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Spin propagation through the C-C and C-H bonds

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The optimized geometry of the radicals.

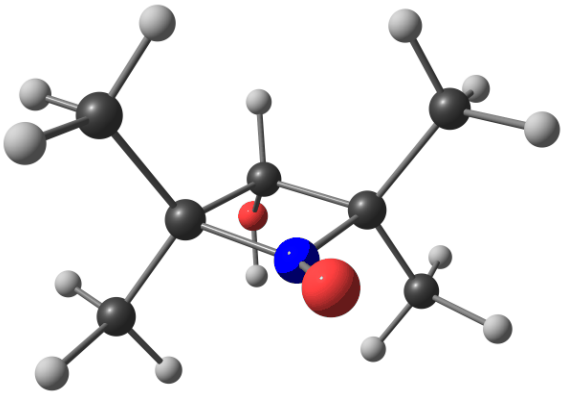

Chart 1

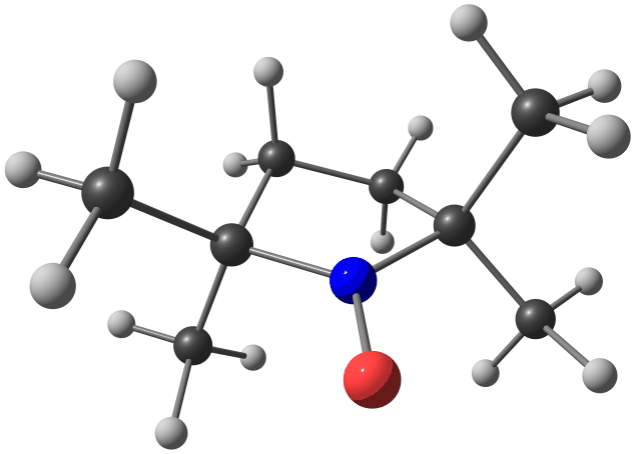

Chart 2

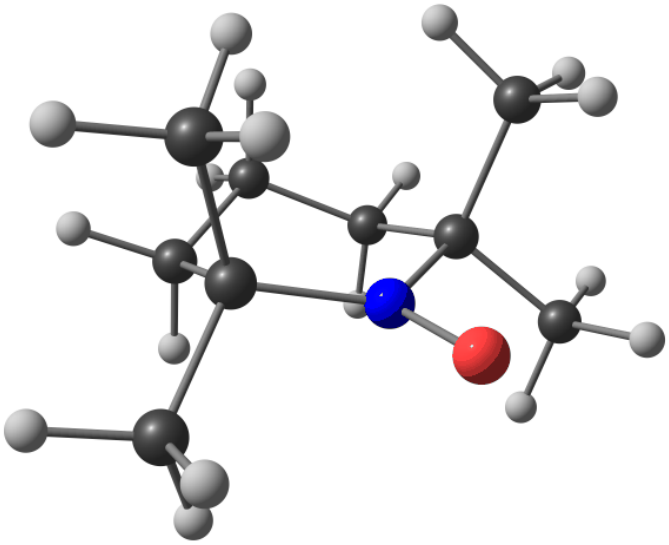

Chart 3

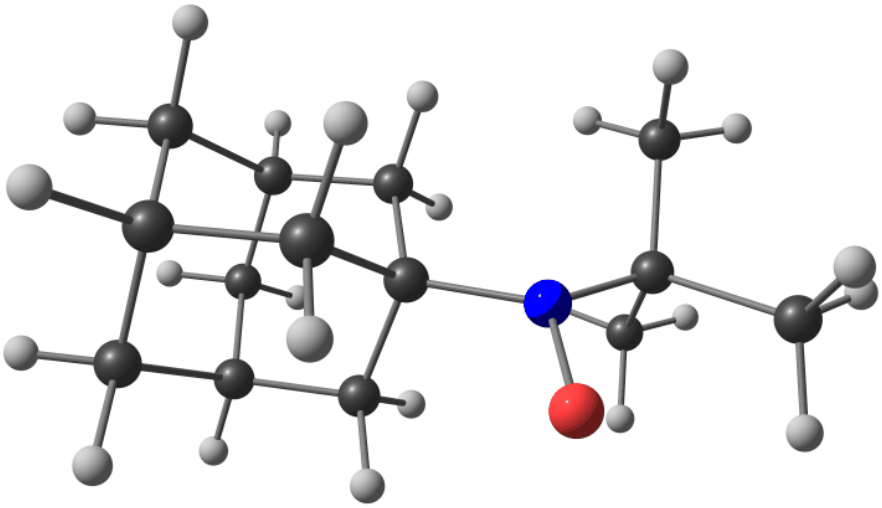

Chart 4

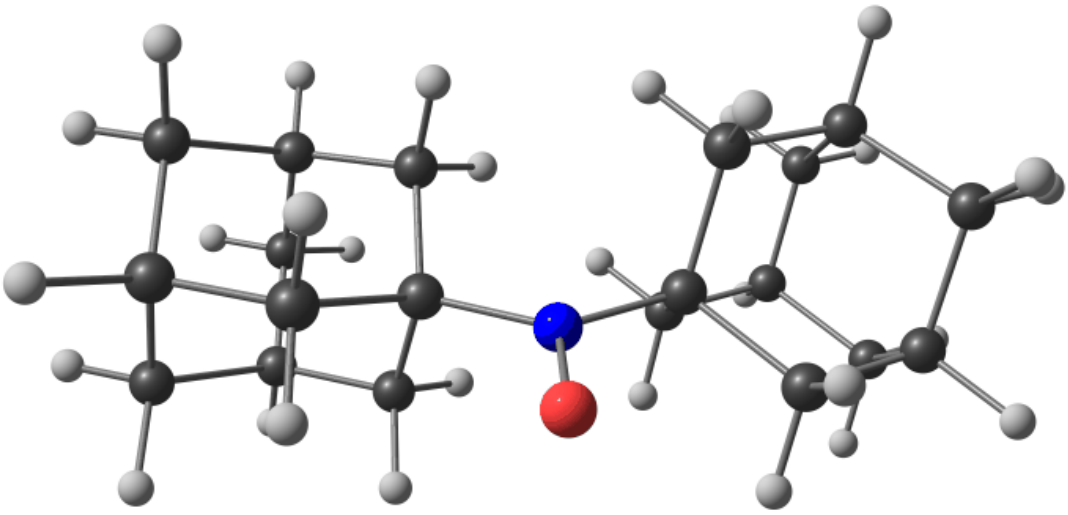

Chart 5

Table 1S Calculated spin densities in the units of (a/a_0) multiplied by 10^4.

	B3LYP/N07D	PBE0/N07D	B3LYP/TZVP	Averaged values
Chart 1				
H (γ-CH_3)	**-5.27**	**-6.74**	**-5.59**	**-5.87**
H (γ-CH_3)	**-4.22**	**-4.65**	**-4.37**	**-4.41**
H (γ-CH)	**-9.49**	**-12.51**	**-10.97**	**-11.0**
H (γ-COH)	**-0.75**	**-0.84**	**-0.93**	**-0.84**
Chart 2				
H (γ-CH_3-equatorial)	**+1.43**	**-0.14**	**+1.03**	**+0.77**
H (γ-CH_3-axial)	**-7.01**	**-8.19**	**-7.18**	**-7.46**
H (γ-CH_2-equatorial)	**-0.85**	**-1.82**	**-0.69**	**-1.12**
H (γ-CH_2-axial)	**-4.08**	**-5.14**	**-4.24**	**-4.49**
Chart 3				
H (γ-CH_3-equatorial)	**-8.79**	**-9.72**	**-8.84**	**-9.12**
H (γ-CH_3-axial)	**+0.09**	**-1.36**	**-0.15**	**-0.47**
H (γ-CH_2-equatorial)	**-10.74**	**-11.84**	**-10.72**	**-11.10**
H (γ-CH_2-axial)	**-4.03**	**-5.22**	**-4.46**	**-4.57**
H (δ-CH_2-equatorial)	**+4.59**	**+4.68**	**+4.70**	**+4.66**
H (δ-CH_2-axial)	**+1.32**	**+1.28**	**+1.02**	**+1.21**
C (β-C)	**-32.76**	**-36.47**	**-29.82**	**-33.02**
C (γ-CH_3-equatorial)	**+55.54**	**+54.40**	**+53.22**	**+54.39**
C (γ-CH_3-axial)	**+25.79**	**+25.21**	**+25.64**	**+25.55**
C (γ-CH_2)	**+4.37**	**+4.04**	**+4.22**	**+4.21**
C (δ-CH_2)	**-2.06**	**-2.35**	**-2.21**	**-2.21**
Chart 4				
H (γ-CH_2)	**-8.58**	**-9.58**	**-8.51**	**-8.89**
H (δ-CH)	**+10.61**	**+10.49**	**+10.44**	**+10.51**
H (ε-CH_2-equatorial)	**-1.05**	**-1.16**	**-1.03**	**-1.08**
H (ε-CH_2-axial)	**-0.38**	**-0.43**	**-0.40**	**-0.40**

Chart 5				
H (γ-CH_2)	**-5.96**	**-6.82**	**-6.30**	**-6.36**
H (δ-CH)	**+10.30**	**+10.18**	**+9.76**	**+10.08**
H (ε-CH_2-equatorial)	**-0.57**	**-0.66**	**-0.58**	**-0.60**
H (ε-CH_2-axial)	**-0.01**	**-0.08**	**-0.02**	**-0.04**

The Cartesian coordinates (Angstroem) of atoms for optimized geometries of the radicals.

Chart 1.

C	1.067593	-0.632422	-6.468318
N	2.276292	0.063366	-7.014962
C	3.278380	-0.902458	-6.463667
C	2.061478	-1.664827	-5.818363
H	1.939992	-2.667481	-6.236838
C	0.177392	-1.191884	-7.576680
H	0.735494	-1.861742	-8.237690
H	-0.660580	-1.750024	-7.146161
H	-0.223161	-0.374260	-8.183791
C	0.274503	0.241582	-5.496388
H	-0.217355	1.051376	-6.044261
H	-0.493274	-0.349627	-4.987359
H	0.915223	0.701977	-4.737188
C	4.254516	-0.245614	-5.488036
H	4.930085	0.421322	-6.033486
H	3.741189	0.357160	-4.731289
H	4.855041	-1.004620	-4.976365
C	4.012430	-1.661137	-7.568384
H	3.312063	-2.169944	-8.237899
H	4.608475	-0.966596	-8.168896
H	4.681814	-2.411179	-7.134056

O	2.365164	0.762596	-8.072232
O	2.036563	-1.837094	-4.422528
H	2.144437	-0.977681	-3.993742

Chart 2.

C	-1.081376	-3.356564	-4.174384
C	-1.989886	-2.128455	-4.390751
N	-2.786907	-2.559792	-5.574781
C	-2.308242	-3.798589	-6.252438
C	-0.939731	-4.005522	-5.568331
H	-1.561333	-4.053499	-3.477960
H	-0.669297	-5.063871	-5.510097
C	-2.933920	-1.843210	-3.217179
H	-3.505837	-2.737596	-2.949707
H	-2.363222	-1.522268	-2.339540
H	-3.639317	-1.052751	-3.486424
C	-1.196545	-0.861370	-4.763809
H	-1.884170	-0.089433	-5.122246
H	-0.660448	-0.474334	-3.890721
H	-0.466483	-1.064692	-5.553737
C	-2.213907	-3.551729	-7.761873
H	-3.194242	-3.274667	-8.158700
H	-1.512622	-2.740440	-7.982121
H	-1.869931	-4.456349	-8.273794
C	-3.299718	-4.939674	-5.954915
H	-3.331926	-5.172987	-4.886053
H	-4.305014	-4.646665	-6.272223

H	-3.012939	-5.847178	-6.496494
O	-3.808950	-1.911148	-5.980257
H	-0.158773	-3.498183	-6.145348
H	-0.114657	-3.078435	-3.745041

Chart 3.

C	-1.138306	-1.260609	-0.339752
C	0.370278	-1.330975	-0.025540
C	0.339390	1.336470	-0.022154
C	-1.167408	1.231678	-0.336432
C	-1.828586	-0.023023	0.237758
H	-1.270664	-1.255907	-1.429854
H	-1.604196	-2.182012	0.029230
H	-1.653576	2.141743	0.034327
H	-1.299171	1.226517	-1.426632
H	-1.777265	-0.023953	1.333912
N	1.010483	0.010671	-0.256167
O	2.295985	0.025405	-0.225896
H	-2.893413	-0.035276	-0.022564
C	0.627880	-1.764025	1.433884
H	0.318358	-2.805036	1.574612
H	1.695534	-1.684081	1.654951
H	0.078127	-1.150415	2.152508
C	1.050743	-2.327241	-0.979181
H	0.593225	-3.315263	-0.864158
H	0.929574	-2.009695	-2.019971
H	2.117799	-2.402358	-0.763178
C	0.996333	2.350601	-0.973450

H	0.515545	3.327237	-0.856270
H	2.061277	2.450552	-0.757177
H	0.882799	2.032566	-2.014921
C	0.586847	1.771773	1.438296
H	1.656114	1.716424	1.659051
H	0.253003	2.804856	1.581548
H	0.051887	1.143647	2.155511

Chart 4.

N	-1.067987	-7.874754	-0.456795
O	-1.603594	-6.714293	-0.627368
C	-1.164963	-8.445406	0.944900
H	-2.187214	-10.327675	0.420344
C	-2.339722	-9.440769	1.040355
H	-2.452359	-9.777675	2.076470
H	-3.274141	-8.959839	0.735697
H	0.333386	-10.071298	0.895825
C	0.159181	-9.109286	1.376669
H	1.009384	-8.451723	1.169155
H	0.128006	-9.288881	2.456291
C	-1.435314	-7.263711	1.893168
H	-1.474907	-7.645268	2.918439
H	-2.379732	-6.769682	1.662628
H	-0.639242	-6.516298	1.830228
C	-1.181524	-8.521810	-4.712673
H	-1.706471	-7.564996	-4.831238
H	-1.055611	-8.946269	-5.717522
C	-2.014442	-9.477751	-3.834172

H	-2.998412	-9.640706	-4.292923
C	0.196286	-8.291623	-4.056707
H	0.788036	-7.602075	-4.672327
C	0.003653	-7.671336	-2.658305
H	-0.504892	-6.706838	-2.726660
H	0.977057	-7.493988	-2.181988
C	-2.210934	-8.858187	-2.435425
H	-2.819198	-9.526689	-1.813961
H	-2.737200	-7.900642	-2.499794
C	-0.838035	-8.611352	-1.754551
C	-0.084063	-9.952838	-1.631762
H	0.901754	-9.794158	-1.181613
H	-0.628879	-10.660943	-0.998581
C	-1.275101	-10.823698	-3.690837
H	-1.143975	-11.293167	-4.674733
H	-1.868700	-11.518152	-3.081004
C	0.934888	-9.637895	-3.923134
H	1.090100	-10.088610	-4.912359
H	1.928571	-9.483906	-3.481725
C	0.100051	-10.582061	-3.035965
H	0.624723	-11.538674	-2.916856

Chart 5.

N	-1.008423	-7.638209	-0.480220
O	-0.531422	-6.471370	-0.745299
C	0.360485	-9.659438	-4.068541
H	0.209519	-8.741629	-4.651699
H	0.744254	-10.421380	-4.760676

C	-0.975106	-10.124162	-3.455686
H	-1.709128	-10.300790	-4.252203
C	1.376521	-9.407236	-2.936247
H	2.324059	-9.052807	-3.361871
C	0.829127	-8.319232	-1.989605
H	0.676295	-7.386338	-2.535953
H	1.550260	-8.103659	-1.192674
C	-1.521799	-9.034250	-2.507126
H	-2.488163	-9.353570	-2.107543
H	-1.688281	-8.096328	-3.051256
C	-0.513900	-8.767430	-1.355556
C	-0.248880	-10.080709	-0.576494
H	0.489088	-9.893169	0.212023
H	-1.156946	-10.448190	-0.091646
C	-0.751273	-11.425432	-2.657119
H	-0.391323	-12.219871	-3.324144
H	-1.699925	-11.774204	-2.227908
C	1.612595	-10.714078	-2.156295
H	2.007539	-11.491367	-2.824090
H	2.360487	-10.555337	-1.368078
C	0.279019	-11.172332	-1.536740
H	0.433800	-12.094575	-0.961792
C	-3.224205	-8.613089	0.347182
H	-3.731958	-8.252094	-0.555128
H	-2.914025	-9.643550	0.155716
C	-4.209300	-8.602666	1.539507
H	-5.046209	-9.272191	1.303236
C	-2.007456	-7.704002	0.651915

C	-2.542287	-6.268126	0.893103
H	-3.018503	-5.900954	-0.023625
H	-1.704124	-5.599789	1.099172
C	-4.732797	-7.171752	1.763120
H	-5.452400	-7.155919	2.592757
H	-5.265365	-6.820309	0.868899
C	-3.540562	-6.246878	2.069025
H	-3.895066	-5.217228	2.205696
C	-2.831354	-6.726185	3.351508
H	-1.998253	-6.054478	3.596497
H	-3.525767	-6.700920	4.202407
C	-3.492818	-9.096113	2.813920
H	-3.134660	-10.124861	2.673008
H	-4.198007	-9.116578	3.655584
C	-1.311424	-8.181001	1.956202
H	-0.915773	-9.193320	1.834585
H	-0.458969	-7.521315	2.160746
C	-2.309866	-8.160123	3.134853
H	-1.795937	-8.510676	4.039591