Dataset for publication “Theoretical Unimolecular Decomposition Kinetics of Dimethyl, Diethyl, and Ethyl Methyl Carbonates and their Fluorinated Counterparts”

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Guide to quantum mechanical data

- smi — SMILES of compound (only for stable compounds, not for TS)
- xyz / Angstrom — geometry of minimum energy conformer / Angstrom
- q / e — charge / e
- multiplicity / - — spin multiplicity / -
- SPE / h/p — single point energy of optimized geometry / h/p
- ZPE / h/p — zero point energy of optimized geometry / h/p
- #Elec.Levels / - — number of electronic levels / states / configurations
- v / cm-1 — harmonic frequencies of internal degrees of freedom / 1/cm
- v_im / cm-1 — imaginary frequency / 1/cm (only for TS)
- normal mode / - — normal modes of internal degrees of freedom
- method — ORCA command line used to obtain results (geometry optimization + frequency calculation)
- scan — dictionary of all one-dimensional hindered rotor scan information (keys are tuples of axis-determining atom IDs)
    - axis — list of atoms determining the rotational axis
    - <step-nr.> — identifier of scan step
        - xyz / Angstrom — geometry of scan step / Angstrom
        - SPE / h/p — single point energy of scan step / h/p
        - method — ORCA command line used to obtain results
- SPE-CC — DLPNO-CCSD(T)/cc-pVXZ results
    - <X> — basis set size; X = 2, 3, 4 for D, T, Q, respectively
        - SPE / h/p — single point energy / h/p
        - T1diag / - — T1 diagnostics for multi-reference check
        - method — ORCA command line used to obtain results