512 **$C_4H_4O_2$** **1,4-Dioxin** **D_{2h}**

ED, *ab initio* calculations

Large-amplitude and anharmonic corrections to the internuclear distances were calculated using new theoretical approaches for ED analysis and quadratic and cubic force constants from MP2/6-31G(d) calculations. The large-amplitude approach was based on the adiabatic separation between large- and small-amplitude motions. In addition to the vibrational terms, the Hamiltonian explicitly included rotational effects as well as interactions between overall rotation and intramolecular motion. These corrections were estimated to amount *ca*. 0.01 Å for the C=C and C–O bond lengths and 0.02 Å for the C–H bond lengths.

Kochikov, I.V., Tarasov, Yu.I., Vogt, N., Spiridonov, V.P.: J. Mol. Struct. **607** (2002) 163.

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