The New Role of 1,1-Diamino-2,2-dinitroethylene (FOX-7): Two Unexpected Reactions

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Supporting materials

Crystal data and structure refinement details

Empirical formula	$C_3H_5N_5O_2$
Formula weight	143.12
Crystal system	*Monoclinic*
Space group	$P_{2(1)/n}$
a (Å)	3.8235(16)
b (Å)	16.595(7)
c (Å)	9.641(4)
β (deg)	99.676(7)
V (Å^3)	603.0(4)
Z	4
F(000)	296
D_{calcd} (g cm^{-3})	1.576
μ (mm^{-1})	0.133
Data/Restraints/Parameters	1078 / 0 / 92
GOF on F^2	0.960
R_1 [$I > 2\sigma(I)$]	0.0493
wR_2 [$I > 2\sigma(I)$]	0.1166
R_1 (all data)	0.0687
wR_2 (all data)	0.1283

Bond length /Å

C1-N2	1.3987	C7-N11	1.4228	C17-N18	1.4245
C1-O3	1.2341	N8-O9	1.295	C17-N21	1.4272
C1-N24	1.4065	N8-O10	1.258	N18-O19	1.2984
N2-N4	1.3874	N11-O12	1.2992	N18-O20	1.2568
N4-C5	1.3681	N11-O13	1.2581	N21-O22	1.2586
C5-N6	1.3392	C15-N14	1.3677	N21-O23	1.2956
C5-C7	1.4312	C15-N16	1.341		
C7-N8	1.4279	C15-C17	1.4303		

Bond angles /(°)

N2-C1-O3	123.5876	C15-C17-N21	121.1504
N2-C1-N24	112.8698	N18-C17-N21	117.0155
O3-C1-N24	123.4915	C17-N18-O19	117.8534
C1-N2-N4	119.7488	C17-N18-O20	120.721
N2-N4-C5	121.6047	O19-N18-O20	121.3893
N4-C5-N6	117.9629	C17-N21-O22	120.3892
N4-C5-C7	119.9054	C17-N21-O23	118.0773
N6-C5-C7	122.1242	O22-N21-O23	121.4833
C5-C7-N8	121.1242	C1-N24-N14	118.2614
C5-C7-N11	121.9461	C7-N11-O13	120.6613
N8-C7-N11	116.9296	O12-N11-O13	121.2597
C7-N8-O9	117.9884	C15-N14-N24	120.6665
C7-N8-O10	120.3535	N14-C15-N16	117.4998
O9-N8-O10	121.6179	N14-C15-C17	120.357
C7-N11-O12	118.0276	N16-C15-C17	122.1333
C15-C17-N18	121.8339		

Mulliken atomic charges /e

C1	0.5123	O9	-0.1172	C17	0.2604
N2	-0.0721	O10	0.1158	N18	-0.4700
O3	-0.4109	N11	-0.4610	O19	-0.0946
N4	-0.0504	O12	-0.0970	O20	0.1385
C5	0.7581	O13	0.1334	N21	-0.4434
N6	0.0516	N14	-0.0383	O22	0.1132
C7	0.1377	C15	0.6476	O23	-0.1139
N8	-0.4222	N16	0.0397	N24	-0.1173

Determination results of energy of combustion

sample	no.	m / g	ΔT / K	$-\Delta_c U$ / J • g^{-1}
MNTzA	1	0.2364	0.2794	12352
	2	0.2309	0.2780	12590
	3	0.2358	0.2796	12397
	4	0.2368	0.2785	12295
	5	0.2358	0.2774	12291
	6	0.2363	0.2795	12367
	mean		**mean**	**12382±45**
BADCh	1	0.20271	0.1622	8116
	2	0.20576	0.1648	8133
	3	0.20559	0.1639	8092
	4	0.20552	0.1638	8089
	5	0.20566	0.1642	8105
	6	0.20495	0.1640	8123
	mean		**mean**	**8110 ±7**

Note: m is mass of sample; ΔT is temperature rise; $\Delta_c U$ is energy of combustion.