq = 0

C	-0.423670	-0.297564	-0.000134
N	0.728457	-0.771685	0.000121
C	-1.657242	0.007860	-0.000239
N	-2.867525	0.237258	0.000164
H	-3.099475	1.231926	0.000107
C	1.813391	0.017094	0.000017
N	2.811154	0.592103	0.000005

Z-1aj

SCF = -391.302844510
Num. Imaginary Freq = 0

C -0.779639 -0.001020 0.420435
N 0.341182 -0.002057 0.943608
C -1.987832 -0.000231 0.010406
N -3.176524 0.000415 -0.285026
H -3.370531 0.002602 -1.286597
N 1.448647 0.000198 -0.043632
O 1.854302 1.081855 -0.348710
O 1.855976 -1.079978 -0.351678

Z-1ak

SCF = -286.002613082
Num. Imaginary Freq = 0

C -0.027303 -0.194906 0.000062
N -1.189419 -0.617265 -0.000094
C 1.239007 -0.028123 0.000112
N 2.453919 0.062347 -0.000020
H 2.838625 1.004858 -0.000358
F -2.106706 0.468638 0.000013

Z-1al

SCF = -646.387078108
Num. Imaginary Freq = 0

C -0.508839 0.415670 -0.000268
N 0.634516 0.877558 0.000129
C -1.718366 0.005998 -0.000049
N -2.920131 -0.231324 0.000133
H -3.164461 -1.221151 -0.000136
Cl 1.913353 -0.343088 0.000012

Z-1bb

SCF = -265.430904481
Num. Imaginary Freq = 0

C -0.637221 -0.458934 0.000079
N -1.866154 -0.555569 0.000002
C 0.637940 -0.461157 -0.000090
N 1.866946 -0.555925 0.000020
C -2.688817 0.642299 -0.000002
H -3.335121 0.612544 -0.878647
H -3.335424 0.612376 0.878399
H -2.105013 1.567260 0.000144
C 2.687881 0.643203 0.000012
H 3.334140 0.614373 -0.878679
H 2.102590 1.567218 0.000261
H 3.334594 0.614220 0.878376

Z-1bc

SCF = -281.458605972
Num. Imaginary Freq = 0

C 0.627321 -0.464501 0.006075
N 1.849489 -0.569006 0.010317
C -0.634750 -0.300446 0.003674
N -1.871177 -0.492684 0.000052
C 2.707804 0.601724 -0.005795
H 3.351829 0.573407 0.874408

H 3.352613 0.548362 -0.884253
H 2.146723 1.541126 -0.019911
N -2.704835 0.563664 -0.075693
H -3.629953 0.341284 0.248598
H -2.337798 1.461344 0.214700

Z-1bd

SCF = -360.081520940
Num. Imaginary Freq = 0

C 1.551909 -0.615390 0.000076
N 2.780879 -0.613846 0.039500
C 0.284006 -0.566174 -0.036555
N -0.935966 -0.879762 -0.086464
C 3.525279 0.632343 0.035914
H 4.144107 0.674670 0.933909
H 4.197669 0.637841 -0.823718
H 2.879767 1.515765 -0.002058
N -1.868978 0.063274 -0.193016
C -3.205970 -0.365231 0.145556
H -3.416354 -0.244652 1.215454
H -3.933149 0.215925 -0.422390
H -3.304128 -1.416242 -0.114885
C -1.512564 1.448315 -0.011676
H -2.391086 2.065474 -0.189244
H -1.134625 1.635398 1.002407
H -0.729704 1.724980 -0.719507

Z-1be

SCF = -340.612600993
Num. Imaginary Freq = 0

C 1.273354 -0.452963 0.000074
N 2.492216 -0.536702 -0.000112
C 0.005222 -0.326164 0.000157
N -1.217114 -0.572930 -0.000025
C 3.344091 0.639478 -0.000012
H 3.987848 0.596514 0.879203
H 3.987340 0.597032 -0.879645
H 2.778278 1.574616 0.000379
O -2.003898 0.557137 0.000070
C -3.371196 0.178423 -0.000082
H -3.930918 1.111419 -0.000241
H -3.612833 -0.401037 -0.893038
H -3.613072 -0.400867 0.892923

Z-1bf

SCF = -663.632539959
Num. Imaginary Freq = 0

C 1.402068 -0.662232 -0.000002
N 2.627043 -0.534692 -0.000060
C 0.149517 -0.874314 0.000006
N -1.050984 -1.193257 0.000002
C 3.227681 0.787546 0.000028
H 3.868921 0.874554 -0.878528
H 2.491402 1.596810 -0.000108
H 3.868535 0.874550 0.878875
S -2.301449 -0.088066 0.000018

C -1.504137 1.517437 -0.000023
H -2.307243 2.254571 0.000037
H -0.890703 1.646817 0.892020
H -0.890916 1.646765 -0.892228

Z-1bf

SCF = -563.221856465
Num. Imaginary Freq = 0

C -1.783613 -0.629964 -0.000042
N -3.008660 -0.552712 0.000005
C -0.512964 -0.716808 -0.000001
N 0.693109 -0.995640 -0.000033
C -3.671477 0.739539 0.000020
H -4.316742 0.784324 -0.878248
H -4.316893 0.784245 0.878170
H -2.975122 1.581191 0.000091
C 1.652246 0.068882 0.000007
F 2.419602 -0.043187 1.079629
F 1.128959 1.299363 0.000132
F 2.419490 -0.042975 -1.079730

Z-1bh

SCF = -339.449375892
Num. Imaginary Freq = 0

C -1.065852 -0.515652 -0.122062
N -2.290772 -0.445113 -0.206276
C 0.200773 -0.632543 -0.056383
N 1.410376 -0.870902 -0.019322
C -2.986701 0.770561 0.178043
H -3.555818 1.118018 -0.685302
H -3.705824 0.514424 0.957363
H -2.316869 1.559801 0.527910
C 2.387418 0.072903 0.348030
O 2.704291 1.006904 -0.324135
H 2.893120 -0.206986 1.286539

Z-1bi

SCF = -318.341352015
Num. Imaginary Freq = 0

C 1.027652 -0.518061 0.000085
N 2.253910 -0.469781 -0.000196
C -0.244660 -0.514325 0.000153
N -1.458278 -0.804548 -0.000041
C 2.955530 0.800421 0.000008
H 3.602862 0.823796 -0.877597
H 2.285135 1.662694 -0.000356
H 3.601859 0.823964 0.878396
C -2.403154 0.146734 0.000039
N -3.295927 0.874462 -0.000070

Z-1bj

SCF = -430.615942594
Num. Imaginary Freq = 0

C -1.427530 -0.556220 -0.004753
N -2.643108 -0.461132 -0.003776

C -0.153041 -0.642662 -0.005829
N 1.034501 -0.995286 -0.009334
C -3.324960 0.820485 0.008088
H -3.969632 0.863577 -0.870054
H -3.968520 0.847869 0.887681
H -2.639055 1.670018 0.015274
N 1.978933 0.140268 0.000966
O 2.341646 0.493815 1.084496
O 2.335618 0.518931 -1.076113

Z-1bk

SCF = -325.314784333
Num. Imaginary Freq = 0

C -0.584922 -0.423903 -0.000123
N -1.790066 -0.543435 0.000163
C 0.688176 -0.275570 -0.000321
N 1.896719 -0.541475 0.000150
C -2.728047 0.563418 0.000005
H -3.364248 0.465942 -0.879448
H -3.363715 0.466536 0.879924
H -2.233337 1.536522 -0.000457
F 2.662609 0.660189 0.000048

Z-1bl

SCF = -685.699093124
Num. Imaginary Freq = 0

C -1.113961 -0.514667 0.000125
N -2.333303 -0.484494 0.000006
C 0.156251 -0.645911 -0.000040
N 1.361809 -0.905313 -0.000079
C -3.084179 0.758488 -0.000017
H -3.728736 0.761599 -0.879412
H -3.729645 0.760734 0.878575
H -2.446688 1.644982 0.000650
Cl 2.409227 0.527875 0.000017

Z-1cc

SCF = -297.480497413
Num. Imaginary Freq = 0

C 0.632220 -0.402184 0.002863
N 1.869517 -0.516800 0.011490
C -0.632187 -0.401952 -0.003060
N -1.869522 -0.516882 -0.011403
N -2.654921 0.598227 -0.082114
H -3.571979 0.402766 0.284537
H -2.239920 1.439961 0.299930
N 2.654848 0.598249 0.082171
H 3.572145 0.402668 -0.283845
H 2.240105 1.439866 -0.300451

Z-1cd

SCF = -376.102269012
Num. Imaginary Freq = 0

C -0.282234 -0.653797 0.050688
N 0.939699 -0.910345 0.115939

C	-1.541519	-0.570040	-0.001735
N	-2.782641	-0.560263	-0.065077
N	-3.444794	0.642405	-0.124577
H	-4.386915	0.527356	0.213273
H	-2.960674	1.408715	0.329560
N	1.854895	0.069755	0.258415
C	3.175089	-0.322714	-0.182822
H	3.284259	-0.256734	-1.273379
H	3.918685	0.322753	0.284806
H	3.350309	-1.350987	0.124722
C	1.448044	1.429743	0.001453
H	2.293486	2.090474	0.183936
H	1.100902	1.562107	-1.033386
H	0.633558	1.706300	0.672059

Z-1ce

SCF = -356.634913907
 Num. Imaginary Freq = 0

C	-0.012671	-0.448266	0.003516
N	1.217607	-0.631280	0.011874
C	-1.275653	-0.412416	0.002039
N	-2.514290	-0.470955	0.003591
N	-3.259643	0.657041	-0.084005
H	-4.188836	0.507285	0.270802
H	-2.816563	1.509111	0.236237
O	1.949585	0.545466	-0.006056
C	3.330713	0.230843	-0.001605
H	3.846842	1.188930	-0.016078
H	3.601117	-0.323598	0.899503
H	3.600712	-0.350066	-0.885941

Z-1cf

SCF = -679.657544530
 Num. Imaginary Freq = 0

C	-0.168301	-0.874621	0.002856
N	1.026276	-1.195008	0.006429
C	-1.395237	-0.564141	0.000620
N	-2.639724	-0.475233	-0.006588
N	-3.224345	0.745019	-0.073145
H	-4.172224	0.717049	0.262430
H	-2.675554	1.525295	0.266412
S	2.298578	-0.107791	0.004215
C	1.524255	1.509214	-0.010492
H	2.340870	2.231522	-0.023118
H	0.910227	1.641461	-0.901798
H	0.919679	1.663167	0.883861

Z-1cg

SCF = -579.252849943
 Num. Imaginary Freq = 0

C	0.524347	-0.737886	-0.004469
N	-0.686939	-0.996435	-0.008659
C	1.764414	-0.523893	-0.003950
N	3.018284	-0.486375	-0.003148
N	3.650733	0.669489	0.042074
H	4.637691	0.625979	-0.130510

H	3.150325	1.534970	-0.104848
C	-1.640279	0.053982	0.000023
F	-2.423092	-0.044386	-1.073790
F	-1.117916	1.290645	-0.001138
F	-2.409376	-0.048583	1.083136

Z-1ch

SCF = -355.480646832
 Num. Imaginary Freq = 0

C	0.240473	-0.706519	0.061807
N	1.454733	-0.950401	0.023794
C	-0.992780	-0.450613	0.059651
N	-2.244902	-0.409318	0.154606
N	-2.894638	0.688266	-0.188507
H	-3.857637	0.715934	0.091525
H	-2.390031	1.554035	-0.322873
C	2.394418	0.062835	-0.238428
O	2.372734	1.161170	0.236621
H	3.206773	-0.293377	-0.889050

Z-1ci

SCF = -334.374416298
 Num. Imaginary Freq = 0

C	0.235104	-0.583740	0.000284
N	1.459052	-0.830343	-0.000556
C	-1.004851	-0.410882	0.001149
N	-2.264170	-0.395944	-0.000377
N	-2.914032	0.738559	-0.000009
H	-3.914762	0.682114	-0.001832
H	-2.436577	1.628676	0.000267
C	2.379508	0.134934	-0.000174
N	3.246690	0.894491	0.000088

Z-1cj

SCF = -446.645214230
 Num. Imaginary Freq = 0

C	-0.133046	-0.766201	-0.017473
N	1.087041	-1.021148	-0.029056
C	-1.371919	-0.558111	-0.007469
N	-2.619544	-0.477694	-0.003839
N	-3.225953	0.683369	0.052948
H	-4.221860	0.665343	-0.059749
H	-2.710599	1.548378	-0.025347
N	1.921036	0.202236	-0.001313
O	1.385474	1.279895	-0.047402
O	3.092550	-0.026794	0.060347

Z-1ck

SCF = -341.337197390
 Num. Imaginary Freq = 0

C	0.680980	-0.407893	0.002349
N	1.911751	-0.558564	0.010000
C	-0.584825	-0.396105	0.001453
N	-1.815938	-0.496424	0.003731
N	-2.626834	0.565229	-0.071776

H -3.562575 0.357902 0.229894
H -2.252305 1.462783 0.204771
F 2.550566 0.714623 -0.005684

Z-1cl

SCF = -701.724577652
Num. Imaginary Freq = 0

C 0.140314 -0.639352 0.003042
N 1.348699 -0.904970 0.008947
C -1.110568 -0.451105 0.001637
N -2.353232 -0.430450 0.001570
N -3.030976 0.717248 -0.065422
H -3.991563 0.626251 0.213294
H -2.553962 1.572053 0.187836
Cl 2.389154 0.510096 -0.002639

Z-1dd

SCF = -454.724026058
Num. Imaginary Freq = 0

C 0.629635 -0.876601 0.043462
N 1.867122 -0.998491 0.161576
C -0.629483 -0.876548 -0.043176
N -1.866970 -0.998446 -0.161410
N -2.665577 0.092436 -0.292123
N 2.665653 0.092486 0.292226
C 4.025622 -0.173211 -0.122957
H 4.134960 -0.171769 -1.216161
H 4.684892 0.586437 0.297373
H 4.319012 -1.149558 0.255941
C 2.117630 1.373886 -0.083903
H 2.863510 2.144408 0.103645
H 1.831607 1.399584 -1.146117
H 1.231930 1.588740 0.514827
C -2.117812 1.373933 0.084041
H -2.863638 2.144390 -0.104048
H -1.832347 1.399876 1.146390
H -1.231838 1.588702 -0.514303
C -4.025675 -0.173347 0.122470
H -4.135503 -0.171875 1.215618
H -4.684869 0.586221 -0.298150
H -4.318817 -1.149719 -0.256517

Z-1de

SCF = -435.257854684
Num. Imaginary Freq = 0

C -0.932087 -0.679352 0.008857
N -2.174887 -0.738644 -0.032596
C 0.327840 -0.731295 0.041314
N 1.562079 -0.912438 0.090220
N 2.416132 0.107773 0.226576
C 1.930266 1.451646 0.021830
H 2.737836 2.152318 0.224236
H 1.570650 1.598283 -1.005842
H 1.103252 1.654534 0.703295
C 3.768384 -0.200571 -0.181784
H 3.905629 -0.095002 -1.265311

H 4.460720 0.469637 0.327594
H 3.989267 -1.226716 0.102150
O -2.779419 0.516492 0.001689
C -4.183064 0.349147 -0.044189
H -4.598502 1.355034 -0.016395
H -4.487402 -0.152279 -0.965775
H -4.537398 -0.222035 0.816969

Z-1df

SCF = -758.280679780
Num. Imaginary Freq = 0

C 0.742908 -1.075816 -0.008832
N 1.968064 -1.245555 0.043085
C -0.509047 -0.907130 -0.052172
N -1.760483 -0.995904 -0.111785
N -2.520888 0.099296 -0.219206
C -1.931715 1.391146 0.036532
H -2.674777 2.162929 -0.154513
H -1.581374 1.474858 1.074744
H -1.078830 1.546580 -0.625043
C -3.902906 -0.104618 0.152475
H -4.055748 -0.010306 1.235044
H -4.528176 0.629269 -0.356247
H -4.198283 -1.103912 -0.157768
S 3.090186 0.001408 0.057356
C 2.111391 1.500847 -0.067986
H 2.821938 2.327292 -0.037354
H 1.563447 1.530827 -1.010024
H 1.418181 1.588506 0.768711

Z-1dg

SCF = -657.879893840
Num. Imaginary Freq = 0

C -0.353067 -0.988791 0.000075
N -1.592146 -1.100256 -0.000091
C 0.897727 -0.926097 0.000142
N 2.163469 -0.999454 0.000104
N 2.878031 0.089608 0.000247
C 2.253989 1.391061 0.000167
H 3.027574 2.154850 0.000975
H 1.619752 1.508099 -0.883459
H 1.618505 1.507492 0.882961
C 4.315579 -0.051551 -0.000325
H 4.747189 0.414722 -0.889218
H 4.747915 0.415540 0.887772
H 4.549803 -1.112379 0.000059
C -2.396166 0.058806 -0.000091
F -3.184355 0.070952 -1.077803
F -1.716474 1.222629 -0.000222
F -3.184125 0.071067 1.077945

Z-1dh

SCF = -434.108250370
Num. Imaginary Freq = 0

C 1.184958 -0.993039 0.000450
N 2.441420 -0.997323 -0.000366

C	-0.061364	-1.000754	0.000089
N	-1.335520	-1.038766	0.000357
N	-1.991642	0.082516	-0.000069
C	-1.304484	1.353737	-0.000620
H	-2.041588	2.152586	-0.000371
H	-0.658019	1.436485	0.877673
H	-0.658933	1.436220	-0.879625
C	-3.434833	0.014626	0.000056
H	-3.839688	0.504856	0.888384
H	-3.839802	0.504960	-0.888154
H	-3.723286	-1.032703	0.000019
C	3.063795	0.263556	-0.000711
O	2.514252	1.334055	0.001249
H	4.159075	0.171415	-0.002950

Z-1di

SCF = -413.002682712
 Num. Imaginary Freq = 0

C	-1.172197	-0.822619	0.000010
N	-2.423340	-0.910689	0.000201
C	0.074381	-0.802677	-0.000299
N	1.340762	-0.927671	-0.000651
N	2.097103	0.126139	-0.001509
C	-3.193746	0.176126	0.000184
N	-3.936827	1.058663	0.000399
C	1.534109	1.456465	-0.000399
H	0.905085	1.600940	-0.883302
H	0.908622	1.601207	0.885036
H	2.342520	2.182901	-0.002133
C	3.528749	-0.076083	0.001372
H	3.978993	0.378188	-0.883969
H	3.974752	0.369991	0.893112
H	3.718367	-1.145591	-0.003032

Z-1dj

SCF = -525.274248313
 Num. Imaginary Freq = 0

C	-0.761023	-1.021118	-0.000255
N	-2.013991	-1.091084	0.000009
C	0.486515	-0.987544	-0.000486
N	1.752518	-1.018101	-0.000128
N	2.424072	0.091027	-0.000179
C	1.746659	1.368112	-0.000270
H	2.488325	2.162472	-0.000098
H	1.104295	1.454987	-0.881247
H	1.103881	1.454950	0.880402
C	3.867321	0.005962	0.000613
H	4.277085	0.491568	-0.887676
H	4.276132	0.491502	0.889385
H	4.144852	-1.044216	0.000729
N	-2.634285	0.227692	0.000131
O	-1.934298	1.215320	-0.000265
O	-3.831902	0.200871	0.000523

Z-1dk

SCF = -419.961902811
 Num. Imaginary Freq = 0

C	-1.576616	-0.579233	-0.007650
N	-2.818204	-0.591094	-0.039478
C	-0.317870	-0.673906	0.025767
N	0.906061	-0.900647	0.074276
N	1.806454	0.059316	0.178556
C	1.398528	1.434201	0.008439
H	2.251518	2.081739	0.197951
H	1.022243	1.614614	-1.006218
H	0.602771	1.673533	0.715862
C	3.166561	-0.326905	-0.125423
H	3.396333	-0.198792	-1.189060
H	3.855366	0.281250	0.460622
H	3.294951	-1.372731	0.141450
F	-3.300775	0.758046	-0.024542

Z-1dl

SCF = -780.349745016
 Num. Imaginary Freq = 0

C	-1.060297	-0.859299	0.000335
N	-2.295655	-0.969126	-0.026990
C	0.199585	-0.814124	0.023189
N	1.447687	-0.936601	0.056626
N	2.237931	0.111917	0.138379
C	1.689874	1.441350	0.018475
H	2.485237	2.167438	0.169567
H	1.237929	1.593882	-0.969114
H	0.913957	1.592357	0.771923
C	3.641930	-0.124610	-0.107945
H	3.908208	0.083173	-1.149909
H	4.242084	0.511928	0.542876
H	3.855984	-1.167338	0.111407
Cl	-3.129393	0.583254	-0.015128

Z-1ee

SCF = -415.786812456
 Num. Imaginary Freq = 0

C	0.631661	-0.462866	-0.000069
N	1.864781	-0.607114	-0.000096
C	-0.631680	-0.462982	0.000037
N	-1.864845	-0.607237	0.000123
O	2.570773	0.573122	-0.000166
C	3.961277	0.288197	0.000122
H	4.453152	1.258576	-0.000908
H	4.241327	-0.271655	0.894212
H	4.241293	-0.273549	-0.892777
O	-2.570726	0.573054	0.000177
C	-3.961248	0.288298	-0.000131
H	-4.241328	-0.273580	0.892667
H	-4.453026	1.258726	0.001093
H	-4.241410	-0.271350	-0.894319

Z-1ef

SCF = -738.812035524
 Num. Imaginary Freq = 0

C	-0.450545	-0.938480	-0.000358
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N	-1.662560	-1.165946	0.000306
C	0.796087	-0.717037	-0.000156
N	2.042075	-0.727317	-0.000196
S	-2.849616	0.005199	0.000509
C	-1.952545	1.557575	0.000322
H	-2.711118	2.340655	0.000387
H	-1.332785	1.650985	0.892136
H	-1.332989	1.650881	-0.891641
O	2.597847	0.537455	-0.000416
C	4.011777	0.426414	-0.000577
H	4.359643	-0.096260	-0.893595
H	4.383246	1.449181	-0.000618
H	4.359829	-0.096256	0.892366

Z-1eg

SCF = -638.402064671
 Num. Imaginary Freq = 0

C	-1.195325	0.582134	0.001529
N	-2.440677	0.661011	-0.001854
C	0.052796	0.788660	0.002705
N	1.266507	0.992958	-0.004554
C	2.190530	-0.094788	-0.000519
F	2.963514	-0.004487	1.077189
F	2.960880	-0.014039	-1.080716
F	1.623722	-1.304566	0.005545
O	-3.073637	-0.539272	0.003071
C	-4.485228	-0.343870	-0.001874
H	-4.911369	-1.344038	0.002545
H	-4.797454	0.202707	0.888501
H	-4.792576	0.192733	-0.899971

Z-1eh

SCF = -414.630652474
 Num. Imaginary Freq = 0

C	-0.833161	-0.647999	-0.077820
N	-2.044218	-0.828386	-0.048582
C	0.420072	-0.455230	-0.080309
N	1.657750	-0.552105	-0.208942
O	2.344965	0.545354	0.213815
C	3.740709	0.344461	0.019815
H	3.963188	0.200120	-1.038121
H	4.214025	1.254332	0.381067
H	4.087771	-0.514069	0.596147
C	-3.016814	0.107704	0.348179
O	-3.334182	1.057092	-0.299066
H	-3.510807	-0.190131	1.286392

Z-1ei

SCF = -393.521978528
 Num. Imaginary Freq = 0

C	-0.896726	-0.596711	0.000014
N	-2.123029	-0.782681	-0.000004
C	0.357256	-0.490792	0.000032
N	1.603743	-0.591424	-0.000004
C	-3.018368	0.207934	-0.000026
N	-3.871083	0.982151	-0.000032

O	2.255485	0.591763	0.000180
C	3.666420	0.376069	-0.000120
H	3.965746	-0.169750	-0.894915
H	4.105396	1.370407	-0.000019
H	3.966076	-0.170071	0.894368

Z-1ej

SCF = -505.792320407
 Num. Imaginary Freq = 0

C	-0.460786	0.767646	0.006578
N	-1.673936	1.002085	0.008698
C	0.792095	0.598202	0.004872
N	2.035164	0.625796	0.004897
N	-2.515289	-0.203201	-0.001298
O	-2.836473	-0.610498	1.075603
O	-2.845818	-0.585305	-1.084541
O	2.631835	-0.590132	-0.005514
C	4.050133	-0.436682	-0.004383
H	4.374925	0.087094	0.894868
H	4.443821	-1.449883	-0.013165
H	4.374676	0.102514	-0.894566

Z-1ek

SCF = -400.485982751
 Num. Imaginary Freq = 0

C	1.314959	-0.388153	-0.000010
N	2.546964	-0.517133	0.000008
C	0.049407	-0.410975	0.000021
N	-1.174849	-0.590314	-0.000047
F	3.171308	0.746881	0.000024
O	-1.933449	0.538861	-0.000108
C	-3.315027	0.189759	0.000083
H	-3.845716	1.138734	-0.000925
H	-3.564556	-0.382503	-0.893983
H	-3.564741	-0.380699	0.895260

Z-1el

SCF = -760.874471030
 Num. Imaginary Freq = 0

C	-0.486987	0.525948	0.001888
N	-1.725598	0.616039	0.000018
C	0.773819	0.648881	0.000480
N	1.989411	0.859602	-0.001330
O	-2.384403	-0.576936	0.001099
C	-3.789828	-0.348933	-0.001222
H	-4.238453	-1.339439	0.002975
H	-4.089470	0.203469	0.890147
H	-4.087891	0.195128	-0.898262
Cl	2.980137	-0.572267	-0.000078

Z-1ff

SCF = -1061.83298457
 Num. Imaginary Freq = 0

C	0.865942	-0.995536	0.000569
N	2.091995	-1.190511	-0.000121

C	-0.391859	-0.861159	0.000266
N	-1.633198	-0.838298	0.000065
S	3.222218	0.035224	-0.000315
C	2.261555	1.548661	0.000271
H	2.983907	2.365097	0.000200
H	1.637401	1.614303	-0.891397
H	1.637981	1.613949	0.892374
S	-2.452942	0.634813	0.000005
C	-4.129463	0.004788	-0.000257
H	-4.317636	-0.586078	0.893900
H	-4.781210	0.879060	-0.000158
H	-4.317490	-0.585772	-0.894647

Z-1fg

SCF = -961.425764940
 Num. Imaginary Freq = 0

C	-1.014728	-1.125225	-0.000431
N	-2.254246	-1.209270	-0.000067
C	0.247519	-1.060303	-0.000385
N	1.485365	-1.125139	-0.000272
C	2.243463	0.081233	-0.000018
F	3.019900	0.114879	1.079589
F	1.509945	1.206121	-0.000884
F	3.021571	0.114333	-1.078131
S	-3.270538	0.091654	0.000385
C	-2.190200	1.520990	-0.000386
H	-2.842704	2.394021	-0.000032
H	-1.562218	1.531209	0.890555
H	-1.563378	1.531008	-0.892145

Z-1fh

SCF = -737.653172740
 Num. Imaginary Freq = 0

C	-1.025165	-0.985323	0.022930
N	-2.262796	-0.970133	0.113800
C	0.233381	-1.066879	-0.047271
N	1.468282	-1.192200	-0.141681
S	2.525235	0.073474	-0.032989
C	1.495485	1.519529	0.209665
H	0.949633	1.453157	1.150982
H	2.173184	2.372636	0.238165
H	0.791695	1.634222	-0.614973
C	-2.942263	0.263044	0.219448
O	-2.692598	1.239140	-0.425518
H	-3.784521	0.205390	0.924331

Z-1fi

SCF = -716.546062014
 Num. Imaginary Freq = 0

C	1.021830	-0.879750	-0.000087
N	2.271461	-0.908212	0.000032
C	-0.229876	-1.011640	-0.000072
N	-1.467488	-1.152321	-0.000030
C	2.988272	0.220298	0.000076
N	3.690158	1.134510	-0.000005
S	-2.545639	0.087157	0.000079

C	-1.550729	1.576366	-0.000072
H	-0.926549	1.623031	-0.892736
H	-2.252849	2.409924	0.000025
H	-0.926280	1.623041	0.892399

Z-1fj

SCF = -828.819488020
 Num. Imaginary Freq = 0

C	-0.653256	-1.098837	0.000065
N	-1.896682	-1.123085	-0.000070
C	0.610108	-1.125595	0.000013
N	1.844428	-1.202986	0.000141
N	-2.477044	0.261943	-0.000089
O	-3.669733	0.270249	-0.000004
O	-1.730450	1.206217	0.000077
S	2.861612	0.090725	-0.000088
C	1.776598	1.516161	0.000043
H	1.147363	1.522539	0.890048
H	2.426747	2.390956	-0.000859
H	1.145954	1.521703	-0.888975

Z-1fk

SCF = -723.513701497
 Num. Imaginary Freq = 0

C	1.440860	-0.559886	-0.002461
N	2.678440	-0.494374	0.001249
C	0.208101	-0.868544	-0.006354
N	-0.979210	-1.172989	0.000413
F	3.085466	0.872361	0.002614
S	-2.267413	-0.130992	0.003122
C	-1.518113	1.497697	-0.003152
H	-2.346548	2.206471	-0.001663
H	-0.908482	1.649023	0.887511
H	-0.915249	1.645058	-0.899166

Z-1fl

SCF = -1083.89978308
 Num. Imaginary Freq = 0

C	0.316370	-1.019760	-0.001236
N	1.539574	-1.176213	0.000602
C	-0.952729	-0.991992	-0.002517
N	-2.188769	-0.965309	0.000392
S	2.653939	0.050725	0.001171
C	1.668870	1.548732	-0.001571
H	2.377765	2.376790	-0.001266
H	1.046577	1.601225	-0.895153
H	1.043961	1.602810	0.890093
Cl	-2.857766	0.669197	0.000739

Z-1gg

SCF = -861.006352180
 Num. Imaginary Freq = 0

C	0.636307	0.987774	-0.000085
N	1.863731	1.086523	0.000433
C	-0.636073	0.986540	0.000002

N -1.863459 1.086196 -0.000372
C 2.671140 -0.108135 -0.000050
F 3.439325 -0.094149 1.079920
F 1.974757 -1.243567 -0.000198
F 3.438863 -0.093463 -1.080022
C -2.671273 -0.108201 0.000029
F -3.438685 -0.094329 -1.080347
F -1.974856 -1.243563 0.000980
F -3.439683 -0.092806 1.079689

Z-1gh

SCF = -637.235493209
Num. Imaginary Freq = 0

C 1.379278 -0.845600 -0.122252
N 2.602031 -0.891469 -0.038989
C 0.108711 -0.833867 -0.207650
N -1.110645 -0.966810 -0.342681
C 3.423744 0.180759 0.385286
O 3.720107 1.096219 -0.313834
H 3.821364 0.010480 1.398410
C -1.980421 0.123819 0.014995
F -2.829958 -0.302670 0.940477
F -2.661896 0.490506 -1.061581
F -1.353678 1.198502 0.494623

Z-1gi

SCF = -616.124082834
Num. Imaginary Freq = 0

C -1.427814 -0.771788 0.000007
N -2.666062 -0.853403 -0.000027
C -0.163212 -0.876332 0.000143
N 1.059585 -1.022045 0.000201
C -3.460031 0.225531 -0.000063
N -4.237243 1.074949 0.000018
C 1.918147 0.137975 0.000033
F 2.682366 0.089652 -1.080413
F 2.683117 0.089460 1.079813
F 1.268239 1.299908 0.000370

Z-1gj

SCF = -728.398368234
Num. Imaginary Freq = 0

C 1.022407 0.950838 -0.000339
N 2.249862 1.077391 -0.000295
C -0.250724 0.958279 -0.000372
N -1.473272 1.045218 -0.000284
N 2.979051 -0.219821 0.000038
O 3.259683 -0.636012 -1.081591
O 3.260339 -0.634987 1.081891
C -2.289852 -0.143460 0.000110
F -3.055968 -0.123059 1.079159
F -3.054043 -0.125232 -1.080462
F -1.594505 -1.278982 0.001859

Z-1gk

SCF = -623.097723981

Num. Imaginary Freq = 0

C 1.805139 -0.471959 -0.000164
N 3.042436 -0.524195 0.000132
C 0.553515 -0.700037 -0.000136
N -0.638037 -0.964672 -0.000008
F 3.592926 0.765136 -0.000006
C -1.642739 0.062629 -0.000011
F -2.395104 -0.082649 1.079862
F -2.396717 -0.084159 -1.078528
F -1.148470 1.299258 -0.001217

Z-1gl

SCF = -983.483847506
Num. Imaginary Freq = 0

C 0.051240 -0.866100 -0.000068
N -1.166048 -1.022032 -0.000190
C 1.322516 -0.824189 0.000033
N 2.553386 -0.910299 -0.000034
Cl 3.398971 0.612058 0.000013
C -2.047376 0.113325 -0.000028
F -2.814740 0.053519 -1.079055
F -2.813635 0.054062 1.079898
F -1.421864 1.290543 -0.000652

Z-1hh

SCF = -413.464487431
Num. Imaginary Freq = 0

C -0.629500 -0.717399 0.094110
N -1.840756 -0.794362 0.288621
C 0.630316 -0.718268 -0.093215
N 1.841521 -0.795259 -0.287919
C -2.707664 0.319259 0.367783
O -3.080400 0.933100 -0.582159
H -3.064431 0.484878 1.396840
C 2.708016 0.318872 -0.368067
O 3.078597 0.935095 0.581094
H 3.066489 0.482125 -1.396893

Z-1hi

SCF = -392.353720928
Num. Imaginary Freq = 0

C -0.676498 -0.617604 -0.089940
N -1.906096 -0.753362 -0.219610
C 0.587903 -0.741665 -0.030857
N 1.808589 -0.826172 0.050286
C -2.762208 0.251333 0.012898
N -3.588549 1.034242 0.186347
C 2.674160 0.248388 0.377898
O 2.970695 1.105017 -0.390938
H 3.096691 0.134194 1.388343

Z-1hj

SCF = -504.628443126
Num. Imaginary Freq = 0

C 0.274505 0.743708 -0.285123
N 1.487970 0.904470 -0.454846
C -0.998021 0.771139 -0.201823
N -2.213638 0.816178 -0.115294
N 2.309865 -0.217719 0.068255
O 2.657066 -1.006883 -0.755928
O 2.588492 -0.147473 1.227585
C -3.053402 -0.189497 0.429287
O -3.369918 -1.166733 -0.167048
H -3.432996 0.096116 1.422272

Z-1hk

SCF = -399.328378256
Num. Imaginary Freq = 0

C -1.114978 -0.312557 -0.073704
N -2.340267 -0.411072 -0.225085
C 0.134690 -0.577028 -0.064600
N 1.324119 -0.812110 -0.035525
F -2.986541 0.768789 0.193885
C 2.381923 0.039032 0.368731
O 2.853657 0.871526 -0.334194
H 2.752837 -0.225723 1.370292

Z-1hl

SCF = -759.713478673
Num. Imaginary Freq = 0

C 0.678844 -0.726978 -0.023519
N 1.892717 -0.825572 0.057804
C -0.591946 -0.710494 -0.116297
N -1.813727 -0.829634 -0.240415
Cl -2.730544 0.625382 0.100490
C 2.804570 0.208004 0.375690
O 3.164843 1.028985 -0.405420
H 3.198779 0.099876 1.398062

Z-1ii

SCF = -371.241811291
Num. Imaginary Freq = 0

C -0.632121 -0.649568 0.000014
N -1.867573 -0.773048 -0.000008
C 0.631493 -0.648349 0.000014
N 1.866699 -0.772012 -0.000010
C -2.700766 0.273611 -0.000005
N -3.507923 1.095000 0.000001
C 2.700799 0.273495 -0.000006
N 3.509307 1.093612 0.000003

Z-1ij

SCF = -483.515425302
Num. Imaginary Freq = 0

C -0.222195 0.831833 -0.000335
N -1.444208 1.010595 -0.000155
C 1.042947 0.734773 -0.000266
N 2.276531 0.785729 -0.000117
N -2.230558 -0.251810 0.000036

O -2.528311 -0.652675 1.082190
O -2.527386 -0.653763 -1.082000
C 3.069291 -0.291298 0.000099
N 3.841852 -1.144562 0.000450

Z-1ik

SCF = -378.215137396
Num. Imaginary Freq = 0

C -1.063428 -0.374089 0.000170
N -2.302661 -0.436757 0.000134
C 0.192709 -0.535621 -0.000044
N 1.396267 -0.784011 -0.000140
F -2.862187 0.841318 0.000129
C 2.377284 0.120829 -0.000210
N 3.295007 0.815256 -0.000089

Z-1il

SCF = -738.601895250
Num. Imaginary Freq = 0

C -0.738860 -0.667605 -0.000173
N -1.968773 -0.793764 -0.000374
C 0.527749 -0.702242 0.000036
N 1.756882 -0.834603 0.000253
Cl 2.659696 0.643313 0.000445
C -2.823692 0.234022 -0.000426
N -3.646110 1.039601 -0.000478

Z-1jj

SCF = -595.788125525
Num. Imaginary Freq = 0

C -0.636612 0.925643 0.000079
N -1.861756 1.034445 0.000137
C 0.636663 0.925581 0.000013
N 1.861809 1.034607 0.000079
N -2.585423 -0.267923 -0.000009
O -2.861033 -0.682626 1.081967
O -2.861348 -0.682293 -1.082039
N 2.585435 -0.267969 -0.000052
O 2.861117 -0.682483 -1.082067
O 2.861168 -0.682532 1.081934

Z-1jk

SCF = -490.485568227
Num. Imaginary Freq = 0

C -1.440101 0.447404 0.000321
N -2.677050 0.417992 0.000234
C -0.195259 0.701760 0.000321
N 0.991134 1.015041 0.000776
F -3.145685 -0.895019 -0.000563
N 1.930904 -0.135077 -0.000100
O 2.275568 -0.494443 -1.081817
O 2.275483 -0.496245 1.081173

Z-1jl

SCF = -850.874037700

Num. Imaginary Freq = 0

C	0.331745	0.844466	-0.000149
N	1.549247	1.030336	-0.000335
C	-0.938445	0.781183	0.000038
N	-2.167931	0.844625	0.000140
Cl	-2.996452	-0.672661	0.000417
N	2.349567	-0.219143	-0.000242
O	2.653640	-0.619687	-1.081535
O	2.654324	-0.618986	1.081115

Z-1kk

SCF = -385.179387651

Num. Imaginary Freq = 0

C	0.633544	-0.378130	0.000015
N	1.858966	-0.542996	0.000029
C	-0.633875	-0.378620	0.000016
N	-1.859182	-0.543915	-0.000052
F	2.530085	0.674547	-0.000024
F	-2.529695	0.675328	0.000021

Z-1kl

SCF = -745.570255110

Num. Imaginary Freq = 0

C	-1.157981	0.421039	0.000048
N	-2.394580	0.469254	0.000096
C	0.100864	0.593292	-0.000034
N	1.298551	0.864294	-0.000114
Cl	2.382001	-0.472813	0.000048
F	-2.942124	-0.820334	-0.000086

Z-1ll

SCF = -1105.95852912

Num. Imaginary Freq = 0

C	-0.636008	0.721005	0.001529
N	-1.859247	0.862521	-0.000564
C	0.635939	0.720842	0.000415
N	1.859185	0.862278	-0.000943
Cl	2.778456	-0.609496	0.000064
Cl	-2.778406	-0.609602	-0.000130

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2aa

SCF = -148.792222093

Num. Imaginary Freq = 0

C	0.000026	-0.012194	0.000210
N	-1.208698	0.076587	-0.101108
H	-1.799594	-0.502190	0.476906
N	1.208726	0.078951	0.099261
H	1.799241	-0.513412	-0.465241

2ab

SCF = -188.097980195

Num. Imaginary Freq = 0

C	-0.676867	-0.118870	-0.011041
N	-1.855090	0.179744	0.128796
H	-2.403804	0.346606	-0.702617
N	0.461593	-0.516544	-0.020852
C	1.691319	0.242225	-0.000342
H	2.293620	-0.082745	0.847961
H	2.256648	0.035330	-0.909266
H	1.521306	1.318286	0.076610

2ac

SCF = -204.104955194

Num. Imaginary Freq = 0

C	-0.641300	0.118517	0.005709
N	-1.820260	-0.188205	-0.116418
H	-2.362882	-0.238952	0.737649
N	0.502105	0.525585	-0.041393
N	1.635242	-0.282815	0.137101
H	1.567919	-1.114307	-0.440642
H	2.423156	0.260195	-0.186289

2ad

SCF = -282.724668339

Num. Imaginary Freq = 0

C	1.428922	0.304109	-0.005229
N	2.590959	-0.034997	0.187697
H	3.199108	-0.017353	-0.622922
N	0.293003	0.734307	-0.039995
N	-0.848380	0.003798	-0.377921
C	-0.777554	-1.382143	0.045347
H	-0.656100	-1.480050	1.133973
H	-1.696767	-1.883053	-0.256067
H	0.059623	-1.877298	-0.448128
C	-2.016140	0.696360	0.134058
H	-2.907020	0.199587	-0.249749
H	-2.054934	0.702473	1.232596
H	-2.004354	1.723975	-0.223236

2ae

SCF = -263.254927623

Num. Imaginary Freq = 0

C	-1.234763	0.111106	0.009139
N	-2.424767	-0.111817	-0.123965
H	-2.962553	-0.242569	0.725580
N	-0.065356	0.483370	0.009901
O	0.900782	-0.522906	-0.007990
C	2.178097	0.084514	0.007922
H	2.886157	-0.742132	-0.009321
H	2.322104	0.716529	-0.871372

H 2.318898 0.676834 0.915118

SCF = -353.274705260
Num. Imaginary Freq = 0

2af

SCF = -586.290170071
Num. Imaginary Freq = 0

C -1.583681 0.193207 0.009453
N -2.785483 0.025794 -0.118688
H -3.349116 -0.058350 0.716486
N -0.400506 0.460064 -0.001292
S 0.888950 -0.632645 -0.000908
C 2.230000 0.552813 0.008549
H 3.146001 -0.039720 0.004175
H 2.201768 1.177818 -0.882104
H 2.202152 1.165442 0.907821

C 1.279442 -0.288305 0.021964
N 2.395250 0.101829 -0.153509
H 3.012565 0.431714 0.572642
N 0.167878 -0.836447 0.078148
N -0.951444 0.056696 0.007098
O -2.011944 -0.489667 -0.045904
O -0.734433 1.245113 0.017581

2ak

SCF = -247.952153164
Num. Imaginary Freq = 0

C 0.572040 -0.131636 0.008540
N 1.729120 0.195358 -0.128599
H 2.271922 0.382243 0.707635
N -0.565932 -0.625453 0.020116
F -1.538497 0.379804 0.000056

2ag

SCF = -485.891867584
Num. Imaginary Freq = 0

C -1.592662 -0.260141 -0.074168
N -2.731304 0.068896 0.137060
H -3.325640 0.470171 -0.571206
N -0.472541 -0.730422 -0.186733
C 0.726483 -0.018945 -0.006619
F 1.442874 -0.565515 0.972122
F 1.456242 -0.059551 -1.119706
F 0.539731 1.273403 0.303545

2al

SCF = -608.351160064
Num. Imaginary Freq = 0

C -1.061519 0.159443 0.010467
N -2.173507 -0.300435 -0.127589
H -2.710236 -0.550133 0.692847
N 0.012640 0.755386 0.019488
Cl 1.423848 -0.211246 0.000062

2ah

SCF = -262.121040337
Num. Imaginary Freq = 0

C 1.141692 -0.129790 0.003211
N 2.307096 0.159457 -0.086582
H 2.940669 0.242463 0.691115
N -0.021093 -0.506565 -0.038975
C -1.140321 0.342956 -0.022969
O -2.256209 -0.063762 0.050084
H -0.901242 1.418394 -0.094345

2ai

SCF = -241.011955897
Num. Imaginary Freq = 0

C -1.047342 0.093144 0.015657
N -2.174333 -0.288711 -0.121219
H -2.802073 -0.556034 0.619158
N 0.060919 0.614156 0.018880
C 1.258879 0.047947 0.004248
N 2.332392 -0.366947 -0.003174

2aj