SUPPLEMENTARY MATERIAL

Insights in the dissociative ionization of glycine by PEPICO experiments

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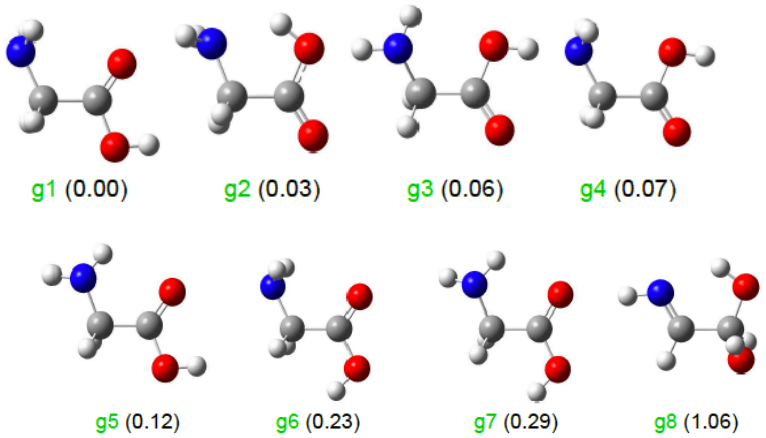

Figure 1: The structure of the eight conformers of neutral glycine. The number in brackets are the energy (eV) of each structure relative to most stable conformer (g1) calculated at the B3LYP/6-311++G(d,p) level [32].

Calculations of the outer valence ionization energies (eV) of glycine.

Table 1: Outer valence ionization energies (eV) of glycine calculated using the OVGF models, for conformers g1-g4.

Orbital	**Conformer g1** pole strength	**Conformer g2** (pole strength)	**Conformer g3** (pole strength)	**Conformer g4** (pole strength)
$16a'$ (HOMO)	10.0(0.93)	10.0(0.91)	9.70(0.91)	10.0(0.91)
$15a'$	11.4(0.91)	11.4(0.91)	12.3(0.90)	11.7(0.90)
$4a''$	12.4(0.91)	12.3(0.90)	11.9(0.91)	11.5(0.91)
$3a''$	13.6(0.90)	13.9(0.92)	13.7(0.92)	13.9(0.92)
$14a'$	14.8(0.92)	14.7(0.91)	14.6(0.92)	13.7(0.91)
$13a'$	15.1(0.92)	15.1(0.90)	14.9(0.92)	15.4(0.91)
$2a''$	15.8(0.91)	15.8(0.90)	15.8(0.90)	15.8(0.91)
$12a'$	17.7(0.91)	16.7(0.91)	17.3(0.90)	16.7(0.91)
$11a'$	17.2(0.90)	17.9(0.91)	17.8(0.91)	18.0(0.90)
$1a''$	17.7(0.91)	18.3(0.90)	17.6(0.91)	18.8(0.91)