

# The electronic ground states potential energy surfaces of small molecules: routine calculations ?

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Complex intramolecular dynamics can occur near the ground state equilibrium geometries of small boron, carbon and silicon clusters. For instance, in the singlet of  $C_2B$ , the linear and cyclic minima lead to complex patterns of rovibrational levels. For the isoelectronic  $C_3^+$ , for which its structure and reactivity lead to many discussions, there are two nearly degenerate vibronically coupled cyclic minima and a close lying linear minimum. Also in cyclic  $C_6^+$  the ground state exhibits vibronic coupling. In  $B_4$  rhombic cluster splittings occur due to two equivalent minima separated by a small barrier. In its radical cation and anion two nearly degenerate rhombic states are vibronically coupled. On the other hand, two stable  $SiC_3$  rhombic isomers are separated by a high barrier related to a bond breaking along the shorter diagonals in both isomers.

The bond formation region of the atmospherically important molecules  $O_3$ ,  $SO_2$  and  $O_2H$  in their electronic ground states will be discussed. The spin-orbit couplings among the spin multiplets resulting from the lowest asymptotes are strongly anisotropic and depend on the orientation of the collision partners. All three molecules possess van der Waals minima on the ground states PES in the spin uncoupling regions.