Excellent results are shown in yellow. Overall, the Many Molecules EA performed better.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Molecule  (many of these can rotate at each bond so often won’t appear like their pictures) | EA Many  Molecules  Average best energy / eV | EA Per Atom Average best energy / eV | EA Many  Molecules  Average shape | EA Per Atom Average shape | EA Many  Molecules  Approx. average time taken / seconds | EA Per Atom Approx. average time taken / seconds |
| Water  H2O | Chemistry of Water | 1.900 | 2.531 | Excellent | Good | 2 | 2 |
| Carbon dioxide | 0.9230 | 0.9720 | Poor | Poor | < 1 | 1 |
| Methane  Ch4 Molecule Images, Stock Photos & Vectors | Shutterstock | 2.993 | 3.890 | Good | Poor | 1 | 3 |
| Dinitrogen tetroxide  Nitrogen tetroxide (dinitrogen tetroxide, N2O4) rocket propellant molecule.  3D rendering. Atoms are represented as spheres with conventional colour  coding: nitrogen (blue), oxygen (red Stock Photo - Alamy | 3.418 | 6.617 | Good | Poor | 10 | 4 |
| Acetonitrile  Acetonitrile | 1.827 | 4.204 | Poor | Poor | 1 | 4 |
| Acetone | 3.455 | 27.69 | Good | Good | 12 | 20 |
| Lattice of 12 carbons  cubic crystal system | NIH 3D Print Exchange | 3.020 | 11.32 | Good | Poor | 2 | 48 |
|  |  |  |  |  |  |  |
| Benzene  Illustrated Glossary of Organic Chemistry - Benzene | 2.416 | 69.32 | Excellent | Good | 39 | 50 |
| Aluminium oxide | 4.467 | 4.139 | Good | Good | 8 | 3 |