

Description of Additional Supplementary Files

File Name: Supplementary Data 1

Description: Excel file with the atomic energies to calculate AIQM1 enthalpies of formation; raw data with reference energies and energies calculated for the article for benchmarks of energies.

File Name: Supplementary Data 2

Description: zip archive file with Cartesian coordinates for species in the CHNO, CATIONS41, and ExGeom data sets used for benchmarks of geometries.