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Accessory Publication

Alkoxy Isothiocyanates as Intermediates in the Flash Vacuum Pyrolysis of Alkoxythioureas

Carl Th. Pedersen, Frank Jensen and Robert Flammang

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Figure S1. Matrix IR spectrum of the product of FVP of thiourea **1b** page S2

Computational data: Tables of Cartesian coordinates, energies and IR spectra of calculated structures. page S3

All geometries, vibrational frequencies and energies were calculated at the B3LYP/6-31G** level. For the structures in schemes 4 and 5, energies are also given at the MP2/cc-pVDZ level at the corresponding optimized geometries.

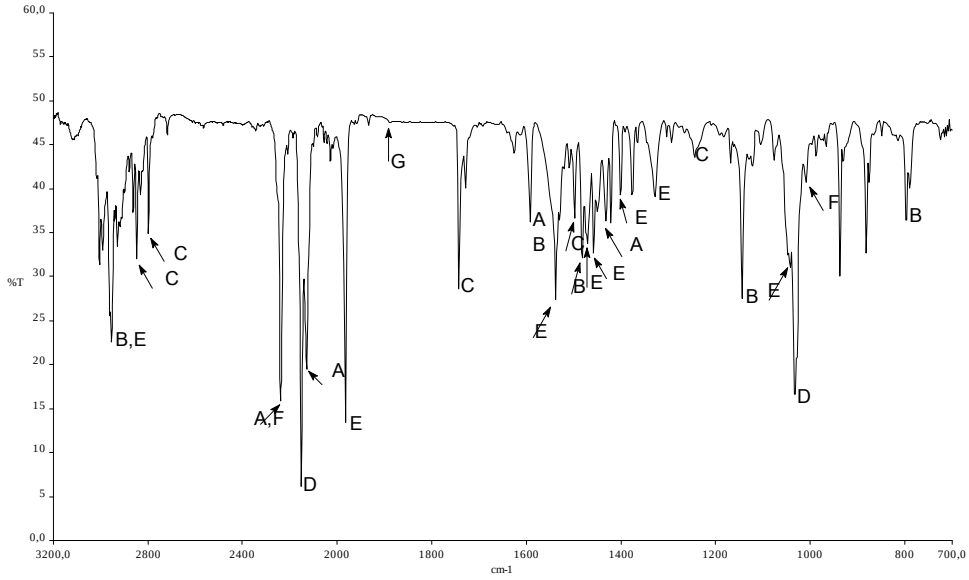
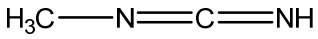


Fig. S1. IR spectrum (10 K, Ar matrix) of the pyrolysis products of compound **1b** at 500^{o}C. (A) Bands due to CH_3NCS **3b**: 2237, 2127, 1592, 1421 cm^{-1}. (B) Bands due to CH_3NH_2: 2954,1592, 1480, 1144, 797 cm^{-1}. (C) Bands due to HCHO: 2863, 2797, 1741, 1498, 1244 cm^{-1}. (D) Bands possibly due to $CH_3ON=C=NCH_3$: 2150 and 1033 cm^{-1}. (E) Bands due to HNCS (3408 and 1982 cm^{-1}) and unpyrolyzed starting material **1b**: 2954, 1537, 1470, 1457, 1401, 1328, 1042 cm^{-1}. (F) Band due to CH_3NHCN **4b**: 2232. (G) Band possibly due to CH_3ONCS **2b**: 1888 cm^{-1}.

Computational Data

Structure 5b



N-(iminomethylene)methanamine

ELECTRONIC ENERGY (B3LYP/6-31G**) = -188.096115133 au.

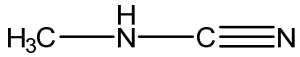
atom type			coordinates [Å]
	x	y	z
C	-1.7163925269	0.1084720911	-0.0301812124
N	-0.4207188136	-0.3744463965	0.4157542338
C	0.6869724665	-0.0656104058	0.0103831341
N	1.8527722705	0.2751021897	-0.2099205491
H	-2.32527978	-0.7400041102	-0.3564650213
H	-2.2311463891	0.5789920852	0.8129581572
H	-1.6501928869	0.8326927957	-0.8496142214
H	2.3587652201	-0.2334414348	-0.9289262375

INFRARED SPECTRUM

mode no.	frequency	absolute intensity	relative intensity[#]
1	83.51	4.81	0.63
2	195.43	13.34	1.74
3	461.29	56.83	7.43
4	568.87	80.68	10.55
5	630.09	14.93	1.95
6	898.86	20.25	2.65
7	959.09	261.00	34.14
8	1144.18	7.39	0.97
9	1146.42	0.86	0.11
10	1409.22	11.54	1.51
11	1469.32	27.97	3.66
12	1504.54	4.39	0.57
13	1518.72	14.69	1.92
14	2260.26	764.53	100.00
15	3035.70	58.13	7.60
16	3110.81	25.04	3.27
17	3115.39	20.56	2.69
18	3576.28	38.59	5.05

[#] normalized to most prominent peak (=100)

Structure 4b



N-methylcyanamide

ELECTRONIC ENERGY (B3LYP/6-31G**) = -188.096542529 au.

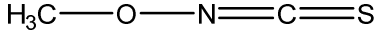
atom type			coordinates [Å]
	x	y	z
N	-0.0632589533	0.3169137235	-0.649650429
C	0.7066917125	-0.3976104552	0.1844046391
N	1.359940042	-1.061225181	0.8889838313
C	-1.4112098401	0.7017554071	-0.2115837086
H	0.4413702575	1.0229744734	-1.171165815
H	-1.9483105087	1.1097692082	-1.0701783149
H	-1.9376603833	-0.190440555	0.1320279036
H	-1.4050582208	1.4430073646	0.5970568264

INFRARED SPECTRUM

mode no.	frequency	absolute intensity	relative intensity[#]
1	157.17	0.53	0.44
2	220.61	5.97	4.94
3	416.68	82.94	68.63
4	527.88	32.10	26.56
5	633.47	33.39	27.63
6	935.52	2.47	2.04
7	1144.08	8.68	7.18
8	1167.82	34.74	28.74
9	1204.73	9.10	7.53
10	1466.21	17.53	14.51
11	1471.92	6.07	5.02
12	1505.06	11.22	9.29
13	1530.26	13.09	10.83
14	2348.82	120.85	100.00
15	3037.44	50.26	41.59
16	3122.41	21.27	17.60
17	3159.70	11.25	9.31
18	3594.52	31.65	26.18

[#] normalized to most prominent peak (=100)

Structure 2b



isothiocyanatooxymethane

ELECTRONIC ENERGY (B3LYP/6-31G**) = -606.093335938 au.

atom type			coordinates [Å]
	x	y	z

H	2.772674	2.224323	0.000000
C	1.682385	2.180416	0.000000
H	1.285944	2.667137	0.896470
H	1.285944	2.667137	-0.896470
O	1.384621	0.780304	0.000000
N	0.000000	0.615483	0.000000
C	-0.549989	-0.476619	0.000000
S	-1.450994	-1.770762	0.000000

INFRARED SPECTRUM

mode no.	**frequency**	**absolute intensity**	**relative intensity**[#]
1	77.05	4.14	0.75
2	140.70	8.26	1.49
3	222.31	1.06	0.19
4	394.79	22.46	4.05
5	399.14	2.81	0.51
6	536.66	41.65	7.50
7	783.77	118.01	21.26
8	987.58	4.69	0.85
9	1102.08	168.71	30.39
10	1177.47	0.61	0.11
11	1223.11	2.31	0.42
12	1471.82	7.58	1.36
13	1484.62	6.15	1.11
14	1520.68	25.84	4.66
15	1985.70	555.11	100.00
16	3045.21	59.35	10.69
17	3122.09	32.28	5.82
18	3163.11	11.98	2.16

[#] normalized to most prominent peak (=100)

Structure 2a

isothiocyanatooxyethane

ELECTRONIC ENERGY (B3LYP/6-31G**) = -645.415969917 au.

atom type			**coordinates [Å]**
	x	**y**	**z**
C	2.189365	-0.171916	0.000000
O	0.803060	-0.571553	0.000000
N	0.000000	0.565860	0.000000
C	-1.221549	0.538651	0.000000
S	-2.788434	0.724703	0.000000
C	2.997439	-1.455160	0.000000
H	2.388903	0.435698	0.890111

H	2.388903	0.435698	-0.890111
H	4.064878	-1.215673	0.000000
H	2.778125	-2.054516	0.887736
H	2.778125	-2.054516	-0.887736

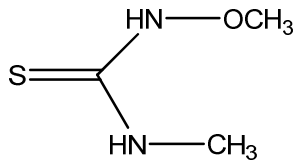
INFRARED SPECTRUM

mode no.	**frequency**	**absolute intensity**	**relative intensity**[#]
1	66.04	2.67	0.45
2	104.37	4.53	0.76
3	117.58	0.04	0.01
4	242.32	0.30	0.05
5	304.70	14.34	2.40
6	388.90	12.72	2.13
7	398.53	2.63	0.44
8	557.05	55.90	9.35
9	813.75	105.42	17.63
10	829.50	0.99	0.17
11	890.65	1.31	0.22
12	1039.50	3.00	0.50
13	1075.38	155.34	25.97
14	1164.08	70.37	11.77
15	1189.91	4.20	0.70
16	1286.65	0.18	0.03
17	1403.46	18.09	3.02
18	1437.74	29.43	4.92
19	1497.61	5.73	0.96
20	1516.49	4.99	0.83
21	1540.57	15.19	2.54
22	1989.39	598.10	100.00
23	3044.05	42.51	7.11
24	3060.57	12.23	2.05
25	3089.24	25.18	4.21
26	3136.49	19.51	3.26
27	3143.03	27.02	4.52

[#] normalized to most prominent peak (=100)

Structures in schemes 4 and 5:

Structure 1b



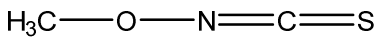
1-methoxy-3-methylthiourea

ELECTRONIC ENERGY (B3LYP/6-31G**) = -701.999054327 au.

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -700.56707700810 au.

atom type			coordinates [Å]
	x	y	z
C	-2.484293	-1.172915	0.142968
N	-1.808139	0.109770	0.048683
C	-0.467483	0.311856	-0.058651
N	0.259014	-0.864810	-0.147023
O	1.573035	-0.770349	-0.619433
C	2.494472	-0.842489	0.474712
H	3.480896	-0.803624	0.007798
S	0.208349	1.840646	0.001274
H	-2.332659	0.957094	0.205610
H	-0.188867	-1.639687	-0.625923
H	2.369363	0.011734	1.145516
H	2.379220	-1.782485	1.027109
H	-2.058705	-1.795716	0.939037
H	-3.535749	-0.994484	0.371401
H	-2.443671	-1.733810	-0.801263

Structure 2b



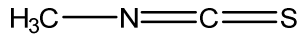
isothiocyanatooxymethane

ELECTRONIC ENERGY (B3LYP/6-31G**) = -606.093335938 au.

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -604.97574040638 au.

atom type			coordinates [Å]
	x	y	z
H	2.772674	2.224323	0.000000
C	1.682385	2.180416	0.000000
H	1.285944	2.667137	0.896470
H	1.285944	2.667137	-0.896470
O	1.384621	0.780304	0.000000
N	0.000000	0.615483	0.000000
C	-0.549989	-0.476619	0.000000
S	-1.450994	-1.770762	0.000000

Structure 3b



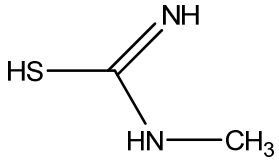
isothiocyanatomethane

ELECTRONIC ENERGY (B3LYP/6-31G**) = -530.953131860 au.

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -530.01597300821 au.

atom type			coordinates [Å]
	x	y	z
C	2.358881	0.137092	0.000000
N	0.997595	-0.280695	-0.000001
C	-0.176824	-0.087731	0.000002
S	-1.765085	0.058264	0.000000
H	3.015564	-0.736456	-0.000009
H	2.575150	0.736477	-0.891045
H	2.575154	0.736461	0.891055

Structure 7



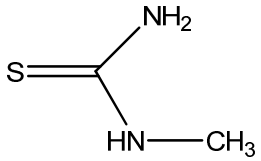
N-methylcarbamimidothioic acid

ELECTRONIC ENERGY (B3LYP/6-31G**) = -587.511219009 au.

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -586.39980092548 au.

atom type			coordinates [Å]
	x	y	z
C	2.307848	-0.328529	0.016676
N	0.899359	-0.672755	-0.059936
C	-0.067524	0.310939	-0.007959
S	-1.727110	-0.407788	-0.017213
N	0.068186	1.578791	-0.010853
H	0.637116	-1.572723	0.315810
H	1.051979	1.851946	0.028174
H	2.579924	0.172293	0.957391
H	2.897050	-1.242938	-0.072864
H	2.580491	0.328141	-0.815771
H	-2.327557	0.751178	0.305883

Structure 8



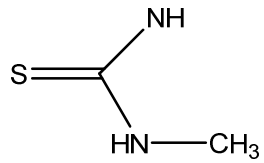
1-methylthiourea

ELECTRONIC ENERGY (B3LYP/6-31G**) = -587.539818134 au.

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -586.42242713831 au.

atom type			coordinates [Å]
	x	y	z
C	2.266336	-0.346258	0.037490
N	0.862286	-0.699915	-0.060402
C	-0.182198	0.164796	-0.014656
S	-1.779603	-0.369152	0.011407
N	0.140536	1.488520	0.038855
H	0.593655	-1.671597	-0.056159
H	1.049678	1.820217	-0.248692
H	-0.633222	2.127401	-0.053917
H	2.853963	-1.263012	0.101690
H	2.615279	0.208210	-0.844702
H	2.469711	0.253752	0.933105

Structure 9

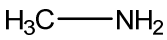


1-methylthiourea radical

ELECTRONIC ENERGY (B3LYP/6-31G**) = -586.869644285 au.

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -585.76104145504 au.

atom type			coordinates [Å]
	x	y	z
C	-2.286114	-0.279144	0.015122
N	-0.888818	-0.668253	-0.046516
C	0.131387	0.236045	-0.049031
N	0.028579	1.536153	-0.035300
S	1.778582	-0.342267	0.016555
H	-0.642114	-1.629247	0.137470
H	-0.884293	1.844084	0.316334
H	-2.504620	0.465927	-0.756769
H	-2.904623	-1.157355	-0.177631
H	-2.571623	0.136167	0.991881

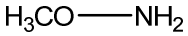


methanamine

ELECTRONIC ENERGY (B3LYP/6-31G**) = -95.8636902239 au.

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -95.547564954881 au.

atom type			coordinates [Å]
	x	y	z
C	0.051369	0.703251	0.000000
N	0.051369	-0.760539	0.000000
H	-0.941991	1.184315	0.000000
H	0.592963	1.064544	0.880333
H	0.592963	1.064544	-0.880333
H	-0.455867	-1.104571	-0.811673
H	-0.455867	-1.104571	0.811673

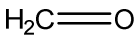


O-methylhydroxylamine

ELECTRONIC ENERGY (B3LYP/6-31G**) = -171.024473298 au.

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -170.53012012705 au.

atom type			coordinates [Å]
	x	y	z
H	-1.997286	0.510357	-0.000003
C	-1.169791	-0.205397	-0.000002
H	-1.237420	-0.842514	0.891573
H	-1.237412	-0.842511	-0.891579
O	0.011544	0.579222	0.000005
N	1.146344	-0.315916	-0.000005
H	1.687058	-0.007633	-0.810881
H	1.687041	-0.007676	0.810899



formaldehyde

ELECTRONIC ENERGY (B3LYP/6-31G**) = -114.503199201 au.

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -114.19323443745 au.

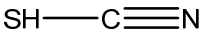
atom type			coordinates [Å]
	x	y	z
C	0.000000	0.000000	-0.528973
O	0.000000	0.000000	0.677675
H	0.000000	0.937762	-1.123780
H	0.000000	-0.937762	-1.123780

ammonia

ELECTRONIC ENERGY (B3LYP/6-31G**) = -56.5577682648 au.

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -56.382505028578 au.

atom type			coordinates [Å]
	x	y	z
N	-0.0241331152	0.0417997816	0.0057667311
H	-0.009679311	0.0167650584	1.0233622664
H	0.949652661	-0.0205546662	-0.2854425916
H	-0.4570254674	-0.8327006623	-0.2854425916

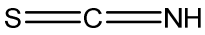


thiocyanic acid

ELECTRONIC ENERGY (B3LYP/6-31G**) = -491.615015464 au.

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -490.82948795429 au.

atom type			coordinates [Å]
	x	y	z
C	0.000000	0.700812	0.000000
S	-0.069452	-1.004648	0.000000
N	-0.022537	1.865164	0.000000
H	1.268996	-1.186650	0.000000



isothiocyanic acid

ELECTRONIC ENERGY (B3LYP/6-31G**) = -491.637503189 au.

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -490.83998116204 au.

atom type			coordinates [Å]
	x	y	z
C	0.000000	0.498523	0.000000
N	-0.151612	1.696215	0.000000
S	0.034102	-1.082242	0.000000
H	0.515656	2.451232	0.000000

Structure TS1

ELECTRONIC ENERGY (B3LYP/6-31G**) = -701.936987402 au. (ν_{imag} = 1568i cm^{-1})

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -700.51149005251 au.

atom type			coordinates [Å]
	x	y	z
C	0.0265912506	-0.0150666863	-0.0032980113

N	-0.0462657356	0.035877805	1.4678678908
C	1.2823570194	0.0163806159	2.1939726247
N	1.0816078859	1.1746040886	2.8092006263
O	1.9560250357	1.5951708764	3.7948002108
C	2.2945542496	2.9662526828	3.5911164138
H	2.9430227943	3.2294622164	4.4286049251
S	2.4299132708	-1.1694003397	2.1127702772
H	-0.6344990506	-0.7154513425	1.8294347296
H	-0.0689897192	1.1351252498	2.1957587965
H	2.8318872727	3.1078188045	2.6463307309
H	1.4007386947	3.6026037661	3.6032015714
H	0.5676171833	0.8655843144	-0.3544932728
H	0.5599254155	-0.9147123993	-0.3231320473
H	-0.9846284239	-0.0077056838	-0.4152498624

Structure TS2

ELECTRONIC ENERGY (B3LYP/6-31G**) = -701.933791782 au. (ν_{imag} = 1561i cm^{-1})

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -700.50764278902 au.

atom type			**coordinates [Å]**
	x	**y**	**z**
C	0.0580254465	-0.0151416635	0.0131393638
N	-0.1129278566	-0.0044251987	1.4490991157
C	0.9018056133	0.0196761087	2.2842016467
N	0.0560258356	0.087445543	3.5568459977
O	0.1007274	-1.0203992304	4.4238448442
C	1.2261291736	-0.968740922	5.3181500314
H	1.1163904515	-1.8570909573	5.9422115593
S	2.5623189453	0.045053438	2.1921987678
H	-0.7924043649	0.0453199417	2.6329861127
H	0.209537492	0.9503603812	4.0927956399
H	2.1703327958	-0.9918930228	4.7711928974
H	1.1754896966	-0.0712373741	5.9511092919
H	-0.9198258884	0.0623247092	-0.4661297619
H	0.6913397699	0.819605085	-0.3121696156
H	0.5434494266	-0.9433369636	-0.3127334715

Structure TS3

ELECTRONIC ENERGY (B3LYP/6-31G**) = -701.942776671 au. (ν_{imag} = 622i cm^{-1})

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -700.51585553475au.

atom type			**coordinates [Å]**
	x	**y**	**z**
C	0.0804148841	0.0280449026	0.0366526593
N	0.037707115	-0.1519717602	1.4767478821

C	1.1213041229	-0.0561577696	2.2944024058
N	2.3488123384	0.2287444807	1.8746173069
S	0.9295541958	-0.207646187	4.0018723726
O	2.7100686498	2.0635567694	2.3847778802
C	2.4006435239	2.344774267	3.6328545926
H	1.6392936244	3.1342956595	3.7518805167
H	-0.8399667243	-0.3724636736	1.9228640412
H	2.3824440375	0.5356061508	0.9019622067
H	1.7824587521	1.3999067614	4.086119999
H	3.2490523303	2.4256843753	4.3326014276
H	0.7575883309	-0.6905326157	-0.4413714239
H	-0.9215265589	-0.1353170579	-0.3622893685
H	0.394396318	1.0428272186	-0.2376054267

Structure TS4

ELECTRONIC ENERGY (B3LYP/6-31G**) = -587.456776429 au. (ν_{imag} = 1418i cm^{-1})

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -586.34689856171 au.

atom type			**coordinates [Å]**
	x	**y**	**z**
C	0.0086586672	-0.0121868072	0.0055556339
N	-0.0282526389	0.0347194815	1.4776649892
C	1.3369456828	-0.0090744834	2.1800477156
S	1.099902371	-1.3900086731	3.226318012
N	2.3129821777	0.7661656575	1.9715759746
H	-0.5623768792	0.8406301713	1.810765921
H	2.1080660431	1.483538504	1.2724235174
H	-0.1824638491	-1.040363883	2.2419509836
H	-1.010879559	0.0072448117	-0.3844813694
H	0.5690878509	0.83164451	-0.4128937956
H	0.4936495509	-0.9429482882	-0.2960953681

Structure TS5

ELECTRONIC ENERGY (B3LYP/6-31G**) = -587.476011715 au. (ν_{imag} = 1600i cm^{-1})

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -586.36350024782 au.

atom type			**coordinates [Å]**
	x	**y**	**z**
C	0.0436408351	0.0284613751	0.0148502665
N	-0.0430963447	0.014688252	1.4643270267
C	1.0400215628	0.029614855	2.2644328423
S	1.0057862655	0.0144282137	4.0225788688
N	2.3069272071	0.057642094	1.9178916049
H	-0.9487048372	-0.0068679257	1.9027767833
H	2.5796832653	0.0711535472	0.9353305817

H	2.464199049	0.0491478784	3.3260514657
H	-0.9652551469	0.0118151214	-0.3997709254
H	0.5491322998	0.932485396	-0.3455283797
H	0.584592119	-0.8486190678	-0.3603209722

Structure TS6

ELECTRONIC ENERGY (B3LYP/6-31G**) = -587.467225644 au. (ν_{imag} = 1653i cm^{-1})

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -586.35684194835 au.

atom type			**coordinates [Å]**
	x	**y**	**z**
C	-0.130529803	-0.1273632128	-0.1255854444
N	0.1633818656	0.1993561287	1.2803840499
C	1.6389885247	0.1221734719	1.6853096529
S	2.5849973058	-1.2323907345	1.5482232651
N	1.7412327715	1.3712837455	2.0877645945
H	-0.3910833199	-0.3850594882	1.9077845621
H	0.4660009134	1.3741358918	1.7073267779
H	2.6263790895	1.70877289	2.4537502739
H	-1.2046837536	-0.0405879718	-0.3019049024
H	0.4006140699	0.579843505	-0.7655939843
H	0.2114152821	-1.1415858287	-0.3519862595

Structure TS7

ELECTRONIC ENERGY (B3LYP/6-31G**) = -587.468613776 au. (ν_{imag} = 1580i cm^{-1})

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -586.35795364678 au.

atom type			**coordinates [Å]**
	x	**y**	**z**
C	-0.0798998183	0.0000729263	-0.088355938
N	0.236866787	-0.0000624073	1.3235144163
C	1.4739434711	-0.0001476049	1.7699614881
N	1.1260064566	-0.0003183133	3.257259258
S	3.0132401475	-0.0001414998	1.1464124845
H	0.0150391324	-0.000281768	2.6795887459
H	1.4687483026	-0.8310742946	3.7401290647
H	1.4686850008	0.8303666662	3.7402973141
H	-1.1646689266	0.0001154708	-0.2133694831
H	0.3388572349	0.8848015017	-0.5839573404
H	0.3388111223	-0.8845837226	-0.5841259015

Structure TS8

ELECTRONIC ENERGY (B3LYP/6-31G**) = -606.042233735 au. (ν_{imag} = 434i cm^{-1})

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -604.93350001771 au.

atom type			coordinates [Å]
	x	y	z
H	-1.701242	-1.596345	0.928312
C	-1.428857	-1.065711	0.000301
O	-1.750440	0.220388	-0.000477
N	-0.348546	1.573988	0.000229
C	0.610203	0.852060	0.000118
S	1.563090	-0.442644	-0.000086
H	-0.251884	-1.223369	0.000121
H	-1.701048	-1.597105	-0.927361

Structure TS9

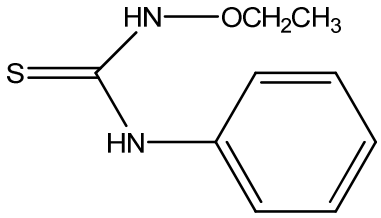
ELECTRONIC ENERGY (B3LYP/6-31G**) = -606.004530574 au. (ν_{imag} = 1292i cm^{-1})

atom type			coordinates [Å]
	x	y	z
H	2.382897	-1.124133	1.157118
C	2.455319	-0.250265	0.484298
H	1.616145	0.492245	0.902341
H	3.381385	0.345646	0.577020
O	1.963828	-0.390830	-0.719932
N	0.286634	1.007478	-0.081232
C	-0.785524	0.452713	-0.012196
S	-2.194766	-0.303384	0.053687

Calculations in relation to thiourea 1a

1a -> TS1a -> EtONCS + PhNH2
1a -> TS2a -> PhNCS + $EtONH_2$

Structure 1a



1-ethoxy-3-phenylthiourea

ELECTRONIC ENERGY (B3LYP/6-31G**) = -933.066997504 au.

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -930.91480835484 au.

atom type			coordinates [Å]
	x	y	z
C	1.738507	0.391582	-0.102482
C	1.796939	-0.904627	-0.638536
C	2.976169	-1.643952	-0.539738
C	4.110380	-1.101116	0.063354
C	4.059202	0.198397	0.572941
C	2.882873	0.938771	0.498905
H	0.936715	-1.317079	-1.153004
H	3.008355	-2.645835	-0.957454
H	5.025907	-1.680032	0.130326
H	4.935966	0.635931	1.040838
H	2.838445	1.941995	0.913358
N	0.585053	1.207285	-0.197733
H	0.734873	2.200684	-0.313903
C	-0.749055	0.907933	-0.070637
S	-1.909113	2.094144	-0.272901
N	-1.025611	-0.418420	0.183042
H	-0.319893	-0.940219	0.695429
O	-2.287047	-0.714672	0.704782
C	-3.140778	-1.264676	-0.319950
H	-3.230768	-0.541128	-1.136366
H	-2.692891	-2.189052	-0.709188
C	-4.482124	-1.523858	0.339311
H	-5.177119	-1.951649	-0.389455
H	-4.380160	-2.224801	1.172957
H	-4.906013	-0.590523	0.718452

TS1a

ELECTRONIC ENERGY (B3LYP/6-31G**) = -932.999279026 au. (ν_{imag} = 1562i cm^{-1})

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -930.85346358726 au.

atom type			coordinates [Å]
	x	y	z
C	-2.88629605	-1.3596122681	0.1816019552
C	-3.9064894574	-0.5568868338	-0.3343902694
C	-5.1414310207	-1.1296313128	-0.6285921579
C	-5.3636547678	-2.4906486646	-0.4049974295
C	-4.3390795668	-3.2832334565	0.1119405622
C	-3.0962869098	-2.7206382847	0.4040024082
H	-3.7263888577	0.4986613135	-0.5073484913
H	-5.933525032	-0.5086473392	-1.0354263711
H	-6.3286842299	-2.9303118353	-0.6363450912
H	-4.5002854358	-4.3429154226	0.2837765505

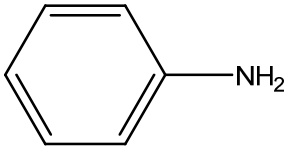
H	-2.2938827795	-3.338951565	0.7983443243
N	-1.6210965577	-0.7636922603	0.5276332737
H	-0.9434644227	-1.4732679793	0.8053363561
C	-0.9563352185	0.2123487683	-0.4526362374
S	-0.3625852489	-0.1418474589	-1.9466953689
N	-1.0261836216	1.2449310188	0.3823829371
H	-1.5167691477	0.3341130537	1.2101839353
O	-0.3339704466	2.4004532022	0.0744264375
C	-1.1357152138	3.5555263103	0.3654303252
H	-2.0381126702	3.5412256622	-0.2600411015
H	-1.4489691544	3.5277115597	1.4182302156
C	-0.2773327072	4.7722842431	0.0736660443
H	-0.845317086	5.6862260015	0.2719452473
H	0.6167068271	4.7753606086	0.7032400474
H	0.0374607754	4.7784019393	-0.9731981013

TS2a

ELECTRONIC ENERGY (B3LYP/6-31G**) = -933.003502975 au. (ν_{imag} = 1566i cm^{-1})

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -930.85645844655 au.

atom type			**coordinates [Å]**
	x	**y**	**z**
C	-3.5959113792	-1.0171059274	-0.0759855486
C	-4.8653221974	-1.1418363211	0.5177677517
C	-5.4647567368	-2.3899085279	0.6438704786
C	-4.808237713	-3.5341785808	0.1823412514
C	-3.5474683498	-3.4138533711	-0.4041661918
C	-2.93419496	-2.1690379937	-0.5380151276
H	-5.3647196105	-0.2458786242	0.8738158624
H	-6.445391721	-2.4708746178	1.1037096248
H	-5.2751104336	-4.5095351366	0.2811675774
H	-3.0301261543	-4.2990553374	-0.7630942916
H	-1.9552301488	-2.0779108672	-0.9911484436
N	-3.0753762324	0.2770606507	-0.1610141304
H	-3.2252345966	1.6140451197	0.0589466076
C	-1.9506337976	0.7219721086	-0.7032767866
S	-0.6119228078	0.1514481951	-1.506536018
N	-2.2225358352	2.2004996804	-0.4160050935
H	-2.2938008892	2.763666462	-1.2721915121
O	-1.3693259268	2.8435090283	0.5003068269
C	-0.1888877496	3.40227145	-0.1275003325
H	0.3834570313	2.6049657363	-0.6081393672
H	-0.5070659004	4.1253078782	-0.8955005046
C	0.5933631739	4.0844711774	0.9779866536
H	1.488941336	4.5518140157	0.558218075
H	-0.007354029	4.8576885392	1.4647512784
H	0.9051526278	3.3574092637	1.7321583606

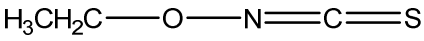


aniline

ELECTRONIC ENERGY (B3LYP/6-31G**) = -287.616504001 au.

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -286.71212084972 au.

atom type			coordinates [Å]
	x	y	z
C	-0.939118	-0.000009	-0.009745
C	-0.221338	1.208161	-0.005102
C	1.171478	1.202325	0.003344
C	1.881286	0.000048	0.008058
C	1.171462	-1.202323	0.003266
C	-0.221268	-1.208202	-0.005068
H	-0.762806	2.151215	-0.012750
H	1.705112	2.148867	0.008770
H	2.966541	-0.000061	0.016181
H	1.705278	-2.148764	0.008523
H	-0.762805	-2.151223	-0.012449
N	-2.335692	-0.000027	-0.076846
H	-2.778199	0.835881	0.280408
H	-2.778293	-0.835728	0.280725



isothiocyanatooxyethane

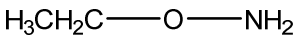
EtONCS , B3LYP/6-31G and MP2/cc-pVDZ data**

ELECTRONIC ENERGY (B3LYP/6-31G**) = -645.415969917 au.

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -644.16158122617 au.

atom type			coordinates [Å]
	x	y	z
C	2.189365	-0.171916	0.000000
O	0.803060	-0.571553	0.000000
N	0.000000	0.565860	0.000000
C	-1.221549	0.538651	0.000000
S	-2.788434	0.724703	0.000000
C	2.997439	-1.455160	0.000000
H	2.388903	0.435698	0.890111
H	2.388903	0.435698	-0.890111
H	4.064878	-1.215673	0.000000
H	2.778125	-2.054516	0.887736

H	2.778125	-2.054516	-0.887736

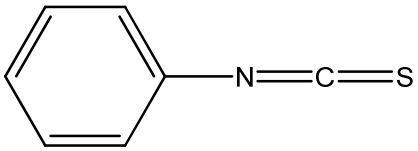


O-ethylhydroxylamine

ELECTRONIC ENERGY (B3LYP/6-31G**) = -210.346437875 au.

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -209.71541382084 au.

atom type			**coordinates [Å]**
	x	**y**	**z**
C	-1.838760	-0.181286	0.000004
H	-2.651614	0.551798	0.000001
H	-1.943671	-0.813227	0.886601
H	-1.943670	-0.813230	-0.886591
C	-0.493302	0.526551	0.000001
H	-0.383180	1.169056	-0.885411
H	-0.383163	1.169042	0.885420
O	0.511870	-0.484997	-0.000015
N	1.808069	0.152515	0.000013
H	2.273113	-0.261372	0.810824
H	2.273110	-0.261288	-0.810844



isothiocyanatobenzene

ELECTRONIC ENERGY (B3LYP/6-31G**) = -722.701125804 au.

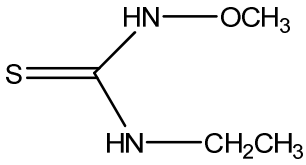
ELECTRONIC ENERGY (MP2/cc-pVDZ) = -721.17638237695 au.

atom type			**coordinates [Å]**
	x	**y**	**z**
C	0.454239	-0.000018	0.000057
C	1.153078	1.218096	0.000031
C	2.545122	1.208439	-0.000013
C	3.245552	0.000019	-0.000066
C	2.545145	-1.208416	-0.000035
C	1.153101	-1.218114	0.000057
H	0.597351	2.149383	0.000052
H	3.084333	2.150711	-0.000024
H	4.330925	0.000017	-0.000130
H	3.084357	-2.150687	-0.000060
H	0.597403	-2.149406	0.000076
N	-0.919236	-0.000015	0.000040
C	-2.105452	-0.000012	0.000089

S	-3.700277	0.000008	-0.000057

Calculations relating to Thiourea 1c.

1c -> TS1c -> MeONCS + $EtNH_2$
1c -> TS2c -> $MeONH_2$ + EtNCS



1-ethyl-3-methoxythiourea
ELECTRONIC ENERGY (B3LYP/6-31G**) = -741.321526363 au.

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -739.75334941406 au.

atom type			coordinates [Å]
	x	y	z
C	-2.806702	-1.397321	0.120832
N	-2.268139	-0.051121	0.027643
C	-0.954223	0.290447	-0.058138
N	-0.106146	-0.801191	-0.128984
O	1.198762	-0.571267	-0.572658
C	2.112340	-0.550082	0.543466
C	3.486234	-0.272336	-0.036691
S	-0.446199	1.883731	0.005864
H	-2.880697	0.736854	0.173731
H	-0.461590	-1.626385	-0.600769
H	1.806268	0.237240	1.239544
H	2.077013	-1.518522	1.060676
H	4.230638	-0.254089	0.765011
H	3.771777	-1.045650	-0.755947
H	3.497088	0.695918	-0.543512
H	-2.329144	-1.968108	0.926458
H	-3.874193	-1.329513	0.334057
H	-2.693985	-1.955360	-0.819240

TS1c
ELECTRONIC ENERGY (B3LYP/6-31G**) = -741.259352464 au. (ν_{imag} = 1566i cm^{-1})

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -739.69774620659 au.

atom type			coordinates [Å]
	x	y	z
C	0.0371792402	0.002542834	-0.0012635776

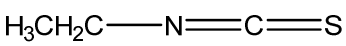
N	-0.0441487622	0.0251201653	1.470204126
C	1.2806970089	0.0262807992	2.2036071275
N	1.0485765379	1.1680240619	2.8378693174
O	1.9081503887	1.5957823683	3.8314306343
C	2.2852483632	2.9648971065	3.6122198722
C	3.1678335998	3.3702979787	4.7780357613
S	2.4576153192	-1.1300995132	2.1071677011
H	-0.6159923834	-0.7464926918	1.8149267668
H	-0.0983091261	1.1100782022	2.2121417946
H	2.8183246797	3.0483401894	2.6562623485
H	1.3821052209	3.5885654728	3.5567397131
H	3.4904342557	4.4090333606	4.6587077563
H	2.6253283852	3.2813998543	5.72329124
H	4.0552269687	2.7338117182	4.8274009854
H	0.5600252109	0.9013584793	-0.3334713383
H	0.5920263208	-0.8789904056	-0.3346868985
H	-0.9719254539	-0.0050760929	-0.4183987997

TS2c

ELECTRONIC ENERGY (B3LYP/6-31G**) = -741.256446153 au. (ν_{imag} = 1566i cm^{-1})

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -739.69396729745 au.

atom type			**coordinates [Å]**
	x	**y**	**z**
C	0.0659379113	-0.011687629	0.0081531024
N	-0.110447794	0.0041404611	1.4434361109
C	0.9007511989	0.0011181979	2.2832551023
N	0.0520111031	0.0882390378	3.5519834479
O	0.0755545781	-1.0198398697	4.4178445901
C	1.1818627303	-0.9704010854	5.3528238643
C	1.0731947002	-2.2208903898	6.2034116396
S	2.5616870422	-0.0207033831	2.1973583794
H	-0.7939070187	0.0674435931	2.6221689025
H	0.2226168928	0.9478975699	4.0876371981
H	2.1242196471	-0.9256831003	4.8008902163
H	1.0839986722	-0.0605386801	5.9664141841
H	1.8708725859	-2.2251685553	6.9520073742
H	0.1105706978	-2.2626333487	6.7206043183
H	1.1765905842	-3.1157696829	5.5844196107
H	-0.9045835617	0.1164787371	-0.4752447315
H	0.7429506463	0.7898307307	-0.3123161079
H	0.5040382153	-0.9631921812	-0.3178141763

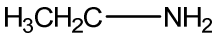


isothiocyanatoethane

ELECTRONIC ENERGY (B3LYP/6-31G**) = -570.273063019 au.

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -569.20010455015 au.

atom type			coordinates [Å]
	x	y	z
C	0.0379932316	0.0000008399	-0.2774180901
N	0.4303402034	0.0000093348	1.1022561436
C	1.2409380097	0.0000181256	1.9747742619
S	2.2416391569	0.0000337912	3.2169083455
C	-1.4819706449	-0.0000014407	-0.4343571438
H	0.4719737644	0.8839001947	-0.7613150902
H	0.4719752093	-0.883903525	-0.7613046295
H	-1.7420766969	-0.0000068007	-1.4967457424
H	-1.9209881153	-0.886551397	0.030624135
H	-1.9209899068	0.8865520971	0.0306156148



ethanamine

ELECTRONIC ENERGY (B3LYP/6-31G**) = -135.183378428 au.

ELECTRONIC ENERGY (MP2/cc-pVDZ) = -134.73121821097 au.

atom type			coordinates [Å]
	x	y	z
C	0.0142175299	-0.0192191865	0.0012227482
N	-0.0260180318	0.0035982791	1.4685051791
H	1.0356981682	0.0027215833	-0.420074532
C	-0.7206067942	-1.2462142346	-0.532777583
H	-0.4869684698	0.8880937287	-0.3574543522
H	0.4490098991	0.8341441752	1.814892605
H	0.4981150052	-0.7900487958	1.8329689002
H	-0.7347465988	-1.250701229	-1.6274343534
H	-0.2316262704	-2.1711800698	-0.203967053
H	-1.7511257451	-1.2634147228	-0.1667465635