Effect of H_2 Binding on the Nonadiabatic Transition Probability between Singlet and Triplet States of the [NiFe]-Hydrogenase Active Site

Danil S. Kaliakin[†,‡], Ryan R. Zaari[†], Sergey A. Varganov[†]*

[†]*Department of Chemistry, University of Nevada, Reno, 1664 N. Virginia Street, Reno, Nevada 89557-0216, United States.*

[‡]*Department of Chemistry, Siberian Federal University, 79 Svobodnyi Prospect, Krasnoyarsk, Krasnoyarskiy kray 660041, Russia.*

*E-mail: svarganov@unr.edu

Supporting Information

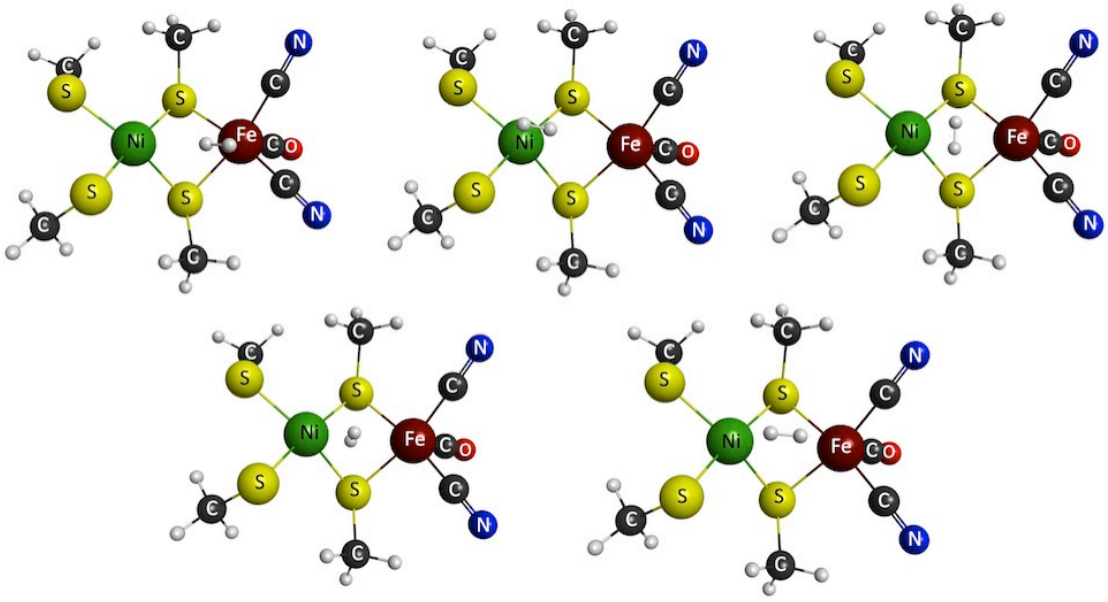

Figure S1. Sampled initial positions of H_2 on the active site of [NiFe]-hydrogenase.

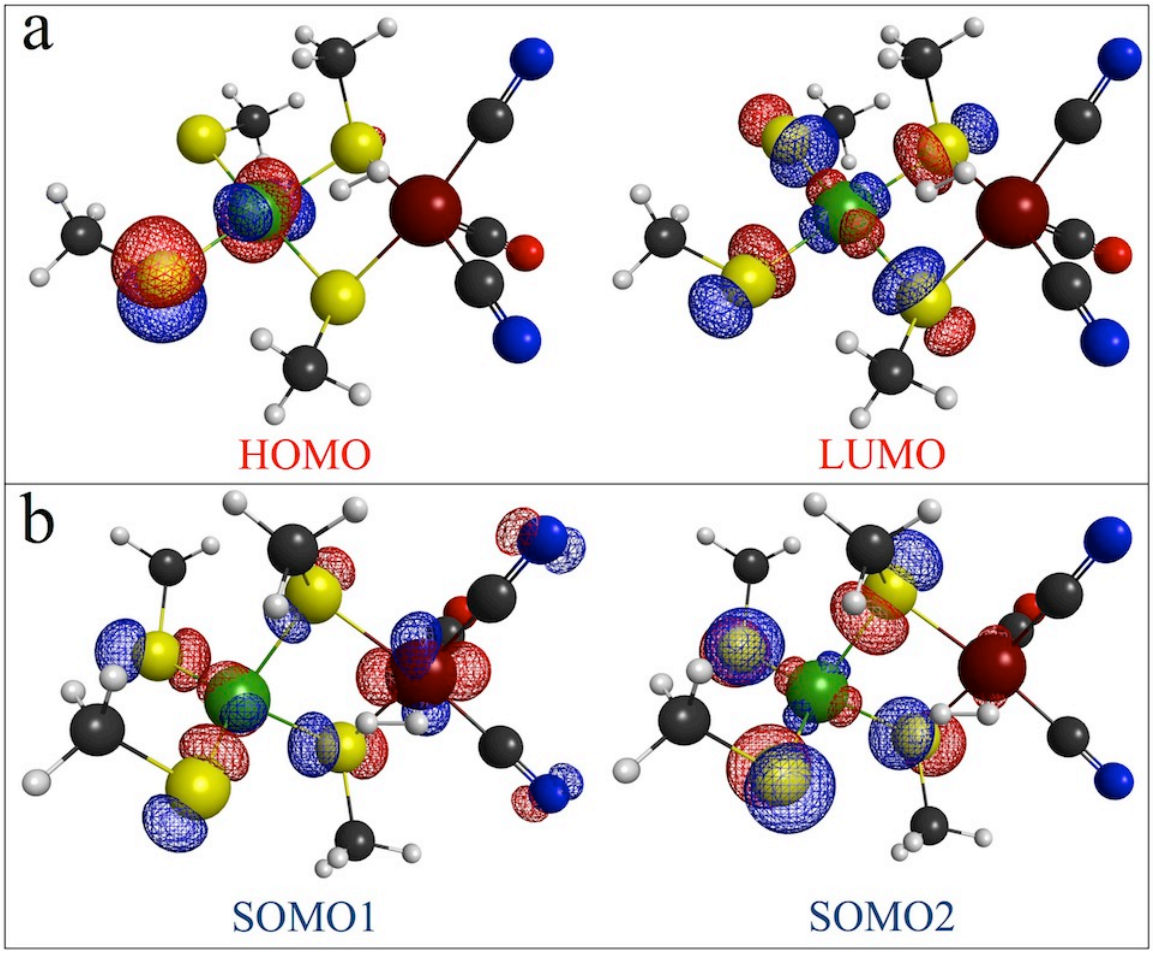

Figure S2. Active space molecular orbitals used in MCQDPT2 calculation of spin-orbit coupling. a) Singlet state orbitals. b) Triplet state orbitals.

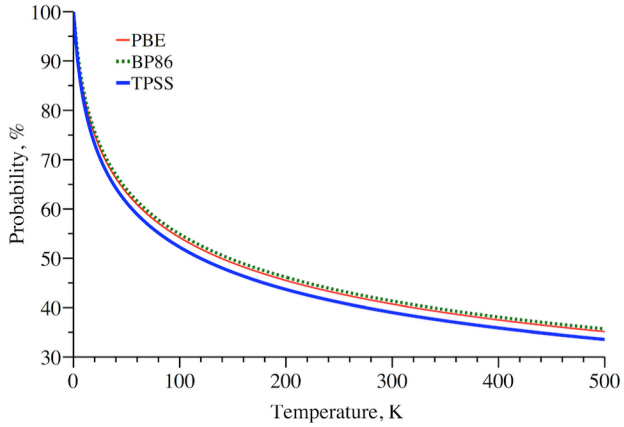

Figure S3. Landau-Zener transition probabilities between the singlet and triplet states of the bare active site and active site with bound H_2 as a function of temperature. Gradients obtained from PBE, BP86 and TPSS calculations with bs1 basis set and spin-orbit coupling calculated with MCQDPT2/6-31G**.

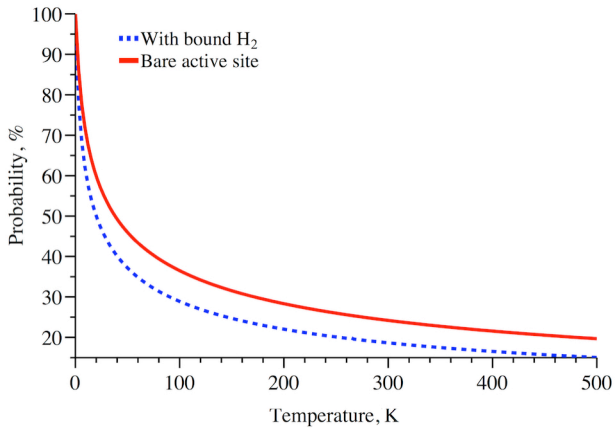

Figure S4. Landau-Zener transition probabilities between the singlet and triplet states of the bare active site and the active site with bound H_2 calculated with normalized probability distribution (Ref. 34) as functions of temperature. The mass-weighted gradients and spin-orbit coupling were calculated with PBE and MCQDPT2, respectively, using def2-TZVP basis set.

Table S1. Binding energies of H_2 (kcal/mol), with and without ZPE correction, to the active site calculated using bs1 basis set.

	PBE	BP86	TPSS	B3LYP
S2	-3.9	-2.4	-4.0	-2.8
S1	-2.6	-1.0	-2.5	-1.5
T2	-8.9	-7.0	-8.8	-6.7
T1	-6.5	-4.7	-6.3	-4.2
ZPE corrected calculations				
S2	0.7	1.9	0.6	2.1
S1	1.5	3.7	1.7	2.8
T2	-3.8	-2.3	-3.3	-2.6
T1	-2.2	0.5	-1.7	-0.5

Table S2. Binding energies of H_2 (kcal/mol), with the ZPE, Grimme's dispersion (D3) and entropy (S) corrections, to the active site calculated with def2-TZVP basis set and different functionals.

	PBE	BP86	TPSS	B3LYP
$E_{binding}$ (no corrections)				
S2	-3.9	-1.9	-3.9	-4.0
S1	-1.7	0.2	-1.6	-2.6
T2	-7.5	-5.9	-7.9	-6.3
T1	-4.6	-3.6	-5.4	-3.9
ΔZPE correction				
S2	4.7	4.3	4.6	4.9
S1	4.1	4.8	4.2	4.3
T2	5.1	4.7	5.5	3.8
T1	4.2	5.2	4.6	4.1
ΔD3 correction				
S2	-4.8	-6.3	-4.0	-5.7
S1	-4.6	-4.8	-3.6	-4.9
T2	-2.5	-4.8	-3.7	-6.7
T1	-4.1	-5.7	-4.7	-5.5
ΔS correction				
S2	8.9	7.9	8.5	9.7
S1	8.4	8.8	7.6	10.1
T2	9.6	9.4	9.8	11.1
T1	9.7	9.4	11.8	10.3
$E_{binding}$ + ΔZPE + ΔD3 + ΔS				
S2	4.9	4.0	5.2	4.9
S1	6.2	9.0	6.6	7.0
T2	4.7	3.4	3.7	2.1
T1	5.2	5.3	6.2	4.7

Table S3. The difference between the singlet and triplet mass-weighted gradients ($E_h\, m_e^{-1/2}\, a_0^{-1}$) for the bare active site and active site with bound H_2 obtained with different levels of theory.

	PBE/bs1	BP86/bs1	TPSS/bs1	PBE/def2-TZVP
Bare active site	1.04×10^{-4}	1.01×10^{-4}	1.12×10^{-4}	1.57×10^{-4}
Active site with H_2 bound	-	-	-	1.71×10^{-4}

Derivation of velocity averaged Landau-Zener transition probability formula

The Landau-Zener (LZ) probability of nonadiabatic transition for the specific mass-weighted velocity is

$$P_{LZ}(\upsilon) = 1 - \exp\left(\frac{-2\pi H_{SO}^2}{\upsilon|\Delta g|}\right). \tag{1}$$

Here we use mass-weighted coordinates and atomic units. The general equation for velocity averaged Landau-Zener (LZ) transition probability can be written as

$$\langle P_{LZ} \rangle = \int_0^\infty P_{LZ}(\upsilon) p(\upsilon) d\upsilon \Big/ \int_0^\infty p(\upsilon) d\upsilon. \tag{2}$$

In the main text we use the Maxwell-Boltzmann velocity distribution,

$$p(\upsilon) = \exp\left(\frac{-\upsilon^2}{2k_B T}\right). \tag{3}$$

After substituting the equations (1) and (3) into (2), the averaged LZ probability reads

$$\langle P_{LZ} \rangle = \frac{\int_0^\infty \exp\left(\frac{-\upsilon^2}{2k_B T}\right) d\upsilon - \int_0^\infty \exp\left(\frac{-2\pi H_{SO}^2}{\upsilon|\Delta g|}\right) \exp\left(\frac{-\upsilon^2}{2k_B T}\right) d\upsilon}{\int_0^\infty \exp\left(\frac{-\upsilon^2}{2k_B T}\right) d\upsilon}. \tag{4}$$

Integration of the denominator gives

$$\int_0^\infty \exp\left(\frac{-\upsilon^2}{2k_B T}\right) d\upsilon = \left(\frac{\pi k_B T}{2}\right)^{1/2}. \tag{5}$$

The substitution of equation (5) into (4) simplifies the final expression to

$$\langle P_{LZ} \rangle = 1 - \left(\frac{2}{\pi k_B T}\right)^{1/2} \int_0^\infty \exp\left(\frac{-2\pi H_{SO}^2}{\upsilon|\Delta g|} - \frac{\upsilon^2}{2k_B T}\right) d\upsilon. \tag{6}$$

Equation (6) is equivalent to equation (1) in Ref. 36.

A slightly different form of the velocity averaged LZ formula can be derived with normalized velocity distribution proposed in Ref. 34,

$$p(\upsilon) = \frac{\upsilon}{k_B T} \exp\left(\frac{-\upsilon^2}{2k_B T}\right). \tag{7}$$

If this form of velocity distribution is used then equation (2) has the following form:

$$\left\langle P_{LZ} \right\rangle = \frac{\int_0^\infty \frac{\upsilon}{k_B T} \exp\left(\frac{-\upsilon^2}{2k_B T}\right) d\upsilon - \int_0^\infty \exp\left(\frac{-2\pi H_{SO}^2}{\upsilon |\Delta g|}\right) \frac{\upsilon}{k_B T} \exp\left(\frac{-\upsilon^2}{2k_B T}\right) d\upsilon}{\int_0^\infty \frac{\upsilon}{k_B T} \exp\left(\frac{-\upsilon^2}{2k_B T}\right) d\upsilon}. \tag{8}$$

The integral in the denominator is equal to 1, and the final expression reads

$$\left\langle P_{LZ} \right\rangle = 1 - \frac{1}{k_B T} \int_0^\infty \upsilon \exp\left(\frac{-2\pi H_{SO}^2}{\upsilon |\Delta g|} - \frac{\upsilon^2}{2k_B T}\right) d\upsilon \ . \tag{10}$$

This equation is identical to equation (A7) in Ref. 34.

The transition probabilities calculated using equation 10 (Figure S4) are somewhat lower than the probabilities obtained using equation 6 (Figure 5). However, in both cases the probabilities are large enough to make the nonadiabatic transitions between the lowest energy singlet and triplet states potentially important for the H_2 activation on [NiFe]-hydrogenase.

Calculation of difference between the singlet and triplet mass-weighted gradients, $|\Delta g|$

All equations are shown in atomic units. The Cartesian components of the singlet and triplet states gradients for each atom were obtained at the minimum energy crossing point geometry, as calculated using GAMESS. The vector gradient g_n, of each atom n, is defined as,

$$g_n = \left(\frac{\partial E}{\partial x_n}, \frac{\partial E}{\partial y_n}, \frac{\partial E}{\partial z_n} \right), \tag{1}$$

with energy derivatives with respect to atomic coordinates, $\frac{\partial E}{\partial x_n}, \frac{\partial E}{\partial y_n}$ and $\frac{\partial E}{\partial z_n}$.

The difference between the triplet and singlet state Cartesian gradients for each atom, Δg_n, can be written as,

$$\Delta g_n = g_n^{\text{triplet}} - g_n^{\text{singlet}}, \tag{2}$$

and the subsequent squared norm,

$$\left|\Delta g_n\right|^2 = \Delta g_n(x)^2 + \Delta g_n(y)^2 + \Delta g_n(z)^2, \tag{3}$$

written in terms of each Cartesian component.

The difference between the singlet and triplet mass-weighted energy gradients, $|\Delta g|$, can be calculated as,

$$\left|\Delta g\right| = \left\{ \sum_{n=1}^{N} \left|\Delta g_n\right|^2 m_n^{-1} \right\}^{1/2}, \tag{4}$$

with corresponding mass of each atom, m_n.

Atomic Cartesian coordinates of different conformers.

Atomic Cartesian coordinates (Å) of conformer S optimized with PBE/bs1 level of theory, E= -2345.248343 Hartree

FE	26.0	-2.2294894074	1.0294984149	0.4466030348
NI	28.0	0.5484338995	0.1092731763	0.0430876407
S	16.0	-1.3619423002	-1.0794671960	0.0170153329
S	16.0	-0.7287443116	1.4866978240	-1.2109149330
C	6.0	-1.4393881674	-2.1422329764	1.5264322081
H	1.0	-0.4538612102	-2.1092985450	2.0157390706
C	6.0	-0.2207400192	3.2543208830	-1.2715427193
H	1.0	-0.1414662416	3.5536603675	-2.3293518754
H	1.0	0.7630831121	3.3173774355	-0.7723267492
H	1.0	-0.9644696447	3.8649048182	-0.7387693728
C	6.0	-3.6928587138	0.8990076624	-0.3738084742
O	8.0	-4.7115025293	0.7968711447	-0.9733324829
C	6.0	-2.9817993340	0.5281677962	2.1022833343
N	7.0	-3.4489990748	0.1819135540	3.1403424956
C	6.0	-2.5070384818	2.8453558627	0.8698453415
N	7.0	-2.6793468844	3.9999611153	1.0991533801
S	16.0	1.9724782193	-1.4845223891	0.6806242576
S	16.0	2.2755832669	1.5364920340	0.2934736149
C	6.0	1.3929510048	-3.0974482787	-0.0171848045
H	1.0	1.0744644549	-2.9816002456	-1.0652805020
H	1.0	0.5577799662	-3.5391790268	0.5502345458
H	1.0	2.2457271861	-3.7993216360	0.0178407857
C	6.0	3.2096928498	1.2209522096	-1.2539300367
H	1.0	4.1582389377	1.7886690854	-1.2291837346
H	1.0	2.6338743058	1.5321145468	-2.1441671505
H	1.0	3.4340345901	0.1427644708	-1.3293172546
H	1.0	-2.2094337750	-1.7400961187	2.2009962033
H	1.0	-1.6860116980	-3.1727859887	1.2221188439

Atomic Cartesian coordinates (Å) of conformer T optimized with PBE/bs1 level of theory, E= -2345.236325 Hartree

Fe	26.0	1.5505926677	-0.4021128432	0.2219150535
Ni	28.0	-1.4606859837	0.4032446448	0.2783057347
S	16.0	-0.4033476154	-1.6573943129	0.0026753316
S	16.0	0.2578645312	0.6869097008	1.8238233369
C	6.0	-0.6810462303	-2.1555441542	-1.7514573074
H	1.0	-1.4193581598	-2.9735542200	-1.7655395740
H	1.0	0.2748113593	-2.4786928506	-2.1904639851
H	1.0	-1.0740253505	-1.2955879281	-2.3140156856
C	6.0	0.6562142289	2.4862832673	1.8932699263

H	1.0	0.3503754771	2.8772308729	2.8774715818
H	1.0	0.1006769641	3.0074185307	1.0992431291
H	1.0	1.7375310174	2.6200683341	1.7385676872
C	6.0	2.4066679903	-1.4372161980	1.2268354182
O	8.0	3.0033828683	-2.1693713842	1.9422179905
C	6.0	2.2924793456	-1.1348951596	-1.3491952549
N	7.0	2.7286278917	-1.6099286381	-2.3488167882
C	6.0	2.8847646184	0.9280412835	0.2718801847
N	7.0	3.7049832252	1.7883504886	0.3212027580
S	16.0	-3.4381454613	0.1555012304	1.3888966519
S	16.0	-2.0432305669	1.8223412252	-1.3767823904
C	6.0	-2.9714651860	-0.9871821280	2.7535104163
H	1.0	-2.2378245548	-0.5135767069	3.4262976617
H	1.0	-2.5220897364	-1.9093730479	2.3502867898
H	1.0	-3.8732263958	-1.2524924682	3.3359057321
C	6.0	-3.8205539999	2.2453223524	-1.1731461103
H	1.0	-4.1743074945	2.8018119466	-2.0595984561
H	1.0	-3.9758402041	2.8679628290	-0.2764195769
H	1.0	-4.4258312958	1.3313064335	-1.0573270556

Atomic Cartesian coordinates (Å) of conformer S1 optimized with PBE/bs1 level of theory, E= -2346.417078 Hartree

FE	26.0	1.7162035924	0.0439025238	0.1393124940
NI	28.0	-1.4839329349	-0.0717554374	-0.1460784674
S	16.0	0.0439163923	1.5270856526	-0.6556047383
S	16.0	0.1759854611	-1.3966122242	-0.9454732629
C	6.0	-0.1036811151	2.8483034843	0.6223518512
H	1.0	-0.6414431183	3.7066270561	0.1908321187
H	1.0	0.9123004870	3.1395690969	0.9277503816
H	1.0	-0.6689362163	2.4626893391	1.4834896962
C	6.0	0.2284609527	-3.0884606773	-0.2226458325
H	1.0	0.1743345137	-3.8156834329	-1.0495536387
H	1.0	-0.6520468415	-3.2011308285	0.4337475560
H	1.0	1.1727202279	-3.2136171874	0.3282631621
C	6.0	2.6935853214	0.1677660312	-1.2583846314
O	8.0	3.3868586385	0.2475808130	-2.2089339245
C	6.0	2.7263887383	1.4055388120	1.0014190233
N	7.0	3.3335458872	2.2838610956	1.5233265563
C	6.0	2.7998126409	-1.3624609746	0.8139216275
N	7.0	3.4407525056	-2.2748415815	1.2250165143
S	16.0	-3.2735605124	1.2114521181	0.1974407998
S	16.0	-2.7492896860	-1.7349915881	0.6911441416
C	6.0	-3.1362766080	2.7700892733	-0.7942299823
H	1.0	-2.4665934126	2.6298777258	-1.6582441746

H	1.0	-2.7595563732	3.6201439880	-0.1988071532
H	1.0	-4.1424052308	3.0337342591	-1.1674781041
C	6.0	-3.7116451362	-2.2254073202	-0.7940579357
H	1.0	-4.4729381271	-2.9730616422	-0.5044758992
H	1.0	-3.0663724773	-2.6636628882	-1.5765558595
H	1.0	-4.2188332107	-1.3346249922	-1.2021136385
H	1.0	1.1254661673	-0.0543519828	1.7858815381
H	1.0	0.4308352542	-0.1255749415	1.3796110819

Atomic Cartesian coordinates (Å) of conformer S2 optimized with PBE/bs1 level of theory, E= -2346.419250 Hartree

FE	26.0	1.8343149123	0.1117640749	0.1237071633
NI	28.0	-1.3954068356	-0.1641435549	-0.7076661814
S	16.0	0.0715340597	1.5418308173	-0.4763292234
S	16.0	0.5048585112	-1.2918046433	-1.2268374334
C	6.0	-0.4360351364	2.3705268114	1.0884057681
H	1.0	-1.3149352783	2.9998768281	0.8828101303
H	1.0	0.4189179530	2.9602364088	1.4533678678
H	1.0	-0.7139221179	1.6170590913	1.8414526121
C	6.0	0.5635458442	-2.9858548228	-0.5153508980
H	1.0	0.1240717235	-3.6891848488	-1.2389226294
H	1.0	-0.0265301278	-3.0217017020	0.4137746346
H	1.0	1.6169213194	-3.2272121590	-0.3087010192
C	6.0	2.8371171482	0.5924441008	-1.1765175975
O	8.0	3.5488789147	0.9207778340	-2.0570327393
C	6.0	2.6410065871	1.4122294229	1.2633670541
N	7.0	3.1080888156	2.2457560736	1.9693002483
C	6.0	3.0740605444	-1.2617675237	0.5865659851
N	7.0	3.8175456162	-2.1486676817	0.8554977114
S	16.0	-3.2063271955	1.1624299372	-0.6652367821
S	16.0	-2.5422038748	-2.0708225779	-0.5036470464
C	6.0	-2.8267379292	2.5934192427	-1.7629931787
H	1.0	-2.6738049347	2.2677288659	-2.8062258775
H	1.0	-1.9214241526	3.1326542864	-1.4403078136
H	1.0	-3.6860191125	3.2883943850	-1.7342401379
C	6.0	-4.3251039468	-1.7920103094	-0.1587853601
H	1.0	-4.5079121908	-1.5503842155	0.9032364119
H	1.0	-4.8792859697	-2.7140987409	-0.4100011862
H	1.0	-4.7030021777	-0.9549750824	-0.7704631577
H	1.0	1.2182343147	-0.2936038279	1.7033140562
H	1.0	0.5932104958	-0.4889129203	1.2353299187

Atomic Cartesian coordinates (Å) of conformer T1 optimized with PBE/bs1 level of theory, E= -2346.411294 Hartree

FE	26.0	1.6694905304	0.0074721981	-0.0464262911
NI	28.0	-1.4818770448	0.0299968338	-0.0441657324
S	16.0	0.0448035960	-1.3543491140	1.0371130470
S	16.0	0.0706323404	1.7214346193	0.3511176037
C	6.0	-0.0673034752	-2.9448168395	0.1126125799
H	1.0	-0.6619662665	-3.6520029688	0.7140834122
H	1.0	0.9495148082	-3.3356875858	-0.0475739851
H	1.0	-0.5713357047	-2.7782175846	-0.8522545110
C	6.0	-0.0223028133	2.7400553042	-1.1818951994
H	1.0	-0.6456973761	3.6256388127	-0.9756406879
H	1.0	-0.4873070495	2.1560437390	-1.9922251734
H	1.0	0.9966078163	3.0431414655	-1.4682562196
C	6.0	2.4639844740	0.3209565151	1.4404949231
O	8.0	3.0314662052	0.5364151208	2.4491304523
C	6.0	2.7938765366	-1.4986158690	-0.3596938176
N	7.0	3.4605885599	-2.4643761570	-0.5428894294
C	6.0	2.8295586969	1.2286415935	-0.9359926029
N	7.0	3.5217025128	2.0175757678	-1.4924056152
S	16.0	-3.3010118241	0.3700550532	1.3076688272
S	16.0	-2.3894924605	-0.5014674958	-2.0771067984
C	6.0	-2.5072979279	0.7893884578	2.9130567940
H	1.0	-1.8299926439	1.6509643217	2.7942943536
H	1.0	-1.9163955718	-0.0620247551	3.2895727560
H	1.0	-3.2817333068	1.0436530326	3.6602442406
C	6.0	-4.2081758134	-0.5442331099	-1.7972682132
H	1.0	-4.7189393903	-0.8779982256	-2.7185169992
H	1.0	-4.5877144858	0.4534260383	-1.5209608499
H	1.0	-4.4582407442	-1.2363239259	-0.9767449953
H	1.0	1.3445800506	-0.2033119191	-1.7325530064
H	1.0	0.6277135116	-0.3988774533	-1.4107279623

Atomic Cartesian coordinates (Å) of conformer T2 optimized with PBE/bs1 level of theory, E= -2346.415063 Hartree

FE	26.0	2.1213691947	0.3085937089	0.8107985704
NI	28.0	-0.9383254369	-0.1537113312	-0.5110866185
S	16.0	0.2627030448	1.6910331190	0.3542236205
S	16.0	1.2024506670	-1.0645687759	-0.8955391853
C	6.0	-0.5115728190	2.0383983214	1.9864918268
H	1.0	-1.3699972153	2.7145932353	1.8374615401
H	1.0	0.2420269153	2.5083199101	2.6376089560
H	1.0	-0.8631904662	1.1009247040	2.4466500972
C	6.0	1.2869901699	-2.7829365825	-0.2490788018

H	1.0	0.9090299374	-3.4699199905	-1.0237630853
H	1.0	0.6617427333	-2.8796020266	0.6529642571
H	1.0	2.3324431682	-3.0157626027	0.0043154547
C	6.0	3.1458326787	1.1590809229	-0.2696163408
O	8.0	3.8666961437	1.7418420234	-0.9970905993
C	6.0	2.6513455867	1.4304527162	2.2583474653
N	7.0	2.9350871723	2.1451484702	3.1639041893
C	6.0	3.5032528721	-0.9575242795	1.1584191256
N	7.0	4.3441538918	-1.7741160082	1.3512119994
S	16.0	-2.3338686965	0.7340202341	-2.0531553820
S	16.0	-1.7834938225	-1.5822612499	1.0398278528
C	6.0	-2.1552999875	2.5654628105	-2.1453757735
H	1.0	-1.8907063947	2.8734645442	-3.1719817786
H	1.0	-1.3588691738	2.9000956005	-1.4603235199
H	1.0	-3.1014757469	3.0644355809	-1.8690901945
C	6.0	-3.2899427421	-0.6614529399	1.5727452124
H	1.0	-4.0524142196	-1.3696582319	1.9442184420
H	1.0	-3.7053390571	-0.0948548455	0.7231728748
H	1.0	-3.0541453274	0.0484725292	2.3852024810
H	1.0	1.4357804605	-0.5368794881	2.1514718115
H	1.0	0.8088741714	-0.5441491824	1.6440138730

Atomic Cartesian coordinates (Å) of MECP(S2/T2) optimized with PBE/bs1 level of theory, E= -2346.410716 Hartree

FE	26.0	2.1440583127	0.3027918249	0.7884657137
NI	28.0	-0.9282634099	-0.0686856895	-0.4075922765
S	16.0	0.4500778895	1.7645162115	0.0558824481
S	16.0	1.1411550438	-1.0683212222	-0.8733958097
C	6.0	-0.3206913122	2.4852124560	1.5642373082
H	1.0	-1.0830698998	3.2203894711	1.2573682974
H	1.0	0.4678527225	2.9667506064	2.1625805899
H	1.0	-0.8024413008	1.6960135741	2.1627823281
C	6.0	1.2296931285	-2.7998654850	-0.2684187250
H	1.0	0.8470613691	-3.4680555543	-1.0570333045
H	1.0	0.6063141013	-2.9121369624	0.6334536218
H	1.0	2.2756302152	-3.0380628252	-0.0234071492
C	6.0	3.2966282155	0.9606837962	-0.2940600914
O	8.0	4.1058137209	1.4085659509	-1.0245212990
C	6.0	2.6863949519	1.5000556157	2.1673263402
N	7.0	2.9809695869	2.2715197258	3.0216668164
C	6.0	3.3939410402	-1.0451656200	1.2921178630
N	7.0	4.1614954834	-1.9084666850	1.5694398784
S	16.0	-2.6982389865	0.9266803240	-1.3834591291
S	16.0	-1.8750407757	-1.7902936469	0.6939996278
C	6.0	-2.5045291794	2.7569792396	-1.4327376199

H	1.0	-3.0446268778	3.1631002595	-2.3068977337
H	1.0	-1.4394403461	3.0310707118	-1.5122636484
H	1.0	-2.9189704473	3.2314296946	-0.5252614792
C	6.0	-3.3737036706	-1.0906376252	1.5074350539
H	1.0	-4.0695650911	-1.9072684465	1.7727033734
H	1.0	-3.8729373150	-0.3856997608	0.8229789522
H	1.0	-3.1052987654	-0.5510185901	2.4324269735
H	1.0	1.3273547112	-0.3503391199	2.1779211943
H	1.0	0.7556031874	-0.4280542919	1.6145162981

Atomic Cartesian coordinates (Å) of conformer S optimized with BP86/bs1 level of theory, E= -2346.854058 Hartree

FE	26.0	1.6595387528	0.0785956125	0.1978870809
NI	28.0	-1.2721472535	-0.0989197598	-0.6027268680
S	16.0	0.1861868979	1.6352951193	-0.6521962341
S	16.0	0.5736261912	-1.1541707268	-1.4083505802
C	6.0	-0.2605746758	2.8291657903	0.6828474251
H	1.0	-1.0276180380	3.5170550146	0.2936557306
H	1.0	0.6531182698	3.3671845749	0.9776608929
H	1.0	-0.6607397565	2.2891087294	1.5503531006
C	6.0	0.6736891418	-2.9677074965	-1.0830273068
H	1.0	0.7544147562	-3.4916476102	-2.0502821679
H	1.0	-0.2499405409	-3.2812166687	-0.5644672126
H	1.0	1.5492957080	-3.1647140083	-0.4458310237
C	6.0	3.0591686076	0.5322875438	-0.6219749494
O	8.0	4.0336407160	0.8504624950	-1.2203962226
C	6.0	2.0757774392	1.1200585085	1.7287174011
N	7.0	2.3351294399	1.7850391423	2.6804380233
C	6.0	2.4808571164	-1.4271258989	1.0016690521
N	7.0	2.9966399910	-2.3900243703	1.4743766281
S	16.0	-3.0766116401	1.2245200400	-0.3187201426
S	16.0	-2.4032257009	-2.0151745113	-0.4466903898
C	6.0	-2.9839599944	2.3706372082	-1.7640329138
H	1.0	-3.0772218201	1.8180222995	-2.7154635989
H	1.0	-2.0319457393	2.9281944566	-1.7842617199
H	1.0	-3.8214537332	3.0906331663	-1.6922139456
C	6.0	-4.0468276529	-1.8004537797	0.3537782204
H	1.0	-3.9515253728	-1.6645111807	1.4458842277
H	1.0	-4.6463317614	-2.7100862721	0.1629323765
H	1.0	-4.5607041278	-0.9181540679	-0.0651319631

Atomic Cartesian coordinates (Å) of conformer T optimized with BP86/bs1 level of theory, E= -2346.842553 Hartree

FE	26.0	1.4079987638	-0.5147738927	1.0245273019
NI	28.0	-1.4156440698	0.4913321121	0.1472584799
S	16.0	0.6397116597	0.4282315735	-0.9643984697
S	16.0	-0.6675281031	-1.5791201081	0.9197776263
C	6.0	1.2379533904	2.1690067420	-1.1590731679
H	1.0	1.1743466412	2.4415828144	-2.2261312869
H	1.0	2.2765321145	2.2328446213	-0.7985052448
H	1.0	0.5980178110	2.8417534236	-0.5676944048
C	6.0	-1.3729270311	-1.8476103818	2.6093696802
H	1.0	-2.1115288265	-2.6654108924	2.5530300482
H	1.0	-1.8699987097	-0.9242726845	2.9447457186
H	1.0	-0.5580039020	-2.1028508281	3.3044551501
C	6.0	2.3623500204	-1.7417629317	0.3814262738
O	8.0	3.0281469428	-2.6078320376	-0.0794142939
C	6.0	2.8528049393	0.7011714138	1.1520567625
N	7.0	3.7475326734	1.4840564080	1.2070691493
C	6.0	1.6878847841	-1.0669728975	2.8120369540
N	7.0	1.8301845076	-1.4217691424	3.9391535509
S	16.0	-3.1156521289	0.1803208381	-1.3518039698
S	16.0	-2.2142251508	2.2255372619	1.3586218073
C	6.0	-2.4793428813	-1.1897113567	-2.4122737318
H	1.0	-2.2721471407	-2.0871914336	-1.8054610513
H	1.0	-1.5433994741	-0.8885589835	-2.9117927368
H	1.0	-3.2333906229	-1.4416181988	-3.1823801847
C	6.0	-3.8801705489	2.6636354904	0.7010972915
H	1.0	-4.2711720910	3.5459372091	1.2413818452
H	1.0	-4.5845740650	1.8241377885	0.8287970996
H	1.0	-3.8257655024	2.8947790727	-0.3763321969

Atomic Cartesian coordinates (Å) of conformer S1 optimized with BP86/bs1 level of theory, E= -2348.032179 Hartree

FE	26.0	1.7587859889	0.0472382661	0.1459540691
NI	28.0	-1.4805574192	-0.1118941648	-0.1582010412
S	16.0	0.0470475882	1.5017824751	-0.6469191408
S	16.0	0.2152747556	-1.4195974930	-0.9162781111
C	6.0	-0.1105016471	2.8304393821	0.6300804612
H	1.0	-0.6563894173	3.6833456226	0.1955756092
H	1.0	0.9046247190	3.1299588594	0.9326653363
H	1.0	-0.6725554709	2.4432198374	1.4932544414
C	6.0	0.2869895888	-3.1093902824	-0.1740664330
H	1.0	0.2940557015	-3.8448327398	-0.9966830706
H	1.0	-0.6207021736	-3.2471326382	0.4395106419

H	1.0	1.2098763416	-3.2009621261	0.4187885927
C	6.0	2.7209009468	0.1810991073	-1.2679016261
O	8.0	3.4011030157	0.2691528874	-2.2280070683
C	6.0	2.7571593239	1.4331370420	0.9976066564
N	7.0	3.3544897542	2.3225324779	1.5133196975
C	6.0	2.8686854391	-1.3455800140	0.8225384837
N	7.0	3.5235424508	-2.2466160988	1.2382808825
S	16.0	-3.2668616005	1.1784869567	0.2049972864
S	16.0	-2.7650537115	-1.7964469308	0.6127504842
C	6.0	-3.1479649210	2.7350353463	-0.8025931440
H	1.0	-2.4846557990	2.5923630458	-1.6720185210
H	1.0	-2.7687291553	3.5916338017	-0.2158444884
H	1.0	-4.1596033936	2.9916516036	-1.1691338425
C	6.0	-3.8427445675	-2.1604888936	-0.8375556283
H	1.0	-4.5977913454	-2.9154169666	-0.5460492419
H	1.0	-3.2613730357	-2.5542990911	-1.6912454422
H	1.0	-4.3564089805	-1.2327706930	-1.1453853889
H	1.0	1.1779873149	-0.0549995585	1.7933756642
H	1.0	0.4850254891	-0.1286654509	1.3900551814

Atomic Cartesian coordinates (Å) of conformer S2 optimized with BP86/bs1 level of theory, E= -2348.034303 Hartree

FE	26.0	1.8451237080	0.1205768905	0.2253425121
NI	28.0	-1.3840478211	-0.1784134772	-0.6704595899
S	16.0	0.0692919353	1.5377882999	-0.4039804869
S	16.0	0.5278918466	-1.3137923585	-1.1178691667
C	6.0	-0.4856065383	2.3475469266	1.1610097585
H	1.0	-1.3625775147	2.9760850206	0.9406242269
H	1.0	0.3568025401	2.9397279785	1.5526342457
H	1.0	-0.7784936643	1.5846363571	1.8996024334
C	6.0	0.5771824090	-3.0006284541	-0.3729090443
H	1.0	0.1360206684	-3.7146802427	-1.0862639673
H	1.0	-0.0120607150	-3.0220701187	0.5583240939
H	1.0	1.6304861556	-3.2422755336	-0.1617783777
C	6.0	2.8487117525	0.5975591110	-1.0822351314
O	8.0	3.5588488801	0.9223710019	-1.9662642244
C	6.0	2.6333102368	1.4443790538	1.3613587558
N	7.0	3.0873235733	2.2881043149	2.0646288915
C	6.0	3.0960218111	-1.2446106190	0.7082543520
N	7.0	3.8438811202	-2.1250595111	0.9882478544
S	16.0	-3.2138720022	1.1256132955	-0.7176543928
S	16.0	-2.5350825600	-2.0802388214	-0.4222289908
C	6.0	-2.8011428318	2.5938894618	-1.7623388454
H	1.0	-2.6288418947	2.3025168125	-2.8138780769
H	1.0	-1.8985579047	3.1166797634	-1.4041587970

H	1.0	-3.6576994854	3.2937033309	-1.7286881650
C	6.0	-4.3358588759	-1.7764061022	-0.1702961172
H	1.0	-4.5318409115	-1.2111617918	0.7573451959
H	1.0	-4.8398594654	-2.7587609696	-0.1008134426
H	1.0	-4.7597340364	-1.2025455940	-1.0111149377
H	1.0	1.2235213751	-0.2783717692	1.8032827265
H	1.0	0.6045144292	-0.4801799059	1.3331476575

Atomic Cartesian coordinates (Å) of conformer T1 optimized with BP86/bs1 level of theory, E= -2348.026431 Hartree

FE	26.0	1.6934414285	0.0073576418	-0.0461025855
NI	28.0	-1.5057964044	0.0299696135	-0.0512028030
S	16.0	0.0434742030	-1.3557032558	1.0147993787
S	16.0	0.0691140366	1.7138739916	0.3327714398
C	6.0	-0.0582181226	-2.9540632245	0.0913989950
H	1.0	-0.6486908789	-3.6647183002	0.6947455165
H	1.0	0.9624136431	-3.3376499664	-0.0665450575
H	1.0	-0.5628305396	-2.7936328082	-0.8747859028
C	6.0	-0.0095766649	2.7456488116	-1.1994613013
H	1.0	-0.6288266873	3.6349941903	-0.9917466982
H	1.0	-0.4728470863	2.1695752659	-2.0170376768
H	1.0	1.0140614996	3.0436644246	-1.4768694854
C	6.0	2.4671127154	0.3252355977	1.4558309732
O	8.0	3.0194809353	0.5426790775	2.4733955021
C	6.0	2.8252097848	-1.5021838908	-0.3471853010
N	7.0	3.4941548647	-2.4683597226	-0.5243338963
C	6.0	2.8604489584	1.2353935413	-0.9286759948
N	7.0	3.5550645308	2.0256391908	-1.4814514464
S	16.0	-3.3124079963	0.3722556616	1.3209633832
S	16.0	-2.4339817503	-0.4964129853	-2.0780184015
C	6.0	-2.5179191702	0.7958869283	2.9313696888
H	1.0	-1.8376364745	1.6556807923	2.8104042309
H	1.0	-1.9310130952	-0.0564170919	3.3141901232
H	1.0	-3.2948763673	1.0561494200	3.6755487840
C	6.0	-4.2568681233	-0.5491033686	-1.7903568387
H	1.0	-4.7693088847	-0.8833973422	-2.7119297992
H	1.0	-4.6399663685	0.4468699936	-1.5100945408
H	1.0	-4.5000438308	-1.2456308543	-0.9706168039
H	1.0	1.3803427018	-0.2096405187	-1.7352346204
H	1.0	0.6642248832	-0.4014049427	-1.4176779622

Atomic Cartesian coordinates (Å) of conformer T2 optimized with BP86/bs1 level of theory, E= -2348.030236 Hartree

FE	26.0	1.6518706137	0.0973001777	0.2168929418
NI	28.0	-1.4503618962	-0.3667736497	-1.0498581272
S	16.0	-0.2357414358	1.4713763312	-0.1824689400
S	16.0	0.6859401404	-1.2881567706	-1.4627256921
C	6.0	-0.9761485780	1.8112369532	1.4734938811
H	1.0	-1.8312313592	2.4974147452	1.3470557963
H	1.0	-0.2041818062	2.2687293912	2.1130202692
H	1.0	-1.3280130874	0.8715260716	1.9304386040
C	6.0	0.7802951388	-3.0037414929	-0.7943465048
H	1.0	0.3854994257	-3.7010780681	-1.5525854412
H	1.0	0.1721505445	-3.0875799640	0.1214250707
H	1.0	1.8314066012	-3.2353524677	-0.5604297713
C	6.0	2.6270700023	0.9661584744	-0.9019760874
O	8.0	3.3140274845	1.5588089496	-1.6546590493
C	6.0	2.2158978801	1.2224504929	1.6583660856
N	7.0	2.5187541972	1.9333270053	2.5613719267
C	6.0	3.0679397285	-1.1557003986	0.5093241295
N	7.0	3.9275424160	-1.9599467784	0.6727111545
S	16.0	-2.8118044549	0.5212611558	-2.6265942967
S	16.0	-2.3035951974	-1.8054450051	0.4880628419
C	6.0	-2.5854238546	2.3504831490	-2.7634523085
H	1.0	-2.3055038856	2.6255537154	-3.7966242047
H	1.0	-1.7862373812	2.6821991725	-2.0791000780
H	1.0	-3.5217638776	2.8798043712	-2.5067840116
C	6.0	-3.8427651313	-0.9157393712	1.0011784986
H	1.0	-4.6098548759	-1.6464216918	1.3199269443
H	1.0	-4.2368200340	-0.3238838592	0.1579872450
H	1.0	-3.6447855966	-0.2334798245	1.8477920891
H	1.0	1.0611159450	-0.8301760676	1.5481917419
H	1.0	0.3839535342	-0.7212499569	1.1274501228

Atomic Cartesian coordinates (Å) of MECP(S/T) optimized with BP86/bs1 level of theory, E= -2346.838510 Hartree

FE	26.0	0.6329261231	-0.2626683674	-1.4377550258
NI	28.0	-0.9213259827	0.2087601876	1.1424123711
S	16.0	-1.6561851937	-0.2588483345	-1.0090681525
S	16.0	0.6340264087	-1.4090526799	0.5855400742
C	6.0	-2.4614594861	1.2872126382	-1.6315687523
H	1.0	-3.5299001343	1.0768387440	-1.8109331340
H	1.0	-1.9617734575	1.6021597104	-2.5611290317
H	1.0	-2.3701602170	2.0822080701	-0.8751359202
C	6.0	2.2042204778	-1.1810882073	1.5333712174

H	1.0	2.3517690235	-2.0623607386	2.1811263118
H	1.0	2.1026111112	-0.2692087608	2.1443060609
H	1.0	3.0379889874	-1.0677083063	0.8231691378
C	6.0	0.6863259381	-1.5644904889	-2.5067557919
O	8.0	0.7139971263	-2.4906776355	-3.2472446538
C	6.0	0.4692302237	1.0223349501	-2.8165653214
N	7.0	0.3250237541	1.8358606292	-3.6734816876
C	6.0	2.5124930426	-0.0449754952	-1.4172249209
N	7.0	3.6969949763	0.0660206740	-1.3817505544
S	16.0	-2.7972599369	0.0124737269	2.4113992845
S	16.0	0.1447962690	1.7849871660	2.3736271161
C	6.0	-3.9517189114	-1.1117804132	1.5105639366
H	1.0	-3.4422446316	-2.0432860329	1.2132378987
H	1.0	-4.3515910539	-0.6376870087	0.5985886652
H	1.0	-4.7970916898	-1.3649316905	2.1783035906
C	6.0	-0.4876032493	1.7298589265	4.1042548135
H	1.0	-0.0952649981	2.5983723122	4.6659633785
H	1.0	-0.1692765563	0.8053815646	4.6181690671
H	1.0	-1.5903739632	1.7638248599	4.1150630225

Atomic Cartesian coordinates (Å) of MECP(S2/T2) optimized with BP86/bs1 level of theory, E= -2348.025924 Hartree

FE	26.0	1.6998281511	0.1096053196	0.2270108213
NI	28.0	-1.4156095789	-0.2450388050	-0.9412906316
S	16.0	-0.0138508165	1.5801205929	-0.4699762396
S	16.0	0.6510442912	-1.2630388831	-1.4168231572
C	6.0	-0.7447145228	2.3173143298	1.0570075038
H	1.0	-1.5063425290	3.0599820403	0.7630539481
H	1.0	0.0631028516	2.7940990187	1.6344662526
H	1.0	-1.2200632802	1.5359430187	1.6717021140
C	6.0	0.7327603901	-2.9992693345	-0.8060933056
H	1.0	0.3416758535	-3.6673868771	-1.5919714090
H	1.0	0.1116120968	-3.1058027702	0.0988533248
H	1.0	1.7797035917	-3.2429045614	-0.5667673745
C	6.0	2.8331320968	0.7587724039	-0.8882957338
O	8.0	3.6276325897	1.1967617439	-1.6416230763
C	6.0	2.2812551591	1.3086297405	1.5961743408
N	7.0	2.6047164086	2.0786862042	2.4420484583
C	6.0	2.9539730123	-1.2486192151	0.7142159509
N	7.0	3.7204482225	-2.1157902611	0.9847718579
S	16.0	-3.1697047377	0.7665249358	-1.9363646197
S	16.0	-2.3745044013	-1.9809099021	0.1292596744
C	6.0	-2.9987618478	2.6053812313	-1.9278888988
H	1.0	-3.4665952219	3.0271789358	-2.8369512605
H	1.0	-1.9335919663	2.8949164324	-1.9080067169

H	1.0	-3.4992097329	3.0507855568	-1.0481214427
C	6.0	-3.9301603787	-1.3318253808	0.8885058564
H	1.0	-3.7218339610	-0.8206636036	1.8458523814
H	1.0	-4.6221907532	-2.1715303726	1.0880347277
H	1.0	-4.4077366974	-0.6127961126	0.2019233311
H	1.0	0.9004179468	-0.5404027381	1.6279208048
H	1.0	0.3227029589	-0.6174003519	1.0742440046

Atomic Cartesian coordinates (Å) of conformer S optimized with TPSS/bs1 level of theory, E= -2346.562297 Hartree

Fe	26.0	1.6046569949	-0.2176741208	0.2133384134
Ni	28.0	-1.2888952035	0.4672057212	0.2314162680
S	16.0	-0.2660037286	-1.4499412978	0.8515481938
S	16.0	0.4195898875	1.3216088098	1.4288340626
C	6.0	-0.6205384380	-2.7872648210	-0.3791309990
H	1.0	-0.8906538579	-3.6974318002	0.1723142644
H	1.0	0.2776508683	-2.9555486532	-0.9803843270
H	1.0	-1.4551538905	-2.4610379737	-1.0116812867
C	6.0	0.9019025517	3.0662915649	1.0696529691
H	1.0	0.9388858511	3.6079297336	2.0235549893
H	1.0	0.1238893429	3.4862957643	0.4189874262
H	1.0	1.8774897113	3.0746167219	0.5740579027
C	6.0	2.7113323907	-0.7986736516	1.3565188973
O	8.0	3.4655956779	-1.2006911873	2.1741557834
C	6.0	2.1487635892	-1.4625794306	-1.1196801913
N	7.0	2.4704810981	-2.2585485687	-1.9392673176
C	6.0	2.8192085365	1.0690287752	-0.4813959017
N	7.0	3.5760796341	1.8891975223	-0.8851785074
S	16.0	-3.2267426390	-0.4492013434	-0.4266881394
S	16.0	-1.9940398061	2.4152409402	-0.6568344003
C	6.0	-3.6437786982	-1.7590542356	0.8156128836
H	1.0	-3.4757985021	-1.3960205251	1.8363482786
H	1.0	-3.0629511816	-2.6798078357	0.6749057484
H	1.0	-4.7111217646	-2.0002733476	0.6975172348
C	6.0	-3.4557775136	2.8881126310	0.3586163782
H	1.0	-3.9487426899	3.7524713765	-0.1121753133
H	1.0	-3.1602977509	3.1662781596	1.3804980828
H	1.0	-4.1536229296	2.0418136419	0.3981282370

Atomic Cartesian coordinates (Å) of conformer T optimized with TPSS/bs1 level of theory, E=-2346.555124 Hartree

FE	26.0	1.4071434967	-0.5120637872	1.0308143537
NI	28.0	-1.4283778301	0.5111798159	0.1539891736
S	16.0	0.6366620463	0.4399332489	-0.9601235353

S	16.0	-0.6747026231	-1.5720799262	0.9279040074
C	6.0	1.2357562773	2.1810478871	-1.1396278391
H	1.0	1.1393703954	2.4684404544	-2.1941490350
H	1.0	2.2801199823	2.2303778342	-0.8154054506
H	1.0	0.6212198882	2.8422038352	-0.5205214984
C	6.0	-1.3744583848	-1.8287665395	2.6211379363
H	1.0	-2.1279889743	-2.6243033992	2.5631216359
H	1.0	-1.8454305816	-0.9007802684	2.9613296780
H	1.0	-0.5654270143	-2.1078522135	3.3035592551
C	6.0	2.3404144156	-1.7475574799	0.3533381354
O	8.0	2.9877063593	-2.6111186794	-0.1259729371
C	6.0	2.8757476224	0.6921802956	1.1434014788
N	7.0	3.7775821111	1.4619020743	1.1902792611
C	6.0	1.7083714178	-1.0984302405	2.8147799975
N	7.0	1.8634655331	-1.4725441101	3.9300969817
S	16.0	-3.1208459997	0.1725612526	-1.3633972942
S	16.0	-2.2406254347	2.2553633854	1.3629389262
C	6.0	-2.4577401073	-1.2009362341	-2.4010919732
H	1.0	-2.2526081636	-2.0841011700	-1.7841024050
H	1.0	-1.5247501694	-0.8937820867	-2.8885079627
H	1.0	-3.1974954363	-1.4637170652	-3.1728900881
C	6.0	-3.9029820581	2.6634225162	0.6785152779
H	1.0	-4.3105842036	3.5354964846	1.2109895586
H	1.0	-4.5884877776	1.8159030704	0.8007515961
H	1.0	-3.8330607870	2.8928920453	-0.3916132346

Atomic Cartesian coordinates (Å) of conformer S1 optimized with TPSS/bs1 level of theory, E= -2347.744463 Hartree

FE	26.0	1.7384193049	0.0385431626	0.0547380431
NI	28.0	-1.4622892473	-0.1001356717	-0.2105552410
S	16.0	0.0514851898	1.5240791029	-0.7091155143
S	16.0	0.2045570342	-1.3998613476	-1.0452221155
C	6.0	-0.0980995361	2.8313660268	0.5905659269
H	1.0	-0.6352695873	3.6881158744	0.1678845710
H	1.0	0.9130166324	3.1193075982	0.8949040946
H	1.0	-0.6606045962	2.4335688595	1.4407525787
C	6.0	0.2842270098	-3.1093918532	-0.3530294156
H	1.0	0.2306071060	-3.8154292650	-1.1917521687
H	1.0	-0.5826507402	-3.2471706224	0.3048451021
H	1.0	1.2318500633	-3.2293201340	0.1813656386
C	6.0	2.7093613976	0.2018301315	-1.3573265653
O	8.0	3.3901328191	0.3093975226	-2.3103117361
C	6.0	2.7460836979	1.3992750094	0.9556842515
N	7.0	3.3480905284	2.2657107281	1.4966577980
C	6.0	2.8472216541	-1.3776776927	0.7124661970

N	7.0	3.5013844372	-2.2839705515	1.1079705413
S	16.0	-3.2399431525	1.1912922790	0.1938317419
S	16.0	-2.7239330494	-1.7924396097	0.5859274221
C	6.0	-3.1404345829	2.7420686916	-0.8227226985
H	1.0	-2.4835027462	2.6021173777	-1.6897098027
H	1.0	-2.7714519183	3.5980062592	-0.2403194320
H	1.0	-4.1523652454	2.9826420762	-1.1815666056
C	6.0	-3.8289485545	-2.1352981731	-0.8475975105
H	1.0	-4.5774142896	-2.8860927391	-0.5514509388
H	1.0	-3.2621676815	-2.5204396857	-1.7069780424
H	1.0	-4.3372922043	-1.2054271540	-1.1336595261
H	1.0	1.1259845363	-0.1154588051	1.7134109469
H	1.0	0.4476015007	-0.1472238247	1.3111837597

Atomic Cartesian coordinates (Å) of conformer S2 optimized with TPSS/bs1 level of theory, E= -2347.746837 Hartree

FE	26.0	1.8338564052	0.1095074565	0.1188329040
NI	28.0	-1.3936261301	-0.1540322272	-0.6903828051
S	16.0	0.0811888423	1.5556846682	-0.4859356184
S	16.0	0.5014423620	-1.2905623101	-1.2353661034
C	6.0	-0.4095170488	2.4054204038	1.0784084724
H	1.0	-1.2850185190	3.0298598104	0.8721694936
H	1.0	0.4459502076	2.9965989385	1.4219485089
H	1.0	-0.6772575732	1.6635224177	1.8384759738
C	6.0	0.5567974822	-2.9905759111	-0.5234991516
H	1.0	0.1094864603	-3.6849687038	-1.2429674386
H	1.0	-0.0223580471	-3.0201170202	0.4057490746
H	1.0	1.6060335891	-3.2349746978	-0.3292791019
C	6.0	2.8427883537	0.5911655103	-1.1904971587
O	8.0	3.5493597647	0.9173333158	-2.0718773993
C	6.0	2.6513783676	1.4043493768	1.2822512278
N	7.0	3.1250381191	2.2237309677	1.9957340114
C	6.0	3.0729633662	-1.2805057273	0.5959780039
N	7.0	3.8126368713	-2.1648706759	0.8714341428
S	16.0	-3.1992547886	1.1836764461	-0.6014899821
S	16.0	-2.5436384876	-2.0649125402	-0.5095030405
C	6.0	-2.8369008030	2.5781218224	-1.7584451935
H	1.0	-2.6796099673	2.2083314748	-2.7799908277
H	1.0	-1.9447387645	3.1400085209	-1.4560389599
H	1.0	-3.7045168369	3.2554000143	-1.7582038640
C	6.0	-4.3313756528	-1.7907850905	-0.1594885296
H	1.0	-4.5081441144	-1.5621956291	0.9009023968
H	1.0	-4.8767018778	-2.7111457538	-0.4165546892
H	1.0	-4.7086573824	-0.9547797239	-0.7614966741
H	1.0	1.1736451833	-0.3023420777	1.7086986876

H	1.0	0.5724063990	-0.4939594858	1.2413049399

Atomic Cartesian coordinates (Å) of conformer T1 optimized with TPSS/bs1 level of theory, E= -2347.743459 Hartree

FE	26.0	1.6691920975	0.0074258155	-0.0416852871
NI	28.0	-1.4878562316	0.0364801107	-0.0394641534
S	16.0	0.0462790450	-1.3581370413	1.0454767280
S	16.0	0.0786570185	1.7324237833	0.3583648036
C	6.0	-0.0669960391	-2.9496217006	0.1127708866
H	1.0	-0.6677775386	-3.6497161433	0.7073451691
H	1.0	0.9446909196	-3.3415893244	-0.0366999775
H	1.0	-0.5591501148	-2.7777471637	-0.8508641242
C	6.0	-0.0156158992	2.7472420306	-1.1835487145
H	1.0	-0.6371159565	3.6281003791	-0.9782394202
H	1.0	-0.4770244498	2.1612945845	-1.9868864158
H	1.0	0.9986788212	3.0483660129	-1.4661757186
C	6.0	2.4705853114	0.3210119464	1.4551293816
O	8.0	3.0355823129	0.5340184816	2.4620063035
C	6.0	2.8010291340	-1.5097038974	-0.3676650429
N	7.0	3.4697927954	-2.4698708306	-0.5552272409
C	6.0	2.8398086463	1.2276156462	-0.9529720264
N	7.0	3.5342393467	2.0053696654	-1.5164074224
S	16.0	-3.3132952304	0.3756498746	1.3232685220
S	16.0	-2.3864176160	-0.4983851577	-2.0880231161
C	6.0	-2.5126918042	0.7944652568	2.9311009748
H	1.0	-1.8426146310	1.6543902852	2.8107069455
H	1.0	-1.9251613118	-0.0549550879	3.3009427506
H	1.0	-3.2861371427	1.0440101307	3.6738389900
C	6.0	-4.2101566662	-0.5454779570	-1.8054891196
H	1.0	-4.7119269796	-0.8756678154	-2.7271246987
H	1.0	-4.5863518856	0.4471661083	-1.5295273036
H	1.0	-4.4545375262	-1.2405177688	-0.9935317542
H	1.0	1.3060334309	-0.2080118561	-1.7453671293
H	1.0	0.6139938838	-0.4030724976	-1.4199618899

Atomic Cartesian coordinates (Å) of conformer T2 optimized with TPSS/bs1 level of theory, E= -2347.747387 Hartree

FE	26.0	1.6446654557	0.0888555212	0.1280635596
NI	28.0	-1.4533798536	-0.3389807962	-1.1306598167
S	16.0	-0.2217755791	1.4945994932	-0.2638668993
S	16.0	0.6839189463	-1.2636064522	-1.5770284552
C	6.0	-0.9506696104	1.7997301226	1.4030980113
H	1.0	-1.8167779992	2.4647610119	1.2915426536
H	1.0	-0.1855425326	2.2627376979	2.0353873862

H	1.0	-1.2748798697	0.8506484789	1.8458422352
C	6.0	0.7643086801	-2.9880142104	-0.9312842824
H	1.0	0.3496528874	-3.6637378428	-1.6899077937
H	1.0	0.1739926718	-3.0729723384	-0.0116782582
H	1.0	1.8101318588	-3.2338629385	-0.7203940642
C	6.0	2.6522738174	0.9547939855	-0.9738950519
O	8.0	3.3527788362	1.5431321545	-1.7117234328
C	6.0	2.2159621830	1.1919996064	1.5942289936
N	7.0	2.5269465044	1.8870819124	2.5025223097
C	6.0	3.0352220905	-1.1983664963	0.4457262106
N	7.0	3.8761779875	-2.0145424334	0.6227385321
S	16.0	-2.8953505825	0.5666917365	-2.6431416935
S	16.0	-2.2567135242	-1.7860016862	0.4426365380
C	6.0	-2.6863471681	2.3996013027	-2.7302686275
H	1.0	-2.4186816289	2.6992321201	-3.7530949782
H	1.0	-1.8901697667	2.7176579149	-2.0467768705
H	1.0	-3.6238234862	2.9047035905	-2.4554288932
C	6.0	-3.7835561551	-0.8922592394	0.9820420845
H	1.0	-4.5276584094	-1.6178623012	1.3423842004
H	1.0	-4.2041063262	-0.3297080646	0.1398624132
H	1.0	-3.5582069359	-0.1925562170	1.7987219518
H	1.0	0.9516693123	-0.7793267974	1.4754531316
H	1.0	0.3312908743	-0.7752556906	0.9898664664

Atomic Cartesian coordinates (Å) of MECP(S2/T2) optimized with TPSS/bs1 level of theory, E= -2347.740315 Hartree

FE	26.0	1.6772121833	0.1000000211	0.1112644656
NI	28.0	-1.4261629791	-0.1908459189	-0.9758378281
S	16.0	0.0018178969	1.6132648450	-0.5719569361
S	16.0	0.6018315313	-1.2328580643	-1.5333580726
C	6.0	-0.6925318600	2.3628015478	0.9650952854
H	1.0	-1.4327808548	3.1216645608	0.6827965416
H	1.0	0.1319112922	2.8142270817	1.5270460804
H	1.0	-1.1769196387	1.5938588080	1.5769404919
C	6.0	0.6784511465	-2.9733596566	-0.9366109593
H	1.0	0.2306386966	-3.6230125931	-1.6988297063
H	1.0	0.1089157839	-3.0660207343	-0.0045851448
H	1.0	1.7259481636	-3.2371676965	-0.7604335846
C	6.0	2.8228382087	0.7407959274	-1.0051012723
O	8.0	3.6181265738	1.1714813935	-1.7560182479
C	6.0	2.2886490983	1.2706640784	1.5055129565
N	7.0	2.6301416166	2.0175166176	2.3604295413
C	6.0	2.9142655700	-1.2887801943	0.5934846579
N	7.0	3.6709227667	-2.1615598889	0.8588969657
S	16.0	-3.2710009827	0.8626892040	-1.7373415802

S	16.0	-2.3717869856	-2.0015461267	0.0045451155
C	6.0	-3.0034706588	2.6845570587	-1.8638870071
H	1.0	-3.5909525775	3.0769714050	-2.7070279119
H	1.0	-1.9427058185	2.9050718981	-2.0331835067
H	1.0	-3.3292563254	3.2010578433	-0.9496409903
C	6.0	-3.8561941559	-1.3976014103	0.9275049926
H	1.0	-3.6030919858	-1.2014810619	1.9793146275
H	1.0	-4.6526712239	-2.1555654020	0.8955354660
H	1.0	-4.2094668802	-0.4715150337	0.4612132077
H	1.0	0.8448841773	-0.5554981490	1.5222945045
H	1.0	0.2752073833	-0.6194492571	0.9833352295

Atomic Cartesian coordinates (Å) of conformer S optimized with B3LYP/bs1 level of theory, E= -2345.860730 Hartree

FE	26.0	1.7416477969	-0.2750844310	0.1939416590
NI	28.0	-1.4470981304	0.5231267203	0.7459645010
S	16.0	-0.2403166348	-1.4801622375	0.6323614273
S	16.0	0.6126068859	1.1966676112	1.6226631638
C	6.0	-0.7753623025	-2.3189813325	-0.9153010714
H	1.0	-1.6436807061	-2.9451078222	-0.6949074028
H	1.0	0.0542239989	-2.9202520762	-1.2906882780
H	1.0	-1.0605149479	-1.5808506085	-1.6660910638
C	6.0	1.0768136140	2.9477411507	1.3164935041
H	1.0	0.8150637955	3.5389601525	2.1984915980
H	1.0	0.5231296816	3.3301150934	0.4562317318
H	1.0	2.1488089641	2.9964631806	1.1195406292
C	6.0	2.7425287275	-1.0651923736	1.3493909925
O	8.0	3.4132402246	-1.5943523586	2.1370429734
C	6.0	2.2811230335	-1.4482515245	-1.2518774549
N	7.0	2.5821821988	-2.1699661610	-2.1274428027
C	6.0	3.1029161946	1.0164134341	-0.2795153685
N	7.0	3.9172069736	1.8199331578	-0.5432302358
S	16.0	-3.5137688719	-0.4237919057	0.4635605264
S	16.0	-2.1367991379	2.6676098789	0.4348642375
C	6.0	-3.5399313225	-1.9141318096	1.5449410645
H	1.0	-3.4451787382	-1.6413261690	2.6023278786
H	1.0	-2.7350186097	-2.6144483114	1.3055407258
H	1.0	-4.5019975390	-2.4249484278	1.4087468822
C	6.0	-3.8230235598	2.7238371419	-0.2933506204
H	1.0	-3.8350362594	2.3375426307	-1.3184664337
H	1.0	-4.1538397298	3.7701726607	-0.3137957160
H	1.0	-4.5255265493	2.1341912358	0.3015595829

Atomic Cartesian coordinates (Å) of conformer T optimized with B3LYP/bs1 level of theory, E= -2345.869613 Hartree

FE	26.0	1.4771794788	-0.5498449713	1.0265001745
NI	28.0	-1.5579603458	0.5327384040	0.1173565317
S	16.0	0.6235155195	0.5828825233	-0.8807346054
S	16.0	-0.6839043577	-1.5459484920	0.9820579949
C	6.0	1.2030154754	2.3310953393	-0.9285351994
H	1.0	1.0774780321	2.7098669724	-1.9476522874
H	1.0	2.2541923203	2.3684155459	-0.6367698814
H	1.0	0.6055728991	2.9396547612	-0.2461994038
C	6.0	-1.3322750018	-1.7488190563	2.6952769040
H	1.0	-2.1964305730	-2.4194770922	2.6616623106
H	1.0	-1.6468157849	-0.7839535648	3.1001475563
H	1.0	-0.5482619967	-2.1688133830	3.3279893318
C	6.0	2.3035368013	-1.8057653977	0.1821614261
O	8.0	2.8580515897	-2.6518604182	-0.3875131935
C	6.0	3.0345784546	0.5949400881	1.1176788979
N	7.0	3.9609266284	1.3150441702	1.1566201015
C	6.0	1.8637773491	-1.2907892717	2.7724006149
N	7.0	2.0601925012	-1.7425275469	3.8380424370
S	16.0	-3.1830237190	0.0672814945	-1.4817389287
S	16.0	-2.3454064715	2.4043163655	1.2529744118
C	6.0	-2.4487198699	-1.3596714847	-2.3844065488
H	1.0	-2.2683406047	-2.2011123616	-1.7088167765
H	1.0	-1.4961235136	-1.0772807350	-2.8434494186
H	1.0	-3.1360234486	-1.6837445963	-3.1766234929
C	6.0	-4.0048118619	2.7501543015	0.5309681557
H	1.0	-4.4116935298	3.6646903679	0.9798017179
H	1.0	-4.6985927903	1.9261399288	0.7221739022
H	1.0	-3.9356391803	2.8872591090	-0.5518287325

Atomic Cartesian coordinates (Å) of conformer S1 optimized with B3LYP/bs1 level of theory, E= -2347.034899 Hartree

FE	26.0	1.7118937536	0.0539937123	-0.0126446290
NI	28.0	-1.7262255248	0.0762765993	-0.2580762147
S	16.0	-0.0160118968	1.6377486366	-0.5193704038
S	16.0	0.0062794774	-1.3876918195	-0.8866098834
C	6.0	-0.1420903038	2.6993216580	0.9781834192
H	1.0	-0.8420782236	3.5162217070	0.7853014280
H	1.0	0.8515046803	3.0947695912	1.1992556483
H	1.0	-0.5069200384	2.1249391104	1.8339993422
C	6.0	0.0122830457	-2.9953024308	0.0075989191
H	1.0	-0.2402584050	-3.7951435880	-0.6964440014
H	1.0	-0.7424501916	-2.9643365817	0.7982701491

H	1.0	1.0115009687	-3.1709563021	0.4106766946
C	6.0	2.4643588930	0.2302243853	-1.5886747246
O	8.0	2.9758228240	0.3449593448	-2.6208246772
C	6.0	2.8792767955	1.4181109253	0.7522942130
N	7.0	3.5475219103	2.2635396698	1.2163734500
C	6.0	2.9208785293	-1.4048237218	0.4564378677
N	7.0	3.6118649947	-2.3087280028	0.7432648667
S	16.0	-3.5050309104	1.4709910492	-0.3477728591
S	16.0	-3.1333596486	-1.5232868308	0.6065097579
C	6.0	-3.0377769535	3.0559938942	-1.1758231302
H	1.0	-2.3477830980	2.8941288268	-2.0086575068
H	1.0	-2.5755766817	3.7723114189	-0.4870152033
H	1.0	-3.9548202478	3.5152952675	-1.5672067455
C	6.0	-3.5360098980	-2.5390193446	-0.8729189024
H	1.0	-4.2123666946	-3.3530369123	-0.5834664927
H	1.0	-2.6364291168	-2.9741254542	-1.3222473226
H	1.0	-4.0368022668	-1.9228051234	-1.6277655918
H	1.0	0.7182399960	-0.3480948371	1.4268708923
H	1.0	1.2942200117	0.0805087225	1.7213529403

Atomic Cartesian coordinates (Å) of conformer S2 optimized with B3LYP/bs1 level of theory, E= -2347.037013 Hartree

FE	26.0	1.8722004239	0.1144765110	0.2439300321
NI	28.0	-1.4122877129	-0.1742103418	-0.6851515702
S	16.0	0.0824317979	1.5573141466	-0.3955989773
S	16.0	0.5404550586	-1.3424835706	-1.0999500506
C	6.0	-0.4704653959	2.3831361112	1.1501612191
H	1.0	-1.3383595728	3.0085059669	0.9292215449
H	1.0	0.3600523734	2.9797783545	1.5345024150
H	1.0	-0.7621557495	1.6421537461	1.8990015193
C	6.0	0.5766593478	-3.0226470162	-0.3595706836
H	1.0	0.1166736978	-3.7276400035	-1.0564040533
H	1.0	0.0132339760	-3.0432976766	0.5765238567
H	1.0	1.6198932448	-3.2852165470	-0.1729409631
C	6.0	2.8658346260	0.6023724890	-1.1170847772
O	8.0	3.5355537818	0.9212433666	-2.0061353533
C	6.0	2.6999680342	1.4603656423	1.3931634078
N	7.0	3.1645518744	2.2900268705	2.0804313234
C	6.0	3.1607338317	-1.2708665055	0.7334904220
N	7.0	3.9111906085	-2.1298421698	1.0087118782
S	16.0	-3.2557030751	1.1467857809	-0.7211607507
S	16.0	-2.5782863899	-2.1004596588	-0.4986995306
C	6.0	-2.8425226296	2.6165248755	-1.7520845051
H	1.0	-2.6530706265	2.3319209964	-2.7934328702
H	1.0	-1.9607625211	3.1472543452	-1.3831921018

H	1.0	-3.7003936333	3.3012649486	-1.7340436656
C	6.0	-4.3688212161	-1.8018674974	-0.2103863866
H	1.0	-4.5425817558	-1.2311900918	0.7076843324
H	1.0	-4.8628455080	-2.7772890503	-0.1143028701
H	1.0	-4.8172550064	-1.2481655348	-1.0392494762
H	1.0	1.2213669395	-0.2918740914	1.8534514609
H	1.0	0.6316527444	-0.4957947177	1.3926542584

Atomic Cartesian coordinates (Å) of conformer T1 optimized with B3LYP/bs1 level of theory, E= -2347.048110 Hartree

FE	26.0	1.7522091662	-0.0029055587	0.0057680667
NI	28.0	-1.5881264217	0.0284953428	0.0613317281
S	16.0	0.0639547677	-1.3823881266	1.0618086792
S	16.0	0.0940665685	1.7224902871	0.3950060566
C	6.0	-0.0304391150	-2.9857581537	0.1629249170
H	1.0	-0.6314653868	-3.6841416826	0.7542913987
H	1.0	0.9800438032	-3.3798751638	0.0332548294
H	1.0	-0.5099518147	-2.8468284566	-0.8094061747
C	6.0	-0.0003595718	2.7781866129	-1.1116005619
H	1.0	-0.6176584758	3.6550153888	-0.8914381707
H	1.0	-0.4561549731	2.2273102265	-1.9396797777
H	1.0	1.0092978064	3.0901743160	-1.3878330689
C	6.0	2.5116699852	0.3303045010	1.5567576295
O	8.0	3.0290970109	0.5484414891	2.5680990120
C	6.0	2.9284155015	-1.5281096639	-0.2860327755
N	7.0	3.6061684212	-2.4719255913	-0.4481085223
C	6.0	2.9477687628	1.2429236596	-0.9020555679
N	7.0	3.6310511464	2.0211384445	-1.4533803604
S	16.0	-3.4119899432	0.3723875309	1.4614026072
S	16.0	-2.4761598480	-0.6601035473	-1.9937323694
C	6.0	-2.6012203678	0.8428070744	3.0463294580
H	1.0	-1.9347659159	1.6986146699	2.9028537461
H	1.0	-2.0109518822	0.0109746910	3.4435924832
H	1.0	-3.3663954630	1.1128021869	3.7855087568
C	6.0	-4.3046000395	-0.5606043149	-1.7848110580
H	1.0	-4.7952363188	-1.0055073149	-2.6594258836
H	1.0	-4.6379812924	0.4772991273	-1.6879656008
H	1.0	-4.6217099217	-1.1013159437	-0.8887055656
H	1.0	1.1485119035	-0.7080941498	-1.5104985795
H	1.0	0.9606476480	0.0407479892	-1.5881644315

Atomic Cartesian coordinates (Å) of conformer T2 optimized with B3LYP/bs1 level of theory, E= -2347.052076 Hartree

FE	26.0	1.7014789000	0.0915910001	0.2503913828
NI	28.0	-1.4465131152	-0.3483671191	-1.0874248442
S	16.0	-0.2109815627	1.4960602720	-0.1550293055
S	16.0	0.7322104322	-1.3078661164	-1.4649323056
C	6.0	-0.9647798188	1.8304098786	1.4883868162
H	1.0	-1.8116207641	2.5129559448	1.3616541126
H	1.0	-0.2090567810	2.2863829302	2.1322502572
H	1.0	-1.3198828746	0.8999054971	1.9399142401
C	6.0	0.7831294094	-3.0233319882	-0.8088204706
H	1.0	0.3890398524	-3.7068994030	-1.5674515368
H	1.0	0.1726091417	-3.1089766788	0.0937370000
H	1.0	1.8185764659	-3.2786115437	-0.5728006000
C	6.0	2.6783340729	0.9769623166	-0.9142424550
O	8.0	3.3364264442	1.5573419808	-1.6688521952
C	6.0	2.2940507472	1.2499707099	1.7073367156
N	7.0	2.6076362719	1.9607623345	2.5865427849
C	6.0	3.1505057613	-1.1842710667	0.5462306254
N	7.0	4.0023194087	-1.9749681473	0.7064849475
S	16.0	-2.9234517110	0.5413071433	-2.6549513178
S	16.0	-2.3438340555	-1.7620575735	0.5171135058
C	6.0	-2.6975441922	2.3695637768	-2.7340073154
H	1.0	-2.4193527035	2.6736701736	-3.7498543321
H	1.0	-1.9085488783	2.6857956198	-2.0465692644
H	1.0	-3.6288108217	2.8839463534	-2.4665885908
C	6.0	-3.9145979657	-0.8969072011	0.9508691271
H	1.0	-4.6719363948	-1.6334422339	1.2465200999
H	1.0	-4.2871224320	-0.3309565633	0.0923448311
H	1.0	-3.7664788301	-0.2058441784	1.7892812970
H	1.0	1.0966788071	-0.8508985137	1.6121697076
H	1.0	0.4380286901	-0.7412556778	1.2146872136

Atomic Cartesian coordinates (Å) of MECP(S2/T2) optimized with B3LYP/bs1 level of theory, E= -2347.034467 Hartree

FE	26.0	1.8586605107	0.1336177384	0.2500580222
NI	28.0	-1.4404534351	-0.1667396353	-0.6878914339
S	16.0	0.0835953593	1.5993576882	-0.4015605266
S	16.0	0.5722498975	-1.3116098074	-1.1630344183
C	6.0	-0.4933310612	2.4485858284	1.1233572266
H	1.0	-1.2484495959	3.1919049801	0.8537587892
H	1.0	0.3657405483	2.9303063262	1.5958662385
H	1.0	-0.9381659717	1.7324152157	1.8189278118
C	6.0	0.6307936155	-3.0196803508	-0.4929262778

H	1.0	0.2162893011	-3.7057879296	-1.2364624474
H	1.0	0.0317285036	-3.0926717197	0.4182085015
H	1.0	1.6718939722	-3.2670746305	-0.2763517954
C	6.0	2.8761561436	0.6565884049	-1.0819327130
O	8.0	3.5608092005	0.9980574328	-1.9506640097
C	6.0	2.6538811281	1.4583689735	1.4435298731
N	7.0	3.0934528375	2.2778648304	2.1589589731
C	6.0	3.1468646486	-1.2525132938	0.7342423337
N	7.0	3.8998872402	-2.1104799259	1.0055718585
S	16.0	-3.3267041985	1.0671504424	-1.0447296896
S	16.0	-2.5599014238	-2.1065157195	-0.2151598619
C	6.0	-2.9001718264	2.7830282533	-1.5629554138
H	1.0	-3.5551681720	3.0811326718	-2.3915653200
H	1.0	-1.8613382943	2.8468960936	-1.8957347533
H	1.0	-3.0450113749	3.5017223062	-0.7461386774
C	6.0	-4.3261432436	-1.7674381380	0.1687379585
H	1.0	-4.4387654144	-1.1456079379	1.0627367722
H	1.0	-4.8308446956	-2.7265077556	0.3423352171
H	1.0	-4.8214330503	-1.2567269038	-0.6621451184
H	1.0	1.1718585714	-0.2750378450	1.8415145881
H	1.0	0.6205302635	-0.5415283939	1.3650733463

Atomic Cartesian coordinates (Å) of conformer S2 optimized with PBE/def2-TZVP level of theory, E= -4823.509835 Hartree

FE	26.0	-1.8718029213	0.0024662296	-0.2020112786
NI	28.0	1.4596306157	-0.0991881343	0.1571877549
S	16.0	-0.1133924783	1.4948501951	0.2137533004
S	16.0	-0.2597894773	-1.3517734362	0.8245754227
C	6.0	0.1362403315	2.4170445907	-1.3470278000
H	1.0	1.0005179774	3.0828311761	-1.2213383892
H	1.0	-0.7843855061	2.9786498698	-1.5565752942
H	1.0	0.3450933923	1.7269024396	-2.1746781440
C	6.0	-0.3113992031	-3.0233465671	0.0865447012
H	1.0	0.3075563113	-3.6914633646	0.7011025716
H	1.0	0.0975233403	-3.0103488356	-0.9334455472
H	1.0	-1.3591014576	-3.3519948346	0.0751679494
C	6.0	-2.6803645735	0.3429874071	1.2733048334
O	8.0	-3.2556743783	0.5694090350	2.2652702713
C	6.0	-2.9281055151	1.3155726775	-1.1000640807
N	7.0	-3.5478077447	2.1494700048	-1.6554566341
C	6.0	-3.0933682668	-1.4281013687	-0.5289624843
N	7.0	-3.8144954149	-2.3403668959	-0.7174967212
S	16.0	3.1804471477	1.3045601606	0.0127622358
S	16.0	2.6422891049	-1.8830346654	-0.4165264576
C	6.0	2.8426869143	2.7165731372	1.1293151295

H	1.0	2.7636446872	2.3912187788	2.1780736529
H	1.0	1.9124392304	3.2444019868	0.8717391042
H	1.0	3.6854993575	3.4233249397	1.0442164207
C	6.0	4.3361049741	-1.4568398566	-0.9490824215
H	1.0	4.3509447195	-0.9553632728	-1.9303604464
H	1.0	4.9165920364	-2.3914188031	-1.0206706117
H	1.0	4.8121196825	-0.7813617563	-0.2214267185
H	1.0	-1.4944325907	-0.2133572328	-1.8768147668
H	1.0	-0.8302755153	-0.5056984144	-1.5120876217

Atomic Cartesian coordinates (Å) of conformer T2 optimized with PBE/def2-TZVP level of theory, E= -4823.495878 Hartree

FE	26.0	-1.7848917133	0.0621662673	-0.1117858918
NI	28.0	1.5556146608	-0.2434677214	0.3026055288
S	16.0	0.0913121045	1.4320261307	-0.4263619422
S	16.0	-0.3482633422	-1.0775964438	1.3713048551
C	6.0	0.3561255662	1.5484842940	-2.2310160526
H	1.0	1.2466017403	2.1692837351	-2.4112837438
H	1.0	-0.5312313435	2.0062867829	-2.6901123747
H	1.0	0.5202202243	0.5497837581	-2.6600313832
C	6.0	-0.5700940708	-2.8613891581	1.0478929098
H	1.0	0.0248366620	-3.4222620566	1.7839412084
H	1.0	-0.2139568191	-3.1108549795	0.0382876504
H	1.0	-1.6354714342	-3.1124733037	1.1396956240
C	6.0	-2.4308782321	1.0656199280	1.1265741460
O	8.0	-2.8960049031	1.7429926887	1.9566472654
C	6.0	-2.7665765692	1.0267644109	-1.4369722228
N	7.0	-3.3331626136	1.6329785791	-2.2728684026
C	6.0	-3.1959479971	-1.1901620852	0.1784744303
N	7.0	-4.0457896059	-1.9821105205	0.3731670917
S	16.0	3.2737431791	0.8780719269	1.1832629116
S	16.0	2.0063274526	-1.9339430288	-1.0953337837
C	6.0	3.1438410911	2.6809204881	0.8921447889
H	1.0	3.2537692456	3.2309817769	1.8411051804
H	1.0	2.1629008397	2.9250765528	0.4565626408
H	1.0	3.9350329361	3.0227164069	0.2042629430
C	6.0	3.3210391908	-1.2486973813	-2.1731388684
H	1.0	3.8742353854	-2.0739478134	-2.6527750445
H	1.0	4.0195286409	-0.6364986499	-1.5839152219
H	1.0	2.8931924431	-0.6161702594	-2.9679001020
H	1.0	-1.5876863615	-0.9995144461	-1.4491932817
H	1.0	-0.8162510074	-0.8708967386	-1.2273014589

Atomic Cartesian coordinates (Å) of MECP(S/T) optimized with PBE/def2-TZVP level of theory, E= -4822.315699 Hartree

FE	26.0	1.5514086659	-0.2673098677	0.1952080360
NI	28.0	-1.3794190365	0.3725631366	0.3227045693
S	16.0	-0.2708482383	-1.6256809708	0.4386516379
S	16.0	0.3471610570	0.9701639472	1.7064468146
C	6.0	-0.6276965666	-2.6112585288	-1.0658901993
H	1.0	-1.2931933496	-3.4402046261	-0.7835171592
H	1.0	0.3152086598	-2.9878123343	-1.4829478926
H	1.0	-1.1252415683	-1.9833085541	-1.8153214567
C	6.0	0.6808781611	2.7662842968	1.5820728663
H	1.0	0.3344199346	3.2450970481	2.5104053333
H	1.0	0.1303059833	3.1680693920	0.7207871235
H	1.0	1.7584034850	2.9221437652	1.4398218246
C	6.0	2.6489087511	-1.0363140151	1.2172982952
O	8.0	3.4047095961	-1.5762861653	1.9391711147
C	6.0	2.1662723386	-1.2209611415	-1.3185999123
N	7.0	2.5266339010	-1.8502451176	-2.2488272684
C	6.0	2.7617317058	1.1457623995	-0.1641254031
N	7.0	3.5163900818	2.0322877170	-0.3522298462
S	16.0	-3.4869349933	-0.0771536446	0.9835616166
S	16.0	-1.8585872205	2.0398665407	-1.0936983456
C	6.0	-3.4234524531	-1.6186025283	1.9649499852
H	1.0	-2.7543942592	-1.5096810804	2.8314695629
H	1.0	-3.0595787219	-2.4658532436	1.3657129249
H	1.0	-4.4389165839	-1.8510862298	2.3281535945
C	6.0	-3.4462123861	2.7929827057	-0.5966332867
H	1.0	-3.7255034573	3.5718624053	-1.3251544737
H	1.0	-3.3772860273	3.2495224902	0.4027399754
H	1.0	-4.2407684091	2.0310787036	-0.5632134014

Atomic Cartesian coordinates (Å) of MECP(S2/T2) optimized with PBE/def2-TZVP level of theory, E= -4823.493347 Hartree

FE	26.0	2.1287143205	0.2918637448	0.8009308459
NI	28.0	-0.9439234360	-0.0725290373	-0.4172830783
S	16.0	0.4360796317	1.7369937955	0.0907460605
S	16.0	1.1206974958	-1.0601303313	-0.8484086325
C	6.0	-0.3191812818	2.4883516548	1.5781249166
H	1.0	-1.0838597584	3.2112924183	1.2552377518
H	1.0	0.4652658345	2.9924711756	2.1592034075
H	1.0	-0.7924701269	1.7167718363	2.2003310022
C	6.0	1.2200850426	-2.7922570755	-0.2785119946
H	1.0	0.8235240432	-3.4412131294	-1.0735061860
H	1.0	0.6147354188	-2.9268562130	0.6292039206

H	1.0	2.2682536690	-3.0374218233	-0.0609969820
C	6.0	3.2774923294	0.9577729813	-0.2881926662
O	8.0	4.0767707929	1.4060839623	-1.0133327109
C	6.0	2.6925217374	1.4966272759	2.1676514928
N	7.0	3.0066225017	2.2644690487	3.0041441547
C	6.0	3.3990393101	-1.0469133571	1.2862759721
N	7.0	4.1758694775	-1.8905925077	1.5550094023
S	16.0	-2.6323390393	0.9176983397	-1.4834436297
S	16.0	-1.8481687896	-1.7489052406	0.7476013799
C	6.0	-2.4960598892	2.7422803251	-1.4496831183
H	1.0	-3.0339643992	3.1671773048	-2.3134468180
H	1.0	-1.4414267168	3.0550768456	-1.4947331094
H	1.0	-2.9391803417	3.1596009169	-0.5305056925
C	6.0	-3.3700176100	-1.0787030063	1.5153176605
H	1.0	-4.0498944986	-1.9091653897	1.7707508937
H	1.0	-3.8716263197	-0.3919075508	0.8174877332
H	1.0	-3.1361770134	-0.5278112283	2.4406824240
H	1.0	1.3328493261	-0.3635197159	2.1920466672
H	1.0	0.7529945917	-0.4429180827	1.6295533456