

Toward Low-sensitive and High-energetic Cocystal I: Evaluation of the Power and the Safety of Observed Energetic Cocystals

Supporting information

The V_D and P_D calculation details using K-J equation.

		Products, in mol												M g/mol	N mol	\bar{M} g/mol	HOF(s) kcal/mol	Q_D kcal/mol	d_{298K} g/cm ³	V_D km/s	P_D GPa
		H ₂ O (g)	CO (g)	CO ₂ (g)	N ₂ (g)	C (s)	H ₂ (g)	O ₂ (g)	HF (g)	HBr (g)	SO ₂ (g)	P ₂ O ₅ (s)	S (g)								
ϵ -CL-20	4 ϵ -CL-20	3	3	3	6	0	0	0	0	0	0	0	0	438	0.034247	29.20	32.4	1294.95	2.044	9.5	43.3
β -CL-20	4 β -CL-20	3	3	3	6	0	0	0	0	0	0	0	0	438	0.034247	29.20	35.5	1301.89	1.985	9.3	41.0
γ -CL-20	4 γ -CL-20	3	3	3	6	0	0	0	0	0	0	0	0	438	0.034247	29.20	37.2	1305.87	1.916	9.1	38.2
1	8α-CL-20/8H₂O	4	3	3	6	0	0	0	0	0	0	0	0	456	0.035088	28.50	-35.1	1222.57	1.981	9.2	40.0
2	2 γ -CL-20/4DMF	10	4	0	7	8	0	0	0	0	0	0	0	584	0.035959	23.24	-79.2	1034.86	1.675	7.6	24.4
3	8 α -CL-20/4CO ₂	3	3	3.5	6	0	0	0	0	0	0	0	0	460	0.033696	29.68	-13.3	1235.84	1.987	9.2	39.7
4	4 β -CL-20/2 β -HMX	5	5	3	8	0	0	0	0	0	0	0	0	586	0.035836	27.90	32.4	1255.15	1.945	9.2	39.5
5	8 β -CL-20/8TNT	5.5	12.5	0	7.5	0.5	0	0	0	0	0	0	0	665	0.038346	25.84	14.2	995.64	1.853	8.5	32.9
6	16 β -CL-20/16BL	6	8	0	6	2	0	0	0	0	0	0	0	524	0.038168	25.00	-70.4	930.52	1.804	8.1	29.5
7	4 β -CL-20/4BTf	3	9	3	9	0	0	0	0	0	0	0	0	690	0.034783	28.75	179.4	1264.57	1.918	9.1	38.0
8	2 γ -CL-20/7DO	17	2	0	6	18	0	0	0	0	0	0	0	746	0.033512	21.20	-310.9	971.18	1.56	6.7	18.2
9	4 β -CL-20/12HMPA	7.5	0	0	10.5	24	22.5	0	0	0	1.5	0	0	975	0.041538	11.70	-320.4	1213.19	1.395	6.3	15.0
	β -HMX	4	4	0	4	0	0	0	0	0	0	0	0	296	0.040541	24.67	-0.7	1135.44	1.903	9.1	38.3
	α -HMX	4	4	0	4	0	0	0	0	0	0	0	0	296	0.040541	24.67	-5.1	1120.68	1.84	8.9	35.6

10	4 α -HMX/4PDA	8	0	0	5	10	0	0	0	0	0	0	0	404	0.032178	21.85	-1.0	1142.03	1.599	7.0	20.2
11	4 β -HMX/4PDCA	9	1	0	5	9	0	0	0	0	0	0	0	428	0.035047	22.00	-100.8	1041.59	1.579	7.1	20.6
12	β -HMX/2PN _{ox}	10	0	0	5	16	1	0	0	0	0	0	0	514	0.031128	20.13	15.0	1153.75	1.533	6.6	17.4
13	4 α -HMX/4FA	6.5	1.5	0	4.5	8.5	0	0	1	0	0	0	0	407	0.03317	22.59	-48.1	1062.65	1.634	7.2	21.4
14	2 β -HMX/4DNDA	12	4	0	8	6	0	0	0	0	0	0	0	624	0.038462	23.00	-41.7	1213.89	1.64	8.0	26.9
15	4 γ -HMX/2H ₂ O	4.5	4	0	4	0	0	0	0	0	0	0	0	305	0.040984	24.40	-58.8	1006.13	1.78	8.5	31.7
16	4 α -HMX/4T ₂	6	2	0	4	8	0	0	0	0	0	0	2	436	0.027523	23.00	31.7	989.31	1.709	6.6	18.9
17	6 α -HMX /6Py	7.5	1.5	0	4.5	6.5	0	0	0	0	0	0	0	381	0.035433	22.44	-73.4	1048.98	1.603	7.3	21.8
18	4 α -HMX/4DAT	8	0	0	5	11	1	0	0	0	0	0	0	418	0.033493	20.43	-18.0	1063.16	1.604	6.9	19.8
	TNT	2.5	3.5	0	1.5	3.5	0	0	0	0	0	0	0	227	0.03304	24.67	-18.7	961.37	1.654	7.2	21.7
19	2TNT/2 1-BN	5.5	0.5	0	1.5	16.5	0	0	0	1	0	0	0	434	0.019585	27.76	4.3	792.91	1.661	5.4	12.5
20	2TNT/2Nap	6	0	0	1.5	17	0.5	0	0	0	0	0	0	355	0.022535	18.88	4.2	988.63	1.43	5.1	9.8
21	2TNT/2 9-BN	6	0	0	1.5	21	0.5	0	0	1	0	0	0	484	0.018595	25.78	23.0	782.05	1.614	5.1	10.7
22	4TNT/4Ant	6	0	0	1.5	21	0	0	0	0	0	0	0	405	0.018519	20.00	21.3	908.99	1.449	4.6	8.2
23	4TNT/4Per	6	0	0	1.5	27	2.5	0	0	0	0	0	0	479	0.020877	15.50	32.8	792.40	1.464	4.5	7.7
24	2TNT/2TT	4.5	1.5	0	1.5	11.5	0	0	0	0	0	0	4	431	0.017401	22.00	27.1	758.21	1.632	4.7	9.3
25	8TNT/8DBZ	6	0	0	1.5	19	0.5	0	0	0	0	0	1	411	0.019465	18.88	13.4	876.45	1.477	4.7	8.5
26	4TNT/4 α -ABA	6	2	0	2	12	0	0	0	0	0	0	0	364	0.027473	22.00	-113.0	787.36	1.506	5.7	12.8
27	4TNT/8 α -ABA	9.5	0.5	0	2.5	20.5	0	0	0	0	0	0	0	501	0.02495	20.40	-138.6	845.71	1.444	5.3	10.6
28	2TNT/2AA	6	2	0	2	12	0	0	0	0	0	0	0	364	0.027473	22.00	-119.4	769.78	1.524	5.7	12.9
29	4TNT/8AA	9.5	0.5	0	2.5	20.5	0	0	0	0	0	0	0	501	0.02495	20.40	-145.3	832.34	1.476	5.3	11.0
30	4TNT/4DMB	7.5	0.5	0	1.5	14.5	0	0	0	0	0	0	0	365	0.026027	20.11	-89.3	979.26	1.435	5.5	11.7
31	2TNT/2DMDBT	6	0	0	1.5	21	2.5	0	0	0	0	0	1	439	0.022779	15.50	-7.0	774.13	1.43	4.6	7.9
32	4TNT/4PA	6	0	0	2	19	1	0	0	0	0	0	1	426	0.021127	18.44	1.8	818.34	1.496	4.8	9.1
33	2TNT/2T ₂	4.5	1.5	0	1.5	11.5	0	0	0	0	0	0	2	367	0.020436	22.00	19.6	870.00	1.604	5.2	11.3

34	4TNT/4PDA	6	0	0	2.5	13	0.5	0	0	0	0	0	0	0	348	0.025862	19.89	-25.4	923.59	1.509	5.6	12.4
35	4TNT/4Phe	6	0	0	1.5	21	1.5	0	0	0	0	0	0	0	405	0.022222	17.00	15.0	893.38	1.422	4.8	8.6
36	4TNT/4TNB	4	8	0	3	5	0	0	0	0	0	0	0	0	440	0.034091	25.33	-28.6	940.36	1.64	7.3	22.0
	BTF	0	6	0	3	0	0	0	0	0	0	0	0	0	252	0.035714	28.00	134.4	1161.90	1.901	8.9	36.3
37	4BTF/4TNA	2	10	0	5	2	0	0	0	0	0	0	0	0	482	0.03527	26.82	112.2	1020.33	1.834	8.3	30.6
38	4BTF/4MATNB	3	9	0	5	4	0	0	0	0	0	0	0	0	494	0.034413	26.24	118.6	1072.06	1.751	7.9	27.6
39	2BTF/2TNAZ	2	8	1	5	0	0	0	0	0	0	0	0	0	444	0.036036	27.75	140.9	1265.20	1.844	8.9	35.8
40	4BTF/4TNB	1.5	10.5	0	4.5	1.5	0	0	0	0	0	0	0	0	465	0.035484	27.09	128.1	1058.06	1.806	8.3	30.5
41	4BTF/4TNT	2.5	9.5	0	4.5	3.5	0	0	0	0	0	0	0	0	479	0.034447	26.48	122.5	1081.00	1.747	8.0	27.7