
Subject: Re: HBD/HBA

Posted by [nbehrnd](#) on Mon, 06 Mar 2023 22:28:01 GMT

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Initially for curiosity, I submitted a few simple molecules to the assignment to H-bond donors, and acceptors

DW assigns last entry 6, diacetamide, 3 acceptors and 1 donor. This contrasts to Etter's paper[1] with two acceptors and one donor only.

Do follow medicinal chemistry and solid state chemistry/crystallography different conventions here?

With regards,

Norwid

[1] Etter, M. C. Encoding and decoding hydrogen-bond patterns of organic compounds. *Acc. Chem. Res.* 1990, 23, 120-126 (DOI <https://doi.org/10.1021/ar00172a005>).

[2] Etter, M. C.; MacDonald, J. C.; Bernstein, J. Graph Set Analysis of Hydrogen-Bond Patterns in Organic Crystals. *Acta Cryst. B* 1990, 46, 256-262 (DOI <https://doi.org/10.1107/S0108768189012929>)

File Attachments

- 1) [H-acceptor_donor.png](#), downloaded 520 times
 - 2) [Etter_graphs_diacetamide.png](#), downloaded 566 times
 - 3) [Etter_graphs_2.png](#), downloaded 586 times
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