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Supporting Information

Energetic 1,5-Diamino-4*H*-tetrazolium Nitro-substituted Azolates

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Geometry Coordinates and Natural charge:

B3LYP/6-31+G(d,p) optimized geometries (Å)

5-Nitrotetrazolate anion

Atom	No	Natural Charge	Coordinates (Angstroms) X	Y	Z
N	1	-0.32350	-0.811497	-1.122530	0.000211
N	2	-0.32351	-0.811508	1.122513	-0.000140
N	3	-0.15640	-2.061212	-0.674370	0.000061
N	4	-0.15629	-2.061082	0.674391	-0.000150
C	5	0.32904	-0.075742	-0.000235	0.000083
N	6	0.45633	1.359581	0.000034	0.000034
O	7	-0.41278	1.946985	1.091610	0.000177
O	8	-0.41290	1.947324	-1.091468	-0.000252

3,5-Dinitrotriazolate anion

Atom	No	Natural Charge	Coordinates (Angstroms) X	Y	Z
C	1	0.37569	1.014001	-0.158541	0.000004
C	2	0.37566	-1.014100	-0.158583	-0.000012
N	3	-0.29413	0.668431	-1.467147	0.000049
N	4	-0.29409	-0.668445	-1.467216	0.000038
N	5	-0.47599	-0.000002	0.712916	0.000036
N	6	0.45629	2.398265	0.262528	-0.000023
O	7	-0.39933	2.637916	1.475518	-0.000244
O	8	-0.40050	3.270872	-0.614473	0.000160
O	9	-0.39935	-2.637819	1.475557	0.000273
N	10	0.45626	-2.398225	0.262533	-0.000020
O	11	-0.40053	-3.270914	-0.614422	-0.000252

2,4,5-Trinitroimidazolate anion

Atom	No	Natural Charge	Coordinates (Angstroms) X	Y	Z
C	1	0.40870	-1.440642	-0.000025	0.000210
C	2	0.21299	0.513840	-0.708232	0.000387
C	3	0.21295	0.513815	0.708253	-0.000246
N	4	-0.44773	-0.747597	1.151300	-0.006944
N	5	-0.44775	-0.747545	-1.151339	0.007155
N	6	0.46984	1.622199	-1.630214	0.107485
N	7	0.46983	1.622101	1.630302	-0.107527
N	8	0.45456	-2.891114	-0.000073	0.000003
O	9	-0.38024	1.508233	2.741356	0.414849
O	10	-0.39042	2.615299	1.248830	-0.737691
O	11	-0.39037	2.615148	-1.249004	0.738178
O	12	-0.38022	1.508630	-2.740963	-0.415603
O	13	-0.39607	-3.469144	-1.091279	0.051209
O	14	-0.39607	-3.469214	1.091085	-0.051355

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	8830(1)	2068(1)	4304(1)	31(1)
N(2)	9316(1)	2213(1)	3754(1)	38(1)
N(3)	9351(1)	3360(1)	3638(1)	39(1)
N(4)	8908(1)	3976(1)	4107(1)	32(1)
C(5)	8577(1)	3171(1)	4528(1)	28(1)
N(6)	8635(1)	947(1)	4593(1)	39(1)
N(7)	8106(1)	3375(1)	5046(1)	36(1)
N(8)	11675(1)	1534(1)	6111(1)	32(1)
N(9)	12152(1)	1999(1)	6596(1)	33(1)
N(10)	12068(1)	3213(1)	6615(1)	35(1)
N(11)	11527(1)	3575(1)	6142(1)	33(1)
C(12)	11313(1)	2527(1)	5855(1)	28(1)
N(13)	10735(1)	2509(1)	5305(1)	35(1)
O(14)	10413(1)	3490(1)	5140(1)	53(1)
O(15)	10609(1)	1523(1)	5037(1)	47(1)
N(1B)	8858(1)	1626(1)	6798(1)	31(1)
N(2B)	9354(1)	1489(1)	6253(1)	39(1)
N(3B)	9355(1)	351(1)	6110(1)	41(1)
N(4B)	8876(1)	-266(1)	6560(1)	35(1)
C(5B)	8559(1)	523(1)	6994(1)	29(1)
N(6B)	8696(1)	2732(1)	7113(1)	37(1)
N(7B)	8059(1)	318(1)	7495(1)	36(1)
N(8B)	8488(1)	5176(1)	6388(1)	35(1)
N(9B)	8014(1)	5546(1)	5880(1)	37(1)
N(10B)	7950(1)	6762(1)	5878(1)	37(1)
N(11B)	8381(1)	7223(1)	6386(1)	34(1)
C(12B)	8690(1)	6226(1)	6675(1)	29(1)
N(13B)	9209(1)	6297(1)	7255(1)	36(1)
O(14B)	9446(1)	5333(1)	7505(1)	53(1)
O(15B)	9379(1)	7336(1)	7456(1)	44(1)

Table 3. Bond lengths [Å] and angles [°] for **2**.

N(1)-C(5)	1.3385(15)	N(1)-N(2)	1.3706(16)
N(1)-N(6)	1.3864(15)	N(2)-N(3)	1.2668(16)
N(3)-N(4)	1.3614(15)	N(4)-C(5)	1.3340(16)
N(4)-H(4)	0.8700	C(5)-N(7)	1.3127(17)
N(6)-H(6A)	0.899(15)	N(6)-H(6B)	0.914(14)
N(7)-H(7A)	0.908(14)	N(7)-H(7B)	0.912(13)
N(8)-C(12)	1.3210(16)	N(8)-N(9)	1.3411(15)
N(9)-N(10)	1.3212(15)	N(10)-N(11)	1.3414(15)
N(11)-C(12)	1.3219(16)	C(12)-N(13)	1.4444(16)
N(13)-O(15)	1.2197(15)	N(13)-O(14)	1.2201(15)
N(1B)-C(5B)	1.3408(16)	N(1B)-N(2B)	1.3711(16)
N(1B)-N(6B)	1.3873(15)	N(2B)-N(3B)	1.2671(16)
N(3B)-N(4B)	1.3623(16)	N(4B)-C(5B)	1.3341(16)
N(4B)-H(4B)	0.8700	C(5B)-N(7B)	1.3105(17)
N(6B)-H(6AB)	0.908(14)	N(6B)-H(6BB)	0.905(14)
N(7B)-H(7AB)	0.898(14)	N(7B)-H(7BB)	0.871(14)
N(8B)-C(12B)	1.3202(16)	N(8B)-N(9B)	1.3403(15)
N(9B)-N(10B)	1.3197(16)	N(10B)-N(11B)	1.3404(16)
N(11B)-C(12B)	1.3223(17)	C(12B)-N(13B)	1.4443(17)
N(13B)-O(14B)	1.2200(15)	N(13B)-O(15B)	1.2275(15)
C(5)-N(1)-N(2)	110.10(10)	C(5)-N(1)-N(6)	124.69(11)
N(2)-N(1)-N(6)	125.21(10)	N(3)-N(2)-N(1)	107.15(10)
N(2)-N(3)-N(4)	108.76(11)	C(5)-N(4)-N(3)	109.76(10)
C(5)-N(4)-H(4)	125.1	N(3)-N(4)-H(4)	125.1
N(7)-C(5)-N(4)	129.46(11)	N(7)-C(5)-N(1)	126.32(11)
N(4)-C(5)-N(1)	104.22(11)	N(1)-N(6)-H(6A)	109.3(12)
N(1)-N(6)-H(6B)	108.5(12)	H(6A)-N(6)-H(6B)	109.8(17)
C(5)-N(7)-H(7A)	116.9(11)	C(5)-N(7)-H(7B)	119.3(10)
H(7A)-N(7)-H(7B)	123.7(15)	C(12)-N(8)-N(9)	102.90(10)
N(10)-N(9)-N(8)	110.08(10)	N(9)-N(10)-N(11)	109.17(10)
C(12)-N(11)-N(10)	103.40(10)	N(8)-C(12)-N(11)	114.45(11)
N(8)-C(12)-N(13)	124.24(11)	N(11)-C(12)-N(13)	121.31(11)
O(15)-N(13)-O(14)	124.74(12)	O(15)-N(13)-C(12)	118.09(11)
O(14)-N(13)-C(12)	117.17(11)	C(5B)-N(1B)-N(2B)	110.04(10)
C(5B)-N(1B)-N(6B)	124.37(11)	N(2B)-N(1B)-N(6B)	125.59(10)
N(3B)-N(2B)-N(1B)	107.46(11)	N(2B)-N(3B)-N(4B)	108.34(11)
C(5B)-N(4B)-N(3B)	110.19(10)	C(5B)-N(4B)-H(4B)	124.9
N(3B)-N(4B)-H(4B)	124.9	N(7B)-C(5B)-N(4B)	129.82(12)
N(7B)-C(5B)-N(1B)	126.20(11)	N(4B)-C(5B)-N(1B)	103.96(11)
N(1B)-N(6B)-H(6AB)	109.3(10)	N(1B)-N(6B)-H(6BB)	105.2(12)
H(6AB)-N(6B)-H(6BB)	109.1(15)	C(5B)-N(7B)-H(7AB)	118.4(11)
C(5B)-N(7B)-H(7BB)	118.7(11)	H(7AB)-N(7B)-H(7BB)	
	122.5(15)		

Table 3. Continued

C(12B)-N(8B)-N(9B)	103.02(10)	N(10B)-N(9B)-N(8B) 109.84(10)
N(9B)-N(10B)-N(11B)	109.51(10)	C(12B)-N(11B)-N(10B)
	103.15(10)	
N(8B)-C(12B)-N(11B)	114.49(11)	N(8B)-C(12B)-N(13B)
	123.48(11)	
N(11B)-C(12B)-N(13B)	122.03(11)	O(14B)-N(13B)-O(15B)
	125.15(12)	
O(14B)-N(13B)-C(12B)	118.16(11)	O(15B)-N(13B)-C(12B)
	116.69(11)	

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	40(1)	20(1)	33(1)	0(1)	-2(1)	3(1)
N(2)	43(1)	33(1)	39(1)	0(1)	5(1)	6(1)
N(3)	42(1)	34(1)	41(1)	3(1)	7(1)	4(1)
N(4)	38(1)	21(1)	36(1)	1(1)	2(1)	1(1)
C(5)	33(1)	19(1)	30(1)	0(1)	-6(1)	0(1)
N(6)	56(1)	18(1)	42(1)	2(1)	-3(1)	0(1)
N(7)	52(1)	22(1)	34(1)	-2(1)	6(1)	-2(1)
N(8)	39(1)	23(1)	34(1)	-2(1)	-2(1)	2(1)
N(9)	40(1)	25(1)	36(1)	-2(1)	-3(1)	4(1)
N(10)	42(1)	25(1)	38(1)	-3(1)	-5(1)	1(1)
N(11)	40(1)	22(1)	36(1)	0(1)	-2(1)	1(1)
C(12)	33(1)	21(1)	31(1)	0(1)	2(1)	0(1)
N(13)	41(1)	28(1)	37(1)	2(1)	-3(1)	0(1)
O(14)	64(1)	36(1)	58(1)	6(1)	-20(1)	10(1)
O(15)	62(1)	35(1)	44(1)	-7(1)	-13(1)	-3(1)
N(1B)	42(1)	20(1)	31(1)	2(1)	-1(1)	0(1)
N(2B)	50(1)	32(1)	35(1)	2(1)	4(1)	0(1)
N(3B)	53(1)	32(1)	38(1)	-3(1)	5(1)	0(1)
N(4B)	48(1)	22(1)	36(1)	-2(1)	0(1)	0(1)
C(5B)	37(1)	19(1)	31(1)	1(1)	-8(1)	1(1)
N(6B)	53(1)	19(1)	39(1)	-1(1)	-4(1)	2(1)
N(7B)	51(1)	22(1)	36(1)	2(1)	4(1)	-1(1)
N(8B)	45(1)	23(1)	37(1)	1(1)	-3(1)	0(1)
N(9B)	47(1)	24(1)	38(1)	-1(1)	-7(1)	0(1)
N(10B)	46(1)	25(1)	40(1)	0(1)	-8(1)	1(1)
N(11B)	40(1)	24(1)	38(1)	-2(1)	-1(1)	0(1)
C(12B)	34(1)	22(1)	32(1)	0(1)	3(1)	-2(1)
N(13B)	39(1)	33(1)	34(1)	-1(1)	1(1)	-3(1)
O(14B)	68(1)	42(1)	48(1)	10(1)	-18(1)	1(1)
O(15B)	49(1)	42(1)	42(1)	-12(1)	-1(1)	-7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **2**.

	x	y	z	U(eq)
H(4)	8849	4774	4129	38
H(6A)	8449(12)	412(16)	4292(8)	60(5)
H(6B)	9134(10)	651(17)	4783(8)	58(5)
H(7A)	7887(11)	2702(15)	5251(8)	51(5)
H(7B)	8022(10)	4167(13)	5182(7)	42(4)
H(4B)	8789	-1060	6563	42
H(6AB)	8576(10)	3328(14)	6819(7)	44(4)
H(6BB)	9203(10)	2920(17)	7317(8)	54(5)
H(7AB)	7892(10)	965(14)	7736(7)	44(4)
H(7BB)	7957(11)	-443(13)	7609(8)	45(4)

Table 6. Torsion angles [°] for **2**.

C(5)-N(1)-N(2)-N(3)	-0.89(15)
N(6)-N(1)-N(2)-N(3)	179.86(12)
N(1)-N(2)-N(3)-N(4)	0.90(15)
N(2)-N(3)-N(4)-C(5)	-0.63(15)
N(3)-N(4)-C(5)-N(7)	-179.67(13)
N(3)-N(4)-C(5)-N(1)	0.06(14)
N(2)-N(1)-C(5)-N(7)	-179.77(12)
N(6)-N(1)-C(5)-N(7)	-0.5(2)
N(2)-N(1)-C(5)-N(4)	0.49(14)
N(6)-N(1)-C(5)-N(4)	179.74(11)
C(12)-N(8)-N(9)-N(10)	-0.16(14)
N(8)-N(9)-N(10)-N(11)	0.22(14)
N(9)-N(10)-N(11)-C(12)	-0.18(14)
N(9)-N(8)-C(12)-N(11)	0.04(15)
N(9)-N(8)-C(12)-N(13)	179.47(11)
N(10)-N(11)-C(12)-N(8)	0.09(15)
N(10)-N(11)-C(12)-N(13)	-179.36(11)
N(8)-C(12)-N(13)-O(15)	-4.11(19)
N(11)-C(12)-N(13)-O(15)	175.28(12)
N(8)-C(12)-N(13)-O(14)	176.35(13)
N(11)-C(12)-N(13)-O(14)	-4.25(18)
C(5B)-N(1B)-N(2B)-N(3B)	0.78(15)
N(6B)-N(1B)-N(2B)-N(3B)	179.78(12)
N(1B)-N(2B)-N(3B)-N(4B)	-0.81(15)
N(2B)-N(3B)-N(4B)-C(5B)	0.60(15)
N(3B)-N(4B)-C(5B)-N(7B)	178.69(13)
N(3B)-N(4B)-C(5B)-N(1B)	-0.10(14)
N(2B)-N(1B)-C(5B)-N(7B)	-179.25(12)
N(6B)-N(1B)-C(5B)-N(7B)	1.7(2)
N(2B)-N(1B)-C(5B)-N(4B)	-0.39(14)
N(6B)-N(1B)-C(5B)-N(4B)	-179.41(11)
C(12B)-N(8B)-N(9B)-N(10B)	0.11(14)
N(8B)-N(9B)-N(10B)-N(11B)	-0.03(15)
N(9B)-N(10B)-N(11B)-C(12B)	-0.06(14)
N(9B)-N(8B)-C(12B)-N(11B)	-0.16(15)
N(9B)-N(8B)-C(12B)-N(13B)	-179.78(11)
N(10B)-N(11B)-C(12B)-N(8B)	0.14(15)
N(10B)-N(11B)-C(12B)-N(13B)	179.77(11)
N(8B)-C(12B)-N(13B)-O(14B)	-2.74(19)
N(11B)-C(12B)-N(13B)-O(14B)	177.66(13)
N(8B)-C(12B)-N(13B)-O(15B)	176.94(12)
N(11B)-C(12B)-N(13B)-O(15B)	-2.65(18)

Table 7. Hydrogen bonds for **2** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(4)-H(4)...N(11)#1	0.87	1.96	2.7814(15)	157.1
N(6)-H(6A)...N(8)#2	0.899(15)	2.275(16)	3.0949(16)	151.6(16)
N(6)-H(6B)...O(15)#2	0.914(14)	2.414(18)	3.0109(15)	123.0(15)
N(7)-H(7A)...N(10B)#3	0.908(14)	2.089(15)	2.9397(16)	155.4(16)
N(7)-H(7B)...N(9B)	0.912(13)	2.083(14)	2.9248(16)	153.0(14)
N(4B)-H(4B)...N(11B)#4	0.87	1.99	2.8435(16)	165.3
N(6B)-H(6AB)...N(8B)	0.908(14)	2.197(14)	3.0622(16)	159.2(14)
N(6B)-H(6BB)...O(15B)#5	0.905(14)	2.300(15)	3.0970(16)	146.8(16)
N(7B)-H(7AB)...N(9)#6	0.898(14)	2.110(14)	2.9651(16)	158.8(15)
N(7B)-H(7BB)...N(10)#5	0.871(14)	2.174(15)	2.9417(16)	146.8(15)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+1,-z+1 #2 -x+2,-y,-z+1 #3 -x+3/2,y-1/2,z
#4 x,y-1,z #5 -x+2,y-1/2,-z+3/2 #6 x-1/2,y,-z+3/2