Supporting Information

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SI 1 Optimized parameters

SI 1 Optimized parameters of title compounds at B3LYP/6-311+G(2d) level of theory

Compound (1)

	HF	b3lyp /6-31g*	b3lyp /6-311g*	b3lyp /6-311+g*	Exp.[a]		HF	b3lyp /6-31g*	b3lyp /6-311g*	b3lyp /6-311+g*	Exp.[a]
Bond length (Å)											
N1-N2	1.434	1.379	1.379	1.377	1.385	C2-C3	1.529	1.532	1.532	1.525	1.527
N2-N3	1.262	1.281	1.281	1.275	1.287	C3-N7	1.488	1.474	1.474	1.474	1.482
N3-N4	1.400	1.366	1.366	1.363	1.360	N6-O1	1.241	1.216	1.216	1.210	1.210
N4-C1	1.361	1.367	1.367	1.363	1.357	N6-O2	1.216	1.207	1.207	1.201	1.205
C1-N1	1.289	1.313	1.313	1.308	1.314	N8-O3	1.225	1.212	1.212	1.206	1.221
N4-N5	1.378	1.372	1.372	1.369	1.384	N8-O4	1.251	1.225	1.225	1.220	1.224
N5-N6	1.464	1.507	1.507	1.505	1.498	C2-H2a	1.075	1.091	1.091	1.087	0.99
C1-N7	1.369	1.384	1.384	1.382	1.386	C2-H2b	1.079	1.096	1.096	1.092	0.99
N7-N8	1.388	1.421	1.421	1.420	1.391	C3-H2a	1.077	1.093	1.093	1.089	0.99
N5-C2	1.492	1.479	1.479	1.476	1.483	C3-H2b	1.073	1.088	1.088	1.084	0.99
Bond angle (°)											
N1-N2-N3	111.9	112.8	112.8	112.6	112.3	N4-N5-N6	109.8	110.5	110.6	111.0	108.6
N2-N3-N4	105.4	105.2	105.4	105.5	105.4	N5-N6-O1	117.2	116.0	116.1	116.3	115.6
N3-N4-C1	108.0	108.4	108.2	108.2	108.6	N5-N6-O2	114.0	114.1	113.9	114.0	115.3
N4-C1-N1	109.9	108.5	108.6	108.6	108.9	N7-C3-C2	109.3	109.8	109.8	110.0	108.9
N4-C1-N7	116.9	118.1	118.0	118.4	117.7	C3-C2-N5	110.3	112.0	112.0	112.1	112.2
C1-N7-N8	121.4	121.0	121.2	121.0	119.6	C2-C3-H3a	110.6	110.1	110.1	109.9	109.9
C1-N7-C3	122.5	120.3	120.2	120.0	120.8	C2-C3-H3b	110.6	110.7	110.9	110.9	109.9
N7-N8-O3	118.2	117.3	117.2	117.3	117.9	C3-C2-H2a	112.1	111.9	111.8	111.9	109.2
N7-N8-O4	114.4	114.2	114.2	114.2	115.2	C3-C2-H2b	110.6	110.3	110.4	110.3	109.2
C1-N4-N5	126.4	127.2	127.4	127.0	127.5	H3a-C3-H3b	109.2	107.9	107.7	107.5	108.3
N4-N5-C2	109.3	109.0	109.0	109.0	108.4	H2a-C2-H2b	110.4	108.8	108.6	108.3	107.9
Dihedral angle (°)											
N1-N2-N3-N4	-1.40	-2.12	-2.10	-2.36	-1.721	N4-N5-N6-O1	-26.11	-22.09	-20.24	-19.06	-28.69
C1-N4-N3-N2	1.24	1.79	1.88	2.31	1.691	C2-N5-N6-O2	34.56	40.23	42.21	42.62	35.87
N5-N4-C1-N7	0.38	0.46	0.76	2.62	-0.342	C1-N7-C3-C2	-19.49	-24.59	-24.53	-22.42	-25.48
C1-N7-N8-O3	2.60	9.15	8.20	8.40	16.60	N4-N5-C2-C3	-55.48	-52.18	-51.99	-52.32	-52.87
C3-N7-N8-O4	-1.56	-7.89	-7.70	-9.35	-2.411	N7-C3-C2-N5	49.87	51.84	51.81	51.21	52.65

[a] The experimental values derived from the Ref. 24.

Compound (2)

Bond length (Å)							
N1-N2	1.379	N4-N5	1.363	C2-C3	1.567	N8-O4	1.201
N2-N3	1.279	N5-N6	1.648	C3-N7	1.408	C2-O5	1.197
N3-N4	1.373	C1-N7	1.383	N6-O1	1.198	C3-O6	1.199
N4-C1	1.358	N7-N8	1.524	N6-O2	1.193		
C1-N1	1.307	N5-C2	1.439	N8-O3	1.202		
Bond angle (º)							
N1-N2-N3	112.7	C1-N7-N8	118.6	N4-N5-C2	113.7	C3-C2-N5	119.0
N2-N3-N4	105.3	C1-N7-C3	120.3	N4-N5-N6	109.3	C3-C2-O5	119.3
N3-N4-C1	107.7	N7-N8-O3	115.0	N5-N6-O1	113.0	C2-C3-O6	120.6
N4-C1-N1	109.5	N7-N8-O4	113.1	N5-N6-O2	113.2	O3-N8-O4	131.8
N4-C1-N7	118.0	C1-N4-N5	128.9	N7-C3-C2	114.9	O1-N6-O2	133.7
Dihedral angle (º)							
N1-N2-N3-N4	-1.86	C1-N7-N8-O3	40.20	C2-N5-N6-O2	57.14	N7-C3-C2-N5	-10.79
C1-N4-N3-N2	1.42	C3-N7-N8-O4	63.57	C1-N7-C3-C2	24.07	O6-C3-C2-O5	-9.83
N5-N4-C1-N7	-3.63	N4-N5-N6-O1	-0.37	N4-N5-C2-C3	-7.66	O3-N8-N7-O4	-179.71

Compound (3)

Bond length (Å)							
N1-N2	1.369	N7-N8	1.715	N1'-N2'	1.379	N7'-N8'	1.524
N2-N3	1.289	N6-O1	1.194	N2'-N3'	1.291	N6'-O1'	1.199
N3-N4	1.357	N6-O2	1.189	N3'-N4'	1.354	N6'-O2'	1.198
N4-C1	1.367	N8-O3	1.188	N4'-C1'	1.359	N8'-O3'	1.201
C1-N1	1.310	N8-O4	1.199	C1'-N1'	1.303	N8-'O4'	1.213
N4-N5	1.367	N5-C2	1.403	N4'-N5'	1.368	N5'-C3	1.432
N5-N6	1.814	N7-C3	1.383	N5'-N6'	1.628	N7'-C2	1.425
C1-N7	1.387	C2-C3	1.372	C1'-N7'	1.403		
Bond angle (º)							
N1-N2-N3	112.4	N7-N8-O4	113.6	N1'-N2'-N3'	112.5	N7'-N8'-O4'	114.7
N2-N3-N4	105.6	C1-N4-N5	129.1	N2'-N3'-N4'	105.0	C1'-N4'-N5'	125.3
N3-N4-C1	108.1	N4-N5-C2	108.5	N3'-N4'-C1'	108.7	N4'-N5'-C3	110.3
N4-C1-N1	108.6	N4-N5-N6	103.4	N4'-C1'-N1'	109.1	N4'-N5'-N6'	108.6
N4-C1-N7	120.8	N5-N6-O1	113.0	N4'-C1'-N7'	117.6	N5'-N6'-O1'	113.7
C1-N7-N8	107.3	N5-N6-O2	111.8	C1'-N7'-N8'	111.5	N5'-N6'-O2'	113.2
C1-N7-C3	111.8	N7-C3-C2	124.9	C1'-N7'-C2	112.3	N7'-C2-C3	119.4
N7-N8-O3	112.3	C3-C2-N5	123.8	N7'-N8'-O3'	114.9	C2-C3-N5'	120.6
Dihedral angle (º)							
N1-N2-N3-N4	0.43	N4-N5-N6-O1	27.40	N1'-N2'-N3'-N4'	-2.08	N4'-N5'-N6'-O1'	-16.84
C1-N4-N3-N2	-1.42	C2-N5-N6-O2	95.69	C1'-N4'-N3'-N2'	1.58	C3-N5'-N6'-O2'	45.49
N5-N4-C1-N7	-11.36	C1-N7-C3-C2	4.68	N5'-N4'-C1'-N7'	0.29	C1'-N7'-C2-C3	32.97
C1-N7-N8-O3	-91.33	N4-N5-C2-C3	2.92	C1'-N7'-N8'-O3'	39.65	N4'-N5'-C3-C2	-25.21
C3-N7-N8-O4	-33.05	N7-C3-C2-N5	-8.98	C2-N7'-N8'-O4'	-13.15	N7'-C2-C3-N5'	-4.36

Compound (4)

Bond length (Å)							
N1-N2	1.379	N8-O3	1.205	N1'-N2'	1.374	N8'-O3'	1.201
N2-N3	1.288	N8-O4	1.206	N2'-N3'	1.292	N8-'O4'	1.213
N3-N4	1.358	N5-C2	1.425	N3'-N4'	1.354	N5'-C3'	1.414
N4-C1	1.362	N7-C3	1.410	N4'-C1'	1.359	N7'-C2'	1.421
C1-N1	1.308	C2-C3	1.366	C1'-N1'	1.306	C3'-C2'	1.371
N4-N5	1.375	C2-N9	1.395	N4'-N5'	1.370	C2'-N9	1.394
N5-N6	1.618	C3-N11	1.410	N5'-N6'	1.713	C3'-N11	1.412
C1-N7	1.394	N10-O5	1.203	C1'-N7'	1.398	N10-O6	1.203
N7-N8	1.491	N12-O7	1.205	N7'-N8'	1.518	N12-O8	1.211
N6-O1	1.200	N9-N10	1.511	N6'-O1'	1.198	N11-N12	1.526
N6-O2	1.200			N6'-O2'	1.190		
Bond angle (º)							
N1-N2-N3	112.8	N4-N5-N6	107.2	N1'-N2'-N3'	112.3	N4'-N5'-N6'	106.1
N2-N3-N4	104.9	N5-N6-O1	113.2	N2'-N3'-N4'	105.2	N5'-N6'-O1'	113.7
N3-N4-C1	108.7	N5-N6-O2	114.1	N3'-N4'-C1'	108.4	N5'-N6'-O2'	112.1
N4-C1-N1	108.8	N7-C3-C2	118.4	N4'-C1'-N1'	109.1	N7'-C2'-C3'	120.8
N4-C1-N7	117.1	C3-C2-N5	121.0	N4'-C1'-N7'	119.0	C2'-C3'-N5'	122.6
C1-N7-N8	118.4	C3-C2-N9	118.7	C1'-N7'-N8'	114.3	C3'-C2'-N9	117.5
C1-N7-C3	116.8	C2-C3-N11	118.7	C1'-N7'-C2	112.2	C2'-C3'-N11	119.7
N7-N8-O3	114.4	C2-N9-N10	118.6	N7'-N8'-O3'	115.6	C2'-N9-N10	122.0
N7-N8-O4	114.8	C3-N11-N12	110.8	N7'-N8'-O4'	113.4	C3'-N11-N12	111.3
C1-N4-N5	125.0	N9-N10-O5	114.2	C1'-N4'-N5'	128.0	N9-N10-O6	114.9
N4-N5-C2	108.0	N11-N12-O7	115.3	N4'-N5'-C3	110.3	N11-N12-O8	114.3
Dihedral angle (º)							
N1-N2-N3-N4	-1.49	C1-N7-C3-C2	15.11	N1'-N2'-N3'-N4'	-2.12	C1'-N7'-C2'-C3'	29.52
C1-N4-N3-N2	1.13	N4-N5-C2-C3	-38.16	C1'-N4'-N3'-N2'	1.23	N4'-N5'-C3'-C2'	-6.12
N5-N4-C1-N7	-7.23	N7-C3-C2-N5	15.54	N5'-N4'-C1'-N7'	-1.53	N7'-C2'-C3'-N5'	-16.45
C1-N7-N8-O3	5.06	N9-C2-C3-N11	17.97	C1'-N7'-N8'-O3'	28.19	N9-C2'-C3'-N11	-16.68
C3-N7-N8-O4	-16.14	C2-N9-N10-O5	33.93	C2'-N7'-N8'-O4'	-25.41	C2'-N9-N10-O6	40.47
N4-N5-N6-O1	-34.54	C3-N11-N12-O7	27.97	N4'-N5'-N6'-O1'	22.08	C3'-N11-N12-O8	-30.49
C2-N5-N6-O2	31.14			C3'-N5'-N6'-O2'	85.19		

SI 2 NBO charges

SI 2 NBO charges of atoms for four title compounds

Compound **(1)**		Compound **(2)**		Compound **(3)**				Compound **(4)**			
Atom	Charge	Atom	Charge	Atom	Charge	Atom	Charge	Atom	Charge	Atom	Charge
C1	0.53	C1	0.53	C1	0.52	C1'	0.52	C1	0.51	C1'	0.50
N1	-0.30	N1	-0.32	N1	-0.28	N1'	-0.25	N1	-0.27	N1'	-0.25
N2	-0.03	N2	-0.02	N2	-0.02	N2'	-0.03	N2	-0.02	N2'	-0.03
N3	-0.03	N3	-0.02	N3	-0.03	N3'	-0.01	N3	-0.01	N3'	-0.02
N4	-0.10	N4	-0.10	N4	-0.09	N4'	-0.09	N4	-0.08	N4'	-0.08
N5	-0.16	N5	-0.24	N5	-0.19	N5'	-0.20	N5	-0.20	N5'	-0.20
N6	0.62	N6	0.64	N6	0.61	N6'	0.62	N6	0.63	N6'	0.64
N7	-0.32	N7	-0.39	N7	-0.38	N7'	-0.37	N7	-0.34	N7'	-0.36
N8	0.64	N8	0.65	N8	0.62	N8'	0.63	N8	0.67	N8'	0.66
C2	-0.21	C2	0.60	O1	-0.25	O1'	-0.27	C2	0.28	C3'	0.26
C3	-0.20	C3	0.61	O2	-0.24	O2'	-0.27	C3	0.30	C2'	0.31
O1	-0.32	O1	-0.28	O3	-0.22	O3'	-0.28	O1	-0.29	O1'	-0.28
O2	-0.36	O2	-0.25	O4	-0.27	O4'	-0.34	O2	-0.29	O2'	-0.24
O3	-0.32	O3	-0.26	C2	0.28	C3	0.30	O3	-0.30	O3'	-0.28
O4	-0.39	O4	-0.26					O4	-0.31	O4'	-0.35
H2a	0.23	O5	-0.43					N9	-0.29	N11	-0.36
H2b	0.25	O6	-0.48					N10	0.67	N12	0.65
H3a	0.24							O5	-0.29	O7	-0.31
H3b	0.22							O6	-0.29	O8	-0.34

SI 3 IR spectrum analysis of four title compounds

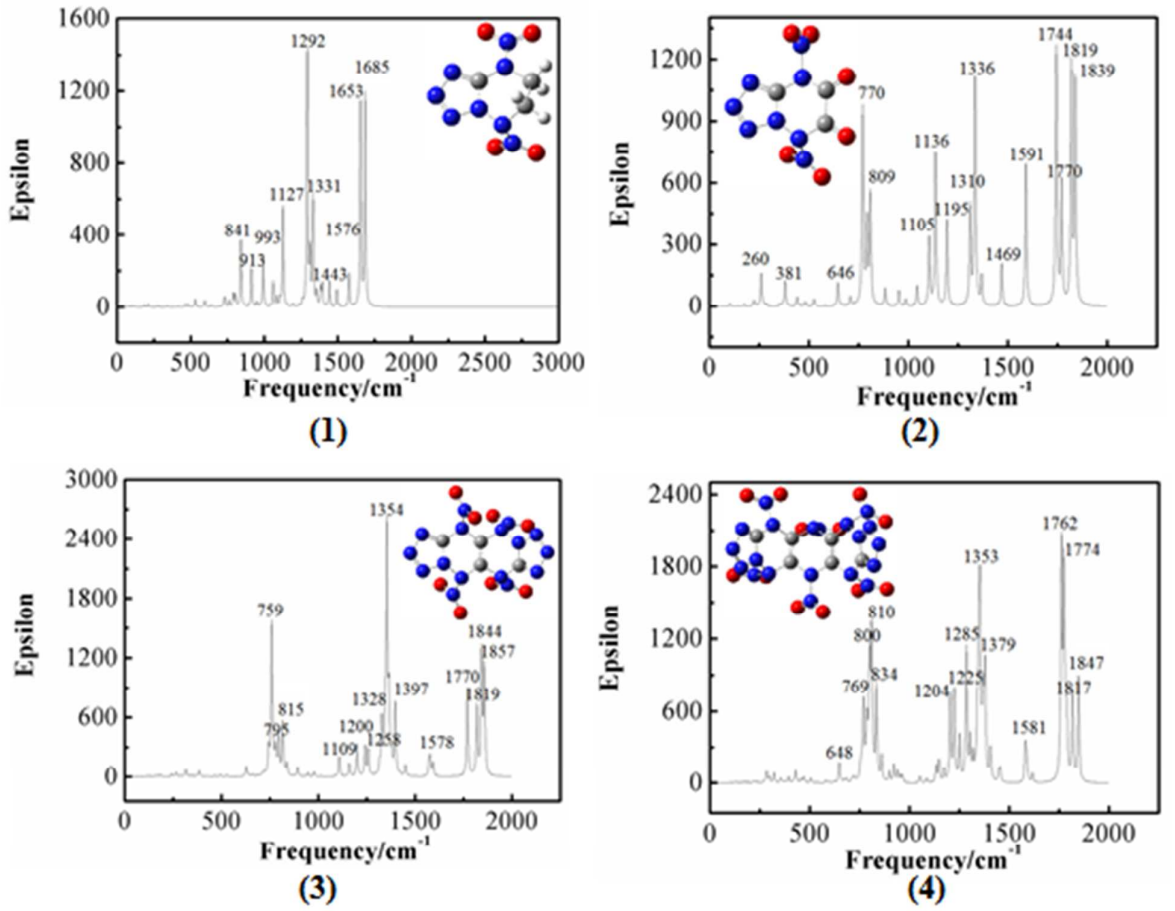

Fig. 6 Calculated IR spectrum of four title compounds

The results show that the strong IR peaks at 1685 cm^{-1} and 1653 cm^{-1} of the compound **(1)** correspond to the asymmetrical stretching modes of the nitro groups. And the stretching vibrations on CN bonds and NN bonds of the tetrazole and trizaine ring are expected in the region 1576 cm^{-1}, 1443 cm^{-1} and 1127 cm^{-1}, 993 cm^{-1}. Again the peaks at 1331 cm^{-1} and 1292 cm^{-1} refer to symmetrical stretching, while the weak peaks at 841 cm^{-1} is belonging to the scissor vibration mode of nitro groups.

As for the compound **(2)**, there are two stronger peaks at 1839 cm^{-1} and 1819 cm^{-1} are assigned to symmetrical stretching of C=O bonds in the triazine ring, while the weaker one at 1591 cm^{-1} and 1469 cm^{-1} are stretching vibration on CN and NN of tetrazoles skeleton. And the corresponding symmetrical and asymmetrical stretching modes on CC, CN and NN bonds of the triazine are expressed in the region 1195 cm^{-1}, 1136 cm^{-1} and 1105 cm^{-1}. Meanwhile, the nitro groups were observed three vibration modes along with

characteristic peaks in the IR spectrum at 1770 cm^{-1}, 1744 cm^{-1} and 1336 cm^{-1}, 1310 cm^{-1} as well as 809 cm^{-1}, 770 cm^{-1}, refer to the asymmetrical and symmetrical stretching and the torsion modes as well. While the weakest one at 646 cm^{-1}, 381 cm^{-1} and 260 cm^{-1} belong to the vibration modes out-of-plane deforming of the rings and nitro groups.

With regard to the compound **(3)**, the strongest peaks at 1354 cm^{-1} is mainly dominated by the symmetrical stretching on nitro groups and the region in 1857 cm^{-1}, 1844 cm^{-1}, 1819 cm^{-1} and 1770 cm^{-1} are belonging to asymmetrical stretching vibration. While the peak at 1578 cm^{-1} and 1397 cm^{-1} correspond to the symmetrical stretching and torsion modes on C=C bond, and the region in 1328 cm^{-1}, 1258 cm^{-1}, 1200 cm^{-1} and 1109 cm^{-1} are vibration nodes on CN and NN bonds of rings. And the nitro groups have additional peaks at 815 cm^{-1}, 795 cm^{-1} and 759 cm^{-1} refer to the torsion modes on N=O bond.

It is similar that the nitro groups of compound **(4)** possess three vibration modes along with the characteristic peaks in the IR spectrum at 1847 cm^{-1}, 1817 cm^{-1}, 1774 cm^{-1}, 1762 cm^{-1} and 1379 cm^{-1}, 1353 cm^{-1} as well as 834 cm^{-1}, 810 cm^{-1}, 800 cm^{-1}, 769 cm^{-1} refer to the asymmetrical and symmetrical stretching and the torsion vibration modes, respectively. And the region in 1285 cm^{-1}, 1225 cm^{-1} and 1204 cm^{-1} as middle peaks are belonging to the symmetrical and asymmetrical stretching modes on CN and NN bonds of rings, and the weakest one at 1581 cm^{-1} refers to the symmetrical stretching on C=C bonds of the central ring. There are similar peaks at 648 cm^{-1}, which is belonging to the vibration modes out-of-plane deforming of the rings and nitro groups as well. It's worth being noticed that the IR spectrum variances of vibrations on nitro groups in different positions can be observed in four title compounds.