Supporting Information

Metal-free Homolytic Hydrogen Activation: A Quest Through Density Functional Theory Computations

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SI1: Frontier orbital energies (hartree) and gaps (hartree) of butadiene analogs

	H_2	**CC**	**SiSi**	**GeGe**	**NN**	**PP**	**AsAs**	**OO**	**SS**	**SeSe**
LUMO	0.06036	0.00375	-0.04347	-0.04852	-0.02614	-0.07229	-0.08773	-0.07912	-0.11419	-0.13271
HOMO	-0.50294	-0.30103	-0.23059	-0.2237	-0.34502	-0.28866	-0.27611	-0.34759	-0.30581	-0.28654
HOMO-1	-	-	–	–	-0.361	-0.33126	-0.33278	-0.41923	-0.30763	-0.30051
HOMO-2	-	–	–	–	-0.38214	-0.35551	-0.361[a]	-0.48233	-0.35788	-0.33429
HOMO-LUMO gap	-	0.30478	0.18712	0.17518	0.31888	0.21637	0.18838	0.26847	0.19162	0.15383
EOFMO-EUFMO gap	-	0.30478	0.18712	0.17518	0.356	0.21637	0.18838	0.40321	0.24369	0.20158
EOFMO'-EUFMO gap	-	0.30478	0.18712	0.17518	0.33486	0.21637	0.18838	0.34011	0.19162	0.15383

[a] Energy of HOMO-3.

SI2: Frontier orbital energies (hartree) and gaps (hartree) of 1,3-dipoles

	$HC{\equiv}N^{+}{-}CH_2^{-}$	**$HC{\equiv}N^{+}{-}NH^{-}$**	**$HC{\equiv}N^{+}{-}O^{-}$**	**$N{\equiv}N^{+}{-}CH_2^{-}$**	**$N{\equiv}N^{+}{-}NH^{-}$**	**$N{\equiv}N^{+}{-}O^{-}$**
EUFMO	0.01157	0.00906	0.03523	0.0436	0.00661	0.02781
EOFMO	-0.26809	-0.29889	-0.35022	-0.28266	-0.40426	-0.42387
Gap	0.27966	0.30795	0.38545	0.32626	0.41087	0.45168
	$H_2C{=}NH^{+}{-}CH_2^{-}$	**$H_2C{=}NH^{+}{-}NH^{-}$**	**$H_2C{=}NH^{+}{-}O^{-}$**	**$HN{=}NH^{+}{-}NH^{-}$**	**$HN{=}NH^{+}{-}O^{-}$**	**$O{=}NH^{+}{-}O^{-}$**
EUFMO	0.02086	0.01249	-0.0024	-0.00084	-0.02074	-0.04633
EOFMO	-0.21093	-0.25241	-0.30342	-0.30019	-0.3567	-0.41796
Gap	0.23179	0.2649	0.30102	0.29935	0.33596	0.37163
	$H_2C{=}O^{+}{-}CH_2^{-}$	**$H_2C{=}O^{+}{-}NH^{-}$**	**$H_2C{=}O^{+}{-}O^{-}$**	**$HN{=}O^{+}{-}NH^{-}$**	**$HN{=}O^{+}{-}O^{-}$**	**$O{=}O^{+}{-}O^{-}$**
EUFMO	-0.01514	-0.03596	-0.06138	-0.06285	-0.09727	-0.14125
EOFMO	-0.22653	-0.27051	-0.32629	-0.32013	-0.3791	-0.44385
Gap	0.21139	0.23455	0.26491	0.25728	0.28183	0.3026
	$H_2C{=}S^{+}{-}CH_2^{-}$	**$H_2C{=}S^{+}{-}NH^{-}$**	**$H_2C{=}S^{+}{-}O^{-}$**	**$HN{=}S^{+}{-}NH^{-}$**	**$HN{=}S^{+}{-}O^{-}$**	**$O{=}S^{+}{-}O^{-}$**
EUFMO	-0.02165	-0.03757	-0.05326	-0.05589	-0.07507	-0.09881
EOFMO	-0.247	-0.28755	-0.33571	-0.33577	-0.39115	-0.45487
Gap	0.22535	0.24998	0.28245	0.27988	0.31608	0.35606

SI3: The activation barriers ($\Delta G^{\ddagger}$ in kcal/mol) and exothermicities (ΔG in kcal/mol) for H_2 activation.

		CC	**SiSi**	**GeGe**	**NN**	**PP**	**AsAs**	**OO**	**SS**	**SeSe**
1,4-H_2 additions	$\Delta G^{\ddagger}$	38.9	9.6	8.1	42.2	19.1	14.5	56.8	21.7	14.1
	ΔG	-25.7	-53.6	-51.5	-28.7	-21.0	-21.6	-19.5	-27.8	-30.4
1,2-H_2 additions	$\Delta G^{\ddagger}$	91.1	60.7	51.1	85.6	73.7	66.7	74.3	63.4	48.5
	ΔG	-19.8	-35.7	21.6	-22.7	-20.5	-22.7	-20.3	-24.8	-29.6

SI4: Cartesian coordinates (Å) and energies of the H_2 activation transition states

CC

M05-2X SCF energy: -157.122216 a.u.

M05-2X enthalpy: -157.015468 a.u.

M05-2X free energy: -157.046693 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.06047900	0.71661000	0.69703600
C	0.06047900	0.71661000	-0.69703600
C	0.06047900	-0.48527600	1.39161000
H	0.69614700	-1.30301400	1.07790900
H	-0.18782100	-0.48977900	2.44521500
C	0.06047900	-0.48527600	-1.39161000
H	-0.18782100	-0.48977900	-2.44521500
H	0.69614700	-1.30301400	-1.07790900
H	-1.01241600	-1.21971300	-0.45220600
H	-1.01241600	-1.21971300	0.45220600
H	-0.22165200	1.62450200	-1.21400600
H	-0.22165200	1.62450200	1.21400600

NN

M05-2X SCF energy: -189.207852 a.u.

M05-2X enthalpy: -189.125096 a.u.

M05-2X free energy: -189.156067 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.70651600	0.65583800	-0.01580200
C	0.70651600	0.65583800	-0.01580200
N	-1.29412000	-0.50818700	-0.15685500
H	-2.26015500	-0.47611400	0.16143900
N	1.29412000	-0.50818700	-0.15685500
H	2.26015500	-0.47611400	0.16143900
H	0.45703300	-1.43724600	0.67366700
H	-0.45703400	-1.43724500	0.67366500
H	1.22374500	1.53564000	0.35769100
H	-1.22374500	1.53564000	0.35769100

OO

M05-2X SCF energy: -228.940349 a.u.

M05-2X enthalpy: -228.883476 a.u.

M05-2X free energy: -228.914091 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.71046700	0.63186600	-0.02546600
C	0.71046700	0.63186500	-0.02546600
O	-1.27362700	-0.48804300	-0.09960300
O	1.27362700	-0.48804300	-0.09960300
H	-0.46584400	-1.38778900	0.59460600
H	0.46584400	-1.38778900	0.59460700
H	1.24948800	1.50093900	0.35501300
H	-1.24948800	1.50093800	0.35501300

SiSi

M05-2X SCF energy: -659.858649 a.u.

M05-2X enthalpy: -659.772119 a.u.

M05-2X free energy: -659.809707 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.70563500	0.99898300	0.00303500
C	-0.70563700	0.99897500	0.00290900
H	-0.38523800	-1.23699900	1.62549600
H	0.38559000	-1.23703700	1.62563900
H	-1.18404300	1.94469800	0.24281500
H	1.18402600	1.94467500	0.24310600
Si	1.81269600	-0.35372700	-0.08699200
H	3.26118100	-0.08478600	-0.01488600
H	1.44403200	-1.66437700	-0.65428800
Si	-1.81272200	-0.35376300	-0.08686400
H	-3.26120600	-0.08460100	-0.01555700
H	-1.44397400	-1.66446700	-0.65399300

PP

M05-2X SCF energy: -762.414228 a.u.

M05-2X enthalpy: -762.343308 a.u.

M05-2X free energy: -762.377703 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.08505900	1.00840100	0.69273300
C	-0.08505900	1.00840100	-0.69273300
H	1.28279400	-1.09299800	-0.43341200

H	1.28279400	-1.09299800	0.43341200
P	-0.08505900	-0.46790400	-1.61460300
H	0.43405100	0.10763700	-2.80981200
P	-0.08505900	-0.46790400	1.61460300
H	0.43405100	0.10763700	2.80981200
H	0.06938800	1.95351200	-1.19818100
H	0.06938800	1.95351200	1.19818100

SS

M05-2X SCF energy: -874.901894 a.u.

M05-2X enthalpy: -874.848518 a.u.

M05-2X free energy: -874.88206 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.70274300	0.97332700	0.02374500
C	0.70274300	0.97332700	0.02374500
H	-0.41735700	-1.32304700	1.05197900
H	0.41735700	-1.32304700	1.05197700
H	1.18528900	1.89280200	0.33776900
H	-1.18528900	1.89280200	0.33776900
S	1.62215700	-0.40060700	-0.09576300
S	-1.62215700	-0.40060700	-0.09576400

GeGe

M06-2X SCF energy: -4234.786751 a.u.

M06-2X enthalpy: -4234.703551 a.u.

M06-2X free energy: -4234.745592 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.70623100	1.19683900	0.02566900
C	-0.70147900	1.19555100	0.00919900
H	-0.39522200	-1.00801000	1.81566900
H	0.36695800	-1.07268100	1.77735900
H	-1.18475700	2.14740100	0.21926900
H	1.18513300	2.14455800	0.26199900
Ge	1.86672900	-0.21111300	-0.05070100
H	3.36949000	0.06241500	0.01839900
H	1.47492800	-1.58845300	-0.58962100
Ge	-1.86698100	-0.21133800	-0.04655100
H	-3.36768000	0.08395400	-0.06206100
H	-1.46933300	-1.60508800	-0.53815100

GeGe

M05-2X SCF energy: -4234.662015 a.u.

M05-2X enthalpy: -4234.577818 a.u.

M05-2X free energy: -4234.620417 a.u.

Cartesian coordinates

ATOM	X	Y	Z	
C		0.69096300	1.17548300	-0.02026100
C		-0.71186700	1.15342300	0.19836900
H		-0.21662800	-0.95473700	2.27182900
H		0.50728200	-0.98299700	2.44832900
H		-1.16722700	2.06887400	0.56072900
H		1.16379300	2.15188300	-0.02680100
Ge		1.86493200	-0.20470800	-0.06329100
H		3.30656200	0.06252100	-0.47906100
H		1.43169200	-1.66581800	-0.03210100
Ge		-1.86896800	-0.20299600	-0.10458100
H		-3.32400800	-0.09857500	0.32834900
H		-1.44690800	-1.50806600	-0.76802100

AsAs

M05-2X SCF energy: -4551.259444 a.u.

M05-2X enthalpy: -4551.190105 a.u.

M05-2X free energy: -4551.227543 a.u.

Cartesian coordinates

ATOM	X	Y	Z	
C		-0.69043400	1.26708700	0.01624000
C		0.69043500	1.26708800	0.01624000
H		0.41445400	-0.97181500	1.40105500
H		-0.41445400	-0.97181600	1.40105400
H		1.19745900	2.20537500	0.20304700
H		-1.19746100	2.20537500	0.20304700
As		1.71077100	-0.27944000	-0.06591100
H		2.97181600	0.38541900	0.47352800
As		-1.71077100	-0.27943900	-0.06591100
H		-2.97181600	0.38541700	0.47352800

SeSe

M05-2X SCF energy: -4881.442013 a.u.

M05-2X enthalpy: -4881.389428 a.u.

M05-2X free energy: -4881.426139 a.u.

Cartesian coordinates

ATOM	X	Y	Z	
C		-0.70184400	1.21711300	0.05676400
C		0.70184400	1.21711300	0.05676400
H		-0.39791000	-1.16059900	1.36678200
H		0.39790800	-1.16059800	1.36677800
H		1.18422200	2.15264700	0.31511800
H		-1.18422200	2.15264700	0.31511900
Se		1.73452200	-0.24396300	-0.05948500
Se		-1.73452200	-0.24396300	-0.05948500

***trans*-1**

M05-2X SCF energy: -2166.699545 a.u.

M05-2X enthalpy: -2165.747398 a.u.

M05-2X free energy: -2165.876096 a.u.

Cartesian coordinates

ATOM	X	Y	Z	
C		-0.71628000	-0.00360500	-0.03469800
H		-1.26617700	0.01480700	0.90419500
C		0.71627000	0.00410800	0.03450400
H		1.26619200	-0.01425700	-0.90437200
P		-1.52984100	-0.03818800	-1.51380300
P		1.52977600	0.03841800	1.51364700
C		-3.29403800	-0.03239200	-0.91619300
C		-5.78234700	-0.02096400	0.41560500
C		-3.95085200	-1.25750700	-0.63733800
C		-3.94914400	1.20322800	-0.65443000
C		-5.16632200	1.16439900	0.02550600
C		-5.17428100	-1.21034700	0.04264100
H		-5.66477200	2.09041600	0.26331500
H		-5.66816700	-2.13346800	0.29002400
C		3.29400900	0.03248500	0.91614100
C		5.78240700	0.02084700	-0.41551600
C		3.95100200	1.25752900	0.63742500
C		3.94899400	-1.20321200	0.65433900
C		5.16619200	-1.16447900	-0.02554300
C		5.17447900	1.21026700	-0.04248200
H		5.66453400	-2.09054100	-0.26342400
H		5.66850200	2.13334800	-0.28974500
C		3.43405600	2.65411200	1.06959800
C		7.10235600	-0.03092800	-1.18576200

C	3.43363800	-2.59057600	1.11638700
C	-3.43377400	-2.65405600	-1.06946200
C	-3.43398600	2.59061600	-1.11658400
C	-7.10228000	0.03068300	1.18589200
C	2.23436800	3.12467800	0.22478500
H	1.33298500	2.55001500	0.41908700
H	2.46723600	3.04761600	-0.83974900
H	2.02262900	4.17242200	0.45428200
C	3.07637500	2.66405500	2.56709000
H	2.24943300	2.00061200	2.81722800
H	2.77890100	3.67376200	2.86080000
H	3.94184800	2.37095200	3.16491100
C	4.51816200	3.73554600	0.90105800
H	5.43893100	3.47530900	1.42681100
H	4.14048100	4.66794300	1.32396000
H	4.75047300	3.92713200	-0.14822900
C	7.63198400	1.36537200	-1.52693100
H	7.84064200	1.94710500	-0.62635300
H	6.92513600	1.92171000	-2.14635000
H	8.56504300	1.26957500	-2.08597200
C	8.16442500	-0.75089400	-0.33810600
H	8.32085200	-0.22649800	0.60653900
H	9.11389400	-0.78293800	-0.87863200
H	7.87121800	-1.77724000	-0.11204400
C	6.89399900	-0.79826300	-2.50177400
H	6.56014700	-1.82133200	-2.32178000
H	7.83233600	-0.84242500	-3.06044200
H	6.14496900	-0.30135200	-3.12142700
C	4.52028500	-3.67239200	0.96896400
H	5.44223600	-3.39659600	1.48479200
H	4.74873300	-3.88706600	-0.07676900
H	4.14749800	-4.59615800	1.41449500
C	3.07937400	-2.56796800	2.61450000
H	3.94520300	-2.25899300	3.20379100
H	2.78544800	-3.57170400	2.93132500
H	2.25083400	-1.90149900	2.85155900
C	2.23298800	-3.08321400	0.28552700
H	1.32888500	-2.51123800	0.47434500
H	2.02916500	-4.12810200	0.53442100
H	2.46025400	-3.02365200	-0.78134600
C	-4.51772000	-3.73562200	-0.90071000
H	-4.74985500	-3.92719100	0.14861700
H	-4.13998800	-4.66798400	-1.32363500
H	-5.43860300	-3.47552600	-1.42632700
C	-2.23391300	-3.12438000	-0.22474000

H	-2.46664300	-3.04720800	0.83981400
H	-1.33265900	-2.54960500	-0.41925100
H	-2.02205200	-4.17211500	-0.45416300
C	-3.07621100	-2.66404700	-2.56697600
H	-2.24942500	-2.00044900	-2.81724000
H	-3.94178200	-2.37116300	-3.16477400
H	-2.77854300	-3.67371700	-2.86063700
C	-6.89404900	0.79825800	2.50178600
H	-6.56043900	1.82138100	2.32165700
H	-6.14487800	0.30161100	3.12147800
H	-7.83236300	0.84227300	3.06051300
C	-8.16450500	0.75029400	0.33814300
H	-7.87150400	1.77665900	0.11191500
H	-9.11398600	0.78223500	0.87866100
H	-8.32083500	0.22574900	-0.60643400
C	-7.63161200	-1.36567500	1.52729900
H	-6.92457800	-1.92180600	2.14668600
H	-7.84025800	-1.94755200	0.62682300
H	-8.56462500	-1.26998300	2.08642700
C	-3.07970700	2.56793600	-2.61469300
H	-3.94549900	2.25878700	-3.20395500
H	-2.25106800	1.90157100	-2.85169500
H	-2.78592000	3.57167900	-2.93161500
C	-4.52079300	3.67227400	-0.96923400
H	-5.44274000	3.39624800	-1.48495400
H	-4.14818000	4.59604100	-1.41491400
H	-4.74919800	3.88704700	0.07648200
C	-2.23342300	3.08348300	-0.28573700
H	-2.46074300	3.02403800	0.78113500
H	-2.02969900	4.12836200	-0.53475600
H	-1.32923300	2.51160200	-0.47443800

TS1

M05-2X SCF energy:	-2166.681683	a.u.
M05-2X enthalpy:	-2165.730053	a.u.
M05-2X free energy:	-2165.861839	a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.72725200	-0.09225100	0.01495700
H	1.27571400	-0.65640500	0.76778100
C	-0.74991700	-0.08504200	0.09990100
H	-1.29736400	-0.75297600	-0.56365000
P	1.55213100	0.73175000	-1.18487800

P	-1.58167300	0.90871900	1.15777000
C	3.31107500	0.31031900	-0.72662400
C	5.77547100	-0.56600100	0.33432700
C	4.02156300	1.13568400	0.18060100
C	3.90578200	-0.88579200	-1.21635800
C	5.11234500	-1.29450600	-0.64875700
C	5.23033500	0.65541400	0.70054900
H	5.56272900	-2.21520000	-0.98460600
H	5.76240900	1.25728000	1.41620700
C	-3.33270500	0.42158200	0.73164000
C	-5.72909700	-0.66215300	-0.28887700
C	-3.94342700	-0.67748800	1.38505100
C	-4.00569600	1.07899700	-0.33545100
C	-5.17446400	0.49666700	-0.82479200
C	-5.11951800	-1.20166200	0.83423800
H	-5.68253700	0.95927200	-1.65608900
H	-5.57395700	-2.06052200	1.29714800
C	-3.42677700	-1.32149000	2.69713200
C	-6.99340600	-1.25445900	-0.91184100
C	-3.56102000	2.42386700	-0.96584400
C	3.58033800	2.55658200	0.61813500
C	3.33561300	-1.75179900	-2.36913800
C	7.07851900	-1.10437200	0.92673100
C	-2.22024800	-2.24756400	2.45802100
H	-1.33494200	-1.70277600	2.14095700
H	-2.45960200	-2.98886100	1.69210100
H	-1.98280100	-2.77671800	3.38486700
C	-3.07809800	-0.24310600	3.73867500
H	-2.23213700	0.37922400	3.44997900
H	-2.81255700	-0.72462900	4.68291800
H	-3.93663300	0.40883800	3.91280100
C	-4.51088400	-2.19330700	3.35933500
H	-5.43983100	-1.63974200	3.50982100
H	-4.14493300	-2.51440500	4.33607200
H	-4.72645700	-3.09629500	2.78525000
C	-7.43658500	-2.54318400	-0.21243700
H	-7.69588500	-2.36490300	0.83342000
H	-6.65793800	-3.30808800	-0.25400400
H	-8.32337800	-2.93797600	-0.71256500
C	-8.14032700	-0.23507200	-0.81109100
H	-8.34600200	0.00729600	0.23338900
H	-9.04857300	-0.64931600	-1.25631300
H	-7.90038000	0.69232300	-1.33348500
C	-6.72859000	-1.58032600	-2.39108000
H	-6.45413400	-0.68875700	-2.95679300

H	-7.62707500	-2.00505300	-2.84578700
H	-5.91700900	-2.30443900	-2.48541200
C	-4.70074400	3.05982700	-1.78536200
H	-5.61680600	3.15882300	-1.19921300
H	-4.92120400	2.49737200	-2.69457900
H	-4.38616700	4.05779900	-2.09515200
C	-3.21681900	3.45550200	0.12338300
H	-4.05772300	3.58115200	0.80870400
H	-3.00679900	4.41916500	-0.34676500
H	-2.33713900	3.18949300	0.70778300
C	-2.37901100	2.25570100	-1.93865400
H	-1.45536500	1.98497400	-1.43452400
H	-2.21184000	3.19771400	-2.46767900
H	-2.60432800	1.48366500	-2.67812400
C	4.73143000	3.31582300	1.30570300
H	4.98515800	2.89033400	2.27835000
H	4.40826700	4.34357800	1.47923500
H	5.62949100	3.34339400	0.68527100
C	2.42547100	2.52150900	1.63691600
H	2.67832100	1.86507000	2.47281200
H	1.49216500	2.17463300	1.20174800
H	2.26189600	3.52831600	2.03062300
C	3.19567000	3.41557400	-0.60034000
H	2.31072400	3.05433700	-1.12204800
H	4.02136300	3.45464700	-1.31392700
H	2.97669800	4.43335700	-0.26840400
C	6.81940100	-2.48112700	1.56069700
H	6.45492700	-3.19998400	0.82535900
H	6.07637100	-2.40379400	2.35684900
H	7.74528300	-2.87498800	1.98745700
C	8.12892800	-1.24634200	-0.18742800
H	7.79813900	-1.93583900	-0.96570900
H	9.06431500	-1.62932100	0.22859400
H	8.32684600	-0.27877400	-0.65274100
C	7.65044600	-0.18276100	2.00827800
H	6.94587800	-0.04821100	2.83194000
H	7.90832000	0.79909100	1.60537800
H	8.56175000	-0.62657100	2.41438100
C	2.93477600	-0.87937100	-3.57226900
H	3.78369100	-0.27923900	-3.90648600
H	2.10510100	-0.20621600	-3.36155300
H	2.62118800	-1.52448600	-4.39661800
C	4.39507600	-2.73094400	-2.91118700
H	5.31462800	-2.21660500	-3.19758200
H	3.98917800	-3.21928100	-3.79868100

H	4.63633600	-3.51761300	-2.19414100
C	2.14809800	-2.62104100	-1.91453700
H	2.42428900	-3.20425400	-1.03308400
H	1.88349300	-3.31609100	-2.71604200
H	1.26842700	-2.03118200	-1.67203800

***cis*-1**

M05-2X SCF energy: -2166.695547 a.u.

M05-2X enthalpy: -2165.742649 a.u.

M05-2X free energy: -2165.872566 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.71611300	-0.04723200	0.38140600
H	1.26331000	0.16122400	1.29763000
C	-0.71658400	0.08922500	0.38563200
H	-1.25950200	-0.13323800	1.30113700
P	1.52756300	-0.57020400	-1.00646500
P	-1.53483800	0.62919900	-0.99165100
C	3.28741900	-0.27274300	-0.47448000
C	5.75819000	0.23841200	0.78687400
C	3.82185300	1.03946500	-0.47980300
C	4.05846000	-1.35518100	0.03269900
C	5.26496900	-1.05805100	0.66495100
C	5.03894200	1.25640600	0.17917300
H	5.85170700	-1.85986600	1.08395700
H	5.43940700	2.25459900	0.21405500
C	-3.29189700	0.31587400	-0.45952100
C	-5.75933700	-0.22823300	0.79493900
C	-4.06898000	1.38085300	0.06090800
C	-3.81720200	-1.00544400	-0.48275700
C	-5.02665200	-1.23503800	0.17328800
C	-5.27990200	1.06964700	0.69115300
H	-5.42676200	-2.23627700	0.19962000
H	-5.86555700	1.86504600	1.11768100
C	-3.68323100	2.87751900	-0.04858200
C	-7.06008600	-0.57826900	1.51881400
C	-3.18138000	-2.20549900	-1.23415700
C	3.19114600	2.25789300	-1.20588000
C	3.66408000	-2.84674500	-0.10426300
C	7.07060500	0.47962500	1.53373500
C	-2.48963400	3.24215000	0.85473600
H	-1.55649900	2.79175100	0.52483600
H	-2.68017200	2.92031000	1.88122700

H	-2.35679400	4.32733500	0.85438200
C	-3.38844200	3.25219700	-1.51292100
H	-2.52626600	2.72913800	-1.92321900
H	-3.18029800	4.32321900	-1.57762700
H	-4.25451900	3.03103300	-2.14015500
C	-4.83806400	3.79634900	0.38941800
H	-5.75147500	3.60093100	-0.17576700
H	-4.54263600	4.83038900	0.20357100
H	-5.05458100	3.70646600	1.45576300
C	-7.73899200	0.65370300	2.12521400
H	-8.01631600	1.37843100	1.35646000
H	-7.09472200	1.14814600	2.85544600
H	-8.65228900	0.34539900	2.63827400
C	-8.04353800	-1.22716800	0.53059800
H	-8.26933700	-0.54367100	-0.29022200
H	-8.97674700	-1.47431600	1.04306600
H	-7.63970500	-2.14690600	0.10479100
C	-6.75493700	-1.56627600	2.65700800
H	-6.30952300	-2.48793000	2.27935500
H	-7.67706900	-1.82660700	3.18274700
H	-6.06079100	-1.12320300	3.37378200
C	-4.22236100	-3.31885900	-1.46952100
H	-5.12556900	-2.93433000	-1.94763100
H	-4.50089900	-3.82826900	-0.54543200
H	-3.78180200	-4.07004700	-2.12699800
C	-2.69579500	-1.79865200	-2.63704300
H	-3.49591600	-1.30704500	-3.19454200
H	-2.39124300	-2.69375800	-3.18449600
H	-1.83097600	-1.13490200	-2.61985100
C	-2.02804200	-2.85602500	-0.44600700
H	-1.14170700	-2.22677100	-0.40966800
H	-1.75268200	-3.79847400	-0.92713800
H	-2.34218000	-3.07399500	0.57736300
C	4.24304800	3.36141900	-1.44125900
H	4.54128700	3.85544700	-0.51508600
H	3.80302700	4.12665500	-2.08274200
H	5.13452000	2.97187300	-1.93683500
C	2.05914600	2.90958100	-0.38853100
H	2.39444600	3.11254600	0.63120600
H	1.16844400	2.28672600	-0.34299700
H	1.78290400	3.86013600	-0.85298800
C	2.67682900	1.88027900	-2.60666900
H	1.79642300	1.23742600	-2.58609000
H	3.45704700	1.37728100	-3.18196100
H	2.38579700	2.78907700	-3.13862100

C	6.92563200	-0.00592700	2.98545900
H	6.69211900	-1.07073700	3.03196300
H	6.12783500	0.53879000	3.49407200
H	7.85952400	0.15967300	3.52863400
C	8.20500900	-0.29861400	0.84638900
H	8.01428900	-1.37295400	0.84689800
H	9.14815500	-0.12308900	1.37014000
H	8.31882800	0.02541000	-0.18990600
C	7.45909500	1.96111900	1.56453800
H	6.69396600	2.56501300	2.05726200
H	7.62189200	2.35559600	0.55915500
H	8.38990000	2.07709300	2.12358700
C	3.37367100	-3.19267100	-1.57650800
H	4.24345700	-2.96421600	-2.19592700
H	2.51569600	-2.65758300	-1.98012000
H	3.16039600	-4.26120900	-1.66211400
C	4.81256300	-3.77841400	0.32223100
H	5.72901900	-3.57728700	-0.23611100
H	4.51342300	-4.80786100	0.11789300
H	5.02479800	-3.70723400	1.39092900
C	2.46465100	-3.22156100	0.78718800
H	2.65024000	-2.91505200	1.81924900
H	2.32946400	-4.30630100	0.77021600
H	1.53415600	-2.76464000	0.45893100

TS2

M05-2X SCF energy:	-2167.840976	a.u.
M05-2X enthalpy:	-2166.874051	a.u.
M05-2X free energy:	-2167.002388	a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.69131800	0.50820000	0.30435400
H	-1.22018300	0.36740100	1.24218700
C	0.69184700	0.50803500	0.30412400
H	1.22098000	0.36717100	1.24179600
P	-1.61199500	0.57976900	-1.18280400
P	1.61211400	0.57934000	-1.18331000
C	-3.31054500	0.14854600	-0.52151200
C	-5.68994700	-0.33915300	0.92553300
C	-3.78528000	-1.17649900	-0.35923000
C	-4.11782700	1.24473000	-0.09441100
C	-5.26429400	0.95586000	0.64724500
C	-4.95924600	-1.38036600	0.37430500

H	-5.86457500	1.76927400	1.02107000
H	-5.30856600	-2.38741200	0.52130800
C	3.31073600	0.14819600	-0.52213900
C	5.68943800	-0.33893200	0.92618300
C	3.78548500	-1.17676300	-0.35935400
C	4.11782600	1.24454700	-0.09512300
C	5.26390400	0.95598800	0.64724800
C	4.95913400	-1.38033400	0.37477400
H	5.86395300	1.76956400	1.02111100
H	5.30853700	-2.38730200	0.52212100
C	3.11549300	-2.42359700	-0.97784200
C	6.94618600	-0.55804300	1.76910800
C	3.86694700	2.73478800	-0.45748300
C	-3.11485800	-2.42312800	-0.97767600
C	-3.86671000	2.73516600	-0.45581700
C	-6.94715200	-0.55853900	1.76770600
C	1.81737400	-2.78052100	-0.23353000
H	1.09534000	-1.97167000	-0.23114100
H	2.04786900	-3.02776200	0.80553100
H	1.35400100	-3.65461800	-0.69912600
C	2.88928100	-2.21316900	-2.48720300
H	2.30912200	-1.32651300	-2.72748400
H	2.36194800	-3.07563500	-2.90267000
H	3.85411800	-2.12483600	-2.99140200
C	4.00704300	-3.67554100	-0.88325700
H	4.98550900	-3.51419100	-1.33991500
H	3.51334400	-4.48612000	-1.42309300
H	4.14623400	-4.00986700	0.14637800
C	7.25570500	-2.04377800	1.97510400
H	7.45538300	-2.54768500	1.02701500
H	6.43331300	-2.55763000	2.47743900
H	8.14595000	-2.14228700	2.59983400
C	8.15338600	0.09095500	1.07156800
H	8.30811900	-0.34956600	0.08473400
H	9.05673900	-0.06565300	1.66677900
H	8.01479800	1.16593300	0.94540400
C	6.74909900	0.08631400	3.15134700
H	6.56599700	1.15891100	3.07197000
H	7.64393300	-0.06005600	3.76174100
H	5.89977900	-0.36554200	3.66751500
C	5.04220900	3.62825700	-0.01700400
H	5.99133400	3.29401700	-0.44011400
H	5.13508200	3.68240300	1.06988800
H	4.85387400	4.64015600	-0.37904200
C	3.78310900	2.89550700	-1.98780100

H	4.70396300	2.53733100	-2.45283200
H	3.66194400	3.95374000	-2.23334400
H	2.94356700	2.35802500	-2.42396100
C	2.61875800	3.33463200	0.22056100
H	1.68533000	2.97797500	-0.20664400
H	2.63943000	4.42121700	0.10341800
H	2.61551900	3.10626500	1.28890400
C	-4.00601200	-3.67536600	-0.88319400
H	-4.14511600	-4.00977800	0.14642800
H	-3.51204000	-4.48573200	-1.42310300
H	-4.98451700	-3.51432900	-1.33987100
C	-1.81675300	-2.77974600	-0.23316600
H	-2.04739000	-3.02712400	0.80582900
H	-1.09489600	-1.97073600	-0.23055800
H	-1.35308900	-3.65369900	-0.69873300
C	-2.88862600	-2.21266100	-2.48704900
H	-2.31028200	-1.32487000	-2.72747700
H	-3.85352400	-2.12641600	-2.99149900
H	-2.35946000	-3.07417800	-2.90216100
C	-6.75071700	0.08520200	3.15032800
H	-6.56738300	1.15780000	3.07149100
H	-5.90175500	-0.36700900	3.66677200
H	-7.64591400	-0.06127200	3.76016500
C	-8.15394800	0.09086000	1.06983800
H	-8.01511100	1.16584300	0.94399900
H	-9.05757100	-0.06573200	1.66464100
H	-8.30835800	-0.34939000	0.08283100
C	-7.25689800	-2.04433900	1.97288500
H	-6.43486400	-2.55846300	2.47552500
H	-7.45601700	-2.54783000	1.02445700
H	-8.14754300	-2.14304600	2.59701600
C	-3.78257800	2.89684100	-1.98601800
H	-4.70343300	2.53914900	-2.45142000
H	-2.94308500	2.35945900	-2.42238300
H	-3.66115800	3.95520400	-2.23086700
C	-5.04189100	3.62856500	-0.01498000
H	-5.99096400	3.29493000	-0.43869000
H	-4.85319100	4.64071400	-0.37612600
H	-5.13511400	3.68182800	1.07192000
C	-2.61858900	3.33440000	0.22285800
H	-2.61603000	3.10599100	1.29119500
H	-2.63870200	4.42099900	0.10574400
H	-1.68509800	2.97733300	-0.20384300
H	0.45073300	-0.68608000	-1.83142900
H	-0.45122600	-0.68590600	-1.83122300

1-PR

M05-2X SCF energy: -2167.899565 a.u.

M05-2X enthalpy: -2166.927721 a.u.

M05-2X free energy: -2167.05506 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.64350500	-0.11674500	0.27831000
H	-1.19651500	0.00644700	1.20580200
C	0.66182800	-0.39990000	0.30867200
H	1.17742300	-0.50409000	1.25961800
P	-1.59655000	0.16895400	-1.27370200
P	1.63775800	-0.62156700	-1.23712600
C	-3.32018800	0.06826400	-0.56435500
C	-5.73655300	0.05212800	0.91304500
C	-4.03969800	-1.14389000	-0.38532900
C	-3.87831200	1.29421900	-0.09357100
C	-5.05806400	1.23628100	0.64996200
C	-5.22536000	-1.11060400	0.35777800
H	-5.47816100	2.14824600	1.04034200
H	-5.76496800	-2.02702900	0.51695500
C	3.34506400	-0.35795000	-0.53840900
C	5.69492400	0.32436100	0.88519200
C	4.11879700	-1.37166000	0.08859600
C	3.81980900	0.98694500	-0.54769800
C	4.96807700	1.28232600	0.18790400
C	5.26920900	-0.99143000	0.78986200
H	5.32289700	2.29885600	0.22369100
H	5.84981600	-1.74925800	1.28473700
C	3.82192800	-2.89100400	0.01825300
C	6.93053800	0.74338200	1.68245000
C	3.19465100	2.14820700	-1.37016400
C	-3.64107600	-2.51138800	-0.99358700
C	-3.30898600	2.71044000	-0.39172500
C	-7.01207800	0.08065000	1.75557900
C	2.56549900	-3.27965400	0.82672600
H	1.64431900	-2.81676600	0.48872300
H	2.71240900	-3.00062500	1.87296400
H	2.43099300	-4.36367100	0.78371300
C	3.77323200	-3.35840200	-1.45312600
H	3.11794700	-2.77427400	-2.09214800
H	3.45063800	-4.40193500	-1.49822000
H	4.77652200	-3.29521100	-1.87999800

C	4.95012500	-3.73725800	0.64276300
H	5.91657900	-3.54203200	0.17498700
H	4.71076200	-4.79047300	0.48269300
H	5.03781200	-3.58164500	1.71977000
C	7.60682700	-0.44354000	2.37554300
H	7.96033400	-1.18221500	1.65285600
H	6.93061500	-0.93660100	3.07736900
H	8.47150500	-0.08568700	2.93832100
C	7.95599500	1.39333300	0.73869500
H	8.25579800	0.69306500	-0.04338800
H	8.84586600	1.68697300	1.30130600
H	7.55179200	2.28561800	0.25821800
C	6.51808400	1.75654800	2.76310500
H	6.06888700	2.64962400	2.32614800
H	7.39436400	2.06545200	3.33886600
H	5.79280000	1.31273900	3.44789000
C	4.00820800	3.44875500	-1.22849200
H	5.04599200	3.32360900	-1.54328200
H	3.98844500	3.83741500	-0.20773900
H	3.55697500	4.20189900	-1.87613800
C	3.22699800	1.80364400	-2.87180700
H	4.25679300	1.63340500	-3.19341000
H	2.82235000	2.64345100	-3.44291600
H	2.63608800	0.92264000	-3.10937100
C	1.76191700	2.51250700	-0.92631200
H	1.01389100	1.80852800	-1.28418500
H	1.49956800	3.49072600	-1.33760000
H	1.69454100	2.57180600	0.16232100
C	-4.71072700	-3.59635300	-0.75283500
H	-4.82195700	-3.84169800	0.30493300
H	-4.39129400	-4.50494700	-1.26725400
H	-5.68356800	-3.31063000	-1.15664800
C	-2.36452600	-3.08844500	-0.34456300
H	-2.55582800	-3.27329400	0.71508400
H	-1.48974200	-2.44994700	-0.40718600
H	-2.12326100	-4.04532100	-0.81518200
C	-3.55926600	-2.40483500	-2.53273700
H	-2.94241300	-1.59034900	-2.89952000
H	-4.56398700	-2.24902100	-2.93149400
H	-3.17097600	-3.33868900	-2.94746400
C	-6.69116900	0.65441100	3.14563900
H	-6.29902700	1.67055400	3.08077700
H	-5.94865400	0.03608100	3.65388600
H	-7.59717300	0.68065700	3.75641200
C	-8.06240000	0.96814400	1.06731900

H	-7.70911000	1.99404600	0.95228600
H	-8.97881500	0.99115400	1.66263300
H	-8.30278800	0.57911400	0.07598900
C	-7.61644500	-1.31431800	1.94487500
H	-6.91801500	-1.98853400	2.44556800
H	-7.90854000	-1.75934000	0.99107900
H	-8.51198600	-1.23711000	2.56492500
C	-3.25889000	2.95565200	-1.91268000
H	-4.25934400	2.85181500	-2.33819900
H	-2.58785500	2.27230900	-2.42624600
H	-2.90993600	3.97451000	-2.10125100
C	-4.21853300	3.82045800	0.16905500
H	-5.23004700	3.76710000	-0.23786000
H	-3.79606800	4.78357100	-0.12155300
H	-4.27075100	3.80072000	1.25988900
C	-1.93003600	2.95616600	0.25270800
H	-1.95660200	2.70721400	1.31631800
H	-1.67656400	4.01547500	0.15900900
H	-1.12593500	2.39459800	-0.21502100
H	1.57655700	-2.02645300	-1.25697500
H	-1.45492400	-1.12004900	-1.81126100

2

M05-2X SCF energy:	-2105.094118	a.u.
M05-2X enthalpy:	-2105.061385	a.u.
M05-2X free energy:	-2105.105471	a.u.

Cartesian coordinates

ATOM	X	Y	Z
S	0.18878800	1.19409100	0.52360100
C	1.44288600	1.32017600	1.74403700
S	0.82710900	1.54852800	3.37034900
C	-0.88862900	1.55466200	3.01504800
C	-1.21650000	1.36274300	1.55656300
S	3.02582300	1.23167600	1.40004700
S	-2.71665000	1.30918600	0.94777600
S	-1.98724500	1.75417600	4.18938400

2-TS

M05-2X SCF energy:	-2106.233339	a.u.
M05-2X enthalpy:	-2106.187543	a.u.
M05-2X free energy:	-2106.231311	a.u.

Cartesian coordinates

ATOM	X	Y	Z
S	-0.74036700	-1.46180800	-0.00404800
C	-1.70761800	-0.00000100	0.01306800
S	-0.74036700	1.46180800	-0.00405600
C	0.83490700	0.70817400	-0.19017300
C	0.83490800	-0.70817400	-0.19017300
S	-3.33530800	0.00000000	0.05379500
H	2.86352400	0.44067700	1.21214300
H	2.86355500	-0.44068700	1.21217500
S	2.23613700	1.60654400	-0.02973700
S	2.23613800	-1.60654300	-0.02974500

3

M05-2X SCF energy:	-6107.431668	a.u.
M05-2X enthalpy:	-6107.399795	a.u.
M05-2X free energy:	-6107.446279	a.u.

Cartesian coordinates

ATOM	X	Y	Z
S	0.20353700	1.18057000	0.52676100
C	1.46574900	1.31803600	1.73901100
S	0.84088900	1.55487800	3.36175800
C	-0.86056700	1.55119700	2.99823100
C	-1.18321100	1.36073500	1.56081400
S	3.04884500	1.23443300	1.39443100
Se	-2.80184100	1.31418400	0.88157700
Se	-2.03781800	1.76120600	4.28422200

3-TS

M05-2X SCF energy:	-6108.59173424	a.u.
M05-2X enthalpy:	-6108.545617	a.u.
M05-2X free energy:	-6108.591939	a.u.

Cartesian coordinates

ATOM	X	Y	Z
S	1.37585800	1.46000300	-0.00537800
C	2.34799600	0.00000600	0.01117300
S	1.37587700	-1.46000000	-0.00545700
C	-0.18920500	-0.70510800	-0.18256700
C	-0.18921100	0.70508900	-0.18257600
S	3.97540000	0.00001200	0.05645000
Se	-1.69039900	1.68379400	-0.02054800

Se	-1.69039300	-1.68381600	-0.02050000
H	-2.25229300	-0.42582400	1.39468300
H	-2.25239800	0.42639700	1.39491700

$HC{\equiv}N^{+}{-}CH_2^{-}$

M05-2X SCF energy: -133.819519837 a.u.

M05-2X enthalpy: -133.7561358 a.u.

M05-2X free energy: -133.7853688 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.20492100	0.11074900	0.00000100
N	-0.12233400	-0.45050500	0.00000500
H	-0.38765300	1.62923300	0.00001700
H	0.48599900	1.58531400	0.00002100
H	-2.17653100	-0.37134300	-0.00002500
C	1.13214800	-0.01948900	-0.00000300
H	1.68559900	-0.11864500	0.92539000
H	1.68555900	-0.11858100	-0.92542700

$HC{\equiv}N^{+}{-}NH^{-}$

M05-2X SCF energy: -149.848847633 a.u.

M05-2X enthalpy: -149.7970036 a.u.

M05-2X free energy: -149.8258566 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.15312500	0.06527100	0.05549500
N	-0.06106800	-0.45437500	0.00986200
H	-0.42018100	1.59718900	0.08656900
H	0.45351000	1.49741500	0.03475200
H	-2.15217300	-0.24712300	-0.19162700
N	1.10297200	0.04020100	-0.12807900
H	1.74426200	-0.33988800	0.56484800

$HC{\equiv}N^{+}{-}O^{-}$

M05-2X SCF energy: -169.710826434 a.u.

M05-2X enthalpy: -169.6713114 a.u.

M05-2X free energy: -169.6997714 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.10703900	-0.00234400	0.00000000

N	0.00000000	0.47129600	0.00000000
O	-1.10528200	-0.07552000	0.00000000
H	0.46957300	-1.52244700	0.00000000
H	-0.41245600	-1.43064300	0.00000000
H	2.14290600	0.27224300	0.00000000

$N{\equiv}N^{+}{-}CH_2^{-}$

M05-2X SCF energy: -149.873414597 a.u.

M05-2X enthalpy: -149.8215256 a.u.

M05-2X free energy: -149.8503316 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	-0.16825900	-0.46295800	0.00000500
H	-0.55089100	1.51745600	0.00001100
H	0.37740300	1.45963900	0.00002400
N	-1.21238000	0.02477000	-0.00000300
C	1.09275300	0.06022700	0.00000000
H	1.64069700	-0.13554500	-0.91544600
H	1.64074700	-0.13559200	0.91540500

$N{\equiv}N^{+}{-}NH^{-}$

M05-2X SCF energy: -165.912643538 a.u.

M05-2X enthalpy: -165.8719335 a.u.

M05-2X free energy: -165.9004085 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	0.10002800	-0.46592400	-0.00012500
H	0.57957100	1.44359100	0.08538100
H	-0.35902200	1.40966600	0.06930300
N	1.15800200	0.01040700	0.00919700
N	-1.03674400	0.09840100	-0.09457900
H	-1.76955300	-0.35344100	0.44386700

$N{\equiv}N^{+}{-}O^{-}$

M05-2X SCF energy: -185.776055461 a.u.

M05-2X enthalpy: -185.7471635 a.u.

M05-2X free energy: -185.7750595 a.u.

Cartesian coordinates

ATOM	X	Y	Z

N	0.00000000	0.47648600	0.00000000
O	-1.02996600	-0.19708900	0.00000000
H	0.71399700	-1.31418800	0.00000000
H	-0.22480000	-1.38228400	0.00000000
N	1.10721800	0.13396900	0.00000000

$H_2C=NH^+–CH_2^-$

M05-2X SCF energy: -135.053618324 a.u.

M05-2X enthalpy: -134.9642083 a.u.

M05-2X free energy: -134.9937183 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	0.00000000	-0.54741300	-0.02894300
C	-1.16638900	0.14002100	-0.07528900
H	-1.25349900	0.88333500	-0.85439400
H	-2.06266700	-0.40778000	0.17635800
H	0.00000000	-1.36343100	0.56231300
C	1.16638900	0.14002100	-0.07528900
H	2.06266600	-0.40778000	0.17636100
H	1.25350100	0.88333300	-0.85439600
H	0.45002800	1.28198600	0.94990700
H	-0.45003000	1.28198400	0.94991100

$H_2C=NH^+–NH^-$

M05-2X SCF energy: -151.080263606 a.u.

M05-2X enthalpy: -151.0021216 a.u.

M05-2X free energy: -151.0312366 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	0.02405800	-0.54764300	-0.01211600
C	-1.12569000	0.12635000	-0.07997900
H	-1.21548900	0.84501400	-0.87853700
H	-2.01551400	-0.36613500	0.28246400
H	0.05179900	-1.28437800	0.68190300
N	1.10255600	0.22310800	-0.17823100
H	1.91781500	-0.28400600	0.15306800
H	-0.39147700	1.34999500	0.88719500
H	0.52071300	1.25315100	0.68620600

$H_2C=NH^+–O^-$

M05-2X SCF energy: -170.945242683 a.u.
M05-2X enthalpy: -170.8794637 a.u.
M05-2X free energy: -170.9082737 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	0.03564900	-0.56057400	-0.01703600
C	-1.07924200	0.15364600	-0.08082900
H	-1.14614200	0.88689000	-0.86816500
H	-1.98952800	-0.29787900	0.29106000
H	0.07138900	-1.30563600	0.67016200
O	1.12337300	0.15127900	-0.12157900
H	0.59850000	1.15586600	0.61292100
H	-0.29529700	1.35266700	0.87087600

$HN{=}NH^{+}{-}NH^{-}$

M05-2X SCF energy: -167.094425877 a.u.
M05-2X enthalpy: -167.0277419 a.u.
M05-2X free energy: -167.0564909 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	0.00000000	-0.52611400	0.00496300
H	0.00000000	-1.17786000	0.78698500
N	1.07964500	0.19732800	-0.18300100
H	-0.48620100	1.32421100	0.60325700
H	0.48620100	1.32421100	0.60325600
N	-1.07964500	0.19732800	-0.18300100
H	-1.86154900	-0.27517900	0.26688800
H	1.86154900	-0.27517900	0.26688800

$HN{=}NH^{+}{-}O^{-}$

M05-2X SCF energy: -186.95425241 a.u.
M05-2X enthalpy: -186.9004124 a.u.
M05-2X free energy: -186.9289134 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	0.00713100	-0.53206000	0.01030800
H	-0.00582200	-1.17987900	0.79924700
H	-0.37559400	1.35217500	0.59727600
H	0.59824900	1.21450400	0.52924900
N	-1.02980100	0.22650800	-0.19280600

O	1.09731600	0.11993400	-0.11369800
H	-1.83666900	-0.20740800	0.26129700

$O{=}NH^{+}{-}O^{-}$

M05-2X SCF energy: -206.809260375 a.u.

M05-2X enthalpy: -206.7681574 a.u.

M05-2X free energy: -206.7964704 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	-0.00000300	-0.53274700	0.01893100
H	-0.00001200	-1.17335700	0.81775100
H	-0.49788100	1.25351900	0.53148800
H	0.49788200	1.25350500	0.53150200
O	1.04956900	0.14972100	-0.12581700
O	-1.04956500	0.14972400	-0.12584000

$H_2C{=}O^{+}{-}CH_2^{-}$

M05-2X SCF energy: -154.895213507 a.u.

M05-2X enthalpy: -154.8190835 a.u.

M05-2X free energy: -154.8490105 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.15315400	0.02386500	0.13072300
H	1.21130300	0.63030700	1.02254100
H	2.00363200	-0.49589800	-0.27283800
C	-1.15315400	0.02386500	0.13072300
H	-2.00363200	-0.49589800	-0.27283800
H	-1.21130300	0.63030700	1.02254100
H	-0.39357700	1.66820600	-0.71694500
H	0.39357700	1.66820600	-0.71694500
O	0.00000000	-0.48645200	-0.20427500

$H_2C{=}O^{+}{-}NH^{-}$

M05-2X SCF energy: -170.908658751 a.u.

M05-2X enthalpy: -170.8432398 a.u.

M05-2X free energy: -170.8722738 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.09095400	0.07036600	0.10915200

H	1.12568400	0.70475200	0.98295700
H	1.97530400	-0.39060700	-0.30275500
H	-0.42812200	1.40462700	-0.55746700
H	0.39441800	1.50793600	-0.73013100
O	-0.00750100	-0.54384200	-0.16230500
N	-1.10107600	0.15099900	0.21593300
H	-1.84546800	-0.35515800	-0.26060400

$H_2C{=}O^+{-}O^-$

M05-2X SCF energy: -190.751239536 a.u.

M05-2X enthalpy: -190.6989225 a.u.

M05-2X free energy: -190.7277375 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.02830200	0.11845100	0.12875700
H	0.98809300	0.76825600	0.99114400
H	1.96502500	-0.24518600	-0.27431400
H	-0.49710900	1.27721700	-0.53926400
H	0.30404800	1.49474400	-0.74398200
O	0.00880500	-0.58807700	-0.16630100
O	-1.12503900	0.08736000	0.14053600

$HN{=}O^+{-}NH^-$

M05-2X SCF energy: -186.902213137 a.u.

M05-2X enthalpy: -186.8491341 a.u.

M05-2X free energy: -186.8777941 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	1.06877700	0.13775200	-0.20909000
H	1.80360600	-0.31887500	0.33681300
H	-0.44135600	1.43765900	0.45743900
H	0.44138200	1.43763300	0.45741200
N	-1.06877800	0.13775600	-0.20909000
O	-0.00000200	-0.52076300	0.16734800
H	-1.80361000	-0.31887100	0.33681000

$HN{=}O^+{-}O^-$

M05-2X SCF energy: -206.734902001 a.u.

M05-2X enthalpy: -206.695219 a.u.

M05-2X free energy: -206.723697 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	-0.31975200	1.47557500	0.45569000
H	0.55263700	1.31970100	0.41432400
N	-1.00490800	0.17745800	-0.23071300
O	-0.01919700	-0.53755000	0.18761400
O	1.09409200	0.05969100	-0.13124700
H	-1.79768200	-0.21460700	0.29404300

$O{=}O^{+}{-}O^{-}$

M05-2X SCF energy: -226.558842155 a.u.

M05-2X enthalpy: -226.5324472 a.u.

M05-2X free energy: -226.5607972 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	-0.44394800	1.37400500	0.41857000
H	0.44394900	1.37400300	0.41857000
O	0.00000000	-0.54489500	0.20638700
O	1.03648700	0.10069700	-0.15551500
O	-1.03648700	0.10069700	-0.15551500

$H_2C{=}S^{+}{-}CH_2^{-}$

M05-2X SCF energy: -477.871091867 a.u.

M05-2X enthalpy: -477.7986729 a.u.

M05-2X free energy: -477.8294829 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.29852000	0.41257300	-0.08562900
H	-1.27659800	1.17328600	-0.85326100
H	-2.26476700	-0.02312200	0.13034100
C	1.29852100	0.41257300	-0.08562900
H	2.26476600	-0.02312300	0.13034200
H	1.27659900	1.17328500	-0.85326300
H	0.43016000	1.55267500	0.91665000
H	-0.43016000	1.55267600	0.91665300
S	0.00000000	-0.64728500	0.04000500

$H_2C{=}S^{+}{-}NH^{-}$

M05-2X SCF energy: -493.909250336 a.u.

M05-2X enthalpy: -493.8486383 a.u.

M05-2X free energy: -493.8790593 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.27203000	0.36281300	-0.09602100
H	-1.25511700	1.11572100	-0.86937800
H	-2.22899500	-0.04768800	0.19682200
H	0.42137800	1.51465500	0.68459400
H	-0.46101400	1.56717800	0.87434400
N	1.17516700	0.52836800	-0.18219800
H	2.08680700	0.16179300	0.08713900
S	0.05268500	-0.63669500	0.05487400

$H_2C=S^+–O^-$

M05-2X SCF energy: -513.785072938 a.u.

M05-2X enthalpy: -513.7365459 a.u.

M05-2X free energy: -513.7666289 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.25357000	0.32039700	-0.09288100
H	-1.28041400	1.07708400	-0.86229100
H	-2.20033400	-0.09401800	0.23520500
H	0.42315100	1.44732200	0.60485500
H	-0.46758400	1.54561200	0.84687800
S	0.11136100	-0.62833600	0.04988600
O	1.15810300	0.51937300	-0.13319300

$HN=S^+–NH^-$

M05-2X SCF energy: -509.933713009 a.u.

M05-2X enthalpy: -509.884789 a.u.

M05-2X free energy: -509.9148 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	-2.05858700	0.08255600	0.16675600
H	0.47628500	1.54226300	0.61863000
H	-0.47631300	1.54224500	0.61860600
N	1.18116900	0.46277900	-0.19282700
H	2.05858700	0.08256800	0.16675000
S	0.00000400	-0.60803000	0.07055200
N	-1.18117400	0.46277100	-0.19282800

HN=S^{+}–O^{-}

M05-2X SCF energy: -529.804648485 a.u.

M05-2X enthalpy: -529.7683725 a.u.

M05-2X free energy: -529.7981615 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	-2.03882800	0.06103300	0.18149500
H	0.51454200	1.46774200	0.54974000
H	-0.46729500	1.53131800	0.60246100
S	0.04860500	-0.59949500	0.07007100
N	-1.16173100	0.43408100	-0.19510000
O	1.16825300	0.43665700	-0.13614000

O=S^{+}–O^{-}

M05-2X SCF energy: -549.67193136 a.u.

M05-2X enthalpy: -549.6483814 a.u.

M05-2X free energy: -549.6780684 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	0.51505700	1.45982800	0.54241100
H	-0.51501700	1.45984700	0.54241700
S	-0.00000100	-0.58855900	0.07183200
O	1.14818900	0.40607600	-0.13963500
O	-1.14819200	0.40608200	-0.13963200