Link:

<http://quantum-machine.org/datasets/>

<https://www.nature.com/articles/sdata201422#MOESM27>

Abstract:

Computational de novo design of new drugs and materials requires rigorous and unbiased exploration of chemical compound space. However, large uncharted territories persist due to its size scaling combinatorially with molecular size. We report computed geometric, energetic, electronic, and thermodynamic properties for 134k stable small organic molecules made up of CHONF. These molecules correspond to the subset of all 133,885 species with up to nine heavy atoms (CONF) out of the GDB-17 chemical universe of 166 billion organic molecules. We report geometries minimal in energy, corresponding harmonic frequencies, dipole moments, polarizabilities, along with energies, enthalpies, and free energies of atomization. All properties were calculated at the B3LYP/6-31G(2df,p) level of quantum chemistry. Furthermore, for the predominant stoichiometry, C7H10O2, there are 6,095 constitutional isomers among the 134k molecules. We report energies, enthalpies, and free energies of atomization at the more accurate G4MP2 level of theory for all of them. As such, this data set provides quantum chemical properties for a relevant, consistent, and comprehensive chemical space of small organic molecules. This database may serve the benchmarking of existing methods, development of new methods, such as hybrid quantum mechanics/machine learning, and systematic identification of structure-property relationships.

**gap - target**

gm9.csv:

| Property | Unit | Description |
| --- | --- | --- |
| smiles | - | Representation of molecule |
| A | GHz | Rotational constant |
| B | GHz | Rotational constant |
| C | GHz | Rotational constant |
| mu | D | Dipole moment |
| alpha |  | Isotropic polarizability |
| homo | Ha | Energy of HOMO |
| lumo | Ha | Energy of LUMO |
| **gap** | **Ha** | **Gap (ϵLUMO−ϵHOMO)** |
| r2 |  | Electronic spatial extent |
| zpve | Ha | Zero point vibrational energy |
| u0 | Ha | Internal energy at 0 K |
| u298 | Ha | Internal energy at 298.15 K |
| h298 | Ha | Enthalpy at 298.15 K |
| g298 | Ha | Free energy at 298.15 K |
| cv |  | Heat capacity at 298.15 K |