

Table 1S. Relative energies (ΔH) including ZPE corrections of the gas-phase conformers relevant for $[\text{Proline} + \text{K}]^+$

Conformer	B3LYP [kJmol ⁻¹]	MP2 [kJmol ⁻¹]
SB1	0	5.5
SB1a	4.3	0
CS1	18.9	15.6
CS1a	20.5	17.6
CS2	26.0	22.3
CS2a	29.8	25.1
CS3	39.7	36.2
CS4	46.6	42.9
CS4a	49.8	45.5
CS5	55.0	52.3
CS5a	55.0	52.3

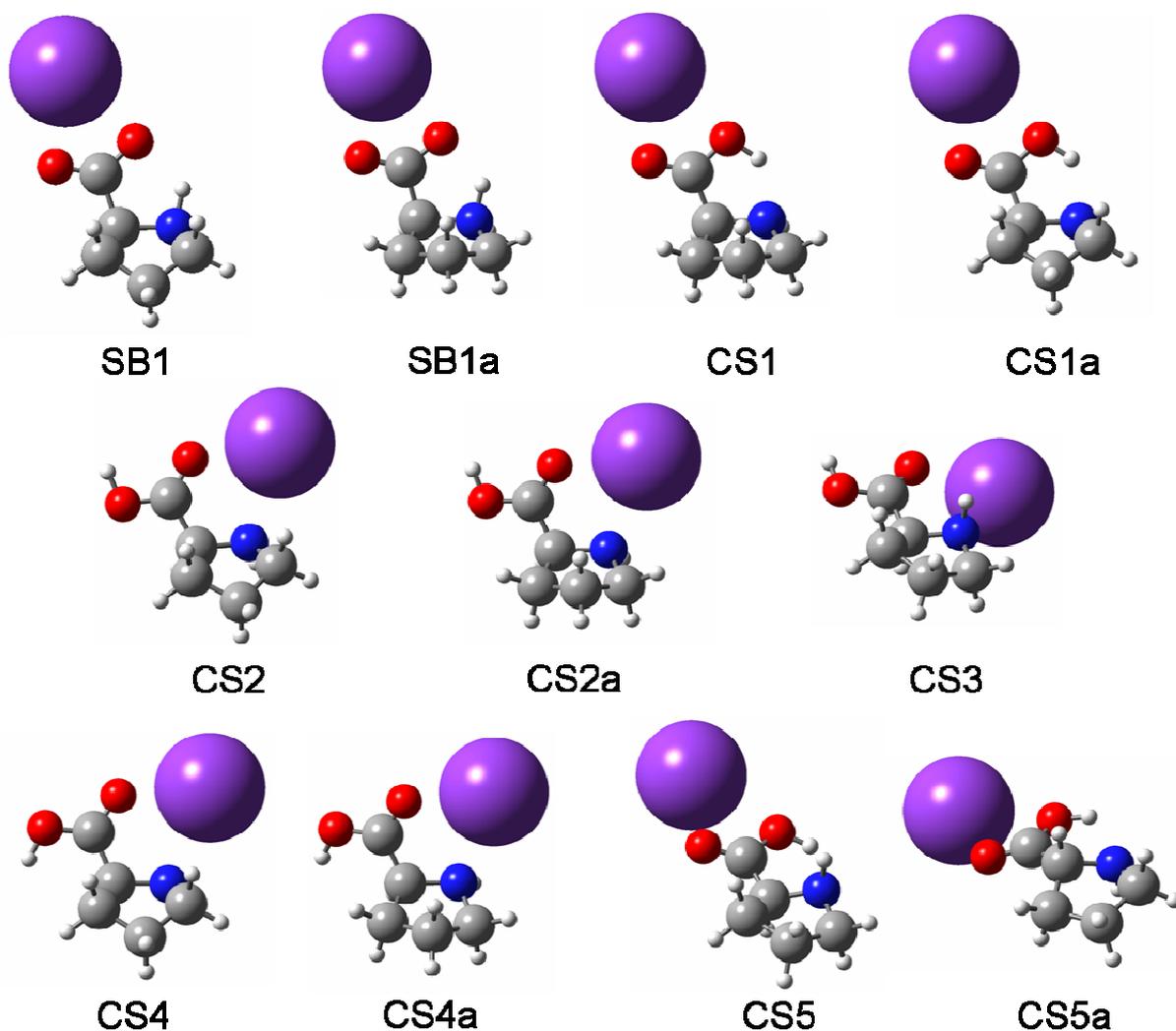


Figure 1S. Structures of $[\text{Proline} + \text{K}]^+$ complexes calculated at the B3LYP/6-311++G(2d,2p) level of theory. Potassium is depicted as brown, nitrogen as blue and oxygen as red balls.