Molecular Design of Long Intra-annular Nitrogen Chains : 3H-tetrazolo[1,5-d]tetrazole-Based High-Energy-Density Materials

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Table 1 Physicochemical and energetic properties of compounds **1**–**8**, RDX, HMX, and CL-20

compound	N[a]	OB[b]	ρ[c]	$\Delta H_{f,solid}$[d]	D[e]	P[f]
1	88.3	-36.01	1.71	641.36	9.05	31.25
2	88.9	-38.07	1.67	736.20	9.21	32.22
3	71.8	0.00	1.86	757.27	9.86	41.77
4	92.1	-21.04	1.75	1129.54	9.50	36.66
5	69.1	-9.87	1.97	731.79	9.16	38.44
6	82.3	-47.03	1.70	877.98	8.35	26.53
7	65.1	9.30	1.88	735.95	9.59	39.66
8	73.7	-4.68	1.82	781.38	9.78	40.72
RDX[g]	37.8	-21.61	1.81	86.3	8.87	34.80
HMX[g]	37.8	-21.62	1.90	116.1	9.26	39.40
CL-20[g]	38.3	-10.95	2.04	365.4	9.73	44.4

a Nitrogen content (%). b Oxygen balance (OB = (xO−2yC−1/2zH)1600/M) (%). c Calculated density (g cm^{-3}). d Calculated enthalpy of formation (kJ mol^{-1}). e Detonation velocity (km s^{-1}). f Detonation pressure (GPa). g Ref.[19] (detonation pressures and detonation velocities were recalculated with EXPLO5 v6.01).

Table 2 BDEs (kJ mol^{-1}) for N-R of **2**-**8** and predicted energy required (kJ mol^{-1}) for the decomposition of **1**–**8**

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**

BDE		218.42	41.06	107.82	60.34	359.16	96.87	177.30
Predicted energy requirements	40.36	40.90	40.19	37.76	37.46	35.73	39.30	38.02