Electronic Supplementary Information

Crystal structure prediction for cyclotrimethylene trinitramine (RDX) from first principles

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Table 1S. Maximum absolute deviations of molecular parameters[a] from corresponding values in an ideal RDX crystal.

Space group	Coordination Geometry	Solution number	Δs_{xMax}	Δs_{yMax}	Δs_{zMax}	$\Delta\Theta_{Max}$ (°)	$\Delta\Phi_{Max}$ (°)	$\Delta\Psi_{Max}$ (°)
Pbca	CB	1	3.1e-04	2.5e-04	1.9e-04	0.16	0.07	0.13
Pbca	CB	2	2.3e-04	5.2e-04	3.0e-04	0.13	0.14	0.12
P21/c	AM	1	6.8e-04	2.5e-04	2.4e-04	0.19	0.64	0.97
P21/c	AM	2	3.2e-03	1.8e-04	7.8e-04	0.34	0.02	0.97
P21/c	AM	3	7.2e-04	1.0e-04	8.0e-05	0.13	0.20	0.49
P21/c	AM	4	5.6e-04	9.0e-05	3.1e-04	0.44	0.25	0.61
P21/c	AI	1	1.9e-03	9.0e-05	1.1e-03	1.22	0.05	0.60
P21/c	AK	1	7.2e-04	2.0e-05	4.2e-04	0.61	0.03	3.01
P21/c	AM	5	1.9e-04	1.5e-04	9.0e-04	0.11	0.64	3.00
Pbca	CB	3	4.0e-04	3.2e-04	2.7e-04	0.07	0.16	0.18
Pbca	CB	4	4.9e-04	5.5e-04	2.2e-04	0.14	0.09	0.13
P212121	AQ	1	3.0e-04	2.1e-04	9.2e-04	0.02	0.10	0.11
Pna21	AV	1	2.5e-04	9.4e-04	1.1e-04	0.13	0.05	0.34

a. From time-averaged unit cells generated through NsT-MD simulations at 298 K, 1 atm.

Table 2S. Experimental and NsT-MD orientational parameters (center of mass fractionals and Euler angles) for the eight symmetry-equivalent molecules in the unit cell of RDX (T=298 K, P= 1 atm)[a]

	Molecule 1			Molecule 2			Molecule 3			Molecule 4		
	Expt.	**NsT-MD**	**Δ [b]**	**Expt.**	**NsT-MD**	**Δ [b]**	**Expt.**	**NsT-MD**	**Δ [b]**	**Expt.**	**NsT-MD**	**Δ [b]**
s_x	0.08172	0.08076	-0.00771	0.41828	0.41950	0.03870	0.08172	0.08078	-0.00690	0.58172	0.58070	0.01712
s_y	0.40516	0.40291	-0.01183	0.90516	0.90306	0.00732	0.09484	0.09704	0.02958	0.40516	0.40303	-0.01052
s_z	0.35212	0.35054	-0.01318	0.35212	0.35032	-0.01560	0.85212	0.85037	-0.00974	0.14788	0.14945	0.01835
θ (°)	101.42	102.31	0.88	101.42	102.25	0.82	78.58	77.76	-0.81	78.58	77.75	-0.82
ϕ (°)	32.44	30.93	-1.51	-32.44	-31.00	1.44	-32.44	-30.96	1.47	32.44	30.90	-1.54
ψ (°)	-6.15	-3.52	2.63	6.15	3.44	-2.72	-6.15	-3.54	2.61	6.15	3.53	-2.62
	Molecule 5			**Molecule 6**			**Molecule 7**			**Molecule 8**		
	Expt.	**NsT-MD**	**Δ [b]**	**Expt.**	**NsT-MD**	**Δ [b]**	**Expt.**	**NsT-MD**	**Δ [b]**	**Expt.**	**NsT-MD**	**Δ [b]**
s_x	0.58172	0.58096	0.02114	0.91828	0.91951	0.06447	0.41828	0.41946	0.03877	0.91828	0.91956	0.06575
s_y	0.09484	0.09693	0.02810	0.90516	0.90292	0.00554	0.59484	0.59703	0.04673	0.59484	0.59685	0.04458
s_z	0.64788	0.64931	0.02220	0.14788	0.14955	0.01943	0.85212	0.85062	-0.00710	0.64788	0.64940	0.02312
θ (°)	101.42	102.24	0.82	78.58	77.69	-0.88	78.58	77.78	-0.79	101.42	102.15	0.73
ϕ (°)	-32.44	-30.97	1.47	-32.44	-30.99	1.45	32.44	30.89	-1.55	32.44	30.89	-1.55
ψ (°)	6.15	3.42	-2.73	-6.15	-3.54	2.61	6.15	3.49	-2.66	-6.15	-3.49	2.66

a. Values are averaged over time and unit cells within the 3 x 3 x 3 simulation supercell of the Pbca low-energy structure resulting from the MOLPAK/WMIN calculations (Solution CB-1)

b. Values correspond to deviations from experimental values of predicted center-of-mass coordinates (in Å) and Euler Angles (°)