

Structure and stability of HSNO, the simplest S-nitrosothiol

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Electronic Supplementary Information:

Cartesian coordinates and energies of molecules calculated.

CCSD/AVDZ cis-HSNO E=-527.884629 Hartree

Coordinates in bohr:

O	-2.8838594129	-0.5880550470	0.0000000000
N	-1.3256420347	1.0318231268	0.0000000000
H	1.4050400425	-2.5575042057	0.0000000000
S	1.9843750650	-0.0663596566	0.0000000000

CCSD/AVDZ trans-HSNO E=-527.886207 Hartree

Coordinates in bohr:

O	-2.9344026416	-0.8723341510	0.0000000000
N	-1.3844028942	0.7495635032	0.0000000000
H	2.8102768252	1.9495155766	0.0000000000
S	1.9162187105	-0.4351629288	0.0000000000

CCSD/AVTZ cis-HSNO E=-528.029340 Hartree

Coordinates in bohr:

O	-2.8538603664	-0.5888387971	0.0000000000
N	-1.2934199660	1.0106823040	0.0000000000
H	1.3874537946	-2.5392554708	0.0000000000
S	1.9397401978	-0.0626838185	0.0000000000

CCSD/AVTZ trans-HSNO E=-528.030748 Hartree

Coordinates in bohr:

O	-2.9002331887	-0.8622606283	0.0000000000
N	-1.3527417363	0.7428360646	0.0000000000
H	2.7852584745	1.9332262940	0.0000000000
S	1.8754064505	-0.4222197302	0.0000000000

CCSD/AVQZ trans-HSNO E=-528.07437982 Hartree

Coordinates in bohr:

O	-2.862611844	0.560539005	0.0000000000
N	-1.281974964	-1.004750984	0.0000000000
S	1.898424057	0.225368799	0.0000000000
H	2.870047222	-2.103662752	0.0000000000

CCSD/AVQZ cis-HSNO E=-528.074379823960 Hartree

Coordinates in bohr:

O	-2.842604059	-0.574329785	0.0000000000
N	-1.272551910	1.009181653	0.0000000000
S	1.931208450	-0.074122614	0.0000000000
H	1.378722267	-2.549756631	0.0000000000

CCSD/AV5Z cis-HSNO E=-528.088556304985 Hartree

Coordinates in bohr:

O	-2.838509992	-0.573284635	0.0000000000
N	-1.267740523	1.008491253	0.0000000000
S	1.927173072	-0.074351610	0.0000000000
H	1.375229926	-2.549468849	0.0000000000

CCSD/AV5Z trans-HSNO E=-528.089865956810 Hartree

Coordinates in bohr:

O	-2.858215949	0.559669478	0.0000000000
N	-1.277315481	-1.004481849	0.0000000000
S	1.894189998	0.225592621	0.0000000000
H	2.870194324	-2.100719647	0.0000000000

CCSD(T)/AVDZ cis-HSNO E=-527.911100 Hartree

Coordinates in bohr:

O	-2.9177966860	-0.5838109699	0.0000000000
N	-1.3604926821	1.0437895016	0.0000000000
H	1.4199080995	-2.5632164198	0.0000000000

S	2.0382949285	-0.0768578943	0.0000000000
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CCSD(T)/AVDZ trans-HSNO E=-527.912777 Hartree			
Coordinates in bohr:			
O	-2.9729076459	-0.8673446480	0.0000000000
N	-1.4118005837	0.7496224866	0.0000000000
H	2.8149298730	1.9597425682	0.0000000000
S	1.9774683566	-0.4504384068	0.0000000000
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CCSD(T)/AVTZ cis-HSNO E=-528.065296 Hartree			
Coordinates in bohr:			
O	-2.8833225081	-0.5876490548	0.0000000000
N	-1.3242884594	1.0238031459	0.0000000000
H	1.3988615263	-2.5445254260	0.0000000000
S	1.9886631011	-0.0717244476	0.0000000000
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CCSD(T)/AVTZ trans-HSNO E=-528.066835 Hartree			
Coordinates in bohr:			
O	-2.9360457133	-0.8604048815	0.0000000000
N	-1.3784369105	0.7434390451	0.0000000000
H	2.7894156250	1.9446738267	0.0000000000
S	1.9327569989	-0.4361259903	0.0000000000
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CCSD(T)/AVQZ cis-HSNO E=-528.112573047138 Hartree			
Coordinates in bohr:			
O	-2.877539902	-0.584690278	0.0000000000
N	-1.315052599	1.018038747	0.0000000000
S	1.966837706	-0.072872266	0.0000000000
H	1.390600908	-2.548152514	0.0000000000
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CCSD(T)/AVQZ trans-HSNO E=-528.114059705869 Hartree			
Coordinates in bohr:			
O	-2.907170860	0.567607702	0.0000000000
N	-1.324601140	-1.005519872	0.0000000000
S	1.939919093	0.223201900	0.0000000000
H	2.849846341	-2.136258490	0.0000000000
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CCSD(T)/AV5Z cis-HSNO E=-528.127616375192 Hartree			
Coordinates in bohr:			
O	-2.872597887	-0.583657461	0.0000000000
N	-1.309067404	1.017638577	0.0000000000
S	1.961890107	-0.073214538	0.0000000000
H	1.386352570	-2.548099085	0.0000000000
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CCSD(T)/AV5Z trans-HSNO E=-528.12907128 Hartree			
Coordinates in ang:			
O	-1.5357804925	0.3000146963	0.0000000000
N	-0.6984754913	-0.5321015376	0.0000000000
S	1.0241603160	0.1182397496	0.0000000000
H	1.5083470692	-1.1288716575	0.0000000000

NO, CCSD

AVDZ	R=1.15960686	Ang	E=-129.6106584	Hartree
AVTZ	R=1.14670583	Ang	E=-129.7057561	Hartree
AVQZ	R=1.14289033	Ang	E=-129.7364363	Hartree
AV5Z	R=1.14190477	Ang	E=-129.7461713	Hartree

NO, CCSD(T)

AVDZ	R=1.16846762	Ang	E=-129.6251255	Hartree
AVTZ	R=1.15651451	Ang	E=-129.7259903	Hartree
AVQZ	R=1.15266708	Ang	E=-129.7579254	Hartree
AV5Z	R=1.15171566	Ang	E=-129.7681761	Hartree

SH, CCSD

AVDZ	R=1.35509105	Ang	E=-398.2434530	Hartree
AVTZ	R=1.34344543	Ang	E=-398.2930907	Hartree
AVQZ	R=1.34251893	Ang	E=-398.3066809	Hartree
AV5Z	R=1.33952391	Ang	E=-398.3026217	Hartree

SH, CCSD(T)

AVDZ	R=1.35509105	Ang	E=-398.2434530	Hartree
AVTZ	R=1.34344543	Ang	E=-398.2930907	Hartree
AVQZ	R=1.34251893	Ang	E=-398.3066809	Hartree
AV5Z	R=1.34204428	Ang	E=-398.3108359	Hartree