
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,


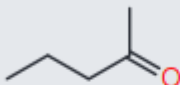
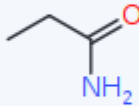
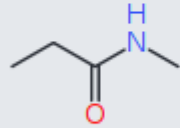
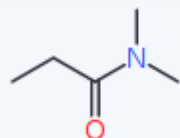
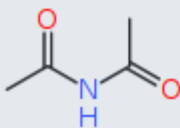
Norwid

[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>).

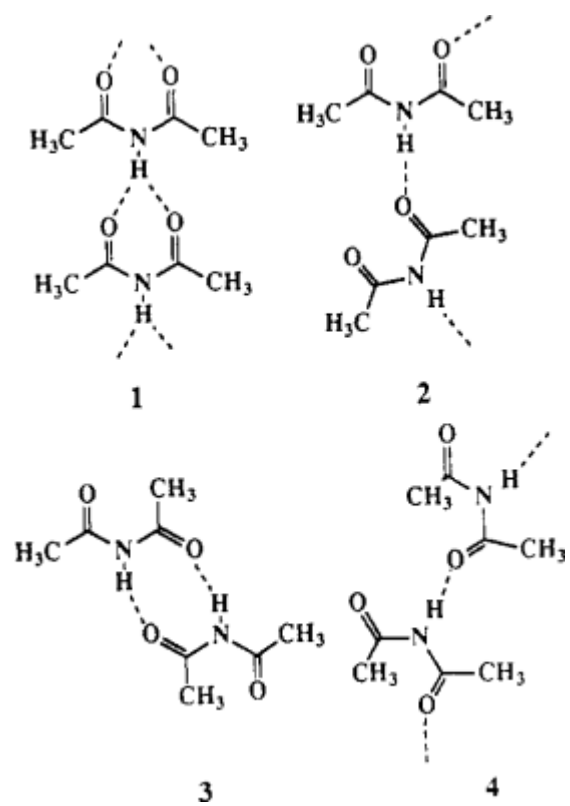
[2] Etter, M. C.; MacDonald, J. C.; Bernstein, J. Graph Set Analysis of Hydrogen-Bond Patterns in Organic Crystals. *Acta Cryst. B* 1990, 46, 256-262 (DOI <https://doi.org/10.1107/S0108768189012929>)

File Attachments

1) [H-acceptor_donor.png](#), downloaded 1351 times

	Structure	H-Acceptors	H-Donors
1		1	1
2		1	0
3		2	1
4		2	1
5		2	0
6		3	1

2) [Etter_graphs_diacetamide.png](#), downloaded 1366 times



3) [Etter_graphs_2.png](#), downloaded 1430 times

Table 1. *Examples of graph-set assignments*

The hexagons are meant to represent any organic ligand. This specific form is given so the degrees of the patterns can be assigned in this table. If the organic ligands were other kinds of groups, then the degrees of some of the patterns would change.

