

**ELECTRONIC SUPPLEMENTARY MATERIAL (ESI) FOR NEW
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Supporting Information

**Conformational studies on substituted
 ϵ -caprolactams by X-ray crystallography and NMR
spectroscopy**

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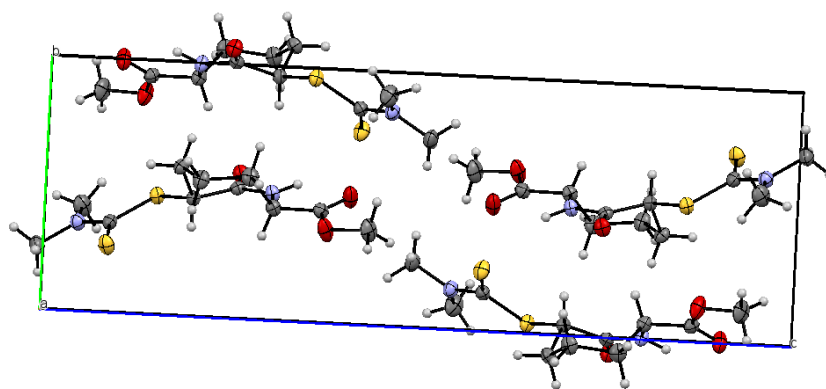
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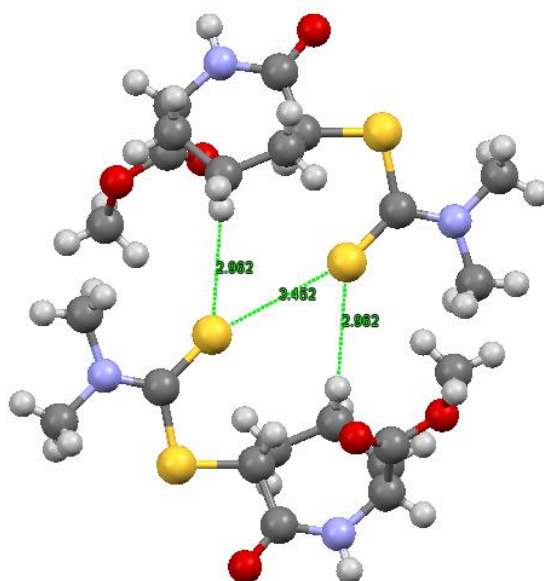
Table S1

Distances (Å) and angles (°) of hydrogen bond type interactions in the here discussed X-ray structures

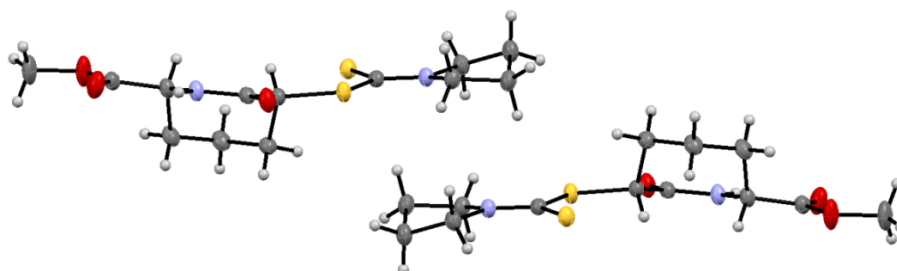
Atoms involved	Distance (Å)			Angle (°)	
	Symmetry	d(D-H)	d(H...A)	d(D...A)	<(DHA)
1					
N(1)-H(11)...O(1)	$-x+2, -y, -z+2$	0.85	2.25	3.056(3)	160
C(6)-H(61)...O(1)	$x-1, y, z$	0.98	2.52	3.498(3)	174
C(8)-H(81)...O(2)	$x-1, y, z$	0.95	2.52	3.258(3)	134
2					
$\hat{N}(1A)$ -H(1A)...O(2C)	x, y, z	0.85	2.14	2.970(4)	164
O(3A)-H(3A)...O(1A)	x, y, z	0.82	1.75	2.555(4)	169
N(1B)-H(1B)...O(2A)	x, y, z	0.85	2.18	2.996(4)	162
O(3B)-H(3B)...O(1C)	x, y, z	0.84	1.72	2.543(4)	170
N(1C)-H(1C)...O(2B)	x, y, z	0.85	2.25	3.074(4)	162
O(3C)-H(3C)...O(1A)	x, y, z	0.85	1.72	2.553(4)	170
3					
C(6)-H(61)...O(2)	$-x+1, -y, -z+1$	0.95	2.57	3.341(2)	139
5 cis					
C(2)-H(21)...O(1)	$-x+2, y+1/2, -z+3/2$	0.97	2.52	3.392(2)	150
C(4)-H(42)...O(3)	$-x+1, y-1/2, -z+3/2$	0.96	2.50	3.331(2)	144
C(5)-H(52)...O(1)	$x-1, y, z$	0.98	2.44	3.279(2)	143
C(6)-H(61)...O(1)	$-x+2, y+1/2, -z+3/2$	0.95	2.51	3.363(2)	150
5 trans					
N(1)-H(11)...O(1)	$-x+1, -y+1, -z+2$	0.87	2.00	2.868(4)	176
C(6)-H(61)...O(2)	x, y, z	0.97	2.42	3.157(4)	132
C(10)-H(101)...O(2)	$-x+2, -y, -z+1$	0.95	2.40	3.235(4)	147
6 cis					
C(2)-H(21)...O(1)	$-x+3/2, y+1/2, -z+1/2$	0.94	2.56	3.4627(2)	162
C(4)-H(42)...O(3)	$-x+1/2, y-1/2, -z+1/2$	0.94	2.51	3.3072(2)	143
C(5)-H(52)...O(1)	$x-1, y, z$	0.95	2.55	3.4293(2)	154
7					
N(1)-H(11)...O(1)	$-x+2, -y+2, -z+1$	0.88	1.98	2.862(2)	179
C(2)-H(21)...O(1)	$-x+2, -y+1, -z+1$	0.96	2.47	3.410(2)	168
C(6)-H(61)...O(2)	$-x+1, -y+2, -z+2$	0.97	2.50	3.277(2)	138



a)



b)



c)

Fig. S1 Packing behaviour of dithiocarbamates *cis*-5 (a), *trans*-5 (b) and *cis*-6 (c).