Electronic supplementary information

Design and theoretical studies of FOX-7-like novel energetic compounds

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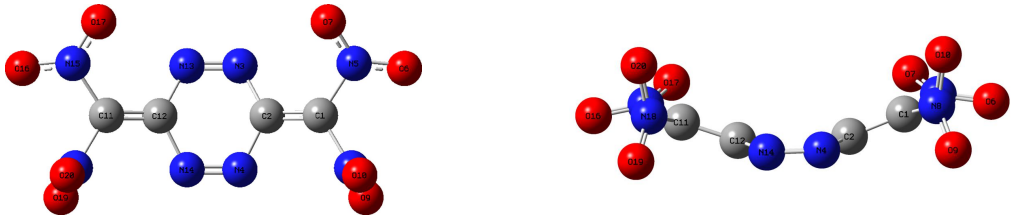
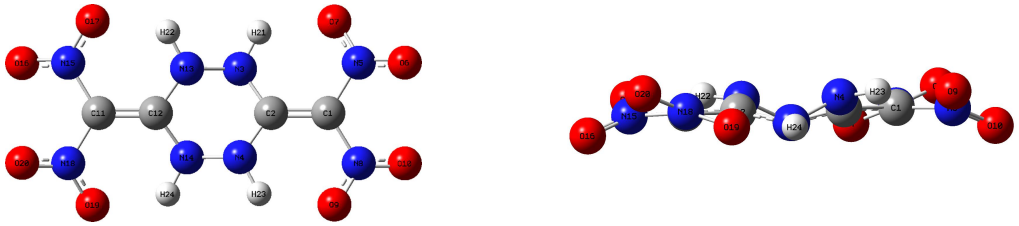


2a



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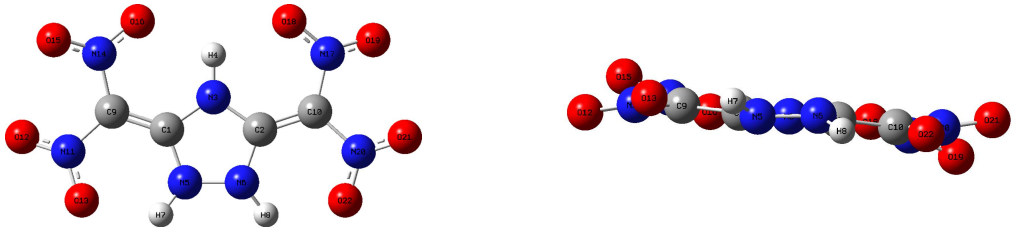

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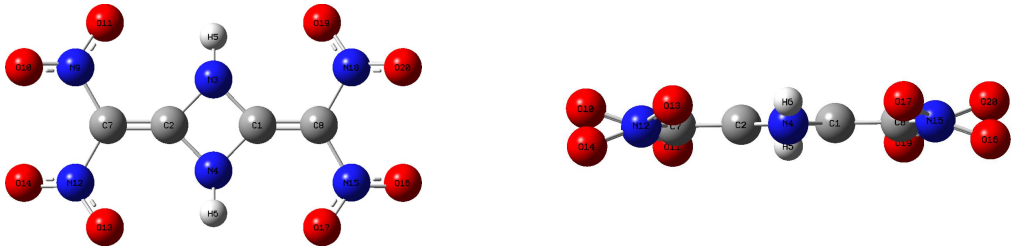

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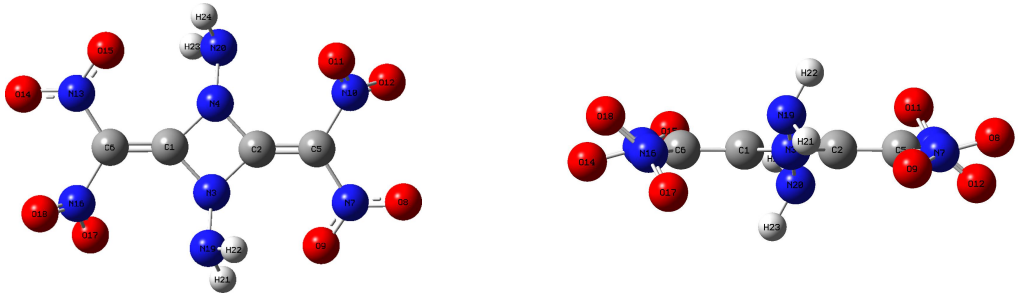


2e

Fig. S1. The optimized structures of compounds **2a**~**2e** demonstrated from different viewpoints.

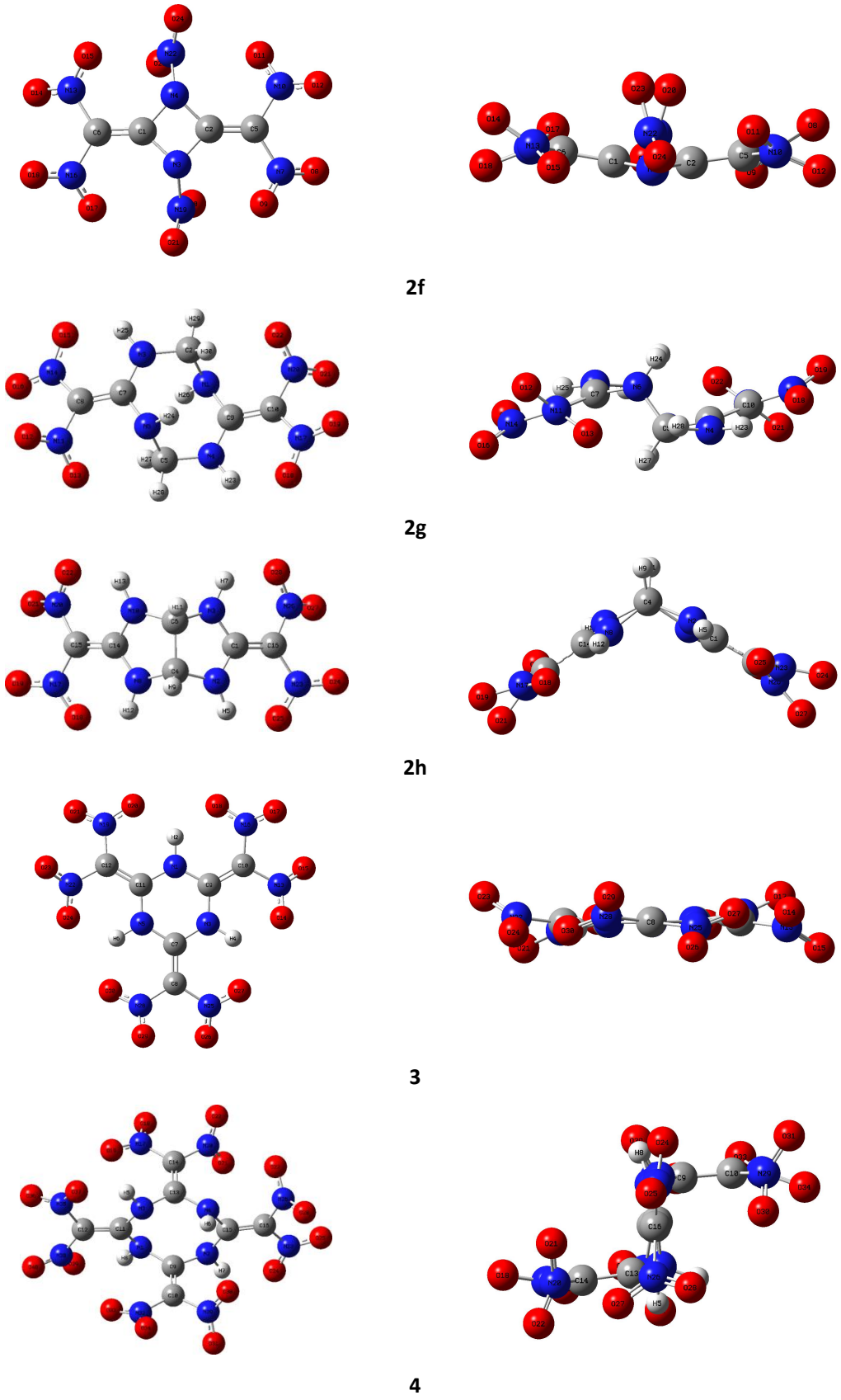


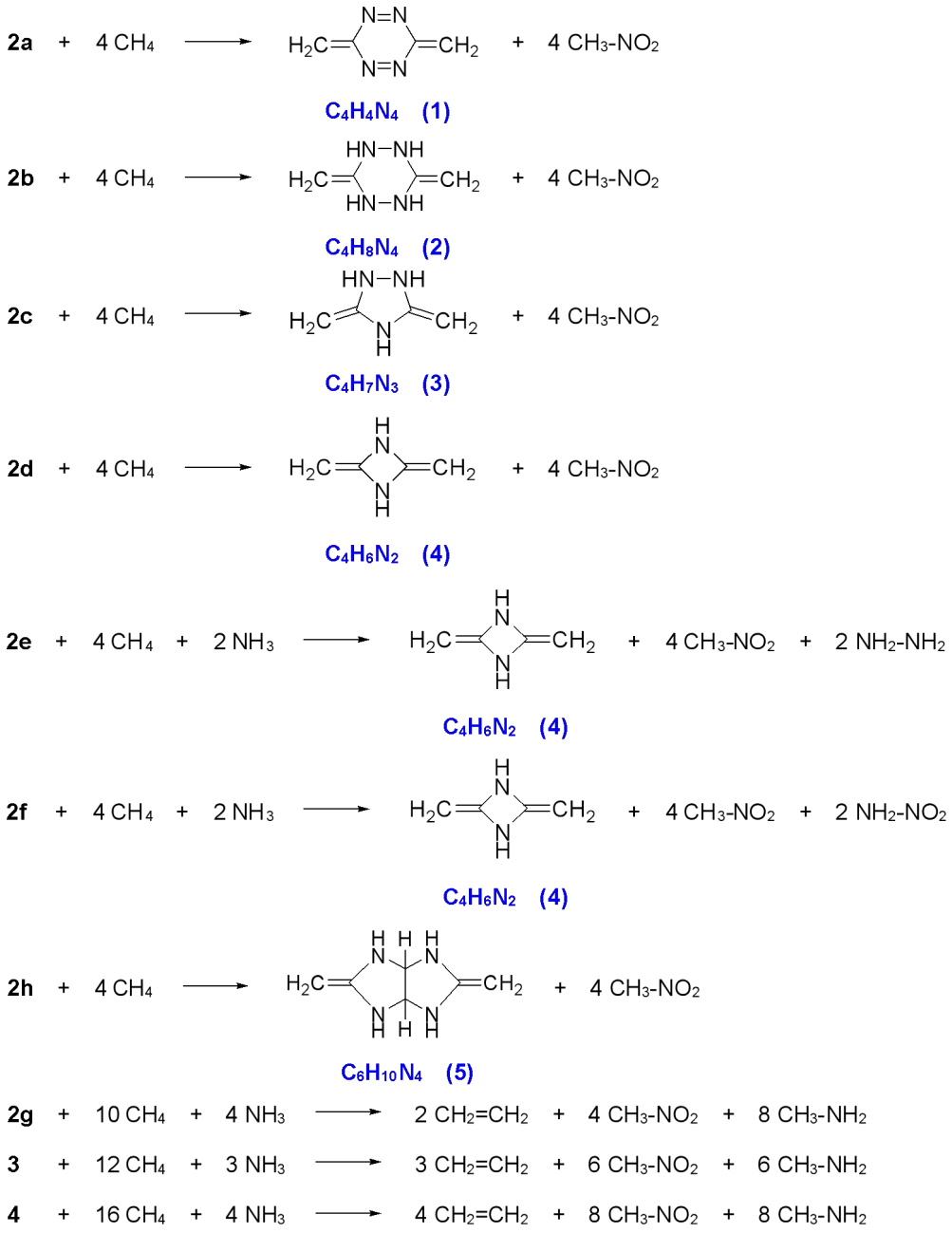
Fig. S2. The optimized structures of compounds **2f**~**4** demonstrated from different viewpoints.

Table S1. Bond lengths, bond orders and nitro group charges of the optimized title molecules.

Bonds	bond lengths/Å	LBO	Mayer	Q_{NO2}	Bonds	bond lengths/Å	LBO	Mayer	Q_{NO2}
2a					2b				
C1=C2	1.3335	1.8543	1.6808		C1=C2	1.3963	1.4743	1.4211	
C1-N5(O_2)	1.4702	0.7620	0.9350	-0.073	C1-N5(O_2)	1.4359	0.8207	1.0290	-0.223
C1-N8(O_2)	1.4765	0.7515	0.9637	-0.088	C1-N8(O_2)	1.4358	0.8208	1.0290	-0.223
C2-N3	1.4109	0.9520	1.0683		C2-N3	1.3514	1.1728	1.2513	
C2-N4	1.4208	0.9008	1.0288		C2-N4	1.3514	1.1730	1.2515	
N3=N13	1.2449	1.4943	1.6946		N3-N13	1.4051	0.6050	0.8796	
N4=N14	1.2422	1.5143	1.7006		N4-N14	1.4053	0.6045	0.8796	
C11=C12	1.3335	1.8544	1.6808		C11=C12	1.3963	1.4744	1.4210	
C11-N15(O_2)	1.4702	0.7620	0.9350	-0.073	C11-N15(O_2)	1.4359	0.8207	1.0290	-0.223
C11-N18(O_2)	1.4765	0.7515	0.9637	-0.088	C11-N18(O_2)	1.4359	0.8206	1.0289	-0.223
C12-N13	1.4109	0.9520	1.0683		C12-N13	1.3513	1.1731	1.2517	
C12-N14	1.4208	0.9007	1.0288		C12-N14	1.3515	1.1724	1.2512	
2c					2d				
C1-N3	1.3660	1.0666	1.1888		C1-N3	1.3888	0.9546	1.1299	
C1-N5	1.3454	1.1850	1.2680		C1-N4	1.3886	0.9553	1.1302	
C1=C9	1.3916	1.5022	1.4299		C1=C8	1.3461	1.7849	1.5954	
C2-N3	1.3660	1.0665	1.1887		C2-N3	1.3888	0.9546	1.1299	
C2-N6	1.3454	1.1849	1.2679		C2-N4	1.3886	0.9553	1.1302	
C2=C10	1.3916	1.5024	1.4299		C2=C7	1.3461	1.7849	1.5953	
N5-N6	1.3802	0.7012	0.9284		C7-N9(O_2)	1.4497	0.7935	0.9767	-0.149
C9-N11(O_2)	1.4310	0.8413	1.0553	-0.218	C7-N12(O_2)	1.4497	0.7936	0.9768	-0.149
C9-N14(O_2)	1.4366	0.8241	1.0324	-0.203	C8-N15(O_2)	1.4497	0.7936	0.9768	-0.149
C10-N17(O_2)	1.4366	0.8240	1.0323	-0.203	C8-N18(O_2)	1.4497	0.7935	0.9767	-0.149
C10-N20(O_2)	1.4310	0.8414	1.0552	-0.218					
2e					2f				
C1-N3	1.3991	0.9112	1.1167		C1-N3	1.4182	0.7966	1.0659	
C1-N4	1.4030	0.8691	1.1174		C1-N4	1.4157	0.8259	1.0358	
C1=C6	1.3411	1.7932	1.6059		C1=C6	1.3355	1.8354	1.6659	
C2-N3	1.4031	0.8688	1.1173		C2-N3	1.4157	0.8261	1.0359	
C2-N4	1.3990	0.9113	1.1168		C2-N4	1.4183	0.7965	1.0658	
C2=C5	1.3411	1.7933	1.6059		C2=C5	1.3355	1.8354	1.6659	
N3-N19	1.3858	0.6642	0.9729		N3-N19(O_2)	1.5474	0.2438	0.7919	0.054
N4-N20	1.3858	0.6641	0.9730		N4-N22(O_2)	1.5477	0.2434	0.7918	0.054
C5-N7(O_2)	1.4442	0.8090	0.9840	-0.165	C5-N7(O_2)	1.4617	0.7654	0.9407	-0.110
C5-N10(O_2)	1.4648	0.7511	0.9388	-0.126	C5-N10(O_2)	1.4599	0.7719	0.9330	-0.103
C6-N13(O_2)	1.4441	0.8091	0.9841	-0.165	C6-N13(O_2)	1.4617	0.7654	0.9407	-0.110
C6-N16(O_2)	1.4648	0.7510	0.9388	-0.126	C6-N16(O_2)	1.4599	0.7720	0.9330	-0.103

Continued to Table S1.

Bonds	bond lengths/Å	LBO	Mayer	Q_{NO2}	Bonds	bond lengths/Å	LBO	Mayer	Q_{NO2}
2g					2h				
C2-N1	1.4644	0.6595	0.8653		C1-N2	1.3517	1.1340	1.2450	
C2-N3	1.4640	0.6720	0.8981		C1-N3	1.3477	1.1538	1.2592	
C5-N4	1.4640	0.6719	0.8981		C1=C16	1.3955	1.4939	1.4184	
C5-N6	1.4644	0.6595	0.8653		C4-N2	1.4431	0.7402	0.9397	
C7-N3	1.3468	1.1729	1.2926		C4-C6	1.5527	0.9221	0.9887	
C7-N6	1.3935	0.9724	1.0867		C4-N8	1.4526	0.7053	0.8925	
C7=C8	1.3767	1.5932	1.5455		C6-N3	1.4526	0.7008	0.9023	
C8-N11(O_2)	1.4654	0.7421	0.9779	-0.155	C6-N10	1.4412	0.7507	0.9203	
C8-N14(O_2)	1.4270	0.8603	1.0488	-0.227	C14-N8	1.3462	1.1585	1.2812	
C9-N1	1.3935	0.9723	1.0867		C14-N10	1.3494	1.1453	1.2605	
C9-N4	1.3468	1.1730	1.2925		C14=C15	1.3982	1.4797	1.4126	
C9=C10	1.3767	1.5933	1.5456		C15-N17(O_2)	1.4333	0.8324	1.0437	-0.233
C10-N17(O_2)	1.4270	0.8604	1.0489	-0.227	C15-N20(O_2)	1.4349	0.8267	1.0399	-0.230
C10-N20(O_2)	1.4654	0.7420	0.9778	-0.155	C16-N23(O_2)	1.4338	0.8263	1.0433	-0.229
					C16-N26(O_2)	1.4354	0.8202	1.0391	-0.226
3					4				
C7-N3	1.3654	1.0705	1.1502		C9-N1	1.4111	0.8672	0.9943	
C7-N5	1.3654	1.0707	1.1501		C9-N2	1.4183	0.8484	0.9488	
C7=C8	1.3769	1.5874	1.5141		C9=C10	1.3316	1.8680	1.8499	
C8-N25(O_2)	1.4512	0.7849	0.9964	-0.154	C10-N29(O_2)	1.4786	0.7306	0.9605	-0.066
C8-N28(O_2)	1.4513	0.7851	0.9963	-0.154	C10-N32(O_2)	1.4762	0.7300	0.9319	-0.054
C9-N1	1.3647	1.0758	1.1647		C11-N1	1.3785	1.0024	1.1126	
C9-N3	1.3660	1.0688	1.1484		C11-N3	1.3810	0.9998	1.1322	
C9=C10	1.3776	1.5877	1.5176		C11=C12	1.3669	1.6425	1.5454	
C10-N13(O_2)	1.4536	0.7735	0.9916	-0.153	C12-N35(O_2)	1.4500	0.7863	0.9822	-0.172
C10-N16(O_2)	1.4497	0.7855	0.9946	-0.156	C12-N38(O_2)	1.4551	0.7712	0.9924	-0.168
C11-N1	1.3647	1.0758	1.1646		C13-N3	1.4235	0.8309	0.9975	
C11-N5	1.3661	1.0687	1.1485		C13-N4	1.3995	0.9148	1.0081	
C11=C12	1.3775	1.5879	1.5177		C13=C14	1.3360	1.8378	1.8429	
C12-N19(O_2)	1.4498	0.7851	0.9945	-0.156	C14-N17(O_2)	1.4689	0.7398	0.9443	-0.079
C12-N22(O_2)	1.4535	0.7734	0.9917	-0.153	C14-N20(O_2)	1.4776	0.7379	0.9514	-0.090
					C15-N2	1.3711	1.0320	1.1303	
					C15-N4	1.4142	0.8527	1.0155	
					C15=C16	1.3492	1.7587	1.6535	
					C16-N23(O_2)	1.4398	0.8253	1.0129	-0.145
					C16-N26(O_2)	1.4732	0.7261	0.9530	-0.115



Scheme S1 Isodesmic reactions for title compounds.