Radicals formed in N-Acetyl-Proline by Electron Attachment: ESR Spectroscopy and Computational Studies

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Table S1. Cartesian coordinates (in Å) for the RAD3 geometry optimized at the B3LYP/6-31++G(d,p) level with the $C_{carboxyl}$-C2-C3-C4 dihedral frozen at 23°.

atom	x	y	z
C	-0.0393	0.0054	0.0107
C	-0.0217	-0.0097	1.5278
N	1.1941	0.0032	2.1126
C	1.3832	-0.0236	3.5599
C	2.8147	0.3539	3.9548
C	3.2230	1.8126	3.6225
C	4.1808	2.0849	2.5120
C	4.4798	1.2466	1.3740
O	3.9047	0.2015	1.0489
O	-1.0802	-0.0292	2.1829
O	5.5065	1.7377	0.6305
H	4.7068	3.0347	2.5375
H	5.6439	1.1380	-0.1231
H	-0.5560	-0.8901	-0.3473
H	-0.6106	0.8744	-0.3286
H	0.9589	0.0404	-0.4320
H	2.3150	2.4125	3.4298
H	3.6575	2.2810	4.5146
H	3.5216	-0.3564	3.5163
H	2.8817	0.2227	5.0394
H	1.1516	-1.0239	3.9490
H	0.6677	0.6684	4.0175
H	2.0341	-0.0175	1.5392