

# OGHAM

Since Kekule's dreams of benzene, molecular structures have been conceived, defined and shared by drawing lines between points to represent bonds and atoms. Ogham [1] is designed to artfully render these 2D Kekule drawings from molecular connectivity information. In conjunction with LexiChem, Ogham helps bridge the communication gap between 3D structure methods and traditional forms of chemical representation.

The utility of Ogham is not lost on third-party vendors, such as Dimension5, which has relied on Ogham to display chemical information more usefully in Miner3D, its visual data-analysis product. "We have found OGHAM extremely fast and reliable and were impressed at how seamlessly the chemical depiction libraries integrated within Miner3D", said Dusan Toman, CEO of Dimension5.

The primary features of OGHAM include:

- Generates structure diagrams (2D coordinates) suitable for rendering from connection tables (e.g. SMILES) or 3D structures [2]
- Renders images (GIF, BMP or EPS) from either generated or user supplied structure diagrams (2D coordinates)
- Provides consistent (and specifiable) orientation of core substructures
- Offers a variety of display controls (color, size, optional use of superatoms or display hydrogens, style of representation for aromatic and dative bonds)
- OEChemplete – all I/O and molecular information processing by OEChem
- OEChempatible C++ toolkit for embedded applications
- Robust reading of SMILES, SLN, SDF, MOL, MOL2, PDB, FASTA, MOPAC, MacroModel, XYZ, and OEBinary file formats
- Support for LINUX, IRIX, Windows, OS X, AIX, HP-UX, Solaris, Tru64UNIX



[1] The Ogham alphabet system of the ancient Irish is represented by lines, hashes and wedges; it is principally known for the inscription of names on standing stones.

[2] Structure Diagram Generation: Helson, H.E., in "Reviews in Computational Chemistry", 1999, **13**, 313–98, Eds. Lipkowitz, K.B, Boyd, D.B., Wiley-VCH Press.

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