Extensive Theoretical Studies on Two New members of the FOX-7 family: 5-(dinitromethylene)-1,4-dinitramino-Tetrazole and 1,1'-dinitro-4,4'-diamino-5,5'-Bitetrazole as Energetic Compounds

Piao He[a], Jian-Guo Zhang**[a], Kun Wang[a,b], Xin Yin[a], Xin Jin[a], Tong-Lai Zhang[a]

Supporting Information

SI 1 Table 1 Selected parameters of the optimized geometry for DNAT and DNABT

DNAT						DNABT					
Bond lengths	Å	Bond angles	(º)	Dihedral angle	(º)	Bond lengths	Å	Bond angles	(º)	Dihedral angle	(º)
N1-N2	1.384	N1-N2-N3	108.8	N1-N2-N3-N4	123.1	N1-N2	1.437	N1-N2-N3	108.1	N1-N2-N3-N4	0.947
N2-N3	1.245	N2-N3-N4	108.2	N1-C5-N4-N3	0.700	N2-N3	1.251	N2-N3-N4	111.5	N1-C5-N4-N3	-1.000
N3-N4	1.391	N3-N4-C5	110.8	N4-N1-C5-C6	0.169	N3-N4	1.356	N3-N4-C5	109.7	N4-N1-C5-C5'	-167.2
N4-C5	1.374	N4-C5-N1	101.3	C5-C6-N5-N6	-179.2	N4-C5	1.404	N4-C5-N1	102.9	N4'-N1'-C5'-C5	167.2
C5-N1	1.376	N1-C5-C6	131.5	O1-O2-N5-C6	-179.9	C5-N1	1.409	C5-N1-N2	107.6	N2-N1-N5-C5	-124.8
C5-C6	1.381	C5-C6-N5	123.3	C5-C6-N6-O3	137.1	C5-C5'	1.355	N1-C5-C5'	127.7	C5-N1-N5-O1	-14.9
C6-N5	1.426	C6-N5-O1	116.6	N2-N1-C5-N7	-166.7	N1-N5	1.492	C5-N1-N5	118.7	N2-N1-N5-O2	45.1
N1-N7	1.357	O1-N5-O2	124.1	N2-N1-N7-N8	95.2	N5-O1	1.213	N1-N5-O1	115.0	O1-O2-N5-N1	174.3
N7-N8	1.488	C5-N1-N7	130.6	N7-N8-O5-O6	-175.8	N5-O2	1.201	O1-N5-O2	129.3	N3-N4-N6-C5	157.6
N5-O1	1.215	N1-N7-N8	112.5	N3-N4-C5-N9	-164.5	N4-N6	1.383	C5-N4-N6	125.0	C5-N4-N6-H2	128.5
N8-O5	1.205	N7-N8-O5	116.5	N3-N4-N9-N10	63.2	N6-H1	1.016	N4-N6-H1	110.5	N3-N4-N6-H1	48.9
N7-H1	1.027	O5-N8-O6	130.2	N9-N10-O7-O8	175.9	N6-H2	1.014	H1-N6-H2	111.1	H1-H2-N6-N4	122.5

SI 2 Table 2 NBO charges of partial atoms for DNAT and DNABT

DNAT				DNABT			
Atom	Charge	Atom	Charge	Atom	Charge	Atom	Charge
N1	-0.094	N10	0.616	N1	-0.192	N1'	-0.192
N2	0.050	O1	-0.318	N2	-0.039	N2'	-0.039
N3	0.011	O2	-0.468	N3	0.009	N3'	0.009
N4	-0.104	O3	-0.312	N4	-0.108	N4'	-0.108
C5	0.421	O4	-0.378	C5	0.259	C5'	0.259
C6	0.071	O5	-0.340	N5	0.619	N5'	0.619
N5	0.468	O6	-0.316	N6	-0.613	N6'	-0.613
N6	0.477	O7	-0.329	O1	-0.370	O1'	-0.370
N7	-0.294	O8	-0.320	O2	-0.311	O2'	-0.311
N8	0.606	H1	0.434	H1	0.367	H1'	0.367
N9	-0.296	H2	0.418	H2	0.379	H2'	0.379

* The type of article: Research paper

Corresponding authors: Jian-Guo Zhang, Tel & Fax: +86 10 68918091.
E-mail: zjgbit@bit.edu.cn