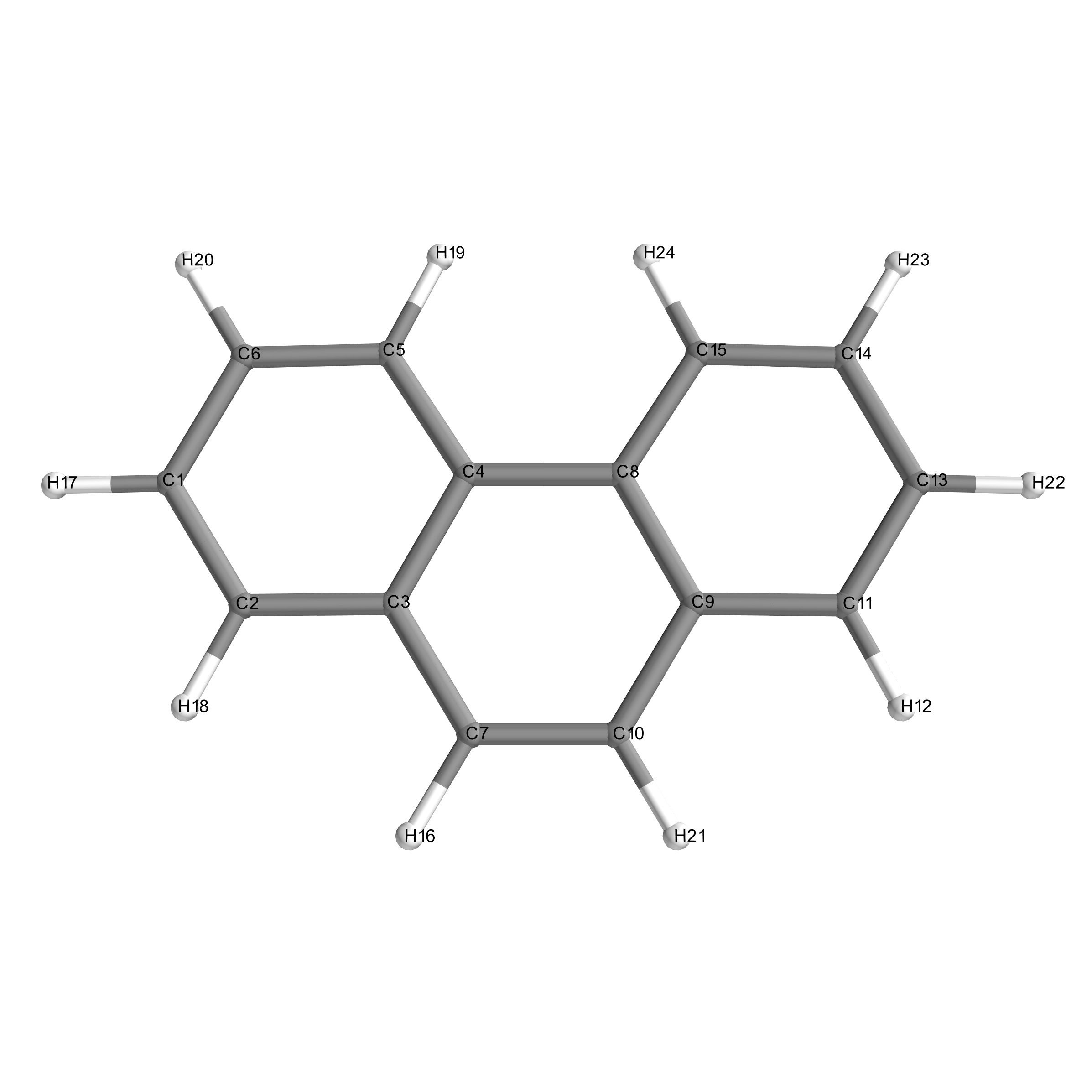
**MOLECULAR CALCULATION REPORT**

**1. MOLECULE**



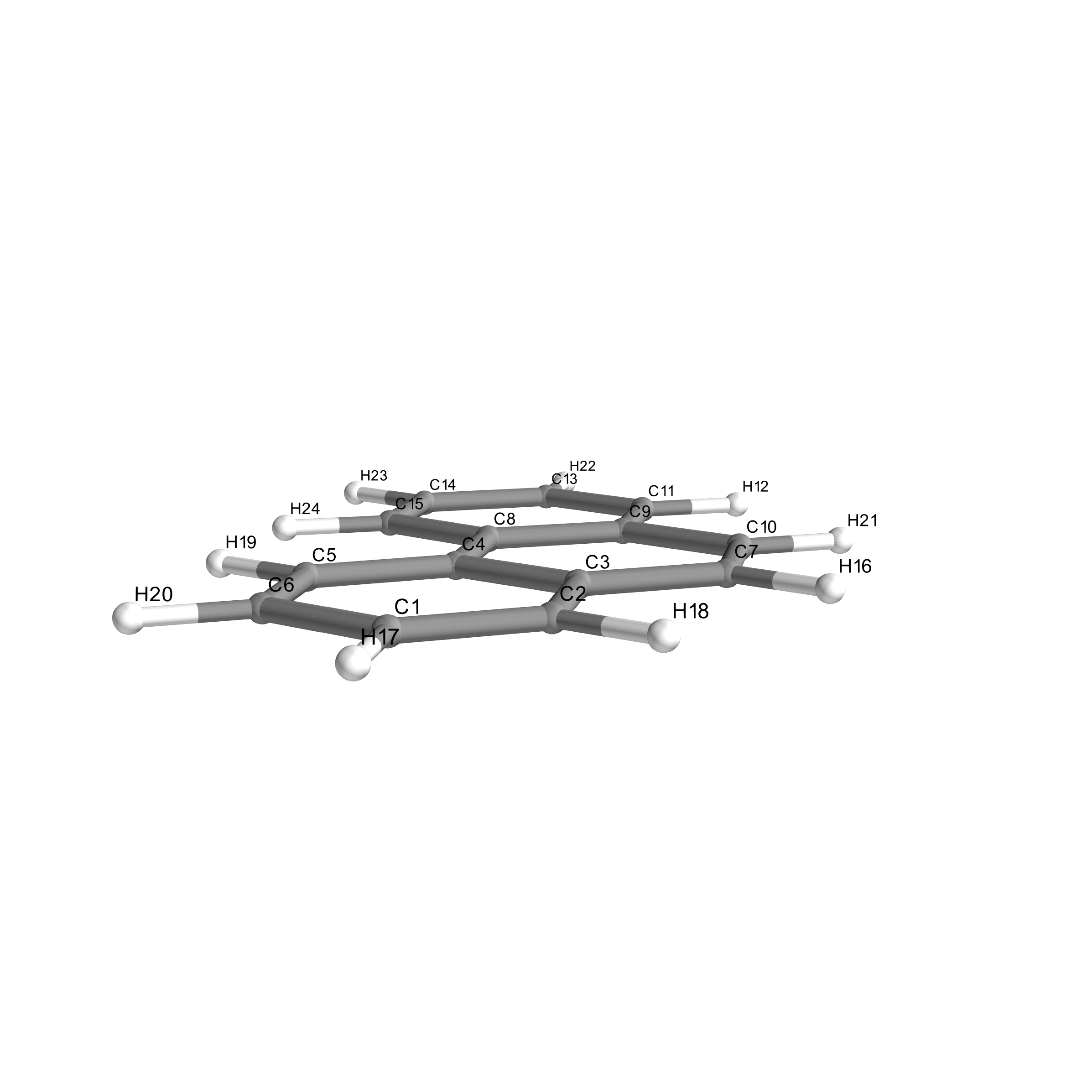


Figure 1: Chemical structure diagram with atomic numbering from two points of view.

|  |  |
| --- | --- |
| Directory name | QuChemReport |
| Formula | C14H10 |
| Charge | 0 |
| Spin multiplicity | 1 |
| Monoisotopic mass | 178.07825 Da |
| InChI | 1S/C14H10/c1-3-7-13-11(5-1)9-10-12-6-2-4-8-14(12)13/h1-10H |
| SMILES | c1cc2c(cc1)c1c(cc2)cccc1 |