Electronic Suplementary Information (ESI)

Unexpected Transalkylation on 3-Alkyl-2-alkylthio-1,3,4-thiadiazolium-5-thiolates: A Computational and Experimental Mechanistic Study.

Arturo Espinosa,* Rafaela García, Pedro Molina and Alberto Tárraga.

Departamento de Química Orgánica. Facultad de Química. Universidad de Murcia.

Campus de Espinardo, E-30100 Murcia, Spain.

E-mail: ***artuesp@um.es***

Table of contents

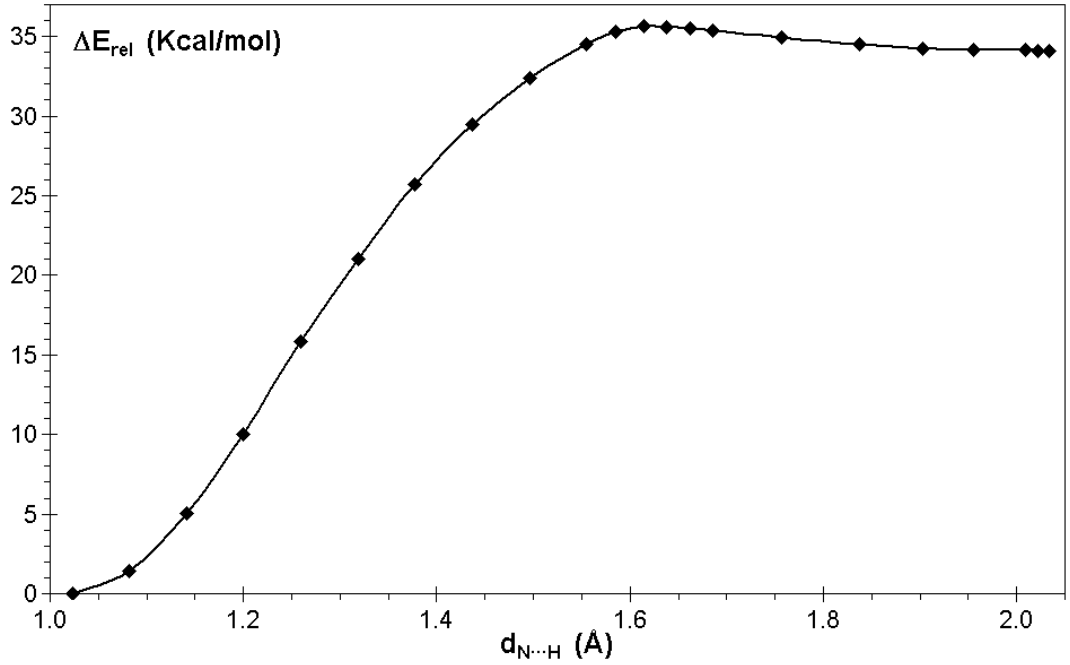


Figure SI 1: Evolution of the calculated total electronic energy for the transformation **1a→10** along the N···H distance as reaction coordinate.

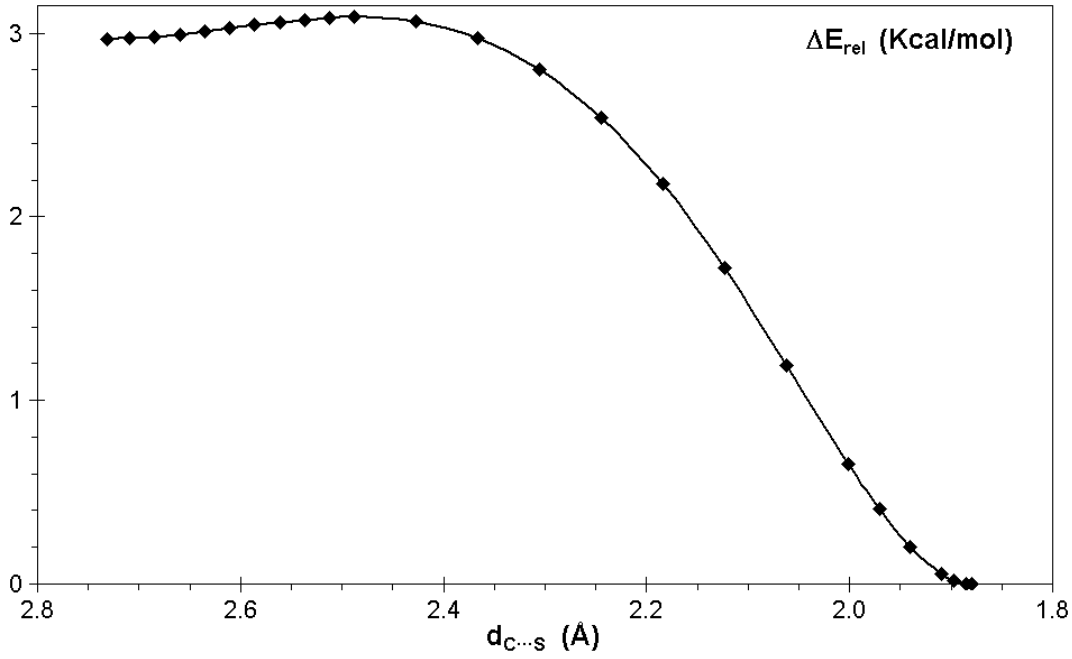


Figure SI 2: Evolution of the calculated total electronic energy for the transformation **15*syn*→2a** along the C···S distance as reaction coordinate.

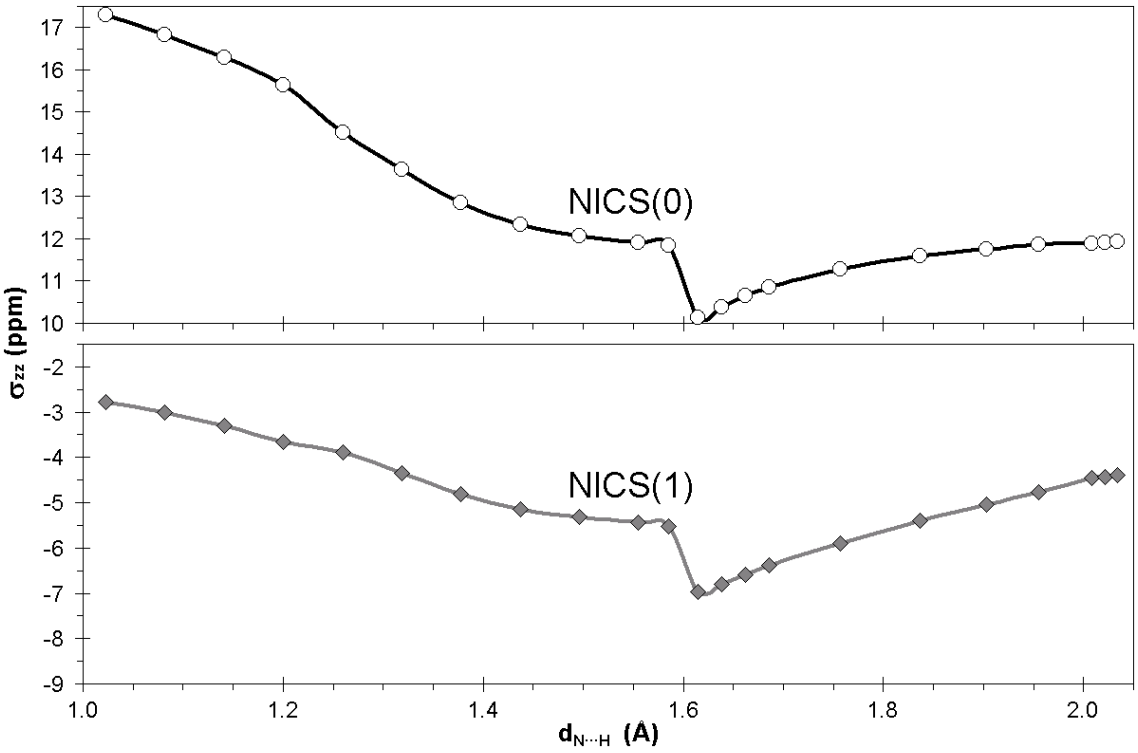


Figure SI 3: Evolution of the calculated $NICS_{zz}$ for the transformation **1a→10** along the N···H distance as reaction coordinate.

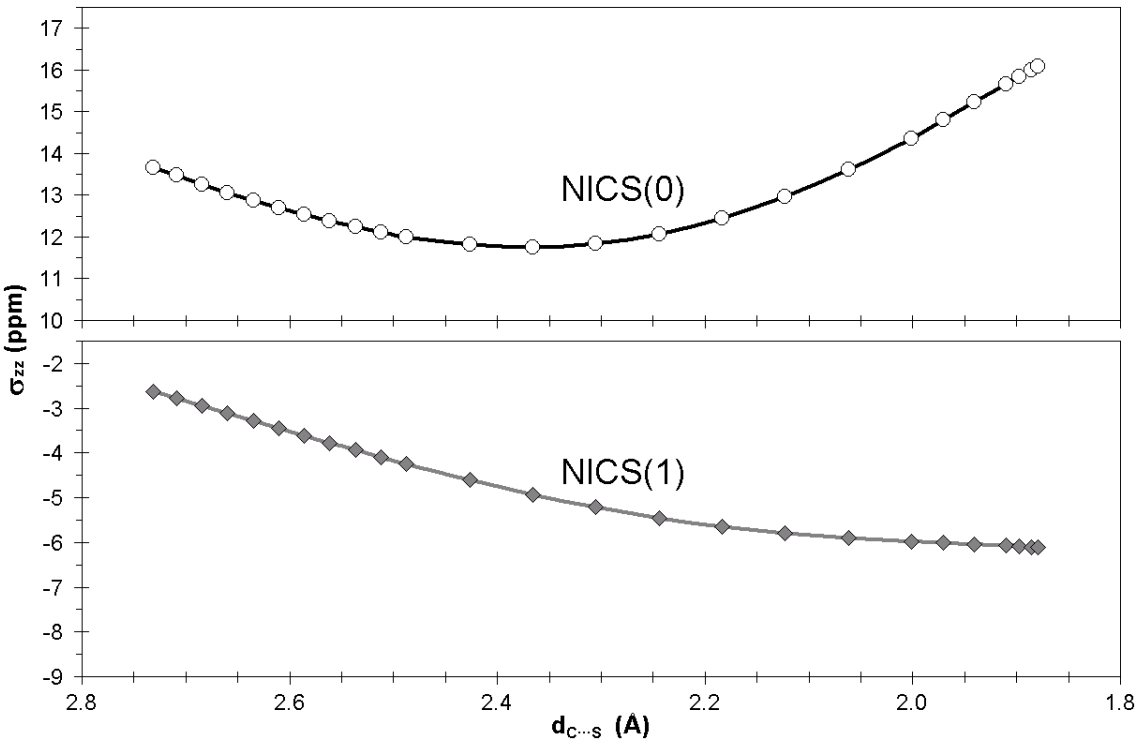
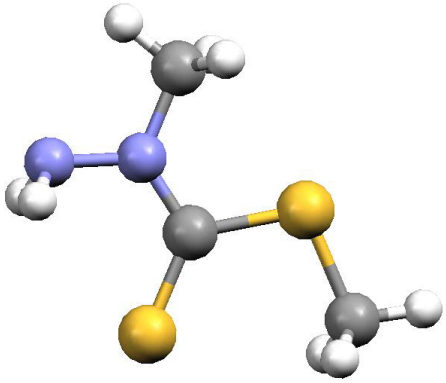


Figure SI 4: Evolution of the calculated $NICS_{zz}$ for the transformation **15*syn*→2a** along the C···S distance as reaction coordinate.

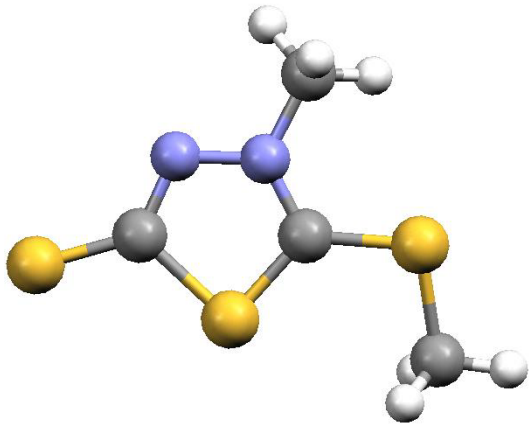
Calculated structures. Energy (au), imaginary vibration mode (cm^{-1}) and cartesian coordinates (Å) for all reported compounds and transition states**.**



Compound **1a**$_{syn}$: E = -1025.109846 au

$G^{o}_{CS_2}$ = -1025.022934 au

C	0.097774	0.199625	-0.000013	S	-1.148268	-1.087874	-0.000034
N	1.359220	-0.297896	-0.000035	C	-2.697452	-0.138544	-0.000012
N	2.477315	0.567159	0.000064	H	-2.767477	0.481797	0.891114
C	1.679188	-1.726259	-0.000003	H	-3.485069	-0.894250	-0.000024
H	2.762164	-1.806612	-0.000272	H	-2.767482	0.481831	-0.891113
H	1.276710	-2.219639	-0.889452	H	2.390426	1.182585	-0.808639
H	1.277163	-2.219520	0.889720	H	2.390343	1.182517	0.808810
S	-0.252331	1.832719	0.000023				



Compound **2a**: E = -1460.213030 au

$G^{o}_{CS_2}$ = -1460.146508 au

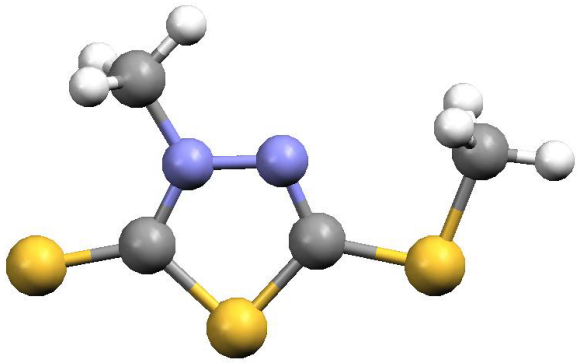
S	0.323997	-1.207056	-0.051588	C	-0.686824	2.600983	0.045060
C	1.765155	-0.000959	0.003968	H	-1.650610	2.566415	0.552581
N	1.280211	1.233299	0.042092	H	-0.816324	2.954762	-0.979729
N	-0.085805	1.267543	0.041561	H	-0.004718	3.260205	0.575809
C	-0.760497	0.126138	-0.017924	S	-2.515059	0.091532	-0.107873
S	3.328930	-0.539770	0.004163	C	-2.856927	-1.683565	0.157834

H	-2.494587	-2.006525	1.132333	H	-3.943299	-1.767214	0.124293
H	-2.422626	-2.284414	-0.639719				

Compound **2a** (MP2/6-311+G**): E = -1456.447618 au

$G_{gas\text{-}phase}$ = -1457.733117 au

S	0.454106	-1.216898	-0.315232	H	-0.848062	2.938165	-0.876146
C	1.744470	-0.012678	0.024525	H	-0.256154	3.099152	0.803053
N	1.183017	1.236215	0.153206	S	-2.456275	-0.194258	-0.507565
N	-0.145456	1.187414	0.037495	C	-2.923788	-1.187530	0.944601
C	-0.750512	-0.003503	-0.203849	H	-2.728502	-0.642549	1.869810
S	3.339251	-0.391539	0.154012	H	-2.397186	-2.143119	0.949239
C	-0.833532	2.482722	0.116059	H	-3.997224	-1.375167	0.855272
H	-1.848940	2.327183	0.476420				



Compound **3a**: E = -1460.239741 au

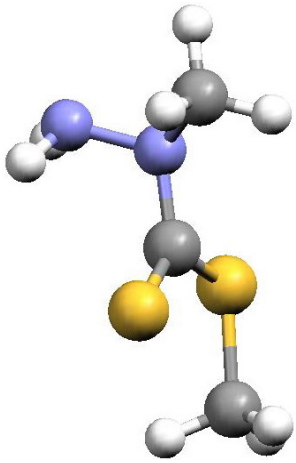
$G^{o}_{CS_2}$ = -1460.166744 au

S	1.511214	0.103835	0.000000	H	-2.758224	-1.471794	0.000000
C	0.574414	-1.414120	0.000000	H	-1.758196	-2.663633	0.886100
N	-0.738014	-1.058424	0.000000	H	-1.758196	-2.663633	-0.886100
N	-1.064760	0.276851	0.000000	C	-1.793046	3.093203	0.000000
C	0.000000	1.008025	0.000000	H	-2.255887	2.677611	-0.893175
S	1.207883	-2.943581	0.000000	H	-2.255887	2.677611	0.893175
S	0.003291	2.764397	0.000000	H	-1.885961	4.179161	0.000000
C	-1.825776	-2.030230	0.000000				

Compound **3a** (MP2/6-311+G**): E = -1456.489787 au

$G_{gas\text{-}phase}$ = -1457.759211 au

S	1.498309	0.137170	0.000000	H	-2.724073	-1.526605	0.000000
C	0.605730	-1.382967	0.000000	H	-1.673288	-2.685097	0.888061
N	-0.721632	-1.049764	0.000000	H	-1.673288	-2.685097	-0.888061
N	-1.080301	0.265374	0.000000	C	-1.828725	2.986662	0.000000
C	0.000000	1.014254	0.000000	H	-2.274034	2.546774	-0.892369
S	1.239467	-2.902447	0.000000	H	-2.274034	2.546774	0.892369
S	-0.038052	2.756378	0.000000	H	-1.988558	4.066719	0.000000
C	-1.772800	-2.056345	0.000000				

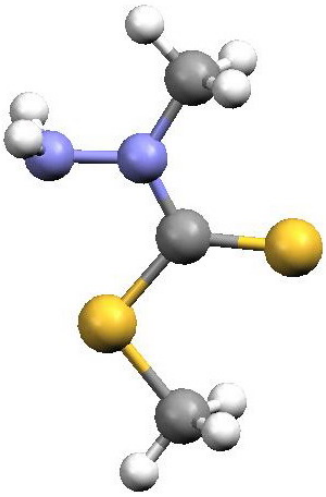


Transition state $\mathbf{TS_{1a}}^{s/a}$: E = -1025.088807 au

$G^{o}_{CS_2}$ = -1024,997226 au

ν = -67.7 cm^{-1}

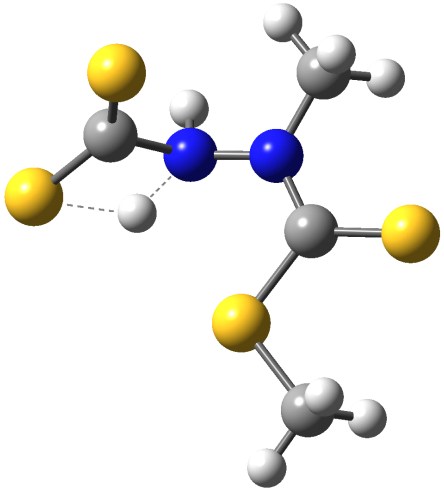
C	-0.049938	0.100787	-0.029975	S	1.237990	-1.070734	-0.121630
N	-1.293938	-0.630142	-0.050633	C	2.749830	-0.065889	-0.001784
N	-1.959117	-0.599989	1.215799	H	2.804613	0.635050	-0.833895
C	-2.209383	-0.217833	-1.117556	H	3.583133	-0.768318	-0.044094
H	-3.060008	-0.898222	-1.099811	H	2.765776	0.483202	0.939202
H	-1.695406	-0.306158	-2.076615	H	-1.484945	-1.244497	1.839781
H	-2.561000	0.814640	-0.995406	H	-1.921607	0.339301	1.617253
S	0.099371	1.736580	0.083712				



Compound $\mathbf{1a}_{anti}$: E = -1025.108135 au

$G^{o}_{CS_2}$ = -1025.021736 au

C	0.076190	0.187066	0.000000	S	-1.183184	-1.081206	-0.000001
N	1.335272	-0.324720	-0.000001	C	-2.700665	-0.075319	-0.000001
N	1.480845	-1.721536	-0.000001	H	-2.758307	0.548559	0.890096
C	2.518731	0.539140	0.000000	H	-3.512785	-0.805292	-0.000002
H	3.398595	-0.104010	-0.000004	H	-2.758306	0.548559	-0.890100
H	2.530150	1.181460	0.883515	H	1.977656	-2.027194	0.831838
H	2.530146	1.181467	-0.883509	H	1.977657	-2.027194	-0.831839
S	-0.220763	1.826338	0.000002				

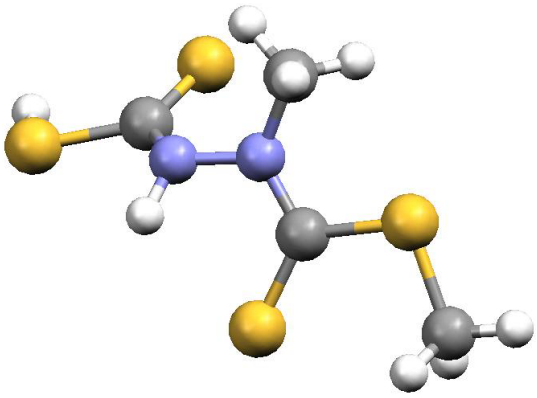


Transition state **$TS_{1anti-6}$**: E = -1859.587316 au

$G^{o}_{CS_2}$ = -1859.501829 au

ν = -1480.3 cm^{-1}

C	-1.362234	-0.275583	-0.174475	C	-2.766006	2.018261	0.599063
N	-0.267498	-0.922420	-0.680424	H	-3.554390	1.773265	-0.109685
N	0.913978	-0.205118	-0.978012	H	-2.674993	3.100071	0.709276
C	-0.239068	-2.381120	-0.856645	H	-2.970671	1.555956	1.562540
H	0.727489	-2.655140	-1.278632	H	1.358194	-0.677689	-1.766750
H	-1.045360	-2.688774	-1.523781	H	1.197883	1.040277	-1.216875
H	-0.356239	-2.881640	0.104213	C	2.029967	-0.003037	0.105500
S	-2.744821	-1.096634	0.231802	S	2.625999	1.511096	-0.421494
S	-1.147338	1.486110	-0.029337	S	2.317209	-1.077115	1.287035

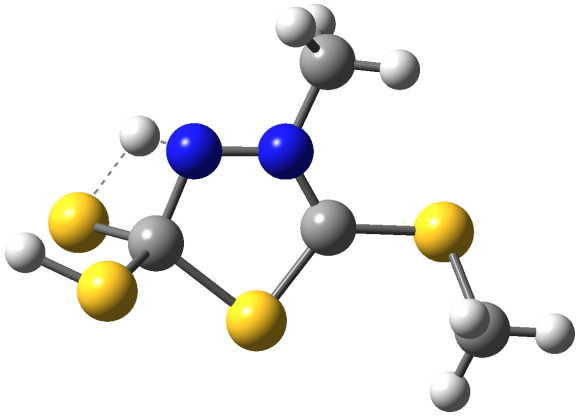


Compound **6**: E = -1859.650715 au

$G^{o}_{CS_2}$ = -1859.561243 au

S	1.229861	1.829925	0.248045	H	0.812254	-1.826004	-2.080752
C	1.302786	0.203437	-0.114389	H	-0.721705	-2.220345	-1.252323
N	0.221367	-0.519893	-0.519999	H	0.808207	-2.535647	-0.437572
N	-0.965576	0.174367	-0.727400	S	2.793180	-0.773252	-0.061134
C	-2.065347	-0.083816	0.048618	C	4.027140	0.433748	0.506658
C	0.293172	-1.858119	-1.117984	H	4.115750	1.254814	-0.201671

H	3.765676	0.814883	1.491626	H	-4.180054	0.662820	0.606962
H	4.960312	-0.130055	0.554136	S	-2.211927	-1.306662	1.143090
S	-3.367826	1.067770	-0.385411	H	-0.790077	1.142230	-0.999465

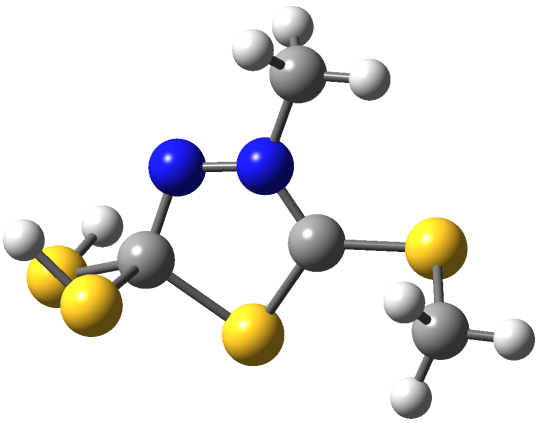


Transition state **TS_{6-7}**: E = -1859.56447967 au

$G^{o}_{CS_2}$ = -1859.557468 au

ν = -1505.5 cm^{-1}

S	0.00000000	0.00000000	0.00000000	C	1.41670572	-2.79536344	0.13784298
C	1.65284733	0.00000000	0.00000000	H	0.82310805	-2.68806074	1.04356162
N	2.41450003	1.15263261	0.00000000	H	0.76803707	-2.78059317	-0.73548780
N	1.76639042	2.34075653	-0.35945088	H	1.99466284	-3.72068048	0.16841061
C	3.85911923	1.16815492	-0.28110853	S	0.71321958	4.54986052	-0.35408243
H	4.36641023	0.42485559	0.33305369	C	1.43869683	3.26297151	0.52716061
H	4.23801119	2.15482251	-0.02083181	S	1.66552506	3.21805377	2.25007382
H	4.06027505	0.96885980	-1.33808926	H	2.16510511	1.95906302	2.26553219
S	2.66169370	-1.47756515	0.02867754	H	1.20203695	3.22238915	-1.25837410

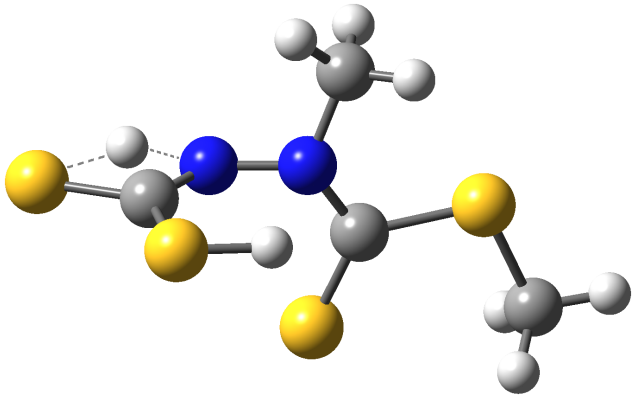


Compound **7**: E = -1859.60184215 au

$G^{o}_{CS_2}$ = -1859.594388 au

S	0.00000000	0.00000000	0.00000000	C	1.73848104	3.45959798	-0.89748621
C	1.89403773	0.00000000	0.00000000	H	2.56398828	3.39132113	-1.60443193
N	2.28991623	1.34536348	0.00000000	H	2.08275050	3.95096636	0.01266865
N	1.32481692	2.09665979	-0.54911808	H	0.89827904	3.99650236	-1.32755329
C	0.08786371	1.62023371	-0.66408264	S	2.36467221	-0.94718037	-1.60803583

H	3.69263132	-0.73629220	-1.47773473	H	-2.09663590	0.61446759	-2.41891014
S	-1.31709225	2.54819171	-1.14240765	H	-1.10000300	1.70729690	-3.42916922
C	-1.86318049	1.65098900	-2.65488068	S	2.63064243	-0.95813187	1.36978910
H	-2.76762919	2.16296150	-2.98605902	H	2.40359978	-0.01979644	2.31574464

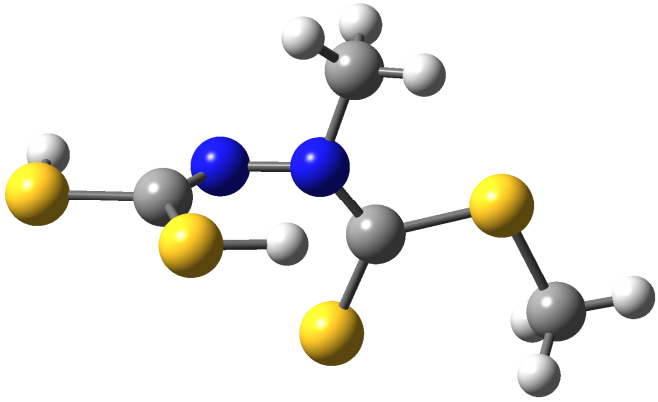


Transition state **$TS_{6\text{-}8}$**: E = -1859.59379173 au

$G^{o}_{CS_2}$ = -1859.583004 au

ν = -1590.8 cm^{-1}

S	0.00000000	0.00000000	0.00000000	C	1.41670572	-2.79536344	0.13784298
C	1.65284733	0.00000000	0.00000000	H	0.82310805	-2.68806074	1.04356162
N	2.41450003	1.15263261	0.00000000	H	0.76803707	-2.78059317	-0.73548780
N	1.76639042	2.34075653	-0.35945088	H	1.99466284	-3.72068048	0.16841061
C	3.85911923	1.16815492	-0.28110853	S	0.71321958	4.54986052	-0.35408243
H	4.36641023	0.42485559	0.33305369	C	1.43869683	3.26297151	0.52716061
H	4.23801119	2.15482251	-0.02083181	S	1.66552506	3.21805377	2.25007382
H	4.06027505	0.96885980	-1.33808926	H	2.16510511	1.95906302	2.26553219
S	2.66169370	-1.47756515	0.02867754	H	1.20203695	3.22238915	-1.25837410

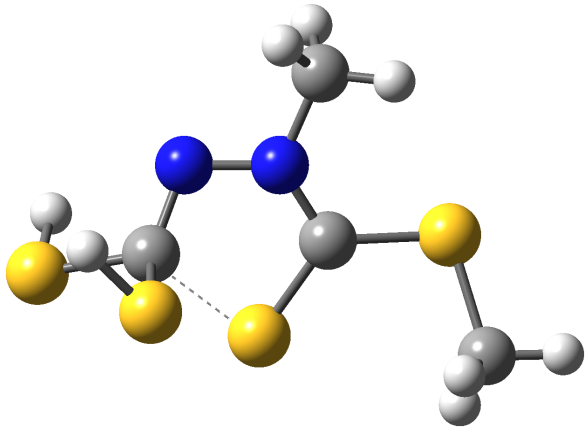


Compound **8**: E = -1859.63320246 au

$G^{o}_{CS_2}$ = -1859.624701 au

S	0.00000000	0.00000000	0.00000000	H	4.35947668	0.38831898	0.27434856
C	1.65656389	0.00000000	0.00000000	H	4.24382721	2.13448916	0.01449345
N	2.41341565	1.14354911	0.00000000	H	4.03706575	1.02420808	-1.36330059
N	1.77193593	2.33356921	-0.44227084	S	2.66005497	-1.48779187	0.03959476
C	3.85206046	1.16629477	-0.29412307	C	1.40779962	-2.79454810	0.18985987

H	0.82193241	-2.66297035	1.09746812	C	1.48894078	3.19022139	0.46648707
H	0.75168470	-2.79717814	-0.67787843	S	1.72936397	3.07160970	2.22316000
H	1.98094751	-3.72228670	0.23768496	H	2.14457445	1.78750398	2.16052060
S	0.75043220	4.72647886	-0.01636387	H	0.75982784	4.41321306	-1.32936328

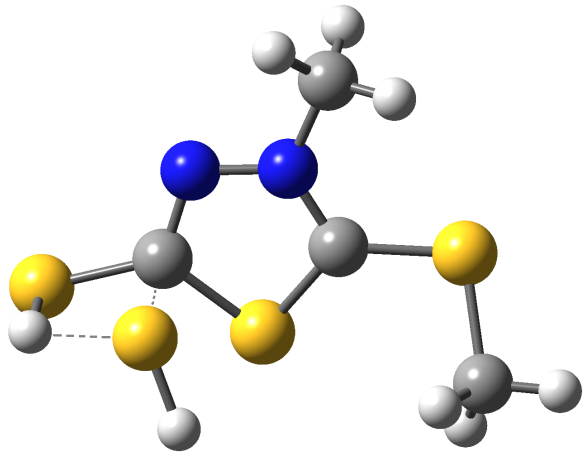


Transition state **$TS_{8\text{-}7}$**: E = -1859.59995826 au

$G^{o}_{CS_2}$ = -1859.593012 au

ν = -198.7 cm^{-1}

S	0.00000000	0.00000000	0.00000000	S	2.70754736	-1.44184538	-0.21270092
C	1.72420310	0.00000000	0.00000000	C	1.76552624	-2.70200552	0.72569925
N	2.27347949	1.21146722	0.00000000	H	1.61833365	-2.37779600	1.75428995
N	1.46274744	2.30831574	-0.16429650	H	0.81284464	-2.91127290	0.24451895
C	0.24102378	2.05873544	0.35878970	H	2.39103787	-3.59539095	0.70483550
C	3.70373541	1.49296574	-0.09925421	S	0.03580412	1.99598650	2.25132499
H	3.92584485	2.32503552	0.56620962	H	0.33370217	3.30276444	2.43487993
H	3.94560103	1.77812762	-1.12545902	S	-1.07878848	3.09523304	-0.29688958
H	4.27241910	0.61207818	0.18976258	H	-0.57374007	3.15957288	-1.54887842



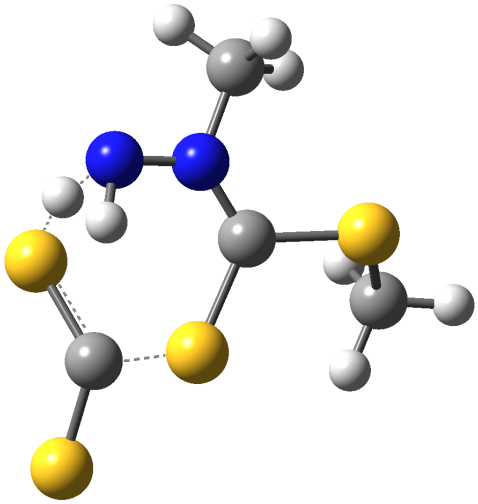
Transition state **$TS_{7\text{-}2a}$**: E = -1859.58530665 au

$G^{o}_{CS_2}$ = -1859.581651 au

ν = -254.3 cm^{-1}

S	0.00000000	0.00000000	0.00000000	C	1.79906640	0.00000000	0.00000000

N	2.28676347	1.21905468	0.00000000	H	1.04285686	-1.36190365	-2.89847969
N	1.33318571	2.09810722	-0.39870664	S	-1.26506184	2.67911749	-0.92087834
C	0.08275369	1.65085867	-0.50056883	C	-2.37045052	1.48771450	-1.77162163
C	1.78416835	3.45931654	-0.69686701	H	-3.17075409	2.09811817	-2.19017080
H	2.78829228	3.38319697	-1.10551872	H	-2.79169446	0.77284342	-1.06734955
H	1.79516293	4.05429337	0.21803091	H	-1.82809034	0.98592261	-2.57100095
H	1.10965633	3.90352800	-1.42664923	S	2.70975130	-1.39186942	0.60941401
S	2.16676199	-0.65667391	-2.63932432	H	2.87144995	-1.80979847	-0.69470364

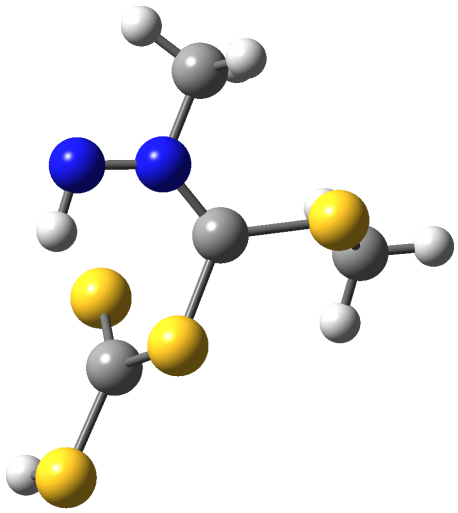


Transition state $\mathbf{TS_{1a\text{-}9}}$: E = -1859.58517643 au

$G^{o}_{CS_2}$ = -1859.577186 au

ν = -607.8 cm^{-1}

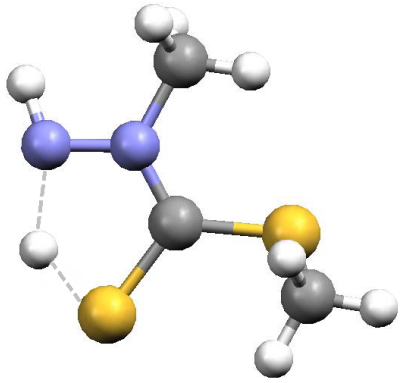
C	0.00000000	0.00000000	0.00000000	H	2.99345657	-0.97736381	-0.72760424
N	1.32852162	0.00000000	0.00000000	H	1.52313382	-2.01112542	-0.63677155
N	2.10959281	1.09841989	0.00000000	H	2.42767067	-1.58340300	0.84158538
C	-0.58250801	2.37895660	-1.62197659	S	-0.89271978	-1.46444664	0.42176193
S	-1.71655799	3.47484044	-2.07524700	C	-2.16111953	-1.53760112	-0.90123102
S	0.86533767	2.03087227	-2.52724591	H	-2.80136608	-2.38065622	-0.63995409
H	1.71659556	1.57563029	-1.39891733	H	-2.74825490	-0.62143089	-0.91335903
S	-0.94418376	1.51144944	-0.06069514	H	-1.69503013	-1.71177837	-1.86958515
C	2.11382245	-1.24317676	-0.14599622	H	1.55731725	1.84349415	0.43569133



Compound **9**: E = -1859.59455335 au

$G^{o}_{CS_2}$ = -1859.585623 au

C	0.00000000	0.00000000	0.00000000	H	3.12470198	-1.06542994	-0.13840141
N	1.35986905	0.00000000	0.00000000	H	1.69774794	-1.92590359	-0.80568851
N	2.17131874	1.00418523	0.00000000	H	1.91432821	-1.80777832	0.95329310
C	-0.72767552	2.22903074	-1.56284343	S	-0.93055259	-1.47886834	0.19716422
S	0.00125179	1.53565363	-2.85327043	C	-1.74967028	-1.67177592	-1.43746377
S	-1.52159305	3.82065077	-1.55613436	H	-2.36612100	-2.56865781	-1.35497721
H	-1.30642263	4.05767073	-2.86553942	H	-2.38749385	-0.81284935	-1.64264306
S	-0.84086363	1.54207471	0.09264908	H	-1.01517026	-1.79445623	-2.23172161
C	2.07572161	-1.30428081	0.00207346	H	1.60747251	1.85852950	-0.00657381

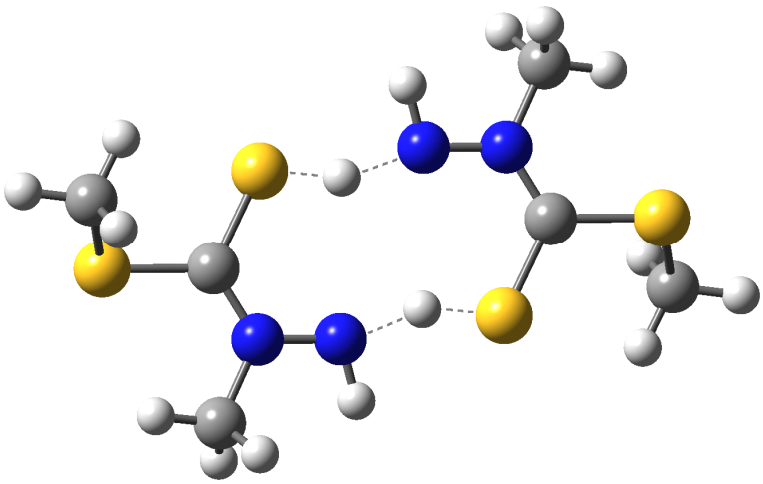


Transition state $\mathbf{TS_{1a\text{-}10}}^{u}$: E = -1025.055939 au

$G^{o}_{CS_2}$ = -1024.972084 au

ν = -554.6 cm^{-1}

C	0.090129	0.150054	-0.164513	S	-1.416139	-0.677293	-0.558335
N	1.231539	-0.495781	0.083192	C	-2.505106	-0.148848	0.826048
N	2.327469	0.229397	0.384555	H	-2.130694	-0.520988	1.778731
C	1.362731	-1.959835	0.043695	H	-2.592382	0.936074	0.845842
H	1.818891	-2.281742	0.980680	H	-3.480543	-0.589219	0.614863
H	2.012058	-2.229906	-0.792237	H	3.148400	-0.354946	0.246820
H	0.389156	-2.423019	-0.082138	H	1.599777	1.641899	0.106133
S	0.205873	1.892187	-0.141934				

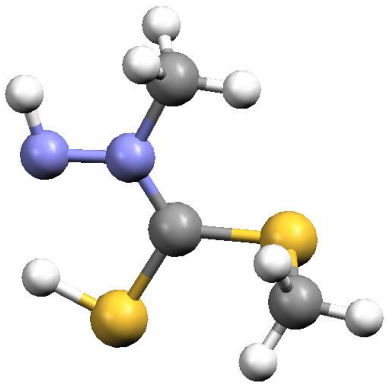


Transition state $\mathbf{TS_{1a\text{-}10}}^{b}$: E = -2050.11598885 au

$G^{o}_{CS_2}$ = -2050.099589 au

ν = -226.5 cm^{-1}

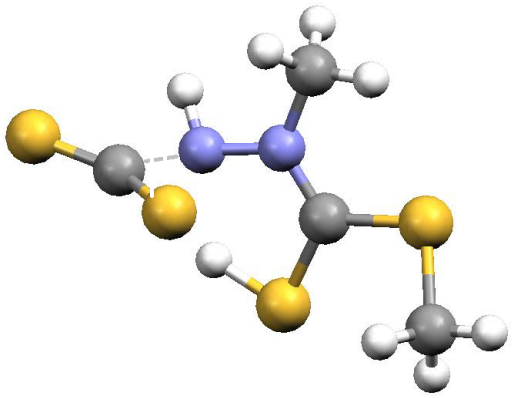
C	0.00000000	0.00000000	0.00000000	C	2.10334066	4.53391169	2.12065827
N	1.32791740	0.00000000	0.00000000	N	0.77542326	4.53391169	2.12065827
N	2.02392103	1.15592052	0.00000000	N	0.07941962	3.37799117	2.12065827
C	2.12123539	-1.24689086	0.00332570	C	-0.01789474	5.78080255	2.11733257
H	2.65265048	-1.31771397	-0.94813861	H	-0.54930983	5.85162566	3.06879688
H	1.48019438	-2.11326315	0.13003145	H	0.62314628	6.64717484	1.99062682
H	2.83878173	-1.18135778	0.82204482	H	-0.73544107	5.71526947	1.29861345
S	-0.90046840	1.49749196	-0.04522021	S	3.00380905	3.03641972	2.16587848
S	-0.92098991	-1.50493206	-0.18095410	S	3.02433056	6.03884375	2.30161237
C	-2.00292398	-1.46995797	1.30097587	C	4.10626464	6.00386966	0.81968240
H	-1.41793332	-1.59378393	2.21152843	H	3.52127397	6.12769561	-0.09087016
H	-2.68935063	-2.30967224	1.18406178	H	4.79269128	6.84358393	0.93659649
H	-2.56140137	-0.53621538	1.32695374	H	4.66474203	5.07012707	0.79370453
H	2.26332722	2.20541043	1.25122840	H	-0.15998656	2.32850126	0.86942987
H	2.99066351	0.90029900	-0.19630219	H	-0.88732285	3.63361268	2.31696046



Compound **10**: E = -1025.057539 au

$G^{o}_{CS_2}$ = -1024.972887 au

S	0.365352	1.936081	-0.063436	S	-1.470702	-0.380597	-0.648379
C	0.125990	0.195843	-0.186840	C	-2.390373	-0.296303	0.947148
N	1.176230	-0.596512	0.043013	H	-2.007809	-1.026551	1.659773
N	2.355948	-0.075305	0.367594	H	-2.329322	0.709103	1.361010
C	1.074533	-2.069182	-0.057181	H	-3.428914	-0.528130	0.705628
H	1.355347	-2.490479	0.909199	H	3.009207	-0.849093	0.464713
H	1.777996	-2.400798	-0.822293	H	1.655999	1.787454	0.342235
H	0.066954	-2.368692	-0.324251				

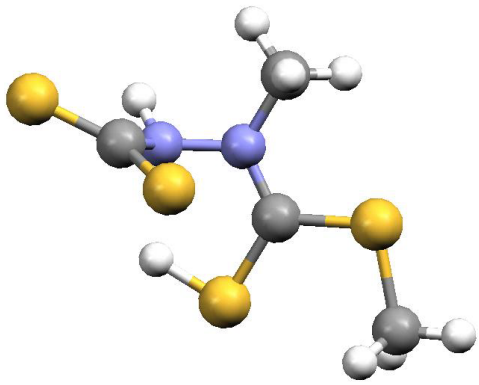


Transition state **TS$_{10\text{-}11}$** (B3LYP/6-31+G*): E = -1859.606097 au

(B3LYP/6-311+G**) $G^{o}_{CS_2}$ = -1859.505356 au

ν = -723.8 cm^{-1}

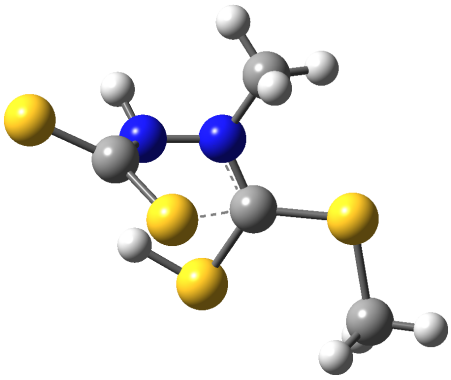
S	1.104133	-1.442692	-1.230210	C	3.359328	-0.876536	0.973496
C	1.213114	0.143092	-0.502202	H	2.607919	-1.305197	1.639212
N	0.175922	0.971347	-0.609182	H	3.663931	-1.598766	0.213931
N	-0.995839	0.477524	-1.100267	H	4.235524	-0.572882	1.553065
C	0.168671	2.343888	-0.077578	H	-1.563050	1.264002	-1.421552
H	1.094226	2.564017	0.452445	S	-3.686348	-0.198765	-0.280458
H	-0.676790	2.428072	0.609312	C	-2.234128	-0.198159	0.414964
H	0.048229	3.040852	-0.913347	S	-1.311061	-0.486140	1.705968
S	2.734930	0.672845	0.218072	H	-0.178951	-1.159875	-1.632952



Compound **11**: E = -1859.608221 au

$G^{o}_{CS_2}$ = -1859.527618 au

S	1.165878	-1.708181	-0.674963	C	3.677437	-0.497854	0.585548
C	1.111942	0.012683	-0.417326	H	3.244727	-1.173927	1.321319
N	0.071009	0.740546	-0.816188	H	3.985109	-1.030178	-0.312633
N	-1.139685	0.055826	-0.979887	H	4.539443	0.009009	1.019794
C	-0.000058	2.190275	-0.578362	H	-1.666991	0.414924	-1.771837
H	0.932475	2.665967	-0.881803	S	-3.622950	-0.232373	-0.222946
H	-0.207305	2.369592	0.480490	C	-2.014462	-0.080857	0.213507
H	-0.814878	2.583743	-1.182928	S	-1.246332	-0.127735	1.709243
S	2.513187	0.852729	0.198227	H	-0.137537	-1.710264	-1.073048

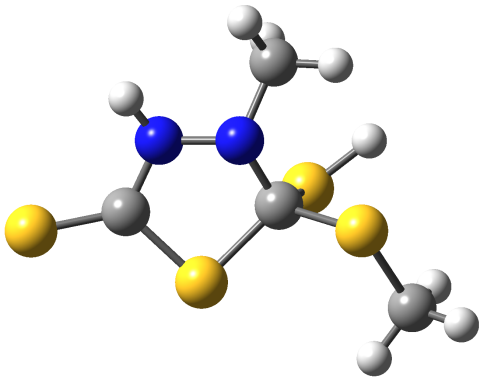


Transition state **$TS_{11\text{-}12}$**: E = -1859.6081735 au

$G^{o}_{CS_2}$ = -1859.609215 au

ν = -31.7 cm^{-1}

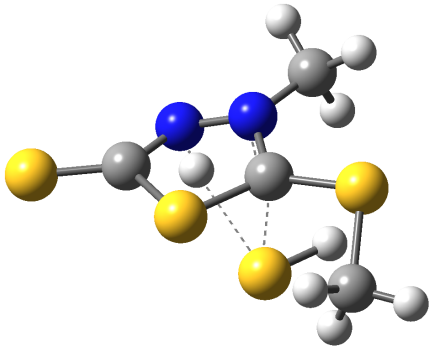
S	0.00000000	0.00000000	0.00000000		C	1.30778515	-2.75405809	-0.25777897
C	1.74881843	0.00000000	0.00000000		H	0.84963100	-2.74160754	0.73006555
N	2.44406494	1.14416234	0.00000000		H	0.56384958	-2.63912608	-1.04394284
N	1.83017431	2.20298889	0.67483442		H	1.84228378	-3.69353543	-0.40003766
C	3.91446658	1.14053238	-0.03113693		H	2.07914779	3.10527557	0.27960881
H	4.26895831	0.52157749	-0.85507668		C	1.92885015	2.21198431	2.14726545
H	4.29765560	0.77455617	0.92645754		S	1.81564274	3.75412208	2.78276656
H	4.24298905	2.16569734	-0.19149357		S	2.06274133	0.70395796	2.89231169
S	2.60757937	-1.47832426	-0.36730831		H	-0.04542615	1.31184701	0.34672998



Compound **12**: E = -1859.627807 au

$G^{o}_{CS_2}$ = -1859.624469 au

S	0.00000000	0.00000000	0.00000000		C	1.72356094	-2.47349095	-1.44280352
C	1.88339667	0.00000000	0.00000000		H	1.88486632	-3.03008756	-0.51920702
N	2.52731443	1.30585219	0.00000000		H	0.65928464	-2.32493851	-1.61316949
N	2.50099089	1.81729895	1.33765173		H	2.15367188	-3.03564687	-2.27313029
C	2.02030128	2.30729659	-0.94009318		H	2.96747348	2.70908412	1.45191003
H	1.01579620	2.65617142	-0.67586437		C	2.65829875	0.90722166	2.32817984
H	2.01645163	1.86718923	-1.93602271		S	3.06857233	1.22243305	3.89360949
H	2.71184222	3.15222310	-0.94933054		S	2.35138133	-0.70346711	1.65902423
S	2.63643979	-0.89366128	-1.42479699		H	-0.15498216	0.35497883	-1.29550524

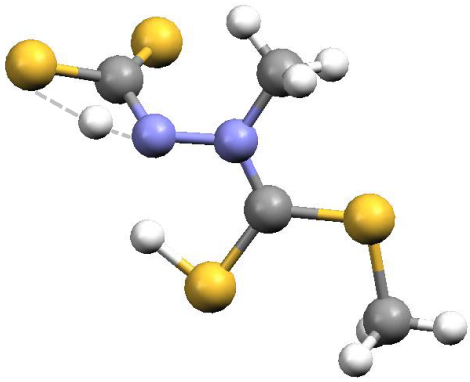


Transition state **$TS_{12\text{-}2a}$**: E = -1859.58774845 au

$G^{o}_{CS_2}$ = -1859.582646 au

ν = -220.9 cm^{-1}

S	0.00000000	0.00000000	0.00000000	C	3.12550894	-2.58846432	-0.88547754
C	2.96749842	0.00000000	0.00000000	H	3.78334692	-2.91785451	-0.08269318
N	2.84266232	1.33043641	0.00000000	H	2.07489126	-2.63782158	-0.60003798
N	2.15312671	1.80435752	1.14395240	H	3.30075034	-3.19736387	-1.77201211
C	2.65468581	2.13443122	-1.19741125	H	1.10958110	1.55894766	0.88369435
H	1.65978615	1.94359546	-1.61545433	C	2.45157762	0.99730376	2.24662232
H	3.42294205	1.88484030	-1.92786876	S	2.13320517	1.32755208	3.80488122
H	2.74997898	3.17958513	-0.91187710	S	3.07788845	-0.58791108	1.65003525
S	3.51036526	-0.87684204	-1.40410941	H	-0.19551176	0.51696214	-1.23177184

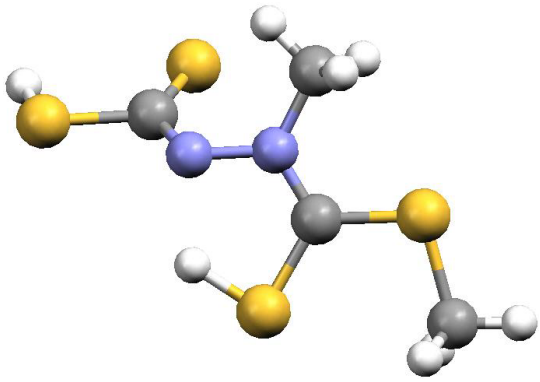


Transition state **$TS_{11\text{-}13}$**: E = -1859.574033 au

$G^{o}_{CS_2}$ = -1859.493797 au

ν = -1522.8 cm^{-1}

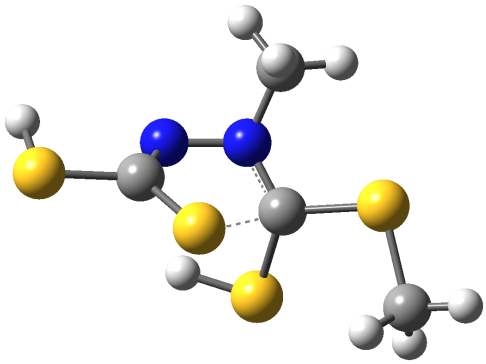
S	1.309482	1.756183	0.420677	S	2.747690	-0.841773	-0.288945
C	1.283804	0.109617	-0.135843	C	4.040870	0.289883	0.326974
N	0.135558	-0.437928	-0.493617	H	4.106579	1.183194	-0.291840
N	-1.006007	0.377882	-0.546883	H	3.870195	0.545293	1.371184
C	-2.150951	-0.019331	0.176895	H	4.964760	-0.282327	0.239441
C	0.041761	-1.818515	-0.997167	S	-3.394466	0.772737	-0.766373
H	0.469252	-1.875602	-2.001919	H	-1.850451	0.860632	-1.429320
H	-1.009510	-2.089109	-1.019493	S	-2.178714	-0.972502	1.529082
H	0.564647	-2.496385	-0.322147	H	-0.059113	1.770382	0.201395



Compound **13**: E = -1859.621341 au

$G^{o}_{CS_2}$ = -1859.536870 au

S	1.245699	1.809617	0.289675	S	2.785223	-0.806297	-0.134687
C	1.293187	0.121570	-0.138941	C	4.011616	0.406659	0.461263
N	0.182822	-0.468352	-0.527247	H	4.101423	1.245223	-0.226828
N	-0.958280	0.326135	-0.698288	H	3.767785	0.747651	1.466045
C	-2.020074	-0.058618	0.021505	H	4.950209	-0.147587	0.485671
C	0.180224	-1.845296	-1.053671	S	-3.405368	0.999793	-0.434145
H	0.789648	-1.884641	-1.960834	H	-4.230104	0.505315	0.506997
H	-0.846772	-2.113564	-1.274970	S	-2.149746	-1.275957	1.171177
H	0.566820	-2.531072	-0.299920	H	-0.073443	1.793819	-0.130662

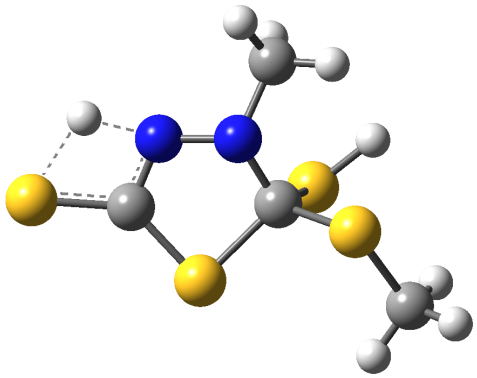


Transition state $\mathbf{TS_{13\text{-}14}}$: E = -1859.60472021 au

$G^{o}_{CS_2}$ = -1859.597800 au

ν = -176.6 cm^{-1}

S	0.00000000	0.00000000	0.00000000	C	1.39930865	-2.68536022	-0.72378220
C	1.80115295	0.00000000	0.00000000	H	1.26446422	-2.86126236	0.34265623
N	2.43639406	1.20161828	0.00000000	H	0.44182367	-2.53389831	-1.21872339
N	2.13746991	2.05419776	1.09462515	H	1.90548975	-3.54053616	-1.17262757
C	3.83221337	1.32573868	-0.42208776	H	2.08846864	3.52749132	3.11123488
H	3.95895152	0.91597078	-1.42439808	C	2.14313280	1.38608753	2.22738387
H	4.50342080	0.81826083	0.28068853	S	1.96998501	2.32448387	3.71785424
H	4.06032282	2.38978665	-0.44016714	S	2.25542389	-0.32485094	2.36933469
S	2.53797961	-1.28340784	-0.99271042	H	-0.10408097	1.15036952	0.69734621

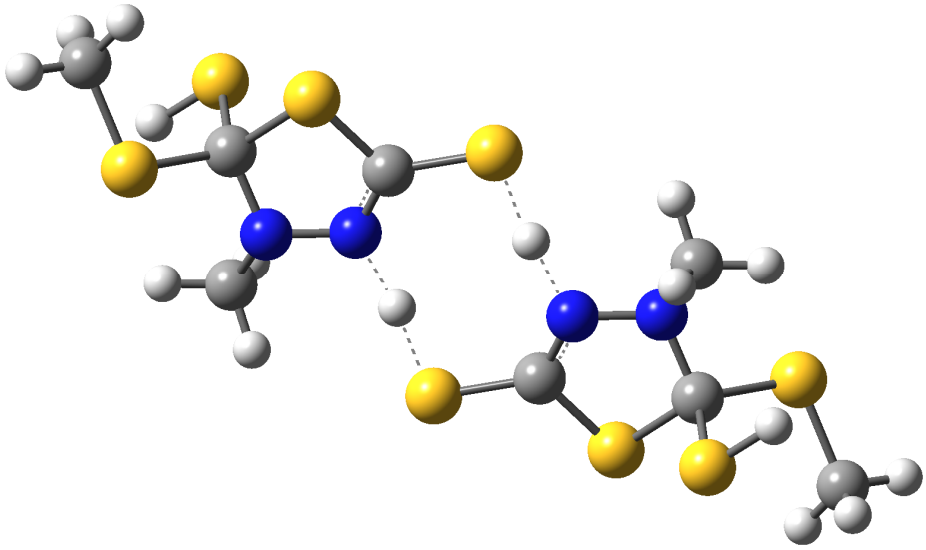


Transition state $\mathbf{TS_{12\text{-}14}}^{\mathbf{u}}$: E = -1859.56755643 au

$G^{o}_{CS_2}$ = -1859.559194 au

ν = -1699.2 cm^{-1}

S	0.00000000	0.00000000	0.00000000		C	1.68646600	-2.46334499	-1.47447526
C	1.88803909	0.00000000	0.00000000		H	1.79811139	-3.03522052	-0.55289923
N	2.52910659	1.31008167	0.00000000		H	0.63358769	-2.28344482	-1.68077965
N	2.59036093	1.81368651	1.32461580		H	2.13049986	-3.02827589	-2.29573334
C	2.04970539	2.31780703	-0.94488344		H	3.02368461	2.62261622	2.30131532
H	1.04379585	2.67441208	-0.69665925		C	2.62278305	0.90420780	2.25906531
H	2.05977044	1.88865309	-1.94593277		S	3.06846452	1.65417388	3.74496892
H	2.74712303	3.15505737	-0.92039113		S	2.33890002	-0.71682730	1.68798936
S	2.64356975	-0.91026926	-1.40698797		H	-0.15001429	0.36898551	-1.29159638



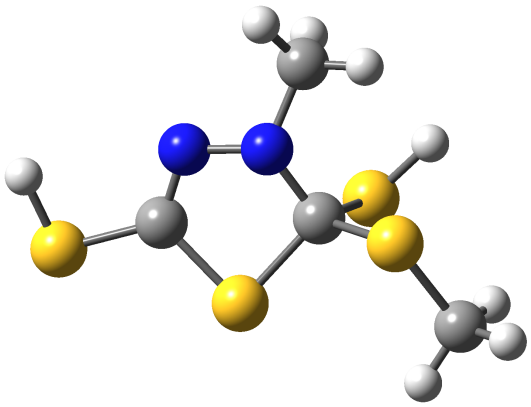
Transition state $\mathbf{TS_{12\text{-}14}}^{\mathbf{b}}$: E = -3719.24297511 au

$G^{o}_{CS_2}$ = -3719.224519 au

ν = -1136.4 cm^{-1}

S	0.00000000	0.00000000	0.00000000		S	2.63752755	-0.91201454	-1.41851125
C	1.89435957	0.00000000	0.00000000		C	1.72463166	-2.49210213	-1.42023726
N	2.52159677	1.31009081	0.00000000		H	1.91053800	-3.05491715	-0.50498548
N	2.60375167	1.85729653	1.29685391		H	0.65624254	-2.33952686	-1.55901182
C	2.06405546	2.29099449	-0.98513434		H	2.12945362	-3.04952460	-2.26643909
H	1.08174126	2.70468269	-0.73245669		H	3.08034616	3.18294161	1.40012903
H	2.02405582	1.80441373	-1.95850149		C	2.61461989	0.97534980	2.24217155
H	2.79602482	3.09645948	-1.04193068		S	2.86379468	1.24103596	3.93168870

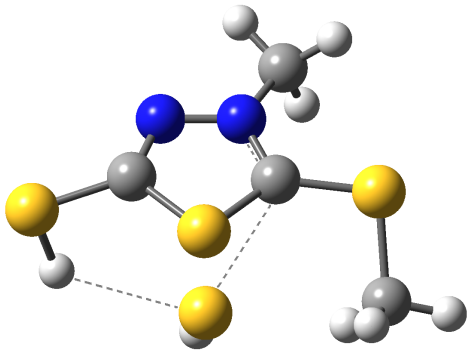
S	2.37209015	-0.68201894	1.65730919	S	3.84809572	6.79943599	6.70754624
H	-0.15450106	0.37375084	-1.28960204	C	4.76099161	8.37952359	6.70927225
S	6.48562327	5.88742145	5.28903499	H	4.57508527	8.94233860	5.79402047
C	4.59126370	5.88742145	5.28903499	H	5.82938073	8.22694832	6.84804681
N	3.96402651	4.57733064	5.28903499	H	4.35616966	8.93694605	7.55547408
N	3.88187161	4.03012492	3.99218108	H	3.40527711	2.70447984	3.88890596
C	4.42156781	3.59642696	6.27416933	C	3.87100338	4.91207165	3.04686344
H	5.40388201	3.18273877	6.02149168	S	3.62182859	4.64638550	1.35734629
H	4.46156745	4.08300773	7.24753648	S	4.11353312	6.56944040	3.63172580
H	3.68959845	2.79096197	6.33096567	H	6.64012433	5.51367061	6.57863703



Compound **14**: E = -1859.62353746 au

$G^{o}_{CS_2}$ = -1859.616508 au

S	0.00000000	0.00000000	0.00000000	C	1.73714181	-2.51201293	-1.38556056
C	1.90096767	0.00000000	0.00000000	H	1.95177105	-3.06572733	-0.47086133
N	2.52071789	1.31329519	0.00000000	H	0.66408183	-2.36943360	-1.49720977
N	2.65602623	1.87825958	1.26703171	H	2.12463533	-3.07255015	-2.23777215
C	2.10503832	2.29247846	-1.00122891	H	3.37566599	2.57887005	3.68899281
H	1.10664672	2.69409516	-0.79372414	C	2.64792900	0.99830509	2.18790532
H	2.11896101	1.82180004	-1.98361498	S	2.92288915	1.32559150	3.90110160
H	2.82810485	3.10679689	-0.99079572	S	2.38472999	-0.68176095	1.65972815
S	2.63267195	-0.92253588	-1.41672766	H	-0.15185211	0.37697133	-1.28880839



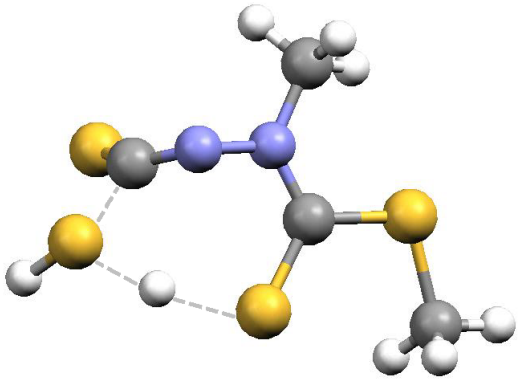
Transition state $\mathbf{TS_{14\text{-}2a}}$: E = -1859.59173701 au

$G^{o}_{CS_2}$ = -1859.588973 au

ν = -73.7 cm^{-1}

S	0.00000000	0.00000000	0.00000000	N	2.84266232	1.33043641	0.00000000
C	2.96749842	0.00000000	0.00000000	N	2.15312671	1.80435752	1.14395240

C	2.65468581	2.13443122	-1.19741125	H	2.07489126	-2.63782158	-0.60003798
H	1.65978615	1.94359546	-1.61545433	H	3.30075034	-3.19736387	-1.77201211
H	3.42294205	1.88484030	-1.92786876	H	1.10958110	1.55894766	0.88369435
H	2.74997898	3.17958513	-0.91187710	C	2.45157762	0.99730376	2.24662232
S	3.51036526	-0.87684204	-1.40410941	S	2.13320517	1.32755208	3.80488122
C	3.12550894	-2.58846432	-0.88547754	S	3.07788845	-0.58791108	1.65003525
H	3.78334692	-2.91785451	-0.08269318	H	-0.19551176	0.51696214	-1.23177184

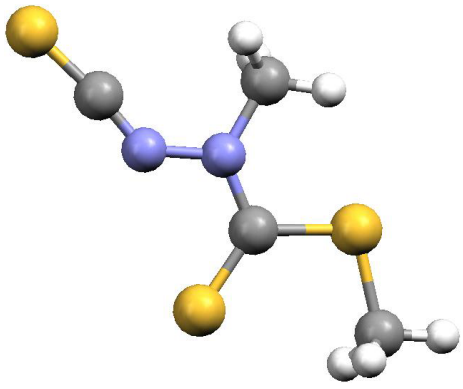


Transition state **$TS_{13\text{-}15}$**: E = -1859.580337 au

$G^{o}_{CS_2}$ = -1859.497502 au

ν = -609.3 cm^{-1}

S	-0.568052	-1.641250	0.007950	S	-2.784911	0.453049	0.044597
C	-1.093501	-0.022462	-0.221677	C	-3.545869	-1.052257	0.731816
N	-0.279818	0.947878	-0.630844	H	-3.515430	-1.866792	0.011770
N	0.992580	0.496685	-1.025808	H	-3.056721	-1.344053	1.658813
C	1.842758	0.442864	-0.044293	H	-4.579761	-0.764079	0.928380
C	-0.643576	2.328149	-0.943120	S	2.729893	-1.275036	-0.548640
H	-0.887738	2.422676	-2.005010	H	3.260719	-1.565704	0.659100
H	0.212447	2.956584	-0.703530	S	2.151499	1.146324	1.402357
H	-1.493973	2.639375	-0.337451	H	1.257374	-1.697103	-0.252103

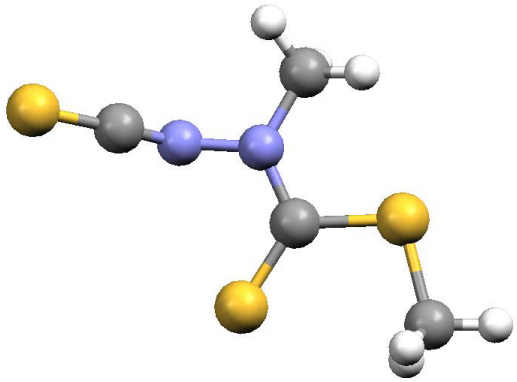


Compound **15_{anti}**: E = -1460.204295 au

$G^{o}_{CS_2}$ = -1460.133465 au

N	-1.334933	0.372086	-0.006864	C	-0.504384	-1.884746	-0.022169
C	-2.526936	0.180127	0.000434	C	0.980142	0.180586	-0.018926
S	-4.102543	0.102120	0.022432	S	1.158890	1.821304	-0.004065
N	-0.247193	-0.440968	-0.071917	S	2.330257	-0.991766	0.033156

C	3.782270	0.098556	0.005074	H	3.784636	0.752714	0.874345
H	0.373331	-2.425847	-0.365847	H	4.636094	-0.580591	0.035886
H	-1.335792	-2.110669	-0.691066	H	3.800023	0.689718	-0.908170
H	-0.755631	-2.196833	0.995462				

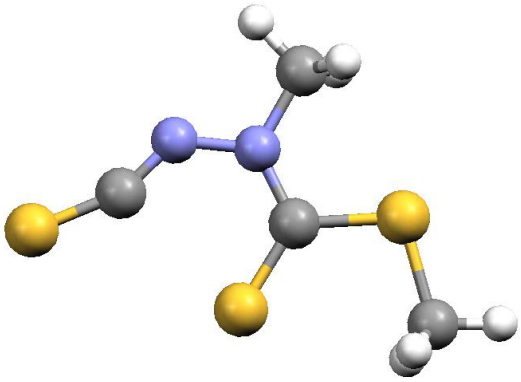


Transition state $\mathbf{TS_{15}}^{a/s}$: E = -1460.200673 au

$G^{o}_{CS_2}$ = -1460.127413au

ν = -53.0 cm^{-1}

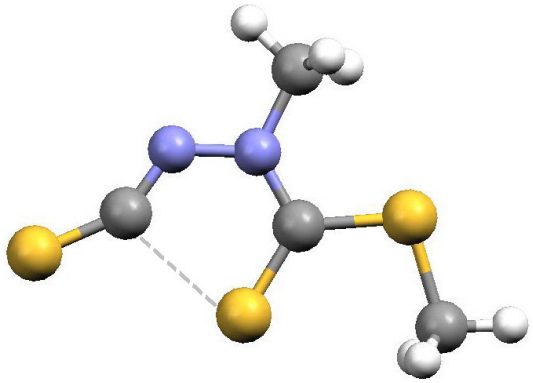
S	-0.672085	-1.728629	0.260399	H	-0.202221	2.584879	1.186737
C	-0.877962	-0.099947	0.077985	H	-0.779884	2.579224	-0.503613
N	0.161864	0.801729	0.087033	S	-2.455249	0.705060	-0.182850
N	1.378526	0.346578	0.530893	C	-3.589031	-0.709007	-0.299061
C	2.452183	0.054085	0.066866	H	-3.585105	-1.278846	0.627648
S	3.920977	-0.355267	-0.323217	H	-3.315716	-1.351334	-1.133777
C	0.018092	2.261772	0.165127	H	-4.570145	-0.261844	-0.468425
H	0.952353	2.709720	-0.168868				



Compound $\mathbf{15}_{syn}$: E = -1460.208288 au

$G^{o}_{CS_2}$ = -1460.135882 au

S	0.002555	-1.482061	0.000000	H	-1.220046	2.651126	-0.891983
C	-0.728409	0.008001	0.000000	H	0.210751	3.220182	-0.000001
N	-0.010459	1.164887	0.000000	S	-2.490464	0.288918	0.000001
N	1.353434	1.167071	0.000000	C	-3.148438	-1.405892	-0.000001
C	2.143126	0.216237	0.000000	H	-2.830042	-1.940288	0.892793
S	3.535741	-0.533700	-0.000001	H	-2.830042	-1.940287	-0.892795
C	-0.606980	2.505920	0.000001	H	-4.232528	-1.281664	-0.000001
H	-1.220042	2.651127	0.891986				

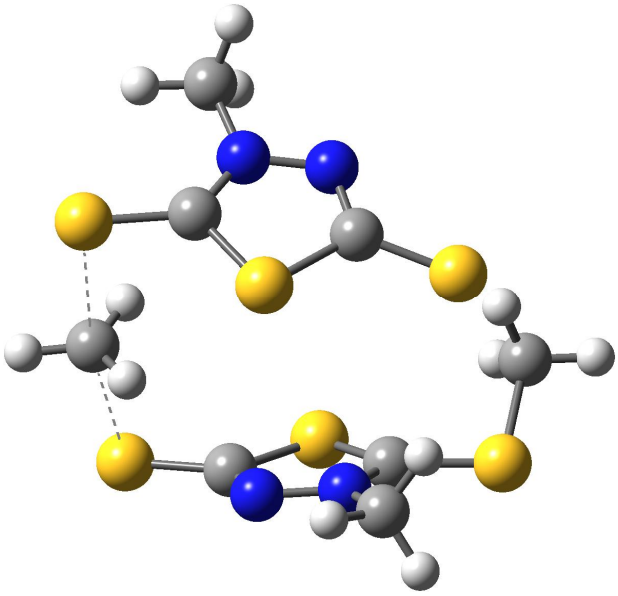


Transition state **$TS_{15syn\text{-}2a}$**: E = -1460.208113 au

$G^{o}_{CS_2}$ = -1460.136736 au

ν = -100.9 cm^{-1}

S	-0.096253	-1.407888	-0.006544	H	1.004886	2.763032	1.006083
C	-2.036161	0.151373	-0.000421	H	-0.144089	3.242931	-0.268107
N	-1.334314	1.193407	-0.008894	S	2.496277	0.234641	0.020606
N	0.033465	1.198003	-0.034069	C	3.070700	-1.492409	-0.007653
C	0.731495	0.042254	-0.012088	H	2.745151	-1.990751	-0.918623
S	-3.475953	-0.533656	0.011499	H	2.712539	-2.029289	0.868508
C	0.632649	2.534149	0.004227	H	4.159216	-1.422847	0.013607
H	1.451012	2.595280	-0.714095				



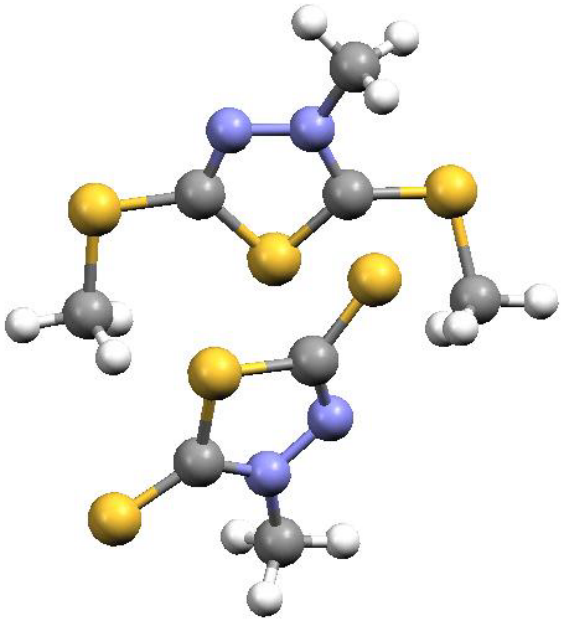
Transition state **$TS_{2a\text{-}16}$**: E = -2920.403831 au

$G^{o}_{CS_2}$ = -2920.240785 au

ν = -439.3 cm^{-1}

S	1.584309	-1.039351	1.373237	N	2.602132	-1.312032	-0.892009
C	0.849460	-2.183921	0.180784	C	2.787302	-0.567570	0.205602
N	1.556997	-2.202495	-0.934064	S	-0.562008	-3.046427	0.537441

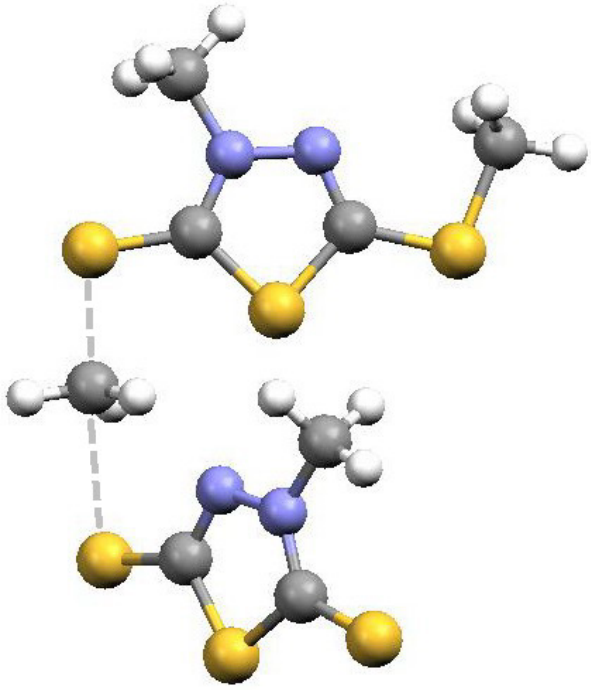
C	3.439110	-1.272171	-2.088371	N	-1.959976	0.689718	1.132863
H	4.179933	-0.486176	-1.969007	C	-2.512990	0.394428	-0.038683
H	2.805455	-1.081135	-2.954575	S	0.087103	3.618510	-0.364299
H	3.926676	-2.240562	-2.208303	C	-2.163735	-0.076254	2.373522
S	3.903161	0.720140	0.420792	H	-1.960863	-1.129105	2.161588
C	2.074953	2.343109	0.069756	H	-3.182681	0.062357	2.735930
H	1.612843	1.948489	0.954972	H	-1.454418	0.314847	3.096608
H	1.947525	1.876592	-0.887376	S	-3.736434	-0.835517	-0.217069
H	2.721872	3.202001	0.148978	C	-3.221840	-1.636209	-1.787162
S	-1.938482	1.492877	-1.243607	H	-3.237128	-0.927605	-2.613713
C	-0.950685	2.315964	0.011783	H	-2.244254	-2.095746	-1.639096
N	-1.106956	1.752836	1.188250	H	-3.972175	-2.408096	-1.958593



Compound **16**: E = -2920.440237 au

$G^{o}_{CS_2}$ = -2920.277254 au

S	-1.879055	-0.228324	1.694214	H	-3.118569	-1.144348	-2.422216
S	0.969506	0.591170	-1.217244	H	-4.036540	-2.290922	-1.437307
C	-2.998393	-0.509000	0.356473	H	-2.410214	-2.742981	-2.034718
C	2.333205	-0.069144	-0.346629	C	3.825185	0.579133	1.522543
N	-2.406316	-1.416970	-0.457919	H	4.752755	0.278631	1.037296
N	2.791195	0.846082	0.521637	H	3.975391	1.500113	2.078373
N	-1.138035	-1.868113	-0.156552	H	3.466785	-0.213435	2.184436
N	2.040815	1.972671	0.687333	C	-1.371772	2.762228	-1.291943
C	-0.695909	-1.353408	0.963676	H	-0.991852	2.539105	-2.289430
C	1.049818	1.998459	-0.146128	H	-2.067399	3.598314	-1.363218
S	-4.485606	0.221418	0.128063	H	-1.895237	1.912247	-0.856680
S	3.355477	-1.377766	-0.898489	C	2.128295	-2.564900	-1.548077
S	0.841532	-1.648070	1.664516	H	1.409376	-2.784798	-0.757854
S	-0.043919	3.364513	-0.190008	H	2.708990	-3.451611	-1.803302
C	-3.033420	-1.931074	-1.668279	H	1.643886	-2.176805	-2.443508

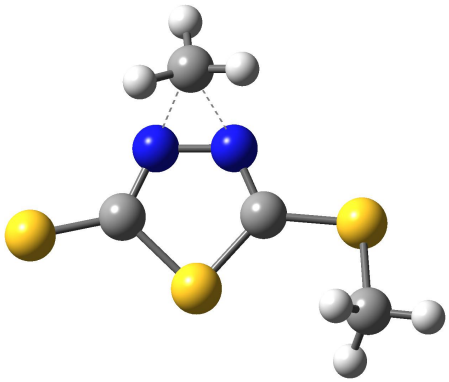


Transition state **$TS_{16\text{-}3a}$**: E = -2920.420001 au

$G^{o}_{CS_2}$ = -2920.265216 au

ν = -331.4 cm^{-1}

S	4.350847	-0.236219	-0.789025	S	-1.579561	0.030005	-0.506402
C	2.790646	-1.048082	-0.499515	C	-2.986882	1.092247	-0.404742
N	2.058596	-0.408988	0.377290	N	-4.013860	0.576687	0.192525
N	2.703869	0.719660	0.853527	N	-3.735710	-0.707537	0.595834
C	3.931489	1.031526	0.369650	C	-2.516408	-1.199404	0.328414
S	2.377120	-2.504077	-1.319679	S	-2.913155	2.704472	-1.076040
C	1.991007	1.500314	1.848447	C	-4.788312	-1.449057	1.291592
H	2.677576	2.242798	2.249282	H	-4.457677	-1.704007	2.299679
H	1.642541	0.835893	2.640899	H	-5.017051	-2.364619	0.744247
H	1.133966	2.005097	1.392975	H	-5.661212	-0.803571	1.331996
S	4.894329	2.341707	0.759027	S	-1.993877	-2.757059	0.742116
C	-4.586853	3.307710	-0.660236	C	-0.044127	-2.716439	-0.155512
H	-5.343872	2.693747	-1.144208	H	-0.311304	-2.607026	-1.194892
H	-4.730992	3.315976	0.418408	H	0.397376	-1.874377	0.360487
H	-4.623589	4.324496	-1.050520	H	0.289335	-3.697290	0.148877

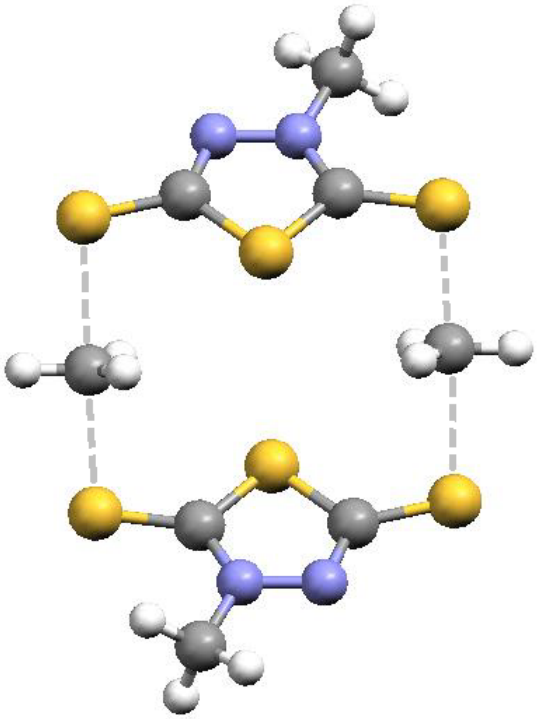


Transition state **$TS_{2a\text{-}3a}^{u}$**: E = -1460.111684 au

$G^{o}_{CS_2}$ = -1460.044815 au

ν = -724.80 cm^{-1}

S	-0.098540	-1.255672	-0.089970	H	-1.422503	2.171162	1.417495
C	-1.611473	-0.231031	-0.165552	H	-0.989435	3.295024	0.043872
N	-1.251929	1.028708	-0.490795	S	2.615118	0.317772	-0.301313
N	0.127835	1.247981	-0.506491	C	3.112081	-1.150682	0.669806
C	0.861439	0.187184	-0.284066	H	2.844381	-2.072113	0.154298
S	-3.136784	-0.796843	0.148658	H	2.677432	-1.127055	1.668312
C	-0.666788	2.522175	0.724661	H	4.197907	-1.088791	0.745259
H	0.312603	2.674944	1.164676				

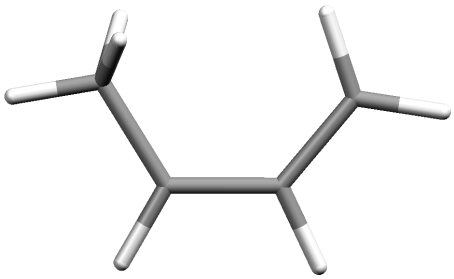


Transition state $\mathbf{TS_{2a\text{-}3a}}^{b}$: E = -2920,378853 au

$G^{o}_{CS_2}$ = -2920.216086 au

ν = -511.6 and -358.0 cm^{-1}

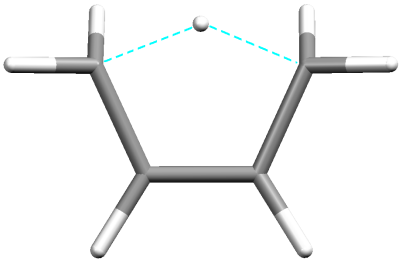
S	-1.968601	0.000000	0.000000	H	-3.492926	3.317106	-2.671492
S	1.968601	0.000000	0.000000	H	-2.860043	4.060955	-1.161493
C	-2.420197	1.684222	0.000000	H	-4.506755	3.378549	-1.198692
C	2.420197	-1.684222	0.000000	C	3.487471	-3.273666	1.583112
N	-2.941341	1.969946	-1.204659	H	3.492926	-3.317106	2.671492
N	2.941341	-1.969946	1.204659	H	2.860043	-4.060955	1.161493
N	-2.981678	0.984677	-2.162285	H	4.506755	-3.378549	1.198692
N	2.981678	-0.984677	2.162285	C	-0.038376	2.199787	1.950368
C	-2.477971	-0.143977	-1.716018	H	0.336379	2.388839	0.959700
C	2.477971	0.143977	1.716018	H	0.005094	2.989437	2.685876
S	-2.228930	2.782451	1.299393	H	-0.309473	1.207054	2.267043
S	2.228930	-2.782451	-1.299393	C	0.038376	-2.199787	-1.950368
S	-2.315612	-1.600616	-2.606892	H	-0.336379	-2.388839	-0.959700
S	2.315612	1.600616	2.606892	H	-0.005094	-2.989437	-2.685876
C	-3.487471	3.273666	-1.583112	H	0.309473	-1.207054	-2.267043



Compound **17**: E = -156.598794472 au

G = -156.534490 au

C	0.000000	0.000000	0.000000	H	2.024707	-0.955927	-0.000000
C	1.501801	0.000000	0.000000	H	3.321627	1.065960	-0.000000
C	2.230094	1.188566	0.000000	H	2.485270	3.346831	0.000000
C	1.780415	2.517024	0.000000	H	0.721166	2.770692	0.000000
H	-0.434236	0.522043	0.880428	H	-0.434234	0.522088	-0.880405
H	-0.408533	-1.022955	-0.000000				



Transition state $\mathbf{TS_{17\text{-}17}}$: E = -156.541814896 au

G = -156.480070 au

ν = -1600.3 cm^{-1}

C	0.000000	0.000000	0.000000	H	2.059877	-0.899777	-0.198236
C	1.468749	0.000000	0.000000	H	3.108527	1.396387	-0.198236
C	2.041411	1.253924	0.000000	H	1.452331	3.310572	-0.429318
C	1.079606	2.363949	0.000000	H	0.562954	2.582804	0.948674
H	-0.503730	0.247150	0.948674	H	0.032097	1.413842	-0.462039
H	-0.471345	-0.901584	-0.429318				