

Triplos Mol2 format

Triplos Mol2 import/export is alpha level in the current version of Marvin.

Only the following records are imported and exported:

- @<TRIPOS>MOLECULE
- @<TRIPOS>ATOM
Import: x, y, z, atom_type, charge rounded to integer
Export: atom_id(=atom index), atom_name, x, y, z, atom_type, subst_id=1, subst_name="noname", charge (integer)
- @<TRIPOS>BOND

Reference

- <http://www.tripos.com/data/support/mol2.pdf>

Code: **mol2**

See also

- Triplos SYBYL MOL format
- Basic export options