Electronic Supporting Information (ESI)

Theoretical study of a series of 4,4′-Azo-1*H*-1,2,4-triazol-5-one based nitrogen-rich salts as potential energetic compounds

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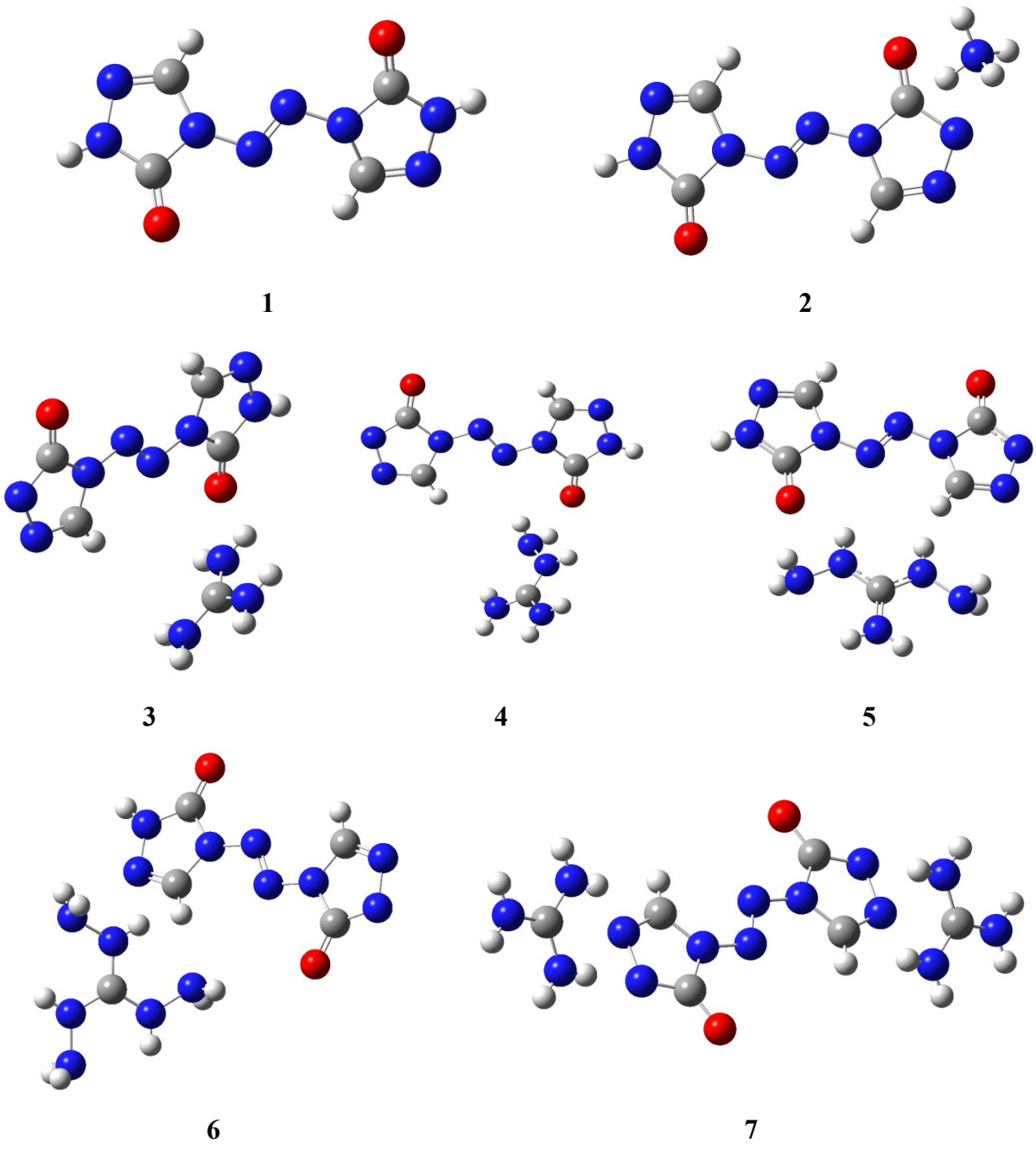

Fig. S1. The starting geometries extracted from the single crystal X-ray data plotted by GaussianView of **1**-**7**.

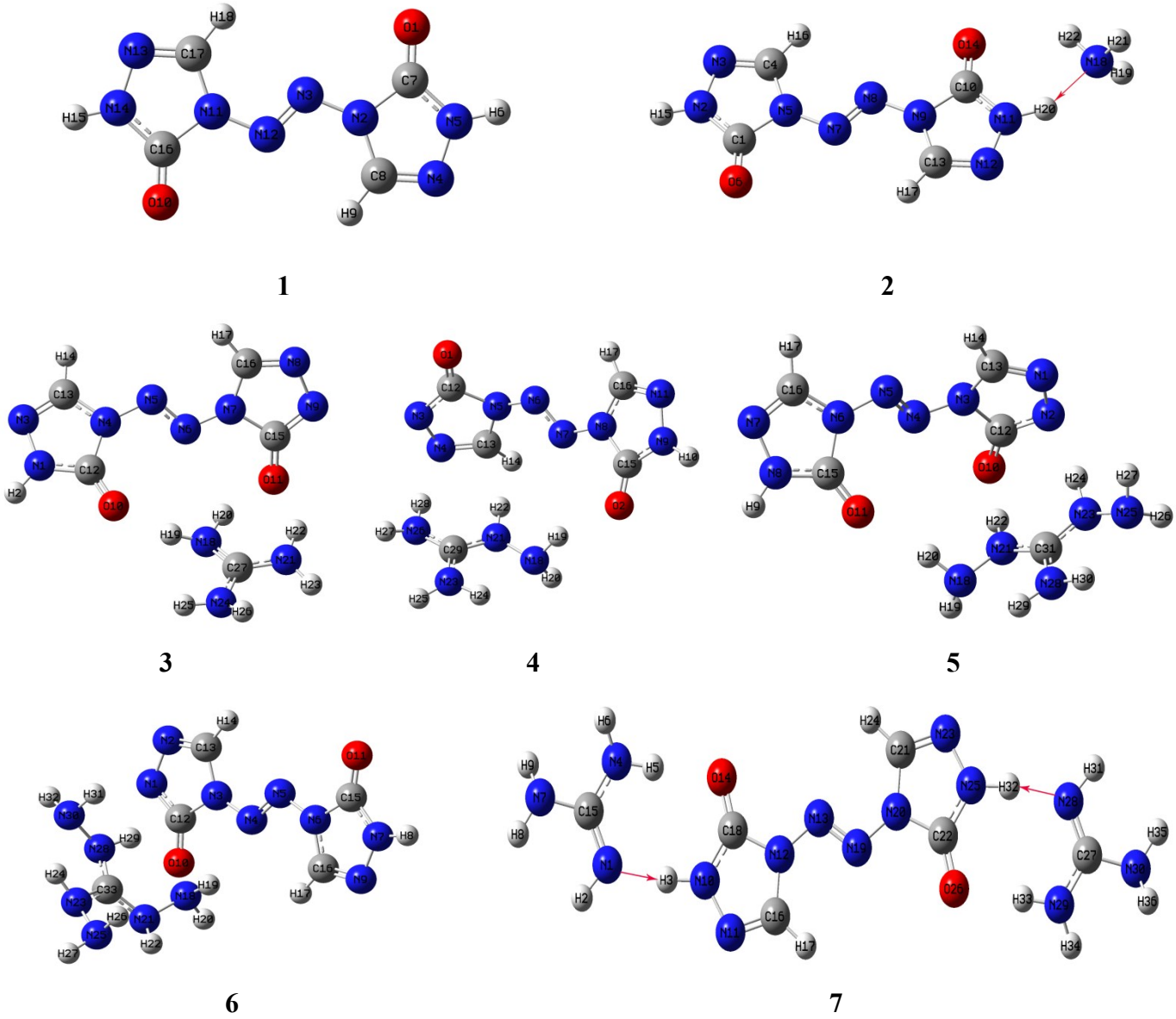

Fig. S2. Optimized geometries of **1-7** at DFT-B3PW91/6-31G(d,p) level.

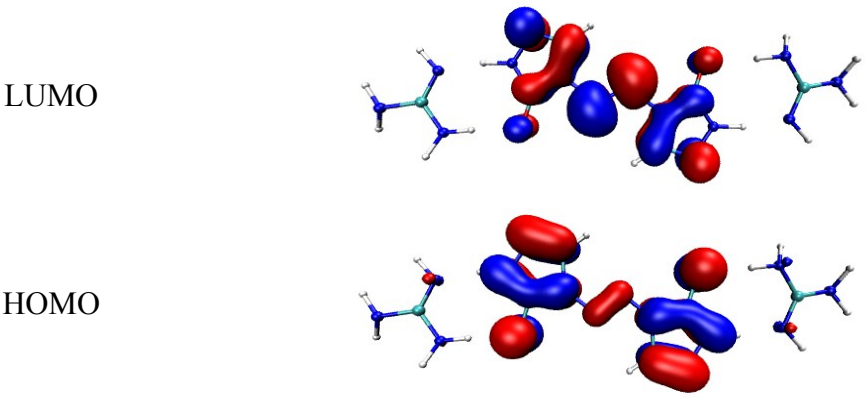

Fig. S3. The pictorial illustration of HOMO and LUMO at B3PW91/6-31G(d,p) level for **7**.

Table S1. The selected electrostatic potential parameters of compound **1**-**7**.

	1		**2**		**3**		**4**	
	B3LYP	B3PW91	B3LYP	B3PW91	B3LYP	B3PW91	B3LYP	B3PW91
A_S^+ (Å^2)	119.075	117.604	133.352	130.174	150.697	136.209	148.876	153.865
A_S^- (Å^2)	82.220	82.687	99.366	101.684	103.475	122.384	120.089	116.174
	5		**6**		**7**			
	B3LYP	B3PW91	B3LYP	B3PW91	B3LYP	B3PW91		
A_S^+ (Å^2)	151.983	147.495	141.222	143.709	161.009[1]	130.759		
A_S^- (Å^2)	134.410	138.207	155.182	155.117	158.670[1]	212.133		

Table S2. The data of electrostatic potential parameters of ions used by densities calculation.

	$\bar{V}_S^+$ / kcal·mol^{-1}		$\bar{V}_S^-$ / kcal·mol^{-1}		A_S^+ / Å^2		A_S^- / Å^2	
	B3LYP	B3PW91	B3LYP	B3PW91	B3LYP	B3PW91	B3LYP	B3PW91
2	171.23	171.77	-81.47	-81.72	47.80	47.44	202.36	201.41
3	122.57	122.85	-81.47	-81.72	95.40	94.83	202.36	201.41
4	113.86	114.13	-81.47	-81.72	110.16	109.37	202.36	201.41
5	106.74	106.99	-81.47	-81.72	125.16	124.18	202.36	201.41
6	101.02	101.23	-81.47	-81.72	139.87	138.71	202.36	201.41

Table S3. The densities, detonation pressures (P) and detonation velocities (D) of 1-7 based on optimized geometries at B3PW91/6-31G(d,p) level.

	1	**2**	**3**	**4**	**5**	**6**	**7**
ρ_{cal}[a]/ g·cm^{-3}	1.775	1.816	1.680	1.668	1.659	1.653	1.640
P[b]/ GPa	22.37	27.07	20.94	21.85	22.80	23.71	18.06
D[c]/ ms^{-1}	7131	7792	7107	7185	7352	7505	6568

[a] Calculated density. [b] Detonation pressure. [c] Detonation velocity.

1. W. L. Cao, J. J. Guo, X. Chen, Z. M. Ding, K. Z. Xu, J. R. Song, A. Fan and J. Huang, *J. Mol. Struct.*, 2017, 1147, 754-762.