Supporting Information

Synthesis and characteristics of novel energetic salts based on bis(*N*-dinitroethyl)aminofurazan

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X-ray crystallography: Crystals of **7** was removed from the flask and covered with a layer of hydrocarbon oil. A suitable crystal was then selected, attached to a glass fiber, and placed in the low-temperature nitrogen stream. Data for **7** was collected at 153(2) K using a Rigaku Saturn724 CCD (AFC10/Saturn724+ for 7) diffractometer equipped with a graphite-monochromatized MoKα radiation (λ = 0.71073 Å) using omega scans. Data collection and reduction were performed and the unit cell was initially refined by using CrystalClear -SM Expert 2.0 r2[i] software. The reflection data were also corrected for Lp factors. The structure was solved by direct methods and refined by the least squares method on F2 using the SHELXTL-97 system of programs.[ii] Structure was solved in the space group *P*ī by analysis of systematic absences. In this all-light-atom structure the value of the Flack parameter did not allow the direction of polar axis to be determined and Friedel reflections were then merged for the final refinement. Band angles and dihedral angles of the data collection and refinement are given in Table S1.

Table S1. Band angles and dihedral angles for the structure of **7**.

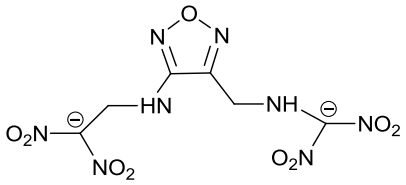
N1—O1—N2	110.24(18)	C2—N3—H3N	109.6(17)
H0A—O10—H0B	108.5	C3—N3—H3N	127.4(17)
N1—C1—N6	124.7(2)	O3—N4—O2	120.17(19)
N1—C1—C2	109.7(2)	O3—N4—C4	122.9(2)
N6—C1—C2	125.6(2)	O2—N4—C4	116.94(19)
N2—C2—N3	125.6(2)	O4—N5—O5	120.12(19)
N2—C2—C1	109.1(2)	O4—N5—C4	124.51(19)
N3—C2—C1	125.3(2)	O5—N5—C4	115.37(19)
N3—C3—C4	113.38(19)	C1—N6—C5	122.9(2)
N3—C3—H3A	108.9	C1—N6—H6N	114.1(18)
C4—C3—H3A	108.9	C5—N6—H6N	122.9(18)
N3—C3—H3B	108.9	O7—N7—O6	120.47(19)
C4—C3—H3B	108.9	O7—N7—C6	124.09(19)
H3A—C3—H3B	107.7	O6—N7—C6	115.44(19)
N5—C4—N4	120.8(2)	O8—N8—O9	119.44(18)
N5—C4—C3	118.5(2)	O8—N8—C6	123.04(19)
N4—C4—C3	120.7(2)	O9—N8—C6	117.52(19)
N6—C5—C6	114.64(19)	C7—N9—H9A	117(2)
N6—C5—H5A	108.6	C7—N9—H9B	123(2)
C6—C5—H5A	108.6	H9A—N9—H9B	120(3)
N6—C5—H5B	108.6	C7—N10—H10A	119(3)
C6—C5—H5B	108.6	C7—N10—H10B	117(2)
H5A—C5—H5B	107.6	H10A—N10—H10B	124(3)
N8—C6—N7	120.8(2)	C7—N11—H11A	117(2)
N8—C6—C5	120.9(2)	C7—N11—H11B	121(2)
N7—C6—C5	118.18(19)	H11A—N11—H11B	121(3)

N10—C7—N11	120.4(2)	C8—N12—H12A	123.9(19)
N10—C7—N9	119.3(2)	C8—N12—H12B	118(2)
N11—C7—N9	120.3(2)	H12A—N12—H12B	117(3)
N13—C8—N14	119.9(2)	C8—N13—H13A	116(2)
N13—C8—N12	120.1(2)	C8—N13—H13B	117(2)
N14—C8—N12	120.0(2)	H13A—N13—H13B	127(3)
C1—N1—O1	105.2(2)	C8—N14—H14A	119(3)
C2—N2—O1	105.7(2)	C8—N14—H14B	121(3)
N4—N5—N6—C3	−0.26(16)	N5—N6—C3—N3	0.17(16)
C2—N3—C3	122.6(2)	H14A—N14—H14B	119(4)
N1—C1—C2—N2	−0.8(3)	C3—C4—N4—O3	177.1(2)
N6—C1—C2—N2	179.6(2)	N5—C4—N4—O2	178.2(2)
N1—C1—C2—N3	−180.0(2)	C3—C4—N4—O2	−2.9(3)
N6—C1—C2—N3	0.4(4)	N4—C4—N5—O4	0.1(3)
N3—C3—C4—N5	−69.8(3)	C3—C4—N5—O4	−178.9(2)
N3—C3—C4—N4	111.3(2)	N4—C4—N5—O5	180.0(2)
N6—C5—C6—N8	−116.7(2)	C3—C4—N5—O5	1.0(3)
N6—C5—C6—N7	66.0(3)	N1—C1—N6—C5	2.3(4)
N6—C1—N1—O1	−179.5(2)	C2—C1—N6—C5	−178.1(2)
C2—C1—N1—O1	0.9(3)	C6—C5—N6—C1	63.2(3)
N2—O1—N1—C1	−0.7(3)	N8—C6—N7—O7	1.6(3)
N3—C2—N2—O1	179.5(2)	C5—C6—N7—O7	178.9(2)
C1—C2—N2—O1	0.3(3)	N8—C6—N7—O6	−178.3(2)
N1—O1—N2—C2	0.3(3)	C5—C6—N7—O6	−1.0(3)
N2—C2—N3—C3	1.6(4)	N7—C6—N8—O8	0.2(3)
C1—C2—N3—C3	−179.3(2)	C5—C6—N8—O8	−177.0(2)
C4—C3—N3—C2	117.4(2)	N7—C6—N8—O9	179.9(2)
N5—C4—N4—O3	−1.8(3)	C5—C6—N8—O9	2.7(3)

Theoretical study: Calculations were carried out by using the Gaussian 03 (Revision E.01) suite of programs. [1] The geometric optimization of the structures and frequency analyses were carried out by using the B3LYP functional with the 6-31+G** basis set, [2] and single-point energies were calculated at the MP2(full)/6-311++G** level. All of the optimized structures were characterized to be true local energy minima on the potential-energy surface without imaginary frequencies.

Geometry coordinates

The optimized structure of the following structure



O	0.464221	3.185415	-0.737204
C	-0.549862	1.332506	-0.288509
C	0.837945	1.254948	0.159481
N	-0.747043	2.503006	-0.844319
N	1.436427	2.384874	-0.129323
N	-1.534395	0.395313	-0.080408
H	-1.249128	-0.573743	-0.189649
N	1.399163	0.221910	0.858024
H	1.031121	-0.709752	0.708329
C	-2.853271	0.632659	-0.698472
H	-2.775387	0.525099	-1.791224
H	-3.145616	1.655767	-0.475291
C	2.808513	0.223106	1.266262
H	2.845409	-0.231780	2.265196
H	3.142831	1.254917	1.346872
C	-3.919968	-0.281068	-0.175367
C	3.758980	-0.501191	0.347045
N	-4.992444	0.237713	0.555627
O	-5.047587	1.496841	0.685783
O	-5.859346	-0.499349	1.072173
N	-3.833958	-1.630906	-0.497903
O	-2.748167	-1.978987	-1.068279
O	-4.740427	-2.460144	-0.282414
N	4.948112	0.120534	-0.049523
O	5.703606	-0.378473	-0.909011
O	5.227682	1.222879	0.508109
N	3.533042	-1.850607	0.113637
O	2.470947	-2.323263	0.643124
O	4.303374	-2.584810	-0.538225

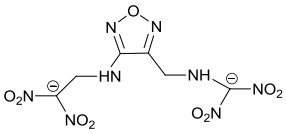
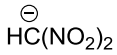
O	-0.768830	-0.794977	-0.032344

C	-0.012025	1.097718	-0.106360
C	1.225138	0.292063	-0.015933
H	0.133000	2.443525	0.226355
H	2.530927	0.662188	0.101932
N	-1.279744	0.368556	0.061439
N	0.738035	-1.094925	0.033449

$HC(NO_2)_2^{\ominus}$

C	-6.568211	0.113431	0.245351
N	-5.759917	1.225093	0.122244
O	-6.351687	2.339781	0.277897
O	-4.536838	1.159207	-0.123328
N	-6.177358	-1.204282	0.122242
O	-7.107273	-2.057497	0.277908
O	-5.002440	-1.550446	-0.123330
H	-7.605684	0.291699	0.457303

Table S2. Ab Initio computional data (B3LYP/6-31+G(d,p)/MP2(full)/6-311++G**)

	E_0	ZPE	H_T	HOF ^{Exp}	HOF ^{Calcd}
	-1344.192081	0.177415	0.021583	-	-122.3
	-448.1640811	0.039725	0.00688	-	-222.8
	-261.5324597	0.045703	0.004418	196[a]	-
CH_4	-40.39849	0.044791	0.003812	-74.6[b]	-
CH_3CH_3	-79.6068548	0.074609	0.00443	-84.68[c]	-
CH_3NH_2	-95.6318759	0.064032	0.004369	-23.0[b]	-
NH_3	-56.43462	0.034377	0.003818	-45.9[b]	-

[a] Struct Chem. **2011**, 22, 149-159 [b]Eur. J. Inorg. Chem. **2008**, 2560-2568; [c]Data calculated with the G2 method by using the Gaussian 03 program. 32, 317-322

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(1) Gaussian 03, Revision E.01, M. J.Frisch, G. W.Trucks, H. B.Schlegel, G. E.Scuseria, M. A.Robb, J. R.Cheeseman, J. A.Montgomery, J. T.Vreven, K. N.Kudin, J. C.Burant, J. M.Millam, S. S.Iyengar, J.Tomasi, V.Barone, B.Mennucci, M.Cossi, G.Scalmani, N.Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K .Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G .Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, J. A. Pople, Gaussian, Inc., Wallingford CT, **2004**.

(2) R. G. Parr, W. Yang, *Density Functional Theory of Atoms and Molecules*, Oxford University Press, New York, **1989**.

[i] CrystalClear: SM Expert 2.0 r2, An Integrated Program for the Collection and Processing of Area Detector Data, Rigaku Corporation, 2009.

[ii] G. M. Sheldrick, SHELXTL-97, Structure Determination Software Suite. Bruker AXS, Madison WI, 2008.