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 accptors and one donor only.

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

With regards,

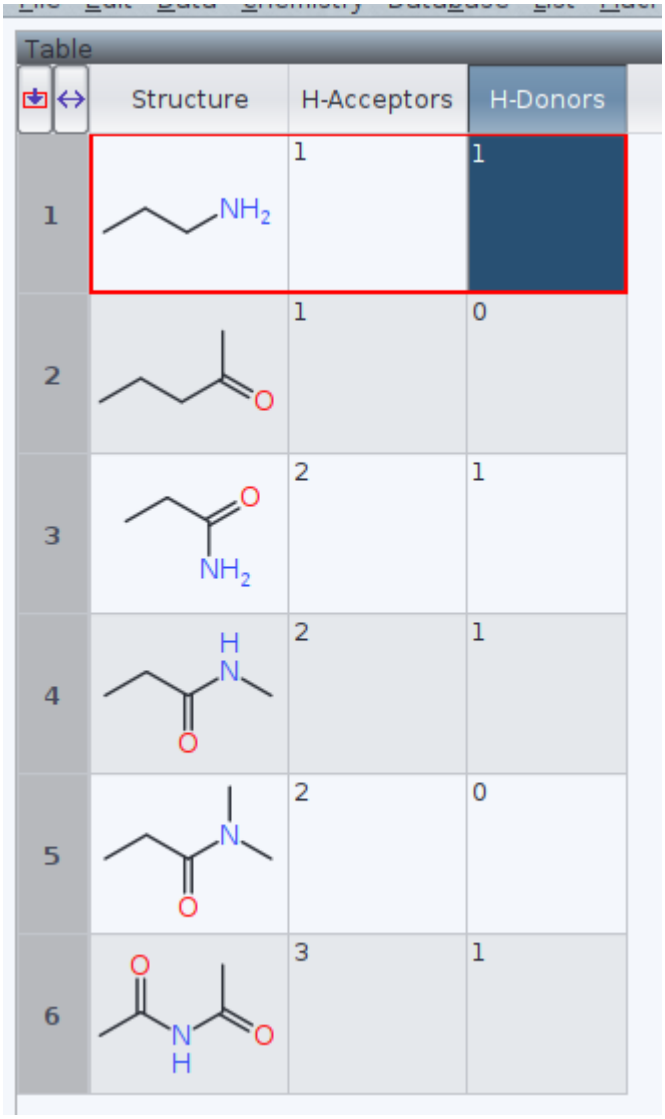
Norwid

[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).

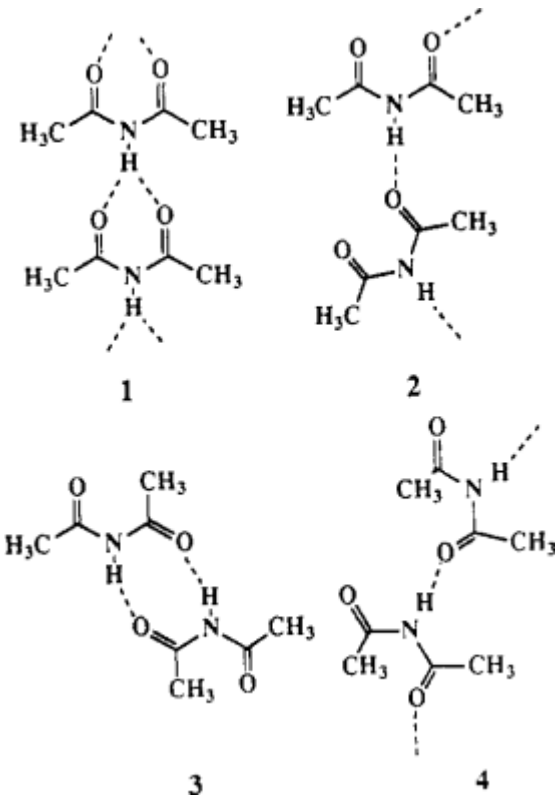
[2] Etter, M. C.; MacDonald, J. C.; Bernstein, J. Graph Set Analysis of Hydrogen-Bond Patterns in Organic Crystals. Acta Cryst. B 1990, 46, 256-262 (DOI https://doi.org/10.1107/S0108768189012929)

File Attachments

1) H-acceptor_donor.png, downloaded 1220 times



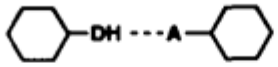
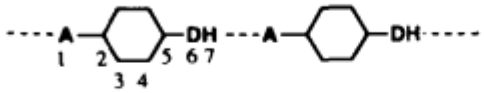
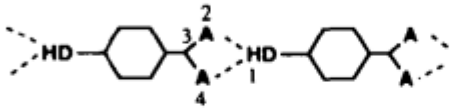
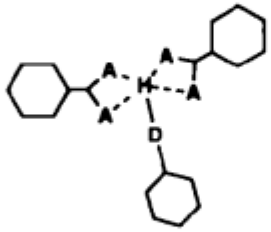
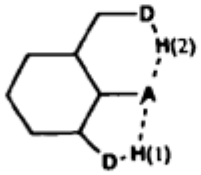
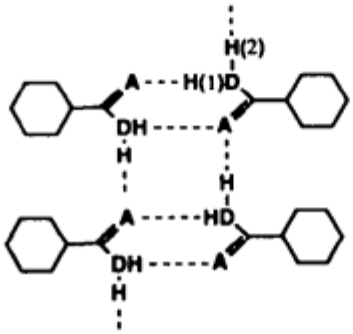
2) Etter_graphs_diacetamide.png, downloaded 1239 times



3) Etter_graphs_2.png, downloaded 1306 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.

(I)		$N_1 = D$
(II)		$N_1 = C(7)$
(III)		$N_1 = C_1^2(8)[R_1^2(4)]$
(IV)		$N_1 = 2R_1^2(4)$
(V)		$N_1 = S(6)S(5)$ $N_2 = S_2^1(9)$
(VI)		$N_1 = C(4)R_2^2(8)$ $N_2 = R_4^2(8)$