Electronic Supplementary Information

Sulfamoyl Nitrenes: Singlet or Triplet Ground State?

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Experimental details

Caution! *Covalent azides are potentially hazardous explosive. Although we have not experienced any incident during this work, safety precautions (face shields, leather gloves, and protective leather clothing) are recommended for handling the azides.*

Synthesis of $H_2NS(O)_2–N_3$ and $Me_2NS(O)_2–N_3$

Sulfamoyl azides ($H_2NS(O)_2N_3$) was prepared according to the reference[1] with modifications. Briefly, a solution of 0.012 mol sulfamoyl chloride ($H_2NS(O)_2Cl$) in 4 mL of acetonitrile (CH_3CN) was added to a stirred mixture of 0.018 mol sodium azide (NaN_3) in 4 mL of acetonitrile. The reaction was completed after 24 h at 45 °C. After filtration, the solvent (CH_3CN) was removed by distillation with a rotary evaporator. Then the residue was purified by trap-to-trap condensation (0, −95, and −196 °C) in vacuum. The product $H_2NS(O)_2N_3$ was collected in the 0 °C trap as white solid. The azide has a melt point of about 29 °C. Its purity was checked by liquid IR spectroscopy (3386, 3282, 2134, 1548, 1364, 1159, 920, 748, and 605 cm^{-1}) and ^1H (7.26, 5.43 ppm) NMR spectroscopy (600 MHz, $CDCl_3$). 1-^{15}N sodium azide (98 atom % ^{15}N, EURISO-TOP GmbH) was used for the preparation of ^{15}N labeled sample.

N,N-Dimethylsulfamoyl azide ($Me_2NS(O)_2N_3$) was prepared according to published protocols[2] with modifications. Which is in the similar manner to that of $H_2NS(O)_2N_3$. Briefly, a solution of 0.014 mol sulfamoyl chloride ($Me_2NS(O)_2Cl$) in 4 mL of acetonitrile (CH_3CN) was added to a stirred mixture of 0.020 mol sodium azide (NaN_3) in 4 mL of acetonitrile. The reaction was completed after 48 h at 50 °C. After filtration, the solvent (CH_3CN) was removed by distillation with a rotary evaporator. Then the residue was purified by repeated trap-to-trap condensation (−45, −95, and −196 °C) in vacuum. The product $Me_2NS(O)_2N_3$ was collected in the −45 °C trap as colorless liquid. Its purity was checked by liquid IR spectroscopy (2981, 2938, 2126, 1462, 1416, 1375, 1271, 1197, 1161, 1052, 962, and 727 cm^{-1}) and ^1H (7.28, 2.97 ppm) and ^{13}C (77.34, 77.13, 76.92, 39.58 ppm) NMR spectroscopy (600 MHz, $CDCl_3$).

Matrix isolation spectroscopy

Matrix IR spectra were recorded on a FT-IR spectrometer (Bruker 70 V) in a reflectance mode by using a transfer optic. A KBr beam splitter and MCT detector were used in the mid-IR region (4000-500 cm^{-1}). For each spectrum, 200 scans at a resolution of 0.5 cm^{-1} were co-added.

The gaseous sample was mixed by passing a flow of matrix gas (N_2, Ar, Ne) through an U-trap (about 25 °C for $H_2NS(O)_2N_3$, about −25 °C for $Me_2NS(O)_2N_3$) containing ca. 50 mg of the azide. Then the mixture (azide : inert gas ≈ 1 : 1000 estimated) was passed through an aluminum oxide furnace (o.d. 2.0 mm, i.d. 1.0 mm), which can be heated over a length of approximately 25 mm by a tantalum wire (o.d. 0.4 mm, resistance 0.4 Ω) deposited (rate about 2 mmol/h) at a high vacuum onto the Rh-plated copper block matrix support (2.8 K) in a high vacuum (≈ 10^{-6} Pa). While not directly measured, the expected residence time of the mixture in the pyrolysis tube is about a few milliseconds, and the pressure inside the pyroysis tube is about 10 mbar. Photolysis experiments were performed by using an ArF excimer laser (193 nm, Gamlaser EX5/250, 3Hz) and Nd^{3+}:YAG laser (266 nm, MPL-F-266, 10 mW).

EPR spectra were recorded using a Bruker ELEXSYS E500 spectrometer operating at the X-band equipped with a digital temperature controller. For the measurements under the organic glassy matrix conditions, the sample solution (20 mg mL^{-1}) in a quartz tube (4.0 mm) was degassed by the freeze-pump-thaw cycle for three times. After the sample deposition, the cryostat cold head was cooled to 5 K for photolysis (266 nm laser) and measurement.

Quantum chemical calculation methods

Structures and IR frequencies of stationary points and transient states were calculated using the DFT methods (B3LYP)[3] with the 6-311++G(3df,3pd)[4] basis set. Accurate relative energies calculation were performed by applying several sophisticated theoretical methods, such as CBS-QB3[5] and CCSD(T).[6] All reaction energies calculated at the CCSD(T)/aug-cc-pVTZ[7] level are corrected with B3LYP/6-311++G(3df,3pd) zero-point vibrational energy (ZPVE) at 298.15 K. Transition states were further confirmed by intrinsic reaction coordinate (IRC) calculations.[8] The *D* values were calculated by the linear correlation with the natural spin density

(D=1.96673ρ – 2.0577, [9] M06-2X[10]/6-311++G(3df,3pd)//CASPT2(8,8)[11]/6-311++G(3df,3pd)). The minimum energy crossing point (MECP) is located at the B3LYP/6-311++G(3df,3pd) level using the Newton-Lagrange method, which was introduced by Koga and Morokuma.[12] The algorithm is based on the minimization of the Lagrangian function $L(R\lambda) = E_1(R) – \lambda[E_1(R) – E_2(R)]$, where R is nuclear coordinates, $E_1(R)$ and $E_2(R)$ are the energies of the states presently considered as functions of R, and λ is Lagrange multiplier. The energies, energy gradients, and Hessian matrixes of both the two states need to be calculated, and the minimum point is found on the seam of intersection. These calculations are treated using a homemade program LookForMECP (version 1.0). This program can be obtained from the authors upon request. The early version of this program has been used successfully to search the MECP.[13-15] These calculations performed were performed using the Gaussian 09 software package.[16] The CCSD(T)/aug-cc-pVTZ//B3LYP/6-311++G(3df,3pd) and CASPT2(8,8)/6-311++G(3df,3pd) calculations were performed with the MOLPRO 2012 program.[17]

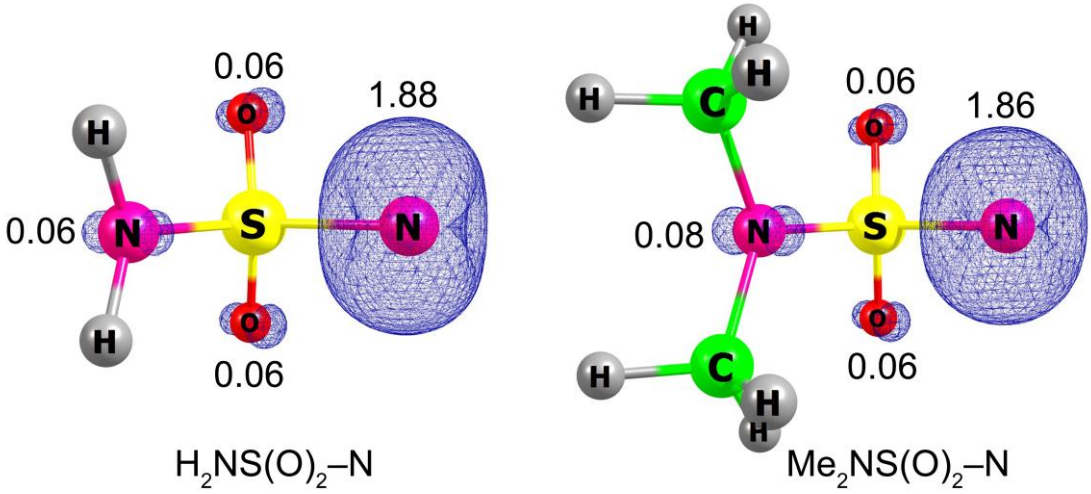


Figure S1. Natural spin densities of H_2NSO_2N and Me_2NSO_2N computed at the M06-2X/6-311++G(3df,3pd)//CASPT2(8,8)/6-311++G(3df,3pd) level.

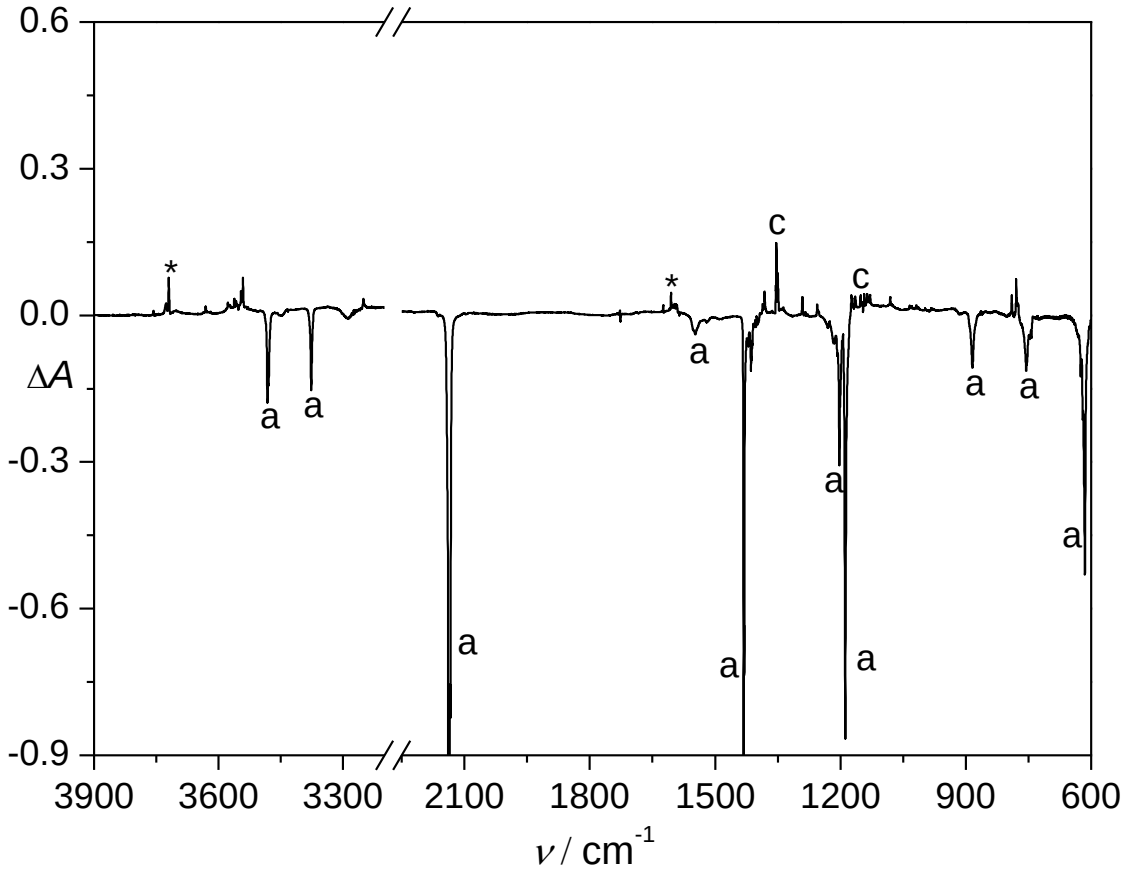


Figure S2. IR difference spectrum showing the changes of Ar-matrix isolated $H_2NS(O)_2$–N_3 (a) upon a 266 nm laser photolysis. The IR bands of SO_2 (c), H_2O (*) are labeled.

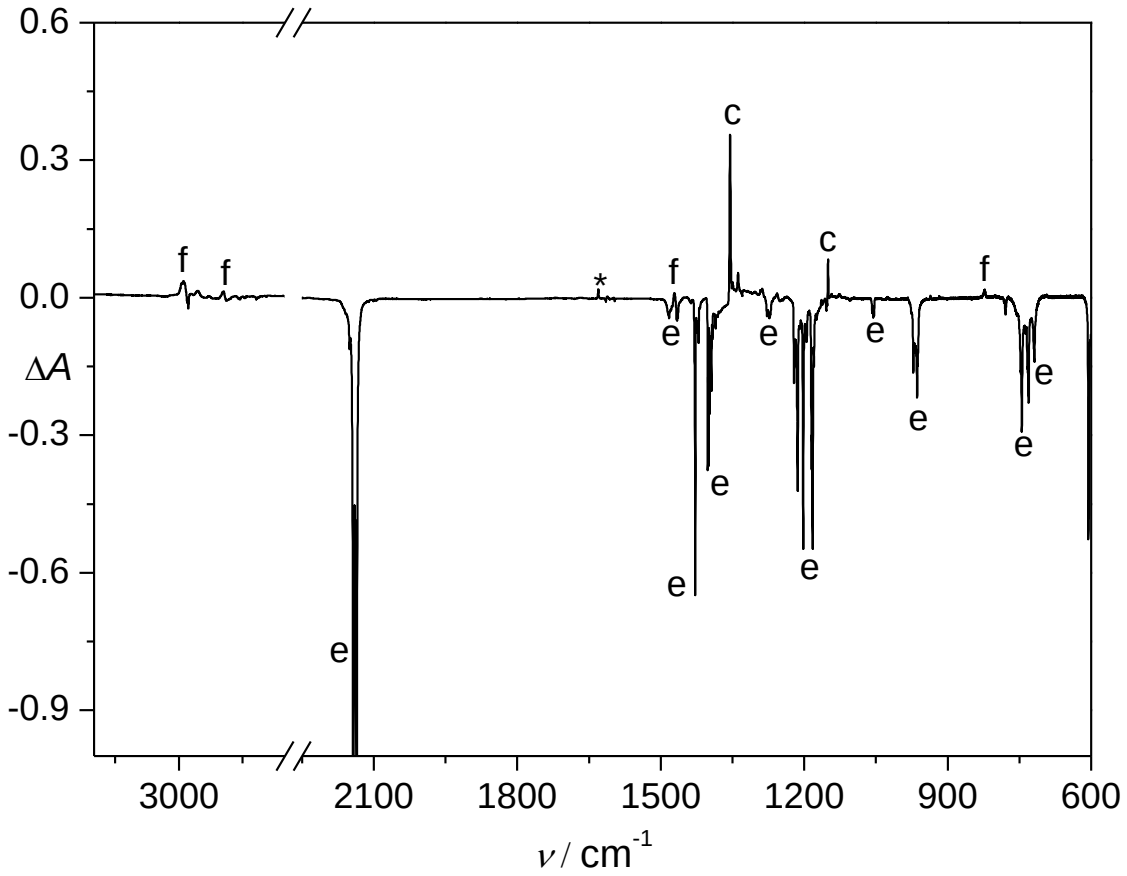


Figure S3. IR difference spectrum showing the changes of Ne-matrix isolated $Me_2NS(O)_2–N_3$ (e) upon a 266 nm laser photolysis. The IR bands of SO_2 (c), C_2H_6 (f), H_2O (*) are labeled.

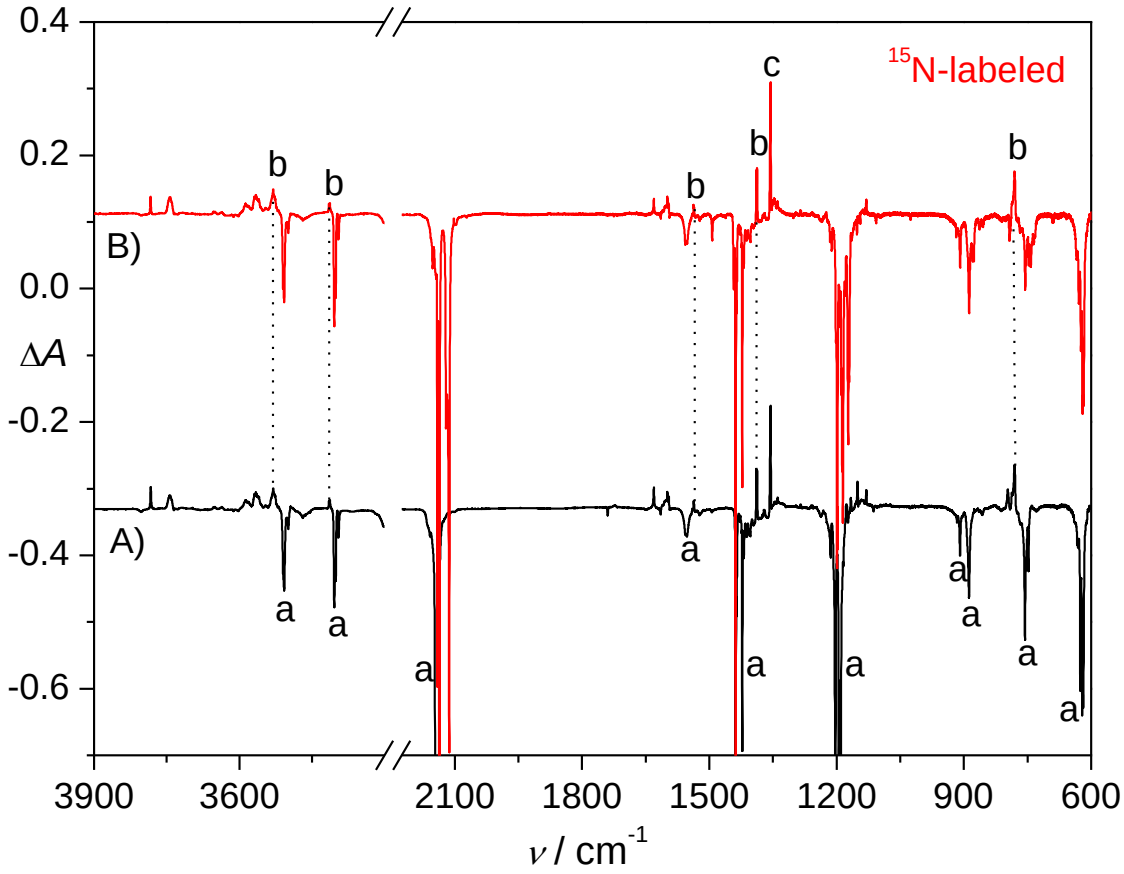


Figure S4. A): IR difference spectrum showing the changes of Ne-matrix isolated $H_2NS(O)_2$–N_3 (a) upon a 193 nm laser photolysis; B): IR difference spectrum showing the changes of Ne-matrix isolated ^{15}N-labled label sample (1:1 mixture of $H_2NS(O)_2$–$^{15}N_\alpha N_\beta N_\gamma$ and $H_2NS(O)_2$–$N_\alpha N_\beta {}^{15}N_\gamma$) upon a 193 nm laser photolysis. The IR bands of $H_2NS(O)_2$–N_3 (a), $H_2NS(O)_2$–N (b) and SO_2 (c) are labeled.

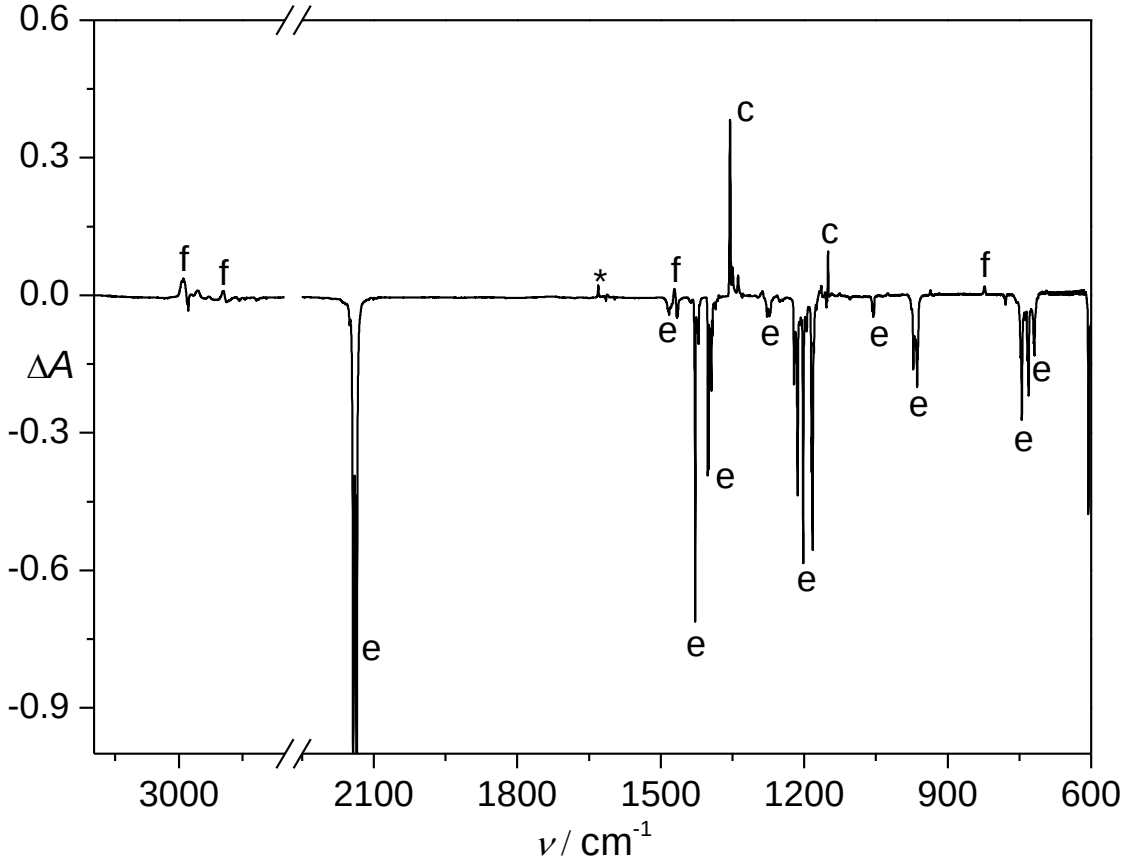


Figure S5. IR difference spectrum showing the changes of Ne-matrix isolated $Me_2NS(O)_2–N_3$ (e) upon a 193 nm laser photolysis. The IR bands of SO_2 (c), C_2H_6 (f), H_2O (*) are labeled.

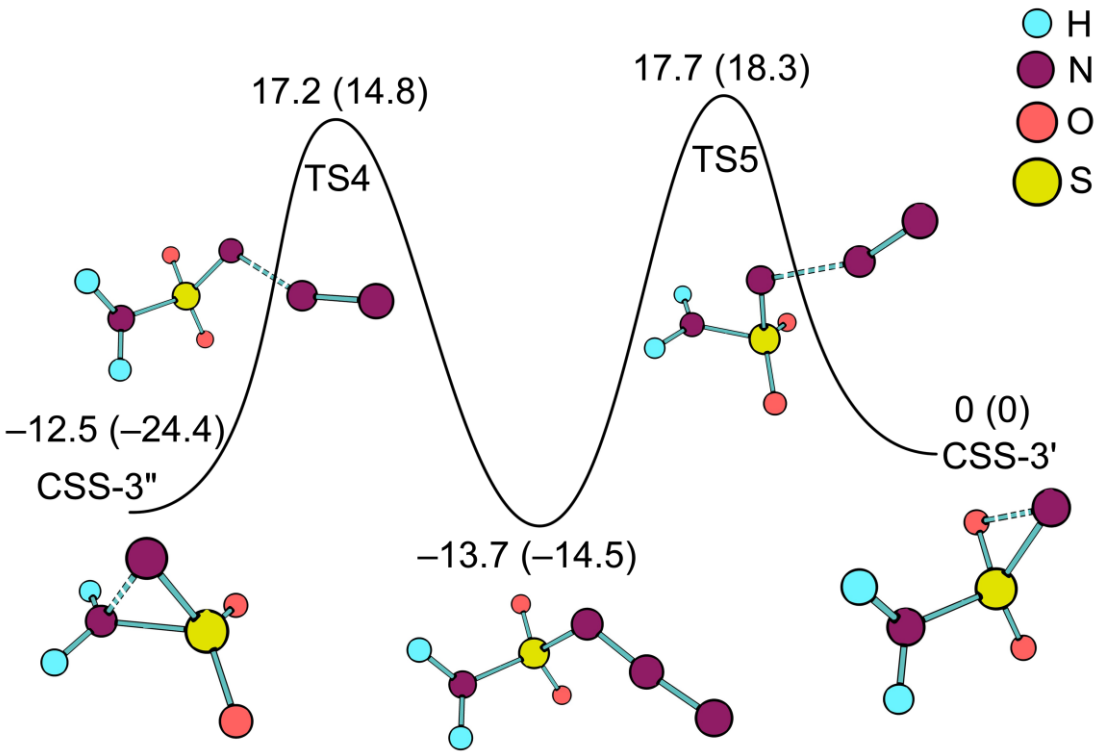


Figure S6. Calculated potential energy profiles (Gibbs free energy, kcal mol^{-1}, ZPVE corrected) for the decomposition of $H_2NS(O)_2–N_3$ and $Me_2NS(O)_2–N_3$ (in parentheses) at the CCSD(T)/aug-cc-pVTZ//B3LYP/6-311++G(3df,3pd) level. For clarity, only the molecular structures of $H_2NS(O)_2–N_3$ are depicted.

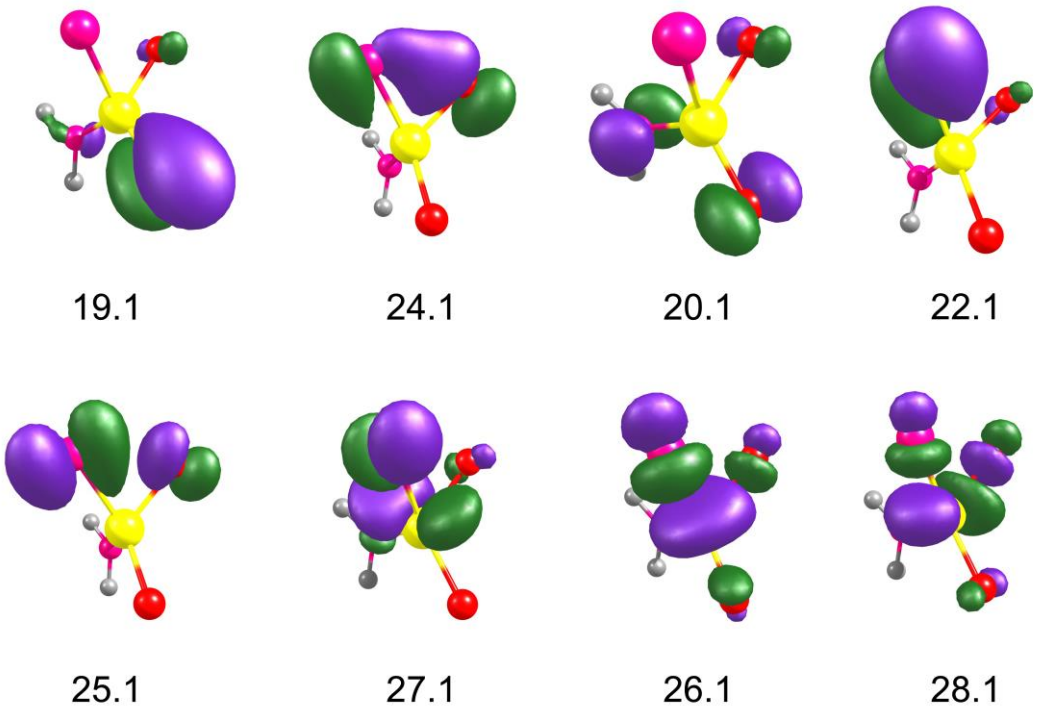


Figure S7. Molecular orbitals included in the (8,8) active space of the CASPT2 calculation at geometry of $H_2NS(O)_2$–N (*CSS-3'*).

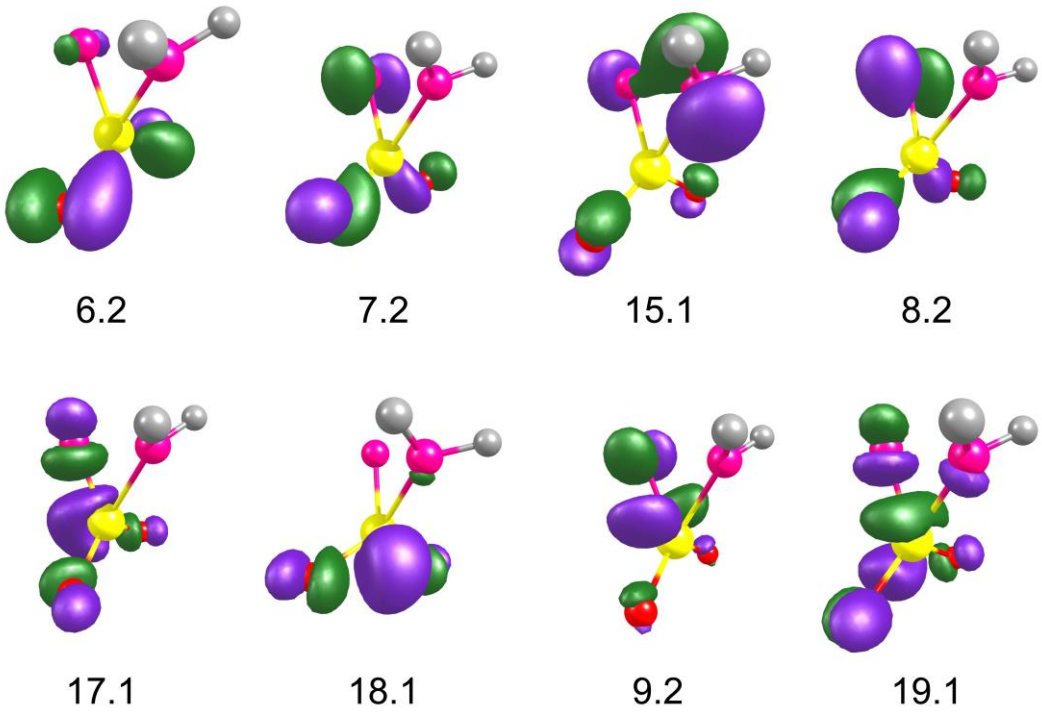


Figure S8. Molecular orbitals included in the (8,8) active space of the CASPT2 calculation at geometry of $H_2NS(O)_2$–N (*CSS-3''*).

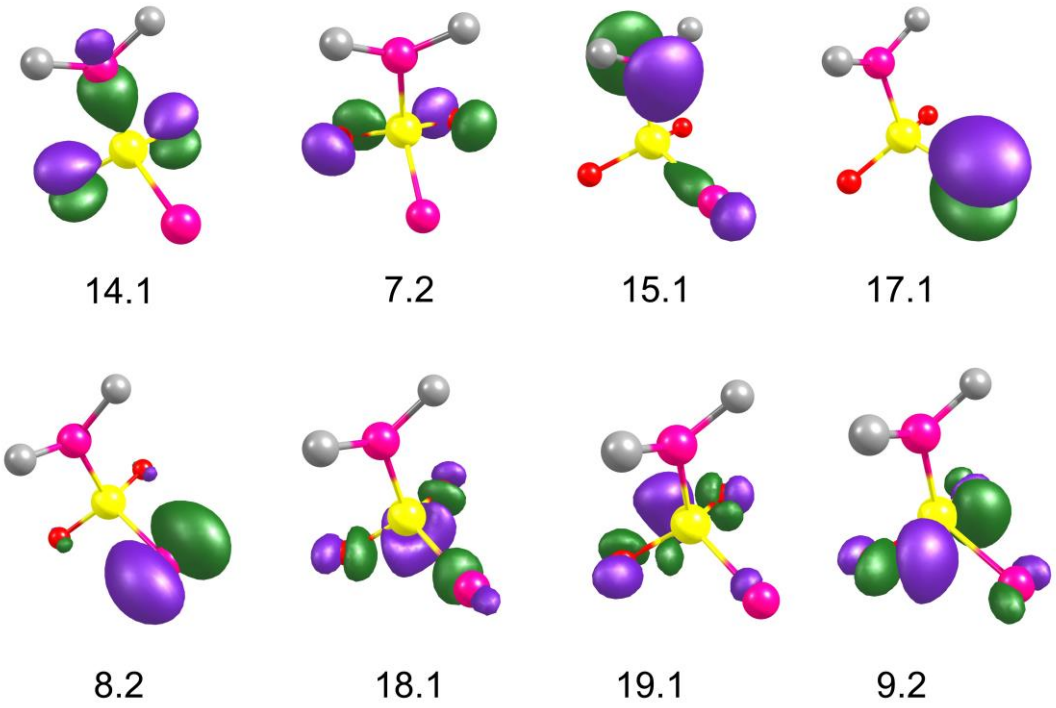


Figure S9. Molecular orbitals included in the (8,8) active space of the CASPT2 calculation at geometry of $H_2NS(O)_2$–N (*Triplet*).

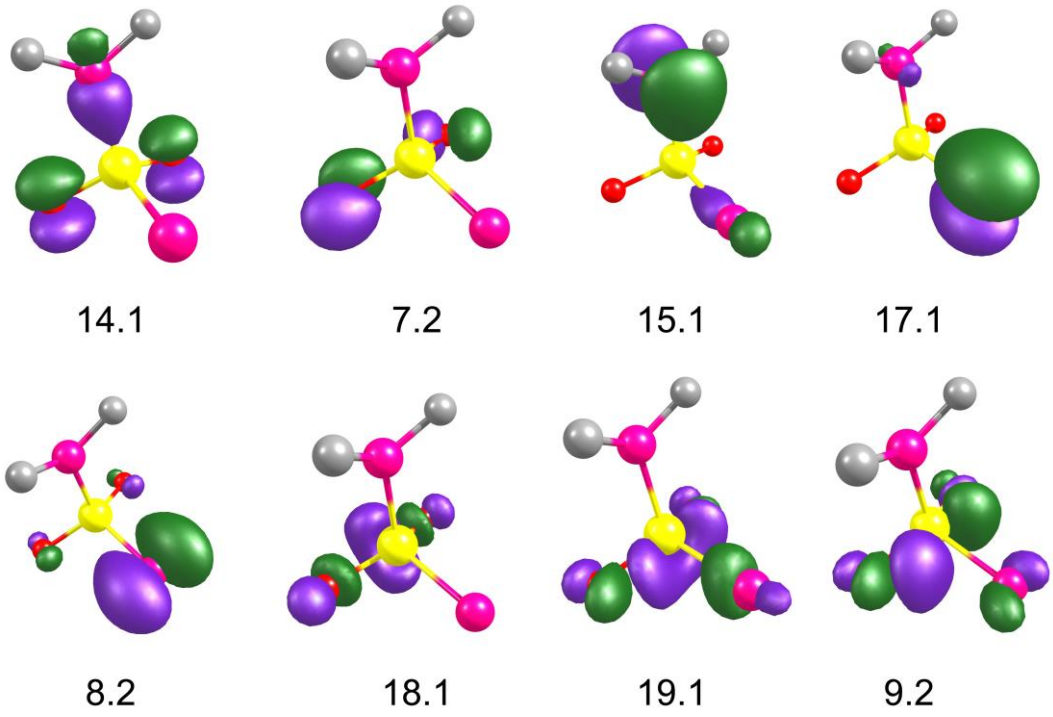


Figure S10. Molecular orbitals included in the (8,8) active space of the CASPT2 calculation at geometry of $H_2NS(O)_2$–N (*OSS-3*).

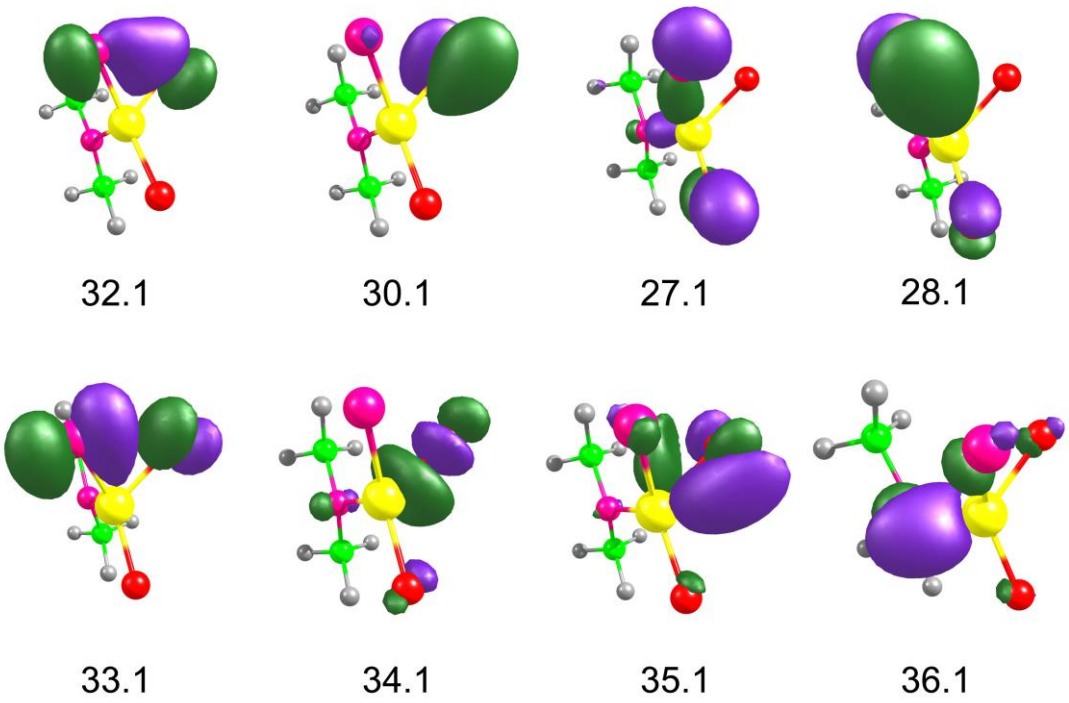


Figure S11. Molecular orbitals included in the (8,8) active space of the CASPT2 calculation at geometry of $Me_2NS(O)_2$–N (*CSS-3′*).

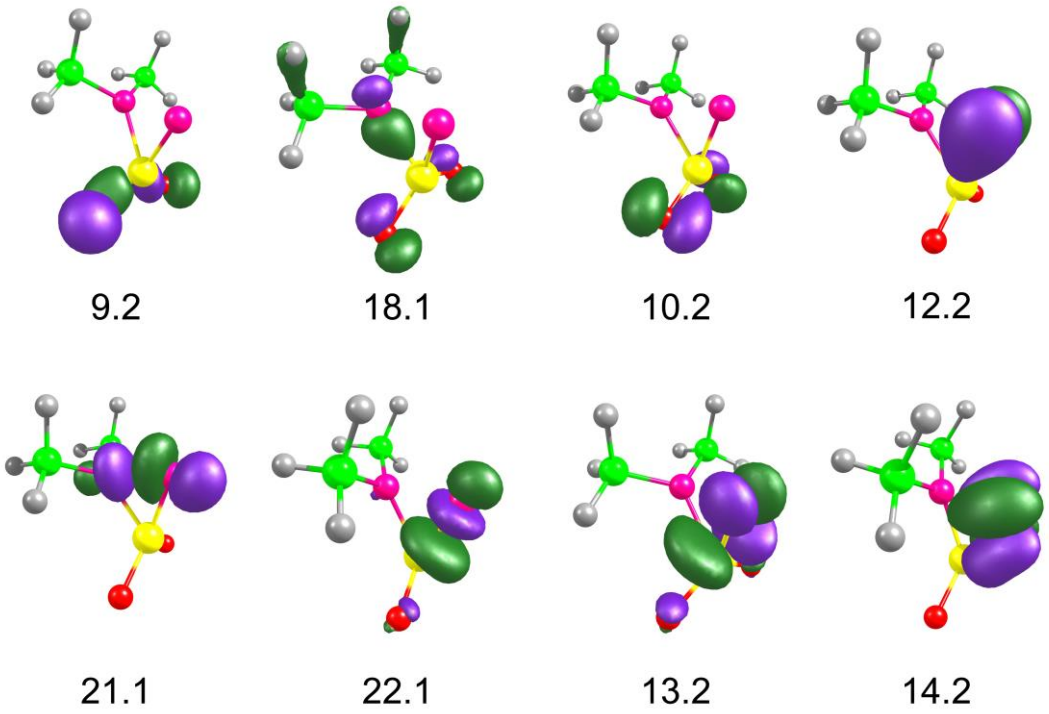


Figure S12. Molecular orbitals included in the (8,8) active space of the CASPT2 calculation at geometry of $Me_2NS(O)_2$–N (*CSS-3″*).

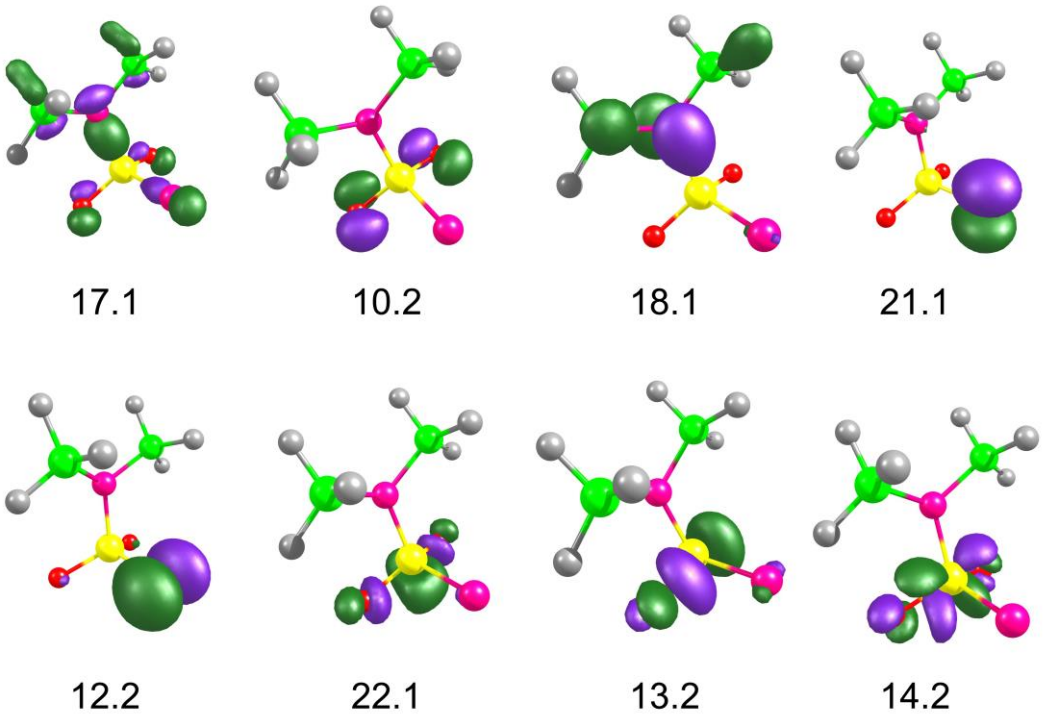


Figure S13. Molecular orbitals included in the (8,8) active space of the CASPT2 calculation at geometry of $Me_2NS(O)_2$–N (*Triplet*).

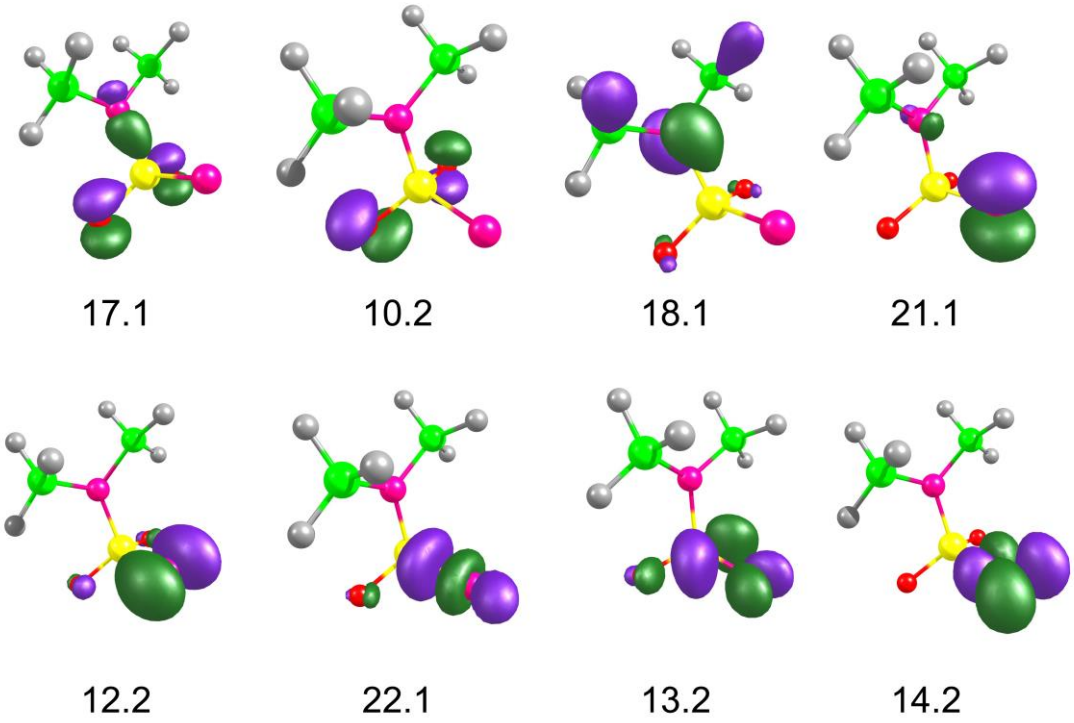


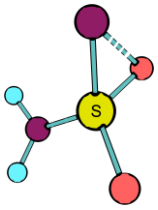
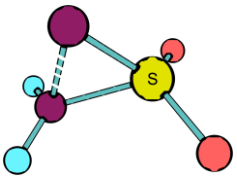
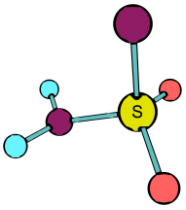
Figure S14. Molecular orbitals included in the (8,8) active space of the CASPT2 calculation at geometry of $Me_2NS(O)_2$–N (*OSS-3*).

Table S1. Calculated energy gaps (ΔG_{ST}, kcal mol^{-1}, ZPVE corrected)[a] for sulfamoylnitrenes

Method	$H_2NS(O)_2$–N			$Me_2NS(O)_2$–N		
	CSS-3'	CSS-3''	OSS-3	CSS-3'	CSS-3''	OSS-3
B3LYP[b]	18.4	4.7	10.4	19.5	–4.7	8.8
CBS-QB3	12.0	–0.1		11.2	–12.5	
M06-2X[b]	17.1	0.7		17.5	–9.8	
CCSD(T)[c]	13.9	1.4		13.5	–10.9	
CASPT2[d]	14.1	–1.5	30.3	16.7	–16.0	30.8

[a] Relative Gibbs free energies to the triplet, and positive values refer to the triplet being more stable. [b] At the 6-311++G(3df,3pd) basis set. [c] At the aug-cc-pVTZ basis set and the B3LYP/6-311++G(3df,3pd) optimized structures. [d] At the 6-311++G(3df,3pd) basis set with the (8,8) active space.

Table S2. Calculated (B3LYP/6-311++G(3df,3pd)) and observed IR data of sulfamoylnitrene $H_2NS(O)_2$–N.

calculated						observed[d]	
CSS-3'		CSS-3''		Triplet		Triplet	
(-659.301075)[a]		(-659.322861)[a]		(-659.330426)[a]		Ne-matrix	
							
ν[b]	Δν[c]	ν[b]	Δν[c]	ν[b]	Δν[c]	ν	Δν
3688 (90)	0	3579 (64)	0	3664 (75)	0	3530.6	< 0.5
3559 (72)	0	3455 (45)	0	3540 (69)	0	3414.1	< 0.5
1568 (64)	0	1578 (32)	0.2	1570 (57)	0	1537.7	< 0.5
1399 (222)	2.7	1366 (228)	0	1382 (190)	0	1387.6	< 0.5
1091 (121)	4.9	1237 (218)	3.4	1175 (94)	0	1166.5	< 0.5
1051 (15)	2.6	1033 (3)	1.1	1036 (1)	0.1		
984 (15)	10.5	988 (35)	10.1	855 (49)	0.1	781.3	< 0.5
869 (45)	4.4	910 (45)	11.3	723 (1)	13.8		
518 (56)	2.7	785 (5)	0.8	525 (85)	4.6		
478 (22)	1.2	708 (55)	6.1	487 (34)	0.7		
432 (17)	0.6	548 (87)	2.3	455 (7)	0		
416 (5)	3.0	505 (38)	3.0	439 (145)	0.4		
385 (8)	4.8	437 (12)	5.3	361 (<1)	1.7		
326 (165)	1.1	360 (5)	1.4	281 (11)	3.2		
156 (29)	1.2	222 (5)	1.0	273 (23)	4.1		

[a] Calculated total energies (Hartree) in parentheses. [b] Calculated harmonic frequencies (cm^{-1}, unscaled) and intensities (km mol^{-1}) in parentheses. [c] Calculated ^{15}N isotopic shifts (cm^{-1}). [d] Observed data (cm^{-1}) for the most intense band in cryogenic matrices.

Table S3. Calculated vertical transitions for $H_2NS(O)_2$–N at the TD-B3LYP/6-311++G(3df,3pd) level.

CSS-3'		CSS-3"		Triplet	
energy (nm)	oscillator strength	energy (nm)	oscillator strength	energy (nm)	oscillator strength
586	0.0009	268	0.0023	475	0.0002
268	0.0049	241	0.0001	332	0.0003
239	0.0028	220	0.0006	327	0.0060
218	0.0049	196	0.0309	310	0.0232
217	0.0041	186	0.0121	308	0.0022
202	0.0017	184	0.0001	296	0.0020
187	0.0068	183	0.0201	277	0.0489
177	0.0037	176	0.0105	263	0.0054
170	0.0150	170	0.0018	258	0.0022
164	0.0093	166	0.0012		

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Calculated Atomic Coordinates (in Angstroms) and Energies (in Hatrees) for All Optimized Structures

$H_2NS(O)_2–N_3$
B3LYP/6-311++G(3df,3pd)

H	1.60921200	-1.16376100	-1.47729800
H	0.76739000	-2.09666400	-0.32971400
S	0.68835600	0.10540000	0.13004500
O	0.28218000	-0.20589300	1.46318600
O	1.57486100	1.16252300	-0.20949400
N	-0.72852100	0.45390500	-0.79174000
N	-1.79583000	0.10432000	-0.27452600
N	-2.81434700	-0.16591600	0.11286200
N	1.30346600	-1.26074000	-0.51848800

Zero-point correction=	0.050104
Thermal correction to Energy=	0.057063
Thermal correction to Enthalpy=	0.058007
Thermal correction to Gibbs Free Energy=	0.017899
Sum of electronic and zero-point Energies=	-768.880961
Sum of electronic and thermal Energies=	-768.874003
Sum of electronic and thermal Enthalpies=	-768.873059
Sum of electronic and thermal Free Energies=	-768.913167

$H_2NS(O)_2–N$ (*CSS-3'*)
B3LYP/6-311++G(3df,3pd)

H	-0.87899500	-1.95829700	-0.21312600
H	-2.10200400	-0.74575300	-0.06586200
S	-0.02637400	0.12794800	-0.05728200
O	-0.73275600	1.36469300	-0.01659800
O	1.10924500	-0.16166800	0.89166700
N	1.20348800	-0.24860300	-0.91275300
N	-1.14761900	-1.03244300	0.08345900

Zero-point correction=	0.038551
Thermal correction to Energy=	0.043921
Thermal correction to Enthalpy=	0.044865
Thermal correction to Gibbs Free Energy=	0.010109
Sum of electronic and zero-point Energies=	-659.272632
Sum of electronic and thermal Energies=	-659.267263
Sum of electronic and thermal Enthalpies=	-659.266319
Sum of electronic and thermal Free Energies=	-659.301075

$H_2NS(O)_2$–N (*CSS-3"*)

B3LYP/6-311++G(3df,3pd)

S	-0.28737600	-0.00004800	0.10407700
O	-0.97894500	1.22847000	-0.15033300
O	-0.98043500	-1.22754000	-0.15085000
N	1.03541500	-0.00075100	0.95296600
H	1.78723000	0.86054600	-0.90065400
H	1.78736300	-0.86075400	-0.90092200
N	1.35008100	-0.00017300	-0.58928000

Zero-point correction=	0.040352
Thermal correction to Energy=	0.045090
Thermal correction to Enthalpy=	0.046034
Thermal correction to Gibbs Free Energy=	0.012414
Sum of electronic and zero-point Energies=	-659.294924
Sum of electronic and thermal Energies=	-659.290185
Sum of electronic and thermal Enthalpies=	-659.289241
Sum of electronic and thermal Free Energies=	-659.322861

$H_2NS(O)_2$–N (*Triplet*)

B3LYP/6-311++G(3df,3pd)

S	0.12528400	-0.07071100	0.00000000
O	0.54077800	-0.61524000	1.25586500
O	0.54077800	-0.61524000	-1.25586500
N	0.54077800	1.53495100	0.00000000
H	-1.95165000	0.24799200	0.85970200
H	-1.95165000	0.24799200	-0.85970200
N	-1.50559100	-0.03791800	0.00000000

Zero-point correction=	0.038190
Thermal correction to Energy=	0.043476
Thermal correction to Enthalpy=	0.044420
Thermal correction to Gibbs Free Energy=	0.008889
Sum of electronic and zero-point Energies=	-659.301125
Sum of electronic and thermal Energies=	-659.295840
Sum of electronic and thermal Enthalpies=	-659.294895
Sum of electronic and thermal Free Energies=	-659.330426

$H_2NS(O)_2$–N (*OSS-3)*

B3LYP/6-311++G(3df,3pd)

S	0.13186300	-0.06564400	0.00000000

O	0.53549200	-0.62693700	1.25368100
O	0.53549200	-0.62693700	-1.25368100
N	0.53549200	1.52025600	0.00000000
H	-1.94769500	0.27524200	0.85992500
H	-1.94769500	0.27524200	-0.85992500
N	-1.50439000	-0.01585500	0.00000000

Zero-point correction=	0.038003
Thermal correction to Energy=	0.043342
Thermal correction to Enthalpy=	0.044286
Thermal correction to Gibbs Free Energy=	0.009680
Sum of electronic and zero-point Energies=	-659.285495
Sum of electronic and thermal Energies=	-659.280156
Sum of electronic and thermal Enthalpies=	-659.279212
Sum of electronic and thermal Free Energies=	-659.313818

H_2NNSO_2

B3LYP/6-311++G(3df,3pd)

N	-2.01175100	-0.07152900	-0.12082200
H	-1.91106600	0.93849100	-0.10945100
H	-2.69861600	-0.41133100	0.53857200
N	-0.84848800	-0.78999400	-0.02547800
S	0.47663900	0.00110100	0.10328300
O	0.44489000	1.44076600	-0.03856500
O	1.68075200	-0.75503000	-0.09362900

Zero-point correction=	0.039705
Thermal correction to Energy=	0.045136
Thermal correction to Enthalpy=	0.046080
Thermal correction to Gibbs Free Energy=	0.010764
Sum of electronic and zero-point Energies=	-659.335919
Sum of electronic and thermal Energies=	-659.330488
Sum of electronic and thermal Enthalpies=	-659.329544
Sum of electronic and thermal Free Energies=	-659.364860

$HNSO_2NH$

B3LYP/6-311++G(3df,3pd)

S	-0.26026300	0.00000100	-0.00009400
O	-0.95489800	-1.24024200	0.12595100
O	-0.95684900	1.23907200	-0.12585000
N	1.18305500	-0.04429800	-0.80098300
H	1.44825500	1.01381300	0.98401200

N	1.18277400	0.04545000	0.80108200
H	1.44912400	-1.01253900	-0.98399800

Zero-point correction= 0.041081
Thermal correction to Energy= 0.045505
Thermal correction to Enthalpy= 0.046449
Thermal correction to Gibbs Free Energy= 0.013445
Sum of electronic and zero-point Energies= -659.320647
Sum of electronic and thermal Energies= -659.316224
Sum of electronic and thermal Enthalpies= -659.315280
Sum of electronic and thermal Free Energies= -659.348284

TS1: $H_2NS(O)_2$–N (*CSS-3′*) → $H_2NS(O)_2$–N (*CSS-3″*)
B3LYP/6-311++G(3df,3pd)

S	0.15229700	0.05893200	0.03341800
O	1.14499000	-0.57351500	-0.80992800
O	0.31234900	1.44827500	0.32964700
N	-0.07749400	-1.02914500	1.14159400
H	-1.75533000	-0.96432600	-0.79868000
H	-1.99530200	0.74256600	-0.48883600
N	-1.40033900	-0.07360200	-0.48515600

Zero-point correction= 0.037665
Thermal correction to Energy= 0.042480
Thermal correction to Enthalpy= 0.043424
Thermal correction to Gibbs Free Energy= 0.009716
Sum of electronic and zero-point Energies= -659.252005
Sum of electronic and thermal Energies= -659.247190
Sum of electronic and thermal Enthalpies= -659.246246
Sum of electronic and thermal Free Energies= -659.279954

TS2: $H_2NS(O)_2$–N (*CSS-3″*) → H_2NNSO_2
B3LYP/6-311++G(3df,3pd)

S	-0.35698300	-0.00637400	0.09566100
O	-0.73573100	1.37086400	-0.00902800
O	-1.31645100	-0.99038600	-0.30459100
N	0.94474400	-0.46901500	0.79862800
H	2.23062500	0.80823500	-0.28376200
H	2.07154700	-0.74782300	-0.91433400
N	1.60197200	0.04012100	-0.48770400

Zero-point correction= 0.039275

Thermal correction to Energy=	0.043857
Thermal correction to Enthalpy=	0.044801
Thermal correction to Gibbs Free Energy=	0.011312
Sum of electronic and zero-point Energies=	-659.290141
Sum of electronic and thermal Energies=	-659.285559
Sum of electronic and thermal Enthalpies=	-659.284615
Sum of electronic and thermal Free Energies=	-659.318104

TS3: $H_2NS(O)_2$–N (*CSS-3″*) → $HNSO_2NH$

B3LYP/6-311++G(3df,3pd)

S	0.25761700	-0.00434700	0.05766100
O	1.01942300	-1.19042600	-0.15709500
O	0.88722200	1.27769900	-0.00414100
N	-1.06079400	-0.09576800	0.98494100
H	-1.60348100	0.91744600	-0.95475300
N	-1.23484200	-0.02234200	-0.80387000
H	-1.70209700	-0.71930700	0.05456200

Zero-point correction=	0.035210
Thermal correction to Energy=	0.039690
Thermal correction to Enthalpy=	0.040635
Thermal correction to Gibbs Free Energy=	0.007508
Sum of electronic and zero-point Energies=	-659.248406
Sum of electronic and thermal Energies=	-659.243926
Sum of electronic and thermal Enthalpies=	-659.242982
Sum of electronic and thermal Free Energies=	-659.276109

TS4: $H_2NS(O)_2$–N_3 → $H_2NS(O)_2$–N (*CSS-3″*)

B3LYP/6-311++G(3df,3pd)

N	0.47409300	0.92595100	-0.00028300
N	2.06015800	0.03702800	0.00025200
N	3.15439800	0.01904500	-0.00006600
O	-0.86022100	-0.91720700	-1.23414000
S	-0.68422200	-0.21336700	0.00001400
O	-0.86059600	-0.91633800	1.23459400
H	-1.87555000	1.58350700	-0.87325600
H	-1.87515000	1.58422300	0.87237700
N	-1.62225100	1.14861900	-0.00033000

Zero-point correction=	0.045798
Thermal correction to Energy=	0.053474
Thermal correction to Enthalpy=	0.054418

Thermal correction to Gibbs Free Energy=	0.013203
Sum of electronic and zero-point Energies=	-768.825553
Sum of electronic and thermal Energies=	-768.817877
Sum of electronic and thermal Enthalpies=	-768.816932
Sum of electronic and thermal Free Energies=	-768.858148

TS5: $H_2NS(O)_2–N_3$ → $H_2NS(O)_2–N$ (*CSS-3′*)

B3LYP/6-311++G(3df,3pd)

H	-1.03455600	0.92218200	-1.89359600
H	-0.85386100	2.07025700	-0.64059700
S	-0.74706000	-0.04095500	0.13051500
O	-0.70186000	0.58898000	1.41077800
O	-1.59334500	-1.19051600	-0.16824100
N	0.48552400	-0.93837200	-0.35166600
N	2.08999200	0.04762800	-0.07422300
N	3.18049100	0.09626600	-0.01365500
N	-1.15557500	1.14806700	-0.91679100

Zero-point correction=	0.045821
Thermal correction to Energy=	0.053523
Thermal correction to Enthalpy=	0.054468
Thermal correction to Gibbs Free Energy=	0.013117
Sum of electronic and zero-point Energies=	-768.823553
Sum of electronic and thermal Energies=	-768.815851
Sum of electronic and thermal Enthalpies=	-768.814906
Sum of electronic and thermal Free Energies=	-768.856257

$Me_2NS(O)_2–N_3$

B3LYP/6-311++G(3df,3pd)

S	-0.02653700	0.07164000	0.57522400
O	0.19297700	1.38568900	1.09207900
O	0.22664100	-1.08972000	1.36880900
N	0.92046000	-0.07753800	-0.87459100
N	2.14300800	-0.07342200	-0.69874000
N	3.26501900	-0.07988100	-0.63739500
N	-1.51697300	-0.01808100	-0.05359100
C	-2.00855900	1.13936300	-0.80804300
H	-1.66894600	1.11465500	-1.84700000
H	-3.09680100	1.11343600	-0.78777900
H	-1.67053800	2.05497500	-0.33550100
C	-1.97139800	-1.32413800	-0.54162700
H	-1.60788300	-2.10718600	0.11462400

H	-3.05996100	-1.32696500	-0.52393500
H	-1.62908800	-1.51181200	-1.56286900

Zero-point correction=	0.106428
Thermal correction to Energy=	0.116328
Thermal correction to Enthalpy=	0.117272
Thermal correction to Gibbs Free Energy=	0.069627
Sum of electronic and zero-point Energies=	-847.465516
Sum of electronic and thermal Energies=	-847.455617
Sum of electronic and thermal Enthalpies=	-847.454672
Sum of electronic and thermal Free Energies=	-847.502317

$Me_2NS(O)_2$–N (*CSS-3′*)

B3LYP/6-311++G(3df,3pd)

S	0.63687100	0.21094000	-0.08600900
O	0.81488200	1.62609600	-0.14316100
O	1.32162600	-0.58944700	1.00979200
N	1.50568800	-0.87424900	-0.75610600
N	-0.94991300	-0.08732100	-0.18127900
C	-1.92929500	0.95405200	0.14038500
H	-2.23177900	0.90294000	1.18914600
H	-1.51030600	1.93122100	-0.06750800
H	-2.80530100	0.79981200	-0.48811000
C	-1.41005000	-1.47319100	-0.05942900
H	-1.70042400	-1.70022600	0.96827000
H	-2.27016900	-1.60914400	-0.71367000
H	-0.61837600	-2.14701700	-0.36907600

Zero-point correction=	0.095372
Thermal correction to Energy=	0.103405
Thermal correction to Enthalpy=	0.104350
Thermal correction to Gibbs Free Energy=	0.062988
Sum of electronic and zero-point Energies=	-737.856884
Sum of electronic and thermal Energies=	-737.848851
Sum of electronic and thermal Enthalpies=	-737.847906
Sum of electronic and thermal Free Energies=	-737.889268

$Me_2NS(O)_2$–N (*CSS-3″*)

B3LYP/6-311++G(3df,3pd)

S	0.87411400	-0.00000200	0.09350200
O	1.46604200	-1.22719000	-0.36275300
O	1.46593000	1.22726400	-0.36264700

N	-0.09618500	-0.00010200	1.32877200
N	-0.89090200	-0.00002000	-0.03204300
C	-1.63631400	1.24512500	-0.24867800
H	-2.08863700	1.22327400	-1.23897700
H	-2.40779800	1.32515600	0.51693400
H	-0.95145300	2.08209400	-0.17077000
C	-1.63635500	-1.24509400	-0.24869200
H	-2.40728100	-1.32554100	0.51744300
H	-2.08942600	-1.22280600	-1.23864500
H	-0.95138400	-2.08206600	-0.17169500

Zero-point correction=	0.096255
Thermal correction to Energy=	0.103809
Thermal correction to Enthalpy=	0.104753
Thermal correction to Gibbs Free Energy=	0.064750
Sum of electronic and zero-point Energies=	-737.896402
Sum of electronic and thermal Energies=	-737.888848
Sum of electronic and thermal Enthalpies=	-737.887904
Sum of electronic and thermal Free Energies=	-737.927907

$Me_2NS(O)_2$–N (*Triplet*)

B3LYP/6-311++G(3df,3pd)

S	0.09068900	-0.72464100	0.00000000
O	-0.33056900	-1.28327800	1.25117600
O	-0.33056900	-1.28327800	-1.25117600
N	1.72511600	-0.64745600	0.00000000
N	-0.31336200	0.86767600	0.00000000
C	-0.33056900	1.63351400	-1.24364500
H	-0.32157200	0.95849100	-2.09199900
H	-1.24514300	2.22721700	-1.27589500
H	0.52803200	2.30578900	-1.29631800
C	-0.33056900	1.63351400	1.24364500
H	-1.24514300	2.22721700	1.27589500
H	-0.32157200	0.95849100	2.09199900
H	0.52803200	2.30578900	1.29631800

Zero-point correction=	0.094431
Thermal correction to Energy=	0.102688
Thermal correction to Enthalpy=	0.103632
Thermal correction to Gibbs Free Energy=	0.060708
Sum of electronic and zero-point Energies=	-737.886644
Sum of electronic and thermal Energies=	-737.878387
Sum of electronic and thermal Enthalpies=	-737.877443

Sum of electronic and thermal Free Energies= -737.920367

$Me_2NS(O)_2$–N (*OSS-3)*

B3LYP/6-311++G(3df,3pd)

S	0.11370000	-0.74235500	0.00000000
O	-0.33696100	-1.28718900	1.24814200
O	-0.33696100	-1.28718900	-1.24814200
N	1.70727600	-0.59709400	0.00000000
N	-0.31613000	0.87088000	0.00000000
C	-0.33696100	1.63204600	-1.24259300
H	-0.30276000	0.95556600	-2.08895800
H	-1.26441500	2.20589700	-1.28405500
H	0.50601000	2.32436500	-1.28357900
C	-0.33696100	1.63204600	1.24259300
H	-1.26441500	2.20589700	1.28405500
H	-0.30276000	0.95556600	2.08895800
H	0.50601000	2.32436500	1.28357900

Zero-point correction= 0.094090
Thermal correction to Energy= 0.102400
Thermal correction to Enthalpy= 0.103345
Thermal correction to Gibbs Free Energy= 0.061362
Sum of electronic and zero-point Energies= -737.873549
Sum of electronic and thermal Energies= -737.865239
Sum of electronic and thermal Enthalpies= -737.864295
Sum of electronic and thermal Free Energies= -737.906278

Me_2NNSO_2

B3LYP/6-311++G(3df,3pd)

N	-1.52773300	-0.09107000	0.10214700
N	-0.70703200	-0.90467700	0.45789000
S	1.68606700	-0.40189200	0.13928200
O	1.81273600	0.82026200	0.91267800
O	1.60589800	-0.23785300	-1.29987300
C	-2.98645100	-0.42198000	0.04223800
H	-3.35269400	-0.21805600	-0.96298100
H	-3.09135800	-1.47092800	0.29217900
H	-3.52010100	0.20546400	0.75432600
C	-1.22133900	1.31002800	-0.34036400
H	-1.96588000	1.97872300	0.08555100
H	-0.22672900	1.57432900	-0.00499800
H	-1.27928700	1.34341200	-1.42653800

Zero-point correction=	0.093449
Thermal correction to Energy=	0.102810
Thermal correction to Enthalpy=	0.103754
Thermal correction to Gibbs Free Energy=	0.057531
Sum of electronic and zero-point Energies=	-737.947801
Sum of electronic and thermal Energies=	-737.938441
Sum of electronic and thermal Enthalpies=	-737.937497
Sum of electronic and thermal Free Energies=	-737.983720

$MeNSO_2NMe$

B3LYP/6-311++G(3df,3pd)

S	0.00005000	-0.70465400	-0.00000200
O	0.92378200	-1.41133700	-0.83232700
O	-0.92358900	-1.41126800	0.83242700
N	-0.50781800	0.73372300	-0.62199700
N	0.50774100	0.73379400	0.62182800
C	-1.81755900	1.26222800	-0.23629800
H	-2.19371400	0.83911600	0.69435100
H	-1.72614200	2.34273800	-0.14844800
H	-2.50544500	1.03459000	-1.04980700
C	1.81734700	1.26253600	0.23632300
H	2.19376600	0.83958300	-0.69430500
H	1.72581600	2.34305300	0.14855900
H	2.50518600	1.03501400	1.04991400

Zero-point correction=	0.095759 (Hartree/Particle)
Thermal correction to Energy=	0.103377
Thermal correction to Enthalpy=	0.104321
Thermal correction to Gibbs Free Energy=	0.064123
Sum of electronic and zero-point Energies=	-737.917042
Sum of electronic and thermal Energies=	-737.909424
Sum of electronic and thermal Enthalpies=	-737.908480
Sum of electronic and thermal Free Energies=	-737.948678

TS1: $Me_2NS(O)_2$–N (*CSS-3'*) → $Me_2NS(O)_2$–N (*CSS-3''*)

B3LYP/6-311++G(3df,3pd)

S	-0.73180600	0.08901400	0.01693500
O	-1.00926100	1.49444000	-0.03338100
O	-1.34711100	-0.75419900	-0.99730100
N	-1.01191500	-0.76565800	1.28176200
N	0.92317300	-0.02773400	0.03409800
C	1.78150100	1.14531500	-0.01302900

H	2.18090100	1.27738900	-1.02320400
H	1.21141300	2.02662700	0.25676900
H	2.61380900	1.00494300	0.67635400
C	1.55514500	-1.33310000	-0.10656900
H	2.01278100	-1.41611700	-1.09520000
H	2.32990000	-1.44538000	0.65182700
H	0.81239100	-2.11315300	0.01452100

Zero-point correction=	0.094003
Thermal correction to Energy=	0.101693
Thermal correction to Enthalpy=	0.102637
Thermal correction to Gibbs Free Energy=	0.061928
Sum of electronic and zero-point Energies=	-737.845047
Sum of electronic and thermal Energies=	-737.837358
Sum of electronic and thermal Enthalpies=	-737.836414
Sum of electronic and thermal Free Energies=	-737.877123

TS2: $Me_2NS(O)_2$–N (*CSS-3"*) → Me_2NNSO_2
B3LYP/6-311++G(3df,3pd)

S	-1.02128400	0.03104200	0.08163700
O	-1.28618200	1.33614100	-0.45553800
O	-2.01734900	-0.97924100	-0.12777100
N	0.14203400	-0.27516200	1.05123400
N	1.05920700	-0.03131000	-0.14912900
C	1.89531500	1.13903700	0.07380900
H	2.57900800	1.25254100	-0.76664200
H	1.26833500	2.02291700	0.14237900
H	2.46488500	1.02569200	1.00287800
C	1.79161800	-1.26773300	-0.39697500
H	2.41573400	-1.52865600	0.46399700
H	1.09210600	-2.07818400	-0.58098200
H	2.41844100	-1.12870400	-1.27708700

Zero-point correction=	0.094978
Thermal correction to Energy=	0.102187
Thermal correction to Enthalpy=	0.103131
Thermal correction to Gibbs Free Energy=	0.063495
Sum of electronic and zero-point Energies=	-737.886463
Sum of electronic and thermal Energies=	-737.879254
Sum of electronic and thermal Enthalpies=	-737.878310
Sum of electronic and thermal Free Energies=	-737.917946

TS3: $Me_2NS(O)_2$–N (*CSS-3″*) → Me_2NSO_2NMe
B3LYP/6-311++G(3df,3pd)

S	-0.77689700	-0.12390800	0.05815200
O	-1.63227100	1.01373500	0.25977500
O	-1.29108200	-1.25843600	-0.65217800
N	0.38301600	-0.33120600	1.13282700
N	0.77588500	0.32745900	-0.42157200
C	1.78323700	-1.32133400	0.00309400
H	1.13943100	-2.03228300	-0.49012700
H	2.56477200	-0.91539700	-0.62417600
H	2.12534600	-1.61571200	0.98265500
C	1.20280200	1.71496600	-0.30055400
H	0.52541200	2.28727300	0.33167900
H	2.20765800	1.73952300	0.11921800
H	1.22602100	2.14117200	-1.30448800

Zero-point correction=	0.092515 (Hartree/Particle)
Thermal correction to Energy=	0.100198
Thermal correction to Enthalpy=	0.101142
Thermal correction to Gibbs Free Energy=	0.060775
Sum of electronic and zero-point Energies=	-737.796440
Sum of electronic and thermal Energies=	-737.788757
Sum of electronic and thermal Enthalpies=	-737.787813
Sum of electronic and thermal Free Energies=	-737.828180

TS4: $Me_2NS(O)_2$–N_3 → Me_2NSO_2–N (*CSS-3″*)
B3LYP/6-311++G(3df,3pd)

N	-0.74147300	-0.77869200	-0.00092400
N	-2.44286200	-0.47383000	-0.00047300
N	-3.46395800	-0.87670500	-0.00111900
O	-0.02377300	1.37497500	-1.23082900
S	0.04255000	0.64154000	0.00068000
O	-0.02408500	1.37233400	1.23374700
N	1.36167400	-0.36334300	-0.00031800
C	1.98580700	-0.78552300	-1.24839400
H	3.01194800	-0.41356600	-1.28706700
H	1.99812800	-1.87436500	-1.30659100
H	1.43115200	-0.38122900	-2.08762600
C	1.98542200	-0.78865900	1.24686500
H	1.99692000	-1.87764000	1.30283800
H	3.01185000	-0.41756400	1.28632900
H	1.43103900	-0.38565900	2.08689400

Zero-point correction=	0.102580
Thermal correction to Energy=	0.112950
Thermal correction to Enthalpy=	0.113894
Thermal correction to Gibbs Free Energy=	0.066283
Sum of electronic and zero-point Energies=	-847.414490
Sum of electronic and thermal Energies=	-847.404120
Sum of electronic and thermal Enthalpies=	-847.403176
Sum of electronic and thermal Free Energies=	-847.450787

TS5: $Me_2NS(O)_2$–N_3 → Me_2NSO_2–N (*CSS-3'*)

B3LYP/6-311++G(3df,3pd)

S	-0.27888800	-0.71541900	0.24025900
O	-0.02787800	-0.78375800	1.64592500
O	-0.83777100	-1.83622700	-0.51206900
N	0.96920800	-0.78992700	-0.76333300
N	2.26744400	0.48097000	-0.19444600
N	3.29264000	0.86017000	-0.23024900
N	-1.26007000	0.57297200	0.00016500
C	-1.62416300	0.88778800	-1.38147200
H	-2.58325800	1.40400600	-1.37154800
H	-0.87925100	1.52832500	-1.86194900
H	-1.72946900	-0.02916700	-1.95166900
C	-1.17532900	1.71441200	0.90926600
H	-2.13717300	2.22569600	0.90194200
H	-0.96889900	1.36867700	1.91549600
H	-0.40214400	2.42655100	0.60101500

Zero-point correction=	0.102164
Thermal correction to Energy=	0.112731
Thermal correction to Enthalpy=	0.113675
Thermal correction to Gibbs Free Energy=	0.065454
Sum of electronic and zero-point Energies=	-847.406345
Sum of electronic and thermal Energies=	-847.395778
Sum of electronic and thermal Enthalpies=	-847.394834
Sum of electronic and thermal Free Energies=	-847.443056

Minimum energy crossing point calculations for $H_2NS(O)_2$–N

$H_2NS(O)_2$–N (CP1)
B3LYP/6-311++G(3df,3pd)

S	-0.00722100	0.12408000	0.02453700
O	0.61370700	1.40635800	-0.01183800
O	-1.03583800	-0.27944100	-0.96284000
N	-1.14351900	-0.25213600	1.03629900
N	1.20429200	-0.95791100	-0.04493400
H	0.96581300	-1.90918700	0.19508700
H	2.10135700	-0.62109800	0.27018600

Zero-point correction=	0.038384
Thermal correction to Energy=	0.043772
Thermal correction to Enthalpy=	0.044716
Thermal correction to Gibbs Free Energy=	0.009963
Sum of electronic and zero-point Energies=	-659.268842
Sum of electronic and thermal Energies=	-659.263453
Sum of electronic and thermal Enthalpies=	-659.262509
Sum of electronic and thermal Free Energies=	-659.297262

$H_2NS(O)_2$–N (CP2)
B3LYP/6-311++G(3df,3pd)

S	-0.22643800	0.00000000	0.06871500
O	-0.89879000	1.23732200	-0.17594000
O	-0.89880900	-1.23731200	-0.17593600
N	0.84166900	0.00000000	1.26467200
N	1.23877300	-0.00000900	-0.75530700
H	1.72035700	0.87181500	-0.92499900
H	1.72035100	-0.87183600	-0.92498900

Zero-point correction=	0.038180
Thermal correction to Energy=	0.042781
Thermal correction to Enthalpy=	0.043725
Thermal correction to Gibbs Free Energy=	0.010383
Sum of electronic and zero-point Energies=	-659.270788
Sum of electronic and thermal Energies=	-659.266187
Sum of electronic and thermal Enthalpies=	-659.265243
Sum of electronic and thermal Free Energies=	-659.298586

Minimum energy crossing point calculations for $Me_2NS(O)_2$–N

$Me_2NS(O)_2$–N (CP1)
B3LYP/6-311++G(3df,3pd)

S	0.65583800	0.17450400	-0.03464500
O	0.82286600	1.59367200	-0.05196700
O	1.32648600	-0.64271700	1.01101500
N	1.42834500	-0.78686400	-0.99544100
N	-0.93726200	-0.09624700	-0.05344500
C	-1.44816800	-1.46616700	-0.01117600
H	-1.92631200	-1.66700000	0.94868500
H	-2.17188600	-1.61239600	-0.81294500
H	-0.62980500	-2.16462500	-0.15207900
C	-1.88357800	1.02249500	0.02669300
H	-1.63017700	1.69738000	0.84023500
H	-1.90793300	1.58824500	-0.90352100
H	-2.86921500	0.60250600	0.21066700

Zero-point correction=	0.094344
Thermal correction to Energy=	0.102144
Thermal correction to Enthalpy=	0.103088
Thermal correction to Gibbs Free Energy=	0.061928
Sum of electronic and zero-point Energies=	-737.851471
Sum of electronic and thermal Energies=	-737.843671
Sum of electronic and thermal Enthalpies=	-737.842727
Sum of electronic and thermal Free Energies=	-737.883887

$Me_2NS(O)_2$–N (CP2)
B3LYP/6-311++G(3df,3pd)

S	0.79336300	0.00000100	0.03027600
O	1.29914400	-1.23501600	-0.49421200
O	1.29915000	1.23502400	-0.49419400
N	0.40091500	-0.00001200	1.57271800
N	-0.89355000	0.00000100	-0.07490800
C	-1.60836100	-1.27910200	-0.16265100
H	-2.66179500	-1.07557200	-0.33030000
H	-1.20903000	-1.86728500	-0.98547800
H	-1.49483000	-1.84242200	0.76077100
C	-1.60836900	1.27910200	-0.16265100
H	-1.20904000	1.86729200	-0.98547600
H	-2.66180400	1.07556900	-0.33031100
H	-1.49484600	1.84241700	0.76077200

Zero-point correction=	0.094121
Thermal correction to Energy=	0.101199
Thermal correction to Enthalpy=	0.102144
Thermal correction to Gibbs Free Energy=	0.061715
Sum of electronic and zero-point Energies=	-737.861079
Sum of electronic and thermal Energies=	-737.854001
Sum of electronic and thermal Enthalpies=	-737.853057
Sum of electronic and thermal Free Energies=	-737.893485

CASPT2(8,8)/6-311++G(3df,3pd) calculated energies (in Hartrees) of $H_2NS(O)_2$–N

$H_2NS(O)_2$–N (*CSS-3′*)

==========

22220000 0.9545403

22022000 -0.1857925

H	0.017021	0.098097	0.019159
H	0.014412	-0.459649	1.648026
S	2.054894	0.120043	0.929086
O	2.450026	-0.074591	2.283270
O	2.641733	-0.749733	-0.167867
N	2.616074	1.062909	-0.150064
N	0.446211	0.106526	0.932689

ENERGY= -658.314941

$H_2NS(O)_2$–N (*CSS-3″*)

==========

2000 2220 0.9761048

2000 2202 -0.0765333

2200 2020 -0.0610513

2020 0220 -0.0576765

0002 2220 -0.0503279

S	0.238557	0.094601	0.000000
O	0.939603	-0.121086	1.232601
O	0.939603	-0.121086	-1.232601
N	-1.124901	0.866640	0.000000
H	-1.762886	-1.009764	0.862577
H	-1.762886	-1.009764	-0.862577
N	-1.342643	-0.680983	0.000000

ENERGY= -658.3397005

$H_2NS(O)_2$–N (*Triplet*)

==========

2a00 22a0 0.9787875

2a00 2a20 -0.0703069

H	0.188419	1.945945	-0.858396
H	0.188419	1.945945	0.858396
S	-0.078306	-0.113865	0.000000
O	-0.586509	-0.551095	1.259562
O	-0.586509	-0.551095	-1.259562

N	1.550744	-0.493846	0.000000
N	-0.098828	1.499863	0.000000

ENERGY= -658.3373587

$H_2NS(O)_2$–N (*OSS-3*)

==========

2a00 22b0	-0.6917387		
2b00 22a0	0.6917387		
S	0.036337	0.024910	0.000000
O	0.712430	-0.107169	1.255216
O	0.712430	-0.107169	-1.255216
N	-0.722535	1.442539	0.000000
H	-1.715171	-1.096785	0.857266
H	-1.715171	-1.096785	-0.857266
N	-1.183875	-1.040982	0.000000

ENERGY= -658.2890066

CASPT2(8,8)/6-311++G(3df,3pd) calculated energies (in Hartrees) of $Me_2NS(O)_2$–N

$Me_2NS(O)_2$–N (*CSS-3′*)

==========

22220000 0.9643347

22202000 -0.1546016

02220200 -0.0513456

S	-0.007341	0.095615	0.195991
O	-0.649056	1.362883	0.384967
O	0.835029	-0.529345	1.309154
N	1.388484	-0.142832	-0.386456
N	-1.117905	-0.906621	-0.382032
C	-2.540507	-0.613458	-0.269861
H	-2.969837	-1.078047	0.620535
H	-2.687434	0.460200	-0.229425
H	-3.034042	-1.014262	-1.154028
C	-0.748588	-2.302999	-0.582523
H	-1.069188	-2.911142	0.265300
H	-1.235594	-2.660098	-1.488736
H	0.329297	-2.371774	-0.700272

ENERGY= -736.743822

$Me_2NS(O)_2$–N (*CSS-3″*)

==========

2200 2200 0.9735450

2020 2200 -0.0931888

2200 2020 -0.0656878

0220 2200 -0.0541832

ab20 2200 -0.0523823

ba20 2200 0.0523823

S	-0.749638	0.000000	0.092912
O	-1.351130	1.230339	-0.343549
O	-1.351130	-1.230339	-0.343549
N	0.247457	0.000000	1.310479
N	0.984834	0.000000	-0.084867
C	1.719189	-1.242116	-0.311121
C	1.719189	1.242116	-0.311121
H	2.147406	-1.223507	-1.311166
H	2.147406	1.223507	-1.311166
H	2.502227	-1.312319	0.441962
H	2.502227	1.312319	0.441962
H	1.028219	-2.071912	-0.209695

H	1.028219	2.071912	-0.209695

ENERGY= -736.7969921

$Me_2NS(O)_2$–N (*Triplet*)

==========

22a0 2a00	0.9879824		
22a0 0a20	-0.0664689		
2a20 2a00	0.0602953		
20a2 2a00	-0.0528714		
S	-0.602133	-0.071581	0.000000
O	-1.125819	-0.508722	-1.255428
O	-1.125819	-0.508722	1.255428
N	-0.672887	1.592285	0.000000
N	1.006866	-0.323004	0.000000
C	1.740591	-0.021018	1.230166
C	1.740591	-0.021018	-1.230166
H	1.121014	-0.258729	2.087856
H	1.121014	-0.258729	-2.087856
H	2.628118	-0.649874	1.249821
H	2.628118	-0.649874	-1.249821
H	2.044256	1.026320	1.268774
H	2.044256	1.026320	-1.268774

ENERGY= -736.771438

$Me_2NS(O)_2$–N (*OSS-3*)

==========

22b0 2a00	-0.6973361		
22a0 2b00	0.6973361		
22a2 0b00	-0.0529842		
22b2 0a00	0.0529842		
S	-0.607976	-0.047979	0.000000
O	-1.121276	-0.515669	-1.262476
O	-1.121276	-0.515669	1.262476
N	-0.722103	1.540457	0.000000
N	1.004932	-0.217291	0.000000
C	1.749360	-0.016618	1.240596
C	1.749360	-0.016618	-1.240596
H	1.105055	-0.241574	2.084222
H	1.105055	-0.241574	-2.084222
H	2.593379	-0.705381	1.237331

H	2.593379	-0.705381	-1.237331
H	2.119686	1.006979	1.309211
H	2.119686	1.006979	-1.309211

ENERGY= -736.7223209