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Table S1. Magnitude of the spin contamination, *S(S+1)*, for the open shell systems, at BH&HLYP/6-311G(d,p) level of theory.

	S(S+1)
OH	0.752
RC-I	0.752
RC-II	0.752
RC-III	0.752
RC-IV	0.753
TS-I	0.767
TS-II	0.764
TS-III	0.766
TS-IV	0.761
PC-I	0.755
PC-II	0.755
PC-III	0.764
PC-IV	0.756
R-I	0.755
R-II	0.755
R-III	0.767
R-IV	0.755

RC*=Reactant Complexes,* ***TS****=Transition States,* ***PC****=Product Complexes,* ***R****=Radical Products,* ***Channel I****= abstraction from the amino end,* ***Channel II****= abstraction from the –CH_2- group next to the amino end,* ***Channel III****= abstraction from the –CH_2- group next to the carboxyl end,* ***Channel IV****= abstraction from the –CH_2- group next to the carboxyl end.*

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Table S2. Topological data for N1-H11 intramolecular interaction in the different species involved in β-alanine + OH gas phase reaction.

	Bond Critical Point (1,11)			**Ring Critical Point (1-5,11)**	
	$d_{1\text{-}11}$**(Å)**	$\rho_{1\text{-}11}$ **(a.u.)**	$\nabla^2(\rho)_{1\text{-}11}$ **(a.u.)**	ρ **(a.u.)**	$\nabla^2(\rho)$ **(a.u.)**
β-alanine	1.820	0.0414	-0.0282	0.0172	-0.0253
RC-I	1.744	0.0443	-0.0285	0.0162	-0.0240
RC-II	1.773	0.0464	-0.0289	0.0180	0.0268
RC-III	1.785	0.0449	-0.0287	0.0177	-0.0263
RC-IV	-	-	-	-	-
TS-I	1.913	0.0319	-0.0251	0.0156	-0.0225
TS-II	1.885	0.0354	-0.0259	0.0169	-0.0242
TS-III	1.817	0.0418	-0.0279	0.0175	-0.0254
TS-IV	-	-	-	-	-
PC-I	-	-	-	-	-
PC-II	1.895	0.0336	-0.0255	0.0178	-0.0246
PC-III	1.805	0.0430	-0.0288	0.0170	-0.0254
PC-IV	-	-	-	-	-
P-I	1.883	0.0332	-0.0268	0.0153	-0.0228
P-II	1.971	0.0286	-0.0230	0.0171	-0.0232
P-III	1.829	0.0406	-0.0282	0.0167	-0.0247
P-IV	-	-	-	-	-

Table S3. Topological data for intramolecular interactions (other than N1-H11) in the different species involved in β-alanine + OH gas phase reaction.

	Bond Critical Point			**Ring Critical Point**		
	Atoms	ρ	$\rho(\nabla^2)$	***Atoms***	ρ	$\rho(\nabla^2)$
RC-I	4, 15	0.0133	-0.0115	1, 4, 11, 12, 14, 15	0.0046	-0.0053
	12, 14	0.0051	-0.0054			
RC-II	4, 15	0.0198	-0.0181	2- 5,10, 14, 15	0.0043	-0.0047
	10, 14	0.0067	-0.0052			
RC-III	6, 15	0.0288	-0.0270	3, 5, 6, 7,14, 15	0.0068	-0.0075
	7, 14	0.0070	-0.0072			
RC-IV	6, 15	0.0287	-0.0254	4-6, 11, 14, 15	0.0136	-0.0151
	11, 14	0.0265	-0.0235			
TS-III	6, 15	0.0168	-0.0153	3, 5-7, 14, 15	0.0137	-0.0165
TS-IV	6, 14	0.0508	-0.0537	4-6, 11, 14, 15	0.0338	-0.0478
PC-I	1, 12	0.0298	-0.0245	1-3, 8, 12, 14	0.0069	-0.0080
	8, 14	0.0089	-0.0090	3-5, 8, 11, 14	0.0086	-0.0091
	11, 14	0.0377	-0.0331			
PC-II	4, 15	0.0129	-0.0121	1-3, 8, 12, 14	0.0053	-0.0059
	8, 14	0.0067	-0.0059	3-5, 8, 11, 14	0.0054	-0.0061
	12, 14	0.0163	-0.0166			
PC-III	6, 15	0.0255	-0.0244	3, 5, 6, 8, 14, 15	0.0088	-0.0099
	8, 14	0.0129	-0.0112			
PC-IV	4, 11	0.0228	-0.0217	4-6, 11, 14	0.0124	-0.0145
	6, 14	0.0174	-0.0170			
R-IV	4, 13	0.0108	-0.0101	1-5, 13	0.0104	-0.0119

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Table S4. Variation of the activation energies (kcal mol^{-1}) with temperature, in the 200 – 500 K range.

T	***Ea*** ($k_{tot}^{(2)}$)	***Ea*** ($k_{tot}^{(4)}$)
250	-1.16	-1.20
260	-1.10	-1.13
270	-1.04	-1.07
280	-0.98	-1.01
290	-0.91	-0.95
298.15	**-0.86**	**-0.90**
300	-0.85	-0.89
310	-0.79	-0.83
320	-0.73	-0.77
340	-0.61	-0.64
350	-0.54	-0.58
360	-0.48	-0.52
370	-0.42	-0.46
380	-0.36	-0.40
400	-0.23	-0.27

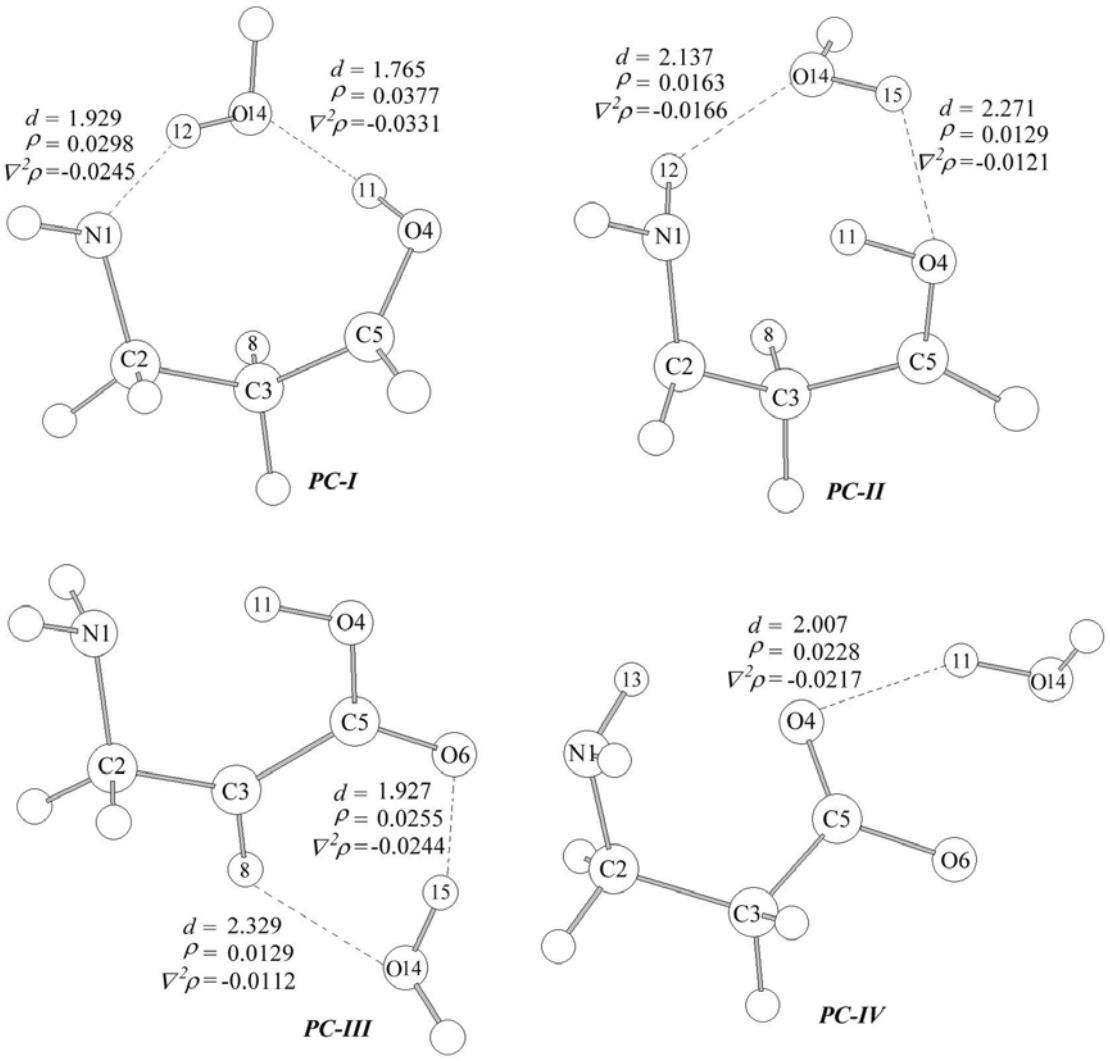

Figure 1S. Fully optimized BH&HLYP/6-311G(d,p) product complexes of the β-alanine + OH reaction. Distances (*d*) are reported in Å.

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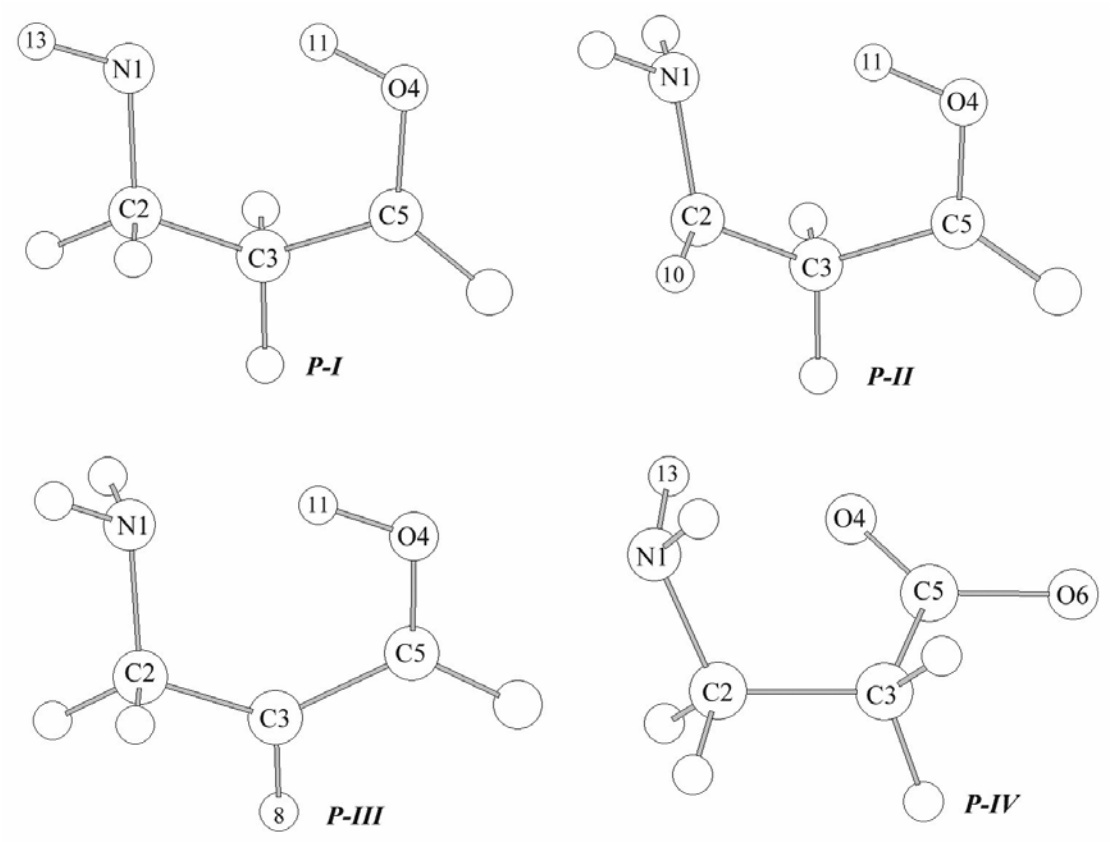

Figure 2S. Fully optimized BH&HLYP/6-311G(d,p) radical products of the β-alanine + OH reaction. Distances (*d*) are reported in Å.