Ab-initio investigation of structure and cohesive energy of crystalline urea

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Supplementary material

Table S1 Lattice parameters (in Å) and atomic fractional coordinates of crystalline urea computed with different Hamiltonians. Basis set: 6-31G(d,p). C and O atoms are on positions (0, 1/2, z), N and H atoms are on positions (x, x+1/2, z). Space group: P-42_1m.

	HF	SVWN	PW91	PBE	PBE0	B3LYP	Exp.[a]
a	5.949	5.257	5.598	5.604	5.588	5.675	5.565
c	4.750	4.521	4.659	4.669	4.649	4.682	4.684
C_z	0.3281	0.3145	0.3282	0.3276	0.3272	0.3287	0.3260
O_z	0.5886	0.5994	0.6035	0.6023	0.5997	0.6001	0.5953
N_x	0.1353	0.1547	0.1460	0.1460	0.1450	0.1435	0.1459
N_z	0.1802	0.1644	0.1771	0.1768	0.1769	0.1784	0.1766
$H1_x$	0.2386	0.2765	0.2595	0.2594	0.2575	0.2543	0.2575
$H1_z$	0.2820	0.2768	0.2821	0.2820	0.2819	0.2824	0.2827
$H2_x$	0.1339	0.1521	0.1433	0.1436	0.1428	0.1412	0.1441
$H2_z$	-0.0295	-0.0640	-0.0423	-0.0424	-0.0410	-0.0383	-0.0380

[a] Swaminathan, S.; Craven, B. N.; McMullan, R. K. *Acta Crystallogr. Sec. B* **1984**, *40*, 300.

Table S2 Lattice parameters (in Å) and atomic fractional coordinates of crystalline urea computed at the B3LYP level of theory with different basis sets. C and O atoms are on positions (0, 1/2, z), N and H atoms are on positions (x, x+1/2, z). Space group: P-42_1m.

	6-31G(d,p)	DZP	6-311G(d,p)	TZP	Exp.[a]
a	5.675	5.700	5.743	5.841	5.565
c	4.682	4.678	4.707	4.710	4.684
C_z	0.3287	0.3303	0.3298	0.3372	0.3260
O_z	0.6001	0.6025	0.5982	0.6013	0.5953
N_x	0.1435	0.1431	0.1415	0.1390	0.1459
N_z	0.1784	0.1796	0.1798	0.1834	0.1766
$H1_x$	0.2543	0.2544	0.2510	0.2467	0.2575
$H1_z$	0.2824	0.2844	0.2826	0.2854	0.2827
$H2_x$	0.1412	0.1398	0.1393	0.1368	0.1441
$H2_z$	-0.0383	-0.0390	-0.0355	-0.0315	-0.0380

[a] Swaminathan, S.; Craven, B. N.; McMullan, R. K. *Acta Crystallogr. Sec. B* **1984**, *40*, 300.

Table S3 CPU time[a] (in sec) for SCF and gradients calculation on the first optimization step and total CPU time of the geometry optimization. The experimental structure[b] was used as starting geometry. Space group: P-42_1m.

	T_{CPU} SCF[c]	T_{CPU} Gradients	T_{CPU} Geom. Opt.[d]
Basis set: 6-31G(d,p)			
HF	376 (19)	132	3570 (11)
SVWN	80 (18)	58	1011 (11)
PW91	97 (17)	61	1308 (13)
PBE	97 (17)	61	1302 (13)
PBE0	326 (16)	162	3849 (13)
B3LYP	327 (16)	161	3928 (13)
Hamiltonian: B3LYP			
6-31G(d,p)	327 (16)	161	3928 (13)
DZP	1493 (16)	393	15869 (14)
6-311G(d,p)	1202 (16)	453	13266 (15)
TZP	4557 (15)	1367	54237 (15)

[a] Calculations carried out on 8 processors Itanium-2 1.3GHz SGI-Altix 350.

[b] Swaminathan, S.; Craven, B. N.; McMullan, R. K. *Acta Crystallogr. Sec. B* **1984**, *40*, 300.

[c] Number of cycles in parentheses

[d] Number of geometry optimization steps in parentheses