

Dataset for publication “Theoretical Kinetics of Propargyl + Aromatics: Abstraction from and Addition to Benzene, Toluene, Naphthalene, and 2-Methyl-Naphthalene”

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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
- H298-G4 G4 results
 - H298 / h/p
 - method Gaussian command line used to obtain results
- SPE-CC-DLPNO DLPNO-CCSD(T)/cc-pVXZ results
 - <X> basis set size; X = 3 and 4 for T and 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