Supporting Information

Regioselectivity of aryl radical attack onto isocyanates and isothiocyanates

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Experimental Procedure

Unless otherwise stated, chemicals from the following suppliers were used without further purification: Aldrich: (i) phenyl isocyanate; (ii) phenyl isothiocyanate; (iii) ethyl isocyanate; (iv) ethyl isothiocyanate; (v) allyl isocyanate; (vi) allyl isothiocyanate; and Merck: (vii) acetonitrile (spectroscopic grade). The diazonium tetrafluoroborates **26** and **29** were available from a previous study.[1]

GC-MS analyses were performed on a Thermo Scientific TSQ 8000 TRACE 1310 GC mass spectrometer using electron ionisation in the positive ion mode with an ionisation energy of 70 eV. The gas chromatography was performed with a SGE SOLGEL-1MS column (30 m x 0.25 mm ID, 0.25 µm film thickness), with a temperature program of 50 °C for 2 minutes, then heating at 23 °C/min to 300 °C where the temperature was held for 7 minutes with a splitless injection, an injector temperature of 300 °C and the transfer line was set to 300°C. High-purity helium was used as carrier gas with a flow rate of 1 ml/min.

Gas Phase Mass Spectrometry Experiments

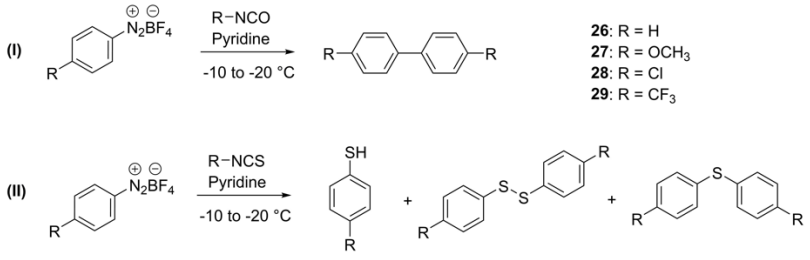
The experiments were conducted in a Thermo Scientific (Bremen, Germany) linear ion trap (LTQ) which was modified to enable the introduction of volatile neutral reagents into the linear ion trap to perform ion−molecule reactions (IMRs) as previously described.[2] Briefly, the iso(thio)cyanate was injected at a rate of 10 ml min^{-1} directly into the helium line which is maintained at a temperature above the boiling point of the corresponding isocyanate.

Typical electrospray source conditions were:

CID: Sheath Gas = 10 arbitrary units, Auxilliary Gas = 5 arbitrary units, Sweep Gas = 0 arbitrary units, Spray Voltage = 4 kV, Capillary Temp. = 250 °C, Capillary Voltage = 2 V, Tube Lens Voltage = 75 V. The precursor ion was mass selected with a window of 1 *m/z* and and collision induced dissociation was carried out using the helium bath gas by activating the ion with an activation time of 30ms. A normalized collision energy (NCE) was chosen to deplete the precursor ion to 10%.

IMR: Sheath Gas = 10 arbitrary units, Auxiliary Gas = 5 arbitrary units, Sweep Gas = 0 arbitrary units, Spray Voltage = 4 kV, Capillary Temp. = 250 °C, Capillary Voltage = 2 V, Tube Lens Voltage = 75 V.

General Procedure for the Reactions of the Iso(thio)cyanates and with the Tetrafluoroborates 26-29.



The aryl radicals were generated following a previously reported procedure[3] from the corresponding diazonium tetrafluoroborates **26** and **29**. In a typical experiment, Iso(thio)cyanate (0.6 mmol, 3 equiv.) was placed in a 4 mL Scintillation vial and taken up in pyridine (1 mL). The tetrafluoroborate salt (0.2 mmol) was added dropwise to the stirred iso(thio)cyanate solution, which was kept at -10 to -20 °C. The reaction mixture was stirred for 5 h and then warmed to the room temperature, after which it was directly analysed via GC-MS using Methyl Stearate (0.2 mmol) as the internal standard.

Generation of γ-NMP radical (m/z 93) via CID

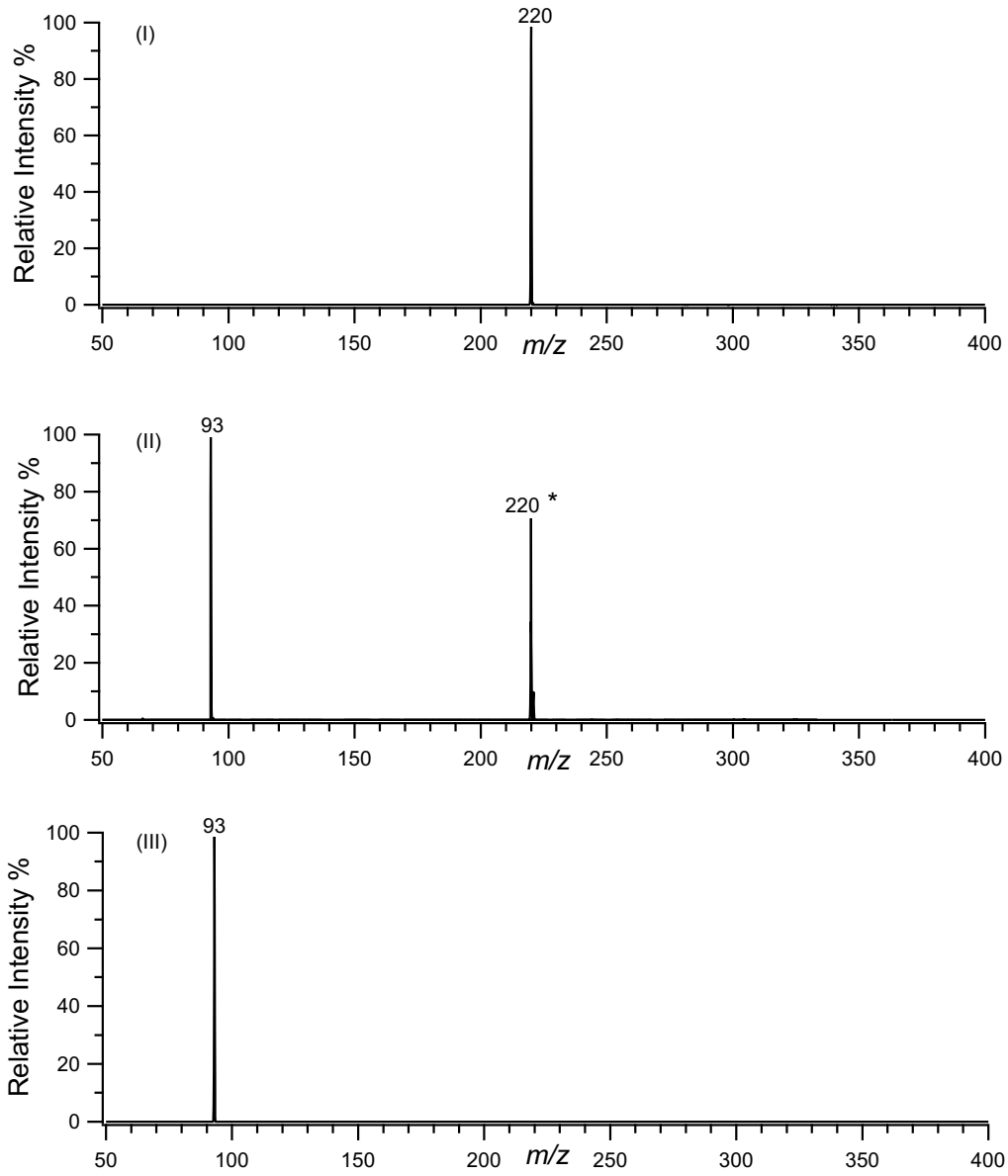


Figure S1 Mass spectrum of (I) methyl 4-Iodopyridinium cation (II) CID at *m/z* 220 (III) Isolation of **γ–NMP** radical. The mass selected precursor ion is highlighted by an asterisk (*).

Isolation of 3a (*m/z* 212) and CID spectrum at *m/z* 212

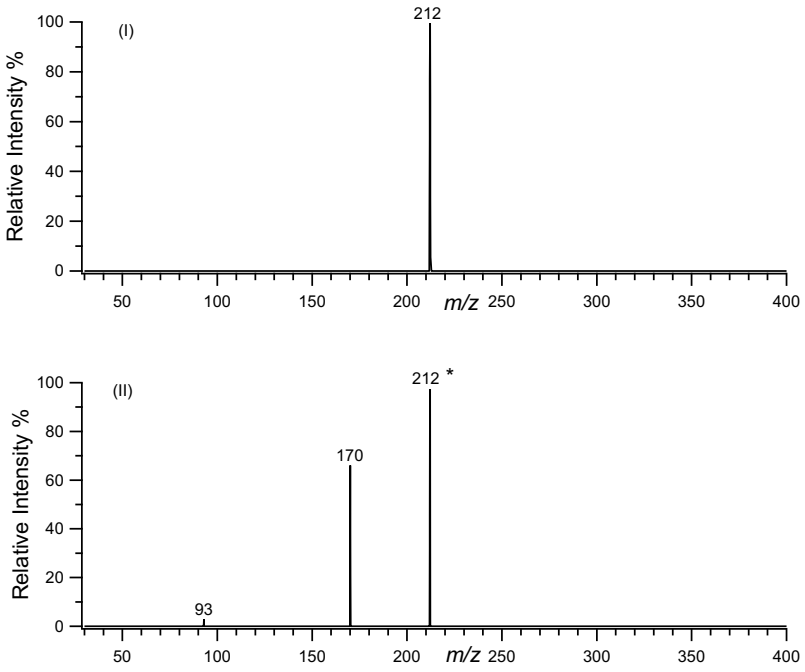


Figure S2 Mass spectrum of (I) *m/z* 212 for **3a** (II) CID at *m/z* 212. The mass selected precursor ion is highlighted by an asterisk (*)

Isolation of 9 (*m/z* 228) and CID spectrum at *m/z* 228

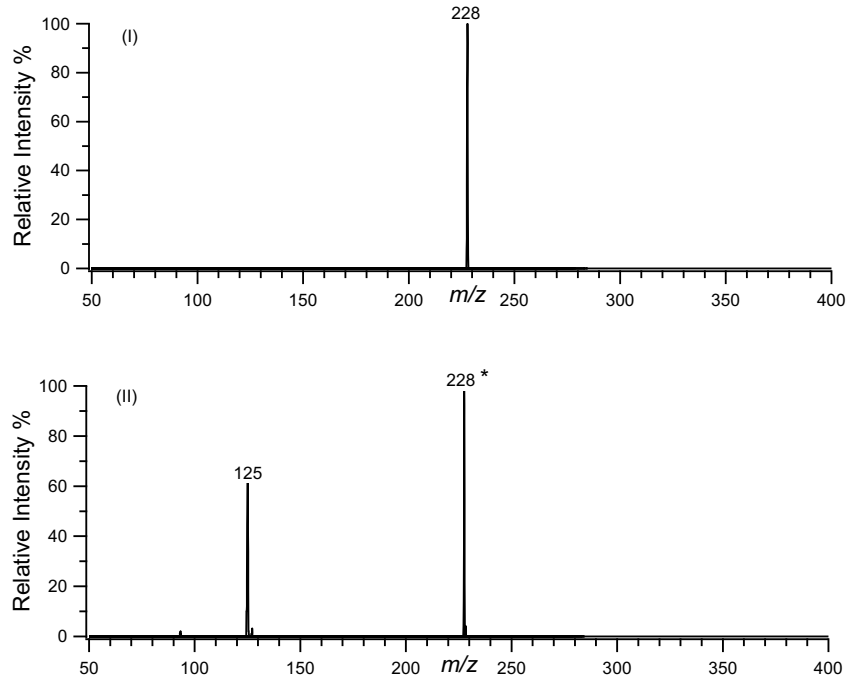


Figure S3 (I) Isolation of **9** at *m/z* 228. (II) CID at *m/z* 228 showing the formation of 12 at *m/z* 125. The mass selected precursor ion is highlighted by an asterisk (*).

Energy profile of 1a calculated at B3LYP level of theory

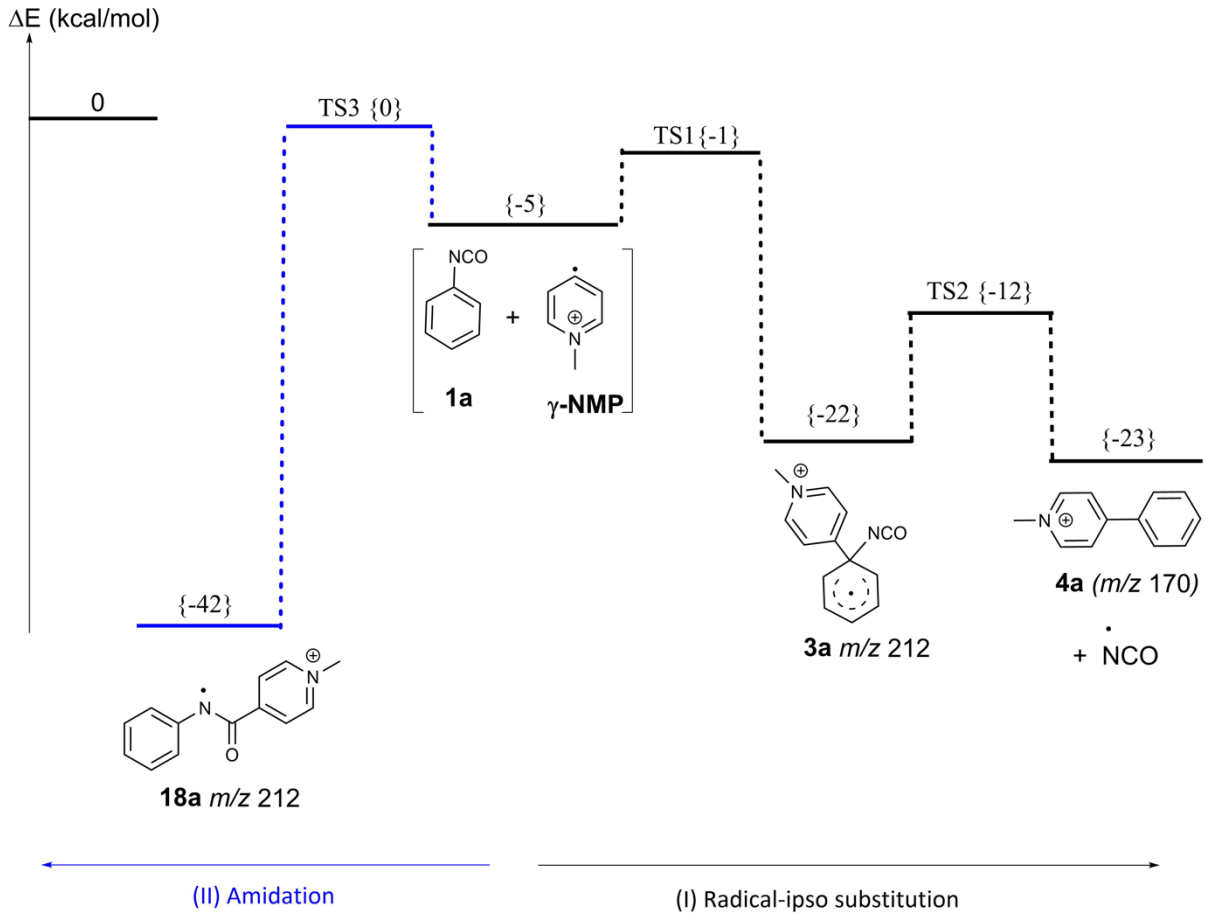
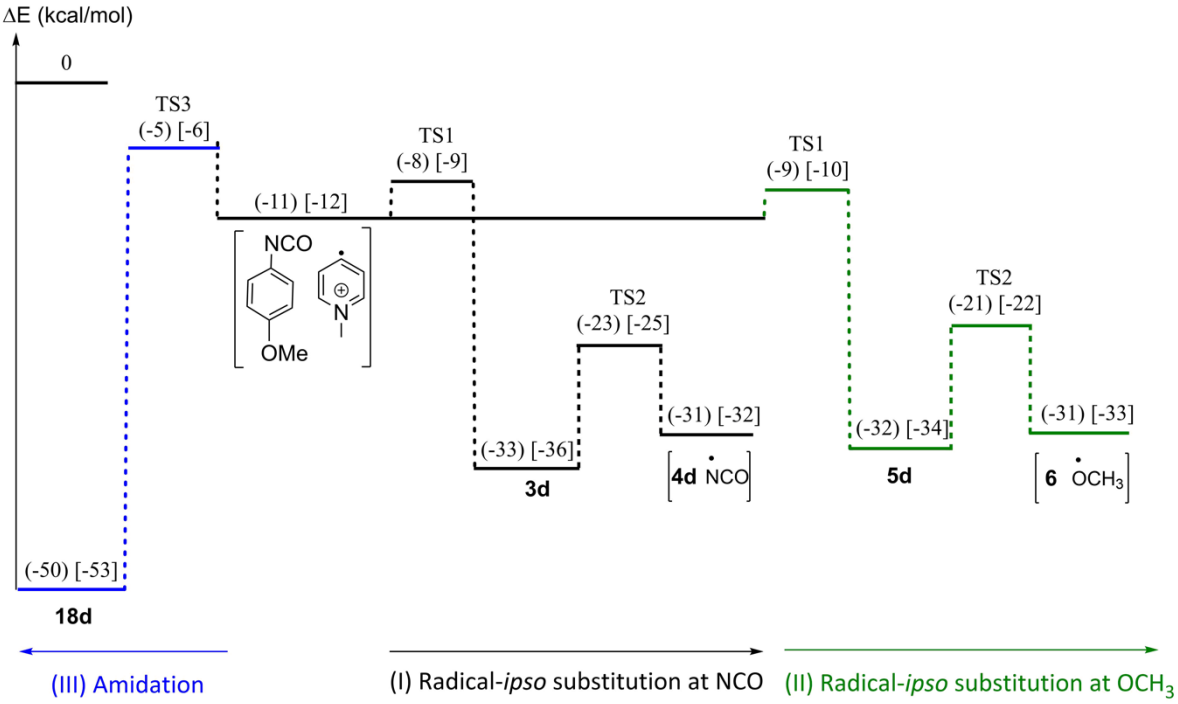


Figure S4 B3LYP calculated potential energy diagram for reacting **γ–NMP** radicals with **1a**. (I) radical-ipso substitution at C with NCO substituent, (II) radical-ipso substitution at C with OMe substituent, (III) amidation at the C-center of NCO moiety. Energies are in kcal/mol and calculated at B3LYP level of theory. Associated complex is shown in square brackets.

Energy profile of 1d



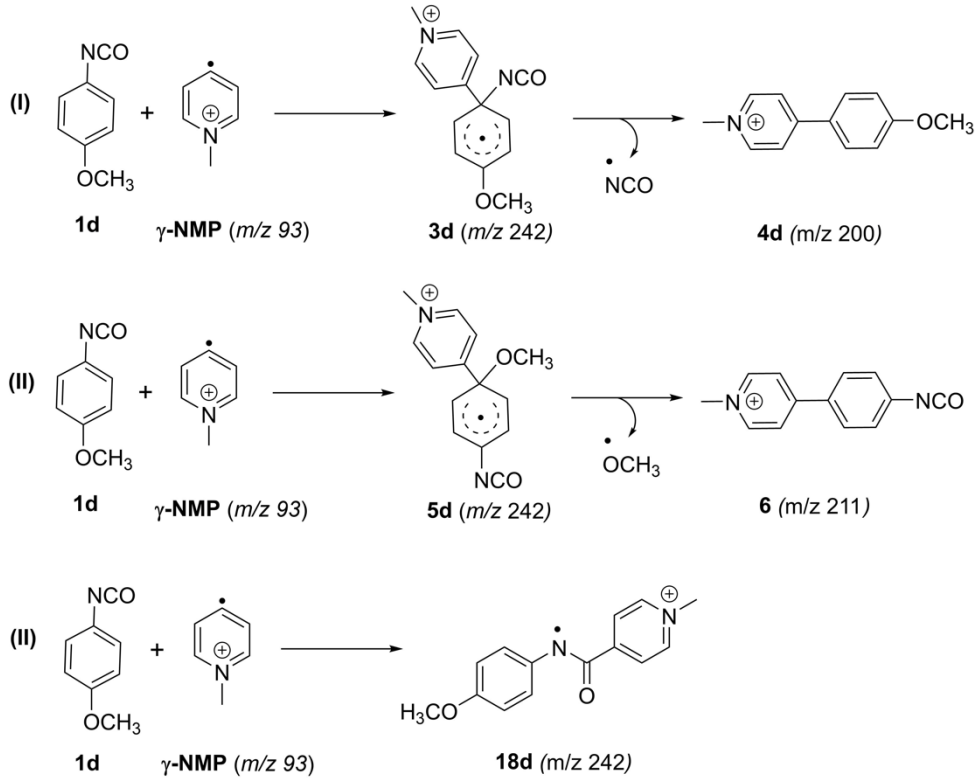


Figure S5 Calculated potential energy diagram for reacting **γ–NMP** radicals with **1d**. (I) radical-ipso substitution at C with NCO substituent, (II) radical-ipso substitution at C with OMe substituent, (III) amidation at the C-center of NCO moiety. Energies are in kcal/mol and calculated at M06-2X (round brackets) and ωB97X-D (square brackets) level of theories. Associated complex is shown in square brackets.

Energy profile of 1e

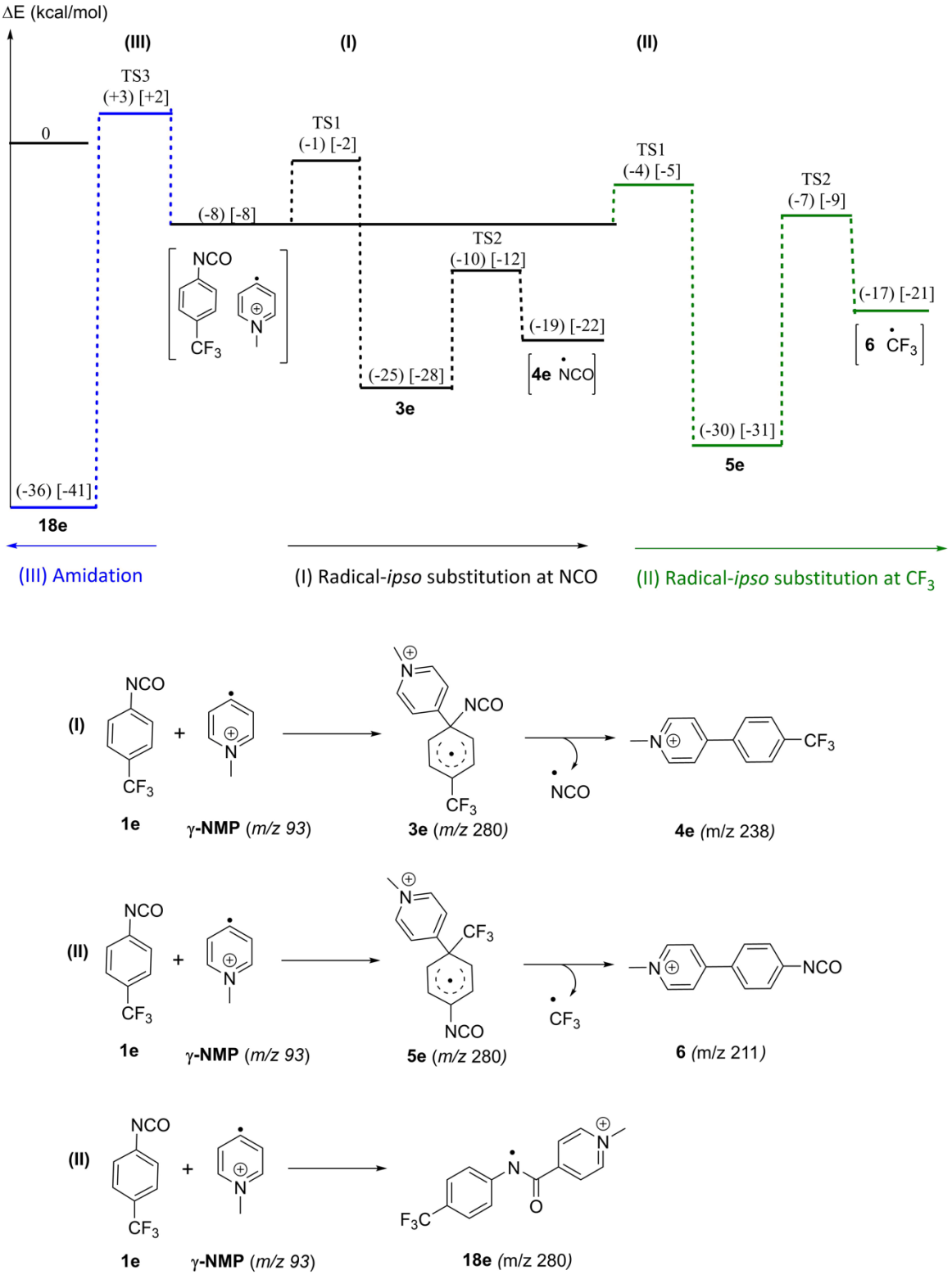


Figure S6 Calculated potential energy diagram for reacting **γ–NMP** radicals with **1e**. (I) radical-ipso substitution at C with NCO substituent, (II) radical-ipso substitution at C with CF3 substituent, (III) amidation at the C-center of NCO moiety. Energies are in kcal/mol and calculated at M06-2X (round brackets) and ωB97X-D (square brackets) level of theories. Associated complex is shown in square brackets.

Energy profile of 2b

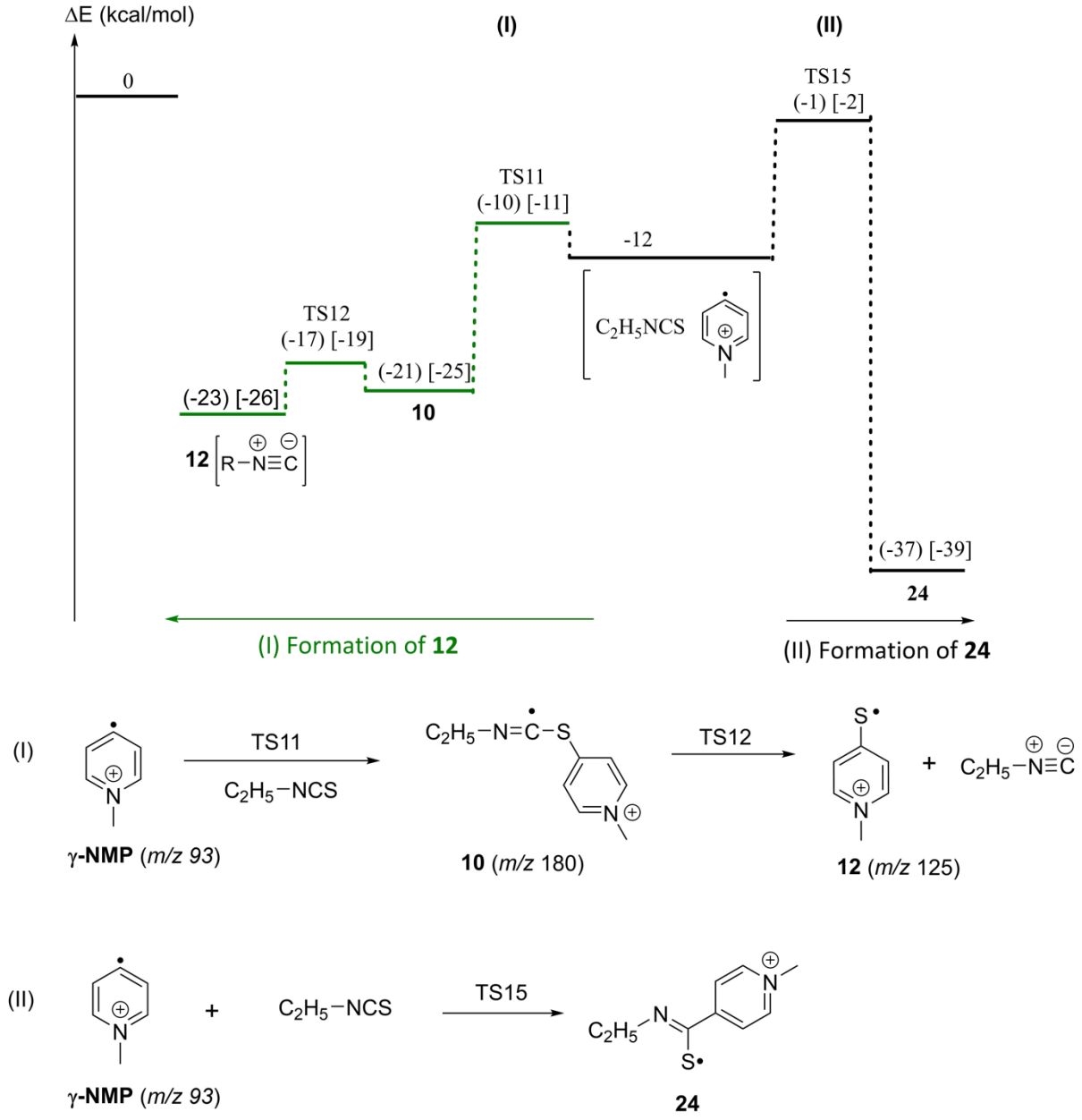


Figure S7 Calculated potential energy diagram for reacting **γ–NMP** radicals with **2b**. Radical addition at (I) formation of **12** (II) formation of S radical intermediate **24**. Energies are in kcal/mol and calculated at M06-2X (round brackets) and ωB97X-D (square brackets) level of theories. Associated complex is shown in square brackets.

Energy profile of 30 reacting with 1a in the gas-phase

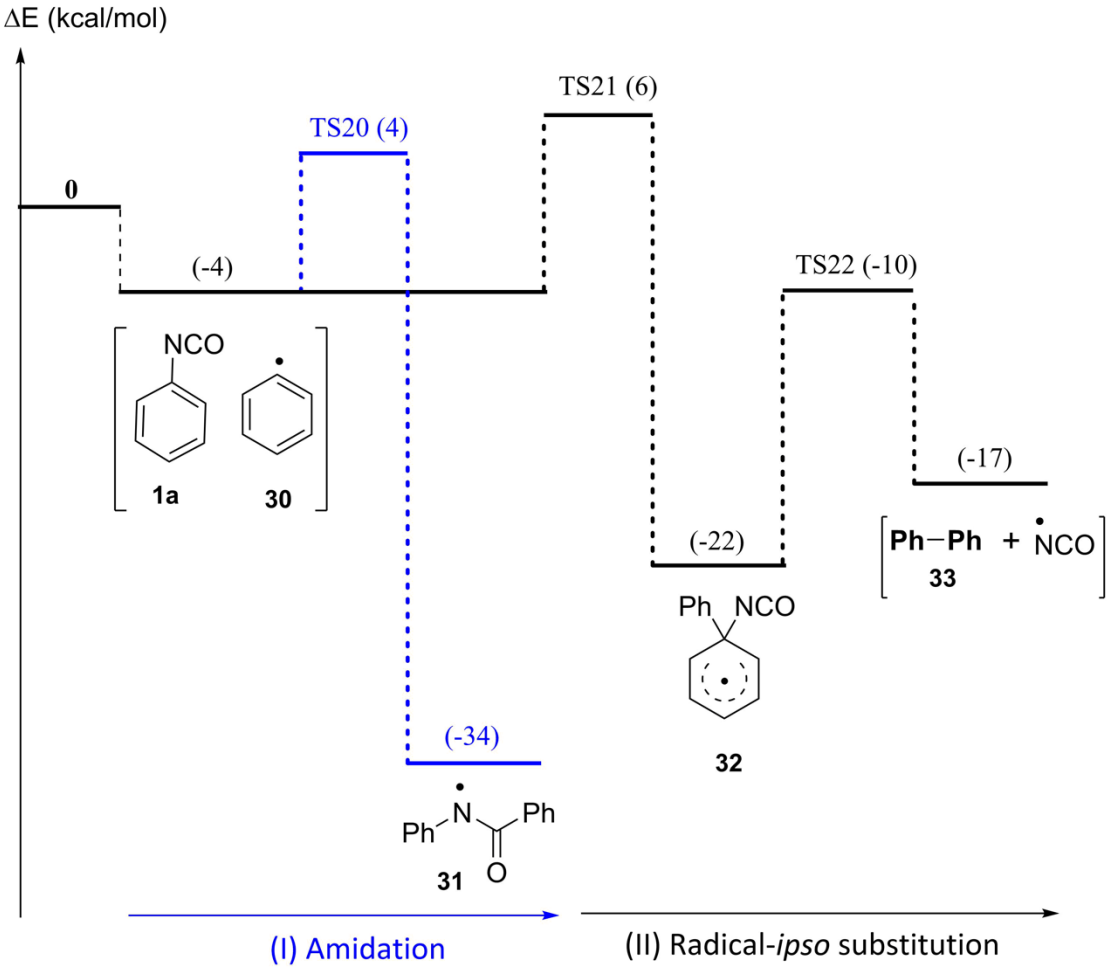


Figure S8: M06-2X calculated potential energy diagram for gas phase reaction of phenyl radical (**30**) with **1a**. (I) amidation (II) radical-ipso substitution. Energies are in kcal/mol and associated complex is shown in square brackets.

Summarized ΔE, ΔG and ΔH for the reactions

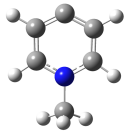
TS / Intermediate	M06-2X/6-31+G(d) - gas phase			ωB97X-D/6-31+G(d) – gas phase		
	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG
1a + γ-NMP	-9	-7	0	-10	-8	0
3a	-29	-28	-16	-32	-30	-19
4a + NCO radical	-25	-23	-12	-27	-25	-16
18a	-41	-39	-27	-46	-43	-31
TS1	-4	-6	7	-5	-5	9
TS2	-16	-15	-3	-17	-16	6
TS3	-2	-1	10	-3	-2	1
1c + γ-NMP	-12	-11	0	-13	-10	-1
20	-27	-25	-13	-30	-29	-18
8a	-46	-45	-33	-48	-46	-36
8	-39	-38	-30	-39	-38	-32
7a	-53	-50	-37	-54	-52	-40
7	-24	-23	-13	-26	-24	-15
TS5	-11	-10	2	-12	-10	0
TS6	-24	-23	-11	-26	-25	-14
TS7	-7	-6	4	-8	-6	3
TS8	-25	-24	-12	-26	-24	-13
TS9	4	5	16	3	3	13
2a + γ-NMP	-11	-11	-3	-12	-10	-2
21	-29	-28	-15	-31	-30	-17
22	-41	-42	-27	-44	-42	-33
9	-24	-23	-12	-26	-26	-16
12 + PhNC	-25	-27	-6	-23	-24	-8
23	-44	-46	-28	-47	-48	-32
TS11	-10	-9	-1	-10	-10	3
TS12	-16	-15	-6	-19	-18	-8
TS13	-4	-4	7	-5	-4	7
TS14	-21	-21	-7	-21	-20	-7
TS15	-1	0	10	-2	-1	9
2c + γ-NMP	-13	-10	-2	-13	-11	-2
14	-54	-51	-40	-56	-53	-41
15 + NCS radical	-41	-38	-30	-44	-43	-36
TS16	-12	-10	1	-13	-11	0
TS17	-33	-31	-19	-33	-32	-19
12 + γ-NMP	-18	-14	-3	-17	-12	-1
16	-23	-22	-8	-25	-21	-8
17 + NCS radical	-10	-9	-1	-13	-11	-4
TS18	-15	-14	-1	-14	-12	-1
TS19	-2	-1	13	-1	-1	14
	M06-2X/6-31+G(d) - acetonitrile					
31	-32	-31	-27			
32	-17	-17	-14			
33 + NCO radical	-15	-14	-12			
TS20	8	7	10			
TS21	10	9	12			
TS22	-8	-9	-5			

Table S1 Calculated energies of the species and transition states for reacting g-NMP radical with iso(thio)cyanates. Energies are in kcal/mol and calculated at M06-2X and ωB97X-D level of theories.

Cartesian coordinates and energies for all DFT calculated structures

The cartesian coordinates and corresponding energies for all optimized ground (including first three analytical frequencies) and transition state structures, including the imaginary frequencies of the transition states at the M06-2X/6-31+G(d) are given below.

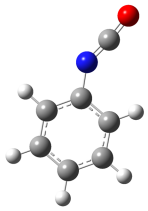
γ-NMP radical



Frequencies 208.81, 380.01, 398.42 cm^{-1}
Zero-point correction= 0.116463 (Hartree/Particle)
Sum of electronic and zero-point Energies= -286.942522
Sum of electronic and thermal Energies= -286.937244
Sum of electronic and thermal Enthalpies= -286.936300
Sum of electronic and thermal Free Energies= -286.972031

C	-0.126788	1.181834	-0.009211
C	-0.126791	-1.181832	-0.009211
C	1.257086	-1.220990	0.003883
C	1.887105	-0.000002	0.008894
C	1.257089	1.220988	0.003883
H	-0.743338	2.078123	-0.013042
H	-0.743343	-2.078120	-0.013042
H	1.783482	-2.172605	0.006701
H	1.783487	2.172602	0.006701
N	-0.786335	0.000002	-0.016951
C	-2.264868	0.000000	0.014269
H	-2.634541	-0.890011	-0.499253
H	-2.603862	-0.000034	1.054749
H	-2.634542	0.890046	-0.499192

1a

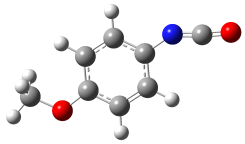


Frequencies 66.73, 82.89, 244.82 cm^{-1}
Zero-point correction= 0.103729 (Hartree/Particle)
Sum of electronic and zero-point Energies= -399.373781
Sum of electronic and thermal Energies= -399.366652
Sum of electronic and thermal Enthalpies= -399.365707
Sum of electronic and thermal Free Energies= -399.406214

C	-0.358622	1.089318	0.000000
C	-1.722970	1.354750	0.000000
C	-2.645324	0.310271	0.000001
C	-2.194396	-1.007544	0.000000
C	-0.832228	-1.285549	0.000000
C	0.085834	-0.235354	0.000000
H	0.367542	1.901269	-0.000001

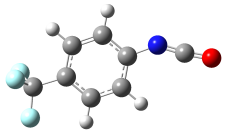
H -2.066133 2.387975 0.000000
H -3.712492 0.523988 0.000001
H -2.908638 -1.829111 0.000001
H -0.462936 -2.309032 0.000000
N 1.444474 -0.543517 -0.000001
C 2.549861 -0.071501 -0.000001
O 3.672301 0.275399 0.000001

1d



Frequencies 10.83, 66.85, 74.68 cm^{-1}
Zero-point correction= 0.135879 (Hartree/Particle)
Sum of electronic and zero-point Energies= -513.807582
Sum of electronic and thermal Energies= -513.797641
Sum of electronic and thermal Enthalpies= -513.796697
Sum of electronic and thermal Free Energies= -513.845241
C -0.570024 -1.076772 -0.000157
C 0.787387 -1.341391 -0.000131
C 1.713700 -0.292099 -0.000113
C 1.261117 1.027475 -0.000141
C -0.107216 1.289374 -0.000134
C -1.027156 0.246877 -0.000117
H -1.288218 -1.895698 -0.000162
H 1.161221 -2.363368 -0.000127
H 1.956965 1.862447 -0.000102
H -0.471011 2.314934 -0.000118
N -2.387610 0.548933 -0.000111
C -3.495298 0.085549 0.000069
O -4.620826 -0.256098 0.000304
O 3.019197 -0.659903 0.000067
C 3.997374 0.353370 0.000280
H 4.963790 -0.156430 0.000515
H 3.922322 0.984613 -0.897694
H 3.921942 0.984686 0.898164

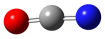
1e



Frequencies 15.39, 47.59, 61.46 cm^{-1}
Zero-point correction= 0.108773 (Hartree/Particle)
Sum of electronic and zero-point Energies= -736.327931
Sum of electronic and thermal Energies= -736.317206
Sum of electronic and thermal Enthalpies= -736.316262
Sum of electronic and thermal Free Energies= -736.367230
C -1.112615 -0.969304 -0.005503
C 0.267613 -1.123526 -0.009906
C 1.091419 -0.002012 -0.011948
C 0.535630 1.277600 -0.006914

C -0.840264 1.438366 -0.003306
C -1.667657 0.312675 -0.002629
H -1.764656 -1.841291 -0.004832
H 0.703097 -2.120186 -0.013311
H 1.186417 2.150774 -0.006724
H -1.292973 2.427254 -0.001634
N -3.043493 0.507899 0.000660
C -4.093642 -0.082382 0.003343
O -5.170679 -0.545142 0.006099
C 2.583102 -0.126237 0.000329
F 2.996884 -1.394278 -0.115124
F 3.145041 0.570837 -1.002517
F 3.108795 0.361020 1.139007

NCO radical



Frequencies 456.91, 1372.03, 2181.03 cm^{-1}
Zero-point correction= 0.009135 (Hartree/Particle)
Sum of electronic and zero-point Energies= -167.909685
Sum of electronic and thermal Energies= -167.906586
Sum of electronic and thermal Enthalpies= -167.905641
Sum of electronic and thermal Free Energies= -167.931764
N 0.965324 0.801280 0.000000
C 0.000000 0.058939 0.000000
O -0.844658 -0.745324 0.000000

OMe radical

Frequencies 970.03, 1151.26, 1345.15 cm^{-1}
Zero-point correction= 0.034798 (Hartree/Particle)
Sum of electronic and zero-point Energies= -114.950169
Sum of electronic and thermal Energies= -114.947252
Sum of electronic and thermal Enthalpies= -114.946308
Sum of electronic and thermal Free Energies= -114.973066
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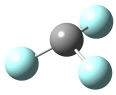
C -0.569671 -0.000155 0.014402
H -0.866836 0.005219 -1.057535
H -1.005736 -0.915565 0.451154
H -1.005319 0.911663 0.459158

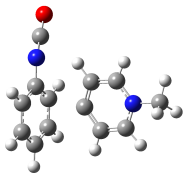
CF_3 radical



Frequencies 510.76, 510.81, 705.34 cm^{-1}
Zero-point correction= 0.012385 (Hartree/Particle)
Sum of electronic and zero-point Energies= -337.451312
Sum of electronic and thermal Energies= -337.447890
Sum of electronic and thermal Enthalpies= -337.446946
Sum of electronic and thermal Free Energies= -337.476961

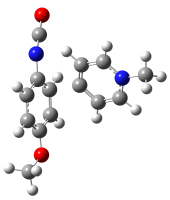
C 0.000000 0.000000 0.328891
F 0.000000 1.253536 -0.073087
F -1.085594 -0.626768 -0.073087
F 1.085594 -0.626768 -0.073087

γ-NMP radical and 1a



Frequencies 18.83, 28.12, 36.92 cm^{-1}
Zero-point correction= 0.220758 (Hartree/Particle)
Sum of electronic and zero-point Energies= -686.330008
Sum of electronic and thermal Energies= -686.314659
Sum of electronic and thermal Enthalpies= -686.313715
Sum of electronic and thermal Free Energies= -686.377614
C 2.089012 -0.527991 1.066000
C 1.903392 -1.894656 1.249654
C 1.715713 -2.735946 0.153295
C 1.718852 -2.204016 -1.135315
C 1.903621 -0.838214 -1.332966
C 2.094543 0.000065 -0.230311
H 2.245236 0.131517 1.919162
H 1.921517 -2.305237 2.257810
H 1.591949 -3.807249 0.301404
H 1.592812 -2.857200 -1.996849
H 1.924718 -0.408351 -2.333146
N 2.242337 1.369093 -0.460177
C 2.649995 2.356083 0.111735
O 2.997924 3.377467 0.559735
C -3.065561 -0.883515 0.396932
C -1.749299 -1.294560 0.313013
C -0.846725 -0.358776 -0.142198
C -1.176552 0.924833 -0.511149
C -2.511723 1.271539 -0.399806
N -3.422886 0.376762 0.047573
H -3.871709 -1.529268 0.739115
H -1.460801 -2.304906 0.596335
H -0.441641 1.643831 -0.872000
H -2.891751 2.256645 -0.659870
C -4.848594 0.752235 0.128927
H -5.253487 0.420686 1.088387
H -4.941204 1.837197 0.055486
H -5.395222 0.279129 -0.692350

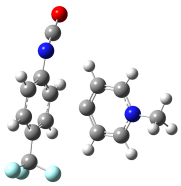
γ-NMP radical and 1d



Frequencies 12.24, 34.94, 36.04 cm^{-1}
Zero-point correction= 0.253616 (Hartree/Particle)
Sum of electronic and zero-point Energies= -800.765295
Sum of electronic and thermal Energies= -800.747496
Sum of electronic and thermal Enthalpies= -800.746552
Sum of electronic and thermal Free Energies= -800.815818

C	1.541149	1.060551	1.104224
C	2.271997	-0.094420	1.308137
C	2.667488	-0.890382	0.220956
C	2.313001	-0.511490	-1.077665
C	1.572789	0.649959	-1.280069
C	1.183273	1.445372	-0.199049
H	1.254197	1.683813	1.950761
H	2.575015	-0.398900	2.308296
H	2.618052	-1.102314	-1.937734
H	1.306908	0.964928	-2.288211
N	0.450131	2.603934	-0.452764
C	0.099780	3.618672	0.105185
O	-0.311052	4.624910	0.537464
C	-2.528398	-1.842942	0.673588
C	-1.237761	-1.358985	0.581382
C	-1.056696	-0.218754	-0.173118
C	-2.077943	0.438976	-0.821874
C	-3.346707	-0.097923	-0.692112
N	-3.551493	-1.214130	0.044477
H	-2.794950	-2.731517	1.242743
H	-0.420530	-1.865479	1.092721
H	-1.917879	1.342899	-1.408098
H	-4.226562	0.337346	-1.160374
C	-4.905612	-1.790486	0.153236
H	-5.124887	-2.002675	1.202859
H	-5.634667	-1.073319	-0.228328
H	-4.955554	-2.712161	-0.434210
O	3.376825	-1.991362	0.531749
C	3.899423	-2.782182	-0.520473
H	4.572385	-2.193580	-1.158732
H	4.463177	-3.585136	-0.042042
H	3.093968	-3.216710	-1.129426

γ-NMP radical and 1e

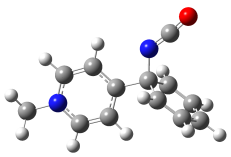


Frequencies 16.18, 25.96, 31.90 cm^{-1}
Zero-point correction= 0.226597 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1023.281355
Sum of electronic and thermal Energies= -1023.262748
Sum of electronic and thermal Enthalpies= -1023.261803
Sum of electronic and thermal Free Energies= -1023.333315

C	-1.300810	1.512830	-0.962686
C	-1.853496	0.243875	-1.052196
C	-2.050452	-0.518753	0.100972

C	-1.703101	-0.005636	1.348597
C	-1.148251	1.266134	1.445091
C	-0.945105	2.027786	0.291365
H	-1.153724	2.115021	-1.858168
H	-2.143149	-0.154071	-2.024012
H	-1.875700	-0.589955	2.249747
H	-0.886135	1.690880	2.412266
N	-0.361184	3.281171	0.427727
C	-0.175400	4.290178	-0.216686
O	0.073148	5.305783	-0.735023
C	2.717846	-1.969422	-0.423916
C	1.429682	-1.473964	-0.350583
C	1.307278	-0.182637	0.111693
C	2.356820	0.617588	0.495948
C	3.618931	0.057740	0.392497
N	3.778259	-1.207113	-0.059816
H	2.949746	-2.975241	-0.768448
H	0.575225	-2.084605	-0.639233
H	2.231572	1.633499	0.866399
H	4.526141	0.592314	0.663748
C	5.128394	-1.800513	-0.141034
H	5.265312	-2.248861	-1.128541
H	5.876208	-1.019407	0.006201
H	5.236367	-2.563290	0.635768
C	-2.586779	-1.910342	-0.046699
F	-2.962303	-2.447885	1.112426
F	-1.628393	-2.728864	-0.564131
F	-3.618184	-1.966600	-0.888862

3a

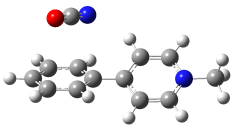


Frequencies 38.00, 41.28, 53.09 cm^{-1}
Zero-point correction= 0.222097 (Hartree/Particle)
Sum of electronic and zero-point Energies= -686.361285
Sum of electronic and thermal Energies= -686.347208
Sum of electronic and thermal Enthalpies= -686.346264
Sum of electronic and thermal Free Energies= -686.404440

C	-1.396131	0.558107	1.257794
C	-2.247222	1.622648	1.232717
C	-2.693017	2.186650	0.013386
C	-2.253802	1.635066	-1.214164
C	-1.402024	0.571571	-1.254875
C	-0.915697	-0.117025	-0.003522
H	-1.071825	0.106234	2.195534
H	-2.602466	2.037849	2.174615
H	-3.380201	3.029056	0.019452
H	-2.614312	2.059629	-2.149874
H	-1.082791	0.129552	-2.199006
N	-1.349148	-1.522207	-0.009601
C	-2.473290	-1.994001	-0.011701
O	-3.493951	-2.555571	-0.013932

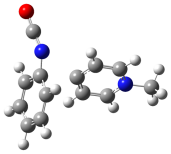
C 2.666394 1.114235 -0.007929
C 1.292409 1.101536 -0.016045
C 0.606382 -0.119942 -0.002885
C 1.355481 -1.295776 0.016781
C 2.732982 -1.230527 0.024263
N 3.372390 -0.042248 0.013467
H 3.250565 2.031065 -0.017627
H 0.747563 2.044392 -0.029649
H 0.856255 -2.260989 0.028483
H 3.362051 -2.117043 0.038186
C 4.844949 0.011381 -0.018293
H 5.188097 0.834332 0.613285
H 5.248695 -0.927682 0.365560
H 5.182805 0.165830 -1.047729

4a + NCO radical



Frequencies 36.59, 52.63, 73.46 cm^{-1}
Zero-point correction= 0.222395 (Hartree/Particle)
Sum of electronic and zero-point Energies= -686.353957
Sum of electronic and thermal Energies= -686.339466
Sum of electronic and thermal Enthalpies= -686.338522
Sum of electronic and thermal Free Energies= -686.397088
C 1.433848 -0.066506 1.333054
C 2.803466 -0.309335 1.445776
C 3.451492 -1.086488 0.493720
C 2.728353 -1.638149 -0.567095
C 1.355328 -1.430704 -0.665176
C 0.689951 -0.644546 0.281189
H 0.930181 0.514081 2.103356
H 3.356804 0.124217 2.275587
H 4.522379 -1.261410 0.568813
H 3.239118 -2.226477 -1.325983
H 0.814340 -1.846945 -1.513984
N 1.456099 2.263606 0.112944
C 2.221326 1.896588 -0.775732
O 2.949428 1.531933 -1.627615
C -2.967395 -1.128075 -0.449522
C -1.618208 -1.375237 -0.352753
C -0.750525 -0.403608 0.173469
C -1.328328 0.810943 0.589734
C -2.681989 1.007965 0.470179
N -3.490658 0.049356 -0.042092
H -3.669344 -1.858660 -0.842805
H -1.247367 -2.348448 -0.664253
H -0.705616 1.625197 0.953436
H -3.168660 1.935945 0.761462
C -4.931370 0.322513 -0.172993
H -5.319611 0.686945 0.782086
H -5.090310 1.075376 -0.951179
H -5.451119 -0.598184 -0.444674

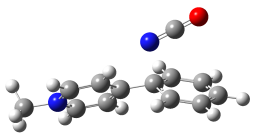
TS1 for 1a



Imaginary Vibrational Frequency = -398.2298 cm^{-1}
Zero-point correction= 0.220015 (Hartree/Particle)
Sum of electronic and zero-point Energies= -686.323181
Sum of electronic and thermal Energies= -686.308848
Sum of electronic and thermal Enthalpies= -686.307904
Sum of electronic and thermal Free Energies= -686.367073

C	-2.060943	-0.580764	-0.959687
C	-2.105716	-1.957914	-1.038064
C	-1.812755	-2.748992	0.083451
C	-1.503804	-2.144390	1.305443
C	-1.459538	-0.765925	1.411911
C	-1.648582	0.043619	0.253563
H	-2.315101	0.041742	-1.817247
H	-2.403832	-2.431595	-1.971802
H	-1.868154	-3.833028	0.011048
H	-1.330743	-2.756732	2.187885
H	-1.266936	-0.269319	2.361790
N	-1.850264	1.411375	0.465150
C	-2.344991	2.341025	-0.137997
O	-2.787004	3.308059	-0.615976
C	2.568669	-0.737762	-0.862651
C	1.187592	-0.746932	-0.898764
C	0.505674	0.172981	-0.120511
C	1.187220	1.072511	0.687224
C	2.564963	1.039836	0.684465
N	3.235025	0.144599	-0.083695
H	3.182683	-1.415148	-1.451819
H	0.671862	-1.461026	-1.540217
H	0.662870	1.799782	1.307505
H	3.183162	1.713308	1.275320
C	4.708169	0.160936	-0.063456
H	5.086240	-0.649429	-0.689315
H	5.067846	1.118196	-0.452280
H	5.059784	0.019324	0.962336

TS2 for 1a

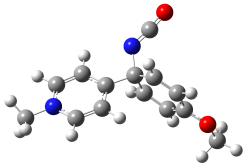


Imaginary Vibrational Frequency = -458.4178 cm-1
Zero-point correction= 0.221334 (Hartree/Particle)
Sum of electronic and zero-point Energies= -686.341106
Sum of electronic and thermal Energies= -686.327182
Sum of electronic and thermal Enthalpies= -686.326238
Sum of electronic and thermal Free Energies= -686.383643

C	1.368815	-0.275935	1.376284
C	2.624539	-0.809011	1.559517

C	3.304521	-1.404752	0.487133
C	2.697685	-1.492343	-0.777542
C	1.438307	-0.979555	-0.979293
C	0.767767	-0.251918	0.066846
H	0.833089	0.177350	2.209373
H	3.086507	-0.775435	2.543595
H	4.301173	-1.813973	0.637842
H	3.224032	-1.973617	-1.598696
H	0.975038	-1.020960	-1.964765
N	1.079427	1.595720	-0.475774
C	2.277837	1.832010	-0.600942
O	3.417931	2.082994	-0.727655
C	-2.865585	-1.041100	-0.582300
C	-1.490164	-1.137773	-0.585763
C	-0.716222	-0.146576	0.024722
C	-1.388495	0.919686	0.639506
C	-2.760816	0.967227	0.621798
N	-3.486043	-0.003014	0.015245
H	-3.506950	-1.784231	-1.048788
H	-1.027157	-2.001330	-1.057273
H	-0.827939	1.733129	1.093152
H	-3.327678	1.777579	1.073223
C	-4.954266	0.113108	-0.032566
H	-5.390159	-0.876470	-0.185130
H	-5.314536	0.521061	0.914860
H	-5.240791	0.774628	-0.856051

3d

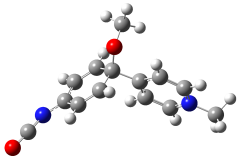


Frequencies 21.79, 40.10, 42.44 cm^{-1}
Zero-point correction= 0.255202 (Hartree/Particle)
Sum of electronic and zero-point Energies= -800.800068
Sum of electronic and thermal Energies= -800.783494
Sum of electronic and thermal Enthalpies= -800.782550
Sum of electronic and thermal Free Energies= -800.846560

C	0.969211	0.322331	1.396845
C	2.069060	-0.464553	1.388011
C	2.598443	-1.000550	0.174628
C	1.988243	-0.676295	-1.053145
C	0.891277	0.144334	-1.096201
C	0.258215	0.733816	0.136281
H	0.584209	0.742643	2.326168
H	2.591512	-0.705494	2.312672
H	2.396278	-1.052107	-1.989209
H	0.440123	0.426004	-2.047794
N	0.208656	2.202195	0.034918
C	1.114225	3.017091	0.009678
O	1.895219	3.882137	-0.020467
C	-2.801826	-1.476444	0.553197
C	-1.511317	-1.010638	0.642297
C	-1.181878	0.242520	0.111868

C	-2.196906	0.979614	-0.510396
C	-3.470472	0.466961	-0.580987
N	-3.766636	-0.744192	-0.051688
H	-3.110509	-2.436602	0.958314
H	-0.755184	-1.621707	1.131957
H	-1.987417	1.966627	-0.916045
H	-4.296108	0.999743	-1.046812
C	-5.134041	-1.274723	-0.175337
H	-5.299248	-2.030257	0.595601
H	-5.850887	-0.461589	-0.037494
H	-5.266825	-1.723022	-1.165124
O	3.676924	-1.777293	0.319162
C	4.311416	-2.304574	-0.836876
H	4.665830	-1.495888	-1.489263
H	5.164149	-2.880586	-0.474655
H	3.630915	-2.965875	-1.389662

5d

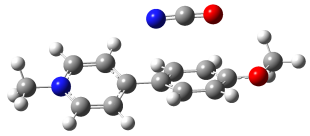


Frequencies 1.98, 31.27, 67.13 cm^{-1}
Zero-point correction= 0.255061 (Hartree/Particle)
Sum of electronic and zero-point Energies= -800.798648
Sum of electronic and thermal Energies= -800.782059
Sum of electronic and thermal Enthalpies= -800.781115
Sum of electronic and thermal Free Energies= -800.847129

C	2.001296	-0.129622	-1.038857
C	0.782341	0.441863	-1.218338
C	0.009528	1.099044	-0.107830
C	0.770940	1.104691	1.188137
C	2.000773	0.547265	1.321006
C	2.640930	-0.103445	0.229638
H	2.517957	-0.586409	-1.882592
H	0.314638	0.473646	-2.202355
H	0.297595	1.580961	2.046996
H	2.529593	0.586730	2.272085
N	3.872165	-0.664521	0.438930
C	4.760349	-1.258481	-0.133397
O	5.673694	-1.835857	-0.574127
C	-3.450341	-0.292661	-0.861661
C	-2.333686	0.505532	-0.894383
C	-1.276432	0.271431	-0.002176
C	-1.409326	-0.787531	0.901825
C	-2.551611	-1.557461	0.898697
N	-3.554227	-1.312159	0.027017
H	-4.298535	-0.153627	-1.528125
H	-2.274397	1.324610	-1.607978
H	-0.615570	-1.016075	1.611169
H	-2.703012	-2.384726	1.587073
C	-4.774294	-2.136453	0.026545
H	-4.907821	-2.587623	-0.960979
H	-4.675596	-2.925623	0.774105

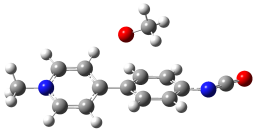
H -5.637912 -1.510780 0.270692
O -0.317058 2.397149 -0.587152
C -0.906948 3.285405 0.345157
H -0.172731 3.657287 1.072044
H -1.284677 4.131624 -0.234306
H -1.749293 2.818973 0.884589

4d and NCO radical



Frequencies 29.83, 47.79, 55.04 cm^{-1}
Zero-point correction= 0.254488 (Hartree/Particle)
Sum of electronic and zero-point Energies= -800.798118
Sum of electronic and thermal Energies= -800.780874
Sum of electronic and thermal Enthalpies= -800.779930
Sum of electronic and thermal Free Energies= -800.844878
C 0.732813 -1.123129 0.960352
C 2.099130 -1.234252 0.984791
C 2.871500 -0.731190 -0.088707
C 2.229944 -0.158056 -1.204804
C 0.857430 -0.039699 -1.208087
C 0.073431 -0.492427 -0.122012
H 0.162840 -1.461995 1.823662
H 2.623738 -1.671981 1.830730
H 2.804132 0.205505 -2.052282
H 0.374756 0.404033 -2.077428
N 0.121008 2.082476 0.813826
C 1.329789 2.020316 0.958999
O 2.506774 1.903794 1.071121
C -3.577060 -1.112966 0.529634
C -2.211043 -1.268182 0.542653
C -1.379833 -0.361855 -0.138589
C -2.021247 0.685201 -0.830330
C -3.386645 0.796000 -0.812846
N -4.157743 -0.092335 -0.138154
H -4.246639 -1.798639 1.041784
H -1.797107 -2.120808 1.074250
H -1.446986 1.459234 -1.330603
H -3.916242 1.603016 -1.313560
C -5.619174 0.072961 -0.150069
H -6.069737 -0.652181 0.530222
H -5.872054 1.083644 0.182885
H -5.999862 -0.091214 -1.162779
O 4.180392 -0.848239 0.048543
C 5.049900 -0.232525 -0.899429
H 4.852802 0.846051 -0.947882
H 6.060067 -0.406855 -0.527494
H 4.936509 -0.694411 -1.887858

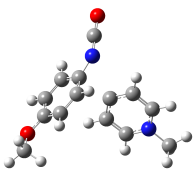
6 and OMe radical



Frequencies 29.11, 44.80, 52.61 cm^{-1}
Zero-point correction= 0.252282 (Hartree/Particle)
Sum of electronic and zero-point Energies= -800.799288
Sum of electronic and thermal Energies= -800.782228
Sum of electronic and thermal Enthalpies= -800.781284
Sum of electronic and thermal Free Energies= -800.846771

C	2.136849	0.022653	-0.992071
C	0.758012	0.113871	-1.034662
C	-0.037719	-0.424769	-0.007112
C	0.604707	-1.042340	1.079164
C	1.983666	-1.114902	1.143339
C	2.761797	-0.591580	0.101791
H	2.739344	0.420581	-1.806939
H	0.293107	0.580555	-1.901386
H	0.022541	-1.435762	1.911155
H	2.483953	-1.577955	1.990763
N	4.132628	-0.702200	0.197541
C	5.134957	-0.425378	-0.424933
O	6.164502	-0.210110	-0.927490
C	-3.522156	0.710948	-0.833717
C	-2.153400	0.678930	-0.770621
C	-1.492409	-0.355175	-0.077270
C	-2.310698	-1.323367	0.534167
C	-3.679106	-1.246188	0.442026
N	-4.279132	-0.241224	-0.235242
H	-4.066937	1.499655	-1.347235
H	-1.593622	1.494101	-1.219290
H	-1.878703	-2.169040	1.062913
H	-4.337524	-1.985427	0.890469
C	-5.743271	-0.181991	-0.359110
H	-6.037534	-0.451941	-1.378191
H	-6.194059	-0.880684	0.348444
H	-6.085621	0.830773	-0.129760
O	-0.073535	2.331515	0.560247
C	1.049404	2.664374	1.252916
H	1.916591	2.897924	0.613999
H	0.793044	3.586312	1.818526
H	1.299412	1.913124	2.024953

TS1 for 1d at C-NCO site

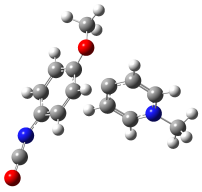


Imaginary Vibrational Frequency = -299.3538 cm^{-1}
Zero-point correction= 0.252842 (Hartree/Particle)
Thermal correction to Energy= 0.269732
Thermal correction to Enthalpy= 0.270677

Thermal correction to Gibbs Free Energy= 0.205583
Sum of electronic and zero-point Energies= -800.762228
Sum of electronic and thermal Energies= -800.745338
Sum of electronic and thermal Enthalpies= -800.744394
Sum of electronic and thermal Free Energies= -800.809487

C	-1.484775	1.086817	-1.037410
C	-2.292354	-0.004187	-1.228319
C	-2.573391	-0.887831	-0.160982
C	-2.032029	-0.641918	1.110111
C	-1.216821	0.458192	1.307394
C	-0.855290	1.301210	0.224520
H	-1.295941	1.787949	-1.849766
H	-2.767977	-0.193308	-2.188911
H	-2.275399	-1.283183	1.953332
H	-0.825204	0.692657	2.296030
N	-0.266073	2.527559	0.541661
C	-0.090392	3.605598	0.016213
O	0.140346	4.678548	-0.380754
C	2.281692	-1.705288	-0.853740
C	1.135820	-0.941242	-0.927415
C	1.065730	0.221668	-0.171818
C	2.115381	0.588229	0.657420
C	3.241603	-0.208172	0.692635
N	3.314936	-1.332737	-0.059308
H	2.430450	-2.621287	-1.422768
H	0.325816	-1.252488	-1.587841
H	2.077865	1.492937	1.265595
H	4.115597	0.020934	1.298430
C	4.513089	-2.186962	-0.006551
H	4.815291	-2.449407	-1.023869
H	5.325434	-1.641991	0.478299
H	4.291748	-3.095130	0.562451
O	-3.381347	-1.910030	-0.460438
C	-3.797789	-2.787755	0.575186
H	-4.338752	-2.239851	1.357740
H	-4.469160	-3.508158	0.105460
H	-2.939275	-3.316547	1.010749

TS1 for 1d at C-OMe site

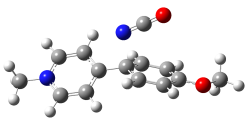


Imaginary Vibrational Frequency = -270.6437 cm^{-1}
Zero-point correction= 0.252875 (Hartree/Particle)
Sum of electronic and zero-point Energies= -800.764570
Sum of electronic and thermal Energies= -800.747747
Sum of electronic and thermal Enthalpies= -800.746803
Sum of electronic and thermal Free Energies= -800.811972

C	-1.855766	0.104053	1.102249
C	-0.856406	1.023669	1.321983
C	-0.348535	1.814233	0.251670
C	-0.981292	1.726537	-1.019047

C -1.975923 0.793258 -1.226439
C -2.422238 -0.030532 -0.179435
H -2.228958 -0.505820 1.923575
H -0.427156 1.172797 2.311644
H -0.665776 2.368219 -1.837905
H -2.451613 0.699200 -2.200787
N -3.423555 -0.941183 -0.446304
C -4.114830 -1.768290 0.104821
O -4.828213 -2.591706 0.523791
C 3.323126 -0.562743 0.697625
C 2.399746 0.458565 0.635492
C 1.308888 0.320322 -0.213508
C 1.147488 -0.830251 -0.970299
C 2.096523 -1.828672 -0.866900
N 3.162888 -1.685723 -0.046523
H 4.212620 -0.535167 1.324768
H 2.536809 1.351375 1.246973
H 0.303405 -0.963719 -1.648089
H 2.049286 -2.757183 -1.431666
C 4.182686 -2.744051 0.048826
H 4.276320 -3.066448 1.089647
H 3.880994 -3.594506 -0.565393
H 5.142024 -2.359755 -0.310325
O 0.462637 2.820976 0.629363
C 0.999300 3.664028 -0.376597
H 0.208305 4.234092 -0.880410
H 1.669205 4.357698 0.135005
H 1.566724 3.077348 -1.116080

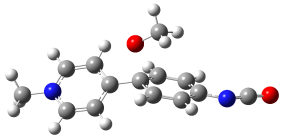
TS2 for 1d – NCO radical removal



Imaginary Vibrational Frequency = -421.9156 cm^{-1}
Zero-point correction= 0.254273 (Hartree/Particle)
Sum of electronic and zero-point Energies= -800.785600
Sum of electronic and thermal Energies= -800.769066
Sum of electronic and thermal Enthalpies= -800.768122
Sum of electronic and thermal Free Energies= -800.831560
C 0.801506 -0.380152 1.313918
C 2.114809 -0.742201 1.296826
C 2.833212 -0.791881 0.073178
C 2.176884 -0.492598 -1.138544
C 0.856029 -0.115070 -1.121645
C 0.136025 0.069345 0.113238
H 0.266425 -0.315902 2.260787
H 2.647283 -1.003145 2.208761
H 2.696575 -0.570322 -2.089643
H 0.346107 0.098625 -2.060084
N 0.129263 1.987590 0.295887
C 1.252423 2.434861 0.490060
O 2.327360 2.877304 0.677298
C -3.399022 -1.121401 0.695668
C -2.029990 -1.002382 0.806216

C	-1.340352	-0.063013	0.033465
C	-2.093235	0.729480	-0.849364
C	-3.452800	0.567247	-0.929017
N	-4.096075	-0.348353	-0.162328
H	-3.972933	-1.834592	1.281099
H	-1.503895	-1.659968	1.493860
H	-1.610559	1.508642	-1.433541
H	-4.081543	1.165609	-1.584175
C	-5.559962	-0.464644	-0.268744
H	-5.901330	-1.298358	0.347620
H	-6.024144	0.462367	0.081059
H	-5.834098	-0.649614	-1.311189
O	4.104695	-1.149702	0.177190
C	4.930782	-1.187233	-0.983635
H	4.994364	-0.192336	-1.441195
H	5.916591	-1.495015	-0.633345
H	4.551366	-1.920926	-1.705698

TS2 for 1d – OMe radical removal



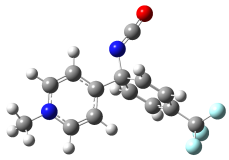
Imaginary Vibrational Frequency = -555.7106 cm^{-1}

Zero-point correction=	0.253202 (Hartree/Particle)
Sum of electronic and zero-point Energies=	-800.782160
Sum of electronic and thermal Energies=	-800.765436
Sum of electronic and thermal Enthalpies=	-800.764492
Sum of electronic and thermal Free Energies=	-800.828431

C	2.069299	-0.407106	-0.751316
C	0.708425	-0.324320	-0.901360
C	-0.119134	0.262412	0.117311
C	0.516316	0.574422	1.366132
C	1.877278	0.499738	1.507661
C	2.677080	0.011682	0.452085
H	2.686533	-0.816608	-1.549605
H	0.245041	-0.674245	-1.822542
H	-0.088866	0.977297	2.177749
H	2.364994	0.801223	2.432148
N	4.034048	-0.055147	0.645672
C	5.049519	-0.375983	0.064514
O	6.087415	-0.650580	-0.388239
C	-3.650280	-0.353947	-1.039392
C	-2.325104	0.001471	-1.052379
C	-1.554182	-0.106493	0.117534
C	-2.189383	-0.596518	1.263893
C	-3.524121	-0.936653	1.226807
N	-4.241359	-0.814282	0.090443
H	-4.290791	-0.276851	-1.914560
H	-1.891597	0.410523	-1.960550
H	-1.644598	-0.730853	2.194839
H	-4.054336	-1.319981	2.094560
C	-5.659746	-1.206561	0.049267
H	-5.761568	-2.158478	-0.480985
H	-6.035751	-1.312972	1.068669

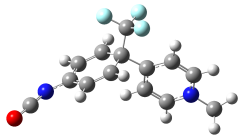
H -6.232692 -0.430466 -0.464926
O -0.480481 1.944606 -0.642114
C 0.611502 2.803503 -0.643268
H 1.488639 2.375714 -1.160084
H 0.299615 3.690949 -1.216590
H 0.904340 3.136330 0.365572

3e



Frequencies 20.18, 25.74, 35.79 cm^{-1}
Zero-point correction= 0.227687 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1023.308328
Sum of electronic and thermal Energies= -1023.290719
Sum of electronic and thermal Enthalpies= -1023.289775
Sum of electronic and thermal Free Energies= -1023.357766
C 0.397216 -0.557390 -1.233723
C 1.606139 0.060701 -1.198497
C 2.232975 0.381330 0.034409
C 1.618311 0.031010 1.257627
C 0.402276 -0.584787 1.278898
C -0.346315 -0.949116 0.020360
H -0.075986 -0.830571 -2.176829
H 2.117891 0.303404 -2.129300
H 2.130780 0.244226 2.193916
H -0.066089 -0.881490 2.217298
N -0.629413 -2.384585 0.004980
C 0.122647 -3.344694 0.007197
O 0.735312 -4.334339 0.008126
C -2.914383 1.840461 0.061141
C -1.712061 1.174143 0.081127
C -1.689017 -0.224094 0.017222
C -2.904910 -0.902039 -0.065303
C -4.084851 -0.187220 -0.083645
N -4.082881 1.160746 -0.021549
H -2.990441 2.923631 0.109167
H -0.788321 1.747512 0.142052
H -2.923727 -1.987602 -0.117385
H -5.059560 -0.664608 -0.149062
C -5.358150 1.900541 0.003486
H -5.226209 2.861986 -0.497976
H -6.120805 1.323267 -0.523369
H -5.665089 2.061869 1.041506
C 3.528626 1.134202 -0.009889
F 4.109664 1.216005 1.186611
F 3.318705 2.388012 -0.450335
F 4.391641 0.562837 -0.856443

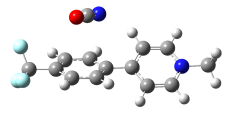
5e



Frequencies 21.19, 26.80, 60.36 cm^{-1}
Zero-point correction= 0.228378 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1023.314909
Sum of electronic and thermal Energies= -1023.297610
Sum of electronic and thermal Enthalpies= -1023.296666
Sum of electronic and thermal Free Energies= -1023.362435

C	-2.029765	0.310814	-0.995229
C	-0.810055	-0.275604	-1.112900
C	-0.009455	-0.729729	0.087440
C	-0.722495	-0.460209	1.392634
C	-1.951593	0.109166	1.448952
C	-2.639177	0.517820	0.272593
H	-2.565862	0.617189	-1.893308
H	-0.366055	-0.443032	-2.093800
H	-0.216182	-0.781990	2.302592
H	-2.442458	0.261824	2.408801
N	-3.873198	1.094642	0.405648
C	-4.799547	1.543433	-0.233496
O	-5.744359	2.002903	-0.741533
C	3.629038	0.347350	-0.553814
C	2.502487	-0.447709	-0.521454
C	1.315706	0.038845	0.039069
C	1.330542	1.353561	0.529015
C	2.477552	2.107266	0.471878
N	3.615180	1.602119	-0.060196
H	4.572544	-0.000562	-0.966340
H	2.575939	-1.451119	-0.928634
H	0.433337	1.788049	0.965994
H	2.534944	3.126400	0.846763
C	4.820438	2.448854	-0.112070
H	4.683351	3.231038	-0.864926
H	4.985469	2.900208	0.869929
H	5.683164	1.834181	-0.375585
C	0.216801	-2.252384	-0.007134
F	1.054732	-2.670460	0.952649
F	0.751966	-2.610260	-1.187736
F	-0.928927	-2.902788	0.125053

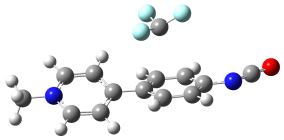
4e and NCO radical



Frequencies 24.97, 36.44, 46.43 cm^{-1}
Zero-point correction= 0.226884 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1023.299620
Sum of electronic and thermal Energies= -1023.281316
Sum of electronic and thermal Enthalpies= -1023.280371
Sum of electronic and thermal Free Energies= -1023.349105

C	-0.272849	0.122318	-1.188893
C	-1.662320	0.055221	-1.211845
C	-2.344093	-0.514139	-0.140934
C	-1.645274	-1.030820	0.948690
C	-0.253879	-0.996314	0.957285
C	0.447850	-0.422452	-0.105534
H	0.252963	0.544532	-2.042685
H	-2.214421	0.455080	-2.060772
H	-2.186328	-1.457059	1.789977
H	0.279158	-1.382791	1.824755
N	0.055772	2.569975	-0.220212
C	-0.746804	2.440953	0.703719
O	-1.507589	2.304330	1.591154
C	4.049162	-1.340816	0.465997
C	2.675242	-1.405761	0.469837
C	1.913939	-0.368098	-0.091669
C	2.614686	0.719887	-0.641887
C	3.988862	0.736800	-0.616830
N	4.694172	-0.282496	-0.072981
H	4.674365	-2.127394	0.880273
H	2.197762	-2.289897	0.885281
H	2.080863	1.579312	-1.043057
H	4.572207	1.563290	-1.015401
C	6.164758	-0.204019	-0.029080
H	6.576724	-1.207517	0.096243
H	6.531757	0.219046	-0.967384
H	6.471551	0.427839	0.810338
C	-3.850696	-0.532701	-0.187785
F	-4.377055	-1.189585	0.844929
F	-4.277291	-1.117737	-1.312889
F	-4.334210	0.714901	-0.178803

6 and CF_3 radical

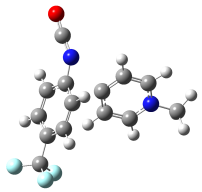


Frequencies 21.38, 31.61, 37.61 cm^{-1}
Zero-point correction= 0.226927 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1023.296517
Sum of electronic and thermal Energies= -1023.277531
Sum of electronic and thermal Enthalpies= -1023.276587
Sum of electronic and thermal Free Energies= -1023.348800

C	1.988701	-0.861808	-1.030038
C	0.610646	-0.786305	-1.108088
C	-0.184370	-0.807685	0.051071
C	0.456082	-0.910521	1.299432
C	1.833954	-0.966175	1.388459
C	2.612876	-0.945263	0.223932
H	2.592335	-0.861857	-1.935977
H	0.147228	-0.737062	-2.092531
H	-0.125998	-0.889627	2.219839
H	2.333049	-1.020817	2.353121
N	3.980839	-1.010944	0.359080
C	4.988301	-1.025130	-0.314943

O	6.021371	-1.047047	-0.853058
C	-3.624730	0.107941	-1.154091
C	-2.257021	-0.001315	-1.097353
C	-1.632842	-0.686753	-0.036716
C	-2.487544	-1.237437	0.940959
C	-3.848055	-1.101828	0.837915
N	-4.412789	-0.435739	-0.198609
H	-4.133505	0.640088	-1.953566
H	-1.672121	0.487400	-1.872677
H	-2.088405	-1.806189	1.776641
H	-4.538310	-1.524018	1.564743
C	-5.878269	-0.327748	-0.270308
H	-6.312770	-1.323644	-0.400748
H	-6.256568	0.125611	0.650427
H	-6.152332	0.300263	-1.120093
C	0.846323	2.178774	0.246827
F	-0.168213	2.378223	1.067876
F	0.522997	2.527801	-0.983680
F	1.924746	2.798478	0.654652

TS1 for 1e at C-NCO

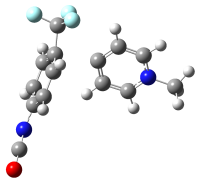


Imaginary Vibrational Frequency = -447.1496 cm^{-1}
Zero-point correction= 0.225112 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1023.271110
Sum of electronic and thermal Energies= -1023.253392
Sum of electronic and thermal Enthalpies= -1023.252448
Sum of electronic and thermal Free Energies= -1023.319674

C	-0.677576	1.613105	-0.926732
C	-1.780239	0.792688	-0.984154
C	-2.195738	0.079857	0.154371
C	-1.537999	0.243861	1.375360
C	-0.432253	1.069710	1.456208
C	0.089568	1.679524	0.276516
H	-0.355893	2.184805	-1.796370
H	-2.347041	0.706591	-1.910353
H	-1.907263	-0.258414	2.266291
H	0.081071	1.245770	2.399836
N	1.057839	2.669416	0.455879
C	1.454050	3.641791	-0.155577
O	1.918815	4.591716	-0.642644
C	1.904886	-2.234190	-0.670141
C	1.037624	-1.161644	-0.692271
C	1.451245	0.022745	-0.101796
C	2.689755	0.129750	0.506145
C	3.520061	-0.974721	0.495060
N	3.123920	-2.129821	-0.087586
H	1.671327	-3.200310	-1.113475
H	0.064564	-1.271209	-1.172709
H	3.022427	1.054187	0.978334

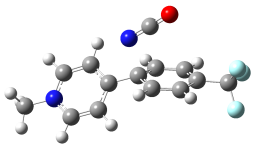
H 4.513795 -0.975766 0.937049
C 4.006455 -3.310989 -0.076583
H 4.053518 -3.736330 -1.082444
H 5.009026 -3.009583 0.232419
H 3.613862 -4.052925 0.625317
C -3.319474 -0.903742 0.001957
F -3.783233 -1.336769 1.172861
F -2.880717 -1.982692 -0.682953
F -4.338232 -0.391806 -0.690600

TS1 for 1e at C-CF_3



Imaginary Vibrational Frequency = -284.8765 cm^{-1}
Zero-point correction= 0.225945 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1023.276266
Sum of electronic and thermal Energies= -1023.258700
Sum of electronic and thermal Enthalpies= -1023.257756
Sum of electronic and thermal Free Energies= -1023.325167
C 2.070228 -0.061465 -1.001349
C 1.018072 0.823057 -1.108817
C 0.398925 1.345734 0.056474
C 0.989559 1.081584 1.318431
C 2.044457 0.202532 1.421347
C 2.591305 -0.385994 0.264842
H 2.524601 -0.485920 -1.895288
H 0.639692 1.107005 -2.089269
H 0.589945 1.568038 2.207297
H 2.496701 -0.022428 2.385108
N 3.646401 -1.255243 0.421493
C 4.424086 -1.910400 -0.239754
O 5.217339 -2.583541 -0.764069
C -3.484518 -0.918715 -0.585528
C -2.583854 0.128755 -0.543269
C -1.382160 -0.071469 0.116635
C -1.080414 -1.288616 0.703819
C -2.016002 -2.299924 0.630651
N -3.196503 -2.105152 -0.004067
H -4.455313 -0.842884 -1.070103
H -2.848130 1.075785 -1.009410
H -0.138551 -1.461603 1.225627
H -1.869797 -3.284887 1.070147
C -4.156640 -3.221914 -0.075400
H -3.779461 -3.982372 -0.765784
H -4.285699 -3.652489 0.921121
H -5.118174 -2.848851 -0.432879
C -0.442659 2.591048 -0.061889
F -1.347416 2.680713 0.922598
F -1.109058 2.636063 -1.228019
F 0.323255 3.680425 0.000723

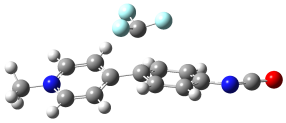
TS2 for 1e – NCO radical removal



Imaginary Vibrational Frequency = -36.4295 cm^{-1}
Zero-point correction= 0.225944 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1023.286277
Sum of electronic and thermal Energies= -1023.269463
Sum of electronic and thermal Enthalpies= -1023.268519
Sum of electronic and thermal Free Energies= -1023.333587

C	-0.338857	-0.221596	-1.202356
C	-1.685946	-0.469335	-1.130890
C	-2.341556	-0.457772	0.114894
C	-1.631823	-0.207675	1.293830
C	-0.279718	0.055276	1.237895
C	0.400652	0.149625	-0.025214
H	0.167671	-0.204158	-2.166610
H	-2.252719	-0.684299	-2.035183
H	-2.142171	-0.233047	2.253251
H	0.280598	0.234931	2.154281
N	0.524293	2.098179	-0.241973
C	-0.586883	2.608610	-0.372040
O	-1.634732	3.119743	-0.499379
C	3.813089	-1.312474	-0.701017
C	2.450291	-1.100802	-0.752255
C	1.874058	-0.067585	-0.009270
C	2.720944	0.717086	0.786709
C	4.070283	0.462191	0.808249
N	4.604487	-0.539709	0.068745
H	4.304467	-2.100490	-1.265369
H	1.842461	-1.758324	-1.369276
H	2.322740	1.555572	1.352407
H	4.772279	1.047782	1.397029
C	6.063528	-0.748994	0.099216
H	6.307381	-1.672014	-0.429903
H	6.560280	0.094832	-0.389103
H	6.395400	-0.828297	1.137856
C	-3.818020	-0.758830	0.132668
F	-4.332485	-0.693809	1.359038
F	-4.042055	-1.989926	-0.346533
F	-4.480460	0.100341	-0.646253

TS2 for 1e – CF_3 radical removal



Imaginary Vibrational Frequency = -454.846 cm^{-1}
Zero-point correction= 0.225914 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1023.281708
Sum of electronic and thermal Energies= -1023.263735
Sum of electronic and thermal Enthalpies= -1023.262791

Sum of electronic and thermal Free Energies= -1023.331355

C	2.231532	-0.595291	-0.991159
C	0.867032	-0.454034	-1.070504
C	0.071570	-0.257554	0.105512
C	0.735528	-0.423861	1.365124
C	2.099402	-0.560794	1.436631
C	2.872174	-0.630745	0.262455
H	2.821914	-0.708477	-1.899003
H	0.395917	-0.470467	-2.051693
H	0.169473	-0.334949	2.291380
H	2.605064	-0.622434	2.397693
N	4.232702	-0.765101	0.387845
C	5.239242	-0.839027	-0.283754
O	6.270523	-0.918956	-0.820739
C	-3.465921	-0.324829	-1.214306
C	-2.109189	-0.129749	-1.150962
C	-1.387113	-0.474315	0.007995
C	-2.128352	-1.027125	1.064779
C	-3.488200	-1.202459	0.953324
N	-4.148908	-0.853100	-0.171784
H	-4.055542	-0.059765	-2.088637
H	-1.620454	0.329913	-2.005454
H	-1.647957	-1.348564	1.984091
H	-4.087707	-1.632094	1.751563
C	-5.598476	-1.079839	-0.294088
H	-5.780551	-1.988285	-0.876773
H	-6.032258	-1.189380	0.701939
H	-6.056742	-0.221070	-0.791121
C	-0.077139	1.920379	0.122898
F	-0.851387	2.285593	1.135687
F	-0.576801	2.382891	-1.017874
F	1.146203	2.368661	0.292209

18a

Frequencies 33.66, 37.74, 62.09 cm^{-1}

Zero-point correction= 0.223819 (Hartree/Particle)

Sum of electronic and zero-point Energies= -686.378389

Sum of electronic and thermal Energies= -686.364905

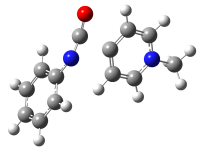
Sum of electronic and thermal Enthalpies= -686.363961

Sum of electronic and thermal Free Energies= -686.420612

C	3.062326	-1.395380	-0.371638
C	4.422146	-1.371955	-0.175050
C	5.032421	-0.210116	0.326635
C	4.264487	0.928187	0.629088
C	2.904002	0.929916	0.427927
C	2.258870	-0.241219	-0.093852
H	2.553810	-2.276794	-0.757240
H	5.025643	-2.247255	-0.404226
H	6.108624	-0.191650	0.488572
H	4.752738	1.816213	1.024824
H	2.311866	1.810772	0.654329
N	0.945716	-0.375901	-0.312575

C	0.092363	0.686555	-0.349691
O	0.345835	1.860960	-0.586040
C	-1.354771	0.291058	-0.162326
C	-2.317635	1.301179	-0.152865
C	-3.644546	0.974431	0.018157
H	-2.011828	2.336530	-0.285389
H	-4.439625	1.715092	0.032325
H	-3.493605	-2.316137	0.299187
C	-3.105459	-1.308658	0.169841
H	-1.034525	-1.837757	-0.007192
C	-5.448832	-0.657463	0.318605
H	-5.827519	-1.038174	-0.635110
H	-5.561735	-1.418966	1.094329
H	-6.008736	0.234366	0.606571
C	-1.765736	-1.033684	0.002628
N	-4.022802	-0.314245	0.177232

TS3 for 1a



Imaginary Vibrational Frequency = -709.5298 cm^{-1}
Zero-point correction= 0.219971 (Hartree/Particle)
Sum of electronic and zero-point Energies= -686.319000
Sum of electronic and thermal Energies= -686.304776
Sum of electronic and thermal Enthalpies= -686.303832
Sum of electronic and thermal Free Energies= -686.362630

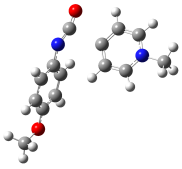
C	-2.300001	0.151108	-1.127515
C	-3.127803	-0.893886	-1.504027
C	-3.779579	-1.661862	-0.534199
C	-3.600265	-1.382352	0.821172
C	-2.770997	-0.342085	1.214974
C	-2.119056	0.430446	0.239731
H	-1.794810	0.763954	-1.874133
H	-3.275959	-1.110469	-2.560005
H	-4.432394	-2.477304	-0.838402
H	-4.115906	-1.975087	1.573594
H	-2.624403	-0.095423	2.264840
N	-1.322169	1.466095	0.668920
C	-0.468414	2.228160	0.199570
O	0.108003	3.216959	-0.075404
C	2.133052	-1.450237	0.233612
C	0.982782	-0.685047	0.262908
C	1.121258	0.675764	0.077158
C	2.345656	1.278696	-0.128916
C	3.461549	0.463093	-0.146174
N	3.342229	-0.872952	0.035227
H	2.136420	-2.529747	0.368792
H	0.014746	-1.161302	0.430711
H	2.440921	2.355201	-0.270602
H	4.470573	0.839126	-0.300155
C	4.542118	-1.729442	-0.020566

H 4.443706 -2.532380 0.713624
H 4.644045 -2.151803 -1.024930
H 5.423662 -1.132075 0.220657

18d

Frequencies 17.08, 37.80, 55.82 cm^{-1}
Zero-point correction= 0.257172 (Hartree/Particle)
Sum of electronic and zero-point Energies= -800.824623
Sum of electronic and thermal Energies= -800.808620
Sum of electronic and thermal Enthalpies= -800.807675
Sum of electronic and thermal Free Energies= -800.870377
C -2.125922 1.542017 -0.265146
C -3.486567 1.570533 -0.194382
C -4.204944 0.369693 0.039240
C -3.512100 -0.851453 0.202204
C -2.142106 -0.881639 0.121483
C -1.389897 0.317224 -0.123381
H -1.552825 2.449604 -0.442610
H -4.053631 2.491494 -0.309969
H -4.054830 -1.774105 0.390901
H -1.612126 -1.821277 0.235721
N -0.057256 0.424296 -0.204856
C 0.759201 -0.662172 -0.244619
O 0.483389 -1.848676 -0.410197
C 2.218404 -0.297427 -0.105442
C 3.158217 -1.330570 -0.088659
C 4.495566 -1.034487 0.045955
H 2.820271 -2.360093 -0.182718
H 5.271309 -1.795254 0.066924
H 4.433533 2.265224 0.239334
C 4.017355 1.265134 0.143692
H 1.955830 1.840237 0.000509
C 6.345602 0.558833 0.271411
H 6.713561 0.932709 -0.689185
H 6.492404 1.316411 1.045581
H 6.892101 -0.345357 0.546441
C 2.668907 1.020454 0.012914
N 4.910904 0.247742 0.161365
O -5.522120 0.497360 0.092144
C -6.345793 -0.643945 0.320911
H -7.371167 -0.272857 0.311222
H -6.212347 -1.383262 -0.478074
H -6.123310 -1.090383 1.297698

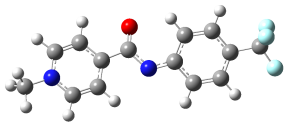
TS3 for 1d



Imaginary Vibrational Frequency = -615.3053 cm-1
Zero-point correction= 0.252495 (Hartree/Particle)
Sum of electronic and zero-point Energies= -800.758352
Sum of electronic and thermal Energies= -800.741384
Sum of electronic and thermal Enthalpies= -800.740440
Sum of electronic and thermal Free Energies= -800.806044

C	1.539871	0.849696	1.066331
C	2.609552	0.036806	1.362809
C	3.431153	-0.464025	0.333122
C	3.150422	-0.143819	-1.003050
C	2.066926	0.668212	-1.299674
C	1.255334	1.178546	-0.275824
H	0.913200	1.250390	1.862968
H	2.854938	-0.226474	2.389523
H	3.776180	-0.514842	-1.810308
H	1.842137	0.938085	-2.329935
N	0.215195	2.005251	-0.619970
C	-0.772370	2.532593	-0.110692
O	-1.584666	3.313687	0.227121
C	-2.475258	-1.734441	-0.313464
C	-1.541784	-0.715919	-0.330622
C	-1.982268	0.560580	-0.040793
C	-3.303620	0.837722	0.251151
C	-4.194295	-0.219056	0.252513
N	-3.773635	-1.475409	-0.026413
H	-2.233554	-2.774150	-0.525335
H	-0.499262	-0.936939	-0.569258
H	-3.642813	1.849922	0.472694
H	-5.253990	-0.106189	0.471176
C	-4.730972	-2.595443	0.026996
H	-4.658865	-3.090444	1.000324
H	-5.742996	-2.211954	-0.117542
H	-4.500669	-3.305802	-0.770420
O	4.448961	-1.234283	0.732781
C	5.355004	-1.740473	-0.234979
H	5.847133	-0.921359	-0.775892
H	6.101516	-2.308171	0.322590
H	4.842668	-2.405913	-0.942625

18e

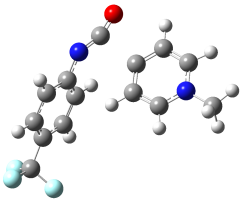


Frequencies 16.57, 34.90, 35.86 cm^{-1}
Zero-point correction= 0.228883 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1023.323821
Sum of electronic and thermal Energies= -1023.306637
Sum of electronic and thermal Enthalpies= -1023.305693
Sum of electronic and thermal Free Energies= -1023.372483

C	-3.870547	1.285191	-0.111169
C	-2.900999	0.284560	-0.211668
C	-3.282436	-1.045399	-0.038102
C	-4.604196	-1.340230	0.229809
H	-3.587501	2.326048	-0.251479

H -4.964684 -2.355480 0.371681
C 1.346584 0.953027 0.220042
C 2.707222 0.964542 0.398834
C 3.484044 -0.150577 0.030225
C 2.891300 -1.295470 -0.517816
C 1.526795 -1.327539 -0.692969
C 0.710981 -0.203817 -0.343390
H 0.748251 1.815822 0.495146
H 3.194734 1.838564 0.827951
H 3.508120 -2.146542 -0.795535
H 1.028708 -2.198150 -1.114401
N -0.603410 -0.350111 -0.535726
C -1.476931 0.699840 -0.499795
O -1.248910 1.874993 -0.747716
H -2.547561 -1.841978 -0.121445
H -5.977279 1.666993 0.250237
C -6.938442 -0.678543 0.600400
H -7.266436 -0.128096 1.486523
H -7.547474 -0.395623 -0.263231
H -7.037590 -1.750235 0.781287
N -5.525714 -0.358050 0.325609
C -5.174502 0.939133 0.158330
C 4.972692 -0.073496 0.253251
F 5.597840 -1.186980 -0.125610
F 5.239510 0.132198 1.548654
F 5.495370 0.950174 -0.430830

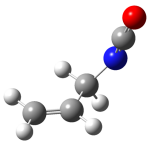
TS3 for 1e



Imaginary Vibrational Frequency = -737.0712 cm^{-1}
Zero-point correction= 0.225273 (Hartree/Particle)
Thermal correction to Energy= 0.242995
Thermal correction to Enthalpy= 0.243939
Thermal correction to Gibbs Free Energy= 0.176206
Sum of electronic and zero-point Energies= -1023.266171
Sum of electronic and thermal Energies= -1023.248448
Sum of electronic and thermal Enthalpies= -1023.247504
Sum of electronic and thermal Free Energies= -1023.315237
C 1.422143 1.016455 1.015237
C 2.450732 0.197257 1.439558
C 3.279691 -0.430367 0.501992
C 3.091400 -0.226297 -0.862557
C 2.057942 0.590302 -1.300281
C 1.214252 1.207768 -0.364476
H 0.773537 1.515368 1.734763
H 2.619582 0.037642 2.503596
H 3.750098 -0.705682 -1.582294
H 1.890146 0.770219 -2.360195
N 0.197452 1.998150 -0.843042
C -0.849095 2.503297 -0.408503

O	-1.666621	3.317252	-0.176033
C	-2.349555	-1.710459	-0.247254
C	-1.453090	-0.665775	-0.365669
C	-1.953271	0.614682	-0.235462
C	-3.288400	0.875381	-0.008044
C	-4.138261	-0.211222	0.097165
N	-3.663327	-1.471690	-0.020396
H	-2.063294	-2.757338	-0.327847
H	-0.397964	-0.872658	-0.553453
H	-3.670400	1.891281	0.089641
H	-5.206319	-0.112559	0.276256
C	-4.575949	-2.625324	0.102539
H	-5.596611	-2.263791	0.238318
H	-4.523098	-3.227474	-0.808718
H	-4.284611	-3.227037	0.968213
C	4.364251	-1.337192	1.016184
F	5.061842	-1.903087	0.030975
F	3.834830	-2.323120	1.759220
F	5.218357	-0.670715	1.800111

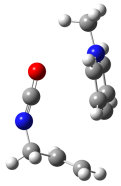
1c



Frequencies 36.38, 65.80, 155.23 cm^{-1}
Zero-point correction= 0.084244 (Hartree/Particle)
Sum of electronic and zero-point Energies= -285.123161
Sum of electronic and thermal Energies= -285.116642
Sum of electronic and thermal Enthalpies= -285.115698
Sum of electronic and thermal Free Energies= -285.154822

C	2.342674	-0.806961	-0.237989
C	1.439683	-0.123701	0.461223
H	2.554542	-0.571439	-1.281936
H	2.908342	-1.625342	0.202718
H	1.233799	-0.379381	1.503325
C	0.650419	1.018221	-0.097833
H	0.887067	1.950216	0.432476
H	0.903267	1.179187	-1.155942
N	-0.773373	0.814691	0.021639
C	-1.603891	-0.052730	-0.030290
O	-2.505840	-0.808131	-0.052847

γ-NMP and 1c

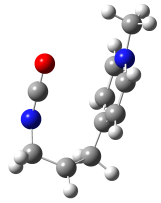


Frequencies 26.27, 37.29, 49.69 cm^{-1}
Zero-point correction= 0.201804 (Hartree/Particle)
Sum of electronic and zero-point Energies= -572.083305

Sum of electronic and thermal Energies= -572.069676
Sum of electronic and thermal Enthalpies= -572.068732
Sum of electronic and thermal Free Energies= -572.127204

C	2.915595	-1.594877	-0.050358
C	2.920566	-0.379925	0.504134
H	2.978354	-1.729045	-1.132176
H	2.913051	-2.501474	0.552642
H	2.884147	-0.264283	1.590142
C	2.980756	0.888715	-0.289137
H	3.860481	1.483756	-0.013265
H	3.059758	0.676292	-1.364623
N	1.816241	1.706485	-0.065866
C	0.651751	1.800946	0.154004
O	-0.502994	1.972162	0.362092
C	-1.694621	-0.367179	-1.241761
C	-0.492222	-1.046268	-1.331209
C	0.007389	-1.556521	-0.154452
C	-0.610961	-1.434834	1.068932
C	-1.807636	-0.740991	1.083181
N	-2.324782	-0.228375	-0.054772
H	-2.178427	0.096691	-2.098391
H	0.009007	-1.151048	-2.291334
H	-0.199540	-1.838936	1.991355
H	-2.375249	-0.558648	1.992690
C	-3.525027	0.625418	0.022714
H	-4.079536	0.554855	-0.915405
H	-4.160016	0.283808	0.842814
H	-3.201838	1.657064	0.196987

7a

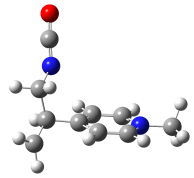


Frequencies 50.48, 58.51, 69.76 cm^{-1}
Zero-point correction= 0.204702 (Hartree/Particle)
Sum of electronic and zero-point Energies= -572.145457
Sum of electronic and thermal Energies= -572.132748
Sum of electronic and thermal Enthalpies= -572.131804
Sum of electronic and thermal Free Energies= -572.185674

C	1.760870	1.567293	-0.410642
C	2.682459	0.824018	0.502801
H	2.050369	1.424284	-1.465849
H	1.837728	2.646802	-0.213683
H	3.325958	1.378760	1.183064
C	3.019937	-0.610266	0.267922
H	3.850874	-0.695551	-0.453164
H	3.375440	-1.082820	1.194213
N	1.918416	-1.365989	-0.269232
C	0.838227	-1.841056	-0.079579
O	-0.249410	-2.294973	-0.012247
C	-1.542165	0.612598	1.175781
C	-0.252888	1.068774	1.028545
C	0.321704	1.156292	-0.246447

C	-0.480281	0.821716	-1.341418
C	-1.760795	0.355041	-1.142495
N	-2.275485	0.247073	0.100261
H	-2.021987	0.501866	2.144862
H	0.323531	1.330381	1.914812
H	-0.090203	0.878696	-2.355523
H	-2.403228	0.035577	-1.959139
C	-3.590579	-0.387705	0.291557
H	-3.451608	-1.471264	0.371016
H	-4.048603	-0.001206	1.204621
H	-4.232439	-0.153560	-0.560602

8a



Frequencies 29.74, 47.47, 67.10 cm^{-1}
Zero-point correction= 0.203099 (Hartree/Particle)
Sum of electronic and zero-point Energies= -572.137264
Sum of electronic and thermal Energies= -572.124002
Sum of electronic and thermal Enthalpies= -572.123058
Sum of electronic and thermal Free Energies= -572.179106

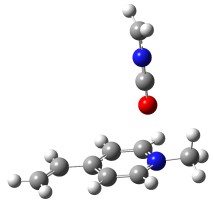
C	-1.022921	2.951987	0.156903
C	-1.089409	1.507044	0.505215
H	-1.792326	3.412573	-0.459329
H	-0.297868	3.603675	0.638504
H	-1.386049	1.377359	1.562922
C	-2.156190	0.797913	-0.347269
H	-3.119464	1.299482	-0.178362
H	-1.901912	0.911206	-1.413752
N	-2.231462	-0.591859	0.002235
C	-2.952672	-1.537033	-0.224372
O	-3.564353	-2.522289	-0.367386
C	2.262051	0.434118	-0.913484
C	1.085978	1.129290	-0.733280
C	0.231824	0.802839	0.324438
C	0.620914	-0.236873	1.177723
C	1.805689	-0.900550	0.960932
N	2.611397	-0.564225	-0.072965
H	2.955224	0.648550	-1.722467
H	0.830368	1.937106	-1.418712
H	-0.010650	-0.534924	2.011638
H	2.152338	-1.715772	1.591874
C	3.865401	-1.312747	-0.274075
H	4.429198	-0.856543	-1.089669
H	4.460967	-1.276649	0.642289
H	3.631469	-2.351088	-0.527118

7 and NCO radical

Frequencies 14.84, 26.21, 53.88 cm^{-1}
Zero-point correction= 0.201761 (Hartree/Particle)
Sum of electronic and zero-point Energies= -572.103621
Sum of electronic and thermal Energies= -572.089667
Sum of electronic and thermal Enthalpies= -572.088723
Sum of electronic and thermal Free Energies= -572.148146

C	-0.553243	1.748917	-0.309259
C	-1.640149	1.444441	0.675856
H	-0.945832	1.608451	-1.329820
H	-0.276960	2.812348	-0.232020
H	-1.340565	1.229177	1.704556
C	-2.948415	1.465553	0.356280
H	-3.716885	1.303294	1.109968
H	-3.284930	1.713641	-0.649828
N	-2.457572	-0.879153	-0.607261
C	-3.555196	-1.291934	-0.229994
O	-4.600150	-1.709532	0.109050
C	3.085217	0.711219	-0.127518
C	1.955551	1.493756	-0.235586
C	0.684869	0.914546	-0.161012
C	0.612649	-0.473227	0.029754
C	1.769005	-1.210751	0.132949
N	2.985966	-0.621943	0.055166
H	4.090644	1.120265	-0.181042
H	2.073868	2.565449	-0.380929
H	-0.357033	-0.971624	0.065431
H	1.769988	-2.289063	0.274499
C	4.193028	-1.456675	0.192032
H	5.074179	-0.862077	-0.056044
H	4.271354	-1.817085	1.222072
H	4.124722	-2.303917	-0.495602

8 and CH_2NCO radical

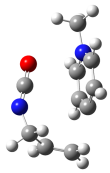


Frequencies 18.29, 45.21, 56.51 cm^{-1}
Zero-point correction= 0.200314 (Hartree/Particle)
Sum of electronic and zero-point Energies= -572.128991
Sum of electronic and thermal Energies= -572.114069
Sum of electronic and thermal Enthalpies= -572.113125
Sum of electronic and thermal Free Energies= -572.174166

C	3.310682	2.593789	-0.503016
C	2.859386	1.773962	0.453652
H	3.882028	3.482968	-0.248974
H	3.142656	2.424030	-1.565758
H	3.074721	2.005789	1.497680
C	-4.990685	1.648791	0.094183
H	-5.635795	1.636647	-0.778792
H	-5.249694	2.189760	0.998775
N	-3.832629	0.976924	0.052111
C	-2.817710	0.369695	-0.011320

O	-1.795716	-0.240463	-0.070061
C	0.963429	-1.047272	-1.170002
C	1.683476	0.113432	-1.040608
C	2.091106	0.557453	0.229566
C	1.720372	-0.236850	1.327435
C	0.999050	-1.392045	1.143341
N	0.636459	-1.795209	-0.092069
H	0.613662	-1.416462	-2.130589
H	1.922889	0.675093	-1.939372
H	2.002076	0.052397	2.337345
H	0.686782	-2.026957	1.968383
C	-0.221231	-2.977187	-0.257294
H	-0.003980	-3.450114	-1.217935
H	-0.015922	-3.688162	0.546191
H	-1.267751	-2.655895	-0.222379

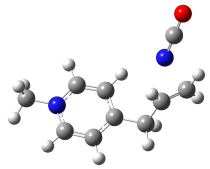
TS5



Imaginary Vibrational Frequency = -176.554 cm^{-1}
Zero-point correction= 0.202152 (Hartree/Particle)
Sum of electronic and zero-point Energies= -572.082280
Sum of electronic and thermal Energies= -572.069205
Sum of electronic and thermal Enthalpies= -572.068261
Sum of electronic and thermal Free Energies= -572.123558

C	-2.586571	-1.664526	0.058448
C	-2.813353	-0.448198	-0.473202
H	-2.585805	-1.819248	1.139172
H	-2.569378	-2.561769	-0.557989
H	-2.878844	-0.323407	-1.556564
C	-2.923856	0.802543	0.341852
H	-3.863318	1.327315	0.129693
H	-2.914803	0.574507	1.417423
N	-1.841150	1.709092	0.045318
C	-0.664434	1.830427	-0.107896
O	0.489470	2.035289	-0.272394
C	1.661274	-0.422778	1.218243
C	0.437285	-1.062572	1.287385
C	-0.109926	-1.498889	0.097294
C	0.511932	-1.328286	-1.122999
C	1.733692	-0.681987	-1.121434
N	2.283129	-0.242908	0.032372
H	2.171713	-0.023452	2.091991
H	-0.049112	-1.196462	2.252204
H	0.078332	-1.665870	-2.062462
H	2.297088	-0.477488	-2.028929
C	3.511611	0.570873	-0.012769
H	4.099272	0.386735	0.889295
H	4.100251	0.290378	-0.888689
H	3.225075	1.626018	-0.072669

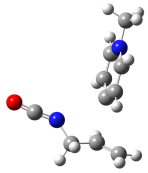
TS6



Imaginary Vibrational Frequency = -163.2956 cm^{-1}
Zero-point correction= 0.202223 (Hartree/Particle)
Sum of electronic and zero-point Energies= -572.103025
Sum of electronic and thermal Energies= -572.090088
Sum of electronic and thermal Enthalpies= -572.089143
Sum of electronic and thermal Free Energies= -572.145031

C	-0.503777	1.905233	-0.273492
C	-1.660880	1.499402	0.585646
H	-0.823102	1.913836	-1.328035
H	-0.206104	2.937327	-0.030011
H	-1.455765	1.271448	1.634163
C	-2.929314	1.384677	0.107135
H	-3.760482	1.175049	0.777765
H	-3.182521	1.686863	-0.906957
N	-2.579005	-0.702715	-0.762130
C	-3.449760	-1.305661	-0.134032
O	-4.278419	-1.909190	0.441825
C	3.049838	0.656647	0.182647
C	1.970096	1.510114	0.098565
C	0.690806	1.002565	-0.147034
C	0.554280	-0.384585	-0.297279
C	1.663143	-1.193758	-0.206354
N	2.891363	-0.674805	0.029689
H	4.061538	1.005589	0.372818
H	2.135090	2.578304	0.222660
H	-0.428113	-0.819479	-0.498348
H	1.614292	-2.274009	-0.320110
C	4.047794	-1.580158	0.158582
H	4.964703	-1.027367	-0.055912
H	4.085887	-1.982007	1.175747
H	3.944961	-2.395946	-0.560717

TS7

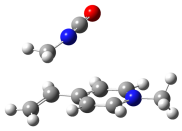


Imaginary Vibrational Frequency = -213.7723 cm^{-1}
Zero-point correction= 0.200834 (Hartree/Particle)
Sum of electronic and zero-point Energies= -572.076664
Sum of electronic and thermal Energies= -572.063023
Sum of electronic and thermal Enthalpies= -572.062078
Sum of electronic and thermal Free Energies= -572.120649

C	1.784881	-2.864966	0.046773
C	1.992699	-1.613861	0.508086
H	1.989095	-3.129412	-0.992189
H	1.403352	-3.654702	0.690141

H 1.874226 -1.400319 1.573791
C 2.694909 -0.556227 -0.291317
H 3.765443 -0.570286 -0.036289
H 2.615153 -0.778253 -1.366702
N 2.147208 0.750465 -0.016478
C 2.454117 1.909578 -0.175394
O 2.622101 3.063667 -0.271617
C -2.171869 -0.380324 -1.098656
C -0.879120 -0.858012 -0.990372
C -0.235498 -0.675060 0.216014
C -0.834875 -0.056541 1.296603
C -2.129582 0.390708 1.131070
N -2.774344 0.226705 -0.050241
H -2.761799 -0.463178 -2.008541
H -0.410055 -1.353290 -1.839542
H -0.324354 0.099608 2.245526
H -2.691642 0.895102 1.914629
C -4.142743 0.759900 -0.189253
H -4.600412 0.347655 -1.090399
H -4.735184 0.466192 0.680994
H -4.102036 1.850716 -0.263699

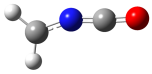
TS8



Imaginary Vibrational Frequency = -489.6765 cm^{-1}
Zero-point correction= 0.200765 (Hartree/Particle)
Sum of electronic and zero-point Energies= -572.104762
Sum of electronic and thermal Energies= -572.091587
Sum of electronic and thermal Enthalpies= -572.090643
Sum of electronic and thermal Free Energies= -572.146754
C -1.693703 2.867424 0.415126
C -1.381241 1.545423 0.665266
H -2.627987 3.290800 0.774583
H -1.057513 3.524336 -0.175886
H -1.967599 1.022159 1.424732
C -2.313000 0.323085 -0.925035
H -3.337834 0.579451 -0.653421
H -1.889003 0.853088 -1.776639
N -1.945488 -0.984542 -0.822317
C -2.047422 -2.038936 -0.243193
O -2.040090 -3.097290 0.258132
C 2.054795 0.890422 -0.731878
C 0.842546 1.497728 -0.518522
C -0.060105 0.976625 0.425921
C 0.350639 -0.174716 1.125794
C 1.572245 -0.746792 0.874062
N 2.415059 -0.220260 -0.045444
H 2.775397 1.264260 -1.454401
H 0.597664 2.378711 -1.107173
H -0.290082 -0.619255 1.885190
H 1.924451 -1.635893 1.392290
C 3.716763 -0.867673 -0.276360

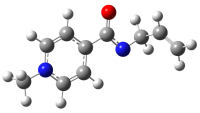
H 4.239137 -0.351177 -1.083782
H 4.318429 -0.816784 0.636063
H 3.557716 -1.912194 -0.559498

CH_2NCO radical



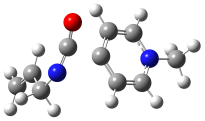
Frequencies 91.27, 222.22, 462.92 cm^{-1}
Zero-point correction= 0.036155 (Hartree/Particle)
Sum of electronic and zero-point Energies= -207.182729
Sum of electronic and thermal Energies= -207.177902
Sum of electronic and thermal Enthalpies= -207.176957
Sum of electronic and thermal Free Energies= -207.209728
C -1.810100 0.093389 0.000068
H -2.135800 1.130280 -0.000118
H -2.517316 -0.728629 -0.000013
N -0.499242 -0.195350 -0.000052
C 0.685446 -0.022165 -0.000016
O 1.861967 0.067307 0.000023

20



Frequencies 22.84, 28.91, 75.85 cm^{-1}
Zero-point correction= 0.203615 (Hartree/Particle)
Sum of electronic and zero-point Energies= -572.105032
Sum of electronic and thermal Energies= -572.092257
Sum of electronic and thermal Enthalpies= -572.091313
Sum of electronic and thermal Free Energies= -572.146812
C 4.377358 -1.172078 0.925388
C 3.808489 -0.062304 0.436835
H 4.406700 -2.098608 0.351571
H 4.857097 -1.180203 1.902146
H 3.714573 0.845683 1.032669
C 3.168640 -0.012459 -0.932846
H 3.255885 0.987442 -1.377550
H 3.593628 -0.773942 -1.594400
N 1.814100 -0.377312 -0.602808
C 1.010617 0.656425 -0.200737
O 1.365441 1.795632 0.082866
C -2.250524 -1.286306 -0.150501
C -0.899465 -1.022579 -0.253630
C -0.446605 0.287318 -0.097395
C -1.374617 1.299868 0.158254
C -2.710879 0.984555 0.247922
N -3.132028 -0.293110 0.094472
H -2.665956 -2.284435 -0.260642
H -0.195157 -1.827132 -0.449389
H -1.036671 2.325608 0.286392
H -3.485592 1.723235 0.440000
C -4.575705 -0.578983 0.188365
H -4.735314 -1.656302 0.119322
H -4.953901 -0.215937 1.148107
H -5.097169 -0.078256 -0.632731

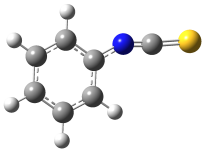
TS9



Imaginary Vibrational Frequency = -696.5624 cm^{-1}
Zero-point correction= 0.200662 (Hartree/Particle)
Sum of electronic and zero-point Energies= -572.058995
Sum of electronic and thermal Energies= -572.045679
Sum of electronic and thermal Enthalpies= -572.044735
Sum of electronic and thermal Free Energies= -572.101168

C	1.818880	-2.428353	0.814299
C	2.543387	-1.331253	0.601926
H	1.322913	-2.952843	-0.004772
H	1.716758	-2.864519	1.805793
H	3.052819	-0.830788	1.429631
C	2.742027	-0.728944	-0.752081
H	3.800265	-0.773614	-1.055099
H	2.189939	-1.285099	-1.525578
N	2.384430	0.672627	-0.834937
C	1.811336	1.437713	-0.033007
O	1.644025	2.402777	0.627917
C	-1.966497	-0.317365	-1.183220
C	-0.626806	0.023746	-1.247459
C	-0.048269	0.546711	-0.108704
C	-0.756775	0.736875	1.064252
C	-2.084267	0.361313	1.071801
N	-2.666169	-0.152730	-0.039184
H	-2.515466	-0.721994	-2.030198
H	-0.078815	-0.109611	-2.178542
H	-0.304997	1.182017	1.949127
H	-2.727726	0.462685	1.943282
C	-4.102452	-0.488492	0.007319
H	-4.361388	-1.094115	-0.863076
H	-4.310303	-1.057713	0.916892
H	-4.690468	0.434234	0.001269

2a

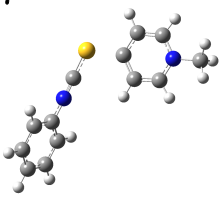


Frequencies 57.40, 64.24, 245.19 cm^{-1}
Zero-point correction= 0.101093 (Hartree/Particle)
Sum of electronic and zero-point Energies= -722.327556
Sum of electronic and thermal Energies= -722.320053
Sum of electronic and thermal Enthalpies= -722.319109
Sum of electronic and thermal Free Energies= -722.361033

C	0.896161	1.103739	0.000000
C	2.261623	1.357950	0.000000
C	3.175740	0.305401	0.000000
C	2.716936	-1.010024	0.000000
C	1.353680	-1.279521	0.000000
C	0.443016	-0.220416	0.000000

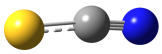
H 0.171248 1.916083 0.000000
H 2.613957 2.388034 0.000000
H 4.244458 0.511301 0.000000
H 3.426215 -1.835781 0.000000
H 0.977292 -2.300387 0.000000
N -0.910402 -0.495171 0.000000
C -2.061918 -0.172564 0.000002
S -3.610737 0.142472 -0.000001

γ-NMP radical and 2a



Frequencies 19.29, 28.13, 34.33 cm^{-1}
Zero-point correction= 0.218134 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1009.286603
Sum of electronic and thermal Energies= -1009.270850
Sum of electronic and thermal Enthalpies= -1009.269906
Sum of electronic and thermal Free Energies= -1009.335094
C -3.648916 -0.003815 -1.209791
C -4.827697 0.723092 -1.304008
C -5.383963 1.311185 -0.168843
C -4.761406 1.172625 1.070979
C -3.581277 0.451047 1.184957
C -3.031272 -0.133658 0.038864
H -3.202238 -0.475376 -2.082643
H -5.316894 0.828882 -2.269931
H -6.309697 1.876915 -0.249653
H -5.200571 1.626555 1.956774
H -3.085293 0.324960 2.145177
N -1.859932 -0.849599 0.142110
C -0.879740 -1.498013 0.237232
C 4.549151 -0.266968 -0.284087
C 3.494610 -1.143404 -0.437737
C 2.206385 -0.641458 -0.334849
C 1.976978 0.697051 -0.058239
C 3.068070 1.529715 0.083553
N 4.328291 1.046149 -0.033179
H 5.591876 -0.568431 -0.359694
H 3.697691 -2.192733 -0.646666
H 0.974461 1.112666 0.037788
H 2.983378 2.595301 0.286214
C 5.475754 1.947593 0.166464
H 6.307285 1.617885 -0.460601
H 5.192746 2.961924 -0.123421
H 5.777015 1.933918 1.218552
S 0.460729 -2.368017 0.367413

NCS radical

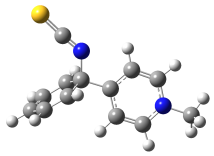


Frequencies 350.17, 775.81, 1985.80 cm^{-1}

Zero-point correction= 0.007089 (Hartree/Particle)
Sum of electronic and zero-point Energies= -490.888027
Sum of electronic and thermal Energies= -490.884747
Sum of electronic and thermal Enthalpies= -490.883803
Sum of electronic and thermal Free Energies= -490.911571

N	0.209062	1.779945	0.000000
C	0.000000	0.612727	0.000000
S	-0.091465	-1.008499	0.000000

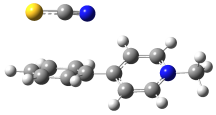
21



Frequencies 36.29, 39.59, 53.27 cm^{-1}
Zero-point correction= 0.219134 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1009.314605
Sum of electronic and thermal Energies= -1009.300933
Sum of electronic and thermal Enthalpies= -1009.299989
Sum of electronic and thermal Free Energies= -1009.357631

C	-0.945239	0.840828	1.279454
C	-1.676682	1.990532	1.333977
C	-2.108750	2.648299	0.158442
C	-1.770238	2.113438	-1.108061
C	-1.030829	0.974766	-1.227094
C	-0.600318	0.171601	-0.027769
H	-0.640276	0.312298	2.183127
H	-1.944621	2.401554	2.306045
H	-2.706932	3.553627	0.226186
H	-2.111731	2.619396	-2.009781
H	-0.794288	0.547038	-2.201587
N	-1.241407	-1.154672	-0.074939
C	-2.421565	-1.458699	-0.071340
C	3.121521	0.859987	-0.189078
C	1.760025	1.046475	-0.214616
C	0.903588	-0.048369	-0.044244
C	1.472926	-1.306350	0.155549
C	2.844641	-1.440695	0.178561
N	3.651047	-0.371569	0.007298
H	3.833620	1.670556	-0.322094
H	1.356423	2.046772	-0.364844
H	0.837327	-2.178503	0.286274
H	3.338013	-2.397920	0.327943
C	5.114712	-0.540431	-0.014214
H	5.583068	0.312331	0.483166
H	5.380277	-1.455444	0.519106
H	5.460373	-0.602768	-1.050733
S	-3.902593	-1.953346	-0.072920

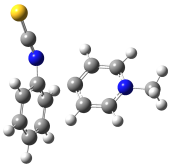
22



Frequencies 35.98, 51.53, 72.48 cm^{-1}
Zero-point correction= 0.220313 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1009.332944
Sum of electronic and thermal Energies= -1009.318086
Sum of electronic and thermal Enthalpies= -1009.317141
Sum of electronic and thermal Free Energies= -1009.376845

C	0.999747	0.781071	-1.464011
C	2.341735	1.114026	-1.558848
C	3.038197	1.521605	-0.421301
C	2.376415	1.628849	0.807538
C	1.022167	1.333551	0.895412
C	0.324684	0.887908	-0.234449
H	0.460360	0.457257	-2.353394
H	2.851709	1.043539	-2.516884
H	4.095947	1.769351	-0.490024
H	2.921683	1.945538	1.694330
H	0.523777	1.391541	1.862382
N	1.052843	-2.085290	-0.254041
C	2.128696	-1.855307	0.185122
C	-3.285557	0.810660	0.816135
C	-1.968710	1.193557	0.724676
C	-1.085816	0.509115	-0.127758
C	-1.612517	-0.566188	-0.865439
C	-2.935732	-0.910770	-0.735830
N	-3.761147	-0.228014	0.092787
H	-4.001476	1.318810	1.456951
H	-1.635227	2.052554	1.301754
H	-0.968069	-1.175403	-1.494396
H	-3.379551	-1.747215	-1.269849
C	-5.161152	-0.655482	0.245863
H	-5.770618	0.202688	0.537715
H	-5.526086	-1.044039	-0.707767
H	-5.226982	-1.433675	1.012856
S	3.594983	-1.458963	0.780778

TS13

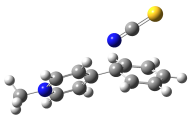


Imaginary Vibrational Frequency = -405.3677 cm^{-1}
Zero-point correction= 0.217358 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1009.277410
Sum of electronic and thermal Energies= -1009.262757
Sum of electronic and thermal Enthalpies= -1009.261812
Sum of electronic and thermal Free Energies= -1009.322211

C	1.688591	-1.188960	-0.927015
C	1.445282	-2.527198	-1.154484
C	0.954108	-3.350033	-0.127476
C	0.734385	-2.823070	1.149698
C	0.975752	-1.486226	1.406382
C	1.372529	-0.618946	0.344470
H	2.101130	-0.544344	-1.702483
H	1.668112	-2.954992	-2.130443

H	0.784661	-4.408246	-0.315607
H	0.407769	-3.474707	1.957519
H	0.857438	-1.060062	2.401509
N	1.876633	0.630378	0.694437
C	2.440623	1.574665	0.183150
C	-2.887219	-0.359866	-0.798057
C	-1.556209	-0.719563	-0.805219
C	-0.665886	0.042042	-0.062016
C	-1.102101	1.127895	0.679582
C	-2.444894	1.448178	0.647433
N	-3.313118	0.710775	-0.083740
H	-3.655892	-0.892151	-1.355327
H	-1.233000	-1.578024	-1.394569
H	-0.416748	1.734032	1.272590
H	-2.869191	2.292000	1.186820
C	-4.747908	1.045110	-0.095868
H	-5.304390	0.287294	0.463770
H	-4.895137	2.022406	0.367838
H	-5.103078	1.081424	-1.129183
S	3.160184	2.855286	-0.352010

TS14

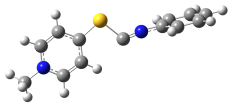


Imaginary Vibrational Frequency = -545.7769 cm^{-1}
Zero-point correction= 0.218743 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1009.301687
Sum of electronic and thermal Energies= -1009.287574
Sum of electronic and thermal Enthalpies= -1009.286630
Sum of electronic and thermal Free Energies= -1009.344574

C	-0.981156	0.674233	1.392382
C	-2.163822	1.356948	1.545137
C	-2.820087	1.901560	0.428913
C	-2.240020	1.804885	-0.850577
C	-1.052881	1.141057	-1.026299
C	-0.451013	0.411910	0.069444
H	-0.466402	0.251911	2.254785
H	-2.588521	1.484828	2.538579
H	-3.765126	2.424904	0.557489
H	-2.731786	2.269653	-1.702517
H	-0.615423	1.036467	-2.019087
N	-1.003659	-1.320954	-0.240776
C	-2.201114	-1.514109	-0.305804
C	3.229965	0.850179	-0.659231
C	1.868458	1.067557	-0.648768
C	1.021332	0.175808	0.015189
C	1.608013	-0.915936	0.670427
C	2.970926	-1.084409	0.638650
N	3.767632	-0.211117	-0.022570
H	3.925217	1.512015	-1.168794
H	1.472737	1.945682	-1.153641
H	0.986674	-1.651358	1.175140
H	3.473501	-1.918456	1.122419
C	5.218464	-0.460976	-0.082355

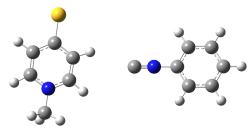
H 5.735201 0.467003 -0.335238
H 5.564842 -0.810734 0.893252
H 5.425087 -1.218801 -0.844499
S -3.757678 -1.768305 -0.391900

9



Frequencies 29.13, 32.28, 35.04 cm^{-1}
Zero-point correction= 0.218842 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1009.307529
Sum of electronic and thermal Energies= -1009.292557
Sum of electronic and thermal Enthalpies= -1009.291613
Sum of electronic and thermal Free Energies= -1009.352729
C 4.464691 -0.843360 -0.011752
C 3.204851 -1.381070 0.000155
C 2.075687 -0.537263 0.005005
C 2.302230 0.851080 -0.000620
C 3.587527 1.329727 -0.012997
N 4.657625 0.498361 -0.020803
H 5.362047 -1.457277 -0.015001
H 3.091436 -2.463022 0.002242
H 1.464587 1.544098 0.000626
H 3.808888 2.394190 -0.017215
C 6.024206 1.040433 0.013805
H 6.674266 0.421730 -0.609932
H 6.018041 2.058647 -0.381002
H 6.394648 1.047452 1.043905
S 0.516535 -1.307719 0.015215
C -5.209481 0.237444 -1.213639
C -3.825537 0.186588 -1.224872
C -3.131650 0.170139 -0.000282
C -3.828420 0.203121 1.222284
C -5.212322 0.253722 1.207205
C -5.907078 0.269518 -0.004202
H -5.752733 0.250816 -2.156126
H -3.265381 0.160093 -2.157113
H -3.270403 0.188989 2.156071
H -5.757744 0.279652 2.148172
H -6.994089 0.307650 -0.005778
N -1.778191 0.103924 0.001877
C -0.577065 0.215671 -0.000057

12 and C_6H_5NC

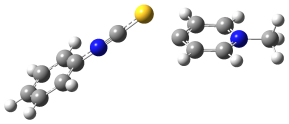


Frequencies 6.58, 32.07, 33.56 cm^{-1}
Zero-point correction= 0.218358 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1009.294114
Sum of electronic and thermal Energies= -1009.278425
Sum of electronic and thermal Enthalpies= -1009.277481

Sum of electronic and thermal Free Energies= -1009.342910

N	2.179573	0.362885	-0.012403
C	1.020824	0.548548	-0.017721
S	-3.466323	-2.820041	-0.088004
C	-2.216558	0.971815	0.015821
C	-2.209660	-0.399568	-0.022359
C	-3.428879	-1.101880	-0.034483
C	-4.624345	-0.350343	-0.005507
C	-4.561329	1.017436	0.032052
H	-1.277819	1.524525	0.025558
H	-1.242525	-0.898359	-0.046079
H	-5.597413	-0.835183	-0.015917
H	-5.452883	1.639833	0.054471
N	-3.373750	1.672239	0.041105
C	-3.357986	3.141289	0.118334
H	-2.362403	3.502044	-0.147007
H	-4.086725	3.550332	-0.586671
H	-3.603834	3.460012	1.136179
C	3.550214	0.137319	-0.003805
C	4.025286	-1.158489	0.201360
C	4.420796	1.209869	-0.199215
C	5.396721	-1.377920	0.209990
H	3.319851	-1.973025	0.350925
C	5.789555	0.973278	-0.187698
H	4.018816	2.208502	-0.355902
C	6.277798	-0.315828	0.016249
H	5.780019	-2.383671	0.368275
H	6.479625	1.800515	-0.338788
H	7.351076	-0.493897	0.023994

TS11



Imaginary Vibrational Frequency = -128.9365 cm^{-1}

Zero-point correction= 0.218118 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1009.285415

Sum of electronic and thermal Energies= -1009.270748

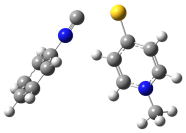
Sum of electronic and thermal Enthalpies= -1009.269804

Sum of electronic and thermal Free Energies= -1009.331420

N	-3.220526	0.071619	0.269176
C	-2.237039	-0.376895	-0.187218
S	-0.902949	-1.025699	-0.847005
C	2.784893	-0.543169	1.023615
C	1.428248	-0.732482	0.965592
C	0.656846	0.046928	0.084244
C	1.320621	0.941658	-0.774942
C	2.679595	1.091518	-0.675111
H	3.426291	-1.076924	1.721513
H	0.970772	-1.463077	1.630622
H	0.776550	1.545137	-1.499549
H	3.241161	1.805511	-1.273724
N	3.407011	0.367214	0.222175
C	4.863766	0.515133	0.272570

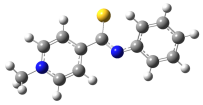
H 5.215644 0.293326 1.283438
H 5.340337 -0.168737 -0.438280
H 5.132382 1.545420 0.024491
C -4.389005 0.563216 0.803658
C -5.042909 1.622049 0.163107
C -4.896840 -0.011836 1.974966
C -6.222635 2.105571 0.709711
H -4.624714 2.044098 -0.748189
C -6.077306 0.487232 2.505024
H -4.366475 -0.835342 2.448103
C -6.738693 1.541896 1.876376
H -6.743878 2.925857 0.221412
H -6.485225 0.050994 3.414063
H -7.665296 1.926418 2.297326

TS12



Imaginary Vibrational Frequency = -62.4491 cm^{-1}
Zero-point correction= 0.218574 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1009.295294
Sum of electronic and thermal Energies= -1009.280479
Sum of electronic and thermal Enthalpies= -1009.279534
Sum of electronic and thermal Free Energies= -1009.342183
C -2.753797 -0.159305 1.288466
C -3.620683 -1.242564 1.232897
C -4.120933 -1.681220 0.007360
C -3.758697 -1.034651 -1.174097
C -2.895153 0.051870 -1.139304
C -2.397537 0.477458 0.096433
H -2.360900 0.207455 2.234412
H -3.913783 -1.743268 2.153070
H -4.804045 -2.527260 -0.026104
H -4.160335 -1.372568 -2.126966
H -2.617343 0.585876 -2.046488
N -1.535629 1.558911 0.135077
C -0.856391 2.520473 0.155021
C 1.702054 -1.213719 -0.729780
C 1.230717 0.071636 -0.655671
C 1.925234 1.042873 0.100121
C 3.106045 0.614405 0.755921
C 3.535330 -0.678406 0.631650
N 2.840570 -1.589266 -0.099284
H 1.196253 -1.983484 -1.306923
H 0.331674 0.330790 -1.208372
H 3.682198 1.308532 1.363171
H 4.439609 -1.044554 1.112612
C 3.351886 -2.962723 -0.201158
H 2.655236 -3.565925 -0.786510
H 4.327473 -2.956167 -0.696981
H 3.448084 -3.394206 0.799777
S 1.448497 2.690555 0.229290

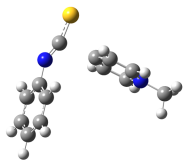
23



Frequencies 34.28, 49.84, 74.64 cm^{-1}
Zero-point correction= 0.221053 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1009.335968
Sum of electronic and thermal Energies= -1009.322867
Sum of electronic and thermal Enthalpies= -1009.321923
Sum of electronic and thermal Free Energies= -1009.377680

C	2.975216	-1.503886	-0.527918
C	4.339243	-1.538612	-0.340436
C	4.966260	-0.530314	0.406845
C	4.216717	0.513008	0.968373
C	2.855245	0.580451	0.762916
C	2.205514	-0.420637	-0.017104
H	2.455711	-2.274766	-1.093525
H	4.928889	-2.350476	-0.759937
H	6.041493	-0.569836	0.570548
H	4.711426	1.268461	1.574752
H	2.267060	1.370192	1.222474
N	0.879528	-0.455531	-0.257204
C	0.056676	0.589224	-0.290795
C	-1.378303	0.209105	-0.108732
C	-2.353411	1.162801	0.204744
C	-3.664519	0.779592	0.367827
H	-2.078837	2.209397	0.315177
H	-4.454085	1.483518	0.616773
H	-3.489612	-2.469210	-0.199657
C	-3.115648	-1.454061	-0.089963
H	-1.060007	-1.895938	-0.476325
C	-5.451748	-0.900366	0.344110
H	-5.886908	-1.031297	-0.651655
H	-5.519355	-1.835645	0.905521
H	-5.993620	-0.119386	0.881178
C	-1.789580	-1.125068	-0.244930
N	-4.037350	-0.511560	0.216353
S	0.438289	2.176076	-0.701812

TS15

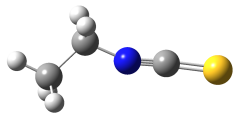


Imaginary Vibrational Frequency = -531.889 cm^{-1}
Zero-point correction= 0.217493 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1009.271011
Sum of electronic and thermal Energies= -1009.256161
Sum of electronic and thermal Enthalpies= -1009.255217
Sum of electronic and thermal Free Energies= -1009.316557

C	-2.022639	-0.523879	1.192853
C	-2.748464	-1.699919	1.333614
C	-3.631573	-2.104852	0.333366

C	-3.795745	-1.326209	-0.810815
C	-3.082364	-0.143931	-0.964521
C	-2.189403	0.247410	0.036532
H	-1.351372	-0.177923	1.978456
H	-2.633824	-2.297915	2.235577
H	-4.201740	-3.023731	0.451857
H	-4.493394	-1.636370	-1.585877
H	-3.211331	0.486903	-1.841581
N	-1.481606	1.428138	-0.117000
C	-0.447895	2.034475	-0.012587
C	2.301948	-0.957244	-1.292576
C	1.340221	0.028884	-1.221433
C	1.157379	0.656371	-0.000452
C	1.892817	0.319367	1.122094
C	2.834320	-0.681431	0.988946
N	3.031406	-1.295954	-0.201889
H	2.523866	-1.507135	-2.204701
H	0.759114	0.290194	-2.104770
H	1.762230	0.819776	2.080234
H	3.459244	-1.019132	1.812552
C	4.023316	-2.381311	-0.312495
H	3.524874	-3.348063	-0.190767
H	4.502815	-2.330688	-1.292830
H	4.783296	-2.257140	0.461670
S	0.615467	3.263358	0.047388

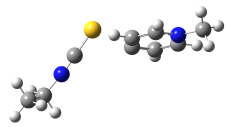
2b



Frequencies 11.28, 50.06, 235.19 cm^{-1}
Zero-point correction= 0.076351 (Hartree/Particle)
Sum of electronic and zero-point Energies= -570.034395
Sum of electronic and thermal Energies= -570.028059
Sum of electronic and thermal Enthalpies= -570.027115
Sum of electronic and thermal Free Energies= -570.066775

C	1.725637	0.603972	0.000019
C	2.768068	-0.498832	0.000021
H	1.841039	1.247085	0.884828
H	1.840542	1.246620	-0.885199
H	2.664317	-1.133484	-0.887558
H	3.774448	-0.064012	-0.000547
H	2.665035	-1.132848	0.888138
N	0.403528	0.074996	0.000533
C	-0.783685	0.040788	0.000161
S	-2.366887	-0.097744	-0.000287

γ-MP radical and 2b



Frequencies 27.40, 39.28, 48.80 cm^{-1}

Zero-point correction= 0.193923 (Hartree/Particle)
Sum of electronic and zero-point Energies= -856.994437
Sum of electronic and thermal Energies= -856.981823
Sum of electronic and thermal Enthalpies= -856.980879
Sum of electronic and thermal Free Energies= -857.037353

C	-4.547879	0.362810	0.789876
C	-4.904712	1.637172	0.046444
H	-4.402646	0.549163	1.861843
H	-5.339722	-0.392149	0.694777
H	-5.053294	1.441825	-1.021156
H	-5.836178	2.046090	0.452857
H	-4.120384	2.393767	0.159433
N	-3.346257	-0.222466	0.287623
C	-2.411786	-0.741550	-0.196595
S	-1.134007	-1.469261	-0.859656
C	2.963789	-0.476763	1.047328
C	1.600422	-0.695681	1.041898
C	0.844680	-0.048143	0.078818
C	1.426816	0.773959	-0.873216
C	2.793434	0.954586	-0.819478
H	3.636451	-0.930211	1.771969
H	1.160137	-1.363927	1.779673
H	0.848237	1.269415	-1.650648
H	3.340520	1.589070	-1.513872
N	3.538808	0.336189	0.129089
C	4.988870	0.592229	0.175909
H	5.482284	-0.213444	0.723228
H	5.382777	0.623419	-0.842840
H	5.176275	1.547383	0.676342

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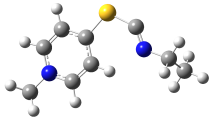
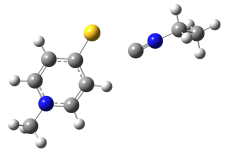


Frequencies 35.22, 43.67, 86.39 cm^{-1}
Zero-point correction= 0.195822 (Hartree/Particle)
Sum of electronic and zero-point Energies= -857.006639
Sum of electronic and thermal Energies= -856.993767
Sum of electronic and thermal Enthalpies= -856.992823
Sum of electronic and thermal Free Energies= -857.047921

C	-3.802702	-0.817119	-0.492963
C	-4.113153	-1.687907	0.707354
H	-3.742541	-1.418342	-1.408224
H	-4.569260	-0.044997	-0.641405
H	-4.170702	-1.088254	1.623335
H	-5.078639	-2.186190	0.565224
H	-3.348516	-2.461458	0.847542
N	-2.497707	-0.168317	-0.325490
C	-2.237327	1.020128	-0.165249
S	-0.770299	1.933610	0.064171
C	1.685564	-1.301932	-0.176166
C	0.527123	-0.561642	-0.157421
C	0.603994	0.827581	0.023875
C	1.876580	1.407987	0.182660

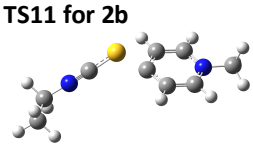
C 2.994967 0.615334 0.155742
H 1.680871 -2.380333 -0.313200
H -0.434385 -1.053954 -0.286385
H 1.992556 2.480724 0.324282
H 3.999207 1.014934 0.274836
N 2.899694 -0.725034 -0.024486
C 4.118901 -1.549826 -0.003612
H 3.929725 -2.485814 -0.533330
H 4.926849 -1.013227 -0.506975
H 4.402040 -1.763012 1.032074

12 and C_2H_5NC



Frequencies 19.07, 37.54, 47.45 cm^{-1}
Zero-point correction= 0.194928 (Hartree/Particle)
Sum of electronic and zero-point Energies= -857.011430
Sum of electronic and thermal Energies= -856.997539
Sum of electronic and thermal Enthalpies= -856.996595
Sum of electronic and thermal Free Energies= -857.055821
C -4.769390 -0.247294 -0.495676
C -5.442424 -1.009946 0.630600
H -4.976342 -0.698468 -1.473694
H -5.103982 0.796878 -0.534966
H -5.234521 -0.546796 1.601166
H -6.526044 -1.004850 0.473108
H -5.104638 -2.051471 0.658838
N -3.345677 -0.227276 -0.335218
C -2.185579 -0.242257 -0.195951
S -0.524796 1.630284 0.086241
C 2.204506 -1.324334 -0.042416
C 0.990196 -0.691417 -0.013297
C 0.928710 0.718705 0.044869
C 2.163711 1.412310 0.074732
C 3.343924 0.720690 0.045571
H 2.289946 -2.407190 -0.086473
H 0.078448 -1.280090 -0.037988
H 2.189632 2.498667 0.117375
H 4.310365 1.218525 0.068439
N 3.371199 -0.634407 -0.016678
C 4.659177 -1.340840 0.001171
H 4.534460 -2.330808 -0.443382
H 5.387977 -0.778388 -0.587939
H 5.015789 -1.442464 1.031319

TS11 for 2b

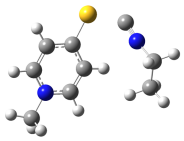


Imaginary Vibrational Frequency = -158.2635 cm^{-1}
Zero-point correction= 0.194192 (Hartree/Particle)

Sum of electronic and zero-point Energies= -856.991905
Sum of electronic and thermal Energies= -856.978963
Sum of electronic and thermal Enthalpies= -856.978019
Sum of electronic and thermal Free Energies= -857.033787

C	-4.350727	0.506434	0.851232
C	-5.048226	1.362194	-0.189681
H	-4.094977	1.081700	1.750282
H	-4.970970	-0.341512	1.169422
H	-5.301004	0.776403	-1.079817
H	-5.977902	1.754884	0.235664
H	-4.424128	2.210871	-0.489320
N	-3.126759	-0.042383	0.349388
C	-2.160057	-0.508502	-0.109276
S	-0.834077	-1.202827	-0.767029
C	2.797091	-0.412856	1.060181
C	1.449117	-0.649807	1.016287
C	0.660530	0.006477	0.049715
C	1.307744	0.817383	-0.904230
C	2.660003	1.016287	-0.814441
H	3.448232	-0.842734	1.818298
H	1.007559	-1.316902	1.754594
H	0.753938	1.321173	-1.694490
H	3.204731	1.675848	-1.486263
N	3.401145	0.421634	0.164345
C	4.851214	0.617689	0.216726
H	5.179188	0.620467	1.259945
H	5.365842	-0.183135	-0.325858
H	5.102746	1.581291	-0.233711

TS12 for 2b

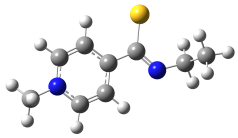


Imaginary Vibrational Frequency = -134.1562 cm^{-1}
Zero-point correction= 0.194632 (Hartree/Particle)
Sum of electronic and zero-point Energies= -857.001451
Sum of electronic and thermal Energies= -856.988529
Sum of electronic and thermal Enthalpies= -856.987585
Sum of electronic and thermal Free Energies= -857.043915

C	-3.263332	-1.394292	-0.626373
C	-2.504475	-2.432305	0.179064
H	-3.163706	-1.566434	-1.704923
H	-4.334045	-1.406701	-0.387389
H	-2.603244	-2.247236	1.255133
H	-2.914348	-3.425941	-0.030959
H	-1.440715	-2.439304	-0.088779
N	-2.792757	-0.066376	-0.366826
C	-2.566710	1.070608	-0.185008
S	-0.835413	2.278804	0.326231
C	1.477213	-0.985197	0.726891
C	0.418218	-0.124905	0.849267
C	0.432511	1.120493	0.177441
C	1.564912	1.404954	-0.618702
C	2.603936	0.512883	-0.689400

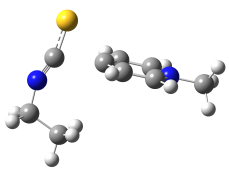
H 1.516816 -1.944547 1.238685
H -0.415033 -0.394293 1.494131
H 1.625495 2.337927 -1.173791
H 3.496836 0.704254 -1.278660
N 2.563195 -0.670291 -0.025023
C 3.672822 -1.628597 -0.120851
H 3.362177 -2.500670 -0.705149
H 4.522347 -1.149055 -0.611150
H 3.972036 -1.942015 0.883511

24



Frequencies 16.43, 61.98, 79.08 cm^{-1}
Zero-point correction= 0.196769 (Hartree/Particle)
Sum of electronic and zero-point Energies= -857.031912
Sum of electronic and thermal Energies= -857.019633
Sum of electronic and thermal Enthalpies= -857.018689
Sum of electronic and thermal Free Energies= -857.072935
C 3.254890 -0.947452 -0.475099
C 3.913607 -1.133140 0.893329
H 3.653032 -0.048651 -0.969089
H 3.463419 -1.829892 -1.094133
H 3.500962 -2.002883 1.416532
H 4.990207 -1.284613 0.761894
H 3.761574 -0.242876 1.516912
N 1.827716 -0.885114 -0.315576
C 1.179719 0.234366 -0.217201
S 1.916231 1.799161 -0.094329
C -2.268395 -1.288896 -0.158421
C -0.902845 -1.158850 -0.249852
C -0.308115 0.102859 -0.114004
C -1.146886 1.199408 0.107357
C -2.510139 1.016414 0.190211
H -2.776316 -2.245355 -0.253851
H -0.281505 -2.032859 -0.425314
H -0.733848 2.199247 0.220918
H -3.202465 1.836019 0.364827
N -3.057665 -0.210921 0.058847
C -4.513762 -0.386840 0.201405
H -4.838793 -1.218790 -0.427204
H -4.754075 -0.596486 1.248501
H -5.020695 0.525587 -0.119974

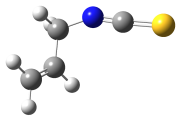
TS15 for 2b



Imaginary Vibrational Frequency = -453.3978 cm^{-1}
Zero-point correction= 0.193377 (Hartree/Particle)
Sum of electronic and zero-point Energies= -856.977669
Sum of electronic and thermal Energies= -856.964367
Sum of electronic and thermal Enthalpies= -856.963422
Sum of electronic and thermal Free Energies= -857.020665

C	-1.770242	-2.417536	0.118742
H	-1.006322	-2.240839	-0.649001
C	-3.016879	-1.595251	-0.148979
H	-3.468755	-1.848894	-1.116507
H	-3.786282	-1.768762	0.613845
N	-2.747451	-0.188630	-0.165784
C	-2.075672	0.789472	-0.138112
C	1.966143	0.315511	1.305215
C	0.617898	0.576218	1.256084
C	-0.001361	0.643418	0.005735
C	0.743315	0.464887	-1.160174
C	2.090346	0.207084	-1.047189
N	2.688665	0.134778	0.168172
H	2.522230	0.234483	2.237256
H	0.064949	0.726341	2.182113
H	0.290025	0.526273	-2.148552
H	2.733763	0.043366	-1.908297
C	4.130336	-0.134240	0.283124
H	4.286996	-1.046422	0.866654
H	4.554523	-0.267638	-0.713891
H	4.623867	0.710101	0.773717
S	-1.615087	2.372224	-0.147055
H	-2.024086	-3.483153	0.106357
H	-1.344440	-2.182164	1.101995

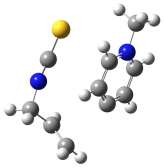
2c



Frequencies 46.51, 115.46, 332.19 cm^{-1}
Zero-point correction= 0.081360 (Hartree/Particle)
Sum of electronic and zero-point Energies= -608.076105
Sum of electronic and thermal Energies= -608.070019
Sum of electronic and thermal Enthalpies= -608.069075
Sum of electronic and thermal Free Energies= -608.107387

C	2.921246	-0.872787	-0.269816
C	1.927601	-0.321243	0.421541
H	3.334738	-0.393199	-1.157997
H	3.363188	-1.822878	0.023271
H	1.514364	-0.819976	1.301175
C	1.306659	0.995111	0.065660
H	1.490424	1.742401	0.852529
H	1.747323	1.393055	-0.859223
N	-0.109681	0.892389	-0.110036
C	-1.133641	0.282926	-0.055466
S	-2.550841	-0.428135	-0.022564

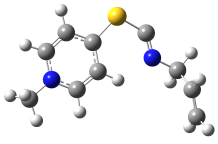
γ-MP radical and 2c



Frequencies 23. 57, 38.90, 55.68 cm^{-1}
Zero-point correction= 0.199185 (Hartree/Particle)
Sum of electronic and zero-point Energies= -895.037207
Sum of electronic and thermal Energies= -895.022523
Sum of electronic and thermal Enthalpies= -895.021579
Sum of electronic and thermal Free Energies= -895.082369

C	-3.143089	-1.729940	-0.122631
C	-2.972822	-0.490501	-0.586408
H	-3.354957	-1.923668	0.930514
H	-3.128214	-2.595983	-0.782233
H	-2.778239	-0.310758	-1.646305
C	-3.033161	0.727481	0.286473
H	-3.794552	1.436324	-0.070069
H	-3.300355	0.458968	1.317733
N	-1.775621	1.409637	0.305674
C	-0.731200	1.833646	-0.059622
C	1.502261	-0.415881	1.216044
C	0.236148	-0.963446	1.326840
C	-0.186911	-1.733825	0.268694
C	0.557647	-1.980969	-0.861617
C	1.821201	-1.416962	-0.897476
N	2.271517	-0.664621	0.130846
H	1.940303	0.228246	1.975461
H	-0.373672	-0.761965	2.205144
H	0.202906	-2.583758	-1.694490
H	2.502429	-1.544372	-1.735125
C	3.581012	0.005137	0.033223
H	4.097444	-0.070787	0.993133
H	4.179803	-0.480507	-0.739360
H	3.416135	1.057305	-0.225124
S	0.695823	2.429212	-0.450378

11

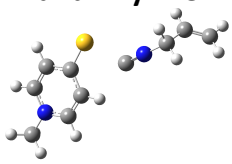


Frequencies 18.03, 30.70, 49.40 cm^{-1}
Zero-point correction= 0.199952 (Hartree/Particle)
Sum of electronic and zero-point Energies= -895.049731
Sum of electronic and thermal Energies= -895.035862
Sum of electronic and thermal Enthalpies= -895.034918
Sum of electronic and thermal Free Energies= -895.093716

C	-4.326455	2.274863	0.190285
C	-3.946466	1.034645	0.488636
H	-4.370750	2.627918	-0.840774
H	-4.630647	2.980132	0.960598

H -3.921386 0.695890 1.526629
C -3.572931 0.019039 -0.543593
H -4.247333 -0.849469 -0.521683
H -3.611448 0.460435 -1.547677
N -2.198679 -0.449026 -0.327062
C -1.771509 -1.578066 -0.107844
C 1.691859 1.382531 -0.030918
C 0.674403 0.458030 0.024183
C 0.991229 -0.907264 0.074947
C 2.350561 -1.275020 0.074902
C 3.318278 -0.305934 0.023330
N 2.991089 1.009005 -0.031791
H 1.498546 2.451304 -0.072051
H -0.360180 0.794066 0.019049
H 2.650309 -2.320466 0.109590
H 4.381332 -0.535712 0.019872
C 4.068145 2.011264 -0.083894
H 3.630595 3.004098 -0.204207
H 4.645089 1.978133 0.845234
H 4.720029 1.798830 -0.936020
S -0.174607 -2.230596 0.155826

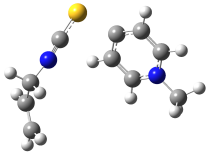
12 and Allyl NC



Frequencies 21.95, 25.29, 39.58 cm^{-1}
Zero-point correction= 0.199516 (Hartree/Particle)
Sum of electronic and zero-point Energies= -895.052679
Sum of electronic and thermal Energies= -895.037944
Sum of electronic and thermal Enthalpies= -895.037000
Sum of electronic and thermal Free Energies= -895.098840
C 4.377856 -0.167567 0.772260
H 4.670337 -1.063511 1.334500
H 4.652751 0.709630 1.374725
N 2.945407 -0.163666 0.671029
C 1.781664 -0.177385 0.565778
S 0.127168 1.648458 0.053270
C -2.585058 -1.321500 0.218616
C -1.380739 -0.670800 0.277079
C -1.311875 0.714404 0.011176
C -2.529551 1.366317 -0.306508
C -3.699929 0.659670 -0.346665
H -2.674074 -2.386815 0.415354
H -0.483355 -1.227318 0.529684
H -2.548824 2.432439 -0.520799
H -4.653452 1.124305 -0.586857
N -3.734530 -0.672057 -0.086930
C -5.010791 -1.393752 -0.179379
H -4.898653 -2.383044 0.269252
H -5.782716 -0.842474 0.364747
H -5.301803 -1.500780 -1.229203
C 5.021368 -0.136501 -0.580479
H 4.770541 0.715883 -1.213649

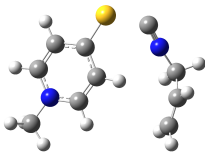
C 5.876940 -1.068382 -0.989984
H 6.139292 -1.924414 -0.367693
H 6.359816 -1.006186 -1.962429

TS11 for 2c



Imaginary Vibrational Frequency = -107.5675 cm^{-1}
Zero-point correction= 0.198749 (Hartree/Particle)
Sum of electronic and zero-point Energies= -895.034621
Sum of electronic and thermal Energies= -895.020576
Sum of electronic and thermal Enthalpies= -895.019632
Sum of electronic and thermal Free Energies= -895.079598
C 3.584731 2.639062 0.008504
C 3.618415 1.338158 -0.266561
H 3.451908 3.009194 1.025733
H 3.713079 3.388485 -0.769353
H 3.767143 0.980699 -1.287002
C 3.509964 0.282561 0.792951
H 4.424964 -0.326637 0.846757
H 3.351674 0.728831 1.783520
N 2.429960 -0.617936 0.528884
C 1.663923 -1.458226 0.228582
C -1.844882 1.102883 -0.894982
C -1.049165 0.017874 -1.185303
C -1.286635 -1.184467 -0.521339
C -2.276264 -1.257414 0.458974
C -3.041844 -0.142023 0.709571
N -2.830833 1.017103 0.033680
H -1.746785 2.063129 -1.396999
H -0.275810 0.114442 -1.946729
H -2.477509 -2.174793 1.010029
H -3.855949 -0.128881 1.431298
C -3.644454 2.199608 0.351252
H -3.693155 2.850617 -0.524742
H -4.656718 1.882507 0.613810
H -3.199253 2.744145 1.190191
S 0.536281 -2.533723 -0.195906

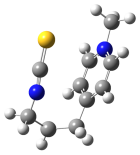
TS12 for 2c



Imaginary Vibrational Frequency = -121.111 cm^{-1}
Zero-point correction= 0.199285 (Hartree/Particle)
Sum of electronic and zero-point Energies= -895.044941
Sum of electronic and thermal Energies= -895.031198
Sum of electronic and thermal Enthalpies= -895.030254
Sum of electronic and thermal Free Energies= -895.088127
C 2.494562 2.791678 -0.287517

C	3.022702	1.572404	-0.363678
H	2.087511	3.183629	0.646077
H	2.484832	3.460631	-1.145532
H	3.449719	1.202019	-1.297811
C	3.126140	0.654955	0.818050
H	4.175498	0.459685	1.082423
H	2.635508	1.083697	1.701462
N	2.519959	-0.615266	0.547869
C	2.147237	-1.707136	0.326099
C	-1.333401	1.144786	-0.475547
C	-0.430947	0.124406	-0.637205
C	-0.760273	-1.186283	-0.226588
C	-2.037438	-1.374979	0.352965
C	-2.904845	-0.322327	0.469206
N	-2.557922	0.927739	0.063066
H	-1.118726	2.163713	-0.788750
H	0.525197	0.340831	-1.107973
H	-2.342136	-2.357813	0.704616
H	-3.899735	-0.425402	0.896673
C	-3.528354	2.020076	0.215481
H	-3.097097	2.944859	-0.172793
H	-4.437268	1.783781	-0.346190
H	-3.770948	2.151413	1.274529
S	0.295025	-2.536696	-0.422391

14

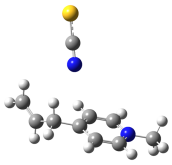


Frequencies 38.69, 42.94, 65. 46 cm^{-1}
Zero-point correction= 0.201472 (Hartree/Particle)
Sum of electronic and zero-point Energies= -895.101464
Sum of electronic and thermal Energies= -895.088122
Sum of electronic and thermal Enthalpies= -895.087177
Sum of electronic and thermal Free Energies= -895.143348

C	-1.944941	-1.686775	0.448792
C	-2.848831	-0.911549	-0.452775
H	-2.203581	-1.516251	1.508981
H	-2.087168	-2.763528	0.273095
H	-3.596764	-1.433791	-1.045683
C	-3.030954	0.561577	-0.285289
H	-3.384440	1.020527	-1.220388
H	-3.809576	0.770149	0.470892
N	-1.833137	1.214010	0.133676
C	-0.799654	1.795885	0.072494
C	1.684543	-0.801612	1.118602
C	0.367302	-1.141323	1.336253
C	-0.486926	-1.365823	0.253481
C	0.057841	-1.270464	-1.033494
C	1.379471	-0.930978	-1.200704
N	2.178901	-0.704591	-0.133448
H	2.377035	-0.584617	1.927979
H	-0.000619	-1.196984	2.358579

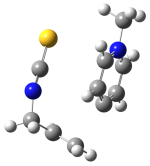
H -0.566297 -1.433402 -1.911062
H 1.841772 -0.819188 -2.178275
C 3.547653 -0.206741 -0.339724
H 4.172954 -0.504712 0.504702
H 3.955262 -0.633597 -1.258867
H 3.517563 0.886248 -0.415422
S 0.613155 2.524377 0.092378

15 and NCS radical



Frequencies 19.55, 34.56, 35.15 cm^{-1}
Zero-point correction= 0.199692 (Hartree/Particle)
Sum of electronic and zero-point Energies= -895.081627
Sum of electronic and thermal Energies= -895.067141
Sum of electronic and thermal Enthalpies= -895.066196
Sum of electronic and thermal Free Energies= -895.127823
C -0.123068 2.042682 0.752840
C 0.263151 2.901884 -0.414730
H 0.779412 1.550087 1.153215
H -0.540106 2.651627 1.568741
H -0.543798 3.463308 -0.893218
C 1.511212 3.018468 -0.863542
H 1.760355 3.669964 -1.698309
H 2.335503 2.476590 -0.397736
N 1.951159 -0.486189 0.130774
C 3.024129 -0.991075 0.143335
C -2.966537 -0.450812 0.990912
C -2.101978 0.573602 1.307220
C -1.094245 0.953804 0.413856
C -1.012266 0.254830 -0.799878
C -1.897365 -0.759216 -1.072682
N -2.862442 -1.103452 -0.186036
H -3.763322 -0.774926 1.655004
H -2.215588 1.079440 2.263807
H -0.239484 0.500237 -1.524722
H -1.873681 -1.334958 -1.995012
C -3.799390 -2.183423 -0.537189
H -4.423698 -2.417238 0.327163
H -4.433253 -1.861854 -1.369047
H -3.233055 -3.074024 -0.823433
S 4.496739 -1.685327 0.162470

TS16

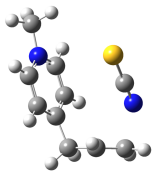


Imaginary Vibrational Frequency = -174.8396 cm^{-1}
Zero-point correction= 0.198941 (Hartree/Particle)

Sum of electronic and zero-point Energies= -895.036625
Sum of electronic and thermal Energies= -895.022982
Sum of electronic and thermal Enthalpies= -895.022037
Sum of electronic and thermal Free Energies= -895.079696

C	-2.649719	-1.898927	-0.147623
C	-2.830808	-0.634112	-0.569784
H	-2.761384	-2.169866	0.903856
H	-2.545885	-2.723842	-0.850794
H	-2.772474	-0.390053	-1.632679
C	-3.027897	0.518763	0.367436
H	-3.892063	1.132355	0.076789
H	-3.212697	0.167129	1.392003
N	-1.867757	1.358325	0.378288
C	-0.830425	1.793917	-0.001476
C	1.492670	-0.467849	1.254261
C	0.232449	-1.035078	1.291655
C	-0.191065	-1.693358	0.155497
C	0.573412	-1.790190	-0.988916
C	1.828664	-1.210924	-0.956987
N	2.268782	-0.575211	0.151457
H	1.920349	0.086468	2.087030
H	-0.375711	-0.942924	2.189932
H	0.233072	-2.294450	-1.891235
H	2.510297	-1.229293	-1.804079
C	3.561680	0.130427	0.127504
H	4.045886	0.029396	1.101682
H	4.201649	-0.308315	-0.640484
H	3.377882	1.187965	-0.093850
S	0.569288	2.429863	-0.416026

TS17

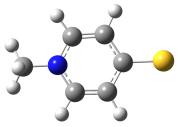


Imaginary Vibrational Frequency = -389.2912 cm^{-1}
Zero-point correction= 0.200322 (Hartree/Particle)
Sum of electronic and zero-point Energies= -895.068356
Sum of electronic and thermal Energies= -895.055532
Sum of electronic and thermal Enthalpies= -895.054588
Sum of electronic and thermal Free Energies= -895.109038

C	-1.722918	-1.964087	-0.008265
C	-2.497095	-0.844847	-0.641969
H	-2.123608	-2.191571	0.987942
H	-1.795995	-2.874897	-0.620374
H	-2.275515	-0.617701	-1.688174
C	-3.324621	-0.005615	0.064494
H	-3.915690	0.748446	-0.448498
H	-3.644772	-0.258852	1.072646
N	-1.985957	1.409326	0.823902
C	-1.064449	1.822740	0.167912
C	1.461372	-0.360711	1.256814
C	0.194067	-0.896887	1.244889
C	-0.286986	-1.524597	0.091330

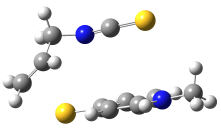
C 0.576187 -1.626421 -1.004344
C 1.840232 -1.080735 -0.940537
N 2.266763 -0.454695 0.175273
H 1.869332 0.168765 2.114332
H -0.436363 -0.784679 2.124118
H 0.260658 -2.117543 -1.923096
H 2.538428 -1.116122 -1.772638
C 3.563891 0.240991 0.187310
H 4.028477 0.124467 1.169381
H 4.216455 -0.190658 -0.574233
H 3.392418 1.302511 -0.023202
S 0.211271 2.398066 -0.611509

12



Frequencies 63.95, 108.33, 223.20 cm^{-1}
Zero-point correction= 0.119313 (Hartree/Particle)
Sum of electronic and zero-point Energies= -685.149779
Sum of electronic and thermal Energies= -685.142345
Sum of electronic and thermal Enthalpies= -685.141401
Sum of electronic and thermal Free Energies= -685.183007
C -1.022685 -1.169591 -0.011375
C 0.347158 -1.207336 -0.003271
C 1.077713 0.000486 0.000658
C 0.349997 1.209122 -0.003281
C -1.020708 1.174779 -0.011099
N -1.700905 0.003676 -0.017161
H -1.627247 -2.073468 -0.013255
H 0.849532 -2.171554 -0.002782
H 0.854145 2.172391 -0.002911
H -1.621090 2.081104 -0.012945
C -3.173169 -0.004227 0.022077
H -3.544784 -0.831016 -0.588041
H -3.514730 -0.120866 1.055467
H -3.550049 0.935961 -0.386332
S 2.794420 -0.002355 0.006792

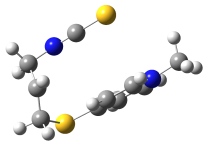
12 and 2c



Frequencies 33.31, 39.40, 51.18 cm^{-1}
Zero-point correction= 0.202531 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1293.248914
Sum of electronic and thermal Energies= -1293.233252
Sum of electronic and thermal Enthalpies= -1293.232308
Sum of electronic and thermal Free Energies= -1293.294917
C 2.023103 -1.155521 -0.943915
C 0.718089 -1.433255 -1.263809
C -0.262829 -1.471847 -0.249555

C 0.160076 -1.212722 1.071160
C 1.476862 -0.921982 1.323843
N 2.399504 -0.909651 0.333240
H 2.807231 -1.095684 -1.694721
H 0.451271 -1.607568 -2.303270
H -0.545896 -1.251767 1.896785
H 1.844760 -0.707249 2.324078
C 3.781995 -0.504491 0.619145
H 4.461885 -1.037426 -0.049590
H 3.875649 0.577088 0.466674
H 4.027165 -0.755320 1.653702
S -1.894787 -1.855522 -0.645463
C -3.660102 -0.177252 0.900758
C -2.747854 0.808320 0.925537
H -3.873733 -0.782232 1.779666
H -4.283768 -0.351046 0.023096
H -2.166856 1.002063 1.830804
C -2.459282 1.702955 -0.240113
H -2.778797 2.734192 -0.022963
H -3.003884 1.370104 -1.133075
N -1.057571 1.715301 -0.529338
C 0.065442 2.076480 -0.366652
S 1.595940 2.480597 -0.233093

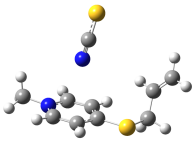
16



Frequencies 36.50, 56.12, 70.79 cm^{-1}
Zero-point correction= 0.203408 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1293.260290
Sum of electronic and thermal Energies= -1293.245617
Sum of electronic and thermal Enthalpies= -1293.244673
Sum of electronic and thermal Free Energies= -1293.303687
C 1.993341 -1.283841 -0.957748
C 0.666886 -1.518187 -1.207467
C -0.287965 -1.336663 -0.186339
C 0.184360 -0.942235 1.077295
C 1.526215 -0.710360 1.262622
N 2.419861 -0.888397 0.265997
H 2.758470 -1.390907 -1.722373
H 0.362628 -1.820173 -2.207170
H -0.480597 -0.804890 1.924305
H 1.929586 -0.376546 2.215511
C 3.829951 -0.529673 0.469976
H 4.459085 -1.157441 -0.165370
H 3.974027 0.525642 0.212678
H 4.098289 -0.696754 1.515650
S -1.947900 -1.632074 -0.604584
C -2.914714 -0.829532 0.775492
C -2.593594 0.593466 0.984703
H -2.819547 -1.429278 1.687838
H -3.940070 -0.976243 0.400132
H -2.254926 0.930877 1.964202

C	-2.599794	1.586150	-0.129302
H	-3.062613	2.532977	0.183495
H	-3.162025	1.217667	-0.997239
N	-1.255438	1.873907	-0.559204
C	-0.110594	2.138548	-0.370026
S	1.436785	2.478353	-0.225069

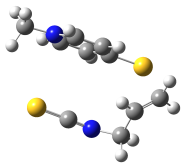
17 and NCS radical



Frequencies 21.17, 25.47, 53.88 cm^{-1}
Zero-point correction= 0.200426 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1293.242091
Sum of electronic and thermal Energies= -1293.226064
Sum of electronic and thermal Enthalpies= -1293.225120
Sum of electronic and thermal Free Energies= -1293.289605

C	-0.256056	2.356398	-0.940259
C	0.742281	1.519349	-1.361444
C	1.424340	0.709792	-0.430139
C	1.043890	0.812532	0.919496
C	0.036817	1.673258	1.277809
N	-0.597737	2.441709	0.367001
H	-0.819569	2.983966	-1.625532
H	0.993973	1.485440	-2.419172
H	1.502484	0.201656	1.691406
H	-0.307106	1.766014	2.304883
C	-1.748899	3.255735	0.773791
H	-1.858705	4.096878	0.085567
H	-2.650144	2.633486	0.752158
H	-1.583462	3.640346	1.783095
S	2.663195	-0.332163	-1.055710
C	3.305568	-1.181960	0.424124
C	2.444256	-2.254680	1.017240
H	3.590093	-0.423823	1.168940
H	4.255150	-1.608610	0.070323
H	2.904673	-2.749959	1.876047
C	1.243300	-2.648498	0.601737
H	0.718540	-3.458213	1.103212
H	0.746606	-2.198283	-0.259544
N	-2.287068	-0.032364	0.057063
C	-2.944484	-1.003624	-0.115186
S	-3.853506	-2.334345	-0.350719

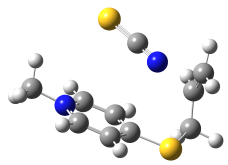
TS18



Imaginary Vibrational Frequency = -172.1776 cm^{-1}
Zero-point correction= 0.202924 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1293.247634
Sum of electronic and thermal Energies= -1293.233109
Sum of electronic and thermal Enthalpies= -1293.232164
Sum of electronic and thermal Free Energies= -1293.291270

C	1.965636	-1.130028	-1.028579
C	0.650067	-1.397620	-1.307509
C	-0.294904	-1.475361	-0.261031
C	0.183816	-1.284927	1.052284
C	1.510521	-1.006278	1.267380
N	2.391870	-0.937827	0.243458
H	2.720765	-1.034760	-1.805189
H	0.340811	-1.526680	-2.341847
H	-0.480099	-1.376178	1.907975
H	1.918082	-0.844659	2.262297
C	3.786072	-0.546166	0.487674
H	4.443157	-1.104097	-0.183962
H	3.892381	0.529962	0.309534
H	4.052068	-0.777125	1.521553
S	-1.941971	-1.829816	-0.635807
C	-3.264752	-0.434198	0.928721
C	-2.520327	0.708726	0.982286
H	-3.299465	-1.119036	1.773897
H	-4.067025	-0.536236	0.197056
H	-1.823252	0.874452	1.807417
C	-2.515557	1.743624	-0.096256
H	-2.951781	2.687703	0.267813
H	-3.113997	1.420280	-0.957975
N	-1.177519	2.003065	-0.528680
C	-0.017858	2.185552	-0.324686
S	1.540230	2.447156	-0.166536

TS19



Imaginary Vibrational Frequency = -358.0168 cm^{-1}
Zero-point correction= 0.201278 (Hartree/Particle)
Sum of electronic and zero-point Energies= -1293.227011
Sum of electronic and thermal Energies= -1293.212634
Sum of electronic and thermal Enthalpies= -1293.211690
Sum of electronic and thermal Free Energies= -1293.269746

C	1.758039	-1.763198	-0.859093
C	0.403566	-1.943331	-0.962249
C	-0.455105	-1.385562	0.004287
C	0.135011	-0.716862	1.089085
C	1.498525	-0.573275	1.142905
N	2.299963	-1.076667	0.176508
H	2.453991	-2.144995	-1.601147
H	0.005751	-2.479343	-1.820883
H	-0.454518	-0.276649	1.888031
H	1.997925	-0.044332	1.951308

C	3.743267	-0.806233	0.240818
H	4.248738	-1.339342	-0.566666
H	3.909289	0.270878	0.129035
H	4.137798	-1.148424	1.201928
S	-2.164603	-1.588341	-0.240038
C	-2.889345	-0.391343	0.947879
C	-2.565534	1.042760	0.680173
H	-2.643882	-0.688391	1.974662
H	-3.968435	-0.575897	0.832293
H	-2.302461	1.655243	1.545641
C	-2.570421	1.625288	-0.564020
H	-2.516704	2.706133	-0.659515
H	-2.919638	1.080875	-1.438412
N	-0.576335	1.412586	-1.238845
C	0.292986	1.998387	-0.645166
S	1.524407	2.708000	0.093796

Notes and references

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