Electronic Supplementary Material (ESI) for CrystEngComm
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CrystEngComm

Supporting Information

Barbiturates with hydrogen-bonded layer and framework structures

Thomas Gelbrich, Denise Rossi, Clemens A. Häfele and Ulrich J. Griesser

1. Geometrical parameters of N–H···O bonds

Table S1. Hydrogen bonds for form II of noctal (**1**; L-4).

#	*D*–H···*A*	*d*(*D*–H) / Å	*d*(H···*A*) / Å	*d*(*D*···*A*) / Å	∠(*D*HA) / °
a	N1–H1···O4^{i}	0.871(19)	2.06(2)	2.934(4)	178(4)
b	N3–H3···O2^{ii}	0.875(19)	1.96(2)	2.832(4)	172(4)

Symmetry transformations used to generate equivalent atoms: (i) *x*, −*y*+1/2, *z*−1/2 (ii) -*x*+2, −*y*, −*z*.

Table S2. Hydrogen bonds for form **A** of 5,5-dichlorobarbituric acid (**2a**; L-5).

#	*D*–H···*A*	*d*(*D*–H) / Å	*d*(H···*A*) / Å	*d*(*D*···*A*) / Å	∠(*D*HA) / °
a	N1A–H1A···O2B	0.866(18)	2.11(2)	2.953(4)	164(3)
b	N3A–H3A···O4D^{i}	0.865(18)	2.19(2)	2.992(4)	155(3)
c	N1B–H1B···O2A	0.866(18)	2.15(2)	2.970(4)	159(3)
d	N3B–H3B···O4C^{ii}	0.849(18)	2.22(2)	3.025(3)	158(3)
e	N1C–H1C···O2D	0.847(18)	2.08(2)	2.920(3)	172(3)
f	N3C–H3C···O4B	0.852(18)	2.23(2)	3.033(3)	157(3)
g	N1D–H1D···O2C	0.864(18)	2.11(2)	2.928(4)	158(3)
h	N3D–H3D···O4A^{iii}	0.886(18)	2.23(2)	3.041(3)	153(3)

Symmetry transformations used to generate equivalent atoms: (i) *x*−1/2, *y*+1/2, *z* (ii) *x*+1/2, *y*+1/2, *z* (iii) *x*, *y*−1, *z*.

Table S3. Hydrogen bonds for form B of 5,5-dibromobarbituric acid (**2b**; L-6).

	D–H···*A*	*d*(*D*–H) / Å	*d*(H···*A*) / Å	*d*(*D*···*A*) / Å	∠(*D*HA) / °
a	N1A–H1A···O4A^{i}	0.846(16)	2.028(17)	2.853(2)	165(2)
b	N3A–H3A···O2B	0.849(15)	1.938(16)	2.786(2)	176(2)
c	N1B–H1B···O4B^{ii}	0.843(16)	1.980(18)	2.765(2)	155(2)
d	N3B–H3B···O2A	0.867(16)	1.964(17)	2.823(2)	170(2)
e	N1C–H1C···O2C^{iii}	0.862(15)	1.961(16)	2.820(2)	174(2)
f	N3C–H3C···O2A	0.859(16)	2.205(18)	3.026(2)	160(2)

Symmetry transformations used to generate equivalent atoms: (i) −*x*+1/2, *y*+1/2, *z* (ii) −*x*+3/2, *y*−1/2, *z* (iii) 1−*x*, 2−*y*, 1−*z*.

Table S4. Hydrogen bonds for form A of 5,5-dibromobarbituric acid (**3a**; L-6).

	D–H···*A*	*d*(*D*–H) / Å	*d*(H···*A*) / Å	*d*(*D*···*A*) / Å	∠(*D*HA) / °
a	N1A–H1A···O4A^{i}	0.88	2.01	2.853(9)	160.5
b	N3A–H3A···O2B	0.88	1.95	2.818(9)	170.0
c	N1B–H1B···O4B^{ii}	0.88	1.99	2.810(9)	153.5
d	N3B–H3B···O2A	0.88	1.96	2.835(9)	174.3
e	N1C–H1C···O2C^{iiI}	0.88	1.94	2.808(9)	167.7
f	N3C–H3C···O2A	0.88	2.21	3.053(9)	160.2

Symmetry transformations used to generate equivalent atoms: (i) −*x*+1/2, *y*+1/2, *z* (ii) −*x*+3/2, *y*−1/2, *z* (iii) 1−*x*, 2−*y*, 1−*z*.

Table S5. Hydrogen bonds for form B of 5,5-dibromobarbituric acid (**3b**; F-2).

	D–H···*A*	*d*(*D*–H) / Å	*d*(H···*A*) / Å	*d*(*D*···*A*) / Å	∠(*D*HA) / °
a	N1A–H1A···O2A^{i}	0.88(2)	1.97(2)	2.840(6)	168(5)
b	N3A–H3A···O4B	0.87(2)	2.02(4)	2.789(6)	146(5)
c	N1B–H1B··· O4A^{ii}	0.89(2)	1.97(2)	2.860(6)	178(6)
d	N3B–H3B··· O2B^{iii}	0.88(2)	1.94(2)	2.820(7)	173(6)

Symmetry transformations used to generate equivalent atoms: (i) −*x*+1, −*y*+1, −*z*+1 (ii) *x*, −*y*+3/2, z−1/2 (iii) −*x*, −*y*+1, −*z*.

2. Second-level graph-set representations[1] of H-bonded structures

Table S6. Graph-set representation[1] of L-4 (crystal structure **1**, $Z' = 1$). For the definition of *a* and *b*, see Table S1.

$C_1^1(6)$	*a*
$R_6^6(28)$	> *b* > *b*
$C_2^2(8)$	> *a* > b
$C_2^2(10)$	> *a* < *b*
$C_4^4(18)$	> *a* > *b* < *a* < *b*
$R_6^6(28)$	> *a* > *a* > *b* > *a* > *a* > *b*
$R_6^6(30)$	> *a* > *a* > *b* > *a* > *a* < *b*
$R_6^6(32)$	> *a* > *a* < *b* > *a* > *a* < *b*

Table S7. Graph-set representation[1] of L-6 (crystal structure **2a**, $Z' = 4$). For the definition of *a*-*h*, see Table S2.

$D_1^1(2)$	*a*
$D_1^1(2)$	*b*
$D_1^1(2)$	*c*
$D_1^1(2)$	*d*
$D_1^1(2)$	*e*
$D_1^1(2)$	*f*
$D_1^1(2)$	*g*
$D_1^1(2)$	*h*
$D_2^2(6)$	> *a* > *d*
$D_2^2(6)$	> *c* > *b*
$D_2^2(6)$	> *e* > *h*
$D_2^2(6)$	> *g* > *f*
$D_2^2(7)$	< *a* > *b*

$D_2^2(7)$	$<c>d$
$D_2^2(7)$	$<e>f$
$D_2^2(7)$	$<g>h$
$D_2^2(7)$	$>a<f$
$D_2^2(7)$	$>b<e$
$D_2^2(7)$	$>c<h$
$D_2^2(7)$	$>d<g$
$D_2^2(8)$	$>b>g$
$D_2^2(8)$	$>d>e$
$D_2^2(8)$	$>f>c$
$D_2^2(8)$	$>h>a$
$C_2^2(8)$	$>b>h$
$C_2^2(8)$	$>\mathrm{d}>f$
$R_2^2(8)$	$>a>c$
$R_2^2(8)$	$>e>g$

Table S8. Graph-set representation[1] of L-5 (crystal structures **2b** and, **3a**, Z' = 3). For the definition of *a-f*, see Tables S3 and S4.

$D_1^1(2)$	*b*
$D_1^1(2)$	*d*
$D_1^1(2)$	*f*
$C_1^1(6)$	*a*
$C_1^1(6)$	*c*
$R_2^2(8)$	> *e* > *e*
$D_2^1(3)$	> *d* < *f*
$D_2^2(6)$	> *f* > *b*
$R_2^2(8)$	> *b* > *d*
$D_3^3(11)$	< *b* > a > *b*
$D_3^3(11)$	< *d* > c > *d*
$D_3^3(11)$	< *f* > e > *f*
$D_3^3(11)$	> *b* > c < *b*
$D_3^3(11)$	> *d* > a < *d*
$D_3^3(11)$	> *f* > a < *f*

Table S9. Graph-set representation[1] of F-2 (crystal structure **3b**, Z' = 2). For the definition of *a-d*, see Table S5.

$D_1^1(2)$	*b*
$D_1^1(2)$	*c*
$R_2^2(8)$	> *a* > *a*
$R_2^2(8)$	> *d* > *d*
$C_2^2(8)$	> *b* > *c*
$D_3^3(11)$	< *b* > *a* > *b*
$D_3^3(11)$	< *c* > *d* > *c*
$D_3^3(13)$	> *b* > *d* < *b*
$D_3^3(13)$	> *c* > *a* < *c*

3. *XPac* comparison between **2a** and **3b**

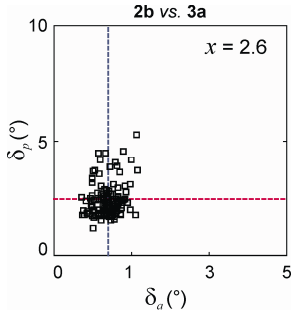

Fig. S1 The isostructural relationship between **2b** and **3a** is indicated by a low *XPac* dissimilarity index, x = 2.6. *XPac* plot[2] for a representative cluster of 37 molecules (n = 36). The δ parameters were calculated from all non-H atomic positions (p = 11).

4. H-bonded structures L-2 and L-3

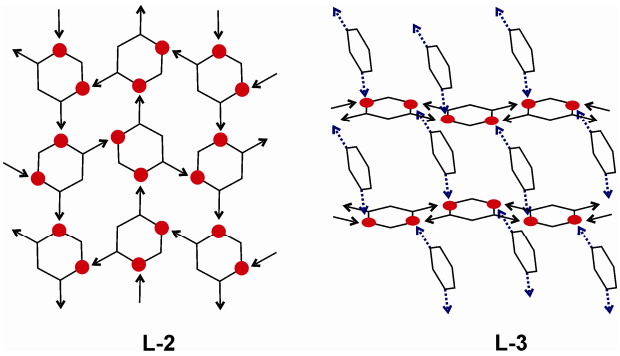

Fig. S2 Schematic representation of the N–H···O=C bonded 2D extended structures L-2 (form II of barbituric acid) and L-3 (phenobarbital I and II). The applied style is explained in the insert of Fig. 1.

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References

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2. (a) T. Gelbrich and M. B. Hursthouse, *CrystEngComm*, 2005, **7**, 324-336; (b) F. P. A. Fabbiani, B. Dittrich, A. J. Florence, T. Gelbrich, M. B. Hursthouse, W. F. Kuhs, N. Shankland and H. Sowa, *CrystEngComm*, 2009, **11**, 1396-1406.