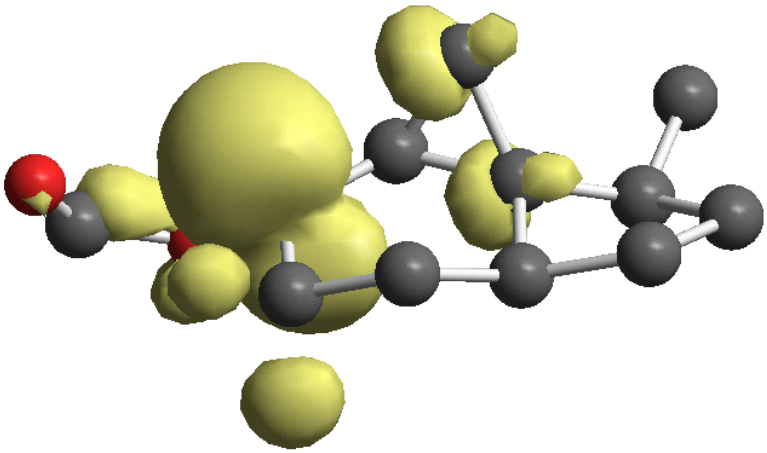
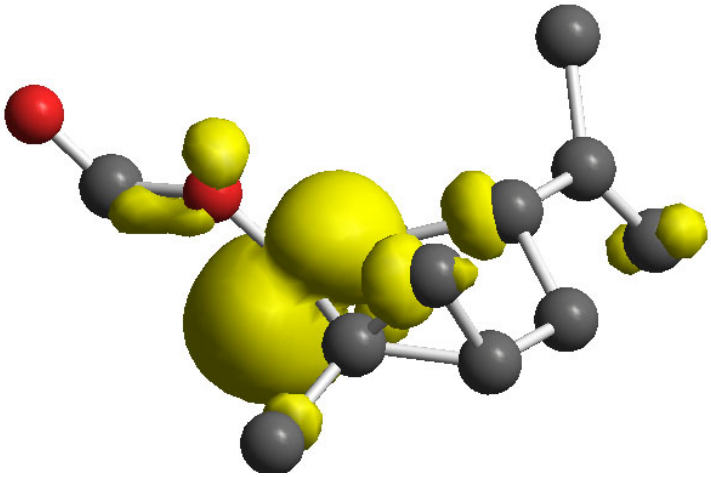
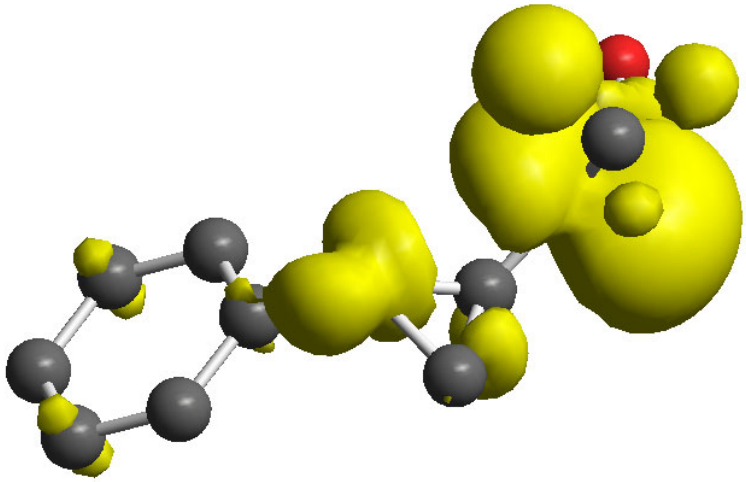


a



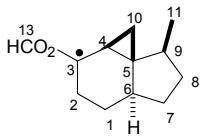
b



c

Figure 2. 3D structures and spin density surfaces from UHF/6-31G** calculations (Gaussian 98; Chem3D Ultra 5.0, Cambridge Soft) for minimum energy conformations of simplified models of intermediate radicals a) **18**, b) **19** and c) **20** (most stable conformer presenting delocalization of spin density on the phenyl ring is shown). Surfaces drawn at 0.002 a.u. for **a**, 0.004 a.u. for **b** and 0.001 a.u. for **c**. See Figure 1 for structures.

Cartesian coordinates, total atomic spin densities and Fermi contact data for UHF/6-31G optimized structure of simplified model of radical 18 (Figure 1a).**



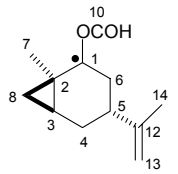
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.177852	1.992241	0.218384
2	6	1.484077	1.347936	-0.274597
3	6	1.533112	-0.138180	-0.027760
4	6	0.309512	-0.960636	0.163271
5	6	-1.013110	-0.262235	0.067770
6	6	-1.014676	1.208958	-0.313991
7	6	-2.434137	1.637905	0.070858
8	6	-3.302152	0.382112	-0.218449
9	6	-2.317933	-0.782870	-0.526908
10	6	-0.516021	-0.703487	1.406824
11	6	-2.817385	-2.146564	-0.063298
12	8	2.537061	-0.830389	-0.710304
13	6	3.797222	-0.695401	-0.332088
14	8	4.198524	-0.023292	0.553145
15	1	0.139473	3.020423	-0.129689
16	1	0.159696	2.036184	1.303331
17	1	2.344304	1.821998	0.185061
18	1	1.572671	1.512841	-1.350107
19	1	0.402184	-1.981940	-0.163642
20	1	-0.948193	1.235921	-1.403637
21	1	-2.768600	2.512181	-0.478261
22	1	-2.472003	1.887895	1.127536
23	1	-3.982372	0.543438	-1.048482
24	1	-3.914580	0.136434	0.643668
25	1	-2.174891	-0.832457	-1.605305
26	1	-0.981562	-1.559461	1.860968
27	1	-0.149106	0.016589	2.115875
28	1	-2.089570	-2.929055	-0.259654
29	1	-3.042899	-2.151978	0.998282
30	1	-3.728683	-2.411041	-0.591619
31	1	4.431281	-1.307213	-0.967155

E(UHF) = -614.010280662 A.U.; Convg = 0.4784D-08; -V/T = 2.0010
Annihilation of the first spin contaminant:
S**2 before annihilation 0.7641, after 0.7502

Atom number	Atom type	Total atomic spin densities	Isotropic Fermi Contact Couplings (au)
1	C	0.008809	0.00314
2	C	-0.139086	-0.03466
3	**C**	**1.125912**	**0.30555**
4	*C*	*-0.191192*	*-0.05826*
5	*C*	*0.064190*	*0.03075*
6	C	-0.007840	-0.00394
7	C	0.000956	0.00150
8	C	0.003308	0.00282
9	C	-0.000756	0.00371
10	*C*	*0.071602*	*0.04135*
11	C	-0.000053	0.00000
12	O	-0.033353	0.00045
13	C	0.015984	0.02222
14	O	0.002792	-0.00069

Bold type indicates predominantly localized radical center; *italic type* indicates cyclopropane carbons.

Cartesian coordinates, total atomic spin densities and Fermi contact data for UHF/6-31G optimized structure of simplified model of radical 19 (Figure 1b).**



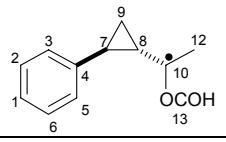
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.011649	0.091546	-0.341653
2	6	-1.225767	-1.346461	-0.025969
3	6	0.015223	-2.171080	0.176208
4	6	1.396914	-1.573542	-0.034916
5	6	1.454324	-0.060834	0.208685
6	6	0.362627	0.627190	-0.644133
7	6	-2.449766	-1.969096	-0.673194
8	6	-0.835551	-1.814983	1.355120
9	8	-1.889090	0.937312	0.328943
10	6	-2.457783	1.932766	-0.342060
11	8	-3.155919	2.730551	0.171146
12	6	2.815974	0.575142	-0.036581
13	6	3.714324	0.099756	-0.881841
14	6	3.085792	1.828186	0.763000
15	1	-0.058078	-3.195686	-0.151473
16	1	1.692763	-1.783287	-1.058983
17	1	2.114243	-2.075540	0.608140
18	1	1.214378	0.122597	1.253591
19	1	0.598447	0.451572	-1.692117
20	1	0.373886	1.700254	-0.490640
21	1	-2.547783	-3.012230	-0.391379
22	1	-2.388082	-1.919280	-1.756763
23	1	-3.352826	-1.454305	-0.359764
24	1	-1.436736	-2.590650	1.797116
25	1	-0.481424	-1.087262	2.062758
26	1	-2.223505	1.932334	-1.405977
27	1	4.655038	0.601013	-1.030120
28	1	3.561828	-0.795918	-1.454789
29	1	4.032834	2.277578	0.490342
30	1	2.306586	2.571510	0.616711
31	1	3.110540	1.602849	1.826636

E(UHF) = -613.985774973 A.U.; Convg = 0.6790D-08; -V/T = 2.0010
Annihilation of the first spin contaminant:
S**2 before annihilation 0.7642, after 0.7502

Atom number	Atom type	Total atomic spin densities	Isotropic Fermi Contact Couplings (au)
1	**C**	**1.141111**	**0.29342**
2	*C*	*-0.152068*	*-0.04844*
3	*C*	*0.000342*	*-0.00054*
4	C	-0.005634	-0.00184
5	C	0.059509	0.04201
6	C	-0.151740	-0.03986
7	C	0.024839	0.02662
8	*C*	*0.067033*	*0.03356*
9	O	-0.020617	0.00680
10	C	0.001496	0.03415
11	O	0.004681	-0.00100
12	C	-0.062123	-0.00959
13	C	0.067741	0.01122
14	C	0.007523	0.00242

Bold type indicates predominantly localized radical center; *italic type* indicates cyclopropane carbons.

Cartesian coordinates, total atomic spin densities and Fermi contact data for UHF/6-31G optimized structure of simplified model of radical 20 (Figure 1c).**



Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.949415	1.112875	-0.038088
2	6	2.767767	1.737565	-0.406240
3	6	1.591310	1.012238	-0.477791
4	6	1.576128	-0.347441	-0.182645
5	6	2.765674	-0.964306	0.182188
6	6	3.945429	-0.239767	0.255370
7	6	0.300176	-1.128825	-0.299799
8	6	-0.892869	-0.787374	0.569901
9	6	-0.153614	-2.077033	0.762615
10	6	-2.266542	-0.708257	0.016955
11	8	-2.638748	0.579668	-0.367848
12	6	-2.880779	-1.750534	-0.861952
13	6	-3.111136	1.411185	0.554362
14	8	-3.400851	2.527685	0.317354
15	1	4.863779	1.676615	0.020264
16	1	2.762042	2.788738	-0.634917
17	1	0.675444	1.501823	-0.761610
18	1	2.770775	-2.016220	0.408766
19	1	4.858179	-0.732330	0.541490
20	1	0.055939	-1.423555	-1.308097
21	1	-0.689636	-0.034403	1.314450
22	1	0.440579	-2.164106	1.654911
23	1	-0.617981	-2.996604	0.454505
24	1	-3.946112	-1.572195	-0.952288
25	1	-2.459753	-1.722756	-1.866277
26	1	-2.732175	-2.743194	-0.456445
27	1	-3.210042	0.957413	1.539956

E(UHF) = -611.670892867 A.U.; Convg = 0.7060D-08; -V/T = 2.0011
Annihilation of the first spin contaminant:
S**2 before annihilation 0.7635, after 0.7501

Atom number	Atom type	Total atomic spin densities	Isotropic Fermi Contact Couplings (au)
1	C	-0.014231	-0.00248
2	C	0.014989	0.00241
3	C	-0.013227	-0.00138
4	C	0.007563	0.00160
5	C	-0.011904	0.00089
6	C	0.015379	0.00315
7	*C*	*0.114792*	*0.05182*
8	*C*	*-0.170427*	*-0.04080*
9	*C*	*0.005298*	*0.00201*
10	**C**	**1.108286**	**0.30397**
11	O	-0.021426	0.00382
12	C	-0.139533	-0.03992
13	C	0.007475	0.03752
14	O	-0.003068	-0.00320

Bold type indicates predominantly localized radical center; *italic type* indicates cyclopropane carbons.