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addenda and errata

Structure predictions allowing more than one molecule in the asymmetric unit. Erratum

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In the paper by van Eijck & Kroon (2000) the fifth and sixth sentences in the third paragraph of §2.1 are incorrect. The correct paragraph is here reprinted in full. Table 6 also contains errors and thus is also reprinted below.

In our procedure the space-group symmetry and the number of independent molecules, G, are chosen in advance. A Cartesian axes system (x, y, z) is used, where the crystallographic a axis coincides with the x axis and the b axis is positioned in the x, y plane. To create a trial structure the components a_x, b_y and c_z are given random values between 4 and 25 Å. For an orthorhombic space group this is sufficient; higher symmetry has not been implemented. In monoclinic space groups the variation of the cell angle β is allowed by assigning a random value (between 0 and a_x) to c_x. In triclinic space groups b_x is similarly chosen between 0 and a_x, and c_y takes a random value between 0 and b_y. So for these three crystal systems the number of lattice parameters to be determined is 3, 4 and 6, respectively.

Table 6
Crystal structure generation for hydrates of carbohydrates and polyalcohols.

N(hydroxyl) is the number of rotatable hydroxyl groups. D is the dimension of the search problem. N(exp) is the number of times the experimental structure was found; numbers between parentheses refer to an extended calculation of 50 000 trials. Only the experimental conformation was used. See text for the investigated space groups.

					UNITAT		*OPLS*	
Substance	Space group	N(hydroxyl)	D	N(exp)	ΔE	R	ΔE	R
DMGALP	$P2_12_12_1$	3	18	6	9.2	23	17.6	32
BAXNAP	$C2$	4	19	1 (3)	4.3	6	0.0	1
*MGALPY*01	$P2_12_12_1$	4	19	4	16.4	142	1.6	2
*RHAMAH*12	$P2_1$	4	19	4	2.7	10	5.1	3
GEHDAY	$P1$	5	20	42	1.3	3	6.3	8
*GLUCMH*11	$P2_1$	5	20	0 (10)	9.4	58	8.5	23
MANHEP	$P2_12_12_1$	6	21	0 (3)	3.8	9	0.0	1
SUNGUD	$C2/c$	7	23	0	13.4		22.1	
MYTOLD	$P2_1/a$	6	28	0	11.9		5.9	
Average					8.0		7.5	

References

Eijck, B. P. van & Kroon, J. (2000). *Acta Cryst.* B**56**, 535–542.