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Supporting Information

Unravelling the factors affecting the stability and reactivity of dehydro- pyrazole, isothiazole and isoxazole radical isomers: A computational study

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Table S1. Electronic and thermodynamic parameters of all parent molecules, their respective radical isomers, ring-opened and fragmented products and transition states at both B3LYP/cc-pVTZ (normal) and M06-2X/cc-pVTZ (italics) levels of theory.

Species	Thermal corrected Electronic energy (E) (Hartree)	ZPVE (Hartree)	Lowest frequency (cm^{-1})	Spin Contamination		Point group	Electronic state	Free Energy (G) (Hartree)	Enthalpy (H) (Hartree)	Entropy (S) (Cal/Mol-Kelvin)
				Before annhilation	After annhilation					
1	-226.209748	0.071140	531.70	0.0000	0.0000	C_S	^{1}A'	-226.239729	-226.208804	65.086
	-226.114545	*0.071914*	*562.04*	*0.0000*	*0.0000*	*C_S*	*$^1A'$*	*-226.144448*	*-226.113601*	*64.922*
1a	-225.538307	0.055377	423.77	0.7663	0.7500	C_{2v}	$^2A_2$	-225.568524	-225.537363	65.585
	-225.442220	*0.056248*	*473.65*	*0.7653*	*0.7500*	*C_{2v}*	*$^2A_2$*	*-225.472331*	*-225.441276*	*65.362*
TS_{1a-4}	-225.467189	0.051063	353.77i	0.7613	0.7501	C_1	^{2}A	-225.500069	-225.466245	71.190
	-225.363794	*0.052613*	*396.35i*	*0.7698*	*0.7502*	*C_1*	*^2A*	*-225.395432*	*-225.362849*	*68.575*
4	-225.483340	0.052217	158.75	0.7649	0.7501	C_S	^{2}A'	-225.517202	-225.482396	73.255
	-225.382007	*0.053213*	*158.98*	*0.7765*	*0.7502*	*C_S*	*$^2A'$*	*-225.415712*	*-225.381063*	*72.925*
$TS_{4-5,6}$	-225.433484	0.047995	461.24i	0.7729	0.7503	C_1	^{2}A	-225.469120	-225.432540	76.989
	-225.326151	*0.048891*	*524.30i*	*0.7767*	*0.7504*	*C_1*	*^2A*	*-225.361386*	*-225.325206*	*76.147*
5	-148.111012	0.018682	484.77	0.7653	0.7501	C_S	^{2}A"	-148.137955	-148.110068	58.694
	-148.042586	*0.018971*	*499.55*	*0.7679*	*0.7501*	*C_S*	*$^2A"$*	*-148.069520*	*-148.041641*	*58.675*
6	-77.333757	0.026986	649.91	0.0000	0.0000	$D_{\infty H}$	$^1\sum_g$	-77.355515	-77.332812	47.782
	-77.294242	*0.027520*	*712.49*	*0.0000*	*0.0000*	*$D_{\infty H}$*	*$^1\sum_g$*	*-77.315896*	*-77.293298*	*47.560*
7	-225.461158	0.050629	96.59	1.7666	0.8063	C_1	^{2}A	-225.495490	-225.460214	74.244
	-225.347915	*0.051291*	*106.59*	*1.7603*	*0.7848*	*C_1*	*^2A*	*-225.382202*	*-225.346970*	*74.152*
7-q	-225.476599	0.050967	125.01	3.8237	3.7517	C_1	^{4}A	-225.511174	-225.475655	74.755
	-225.370200	*0.051388*	*118.74*	*3.8438*	*3.7527*	*C_1*	*^4A*	*-225.404781*	*-225.369256*	*74.768*
$TS_{7-8,9}$	-225.400888	0.044434	230.60i	0.7875	0.7508	C_1	^{2}A	-225.436574	-225.399944	77.095
	-225.288058	*0.045379*	*423.14i*	*0.8034*	*0.7515*	*C_1*	*^2A*	*-225.323227*	*-225.287114*	*76.006*
8	-132.021325	0.029690	221.51	0.7538	0.7500	C_S	^{2}A	-132.049704	-132.020380	61.717
	-131.964919	*0.030955*	*523.54*	*0.7535*	*0.7500*	*C_S*	*^2A*	*-131.992590*	*-131.963974*	*60.227*
9	-93.445024	0.016348	762.08	0.0000	0.0000	$C_{\infty V}$	$^1\sum$	-93.464383	-93.441539	48.079
	-93.403545	*0.016580*	*787.95*	*0.0000*	*0.0000*	*$C_{\infty V}$*	*$^1\sum$*	*-93.425418*	*-93.402601*	*48.022*
TS_{8-10}	-131.931554	0.025019	1405.00i	0.7564	0.7500	C_1	^{2}A	-131.959016	-131.930610	59.785
	-131.877273	*0.025839*	*1284.36i*	*0.7554*	*0.7500*	*C_1*	*^2A*	*-131.904667*	*-131.876329*	*59.644*
10	-132.053915	0.031300	421.99	0.7585	0.7500	C_S	^{2}A'	-132.053915	-132.025176	60.486
	-131.969225	*0.031831*	*512.10*	*0.7584*	*0.7500*	*C_S*	*$^2A'$*	*-131.996865*	*-131.968281*	*60.161*

$TS_{10\text{-}11}$	-132.023658	0.029404	504.58i	0.7754	0.7502	C_S	$^2A'$	-132.051534	-132.022714	60.656
	-131.961440	*0.029717*	*618.90i*	*0.7743*	*0.7502*	*C_S*	*$^2A'$*	*-131.989341*	*-131.960495*	*60.711*
11	-132.110859	0.030977	384.73	0.7672	0.7501	C_{2v}	$^2B_1$	-132.138074	-132.109915	59.267
	-132.047446	*0.031194*	*379.06*	*0.7676*	*0.7501*	*C_{2v}*	*$^2B_1$*	*-132.074697*	*-132.046502*	*59.343*
$TS_{1a\text{-}12,13}$	-225.437212	0.045748	275.60i	1.3403	0.7937	C_1	^2A	-225.472321	-225.436268	75.881
	-225.318436	*0.044772*	*365.67i*	*0.8079*	*0.7519*	*C_1*	*^2A*	*-225.353868*	*-225.317492*	*76.559*
12	-115.870744	0.038945	171.34	0.7863	0.7503	C_1	^2A	-115.900001	-115.869800	63.562
	-115.817001	*0.038918*	*345.28*	*1.7566*	*0.8153*	*C_1*	*^2A*	*-115.846013*	*-115.816056*	*63.048*
13	-109.560487	0.005582	2450.21	0.0000	0.0000	$D_{\infty H}$	$^1\sum_g$	-109.581273	-109.559542	45.735
	-109.524835	*0.005726*	*2513.41*	*0.0000*	*0.0000*	*$D_{\infty H}$*	*$^1\sum_g$*	*-109.545613*	*-109.523891*	*45.718*
$TS_{1a\text{-}1b}$	-225.365177	0.049755	1464.08i	0.7561	0.7500	C_1	^2A	-225.396100	-225.364243	67.071
	-225.273352	*0.050985*	*1345.96i*	*0.7565*	*0.7500*	*C_1*	*^2A*	*-225.304077*	*-225.272407*	*66.653*
1b	-225.525610	0.058101	458.79	0.7552	0.7500	C_S	$^2A'$	-225.556228	-225.524666	66.427
	-225.434250	*0.059118*	*501.24*	*0.7590*	*0.7500*	*C_S*	*$^2A'$*	*-225.464735*	*-225.433306*	*66.148*
$TS_{1b\text{-}14}$	-225.497250	0.053735	579.85i	0.7819	0.7502	C_1	^2A	-225.528412	-225.496306	67.572
	-225.393929	*0.054137*	*727.29i*	*0.7871*	*0.7504*	*C_1*	*^2A*	*-225.425058*	*-225.392984*	*67.505*
14	-225.571171	0.054611	166.09	0.7811	0.7505	C_1	^2A	-225.604577	-225.570227	72.296
	-225.469590	*0.055258*	*169.48*	*0.7804*	*0.7505*	*C_1*	*^2A*	*-225.502984*	*-225.468646*	*72.271*
$TS_{14\text{-}15}$	-225.484907	0.049411	1806.63i	0.7576	0.7500	C_1	^2A	-225.518345	-225.483963	72.364
	-225.383804	*0.050027*	*1775.21i*	*0.7581*	*0.7500*	*C_1*	*^2A*	*-225.417243*	*-225.382859*	*72.367*
15	-225.550883	0.054446	132.04	0.7533	0.7500	C_S	$^2A'$	-225.585210	-225.549939	74.235
	-225.453437	*0.055179*	*148.59*	*0.7544*	*0.7500*	*C_S*	*$^2A'$*	*-225.487587*	*-225.452493*	*73.862*
$TS_{15\text{-}16,11}$	-225.520412	0.049500	413.66i	0.7666	0.7502	C_S	$^2A'$	-225.556409	-225.519468	77.748
	-225.421530	*0.050040*	*467.40i*	*0.7654*	*0.7502*	*C_S*	*$^2A'$*	*-225.457330*	*-225.420586*	*77.335*
16	-93.420183	0.015618	469.89	0.0000	0.0000	$C_{\infty V}$	$^1\sum$	-93.442539	-93.419239	49.040
	-93.939131	*0.016016*	*530.61*	*0.0000*	*0.0000*	*$C_{\infty V}$*	*$^1\sum$*	*-93.405340*	*-93.382187*	*48.729*
$TS_{1b\text{-}17}$	-225.437219	0.052657	299.58i	0.7633	0.7501	C_1	^2A	-225.469333	-225.436274	69.578
	-225.341540	*0.053499*	*380.62i*	*0.7713*	*0.7503*	*C_1*	*^2A*	*-225.373389*	*-225.373389*	*69.018*
17	-225.444293	0.052794	136.07	0.7596	0.7500	C_1	^2A	-225.478580	-225.443349	74.149
	-225.351668	*0.053981*	*146.68*	*0.7661*	*0.7501*	*C_1*	*^2A*	*-225.385567*	*-225.350724*	*73.332*
$TS_{17\text{-}18,6}$	-225.415985	0.048836	543.10i	0.7736	0.7503	C_1	^2A	-225.451774	-225.415040	77.312
	-225.314270	*0.049592*	*622.53i*	*0.7761*	*0.7504*	*C_1*	*^2A*	*-225.349751*	*-225.313326*	*76.661*
18	-148.099919	0.019397	363.80	0.7602	0.7500	C_1	^2A	-148.127316	-148.098974	59.650
	-148.037374	*0.019712*	*383.29*	*0.7624*	*0.7500*	*C_1*	*^2A*	*-148.064693*	*-148.036430*	*59.485*
$TS_{1a\text{-}1c}$	-225.345192	0.049375	1570.96i	0.7541	0.7500	C_1	^2A	-225.376110	-225.34428	67.060
	-225.254441	*0.050932*	*1386.80i*	*0.7556*	*0.7500*	*C_1*	*^2A*	*-225.285116*	*-225.253497*	*66.547*
$TS_{1b\text{-}1c}$	-225.405898	0.051783	1605.51i	0.7674	0.7501	C_1	^2A	-225.436500	-225.404954	66.394
	-225.309543	*0.052749*	*1345.51i*	*0.7660*	*0.7500*	*C_1*	*^2A*	*-225.340086*	*-225.308599*	*66.271*
1c	-225.520154	0.058529	511.55	0.7561	0.7500	C_S	$^2A'$	-225.550681	-225.519210	66.236
	-225.428529	*0.059350*	*548.71*	*0.7592*	*0.7500*	*C_S*	*$^2A'$*	*-225.458953*	*-225.427585*	*66.020*

TS_{1c-29}	-225.453180	0.052712	554.26i	0.7821	0.7503	C_1	^{2}A	-225.484794	-225.452236	68.524
	-225.347765	*0.053068*	*614.19i*	*0.7829*	*0.7503*	*C_1*	*^{2}A*	*-225.379440*	*-225.346820*	*68.655*
29	-225.489908	0.052915	149.82	0.7623	0.7501	C_1	^{2}A	-225.523692	-225.488963	73.094
	-225.385747	*0.053803*	*155.11*	*0.7582*	*0.7500*	*C_1*	*^{2}A*	*-225.419377*	*-225.384803*	*72.767*
TS_{29-30}	-225.381201	0.045496	1603.57i	0.7754	0.7504	C_1	^{2}A	-225.415501	-225.380257	74.177
	-225.270293	*0.046388*	*1609.97i*	*0.7855*	*0.7508*	*C_1*	*^{2}A*	*-225.304518*	*-225.269349*	*74.020*
30	-225.445476	0.051265	36.18	0.7714	0.7501	C_1	^{2}A	-225.481495	-225.444532	77.796
	-225.340307	*0.052373*	*103.16*	*0.7895*	*0.7504*	*C_1*	*^{2}A*	*-225.375307*	*-225.339363*	*75.651*
$TS_{30-6,18}$	-225.412599	0.048577	548.93i	0.7901	0.7505	C_1	^{2}A	-225.448794	-225.411655	78.166
	-225.306668	*0.049242*	*692.73i*	*0.8074*	*0.7510*	*C_1*	*^{2}A*	*-225.342580*	*-225.305724*	*77.570*
TS_{1a-1d}	-225.448258	0.051674	1614.92i	0.7570	0.7500	C_1	^{2}A	-225.478652	-225.447314	65.956
	-225.354859	*0.052837*	*1531.84i*	*0.7580*	*0.7500*	*C_1*	*^{2}A*	*-225.385143*	*-225.353915*	*65.725*
TS_{1b-1d}	-225.324366	0.050729	899.56i	0.7576	0.7500	C_1	^{2}A	-225.355172	-225.323422	66.825
	-225.232119	*0.051895*	*835.92i*	*0.7592*	*0.7501*	*C_1*	*^{2}A*	*-225.262834*	*-225.231175*	*66.633*
TS_{1c-1d}	-225.424126	0.052350	1345.54i	0.7570	0.7500	C_1	^{2}A	-225.454666	-225.423182	66.264
	-225.332171	*0.053578*	*1178.88i*	*0.7581*	*0.7500*	*C_1*	*^{2}A*	*-225.362505*	*-225.331226*	*65.831*
1d	-225.521793	0.058172	444.88	0.7570	0.7500	C_S	^{2}A'	-225.552422	-225.520849	66.452
	-225.429911	*0.059205*	*513.80*	*0.7606*	*0.7500*	*C_S*	*^{2}A'*	*-225.460371*	*-225.428966*	*66.097*
TS_{1d-35}	-225.485375	0.053733	548.14i	0.7925	0.7503	C_1	^{2}A	-225.516400	-225.484431	67.283
	-225.379069	*0.054117*	*710.09i*	*0.7996*	*0.7506*	*C_1*	*^{2}A*	*-225.410064*	*-225.378125*	*67.221*
35	-225.535094	0.053106	145.29	0.7618	0.7501	C_1	^{2}A	-225.569101	-225.534150	73.561
	-225.432604	*0.053629*	*138.31*	*0.7669*	*0.7501*	*C_1*	*^{2}A*	*-225.466636*	*-225.431660*	*73.614*
$TS_{35-36,9}$	-225.491002	0.048243	545.83i	0.7764	0.7504	C_1	^{2}A	-225.527415	-225.490058	78.623
	-225.386664	*0.048892*	*616.67i*	*0.7816*	*0.7507*	*C_1*	*^{2}A*	*-225.422678*	*-225.385720*	*77.784*
36	-132.064425	0.029449	338.99	0.7686	0.7501	C_1	^{2}A	-132.092451	-132.063480	60.974
	-132.998971	*0.029761*	*421.59*	*0.7744*	*0.7502*	*C_1*	*^{2}A*	*-132.026778*	*-132.998027*	*60.511*
TS_{1d-37}	-225.431253	0.051915	427.35i	0.7805	0.7504	C_1	^{2}A	-225.463523	-225.430308	69.905
	-225.330303	*0.052578*	*548.48i*	*0.7858*	*0.7507*	*C_1*	*^{2}A*	*-225.362357*	*-225.329359*	*69.450*
37	-225.448855	0.052307	156.66	0.7555	0.7500	C_1	^{2}A	-225.483308	-225.447911	74.500
	-225.350470	*0.053444*	*164.73*	*0.7593*	*0.7500*	*C_1*	*^{2}A*	*-225.384456*	*-225.349526*	*73.516*
$TS_{37-36,9}$	-225.440801	0.049325	707.06i	0.7692	0.7501	C_1	^{2}A	-225.475566	-225.439856	75.157
	-225.337547	*0.050046*	*827.65i*	*0.7701*	*0.7502*	*C_1*	*^{2}A*	*-225.372004*	*-225.336603*	*74.508*
2	-569.083714	0.054970	485.57	0.0000	0.0000	C_S	^{1}A'	-569.114679	-569.082770	67.158
	-568.979504	*0.055780*	*492.58*	*0.0000*	*0.0000*	*C_S*	*^{1}A'*	*-568.010385*	*-568.978559*	*66.983*
2b	-568.411064	0.042106	463.57	0.7569	0.7500	C_S	^{2}A'	-568.442745	-568.410119	68.667
	-568.308843	*0.042946*	*476.40*	*0.7605*	*0.7501*	*C_S*	*^{2}A'*	*-568.340351*	*-568.307899*	*68.301*
TS_{2b-19}	-568.405425	0.040696	377.18i	0.7739	0.7501	C_S	^{2}A'	-568.437247	-568.404481	68.962
	-568.297535	*0.041293*	*585.38i*	*0.7778*	*0.7502*	*C_S*	*^{2}A'*	*-568.329294*	*-568.296590*	*68.830*
19	-568.441109	0.040654	139.12	0.7823	0.7504	C_S	^{2}A''	-568.475596	-568.440165	74.572
	-568.328971	*0.041040*	*111.34*	*0.7543*	*0.7500*	*C_S*	*^{2}A'*	*-568.363838*	*-568.328027*	*75.369*

$TS_{19\text{-}20}$	-568.364269	0.036139	1521.40i	0.7542	0.7500	C_1	^{2}A	-568.398792	-568.363324	74.647
	-568.255636	*0.036790*	*1478.04i*	*0.7543*	*0.7500*	*C_1*	*^2A*	*-568.290168*	*-568.254692*	*74.666*
20	-568.414385	0.040673	116.35	0.7555	0.7500	C_S	^{2}A'	-568.449700	-568.413441	76.313
	-568.307944	*0.041403*	*113.49*	*0.7571*	*0.7500*	*C_S*	*$^2A'$*	*-568.343180*	*-568.307000*	*76.147*
$TS_{20\text{-}11,21}$	-568.362097	0.035849	225.17i	0.7739	0.7504	C_S	^{2}A'	-568.400127	-568.361152	82.030
	-568.251277	*0.036754*	*338.71i*	*0.7751*	*0.7504*	*C_S*	*$^2A'$*	*-568.288495*	*-568.250332*	*80.219*
21	-436.253980	0.002969	1303.24	0.0000	0.0000	$C_{\infty V}$	$^1\sum$	-436.276927	-436.253036	50.283
	-436.204808	*0.003036*	*1332.73*	*0.0000*	*0.0000*	*$C_{\infty V}$*	*$^1\sum$*	*-436.227741*	*-436.203863*	*50.255*
$TS_{2b\text{-}22}$	-568.330194	0.036514	246.31i	0.7632	0.7501	C_S	^{2}A'	-568.363812	-568.329250	72.743
	-568.174612	*0.037993*	*93.77i*	*0.7577*	*0.7500*	*C_S*	*$^2A''$*	*-568.208004*	*-568.173668*	*72.266*
22	-568.335114	0.036499	117.00	0.7604	0.7501	C_S	^{2}A'	-568.371166	-568.334169	77.866
	-568.233963	*0.037714*	*121.80*	*0.7679*	*0.7501*	*C_S*	*$^2A'$*	*-568.269513*	*-568.233019*	*76.809*
$TS_{22\text{-}6,23}$	-568.324739	0.034885	334.35i	0.7701	0.7502	C_S	^{2}A'	-568.362093	-568.323795	80.605
	-568.219017	*0.035550*	*380.39i*	*0.7721*	*0.7502*	*C_S*	*$^2A'$*	*-568.255915*	*-568.218073*	*79.645*
23	-77.333757	0.026986	649.96	0.0000	0.0000	$D_{\infty H}$	$^1\sum_g$	-77.355516	-77.332813	47.782
	-77.294242	*0.027520*	*712.50*	*0.0000*	*0.0000*	*$D_{\infty H}$*	*$^1\sum_g$*	*-77.315896*	*-77.293298*	*47.560*
$TS_{2b\text{-}2c}$	-568.283406	0.034720	2338.27i	0.7751	0.7502	C_1	^{2}A	-568.315536	-568.282461	69.611
	-568.177599	*0.035288*	*2596.05i*	*0.7739*	*0.7502*	*C_1*	*^2A*	*-568.209846*	*-568.176654*	*69.858*
2c	-568.400778	0.042340	469.17	0.7570	0.7500	C_S	^{2}A'	-568.432331	-568.399833	68.398
	-568.299109	*0.043209*	*481.38*	*0.7612*	*0.7501*	*C_S*	*$^2A'$*	*-568.330535*	*-568.298165*	*68.129*
$TS_{2c\text{-}31}$	-568.364387	0.03965	389.76i	0.7804	0.7503	C_S	^{2}A'	-568.396714	-568.363443	70.024
	-568.254749	*0.040208*	*432.79i*	*0.7789*	*0.7504*	*C_S*	*$^2A'$*	*-568.286994*	*-568.253805*	*69.852*
31	-568.390143	0.040073	108.14	0.7596	0.7501	C_S	^{2}A'	-568.424946	-568.389199	75.237
	-568.279384	*0.040802*	*99.71*	*0.7604*	*0.7501*	*C_S*	*$^2A'$*	*-568.314150*	*-568.278439*	*75.158*
$TS_{31\text{-}32}$	-568.294330	0.031464	1679.91i	0.7730	0.7503	C_S	^{2}A'	-568.329336	-568.293386	75.663
	-568.175250	*0.031773*	*1835.47i*	*0.7809*	*0.7505*	*C_S*	*$^2A'$*	*-568.210153*	*-568.174305*	*75.447*
32	-568.357596	0.038640	98.52	0.7704	0.7501	C_S	^{2}A'	-568.392699	-568.356652	75.868
	-568.245675	*0.039596*	*104.54*	*0.7829*	*0.7503*	*C_S*	*$^2A'$*	*-568.280515*	*-568.244731*	*75.313*
$TS_{32\text{-}6,23}$	-568.313916	0.035579	504.10i	0.7818	0.7503	C_1	^{2}A	-568.351012	-568.312972	80.063
	-568.200039	*0.036152*	*638.18i*	*0.7985*	*0.7506*	*C_1*	*^2A*	*-568.236786*	*-568,199095*	*79.327*
$TS_{2b\text{-}2d}$	-568.205935	0.035140	1007.39i	0.7660	0.7501	C_1	^{2}A	-568.238064	-568.204990	69.608
	-568.105937	*0.036173*	*1027.32i*	*0.7649*	*0.7501*	*C_1*	*^2A*	*-568.137851*	*-568.104993*	*69.155*
$TS_{2c\text{-}2d}$	-568.309703	0.036178	1298.59i	0.7590	0.7500	C_1	^{2}A	-568.341514	-568.308759	68.938
	-568.207550	*0.036851*	*1100.26i*	*0.7600*	*0.7501*	*C_1*	*^2A*	*-568.239198*	*-568.206605*	*68.597*
2d	-568.399299	0.042506	440.47	0.7589	0.7500	C_S	^{2}A'	-568.430850	-568.398355	68.392
	-568.297802	*0.043334*	*465.13*	*0.7635*	*0.7501*	*C_S*	*$^2A'$*	*-568.329231*	*-568.296857*	*68.136*
$TS_{2d\text{-}38}$	-568.368356	0.039869	326.42i	0.8180	0.7507	C_S	^{2}A'	-568.400391	-568.367412	69.411
	-568.254627	*0.040362*	*425.66i*	*0.8296*	*0.7513*	*C_S*	*$^2A'$*	*-568.286589*	*-568.253682*	*69.259*
38	-568.399045	0.039148	122.34	0.7629	0.7501	C_S	^{2}A'	-568.434107	-568.398101	75.781
	-568.286571	*0.039654*	*117.05*	*0.7686*	*0.7501*	*C_S*	*$^2A'$*	*-568.321731*	*-568.285627*	*75.988*

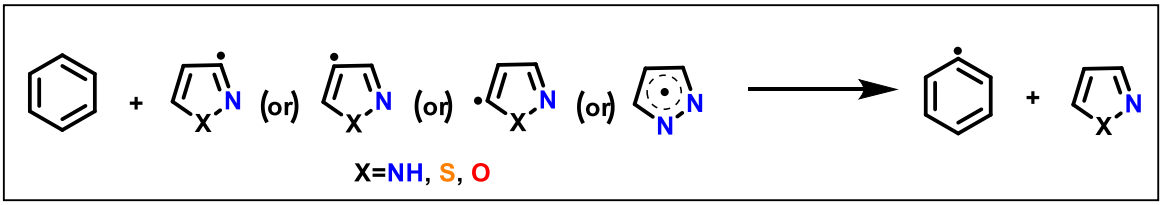
$TS_{38\text{-}39,9}$	-568.366417	0.035540	594.75i	0.7778	0.7504	C_1	^{2}A	-568.402932	-568.365473	78.839
	-568.253009	*0.036035*	*700.09i*	*0.7890*	*0.7508*	*C_1*	*^{2}A*	*-568.289290*	*-568.252065*	*78.348*
39	-474.944279	0.018211	747.72	0.7653	0.7501	$C_{\infty V}$	-	-474.971318	-474.943335	58.895
	-474.871254	*0.018482*	*336.16*	*0.7700*	*0.7501*	*$C_{\infty V}$*	-	*-474.898137*	*-474.870310*	*58.567*
$TS_{2d\text{-}40}$	-568.323304	0.036150	417.08i	0.7684	0.7502	C_S	^{2}A'	-568.356757	-568.322360	72.395
	-568.215718	*0.036931*	*481.68i*	*0.7722*	*0.7503*	*C_S*	*^{2}A'*	*-568.248859*	*-568.214774*	*71.738*
40	-568.338173	0.036257	124.52	0.7564	0.7500	C_S	^{2}A'	-568.374143	-568.337229	77.693
	-568.230802	*0.037495*	*128.91*	*0.7586*	*0.7500*	*C_S*	*^{2}A'*	*-568.266228*	*-568.229858*	*76.547*
$TS_{40\text{-}39,9}$	-568.339075	0.035031	369.66i	0.7613	0.7501	C_S	^{2}A'	-568.374814	-568.338131	77.208
	-568.229868	*0.035656*	*592.40i*	*0.7662*	*0.7501*	*C_S*	*^{2}A'*	*-568.265330*	*-568.228923*	*76.624*
3	-246.064665	0.057820	610.24	0.0000	0.0000	C_S	^{1}A'	-246.094429	-246.063720	64.631
	-245.964623	*0.058834*	*620.50*	*0.0000*	*0.0000*	*C_S*	*^{1}A'*	*-245.994296*	*-245.963678*	*64.439*
3b	-245.381102	0.044512	576.43	0.7568	0.7500	C_S	^{2}A'	-245.411543	-245.380158	66.055
	-245.284065	*0.045843*	*607.49*	*0.7609*	*0.7501*	*C_S*	*^{2}A'*	*-245.314315*	*-245.283121*	*65.655*
$TS_{3b\text{-}24}$	-245.378062	0.042460	492.83i	0.7780	0.7502	C_S	^{2}A'	-245.408660	-245.377118	66.386
	-245.271786	*0.042918*	*633.82i*	*0.7917*	*0.7505*	*C_S*	*^{2}A'*	*-245.302405*	*-245.270841*	*66.431*
24	-245.462041	0.041907	159.49	0.7729	0.7504	C_1	^{2}A	-245.495445	-245.461097	72.291
	-245.358088	*0.042669*	*161.78*	*0.7746*	*0.7504*	*C_1*	*^{2}A*	*-245.391443*	*-245.357144*	*72.188*
$TS_{24\text{-}25}$	-245.391404	0.037807	1606.44i	0.7541	0.7500	C_1	^{2}A	-245.424509	-245.390460	71.663
	-245.287093	*0.038521*	*1572.63i*	*0.7558*	*0.7500*	*C_1*	*^{2}A*	*-245.320151*	*-245.286148*	*71.565*
25	-245.455733	0.042457	129.26	0.7532	0.7500	C_1	^{2}A	-245.489903	-245.454789	73.902
	-245.355890	*0.043227*	*137.73*	*0.7536*	*0.7500*	*C_1*	*^{2}A*	*-245.389916*	*-245.354916*	*73.602*
$TS_{25\text{-}26,11}$	-245.444196	0.039098	402.73i	0.7655	0.7502	C_S	^{2}A'	-245.480529	-245.443251	78.458
	-245.342910	*0.039512*	*446.43i*	*0.7659*	*0.7502*	*C_S*	*^{2}A'*	*-245.378683*	*-245.341966*	*77.277*
26	-113.349855	0.005038	2211.46	0.0000	0.0000	$C_{\infty V}$	$^1\sum$	-113.371334	-113.348911	47.195
	-113.311338	*0.005156*	*2263.37*	*0.0000*	*0.0000*	*$C_{\infty V}$*	*$^1\sum$*	*-113.332811*	*-113.310394*	*47.179*
$TS_{3b\text{-}27}$	-245.286134	0.039232	255.02i	0.7608	0.7501	C_S	^{2}A'	-245.318258	-245.285189	69.599
	-245.188278	*0.040463*	*351.60i*	*0.7692*	*0.7502*	*C_S*	*^{2}A'*	*-245.219981*	*-245.187334*	*68.712*
27	-245.290516	0.039522	134.50	0.7589	0.7500	C_1	^{2}A	-245.324693	-245.289571	73.920
	-245.195892	*0.040700*	*146.96*	*0.7651*	*0.7501*	*C_1*	*^{2}A*	*-245.229665*	*-245.194948*	*73.069*
$TS_{27\text{-}28,6}$	-245.273431	0.036546	510.57i	0.7706	0.7502	C_1	^{2}A	-245.308802	-245.272487	76.432
	-245.166917	*0.037057*	*606.68i*	*0.7752*	*0.7503*	*C_1*	*^{2}A*	*-245.202514*	*-245.165972*	*76.907*
28	-167.956534	0.007880	326.48	0.7574	0.7500	$C_{\infty V}$	^{2}A'	-167.977600	-167.955590	46.325
	-167.889105	*0.009283*	*390.40*	*0.7610*	*0.7500*	*$C_{\infty V}$*	*^{2}A'*	*-167.914116*	*-167.888161*	*54.627*
$TS_{3b\text{-}3c}$	-245.252253	0.037168	2119.66i	0.7758	0.7502	C_1	^{2}A	-245.283200	-245.251309	67.120
	-245.148485	*0.038290*	*3135.72i*	*0.7754*	*0.7502*	*C_1*	*^{2}A*	*-245.179263*	*-245.147540*	*66.767*
3c	-245.373346	0.045212	547.67	0.7566	0.7500	C_S	^{2}A'	-245.403650	-245.372402	65.767
	-245.276616	*0.046379*	*573.47*	*0.7601*	*0.7500*	*C_S*	*^{2}A'*	*-245.306797*	*-245.275671*	*65.509*
$TS_{3c\text{-}33}$	-245.325493	0.041256	601.51i	0.8008	0.7509	C_S	^{2}A'	-245.306797	-245.324549	65.509
	-245.214241	*0.041750*	*838.96i*	*0.8153*	*0.7517*	*C_S*	*^{2}A'*	*-245.245203*	*-245.213297*	*67.152*

33	-245.372816	0.041956	151.42	0.7623	0.7501	C_S	^{2}A'	-245.406073	-245.371871	71.983
	-245.265674	*0.042849*	*152.46*	*0.7667*	*0.7501*	*C_S*	*$^2A'$*	*-245.298768*	*-245.264730*	*71.640*
TS_{33-34}	-245.268474	0.032475	1771.09i	0.7802	0.7505	C_1	^{2}A	-245.302523	-245.267530	73.648
34	-245.339224	0.040699	95.87	0.7654	0.7501	C_S	^{2}A'	-245.373186	-245.338280	73.466
	-245.231472	*0.041738*	*117.58*	*0.7768*	*0.7502*	*C_S*	*$^2A'$*	*-245.265025*	*-245.230528*	*72.605*
$TS_{34-6,28}$	-245.284761	0.037141	347.87i	0.7731	0.7502	C_S	^{2}A'	-245.321049	-245.283817	78.362
	-245.175209	*0.038045*	*461.19i*	*0.7861*	*0.7505*	*C_S*	*$^2A'$*	*-245.210534*	*-245.174265*	*76.336*
TS_{3b-3d}	-245.165290	0.036854	887.15i	0.8542	0.7515	C_1	^{2}A	-245.196309	-245.164346	67.272
	-245.064590	*0.038014*	*930.77i*	*0.9120*	*0.7525*	*C_1*	*^2A*	*-245.095511*	*-245.063646*	*67.065*
TS_{3c-3d}	-245.271510	0.037658	1376.91i	0.7562	0.7500	C_1	^{2}A	-245.302134	-245.270565	66.442
	-245.173564	*0.039535*	*1240.52i*	*0.7588*	*0.7500*	*C_1*	*^2A*	*-245.203831*	*-245.172620*	*65.689*
3d	-245.378335	0.044608	571.45	0.7585	0.7500	C_S	^{2}A'	-245.408754	-245.377391	66.009
	-245.281273	*0.045896*	*602.76*	*0.7619*	*0.7501*	*C_S*	*$^2A'$*	*-245.311505*	*-245.280329*	*65.614*
TS_{3d-41}	-245.374552	0.042302	492.82i	0.7793	0.7502	C_1	^{2}A	-245.405097	-245.373608	66.276
	-245.265975	*0.042452*	*701.25i*	*0.7957*	*0.7504*	*C_1*	*^2A*	*-245.296566*	*-245.265031*	*66.371*
41	-245.378339	0.044605	571.72	0.7586	0.7500	C_1	^{2}A'	-245.408761	-245.377395	66.015
	-245.281340	*0.045842*	*605.65*	*0.7620*	*0.7501*	*C_1*	*$^2A'$*	*-245.311567*	*-245.280396*	*65.604*
$TS_{41-42,9}$	-245.359891	0.037492	685.13i	0.8018	0.7512	C_S	^{2}A''	-245.394316	-245.358947	74.440
	-245.396656	*0.037680*	*456.19i*	*0.7653*	*0.7501*	*C_S*	*2A*	*-245.431936*	*-245.395712*	*76.240*
42	-151.964235	0.018767	476.27	0.7578	0.7500	C_S	^{2}A''	-151.991200	-151.963291	58.741
	-151.896622	*0.018943*	*393.29*	*0.7617*	*0.7501*	*C_S*	*$^2A''$*	*-151.923601*	*-151.895678*	*58.770*

Table S2. Relative energies of the dehydro- pyrazole (**1a-1d**), isothiazole (**2b-2d**) and isoxazole (**3b-3d**) radicals at different levels of theory.

Radicals	Relative Energies (kcal/mol)				
	(U)B3LYP/cc-pVTZ	(U)B3LYP-GD3/cc-pVTZ	(U)M06-2X/cc-pVTZ	(U)CCSD(T)/cc-pVTZ//(U)B3LYP/cc-pVTZ	(U)CCSD(T)/cc-pVTZ//(U)M06-2X/cc-pVTZ
1a	0	0	0	0	0
1b	10.4	8.1	5.2	8.2	8.1
1c	11.5	11.6	8.9	11.4	11.3
1d	10.5	10.6	7.9	10.4	10.3
2b	0	0	0	0	0
2c	6.5	6.6	6.1	6.1	6.1
2d	7.4	7.4	7.0	6.5	6.5
3b	0	0	0	0	0
3c	4.9	5.0	4.7	4.3	4.3
3d	1.7	1.8	1.8	1.7	1.6

Table S3. Radical stabilization energies (RSEs) of the dehydro- pyrazole (**1a-1d**), isothiazole (**2b-2d**) and isoxazole (**3b-3d**) radicals at (U)B3LYP/cc-pVTZ and (U)M06-2X/cc-pVTZ levels of theory.



Radicals	Radical Stabilization Energies (kcal/mol)	
	(U)B3LYP/cc-pVTZ	(U)M06-2X/cc-pVTZ
1a	2.9	0.3
1b	-5.0	-4.7
1c	-8.5	-8.4
1d	-7.4	-7.4
2b	2.2	1.4
2c	-4.3	-4.7
2d	-5.2	-5.6

3b	-4.7	-4.8
3c	-9.5	-9.5
3d	-6.4	-6.6

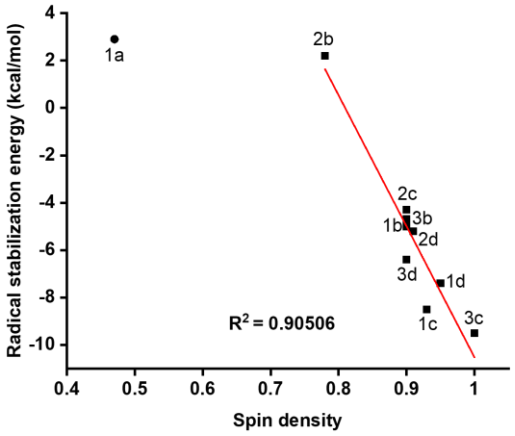


Figure S1. Correlation diagram of Radical stabilization energy with spin density.

Table S4. Bond dissociation energies (BDEs) of the dehydro- pyrazole (**1a-1d**), isothiazole (**2b-2d**) and isoxazole (**3b-3d**) radicals at B3LYP/cc-pVTZ (normal) and M06-2X/cc-pVTZ (italics) levels of theory.

Radicals	**BDE (kcal/mol)**			
	(U)B3LYP/cc-pVTZ	**(U)M06-2X/cc-pVTZ**	**CBS-QB3**	**G4**
1a	107.7	110.7	107.9	107.3
1b	115.7	115.8	115.5	116.6
1c	119.1	119.5	118.9	119.7
1d	118.1	118.5	117.8	118.6
2b	108.5	109.7	108.5	109.5
2c	114.9	115.8	114.9	115.6
2d	115.8	116.7	115.7	116.4
3b	115.3	115.9	115.2	116.3
3c	120.2	120.6	120.1	120.8
3d	117.0	117.3	117.0	117.6

Table S5. Resonance stabilization energies of the dehydro- pyrazole (**1a-1d**), isothiazole (**2b-2d**) and isoxazole (**3b-3d**) radicals at B3LYP/cc-pVTZ (normal) and M06-2X/cc-pVTZ (italics) levels of theory.

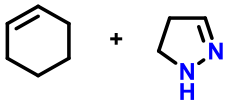
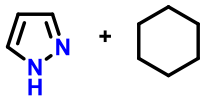
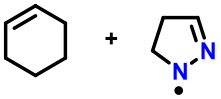
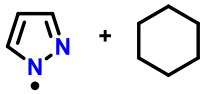
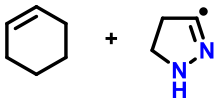
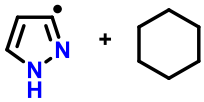
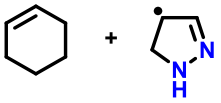
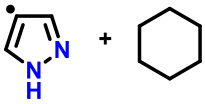
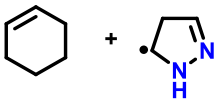
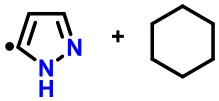
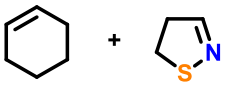
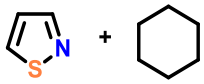
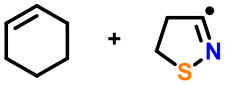
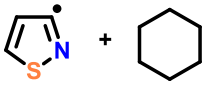
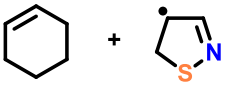
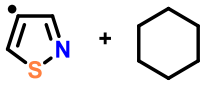
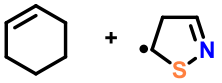
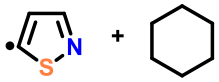
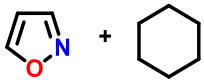
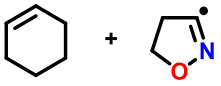
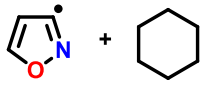
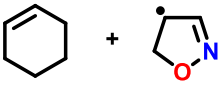
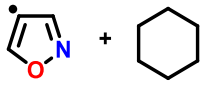
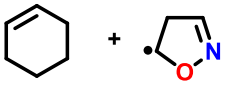
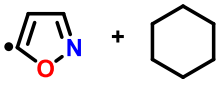
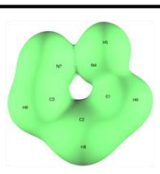
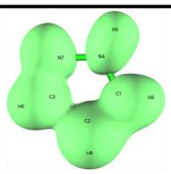
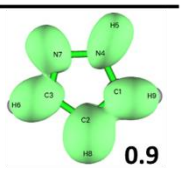
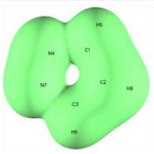
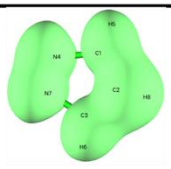
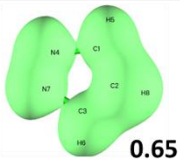
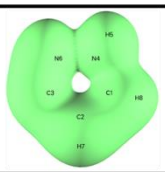
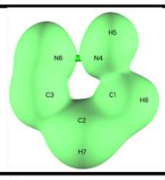
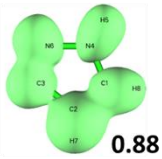
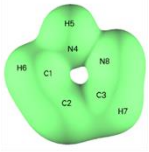
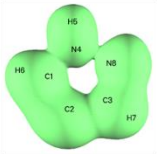
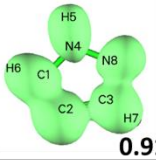
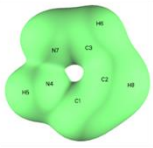
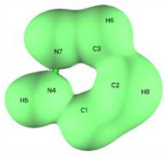
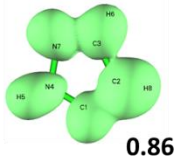
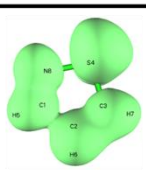
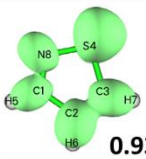
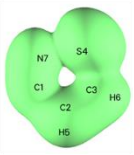
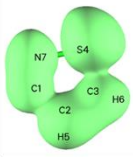
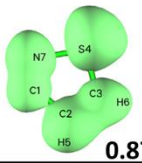
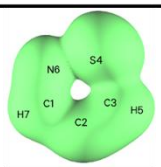
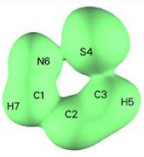
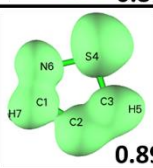
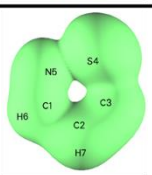
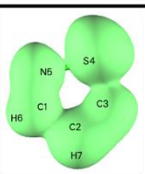
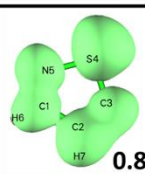
Reactants	Products	Resonance stabilization energy (ΔH) kcal/mol
		-21.6/*-23.6*
		3.1/0.4
		-15.8/*-18.7*
		21.1/*16.3*
		11.0/*6.3*
		-13.8/*-15.1*
		-7.8/*-9.9*
		25.2/*21.3*
		15.1/*11.8*
		-13.7/*-15.1*
		-9.4/*-11.4*
		28.3/*23.8*
		13.5/*10.4*

Table S6. Estimated $NICS_{zz}$ values at various position of probe atom along the perpendicular axis of the molecular plane of pyrazole **1**, isothiazole **2**, isoxazole **3**, and their dehydro- pyrazole (**1a-1d**), isothiazole (**2b-2d**) and isoxazole (**3b-3d**) radical isomers at B3LYP/cc-pVTZ level of theory.

Species	$NICS(0)_{zz}$	$NICS(0.5)_{zz}$	$NICS(1)_{zz}$	$NICS(1.5)_{zz}$	$NICS(2)_{zz}$
1	-17.1495	-29.5972	-33.5581	-24.5152	-15.7563
1a	39.2268	31.5318	12.4949	0.7971	-2.5566
1b	-15.3678	-26.5728	-29.8249	-21.6091	-13.8126
1c	-16.3026	-28.284	-31.2659	-22.3001	-14.1051
1d	-10.3691	-23.3447	-28.5772	-21.0505	-13.4869
2	-20.6192	-30.2524	-33.6632	-25.4424	-16.8545
2b	-17.0657	-25.6837	-28.827	-21.8289	-14.4828
2c	-17.3755	-27.6949	-31.3778	-23.4322	-15.3383
2d	-13.4948	-23.0521	-27.3931	-20.9148	-13.8296
3	-13.279	-25.0438	-29.088	-21.3311	-13.7499
3b	-8.2726	-19.0558	-23.3965	-17.3767	-11.2525
3c	-10.6962	-22.69	-26.5222	-19.1242	-12.1698
3d	-6.0448	-17.0623	-22.2184	-16.7453	-10.8786

Table S7. ELF_{σ}, ELF_{π} and average ELF bifurcation values of the studied systems.

Molecules	ELF_{σ}	ELF_{π}	Average
Parent 1	0.7	0.9	0.8
radical 1a	0.68	0.65	0.665
radical 1b	0.71	0.88	0.795
radical 1c	0.67	0.91	0.79
radical 1d	0.7	0.86	0.78
Parent 2	0.72	0.93	0.825
radical 2b	0.71	0.87	0.79
radical 2c	0.74	0.89	0.815
radical 2d	0.7	0.88	0.79
Parent 3	0.7	0.95	0.825
radical 3b	0.7	0.85	0.775
radical 3c	0.66	0.88	0.77
radical 3d	0.71	0.78	0.745

	0.3	0.7	
Parent 1			 0.9
Radical 1a			 0.65
Radical 1b			 0.88
Radical 1c			 0.91
Radical 1d			 0.86
Parent 2			 0.93
radical 2b			 0.87
radical 2c			 0.89
radical 2d			 0.88

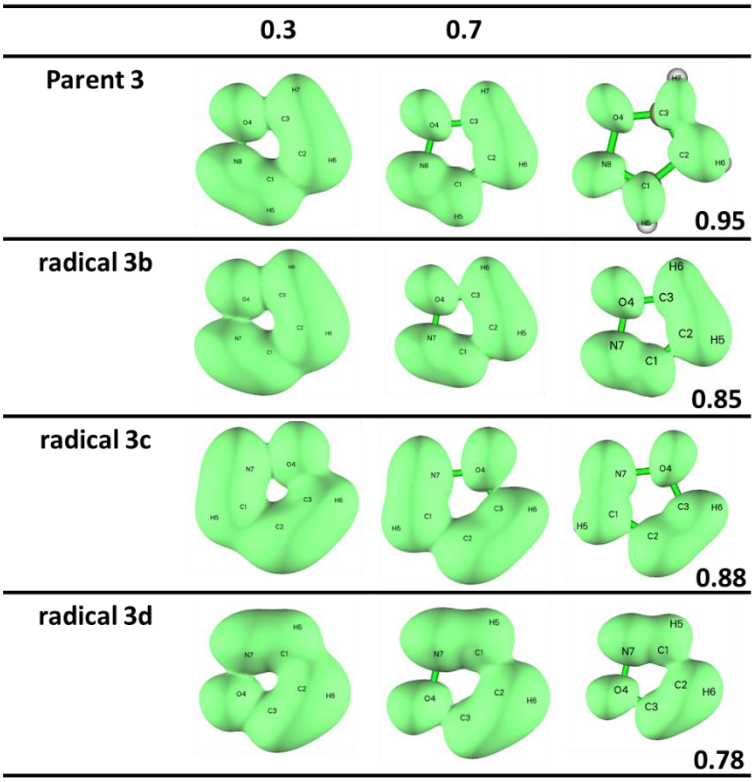
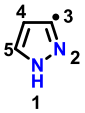


Figure S2. π localization domains of the pyrazole **1**, isothiazole **2**, isoxazole **3**, and their dehydro-pyrazole (**1a-1d**), isothiazole (**2b-2d**) and isoxazole (**3b-3d**) radical isomers for ELF_{π} = 0.3, 0.7, and their respective bifurcation value.

Table S8. The second order perturbation energies (in kcal/mol) for the selected interactions from the natural bond orbital (NBO) analysis for the α and β spins of the dehydro- pyrazole (**1a-1d**), isothiazole (**2b-2d**) and isoxazole (**3b-3d**) radicals at B3LYP/cc-pVTZ level of theory.

 **1b**				 **2b**				 **3b**			
Donor	**Acceptor**	**$E^{(2)}_{\alpha}$**	**$E^{(2)}_{\beta}$**	**Donor**	**Acceptor**	**$E^{(2)}_{\alpha}$**	**$E^{(2)}_{\beta}$**	**Donor**	**Acceptor**	**$E^{(2)}_{\alpha}$**	**$E^{(2)}_{\beta}$**
π_{C4-C5}	π^*_{C3-N2}	13.13	13.99	σ_{C4-C5}	σ^*_{C3-C4}	0.39	0.78	σ_{C4-C5}	n^*_{C3}	-	9.58
σ_{C4-C5}	n^*_{C3}	---	9.47	σ_{C4-C5}	π^*_{C3-N2}	10.78	---	σ_{C4-C5}	σ^*_{C3-C4}	-	0.48
σ_{C4-C5}	σ^*_{C3-C4}	---	0.58	σ_{C4-C5}	n^*_{C3}	---	7.72	π_{C4-C5}	π^*_{C3-N2}	12.23	13.16
π^*_{C4-C5}	π^*_{C3-C4}	---	31.33	π_{C2-C3}	π^*_{C3-N2}	---	11.27	π^*_{C4-C5}	π^*_{C3-N2}	58.37	20.63
σ_{N1-N2}	n^*_{C3}	---	6.30	π^*_{C4-C5}	π^*_{C3-N2}	48.59	23.58	σ_{O1-N2}	n^*_{C3}	-	8.57
σ_{C4-H7}	σ^*_{C3-C4}	0.36	---	σ_{S1-N2}	σ^*_{C3-C4}	0.38	-	σ^*_{O1-N2}	σ^*_{C3-C4}	0.78	---
σ_{C4-H7}	σ^*_{C3-N2}	0.88	0.86	σ_{S1-N2}	n^*_{C3}	-	14.01	n_{C3}	σ^*_{C4-C5}	2.09	---
n_{C3}	σ^*_{C4-C5}	2.59	---	σ^*_{S1-N2}	σ^*_{C3-C4}	0.60	---	n_{C3}	σ^*_{O1-N2}	10.54	---
n_{C3}	σ^*_{N1-N2}	5.77	---	n_{C3}	σ^*_{C4-C5}	3.14	---	$n1_{O1}$	σ^*_{C3-N2}	0.90	1.03
n_{N1}	π^*_{C3-N2}	13.63	10.48	n_{C3}	σ^*_{S1-N2}	11.23	---	$n2_{O1}$	π^*_{C3-N2}	6.39	5.05
n_{N2}	σ^*_{C3-C4}	3.24	2.56	$n1_{S1}$	σ^*_{C3-N2}	1.05	1.35	n_{N2}	σ^*_{C3-C4}	3.21	2.92

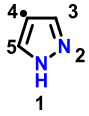
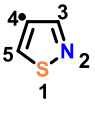
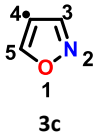
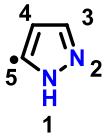
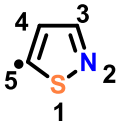
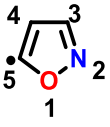
n_{N2}	n^*_{C3}	---	7.32	$n2_{S1}$	π^*_{C3-N2}	6.54	5.11	n_{N2}	n^*_{C3}	-	4.81
				n_{N2}	n^*_{C3}	---	7.05	σ_{C4-H6}	σ^*_{C3-N2}	0.85	0.83
				n_{N2}	σ^*_{C3-C4}	4.49	3.39	σ_{C4-H6}	σ^*_{C3-C4}	0.32	-
				σ_{C4-H6}	σ^*_{C3-N2}	1.16	1.12				
 1c				 2c				 3c			
σ_{C3-N2}	π^*_{C4-C5}	6.77	---	σ_{C3-N2}	σ^*_{C3-C4}	0.39	0.61	σ_{C3-N2}	σ^*_{C1-C2}	0.31	0.49
π_{C3-N2}	π^*_{C4-C5}	---	7.92	σ_{C3-N2}	n^*_{C4}	---	5.0	σ_{C3-N2}	n^*_{C2}	---	5.85
π^*_{C3-N2}	π^*_{C4-C5}	60.33	32.21	π_{C3-N2}	π^*_{C4-C5}	5.31	---	π_{C3-N2}	π^*_{C2-C3}	4.82	5.85
σ_{C5-N1}	n^*_{C4}	---	5.89	π^*_{C3-N2}	π^*_{C4-C5}	57.10	32.23	π^*_{C3-N2}	π^*_{C2-C3}	42.78	24.13
σ_{C5-N1}	σ^*_{C4-C5}	---	0.34	σ_{C5-S1}	σ^*_{C4-C5}	---	0.27	σ_{C5-O1}	n^*_{C2}	---	5.12
σ_{C3-N2}	n^*_{C4}	---	6.33	σ_{C5-S1}	n^*_{C4}	---	10.75	n_{C4}	σ^*_{C1-N7}	3.09	---
σ_{C3-N2}	σ^*_{C3-C4}	---	0.43	n_{C4}	σ^*_{C3-N2}	3.98	---	n_{C4}	σ^*_{C3-O4}	4.50	---
n_{C4}	σ^*_{C5-N1}	3.59	---	n_{C4}	σ^*_{C5-S1}	6.35	---	$n1_{O1}$	σ^*_{C2-C3}	1.53	1.76
n_{C4}	σ^*_{C3-N2}	3.32	---	$n1_{S1}$	σ^*_{C4-C5}	0.67	---	$n2_{O1}$	π^*_{C2-C3}	16.29	13.24
n_{N1}	π^*_{C4-C5}	19.59	15.54	$n1_{S1}$	σ^*_{C3-N2}	-	1.60	n_{N2}	σ^*_{C1-C2}	2.46	3.11
n_{N2}	σ^*_{C3-C4}	2.50	3.15	$n2_{S1}$	π^*_{C4-C5}	10.97	---	n_{N2}	n^*_{C2}	---	0.43
n_{N2}	n^*_{C4}	---	0.65	$n2_{S1}$	π^*_{C3-N2}	---	10.33	σ_{C3-H6}	σ^*_{C4-C5}	0.64	0.64
σ_{C5-H7}	σ^*_{C4-C5}	0.64	0.39	n_{N2}	σ^*_{C3-C4}	3.52	4.19	σ_{C5-H7}	σ^*_{C3-C4}	0.81	0.81
σ_{C5-H7}	σ^*_{C3-C4}	0.76	0.76	n_{N7}	n^*_{C4}	---	0.51	σ_{C5-H7}	σ^*_{C4-C5}	0.52	0.31
σ_{C3-H8}	σ^*_{C4-C5}	0.81	0.80	σ_{C3-H6}	σ^*_{C4-C5}	1.16	1.11				
				σ_{C5-H7}	σ^*_{C3-C4}	1.56	---				
				σ_{C5-H7}	σ^*_{C4-C5}	0.87	0.57				
				σ_{C5-H7}	n^*_{C4}	---	0.46				
 1d				 2d				 3d			
σ_{C3-C4}	σ^*_{C4-C5}	0.31	0.56	σ_{C3-C4}	σ^*_{C4-C5}	0.46	0.74	σ_{C3-C4}	σ^*_{C5-O1}	0.60	---
σ_{C3-C4}	σ^*_{C5-N1}	0.30	---	σ_{C3-C4}	n^*_{C5}	---	9.57	σ_{C3-C4}	n^*_{C5}	---	12.09
σ_{C3-C4}	n^*_{C5}	---	11.29	σ_{S1-N2}	σ^*_{C5-S1}	0.38	---	σ_{C3-C4}	σ^*_{C4-C5}	---	0.52
π^*_{C3-N2}	π^*_{C4-C5}	64.13	23.86	σ_{S1-N2}	n^*_{C5}	---	8.87	π^*_{C3-N2}	π^*_{C4-C5}	59.03	19.06
σ_{N1-N2}	n^*_{C5}	---	6.44	π^*_{C3-N2}	π^*_{C4-C5}	72.42	35.56	σ_{O1-N2}	n^*_{C5}	---	9.49
n_{C5}	σ^*_{C3-C4}	2.30	---	n_{C5}	σ^*_{C3-C4}	3.75	---	n_{C5}	σ^*_{O1-N2}	6.32	---
n_{C5}	σ^*_{N1-N2}	5.26	---	n_{C5}	σ^*_{S1-N2}	2.10	---	n_{C5}	σ^*_{C3-C4}	2.25	---
n_{N1}	π^*_{C4-C5}	21.03	22.39	$n1_{S1}$	σ^*_{C4-C5}	1.63	---	$n1_{O1}$	n^*_{C5}	---	1.62
n_{N2}	σ^*_{C5-N1}	3.25	0.59	$n1_{S1}$	n^*_{C5}	---	1.37	$n1_{O1}$	σ^*_{C4-C5}	2.32	1.93
n_{N2}	n^*_{C5}	---	0.59	$n2_{S1}$	π^*_{C4-C5}	12.89	14.36	$n2_{O1}$	π^*_{C4-C5}	20.21	21.65
σ_{C4-H8}	σ^*_{C4-C5}	0.56	0.29	n_{N2}	σ^*_{C5-S1}	1.06	1.65	n_{N2}	σ^*_{C5-O1}	1.76	2.37
σ_{C4-H8}	σ^*_{C5-N1}	1.06	---	n_{N2}	n^*_{C5}	---	0.55	n_{N2}	n^*_{C5}	---	0.38
σ_{N1-H6}	σ^*_{C4-C5}	0.86	0.77	σ_{C4-H7}	σ^*_{C4-C5}	0.84	0.40	σ_{C4-H7}	σ^*_{C4-C5}	0.68	0.37
				σ_{C4-H7}	σ^*_{C5-S1}	1.82	---	σ_{C4-H7}	σ^*_{C5-O1}	1.20	1.21

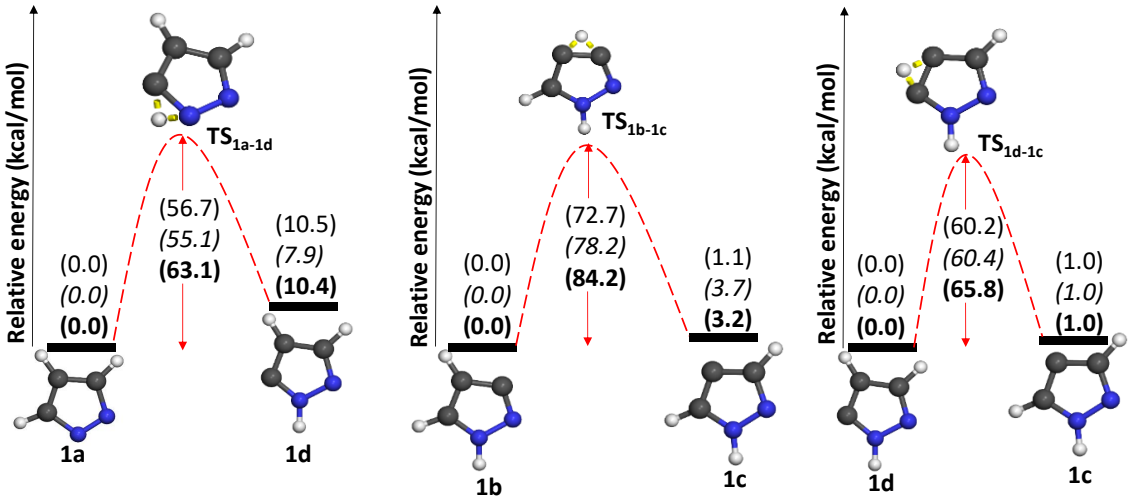
Table S9. Relative electron densities at bond critical points (bcp's) of radical isomers with respect to their corresponding parent and the barrier for the bond cleavage at the B3LYP/cc-pVTZ level of theory. (The radical species having two bond cleavage channels are included.)

Species	Bond	Relative electron densities at bcp w. r. to parent	Bond cleavage barrier (kcal/mol)
1b	N1-N2	-0.0189	15.3
	C3-C4	-0.0080	52.6
2b	S1-N2	-0.0277	3.6
	C3-C4	-0.0104	50.1
3b	O1-N2	-0.0400	1.9
	C3-C4	-0.0076	59.0
1d	N1-N2	-0.0177	22.8
	C3-C4	-0.0049	56.2
2d	S1-N2	-0.0074	19.3
	C3-C4	-0.0041	47.0

Table S10. NICS(1)$_{zz}$ indices for species involving cyclic transition state and their corresponding barrier at B3LYP/cc-pVTZ level of theory.

TS	Reactant NICS(1)$_{zz}$	TS NICS(1)$_{zz}$	Difference of NICS(1)$_{zz}$	Barrier (kcal/mol)
1a-1b	12.4949	-8.8073	-21.3022	108.6
1a-1c	12.4949	-4.8259	-17.3208	121.1
1a-4	12.4949	-12.6074	-25.1023	44.1
1a-12,13	12.4949	-24.2173	-36.7122	62.2
1b-1c	-29.8249	-29.9770	-0.1521	72.7
1b-1d	-29.8249	-12.4252	17.3997	116.7
1b-14	-29.8249	-12.4544	17.3705	15.3
1b-17	-29.8249	-8.5235	21.3014	52.6
1c-1d	-31.2659	-23.6812	7.5847	59.2
1c-29	-31.2659	-5.1854	26.0805	41.7
1d-1a	-28.5772	-28.7131	-0.1359	46.3
1d-35	-28.5772	-11.4171	17.1601	22.8
1d-37	-28.5772	-6.9319	21.6453	56.2
2b-2c	-28.827	-32.6014	-3.7744	79.9
2b-2d	-28.827	0.4364	29.2634	128.5
2b-19	-28.827	-17.8345	10.9925	3.6
2b-22	-28.827	-9.6445	19.1825	50.1
2c-2d	-31.3778	-22.4144	8.9634	57.0
2c-31	-31.3778	-9.6237	21.7541	22.6
2d-38	-27.3931	-11.4575	15.9356	19.3
2d-40	-27.3931	-6.2060	21.1871	47.0

3b-3c	-23.3965	-26.6779	-3.2814	80.6
3b-3d	-23.3965	-0.9772	22.4193	135.2
3b-24	-23.3965	-13.1029	10.2936	1.9
3b-27	-23.3965	-7.0350	16.3615	59.0
3c-33	-26.5222	-2.9606	23.5616	29.8
3d-3c	-22.2184	-20.1398	2.0786	63.7
3d-41	-22.2184	-15.3244	6.894	2.3



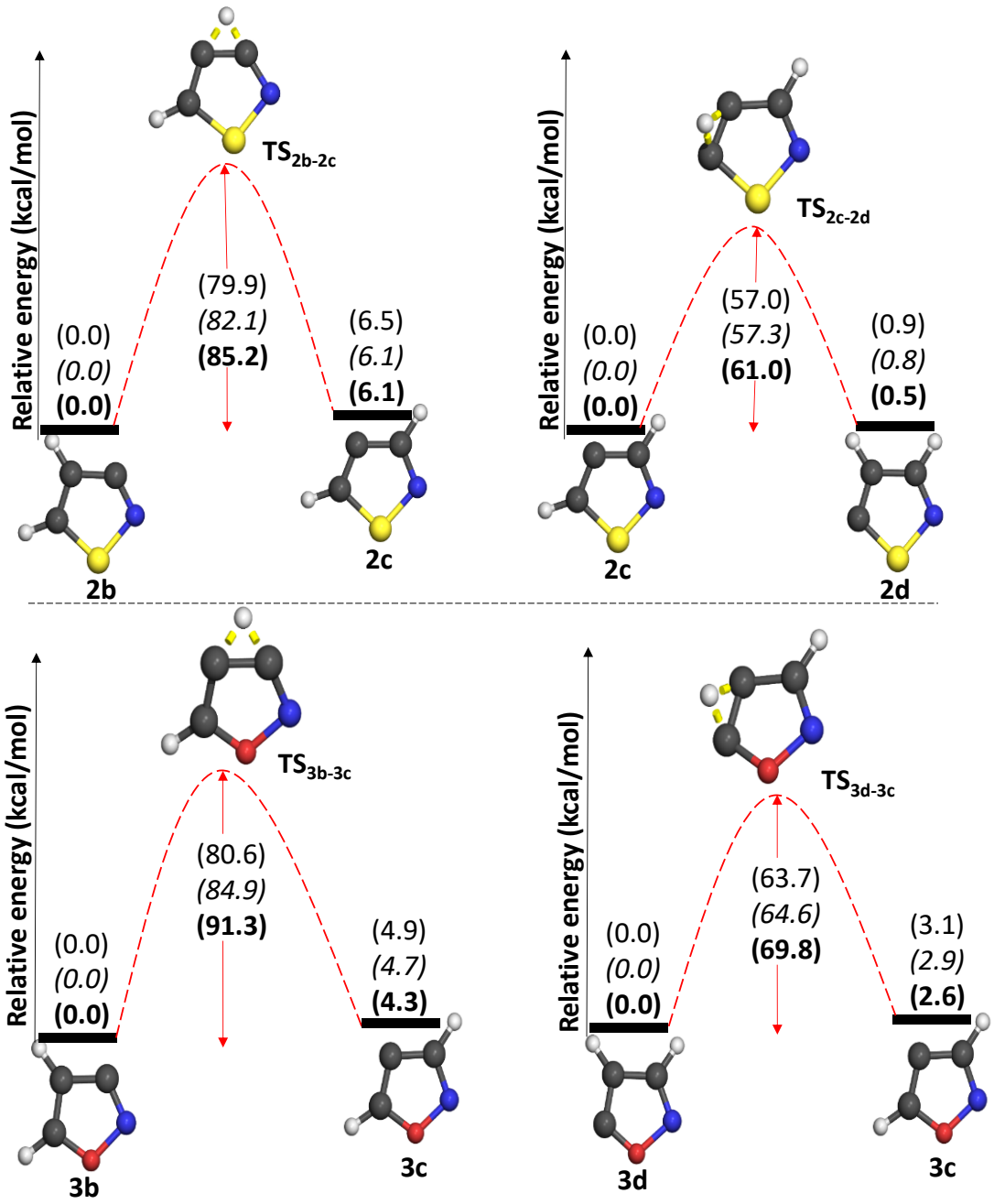


Figure S3. Isomerization pathways through 1,2-H shift in the dehydro- pyrazole (**1a-1d**), isothiazole (**2b-2d**) and isoxazole (**3b-3d**) radical isomers. (Normal font: B3LYP/cc-pVTZ, italics: M06-2X/cc-pVTZ, and bold: CCSD(T)/cc-pVTZ//B3LYP/cc-pVTZ).

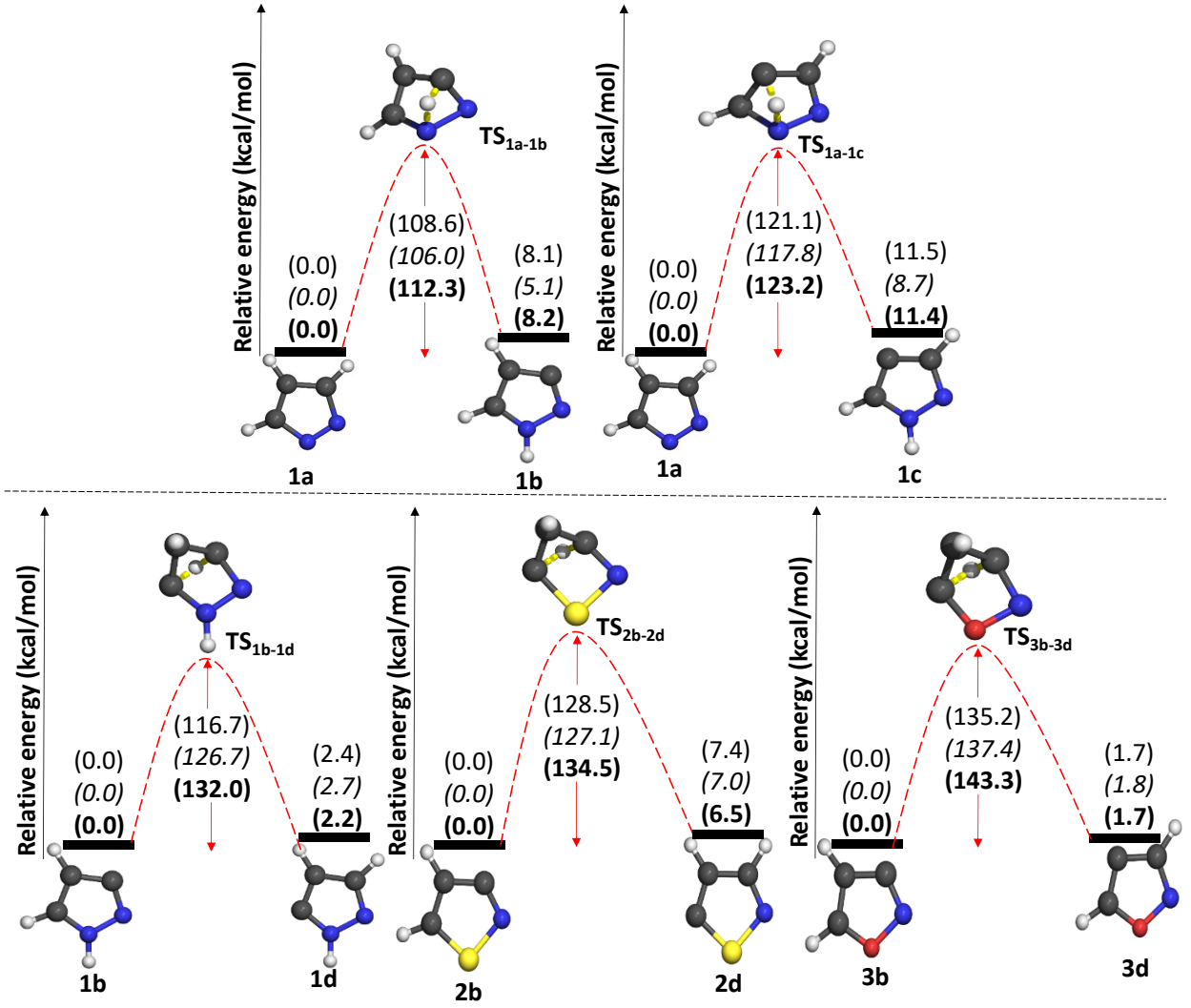


Figure S4. Isomerization pathways through 1,3-H shift in the dehydro- pyrazole (**1a-1d**), isothiazole (**2b-2d**) and isoxazole (**3b-3d**) radical isomers. (Normal font: B3LYP/cc-pVTZ, italics: M06-2X/cc-pVTZ, and bold: CCSD(T)/cc-pVTZ//B3LYP/cc-pVTZ).

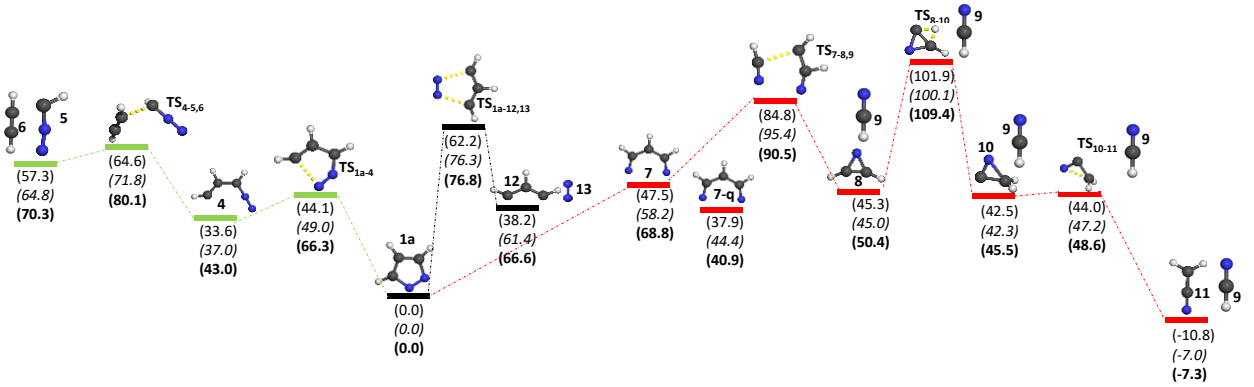


Figure S5. The unimolecular reaction pathways of **1a** depicting three possible ring-opening channels. (Normal font: B3LYP/cc-pVTZ, italics: M06-2X/cc-pVTZ, and bold: CCSD(T)/cc-pVTZ//B3LYP/cc-pVTZ)

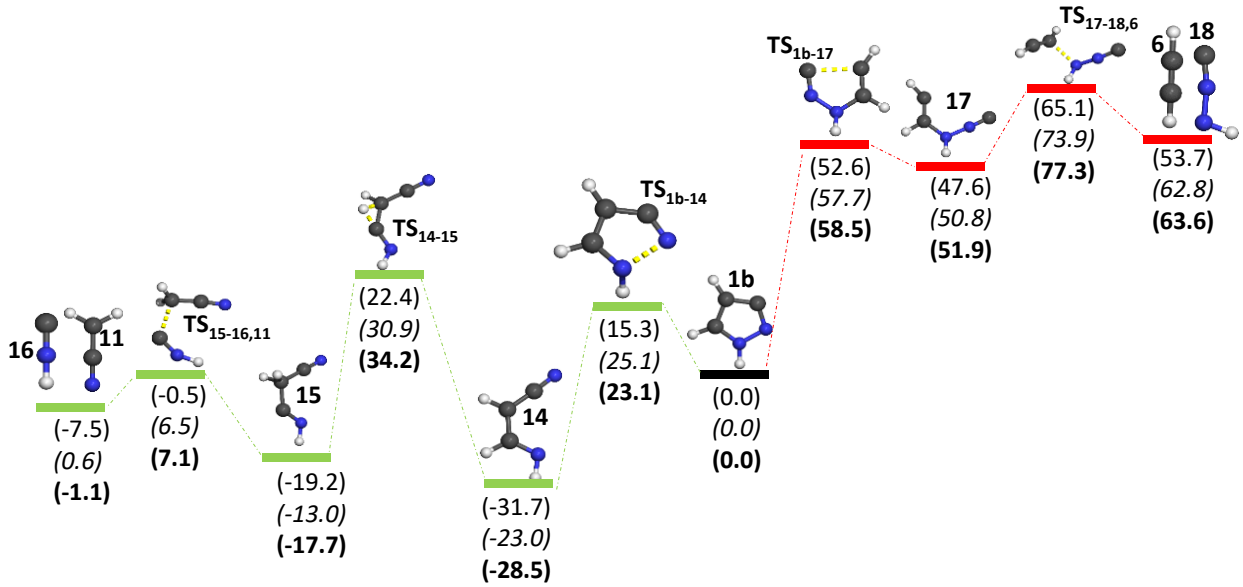


Figure S6. The unimolecular reaction pathways of **1b**. (Normal font: B3LYP/cc-pVTZ, italics: M06-2X/cc-pVTZ, and bold: CCSD(T)/cc-pVTZ//B3LYP/cc-pVTZ)

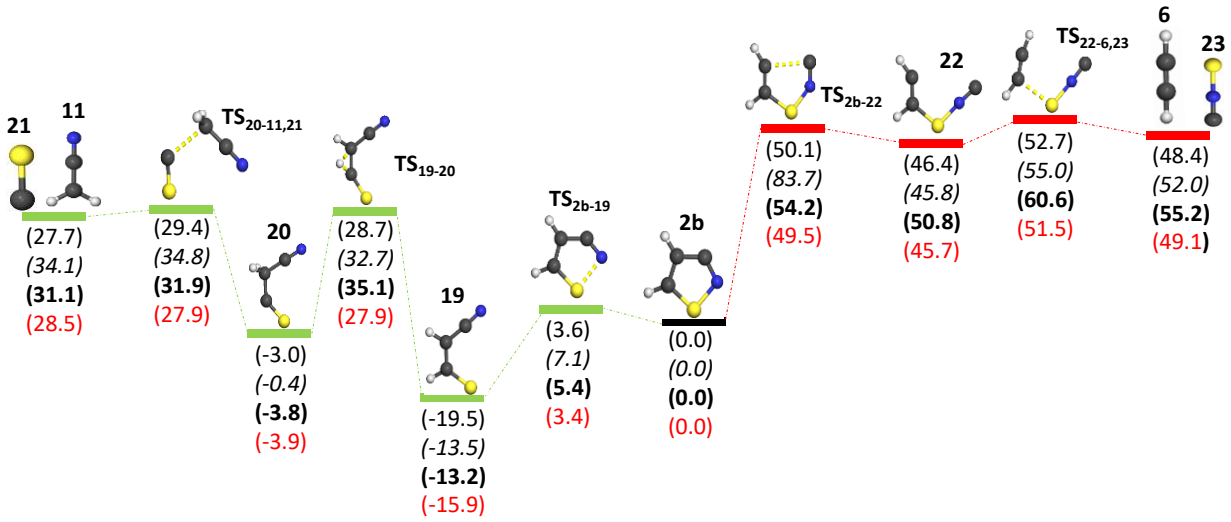


Figure S7. The unimolecular reaction pathways of **2b**. (Normal font: B3LYP/cc-pVTZ, italics: M06-2X/cc-pVTZ, and bold: CCSD(T)/cc-pVTZ//B3LYP/cc-pVTZ), red: B3LYP-GD3/cc-pVTZ.

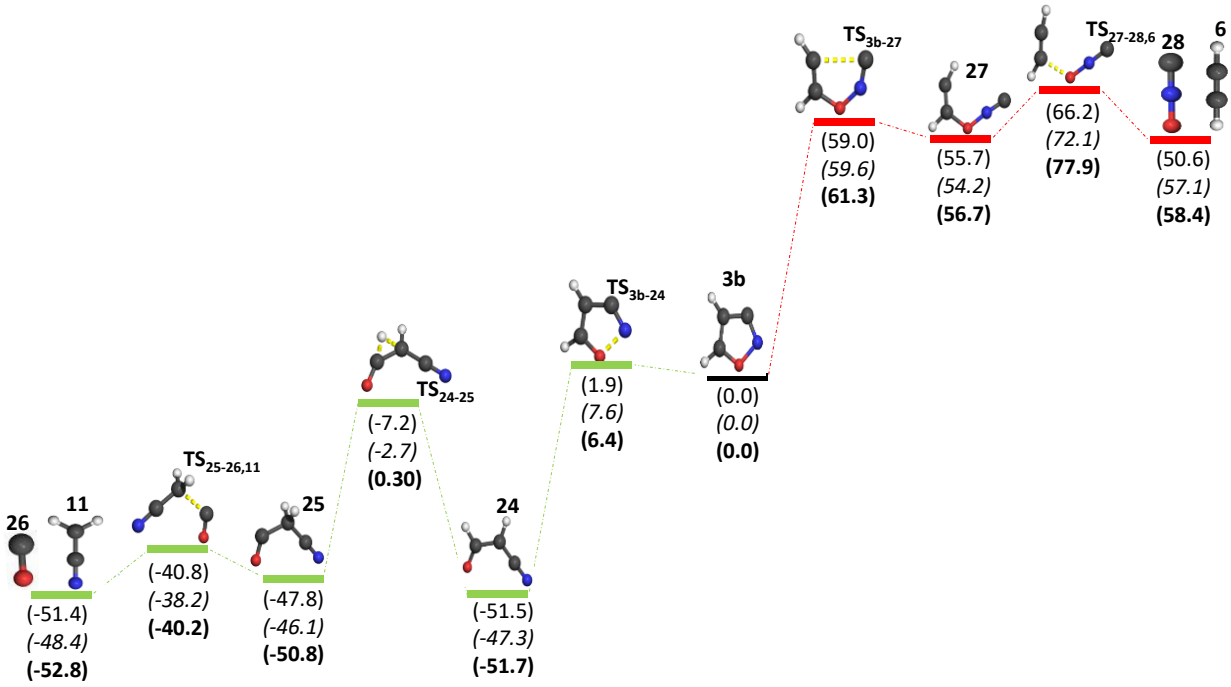


Figure S8. The unimolecular ring pathways of **3b**. (Normal font: B3LYP/cc-pVTZ, italics: M06-2X/cc-pVTZ, and bold: CCSD(T)/cc-pVTZ//B3LYP/cc-pVTZ).

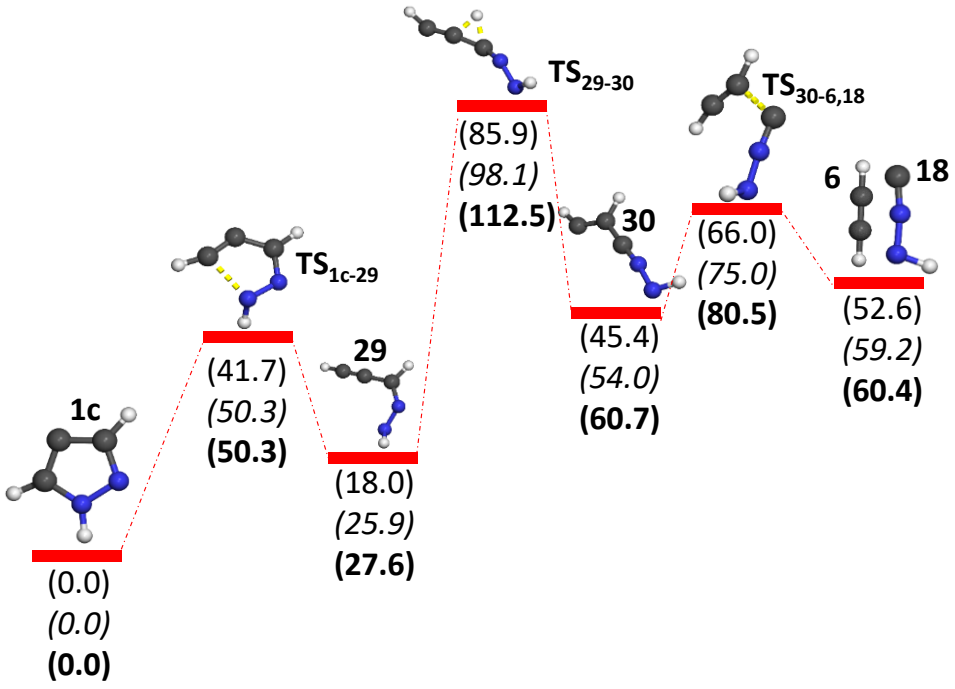


Figure S9. The unimolecular reaction pathways of **1c**. (Normal font: B3LYP/cc-pVTZ, italics: M06-2X/cc-pVTZ, and bold: CCSD(T)/cc-pVTZ//B3LYP/cc-pVTZ).

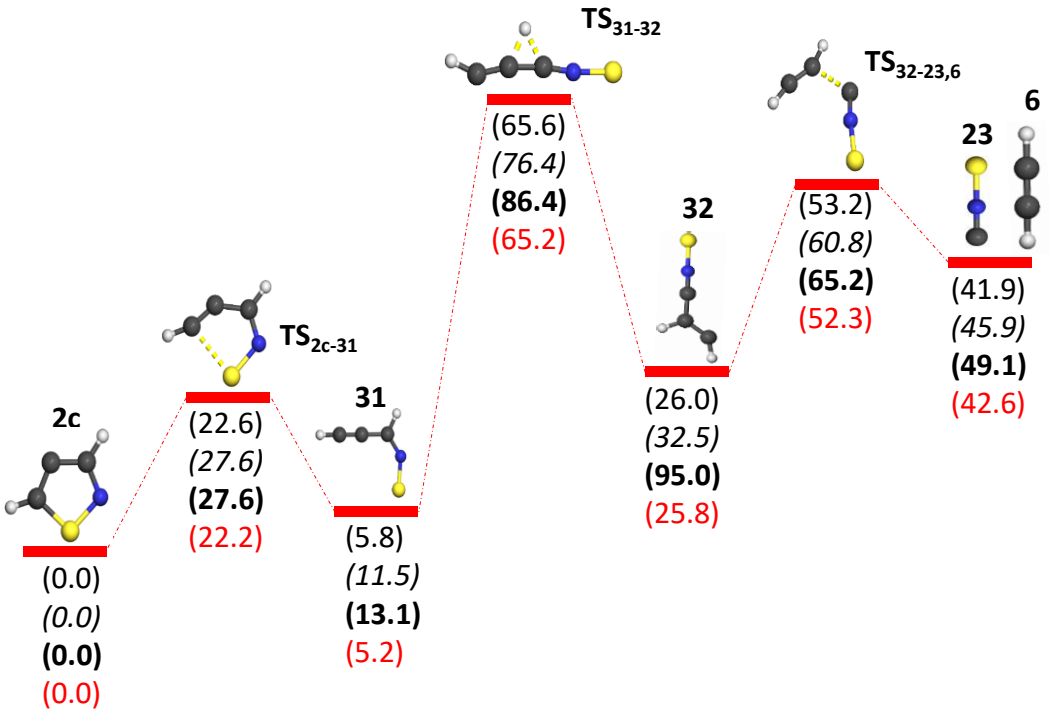


Figure S10. The unimolecular reaction pathways of **2c**. (Normal font: B3LYP/cc-pVTZ, italics: M06-2X/cc-pVTZ, and bold: CCSD(T)/cc-pVTZ//B3LYP/cc-pVTZ) red: B3LYP-GD3/cc-pVTZ.

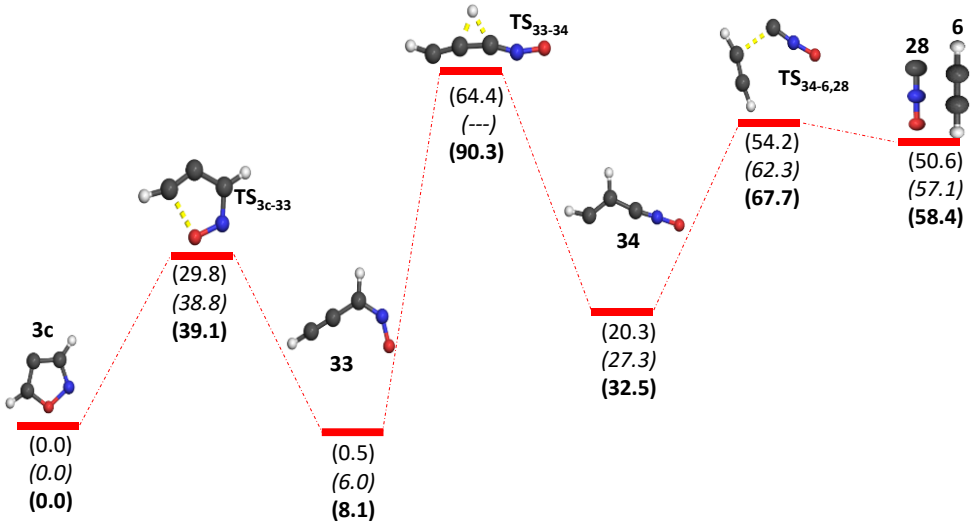


Figure S11. The unimolecular reaction pathways of **3c**. (Normal font: B3LYP/cc-pVTZ, italics: M06-2X/cc-pVTZ, and bold: CCSD(T)/cc-pVTZ//B3LYP/cc-pVTZ).

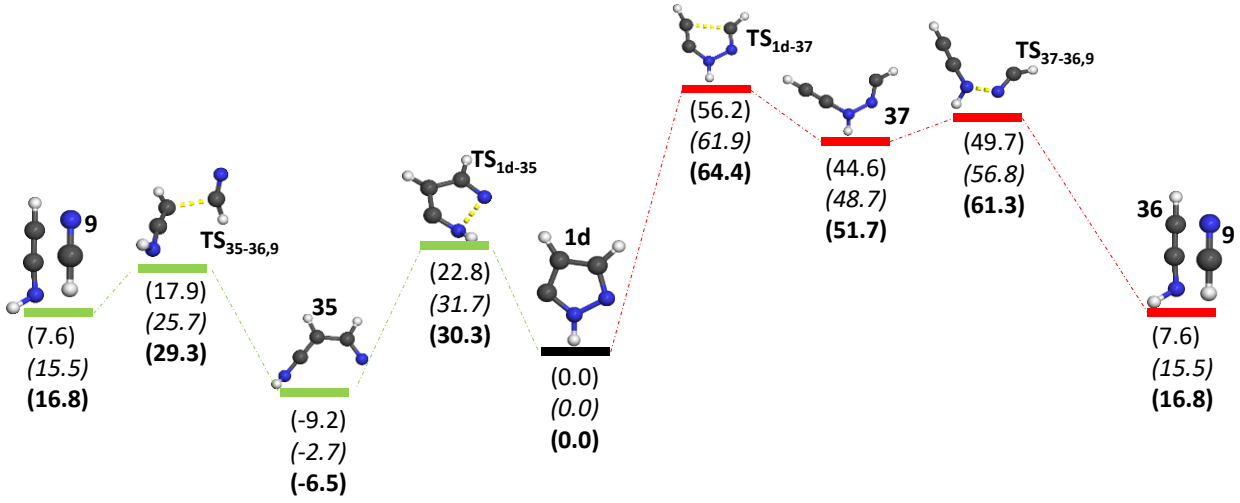


Figure S12. The unimolecular reaction pathways of **1d**. (Normal font: B3LYP/cc-pVTZ, italics: M06-2X/cc-pVTZ, and bold: CCSD(T)/cc-pVTZ//B3LYP/cc-pVTZ).

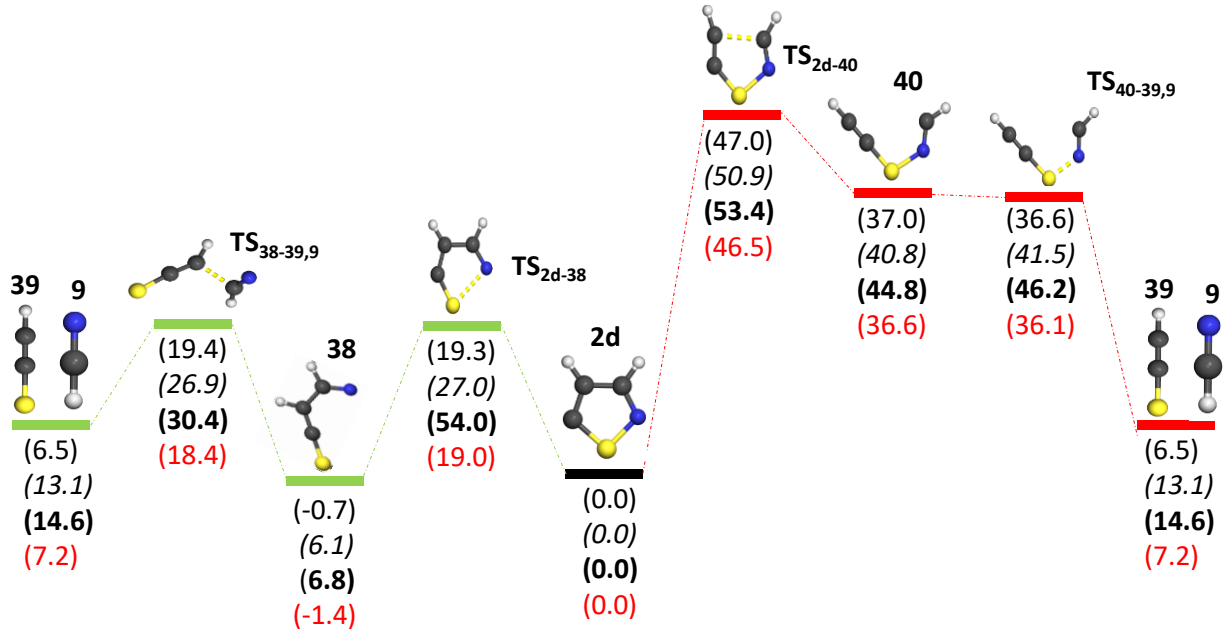


Figure S13. The unimolecular reaction pathways of **2d**. (Normal font: B3LYP/cc-pVTZ, italics: M06-2X/cc-pVTZ, and bold: CCSD(T)/cc-pVTZ//B3LYP/cc-pVTZ) red: B3LYP-GD3/cc-pVTZ.

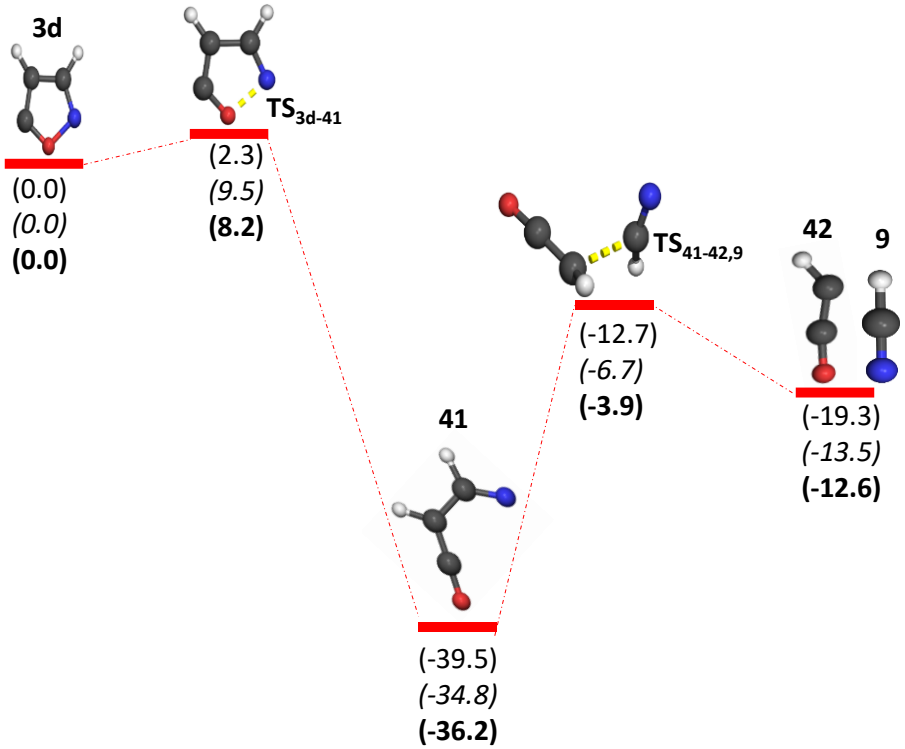


Figure S14. The unimolecular reaction pathways of **3d**. (Normal font: B3LYP/cc-pVTZ, italics: M06-2X/cc-pVTZ, and bold: CCSD(T)/cc-pVTZ//B3LYP/cc-pVTZ).

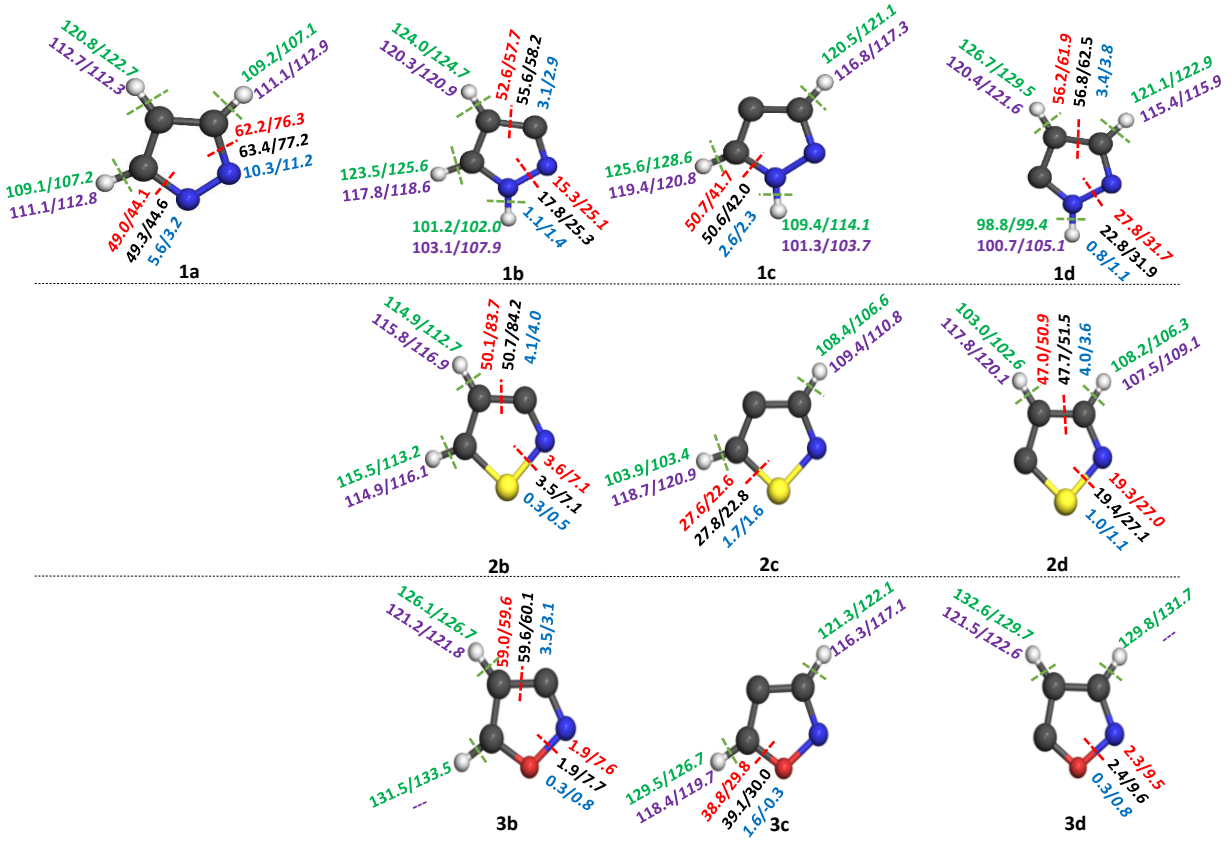
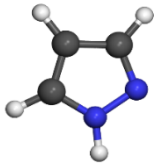


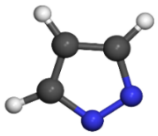
Figure S15. Summary of the unimolecular reaction pathways (energy values indicated in kcal/mol; (normal font = (U)B3LYP/cc-pVTZ; italics = (U)M06-2X/cc-pVTZ level of theory). {Colour codes: red-energy barriers, black-activation enthalpy, blue-activation entropy; all energies correspond to the first step of the unimolecular reaction pathways relative to their corresponding parent radical; the second bond dissociation energy (BDE) values derived from their parent heterocycle for all radicals are indicated; green-singlet and purple-triplet state (B3LYP/cc-pVTZ – normal font and M06-2X/cc-pVTZ – Italics)}.

Appendix 1S. Cartesian Coordinates at B3LYP/cc-pVTZ



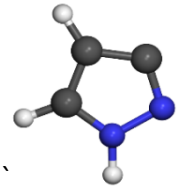
1

C	1.10783800	0.30640200	0.00000000
C	0.66232800	-0.99581500	0.00000000
C	-0.74303900	-0.88948000	0.00000000
N	0.00000000	1.08466300	0.00000000
H	-0.04807700	2.08773000	0.00000000
H	-1.47522200	-1.67992400	0.00000000
N	-1.14284400	0.37629500	0.00000000
H	1.26223500	-1.88801000	0.00000000
H	2.09821000	0.72686100	0.00000000



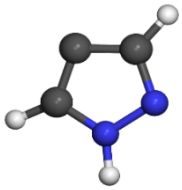
1a

C	0.00000000	1.08465600	0.32791900
C	0.00000000	0.00000000	1.18470600
C	0.00000000	-1.08465600	0.32791900
N	0.00000000	0.63608700	-1.02762400
H	0.00000000	2.14148100	0.54182400
H	0.00000000	-2.14148100	0.54182400
N	0.00000000	-0.63608700	-1.02762400
H	0.00000000	0.00000000	2.25982000



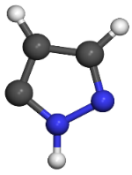
1b

C	1.06994800	0.21093700	0.00000000
C	0.58132900	-1.08102300	0.00000000
C	-0.81048000	-0.87596300	0.00000000
N	0.00000000	1.04315200	0.00000000
H	-0.00808300	2.04768200	0.00000000
N	-1.17904300	0.36290400	0.00000000
H	1.13706500	-1.99937900	0.00000000
H	2.07953400	0.58560600	0.00000000



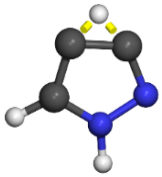
1c

C	1.14693600	0.30429500	0.00000000
C	0.71955300	-0.99666400	0.00000000
C	-0.67758900	-0.99010000	0.00000000
N	0.00000000	1.03113700	0.00000000
H	-0.09991600	2.03118600	0.00000000
H	2.12381500	0.75274800	0.00000000
H	-1.37813800	-1.80623800	0.00000000
N	-1.11130900	0.27130900	0.00000000



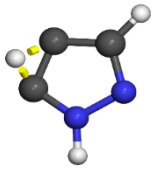
1d

C	0.69946700	0.94902300	0.00000000
C	1.18673800	-0.33150000	0.00000000
C	0.00000000	-1.09983400	0.00000000
N	-0.63635300	0.92743900	0.00000000
H	-1.28286800	1.69489500	0.00000000
H	-0.09517300	-2.17355900	0.00000000
N	-1.09913000	-0.35156400	0.00000000
H	2.20919100	-0.65859900	0.00000000



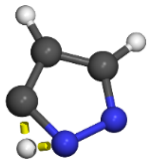
TS_{1b-1c}

C	0.20056200	-1.10866800	-0.02243100
C	-1.11202400	-0.62160700	0.11404900
C	-0.90527200	0.73742400	0.08136700
N	1.01717200	-0.02947300	-0.01470300
H	2.02950100	-0.03353600	0.01884100
N	0.38442600	1.15304800	-0.00274200
H	-1.54518000	0.23207700	-0.86931200
H	0.60490000	-2.10646100	-0.06532800



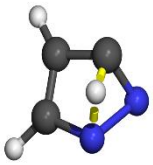
$TS_{1c\text{-}1d}$

C	1.07857600	-0.63123700	-0.11308900
C	-0.17804900	-1.19140400	-0.07587500
C	-1.16577900	-0.15263100	-0.00436500
N	0.78599000	0.69880900	0.00920000
H	1.44007100	1.46212500	0.03818000
H	0.67360700	-1.30746200	0.91634700
H	-2.23973100	-0.20841300	0.01550300
N	-0.54062400	1.00196000	0.01793500



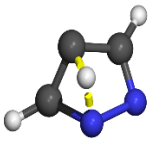
$TS_{1d\text{-}1a}$

C	-0.18376100	-1.14160300	-0.05294700
C	1.08298500	-0.55824900	-0.01443900
C	0.76833000	0.78972000	0.01235400
N	-1.20901400	-0.17452100	-0.11175100
H	-1.06372200	-0.95638300	0.88316100
H	1.43654700	1.63651200	0.03978600
N	-0.56485300	1.00707100	0.02586200
H	2.03892100	-1.04719200	0.00846900



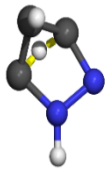
$TS_{1a\text{-}1b}$

C	0.95284800	0.60857200	-0.13753500
C	0.94780700	-0.72861100	-0.04921000
C	-0.48973600	-0.77765500	0.43861800
N	-0.41604700	0.92627900	0.23358700
H	1.68908000	1.38140700	-0.29808400
H	-0.59181100	0.19836800	1.28748900
N	-1.18740700	-0.16595300	-0.56022700
H	1.66140700	-1.51588200	-0.21416100



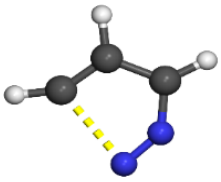
$TS_{1a\text{-}1c}$

C	-1.18777000	0.16546800	-0.47257200
C	-0.32641300	0.92350500	0.40284600
C	1.02316500	0.55155500	-0.12097500
N	-0.43758000	-0.84714300	0.29506500
H	-2.25064900	0.10148300	-0.64744100
H	1.89018200	1.15853100	-0.34082600
N	0.96975300	-0.73261300	-0.17669900
H	-0.41863600	-0.04488900	1.30390800



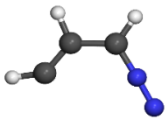
$TS_{1b\text{-}1d}$

C	0.33653700	-0.90480100	0.37428800
C	1.33701800	-0.05571900	-0.33835100
C	0.43441500	0.79619900	0.40018300
N	-0.92658500	-0.50923900	-0.16839500
H	-1.79813600	-1.02849200	-0.22999200
N	-0.88065400	0.79671000	-0.16805600
H	1.47344300	-0.03749300	-1.41023900
H	0.32754500	0.03961600	1.37866800



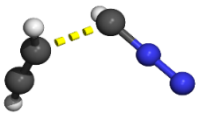
$TS_{1a\text{-}4}$

C	-1.14074200	-0.91318000	-0.01501700
C	-1.12577400	0.40707100	0.00380800
C	0.13248200	1.11181300	0.00063800
N	1.21197000	-0.92957300	-0.00149100
H	-1.70405400	-1.82077700	0.05070600
H	0.31975500	2.16644100	-0.01100700
N	1.10757600	0.22103100	0.00430000
H	-2.04831700	0.97990700	0.00406700



4

C	-1.53099500	-1.02958800	0.00000000
C	-1.29608100	0.26376500	0.00000000

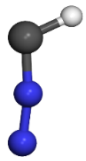


$TS_{4\text{-}5,6}$

C	-1.97707100	-0.60017300	-0.26691500
C	-1.52511900	0.19477800	0.54006800

C	0.00000000	0.91395900	0.00000000
N	1.97340700	-0.49246500	0.00000000
H	-2.40332900	-1.65765900	0.00000000
H	0.15090800	1.97805300	0.00000000
N	1.07704200	0.18336300	0.00000000
H	-2.13826500	0.95449600	0.00000000

C	0.30102500	0.95693500	-0.24971700
N	2.03603200	-0.66543300	0.21091500
H	-2.19755100	-1.25020300	-1.07851200
H	0.05161100	1.22577500	-1.26785400
N	1.23210300	0.08814300	-0.10223300
H	-1.52401200	0.75621800	1.44497500

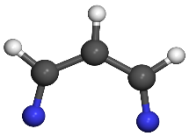


5

C	-0.31466900	-1.16081500	0.00000000
N	0.46695900	1.12140700	0.00000000
H	-1.38069900	-1.37394600	0.0000000
N	0.00000000	0.06985500	0.00000000

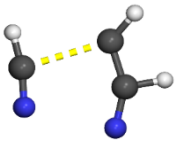
6

C	0.00000000	0.00000000	0.59791600
H	0.00000000	0.00000000	1.65897000
C	0.00000000	0.00000000	-0.59791600
H	0.00000000	0.00000000	-1.65897000



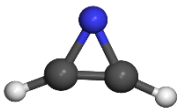
7

C	-1.28465900	0.29854300	-0.00020200
C	-0.00001500	0.94241100	0.00008900
C	1.28454600	0.29861100	0.00007600
N	-1.52322100	-0.94276200	0.00023600
H	-2.15639100	0.96864900	-0.00077800
H	2.15626500	0.96877900	0.00025600
N	1.52336200	-0.94269400	-0.00017400
H	-0.00009600	2.02337200	0.00031600



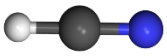
$TS_{7\text{-}8,9}$

C	-1.62444000	0.48329100	-0.02355900
C	0.80968300	1.25590200	-0.04030400
C	1.20578600	-0.07941600	-0.01047700
N	-1.55235500	-0.66871400	0.03858700
H	-1.88060800	1.51442000	-0.08603900
H	2.30743100	0.11862500	-0.09098700
N	0.94796600	-1.27942000	0.00142300
H	1.45772500	2.04523400	0.34298900



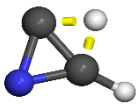
8

C	0.65723100	-0.36951600	-0.00002400
C	-0.63021900	-0.40582600	0.00005900
H	-1.59441100	-0.87716000	-0.00017800
N	-0.03111200	0.90068400	-0.00000800
H	1.65012500	-0.77558300	0.00002000



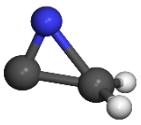
9

C	0.00000000	0.00000000	-0.49704000
N	0.00000000	0.00000000	0.64922600
H	0.00000000	0.00000000	-1.56234300



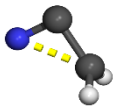
$TS_{8\text{-}10}$

C	0.66642000	-0.17474500	-0.05010000
C	-0.33225800	0.82244100	-0.10510100
H	0.74928800	0.88746300	0.69038900
N	-0.63019100	-0.59857000	0.05780700
H	1.65707900	-0.58365500	-0.16383600



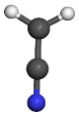
10

C	-0.68588500	0.50251600	0.00000000
C	0.00000000	-0.82349700	0.00000000
N	0.88128100	0.00804900	0.00000000
H	-1.02682700	0.93477200	0.92891200
H	-1.02682700	0.93477200	-0.92891200



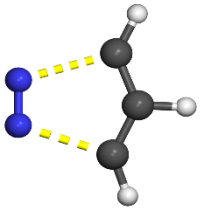
$TS_{10\text{-}11}$

C	0.83977700	-0.51524100	0.00000000
C	0.00000000	0.72126900	0.00000000
N	-1.01987400	0.10957600	0.00000000
H	1.05022800	-1.00159900	0.93764500
H	1.05022800	-1.00159900	-0.93764500



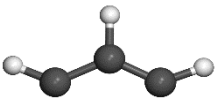
11

C	0.00000000	0.00000000	0.18699400
N	0.00000000	0.00000000	1.35340400
C	0.00000000	0.00000000	-1.18896100
H	0.00000000	0.93327800	-1.73101500
H	0.00000000	-0.93327800	-1.73101500



$TS_{1a\text{-}12,13}$

C	0.75561500	1.23833200	0.00014500
C	1.24867700	-0.03634500	0.00002700
C	0.67307900	-1.24462600	-0.00016800
N	-1.47280600	0.58337800	0.00004900
H	1.23188900	2.20639600	-0.00074500
H	1.01494300	-2.26586000	0.00043800
N	-1.47804500	-0.52752900	-0.00003500
H	2.34490500	-0.07564900	0.00018600

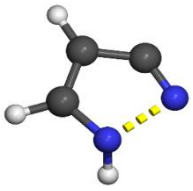


12

C	1.17078300	-0.37558600	-0.05347600
C	-0.00413100	0.42080700	-0.08392200
C	-1.12466200	-0.29695900	-0.00681100
H	1.93994800	0.17272300	0.51965000
H	-2.14884700	-0.17448900	0.31608200
H	-0.04304300	1.51218900	0.02952200

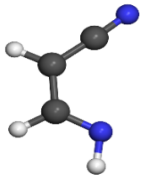
13

N	0.00000000	0.00000000	0.54569200
N	0.00000000	0.00000000	-0.54569200



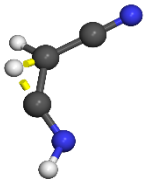
$TS_{1b\text{-}14}$

C	-1.11589100	-0.09312100	-0.02308200
C	-0.48360100	1.11024000	-0.00139800
C	0.90269100	0.76448900	-0.01099100
N	-0.29662100	-1.17876000	0.13895400
H	-0.34643000	-1.91657200	-0.56104200
N	1.38684600	-0.33766300	-0.01880300
H	-0.91879100	2.09154500	0.02430000
H	-2.18554100	-0.24965900	-0.09148700



14

C	1.27660100	0.37581100	0.00002600
C	-0.04750600	0.88855900	-0.00011600
C	-1.18878600	0.08027400	-0.00023200
N	1.50770600	-0.89747600	-0.00012900

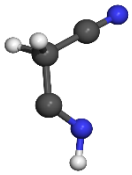


$TS_{14\text{-}15}$

C	1.23553700	0.34954100	-0.01137100
C	-0.08697900	0.86060500	0.07617000
C	-1.25263700	0.04143200	0.04351900
N	1.81498400	-0.74691000	0.11111000

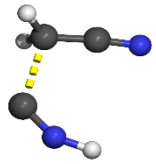
H	2.50973600	-1.08301600	0.00053900
N	-2.16709100	-0.54109500	0.00020300
H	-0.20535400	1.95864100	0.00027200
H	2.06946000	1.12651400	0.00060400

H	2.68904600	-0.88486000	-0.38571700
N	-2.18881600	-0.62634400	-0.05855500
H	-0.19980600	1.89712000	0.36255100
H	0.75205600	1.09105400	-0.99463300



15

C	1.32990500	0.29522800	0.00000000
C	0.00000000	0.99490800	0.00000000
C	-1.16459400	0.10856600	0.00000000
N	1.58228400	-0.90550300	0.00000000
H	2.55210200	-1.21267600	0.00000000
N	-2.07636400	-0.59164500	0.00000000
H	-0.04270700	1.65024900	0.87253700
H	-0.04270700	1.65024900	-0.87253700

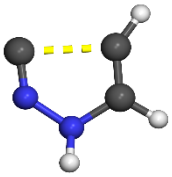


$TS_{15\text{-}16,11}$

C	0.48038000	-1.53940900	0.00000000
C	1.18708700	0.49106000	0.00000000
C	0.00000000	1.23323700	0.00000000
N	-0.66151900	-1.81562800	0.00000000
H	-1.63543600	-1.57665800	0.00000000
N	-1.03514300	1.75654500	0.00000000
H	1.75363300	0.44045400	0.91784400
H	1.75363300	0.44045400	-0.91784400

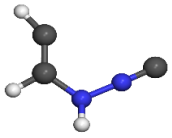
16

C	0.00000000	0.00000000	-0.73526700
N	0.00000000	0.00000000	0.42676500
H	0.00000000	0.00000000	1.42424800



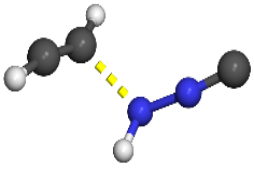
$TS_{1b\text{-}17}$

C	1.09091500	0.39412500	-0.00482500
C	1.18650800	-0.91272400	-0.01667700
C	-1.28182600	-1.04760400	0.00217100
N	-0.16512000	1.02093500	0.09890100
H	-0.31475700	1.88922600	-0.39177500
N	-1.19028700	0.14330900	-0.02353700
H	1.89366100	-1.71689900	-0.00428300
H	1.93537300	1.07518200	-0.01550100



17

C	1.20676200	0.33821800	0.01070800
C	1.46396400	-0.94197800	0.00772300
C	-1.96440700	-0.73514400	0.02109100
N	-0.08164600	0.90918600	-0.10835500
H	-0.23550800	1.73730200	0.45072600
N	-1.10817700	0.05618300	0.00001000
H	2.34278000	-1.55781300	0.02104600
H	1.98356900	1.09636000	0.04951300

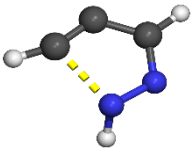


$TS_{17\text{-}18,6}$

C	1.33106600	-0.08185100	-0.58167100
C	2.07966500	-0.39380900	0.34141500
C	-2.19662000	-0.70032400	0.01299800
N	-0.27618500	0.89017800	0.00780100
H	0.00759500	1.13304500	0.95995900
N	-1.28978500	0.04705100	0.10011100
H	2.56403500	-0.56237300	1.27329000
H	1.10549600	-0.07536200	-1.62508100

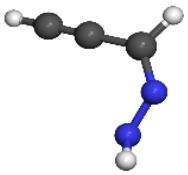
18

C	1.35201200	0.01486900	0.00009400
N	-1.11123100	-0.13952100	0.00006000
H	-1.51909000	0.80322200	0.00007800
N	0.16937600	0.01203000	-0.00015200



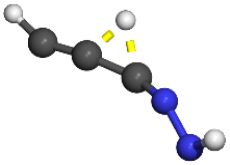
TS_{1c-29}

C	1.44104200	-0.31649700	0.00209200
C	0.92383900	0.81314800	0.03189100
C	-0.49422100	1.04424400	-0.00258600
N	-0.47808000	-1.13814600	-0.12909800
H	-0.77553900	-1.84734600	0.54798000
H	2.18940800	-1.07696000	0.00076100
H	-0.98887300	1.99956000	-0.06946300
N	-1.18605600	-0.05051400	0.03371800



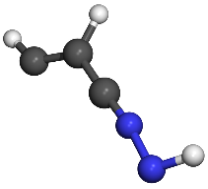
29

C	-2.16255500	0.46726000	-0.02233200
C	-1.12744400	-0.14654400	0.00564700
C	0.07326500	-0.88855500	0.02579200
N	1.59138800	0.84354800	0.12778500
H	2.36601200	1.07202000	-0.50286900
H	-3.07103500	1.01562900	-0.03786300
H	0.02319400	-1.96793900	0.07819700
N	1.26321700	-0.37393000	-0.06951500



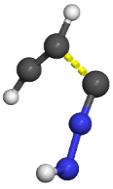
TS_{29-30}

C	-2.49818400	-0.32103200	0.03423600
C	-1.29676500	0.03969000	-0.01301700
C	0.00462300	0.30207600	-0.30779000
N	2.28181000	-0.35394500	-0.05230200
H	2.93462500	0.04812100	0.62904500
H	-3.50234500	-0.16334300	0.35658700
H	-0.82174700	1.23205700	0.31363300
N	1.16553600	0.17662600	0.11232500



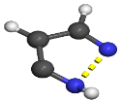
30

C	2.33002800	-0.51701700	-0.00000500
C	1.39661100	0.41185800	0.00002300
C	0.00355400	0.16877600	-0.00011600
N	-2.35988800	-0.29364900	0.00004600
H	-2.91218500	0.56236400	0.00010500
H	3.40585200	-0.50568900	0.00017400
N	-1.14745700	0.02170200	-0.00001900
H	1.67658800	1.46525400	0.00011800



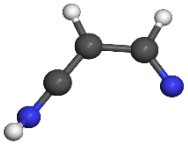
$TS_{30-6,18}$

C	-1.81817600	-0.87736600	-0.02342300
C	-1.74159000	0.34565700	0.07590600
C	0.14566900	1.02821900	-0.10083800
N	2.05447500	-0.51324500	-0.08536600
H	2.45585700	-0.61650600	0.85265500
H	-1.54924600	-1.89859700	-0.15658100
N	1.06112800	0.26367700	-0.00241000
H	-2.23124800	1.28302000	0.20849700



TS_{1d-35}

C	-0.80663200	-0.81597700	-0.03557900
C	0.51371000	-1.09302000	-0.01142300

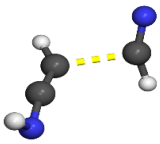


35

C	1.03510400	0.18611000	-0.01104000
C	-0.09556600	0.86468300	-0.02077300

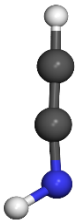
C	1.13502700	0.21463800	-0.00767800
N	-1.32066900	0.31581500	0.13009800
H	-1.88019400	0.77559900	-0.58057400
H	2.21334600	0.35627300	0.00841900
N	0.40713700	1.26694400	-0.00435200
H	1.00894600	-2.04502700	0.02001600

C	-1.42220000	0.23769300	0.00731200
N	2.06995000	-0.42286900	0.13066400
H	2.56110600	-0.76691300	-0.69082500
H	-2.26347800	0.94345000	0.04420100
N	-1.69339000	-0.98434000	-0.00781200
H	-0.03758200	1.94300800	-0.06633400



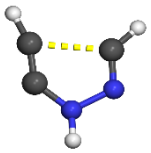
$TS_{35\text{-}36,9}$

C	-1.20609300	0.23467600	0.06142500
C	-0.15876900	0.94804400	-0.03460800
C	1.53236000	-0.26196500	-0.46600900
N	-2.17922800	-0.52264200	-0.06121700
H	-2.54215300	-0.92031100	0.80253600
H	1.29528500	-0.44669400	-1.49365200
N	2.17702600	-0.34196400	0.50386900
H	0.25729300	1.89471600	0.22771100



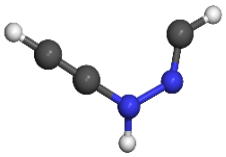
36

C	0.04009900	0.00721100	-0.00079100
C	1.27759400	0.01058700	0.00002500
N	-1.21743500	-0.13012600	0.00036900
H	-1.72119100	0.75674300	0.00038500
H	2.33708100	0.04735200	0.00162600



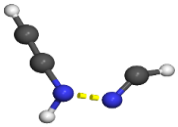
$TS_{1d\text{-}37}$

C	1.00564200	0.56653200	0.00492100
C	1.50970300	-0.56223400	0.02042100
C	-0.83070100	-1.09326300	0.00500000
N	-0.25332800	1.05288400	-0.06964300
H	-0.52269100	1.95747200	0.27231200
H	-1.38568900	-2.01936200	-0.00444600
N	-1.23757100	0.08018500	0.01073700
H	2.23680300	-1.33579900	-0.03757600



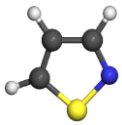
37

C	-1.06301700	0.14972500	-0.00889100
C	-2.06667200	-0.50932300	0.01821700
C	1.56096700	-0.90405900	-0.02734300
N	0.06918600	0.86598900	-0.07527400
H	0.05834000	1.83095900	0.20486100
H	2.54128000	-1.36139700	0.04632700
N	1.32639700	0.30506300	0.04892700
H	-2.95637300	-1.08498000	0.04134600



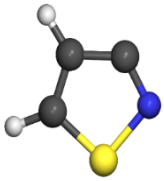
$TS_{37\text{-}36,9}$

C	-1.11019100	0.17756900	-0.02617600
C	-2.01345500	-0.61810700	0.05893400
C	1.63718000	-0.84394000	-0.12493900
N	-0.06476400	0.98044200	-0.21146300
H	-0.04972600	1.78073400	0.41039100
H	2.41829600	-1.57763300	-0.04730100
N	1.40520900	0.27535500	0.22029500
H	-2.83289200	-1.28681500	0.12817400



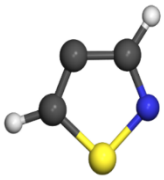
2

C	-0.75971600	-1.15795300	0.00000000
C	0.65445800	-1.27577800	0.00000000
C	1.23303300	-0.03834000	0.00000000
S	0.00000000	1.15058300	0.00000000
H	-1.44753900	-1.99395500	0.00000000
H	1.19508400	-2.20946200	0.00000000
H	2.28090400	0.21274500	0.00000000
N	-1.25644200	0.05910900	0.00000000



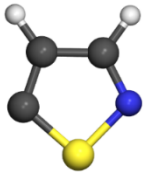
2b

C	-0.81145300	-1.14981800	0.00000000
C	0.59403100	-1.35459700	0.00000000
C	1.19054700	-0.12595700	0.00000000
S	0.00000000	1.12040500	0.00000000
H	1.09819300	-2.30578400	0.00000000
H	2.24471600	0.10217300	0.00000000
N	-1.31166500	0.00848200	0.00000000



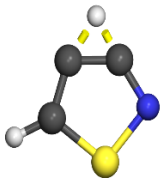
2c

C	-0.71166100	-1.24740900	0.00000000
C	0.69726900	-1.26767600	0.00000000
C	1.28860000	-0.05633400	0.00000000
S	0.00000000	1.09830000	0.00000000
H	-1.36596900	-2.10683800	0.00000000
H	2.32950600	0.21824200	0.00000000
N	-1.22982700	-0.03652800	0.00000000



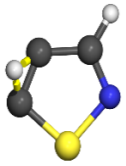
2d

C	-0.63933500	-1.19520800	0.00000000
C	0.78165900	-1.25449100	0.00000000
C	1.24181700	0.02307300	0.00000000
S	0.00000000	1.17383200	0.00000000
H	-1.29119800	-2.05965700	0.00000000
H	1.37861000	-2.15199600	0.00000000
N	-1.19889400	-0.00141300	0.00000000



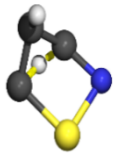
TS_{2b-2c}

C	1.14423400	-0.72415900	-0.06501500
C	1.34035000	0.61079200	-0.10213300
C	0.12267200	1.24827900	0.03304100
S	-1.09429300	0.01476900	-0.00401000
H	2.22042100	-0.25599600	0.53848000
H	-0.13738500	2.29183600	0.11470600
N	-0.03112700	-1.29737200	0.03080400



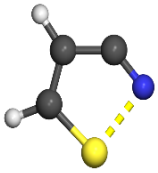
TS_{2c-2d}

C	-1.32773300	0.49006400	-0.00066400
C	-1.07249100	-0.93926200	-0.07346700
C	0.22186800	-1.31631400	-0.11711300
S	1.10525500	0.17288700	0.01235000
H	-2.30228300	0.95620200	0.01791900
H	-0.55009400	-1.62632300	0.88711600
N	-0.25165400	1.21385600	0.00640400



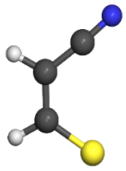
TS_{2b-2d}

C	0.53480800	-0.95553200	0.36108300
C	1.62345200	-0.22823900	-0.33161000
C	0.80129200	0.70565800	0.35351500
N	-0.41064100	1.18679800	-0.11027400
H	1.81236200	-0.27354000	-1.39504600
H	0.67658500	0.11105100	1.38511000
S	-1.08573600	-0.32977600	-0.09475500



TS_{2b-19}

C	1.24084300	-0.67757800	0.00000000
C	1.28882400	0.74027300	0.00000000
C	0.00000000	1.17852400	0.00000000

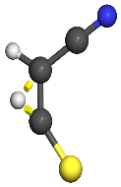


19

C	0.00000000	1.15974400	0.00000000
H	-0.14145900	2.23594100	0.00000000
C	-1.14682100	0.39751400	0.00000000

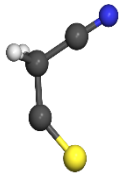
S	-1.20873300	-0.04891300	0.00000000
H	2.17492100	1.34989500	0.00000000
H	-0.30375700	2.21570800	0.00000000
N	0.32722300	-1.46147300	0.00000000

S	1.57273000	0.54751600	0.00000000
C	-1.17773400	-1.01310800	0.00000000
N	-1.28015600	-2.16415600	0.00000000
H	-2.11379900	0.88799000	0.00000000



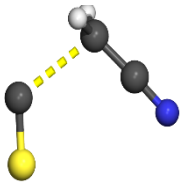
$TS_{19\text{-}20}$

C	0.68971400	0.72791900	0.05179800
H	0.15474500	1.33217600	-0.95189900
C	-0.68705100	0.97899800	0.06469300
S	1.77459300	-0.44943800	0.00468200
C	-1.68905400	-0.04284400	0.03470400
N	-2.48516700	-0.87395000	-0.03811000
H	-1.03371400	1.99205000	0.23659400



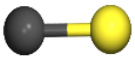
20

C	0.00000000	1.08911300	0.00000000
C	-1.25932200	0.30421300	0.00000000
S	1.54393300	0.83834700	0.00000000
C	-1.10888300	-1.15388800	0.00000000
N	-0.96998000	-2.29515300	0.00000000
H	-1.85192100	0.60794300	0.86850000
H	-1.85192100	0.60794300	-0.86850000



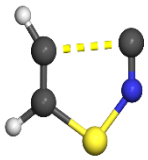
$TS_{20\text{-}11.21}$

C	0.00000000	1.47479900	0.00000000
C	-1.75664700	-0.26504200	0.00000000
S	1.50341600	1.14236400	0.00000000
C	-1.04920800	-1.45765200	0.00000000
N	-0.41810700	-2.43423000	0.00000000
H	-2.14638600	0.12457800	0.92667500
H	-2.14638600	0.12457800	-0.92667500



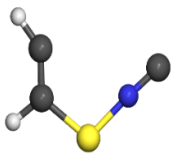
21

C	0.00000000	0.00000000	-1.11796100
S	0.00000000	0.00000000	0.41923500



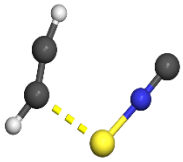
$TS_{2b\text{-}22}$

C	-1.74584600	-0.42606800	0.00000000
C	-1.36712400	-1.59077100	0.00000000
H	-0.81890200	-2.50317700	0.00000000
H	-2.53030300	0.29853500	0.00000000
N	1.28155500	0.08857900	0.00000000
C	2.17602400	-0.67885600	0.00000000
S	0.00000000	1.10992200	0.00000000

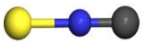


22

C	1.42917600	-0.07023400	0.00000000
C	1.44353900	-1.36722100	0.00000000
H	2.11723600	-2.20285600	0.00000000
H	2.32737900	0.54803700	0.00000000
N	-1.24185000	-0.10057100	0.00000000
C	-2.16465900	-0.82851500	0.00000000
S	0.00000000	0.99716500	0.00000000



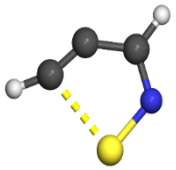
$TS_{22\text{-}6,23}$



23

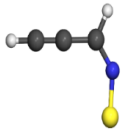
C	-1.48039400	-1.13468400	0.00000000
C	1.05252800	-1.39487200	0.00000000
C	1.30241600	-0.12128300	0.00000000
S	0.00000000	1.10463100	0.00000000
H	1.48427800	-2.37579600	0.00000000
H	2.29109300	0.32920100	0.00000000

S	0.00000000	0.00000000	0.97059700
N	0.00000000	0.00000000	-0.64691000
C	0.00000000	0.00000000	-1.83352900



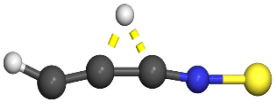
TS_{2c-31}

C	1.20148000	0.73216300	0.00000000
C	1.27964700	-0.69176200	0.00000000
C	0.46185600	-1.62276200	0.00000000
S	-1.23633200	0.13837300	0.00000000
H	2.05553600	1.39377000	0.00000000
H	0.06788000	-2.61232100	0.00000000
N	0.00000000	1.21410600	0.00000000



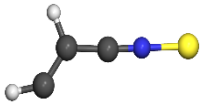
31

C	-1.10274800	-0.37015300	0.00000000
C	-1.20454900	1.04334700	0.00000000
C	-1.30551000	2.24185300	0.00000000
S	1.56788800	-0.79341800	0.00000000
H	-2.02001900	-0.95091300	0.00000000
H	-1.38935800	3.30006800	0.00000000
N	0.00000000	-1.02067800	0.00000000



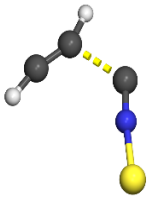
TS_{31-32}

C	-0.61891000	3.09672100	0.00000000
C	-0.20381400	1.91570700	0.00000000
C	0.00000000	0.58233600	0.00000000
H	-0.35401700	4.13157500	0.00000000
H	1.11439400	1.48234700	0.00000000
N	0.01476700	-0.61223700	0.00000000
S	0.25453700	-2.18105300	0.00000000



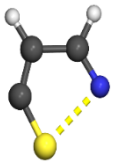
32

C	-0.20300100	-2.93074300	0.00000000
C	0.63226800	-1.90978600	0.00000000
C	0.24345300	-0.55544300	0.00000000
H	-0.13003000	-4.00507000	0.00000000
N	0.00000000	0.58314600	0.00000000
H	1.71047800	-2.09265500	0.00000000
S	-0.35104800	2.14947100	0.00000000



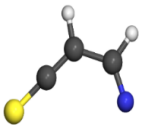
$TS_{35-6,23}$

C	2.26723900	0.96567800	-0.00008000
C	2.34095400	-0.25799200	0.00022800
C	0.47966300	-1.05602400	-0.00026600
H	1.92248700	1.97216000	-0.00042900
N	-0.53611100	-0.43306400	-0.00009300
H	2.90337800	-1.16233900	0.00055100
S	-1.97501400	0.26947800	0.00007800



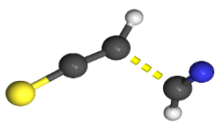
TS_{2d-38}

C	1.30622900	-0.76064000	0.00000000
C	1.28489900	0.69710000	0.00000000
C	0.00000000	1.06695800	0.00000000
S	-1.36310000	0.27235800	0.00000000
H	2.26040100	-1.29125400	0.00000000
H	2.16620900	1.31448400	0.00000000
N	0.26231800	-1.48592300	0.00000000



38

C	-1.29100100	-1.46172100	0.00000000

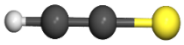


$TS_{38-39,9}$

C	-1.94736700	-0.33379700	0.47030700

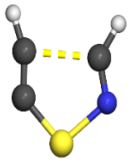
C	-1.14940600	0.00255300	0.00000000
C	0.00000000	0.64397100	0.00000000
S	1.35442700	1.39623300	0.00000000
H	-2.32860300	-1.82126600	0.00000000
H	-2.05735800	0.59361800	0.00000000
N	-0.37749100	-2.31727000	0.00000000

C	-0.51773500	1.03272900	0.05833900
C	0.61662000	0.47808000	-0.03886100
S	1.98792300	-0.31438500	-0.03495200
H	-1.76256600	-0.54580000	1.50547900
H	-1.08281300	1.89291300	-0.22628100
N	-2.55292900	-0.48271700	-0.52266900



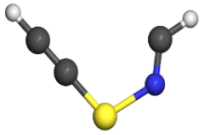
39

S	0.00000000	0.00000000	1.05831500
C	0.00000000	0.00000000	-0.55978700
C	0.00000000	0.00000000	-1.78753900
H	0.00000000	0.00000000	-2.84908400



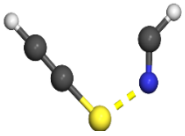
TS_{2d-40}

C	-1.02680600	-1.18476600	0.00000000
C	1.31190300	-1.21355400	0.00000000
C	1.25084800	0.02030100	0.00000000
S	0.00000000	1.16403400	0.00000000
H	-1.56371000	-2.12162200	0.00000000
H	1.71971000	-2.19744500	0.00000000
N	-1.33881100	-0.00533700	0.00000000



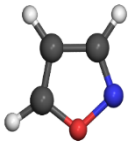
40

C	-1.63408500	-1.11545200	0.00000000
C	2.10979900	-0.96901100	0.00000000
C	1.22879800	-0.14610900	0.00000000
S	0.00000000	1.00510700	0.00000000
H	-2.55149400	-1.69818000	0.00000000
H	2.89200100	-1.68634700	0.00000000
N	-1.50965500	0.09803600	0.00000000



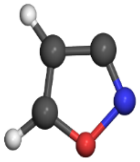
$TS_{40-39,9}$

C	1.59287900	1.18464700	0.00000000
C	-2.10507200	0.92548500	0.00000000
C	-1.23937000	0.08326000	0.00000000
S	0.00000000	-1.03826500	0.00000000
H	2.37157500	1.93377100	0.00000000
H	-2.88089200	1.64950600	0.00000000
N	1.57409900	-0.01876900	0.00000000



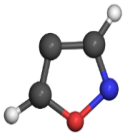
3

C	0.61539600	-0.95936500	0.00000000
C	1.12239600	0.36711100	0.00000000
C	0.00000000	1.12400800	0.00000000
O	-1.09107200	0.34544600	0.00000000
H	1.15890000	-1.89072100	0.00000000
H	2.14584800	0.69387100	0.00000000
H	-0.17588200	2.18593900	0.00000000
N	-0.68957700	-0.99188300	0.00000000

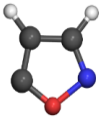


3b

C	0.65752800	-0.96583700	0.00000000
C	1.15734100	0.36106600	0.00000000
C	0.00000000	1.06743100	0.00000000
O	-1.07837700	0.26356900	0.00000000
H	2.17107500	0.71234900	0.00000000
H	-0.20762100	2.12469300	0.00000000
N	-0.60366600	-1.10307800	0.00000000



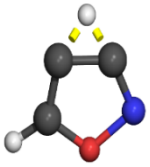
3c



3d

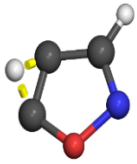
C	-0.66374000	-0.97302400	0.00000000
C	0.74500600	-0.95911200	0.00000000
C	1.11328800	0.33597600	0.00000000
O	0.00000000	1.09470400	0.00000000
H	-1.35154200	-1.80164300	0.00000000
H	2.05562400	0.85331100	0.00000000
N	-1.12448700	0.25252300	0.00000000

C	0.00000000	1.08278000	0.00000000
C	1.17814700	0.28745800	0.00000000
C	0.63804000	-0.95560100	0.00000000
O	-0.65784700	-0.99408800	0.00000000
H	-0.07903200	2.15931800	0.00000000
H	2.20893900	0.58311200	0.00000000
N	-1.10917900	0.38892200	0.00000000



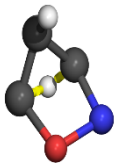
TS_{3b-3c}

C	1.09362800	0.36248000	0.08695400
C	0.03121000	1.21882000	0.09880100
C	-1.05023400	0.36950700	-0.02482000
O	-0.63969800	-0.89176400	-0.00439200
H	1.09753200	1.36336900	-0.72219700
H	-2.11659400	0.51739000	-0.06621100
N	0.81271700	-0.92164200	-0.02029600



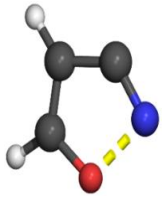
TS_{3c-3d}

C	-1.08754700	-0.41892600	0.00713400
C	0.14597300	-1.17195400	0.07243700
C	1.20683300	-0.31106500	0.11995300
O	0.63959500	0.92326700	-0.01549100
H	-2.10897500	-0.75905600	-0.00574900
H	1.01594800	-1.06790800	-0.92107500
N	-0.80218400	0.83607100	-0.02091300



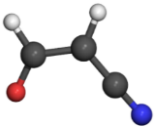
TS_{3b-3d}

C	-0.36561700	0.79556200	0.43052400
C	-1.33184900	0.03887700	-0.31913200
C	-0.35642200	-0.84399100	0.33769200
N	0.94156900	-0.69290600	-0.23507200
H	-1.45194100	0.09996700	-1.39233600
H	-0.26031200	-0.41075100	1.40680400
O	0.93057500	0.65230500	-0.13293300



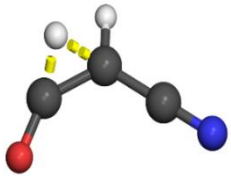
TS_{3b-24}

C	0.63597100	-0.95594000	0.00000000
C	1.15186400	0.36672100	0.00000000
C	0.00000000	1.08496400	0.00000000
O	-1.11833000	0.37584100	0.00000000
H	2.17128700	0.69923400	0.00000000
H	-0.13531400	2.15861500	0.00000000
N	-0.54519200	-1.26272100	0.00000000



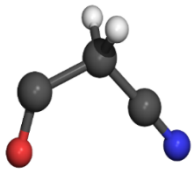
24

O	1.52400000	-0.90391900	-0.00000700
C	1.31647800	0.29561000	0.00001500
C	-0.00909100	0.88428600	0.00000300
C	-1.16803600	0.11461700	-0.00001700
N	-2.15127200	-0.50273600	0.00000800
H	-0.11559700	1.96162300	-0.00000500
H	2.14639900	1.02180600	-0.00000300



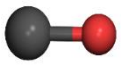
TS_{24-25}

C	-1.26437800	0.29214200	-0.02930100
H	-0.91062900	1.06292900	0.98262500
C	0.03171600	0.85140000	-0.07190500
C	1.22500900	0.06989800	-0.04108000
N	2.17428800	-0.57946300	0.04693500
H	0.10577500	1.90709200	-0.28805100
O	-1.79615600	-0.77430300	-0.02117500



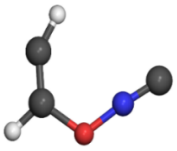
25

C	-1.36718800	0.29051300	-0.00022500
C	0.00226000	0.98831300	0.00006100
C	1.14369300	0.08276400	0.00002200
N	2.02325000	-0.65781000	-0.00004600
H	0.02698700	1.64089100	-0.87433500
H	0.02669900	1.64042400	0.87482600
O	-1.61112800	-0.85577300	0.00008600



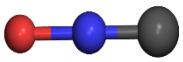
26

C	0.00000000	0.00000000	-0.64351700
O	0.00000000	0.00000000	0.48263800



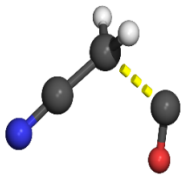
27

C	1.19962600	-0.35425100	0.00074000
O	-0.08369100	-0.92919800	-0.00066800
C	1.46471000	0.91595400	-0.00050500
H	1.91734600	-1.16624000	0.00120000
H	2.28871400	1.60065400	0.00008800
N	-1.06293500	-0.03633300	0.00022300
C	-2.01366700	0.64721400	0.00018000



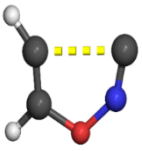
28

N	0.00000000	0.11928500	0.00000000
C	0.00481600	1.32292400	0.00000000
O	-0.00361200	-1.09656800	0.00000000



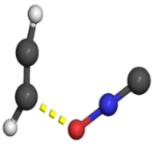
$TS_{25\text{-}26,11}$

C	1.59884000	-0.11221800	0.00000000
C	0.00000000	1.16553600	0.00000000
C	-1.17400100	0.38901300	0.00000000
N	-2.10485700	-0.29905100	0.00000000
H	0.23477800	1.69628500	0.91253500
H	0.23477800	1.69628500	-0.91253500
O	1.46442700	-1.24415000	0.00000000



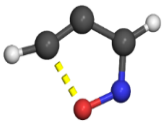
$TS_{3b\text{-}27}$

C	-1.48408900	-0.81261600	0.00000000
C	1.05294600	-1.05171900	0.00000000
C	1.13075700	0.24515200	0.00000000
O	0.00000000	1.07326700	0.00000000
H	1.60605200	-1.96749900	0.00000000
H	2.02233500	0.85840500	0.00000000
N	-1.11800900	0.31972200	0.00000000



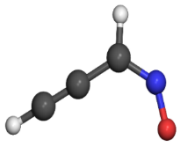
$TS_{27\text{-}28,6}$

C	-1.50797500	0.33320000	-0.00016600
O	0.26165000	0.97772900	-0.00022500
C	-1.64540500	-0.88937000	-0.00009100
H	-1.92393300	1.31590500	-0.00015200
H	-1.52799900	-1.94738500	-0.00045600
N	1.17249300	0.08566000	0.00023000
C	2.01192700	-0.74215900	0.00039000



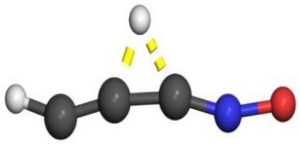
$TS_{3c\text{-}33}$

C	0.00000000	1.15741900	0.00000000
C	1.14695400	0.29271700	0.00000000
C	1.09453600	-0.95573500	0.00000000
O	-0.89952100	-0.80776000	0.00000000
H	-0.02014000	2.23302400	0.00000000
H	1.39867000	-1.97675700	0.00000000
N	-1.09018700	0.46277100	0.00000000



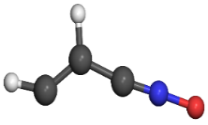
33

C	2.09537100	-0.68467000	0.00000000
O	-1.73287600	-0.64450900	0.00000000
C	0.00000000	0.88124500	0.00000000
C	1.12615700	0.02597300	0.00000000
H	0.11827400	1.95421800	0.00000000
N	-1.21892700	0.45475200	0.00000000
H	2.94804700	-1.31668800	0.00000000



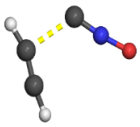
TS_{33-34}

C	-2.54866800	-0.20832900	-0.00001600
C	-1.33320400	0.05534600	0.00004200
C	0.02455700	0.10680400	0.00001200
H	-3.57478700	0.08010500	-0.00015400
H	-0.76076000	1.33634400	0.00000100
N	1.19180300	-0.15112000	0.00003200
O	2.39210200	-0.01019200	-0.00003800



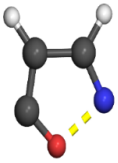
34

C	2.22505900	-0.86277900	0.00000000
C	1.41616500	0.17485100	0.00000000
C	0.00000000	0.10682400	0.00000000
H	3.28950100	-1.02558300	0.00000000
N	-1.15704000	0.19178900	0.00000000
H	1.84038300	1.18241100	0.00000000
O	-2.35974400	0.24840900	0.00000000



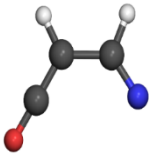
$TS_{34-6,28}$

C	-1.55993400	-1.22552300	0.00000000
C	-1.86442100	-0.04879900	0.00000000
C	0.00000000	1.07058800	0.00000000
H	-1.13611500	-2.20064900	0.00000000
N	1.02646700	0.44783500	0.00000000
H	-2.46856100	0.82576700	0.00000000
O	2.12069300	-0.06719500	0.00000000



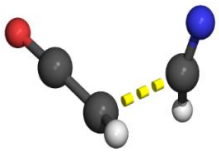
TS_{3d-41}

O	-1.24656800	-0.34105100	0.00027500
C	-0.80492100	0.80143800	-0.00041200
C	0.52388800	1.08361400	-0.00011500
C	1.08046900	-0.23599200	0.00016100
H	1.02956200	2.02815800	0.00123600
H	2.14126400	-0.46439300	-0.00045600
N	0.28644300	-1.24710300	-0.00011300



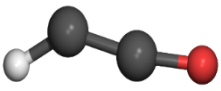
41

C	0.00000000	1.08277700	0.00000000
C	1.17809800	0.28742700	0.00000000
C	0.63797300	-0.95538600	0.00000000
O	-0.65780100	-0.99482500	0.00000000
H	-0.07844600	2.15937800	0.00000000
H	2.20886300	0.58334000	0.00000000
N	-1.10920500	0.38956700	0.00000000



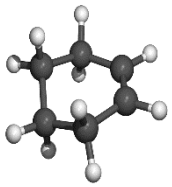
$TS_{41-42,9}$

C	1.42949200	-0.13043200	0.00000000
C	0.00000000	-1.05916700	0.00000000
C	-1.16323000	-0.37956200	0.00000000
O	-1.75972900	0.61538100	0.00000000
H	2.19854400	-0.90532000	0.00000000
H	0.09391100	-2.13263600	0.00000000
N	1.45540200	1.07569600	0.00000000



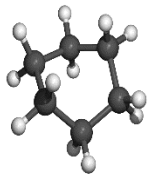
42

C	-1.05982800	0.68514400	0.00000000
H	-2.11865000	0.52999600	0.00000000
C	0.00000000	-0.04550800	0.00000000
O	1.05970200	-0.54597700	0.00000000



Cyclohexene

C	-1.49323900	0.04827800	-0.10977800
C	-0.66272700	1.30214400	-0.05695300
C	0.66251400	1.30227700	0.05673000
C	1.49318700	0.04851100	0.11007200
C	0.69700700	-1.18978200	-0.31585700
C	-0.69674300	-1.19002000	0.31568300
H	-2.37507500	0.16616300	0.52634400
H	-1.19219700	2.24716600	-0.11264800
H	1.19180500	2.24738300	0.11264200
H	2.37529100	0.16646000	-0.52560700
H	0.59533300	-1.19346000	-1.40527100
H	-0.59511600	-1.19399700	1.40509100
H	1.24072000	-2.09795700	-0.04865600
H	1.88311500	-0.08582900	1.12639300
H	-1.88372200	-0.08610200	-1.12585000
H	-1.24015700	-2.09827400	0.04818800



Cyclohexane

C	-1.22493300	0.66371100	0.37979800
C	-0.00024400	1.52373200	0.00007300
C	1.22493300	0.66431200	-0.37992200
C	1.22493300	-0.66371100	0.37979800
C	0.00024400	-1.52373200	0.00007300
C	-1.22493300	-0.66431200	-0.37992200
H	-1.21445100	0.45590800	1.45354700
H	-0.25421100	2.17963000	-0.83568400
H	1.21435800	0.45682800	-1.45367800
H	2.14553700	-1.21797600	0.18866100
H	0.25421100	-2.17963000	-0.83568400
H	-2.14538900	-1.21869700	-0.18850800
H	-1.21435800	-0.45682800	-1.45367800
H	-0.25341200	-2.17959400	0.83596700
H	1.21445100	-0.45590800	1.45354700
H	2.14538900	1.21869700	-0.18850800
H	0.25341200	2.17959400	0.83596700
H	-2.14553700	1.21797600	0.18866100