Prediction of Supramolecular Synthons and Crystal Packings of Supramolecular HMX/Solvent Assemblies

Zhichao Liu,[a] Yu Liu,[b] Jinshan Li,[b] Weihua Zhu[a,*]

[a]Institute for Computation in Molecular and Materials Science and Department of Chemistry, Nanjing University of Science and Technology, Nanjing 210094, China

[b]Institute of Chemical Materials, China Academy of Engineering Physics, P. O. Box 919-327, Mianyang, Sichuan 621900, China

[*] Corresponding author. E-mail: zhuwh@njust.edu.cn

Table S1. Predicted lattice parameters of HMX/solvent supramolecular assemblies with 10 possible space groups by DFTB-D method.

solvent	space group	*a* (Å)	*b* (Å)	*c* (Å)	*α* (Å)	*β* (Å)	*γ* (Å)	*V* (Å^3)	*ρ* (g·cm^{-3})
DMF	*C*2/*c*	21.70	11.11	15.80		62.69		3383.2	1.450
	P-1	7.921	10.15	11.25	107.8	83.35	96.34	852.3	1.439
	$P2_1$	8.042	8.096	12.91		80.55		828.9	1.480
	$P2_12_12_1$	27.52	7.828	7.582				1633.0	1.502
	$P2_1/c$	11.52	20.70	11.84		139.9		1819.3	1.348
	Pbca	21.02	10.68	15.26				3424.1	1.433
	Pbcn	14.87	20.91	10.50				3264.2	1.503
	$Pna2_1$	7.845	26.64	8.071				1686.5	1.503
	R-3	16.10		30.77				6911.6	1.597
	R-3*c*	31.38		22.38				19089.0	1.156
DMSO	*C*2/*c*	12.61	9.553	31.89		54.65		3131.9	1.587
	P-1	7.508	11.35	11.90	98.68	95.23	119.2	858.7	1.447
	$P2_1$	11.44	10.29	7.313		87.97		860.1	1.445
	$P2_12_12_1$	12.64	11.18	10.70				1512.1	1.644
	$P2_1/c$	7.334	14.56	15.71		75.47		1623.8	1.531
	Pbca	27.25	9.979	12.28				3338.9	1.489
	Pbcn	16.41	8.483	22.92				3190.8	1.558
	$Pna2_1$	12.67	11.18	10.69				1513.2	1.643
	R-3	22.08		18.94				7999.3	1.398
	R-3*c*	15.95		76.47				16855.1	1.327
GBL	*C*2/*c*	27.12	7.396	24.45		46.38		3549.7	1.430
	P-1	8.591	10.99	9.616	92.77	85.03	113.0	832.4	1.525
	$P2_1$	10.27	8.260	11.19		112.7		875.6	1.450
	$P2_12_12_1$	19.98	8.272	10.15				1677.1	1.514
	$P2_1/c$	8.463	23.57	8.903		99.95		1749.3	1.451
	Pbca	10.71	18.86	16.31				3293.9	1.542
	Pbcn	21.86	8.230	19.16				3446.3	1.473
	$Pna2_1$	9.330	17.13	10.56				1687.3	1.505
	R-3	32.14		8.631				7719.1	1.480
	R-3*c*	26.75		26.35				16331.8	1.399
HMPA	*C*2/*c*	15.71	7.482	56.53		49.16		5026.3	1.256
	P-1	7.502	8.782	21.25	80.74	76.83	61.80	1199.3	1.317
	$P2_1$	7.703	14.65	12.25		63.39		1235.7	1.277
	$P2_12_12_1$	16.99	9.834	14.45				2413.9	1.308
	$P2_1/c$	8.793	22.83	15.74		51.02		2457.0	1.285
	Pbca	17.21	28.80	9.739				4827.1	1.308
	Pbcn	30.90	11.29	14.50				5058.7	1.248
	$Pna2_1$	40.82	8.435	7.405				2549.8	1.238

	R-3	40.59		8.234				11745.7	1.210
	R-3*c*	31.06		30.64				25599.4	1.110
NMP	*C*2/*c*	11.80	10.87	32.63		110.5		3922.1	1.339
	P-1	7.512	8.507	14.36	94.01	92.42	85.45	912.1	1.439
	$P2_1$	7.449	14.55	8.104		95.05		874.9	1.500
	$P2_12_12_1$	7.985	28.66	7.670				1755.4	1.496
	$P2_1/c$	7.370	29.14	8.025		94.00		1719.5	1.527
	Pbca	11.28	15.48	21.28				3715.2	1.413
	Pbcn	29.97	7.665	15.29				3512.4	1.495
	$Pna2_1$	29.99	8.063	7.527				1820.3	1.443
	R-3	28.75		11.51				8235.4	1.435
	R-3*c*	30.49		23.93				19256.8	1.227

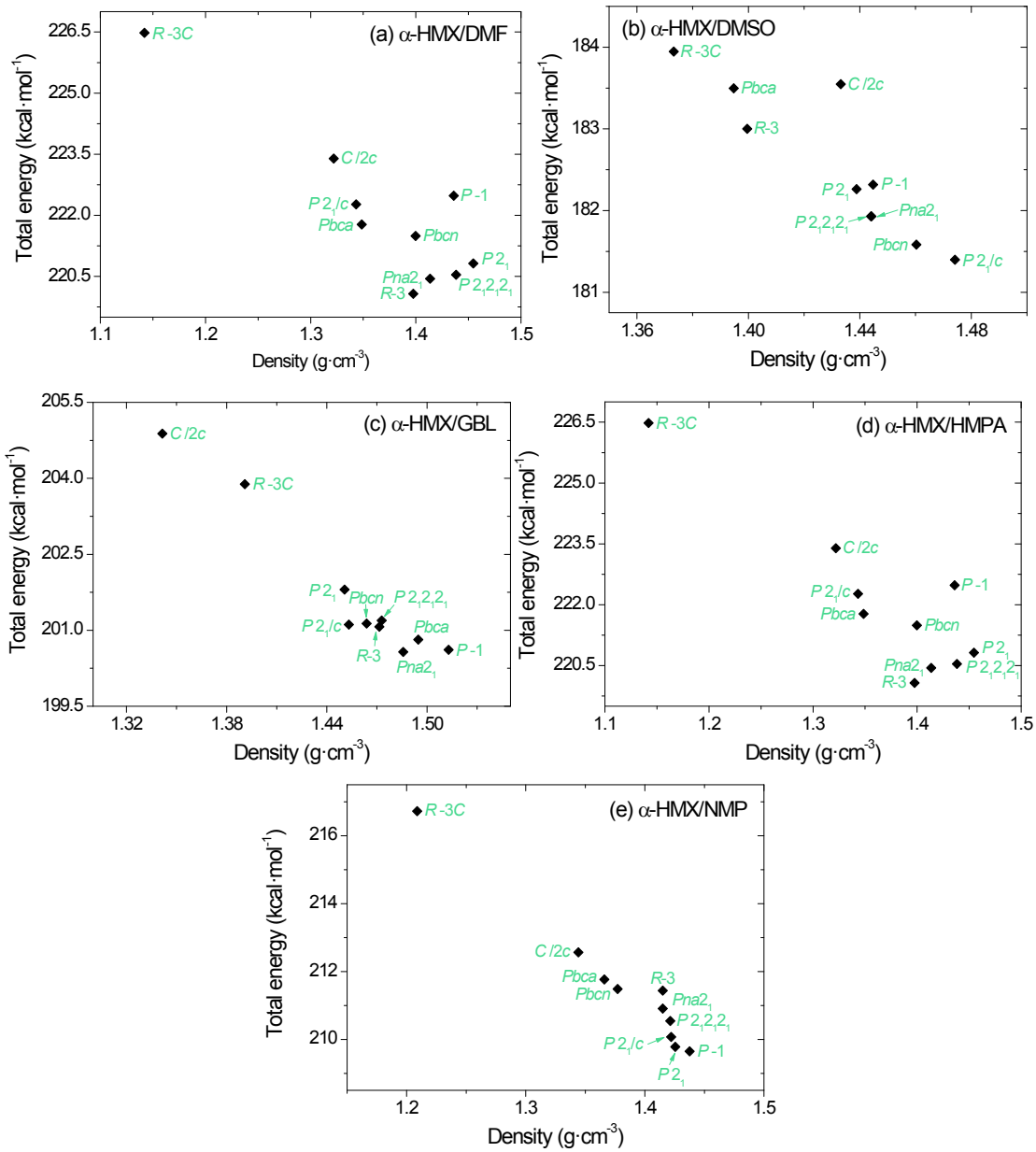

Fig. S1. Relationship between crystal density and total energy of the packings for α-HMX/solvent supramolecular assemblies in different space groups from FF.

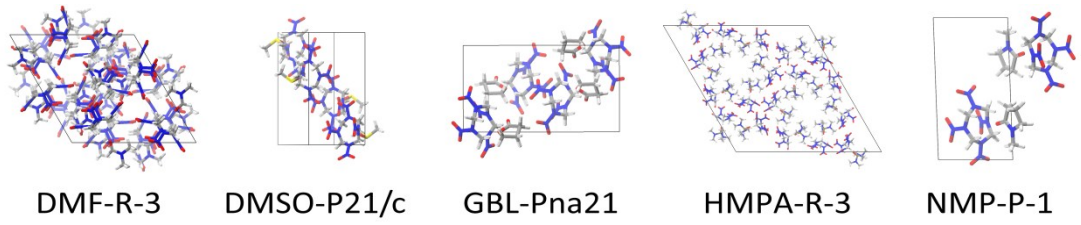

Fig. S2. Packing structures with lowest energy from Dreiding Force Field for the 10 most common space groups for the α-HMX/solvent synthons.