Supplementary Material

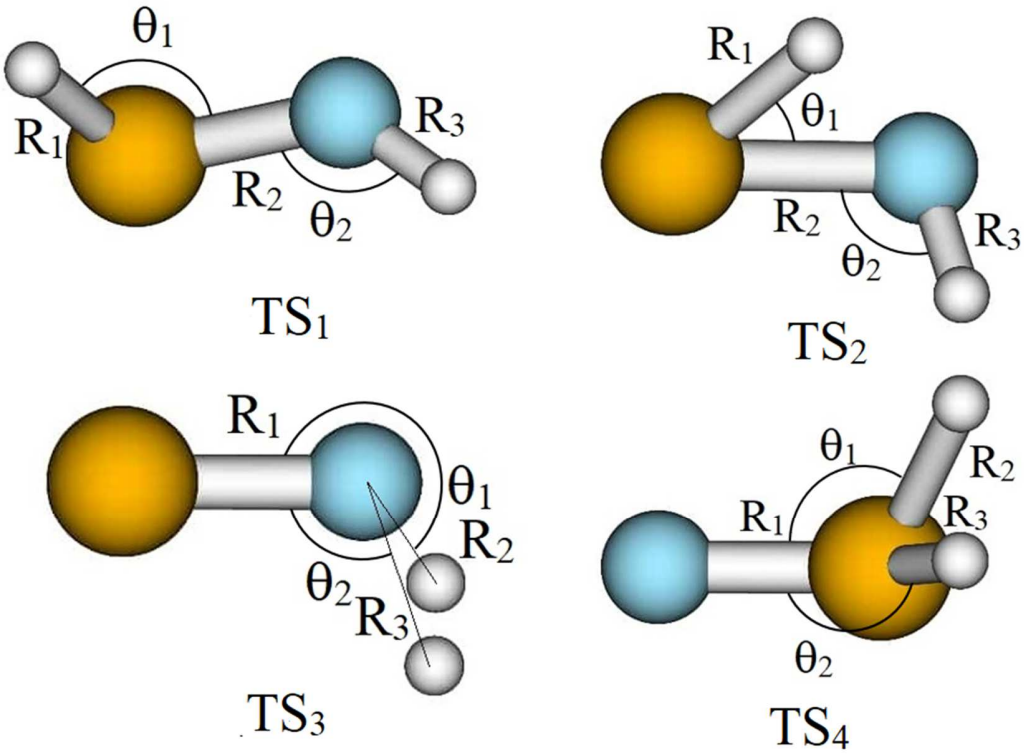

Figure S1: Transition states of the H_2NS species located in the ground potentials and the definition of their internal coordinates given in Table S5.

Table S1: Optimized equilibrium geometries (R_i in Å, angles in degrees), harmonic frequencies (ω_i, in cm^{-1}) and total energies (E, in Hartree) of $H_2NS(X^2B_1)$ calculated with different methods. $\omega_{1\text{-}3}$ are of a_1 symmetry $\omega_{4,5}$ are of b_2 and ω_6 is of b_1 symmetry.

Basis set	R_1	R_2	R_3	θ_1	θ_2	τ	ω_1	ω_2	ω_3	ω_4	ω_5	ω_6	E
RCCSD(T)													
aug-cc-pV(D+d)Z	1.631	1.005	1.005	121.3	121.3	180	3544.23	1611.02	920.37	3678.51	1020.88	86.16	-453.47876894
aug-cc-pV(T+d)Z	1.639	1.007	1.007	121.3	121.3	180	3563.03	1613.80	948.08	3686.38	1017.08	156.62	-453.58065848
aug-cc-pV(Q+d)Z	1.634	1.006	1.006	121.3	121.3	180	3567.14	1613.32	956.83	3691.62	1020.98	230.44	-453.60970487
CBS	1.637	1.006	1.006	121.3	121.3	180							-453.62660484
RCCSD(T)-F12													
cc-pVDZ-F12	1.631	1.005	1.005	121.4	121.4	180	3570.73	1617.99	961.25	3693.74	1022.83	205.21	-453.59495204
cc-pVTZ-F12	1.631	1.005	1.005	121.3	121.3	180	3566.77	1611.99	960.62	3691.32	1023.19	207.89	-453.61744841
cc-pVQZ-F12	1.630	1.005	1.005	121.3	121.3	180	3566.50	1611.06	961.14	3691.40	1022.21	226.06	-453.62310271
CBS	1.630	1.005	1.005	121.3	121.3	180							-453.62704843
CASSCF													
aug-cc-pV(D+d)Z	1.646	1.011	1.011	121.4	121.4	180	3635.25	3509.42	1637.61	1033.72	930.23	157.09	-453.23547061
aug-cc-pV(T+d)Z	1.644	1.010	1.010	121.4	121.4	180	3637.31	3512.21	1639.91	1036.39	931.14	183.37	-453.24233173
aug-cc-pV(Q+d)Z	1.644	1.010	1.010	121.4	121.4	180	3637.65	3512.66	1640.35	1036.56	931.34	187.20	-453.24369133
CBS	1.643	1.010	1.010	121.4	121.4	180							-453.24499779

Table S2: Optimized equilibrium geometries (R_i in Å, angles in degrees), harmonic frequencies (ω_i, in cm^{-1}) and The total energy (E, in Hartree) of trans-HNSH(X^2A'') calculated with different methods. $\omega_{1\text{-}5}$ are of a' symmetry and ω_6 is of a" symmetry.

Basis set	R_1	R_2	R_3	θ_1	θ_2	τ	ω_1	ω_2	ω_3	ω_4	ω_5	ω_6	E
RCCSD(T)													
aug-cc-pV(D+d)Z	1.036	1.669	1.354	103.9	96.5	180	3378.09	2665.88	1248.54	961.51	787.37	652.52	-453.45473576
aug-cc-pV(T+d)Z	1.025	1.640	1.343	104.5	97.1	180	3425.99	2666.17	1250.50	978.92	826.28	657.65	-453.55522469
aug-cc-pV(Q+d)Z	1.023	1.631	1.342	104.7	97.3	180	3437.94	2668.75	1244.20	980.04	836.46	637.89	-453.58402013
CBS	1.021	1.627	1.341	104.8	97.4	180							-453.60064589
RCCSD(T)-F12													
cc-pVDZ-F12	1.023	1.629	1.342	104.6	97.2	180	3441.24	2676.15	1251.94	985.67	842.73	656.03	-453.57048846
cc-pVTZ-F12	1.023	1.628	1.343	104.8	97.3	180	3441.63	2669.15	1250.24	984.42	844.12	662.84	-453.59221949
cc-pVQZ-F12	1.023	1.627	1.343	104.8	97.4	180	3443.39	2671.14	1250.86	984.38	844.86	664.19	-453.59759151
CBS	1.023	1.627	1.343	104.9	97.4	180							-453.60142840
CASSCF													
aug-cc-pV(D+d)Z	1.030	1.668	1.327	105.6	96.8	180	3377.82	2849.48	1267.69	1018.81	776.00	577.32	-453.21242675
aug-cc-pV(T+d)Z	1.029	1.665	1.326	105.7	96.8	180	3384.73	2853.31	1267.56	1020.23	778.25	575.73	-453.21926871
aug-cc-pV(Q+d)Z	1.029	1.664	1.326	105.7	96.9	180	3386.27	2852.52	1267.56	1020.52	778.45	575.94	-453.22068262
CBS	1.029	1.663	1.326	105.8	96.9	180							-453.22196902

Table S3: Optimized equilibrium geometries (R_i in Å, angles in degrees), harmonic frequencies (ω_i, in cm^{-1}) and The total energy (E, in Hartree) of cis-HNSH(X^2A'')) calculated with different methods. $\omega_{1\text{-}5}$ are of a' symmetry and ω_6 is of a" symmetry.

Basis set	R_1	R_2	R_3	θ_1	θ_2	τ	ω_1	ω_2	ω_3	ω_4	ω_5	ω_6	E
RCCSD(T)													
aug-cc-pV(D+d)Z	1.032	1.661	1.363	108.9	104.6	0	3421.12	2589.88	1183.16	947.59	766.31	522.15	-453.45134403
aug-cc-pV(T+d)Z	1.021	1.632	1.353	109.7	105.1	0	3468.10	2587.77	1178.33	962.33	796.73	527.40	-453.55200077
aug-cc-pV(Q+d)Z	1.019	1.622	1.352	110.1	105.2	0	3483.03	2591.61	1178.75	968.88	807.44	532.56	-453.58091115
CBS	1.017	1.618	1.350	110.2	105.3	0							-453.59754579
RCCSD(T)-F12													
cc-pVDZ-F12	1.019	1.620	1.351	110.0	105.2	0	3487.04	2595.94	1181.04	974.62	812.27	521.20	-453.56729391
cc-pVTZ-F12	1.019	1.618	1.352	110.2	105.3	0	3485.75	2589.04	1178.89	972.04	812.60	490.05	-453.58910144
cc-pVQZ-F12	1.019	1.617	1.352	110.3	105.3	0	3487.08	2590.70	1179.07	972.62	813.22	531.73	-453.59450450
CBS	1.019	1.617	1.352	110.3	105.4	0							-453.59835147
CASSCF													
aug-cc-pV(D+d)Z	1.027	1.665	1.333	109.9	104.0	0	3411.00	2817.88	1222.10	1001.35	771.68	204.61	-453.20919974
aug-cc-pV(T+d)Z	1.026	1.661	1.333	110.1	104.1	0	3417.89	2819.96	1222.23	1001.77	773.34	202.15	-453.21607920
aug-cc-pV(Q+d)Z	1.026	1.660	1.333	110.1	104.1	0	3419.44	2819.03	1222.09	1001.70	773.30	198.75	-453.21749868
CBS	1.026	1.660	1.332	110.2	104.1	0							-453.21879275

Table S4: Optimized equilibrium geometries (R_i in Å, angles in degrees), harmonic frequencies (ω_i, in cm^{-1}) and The total energy (E, in Hartree) of $H_2SN(X^2A')$ calculated with different methods. $\omega_{1\text{-}4}$ are of a' symmetry and $\omega_{5,6}$ are of a" symmetry.

Basis set	R_1	R_2	R_3	θ_1	θ_2	τ	ω_1	ω_2	ω_3	ω_4	ω_5	ω_6	E
RCCSD(T)													
aug-cc-pV(D+d)Z	1.583	1.387	1.386	113.9	113.9	103.5	2368.08	1307.31	920.24	773.79	2317.10	791.93	-453.37134543
aug-cc-pV(T+d)Z	1.558	1.373	1.373	114.1	114.1	103.8	2392.21	1315.94	966.14	796.61	2351.08	803.01	-453.47316128
aug-cc-pV(Q+d)Z	1.549	1.372	1.372	114.1	114.1	103.9	2399.76	1319.76	980.18	796.00	2362.16	811.41	-453.50269479
CBS	1.545	1.369	1.369	114.1	114.1	103.9							-453.51943901
RCCSD(T)-F12													
cc-pVDZ-F12	1.542	1.372	1.372	114.5	114.5	104.2	2390.26	1325.46	997.66	807.93	2352.63	825.01	-453.49090382
cc-pVTZ-F12	1.544	1.372	1.372	114.3	114.3	104.1	2393.74	1319.68	990.25	800.37	2356.68	805.14	-453.51135179
cc-pVQZ-F12	1.543	1.372	1.372	114.2	114.2	104.1	2398.18	1320.68	991.24	799.20	2362.75	817.09	-453.51680617
CBS	1.544	1.372	1.372	114.2	114.2	104.1							-453.52030366
CASSCF													
aug-cc-pV(D+d)Z	1.556	1.363	1.363	114.8	114.8	104.8	2475.21	1395.90	985.56	872.81	2454.94	851.60	-453.13883080
aug-cc-pV(T+d)Z	1.552	1.362	1.362	114.9	114.9	104.8	2480.43	1398.71	989.89	876.97	2460.09	854.51	-453.14608162
aug-cc-pV(Q+d)Z	1.551	1.362	1.362	114.9	114.9	104.9	2481.79	1399.48	991.37	877.70	2461.03	854.84	-453.14776004
CBS	1.550	1.362	1.362	114.9	114.9	105.0							-453.14907247

Table S5: Optimized transition geometries (R_i in Å, angles in degrees), harmonic frequencies (ω_i, in cm^{-1}) and The total energy (E, in Hartree) of transition structure T_1 calculated with different methods. All frequencies are of a symmetry. See Figure S1 for the definition of the parameters.

Basis set	R_1	R_2	R_3	θ_1	θ_2	τ	ω_1	ω_2	ω_3	ω_4	ω_5	ω_6	E
TS_1													
RCCSD(T)													
aug-cc-pV(D+d)Z	1.381	1.661	1.006	133.1	107.6	101.8	3734.04	2400.91	1473.69	1076.45	847.50	1646.35i	-453.41660190
aug-cc-pV(T+d)Z	1.369	1.549	0.996	132.4	107.6	101.2	3780.23	2415.01	1230.07	1093.72	812.97	1351.31i	-453.52065762
aug-cc-pV(Q+d)Z	1.374	1.532	1.001	133.5	107.4	104.4	3729.25	2421.26	1181.01	1115.20	896.70	1224.17i	-453.55087992
CBS	1.370	1.509	0.996	133.0	107.5	103.4							-453.56798147
RCCSD(T)-F12													
cc-pVDZ-F12	1.341	1.695	1.039	102.1	96.0	98.8	3222.17	2673.15	1272.51	880.41	800.62	1202.07i	-453.53775582
cc-pVTZ-F12	1.377	1.529	1.007	132.7	106.1	109.2	3641.36	2393.25	1190.62	1116.33	931.20	1155.63i	-453.56053027
cc-pVQZ-F12	1.369	1.538	0.994	132.4	107.8	101.1	3790.70	2430.48	1151.58	1108.42	828.00	1247.52i	-453.56449585
CBS	1.381	1.495	0.989	140.0	109.8	106.0							-453.56898707
TS_2													
RCCSD(T)													
aug-cc-pV(D+d)Z	1.465	1.793	1.038	104.6	49.9	114.8	3332.49	2161.39	1130.41	713.56	564.59	1957.06i	-453.38837133
aug-cc-pV(T+d)Z	1.451	1.759	1.027	105.2	50.7	115.5	3367.08	2205.40	1132.14	735.09	527.23	1966.33i	-453.48811530
aug-cc-pV(Q+d)Z	1.449	1.749	1.025	105.6	50.8	116.6	3380.70	2218.09	1135.24	747.31	523.97	1978.90i	-453.51623645
CBS	1.446	1.744	1.023	105.7	51.0	116.5							-453.53286912
RCCSD(T)-F12													
cc-pVDZ-F12	1.450	1.744	1.025	105.9	50.6	118.1	3387.31	2223.95	1144.21	762.36	558.72	1988.08i	-453.50166119
cc-pVTZ-F12	1.449	1.745	1.025	105.8	50.8	117.4	3382.67	2219.94	1139.99	753.93	528.96	1978.64i	-453.52401170
cc-pVQZ-F12	1.449	1.744	1.025	105.8	50.9	117.3	3380.84	2219.91	1134.29	753.46	521.76	1982.77i	-453.52938526
CBS	1.449	1.744	1.025	105.8	50.9	117.2							-453.533374347
TS_3													
RCCSD(T)													
aug-cc-pV(D+d)Z	1.621	1.396	1.396	109.9	109.9	-97.0	2862.24	978.93	856.79	795.70	156.34	1902.60i	-453.34700271
aug-cc-pV(T+d)Z	1.600	1.387	1.387	109.9	109.9	-96.9	2904.69	1014.74	865.43	766.10	235.00	1894.79i	-453.44528806
aug-cc-pV(Q+d)Z	1.593	1.384	1.384	109.9	109.9	-96.9	2913.31	1022.96	861.21	756.67	236.31	1892.62i	-453.47347187

CBS	1.591	1.383	1.383	109.9	109.9	-96.8							-453.48972745
RCCSD(T)-F12													
cc-pVDZ-F12	1.593	1.379	1.379	109.9	109.9	-97.0	2891.85	1024.53	879.92	787.87	263.46	1920.14i	-453.45958658
cc-pVTZ-F12	1.591	1.382	1.382	109.9	109.9	-96.9	2909.52	1027.03	874.51	774.30	276.94	1898.88i	-453.48156252
cc-pVQZ-F12	1.591	1.382	1.382	109.9	109.9	-96.9	2916.47	1028.49	875.38	777.52	301.76	1893.90i	-453.48691436
CBS	1.591	1.383	1.383	110.0	110.0	-96.9							-453.49081729
TS_4													
RCCSD(T)													
aug-cc-pV(D+d)Z	1.565	1.536	1.536	111.4	111.4	51.7	1762.47	1146.03	954.16	743.56	632.54	1351.07i	-453.32512860
aug-cc-pV(T+d)Z	1.542	1.523	1.523	111.4	111.4	51.0	1775.49	1245.39	1001.02	773.39	759.73	1356.87i	-453.42600909
aug-cc-pV(Q+d)Z	1.534	1.521	1.521	111.4	111.4	50.9	1788.36	1262.05	1016.22	791.81	764.81	1343.81i	-453.45538780
CBS	1.530	1.519	1.519	111.4	111.4	50.8							-453.47194529
RCCSD(T)-F12													
cc-pVDZ-F12	1.528	1.523	1.523	111.6	111.6	51.4	1769.82	1230.86	1030.57	769.36	763.14	1317.45i	-453.44340055
cc-pVTZ-F12	1.529	1.522	1.522	111.5	111.5	51.2	1783.20	1267.37	1026.52	790.14	766.57	1330.60i	-453.46417408
cc-pVQZ-F12	1.529	1.521	1.521	111.4	111.4	51.1	1789.53	1275.58	1027.56	794.88	768.01	1332.92i	-453.46949019
CBS	1.529	1.521	1.521	111.4	111.4	51.1							-453.47310695

Table S6: Harmonic (ω, cm^{-1}) and anharmonic (ν, cm^{-1}) frequencies of [H,H,N,S] species as computed using the RMP2/aug-cc-pV(Q+d)Z approach. Δν (= ν – ω, cm^{-1}) corresponds to the anharmonicity.

Structure	Symmetry	aug-cc-pv(Q+d)z	aug-cc-pv(Q+d)z	
		ω	ν	Δν
H_2NS	a_1	3578.25	3411.67	−166.58
		1611.93	1564.82	−47.11
		964.9	946.96	−17.94
	b_2	3711.88	3523.73	−188.15
		1024.44	1018.88	−5.56
	b_1	294.67	477.19	182.52
***trans*-HNSH**	a'	3462.57	3304.68	−157.89
		2695.02	2584.63	−110.39
		1258.04	1219.96	−38.08
		996.56	977.79	−18.77
		808.00	783.55	−24.45
	a"	718.38	704.69	−13.69
***cis*-HNSH**	a'	3505.83	3348.15	−157.68
		2619.02	2505.09	−113.93
		1185.69	1036.74	−148.95
		990.82	975.32	−15.5
		779.56	757.16	−22.4
	a"	593.97	601.68	7.71
H_2SN	a'	2429.87	2286.43	−143.44
		1336.88	1292.65	−44.23
		995.21	980.46	−14.75
		809.61	785.80	−23.81
	a"	2404.22	2266.59	−137.63
		860.49	838.33	−22.16

Table S7: CASSCF structural parameters and harmonic frequencies (ω_i, cm^{-1}) of the lowest electronic excited states of H_2NS species. Distances are in Å and angles are in degrees. See Figure 1 for the definition of these parameters.

Basis set	R_1	R_2	R_3	θ_1	θ_2	τ	ω_1	ω_2	ω_3	ω_4	ω_5	ω_6	E
$H_2NS(1^2A')$													
aug-cc-pV(T+d)Z	1.786	1.030	1.030	103.7	103.7	105.7	3298.2	1603.7	1026.5	677.6	3372.1	1075.5	-453.20870469
aug-cc-pV(Q+d)Z	1.783	1.029	1.029	103.9	103.9	105.9	3304.3	1604.5	1024.7	679.6	3377.5	1074.8	-453.21524317
aug-cc-pV(5+d)Z	1.783	1.029	1.029	103.9	103.9	105.9	3305.6	1605.2	1024.2	680.0	3378.8	1074.8	-453.21654601
CBS	1.782	1.029	1.029	103.9	103.9	106.0							-453.21778901
$HNSH(2^2A)$													
aug-cc-pV(T+d)Z	1.023	1.608	1.294	115.9	102.6	95.3	3441.5	3292.5	3017.50	1100.6	1001.3	768.6	-453.16683183
aug-cc-pV(Q+d)Z	1.032	1.669	1.350	110.6	105.8	91.1	3352.9	2631.1	2523.60	1050.0	808.1	661.5	-453.17428434
aug-cc-pV(5+d)Z	1.001	1.636	1.340	117.7	101.9	92.2	3676.5	3394.8	2649.37	1004.6	912.8	811.4	-453.17765534
CBS	1.012	1.661	1.357	114.4	103.8	90.9							-453.17853939
$H_2SN(1^2A'')$													
aug-cc-pV(T+d)Z	1.633	1.366	1.366	106.8	106.8	91.7	2454.7	2414.2	1144.8	980.5	930.6	791.4	-453.10582154
aug-cc-pV(Q+d)Z	1.629	1.365	1.365	106.8	106.8	91.8	2459.8	2419.4	1146.1	984.5	933.6	796.4	-453.11279217
aug-cc-pV(5+d)Z	1.628	1.365	1.365	106.8	106.8	91.8	2460.6	2420.7	1146.7	985.4	934.3	797.8	-453.11436334
CBS	1.627	1.365	1.365	106.8	106.8	91.8							-453.11563703
$H_2NS(2^2A')$													
aug-cc-pv(T+d)z	2.129	1.031	1.031	115.6	115.6	128.5	3436.6	3313.4	1500.7	821.9	618.4	283.3	-453.10495252
aug-cc-pv(Q+d)z	2.129	1.030	1.030	115.6	115.6	128.6	3442.2	3319.5	1501.8	822.7	620.2	282.9	-453.11118784
aug-cc-pv(5+d)z	2.128	1.030	1.030	115.6	115.6	128.5	3443.4	3320.6	1502.4	823.1	621.1	284.3	-453.112418363
CBS	2.128	1.030	1.020	115.6	115.6	128.5							-453.1136070
cis-$HNSH(2^2A')$													
aug-cc-pv(T+d)z	1.037	1.648	1.494	116.8	87.9	0	4356.4	2792.1	1185.5	1089.1	821.5	555.9	-453.07250233
aug-cc-pv(Q+d)z	1.036	1.645	1.492	117.0	88.0	0	4347.1	2793.5	1187.3	1092.8	824.8	560.3	-453.07929605
aug-cc-pv(5+d)z	1.035	1.644	1.491	116.89	88.0	0	4335.3	2789.7	1189.5	1096.4	825.3	564.1	-453.08072441
CBS	1.035	1.643	1.491	116.9	88.0	0							-453.08199485
$H_2SN(2^2A')$													
aug-cc-pv(T+d)z	1.516	1.382	1.382	110.3	110.3	93.3	2357.4	2309.6	1350.6	1226.7	1158.2	1142.1	-452.99582000
aug-cc-pv(Q+d)z	1.512	1.381	1.381	110.3	110.3	93.3	2365.1	2317.7	1353.6	1230.8	1163.0	1147.6	-453.00370243
aug-cc-pv(5+d)z	1.512	1.380	1.380	110.3	110.3	93.4	2367.5	2319.9	1354.5	1231.6	1164.2	1148.5	-453.00559103

CBS	1.511	1.380	1.380	110.3	110.3	93.4							-453.00699971

Table S8: Fragmentation energies (E_0, eV) of *cis*-HNSH and of *trans*-HNSH, where the ZPE corrections are also included. These energies correspond to the diatom + diatom fragmentations from the corresponding tetratomic. All molecular species are taken at their equilibrium structure as optimized at the respective theoretical level. See text for more details.

Reaction	Method	Basis set	E_0
trans-HNSH → SH($X^2\Pi$) + HN($X^3\Sigma^-$)	RCCSD(T)	aug-cc-pV(D+d)Z	2.642
		aug-cc-pV(T+d)Z	2.955
		aug-cc-pV(Q+d)Z	3.070
		CBS	3.115
	RCCSD(T)-F12	cc-pVDZ-F12	3.110
		cc-pVTZ-F12	0.114
		cc-pVQZ-F12	3.135
		CBS	3.135
cis-HNSH → SH($X^2\Pi$) + HN($X^3\Sigma^-$)	RCCSD(T)	aug-cc-pV(D+d)Z	2.566
		aug-cc-pV(T+d)Z	2.884
		aug-cc-pV(Q+d)Z	3.001
		CBS	3.046
	RCCSD(T)-F12	cc-pVDZ-F12	3.040
		cc-pVTZ-F12	3.059
		cc-pVQZ-F12	3.069
		CBS	3.071

Table S9: Fragmentation energies (E_0, eV) where the ZPE corrections are also included. These energies correspond to the atom + triatom fragmentations from the corresponding tetratomic. All molecular species are taken at their equilibrium structure as optimized at the respective theoretical level.

Reaction	Method	Basis set	E_0
$H_2NS \rightarrow H_2N(X^2B_1) + S(^3P)$	RCCSD(T)	aug-cc-pV(D+d)Z	2.901
		aug-cc-pV(T+d)Z	3.213
		aug-cc-pV(Q+d)Z	3.330
		CBS	3.374
	RCCSD(T)-F12	cc-pVDZ-F12	3.360
		cc-pVTZ-F12	3.832
		cc-pVQZ-F12	3.556
		CBS	3.750
$H_2NS \rightarrow HNS(X^1A') + H(^2S)$	RCCSD(T)	aug-cc-pV(D+d)Z	3.065
		aug-cc-pV(T+d)Z	3.218
		aug-cc-pV(Q+d)Z	2.839
		CBS	2.984
	RCCSD(T)-F12	cc-pVDZ-F12	3.200
		cc-pVTZ-F12	3.231
		cc-pVQZ-F12	3.240
		CBS	3.245
trans-HNSH $\rightarrow HNS(X^1A') + H(^2S)$	RCCSD(T)	aug-cc-pV(D+d)Z	2.483
		aug-cc-pV(T+d)Z	2.599
		aug-cc-pV(Q+d)Z	2.620
		CBS	2.643
	RCCSD(T)-F12	cc-pVDZ-F12	2.609
		cc-pVTZ-F12	2.620
		cc-pVQZ-F12	2.621
		CBS	2.623
trans-HNSH $\rightarrow HSN(X^1A') + H(^2S)$	RCCSD(T)	aug-cc-pV(D+d)Z	3.399
		aug-cc-pV(T+d)Z	3.483
		aug-cc-pV(Q+d)Z	3.483
		CBS	3.504
	RCCSD(T)-F12	cc-pVDZ-F12	3.424
		cc-pVTZ-F12	3.463
		cc-pVQZ-F12	3.468
		CBS	3.476
cis-HNSH $\rightarrow HNS(X^1A') + H(^2S)$	RCCSD(T)	aug-cc-pV(D+d)Z	2.407
		aug-cc-pV(T+d)Z	2.529
		aug-cc-pV(Q+d)Z	2.551
		CBS	2.575
	RCCSD(T)-F12	cc-pVDZ-F12	2.540
		cc-pVTZ-F12	2.555
		cc-pVQZ-F12	2.555
		CBS	2.559
cis-HNSH $\rightarrow HSN(X^1A') + H(^2S)$	RCCSD(T)	aug-cc-pV(D+d)Z	3.323

		aug-cc-pV(T+d)Z	3.413
		aug-cc-pV(Q+d)Z	3.412
		CBS	3.435
	RCCSD(T)-F12	cc-pVDZ-F12	3.355
		cc-pVTZ-F12	3.398
		cc-pVQZ-F12	3.402
		CBS	3.412
$H_2SN \rightarrow H_2S(X^1A_1) + N(^4S)$	RCCSD(T)	aug-cc-pV(D+d)Z	-0.204
		aug-cc-pV(T+d)Z	0.232
		aug-cc-pV(Q+d)Z	0.382
		CBS	0.447
	RCCSD(T)-F12	cc-pVDZ-F12	0.454
		cc-pVTZ-F12	0.472
		cc-pVQZ-F12	1.343
		CBS	1.101
$H_2SN \rightarrow HSN(X^1A') + H(^2S)$	RCCSD(T)	aug-cc-pV(D+d)Z	1.206
		aug-cc-pV(T+d)Z	1.324
		aug-cc-pV(Q+d)Z	1.341
		CBS	1.365
	RCCSD(T)-F12	cc-pVDZ-F12	1.330
		cc-pVTZ-F12	1.336
		cc-pVQZ-F12	1.343
		CBS	1.342