Comprehensive Structural Insights into Nitro-Substituted Azines as Potential Antioxidant Additives for Biodiesel

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Supplementary Information

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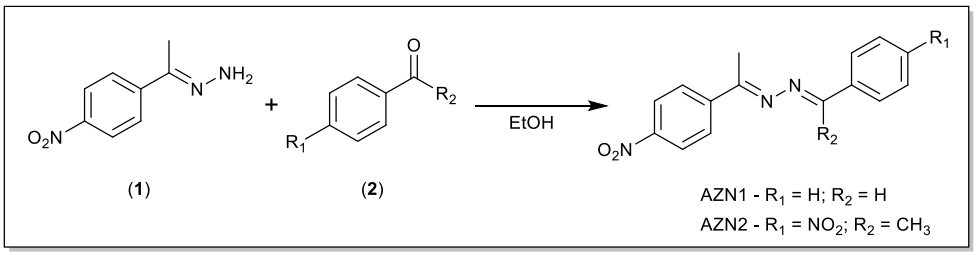
1. Synthesis and Characterization

1.1. Regents and equipment

All reagents were purchased from Sigma-Aldrich, Darmstadt, Germany. All reagents and solvents utilized in the experiments were of analytical grade and were employed without additional purification. The ^{1}H NMR and ^{13}C NMR spectra were recorded in chloroform on a 600 MHz Bruker NMR spectrometer, with TMS utilized as reference.

1.2. Procedure for the synthesis

The azine (1E,2E)-1-benzylidene-2-[1-(4-nitrophenyl)ethylidene]hydrazine (AZN1) was synthesized by the reaction of (E)-1-(1-(4-nitrophenyl) ethylidene) hydrazine (**1**) with benzaldehyde (**2**) in ethanol according to Figueredo and co-workers.[1] The synthetic pathways adopted to prepare the azine (1E,2E)-bis[1-(4-nitrophenyl)ethylidene]hydrazine (AZN2) was via the reaction of an equimolar amount (E)-1-(1-(4-nitrophenyl) ethylidene) hydrazine (**1**) and 4-nitroacetophenone (**2**), as depicted in Scheme S1. The reactions were carried out in a round-bottom flask containing 30 mL of ethanol. The reaction mixture was subjected to reflux for a period of 1 hour, during which it was continuously stirred using a magnetic stirrer. The product was filtered and subsequently air-dried. The resulting residue was then purified by recrystallization in ethanol to yield the pure product. The products were recrystallized in ethanol.



Scheme S1. The synthesis of AZN1 and AZN2 compounds.

1.3. Spectroscopic characterization

AZN1: $C_{15}H_{13}N_3O_2$ (267.28 g/mol); yield 68% obtained as yellow crystals; m.p. 147 °C; ^{1}H NMR (600 MHz, CDCl3) δ 8.46 (s, 1H), 8.31 (d, J = 8.9 Hz, 2H), 8.11 (d, J = 8.8 Hz, 2H), 7.89 (dd, J = 7.4, 2.2 Hz, 2H), 7.57 – 7.40 (m, 3H), 2.58 (s, 3H) (Figure S1). ^{13}C NMR (151 MHz, CDCl3) δ 162.38, 159.08, 148.65, 144.12, 134.28, 131.30,

128.85, 128.55, 127.73, 123.62, 15.32 (Figure S2). ^{1}H-^{15}N HSQC plot (Figure S3); ^{1}H-^{13}C HMBC plot (Figure S4); ^{1}H-^{1}H COSY plot (Figure S5).

AZN2: $C_{16}H_{14}N_{34}O_4$ (326.2 g/mol); yield 92% obtained as orange crystals; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.32 (d, J = 8.9 Hz, 1H), 8.18 (d, J = 8.9 Hz, 1H), 2.32 (s, 2H) (Figure S6). ^{13}C NMR (151 MHz, $CDCl_3$) δ 156.53, 148.58, 143.80, 128.37, 124.15, 15.55 (Figure S7). ^{1}H-^{15}N HSQC plot (Figure S8); ^{1}H-^{13}C HMBC plot (Figure S9); ^{1}H-^{1}H COSY plot (Figure S10).

1.4. Supplementary spectroscopic characterization

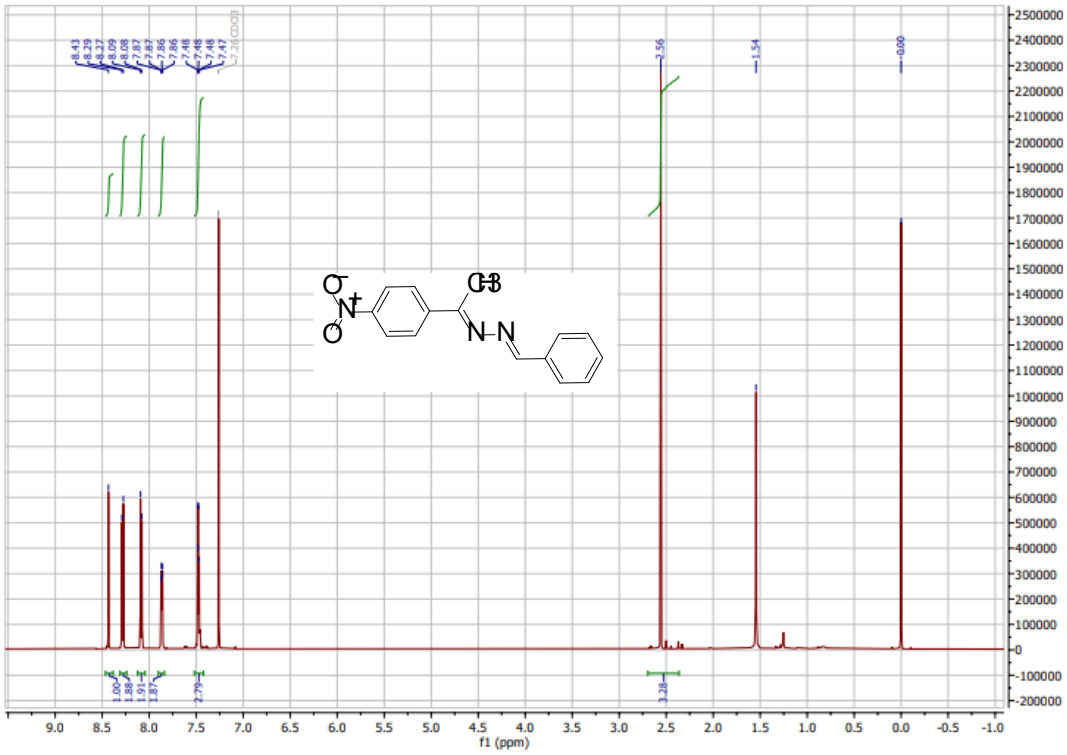


Figure S1. ^{1}H NMR spectrum of AZN1.

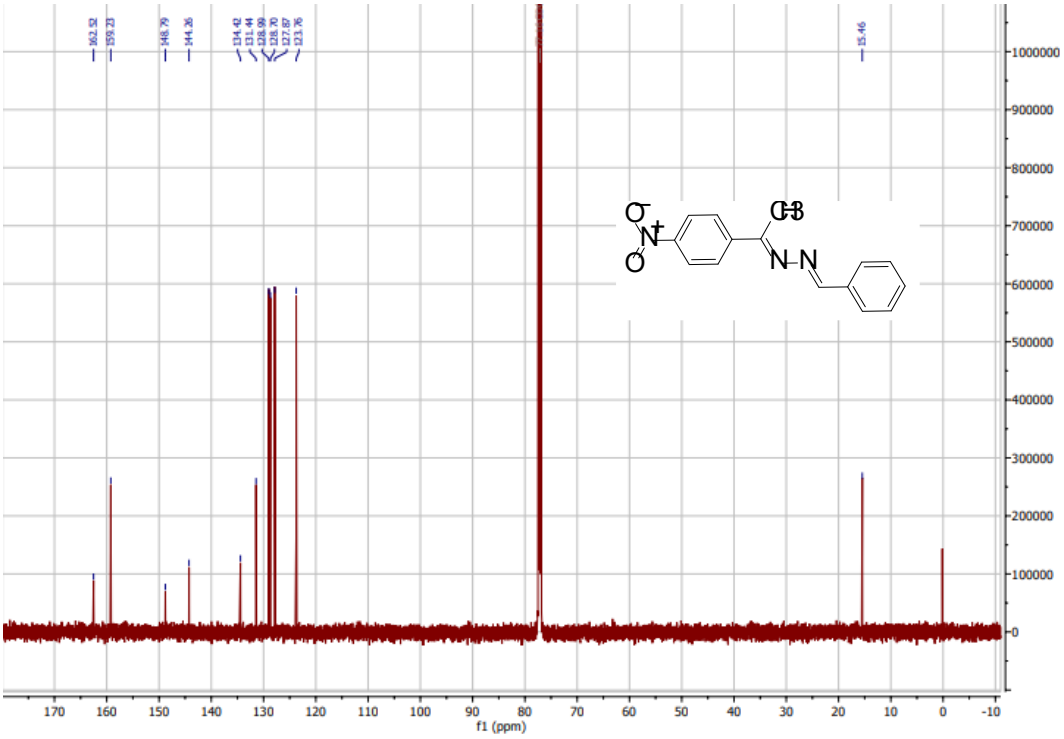


Figure S2. ^{13}C NMR spectrum of AZN1.

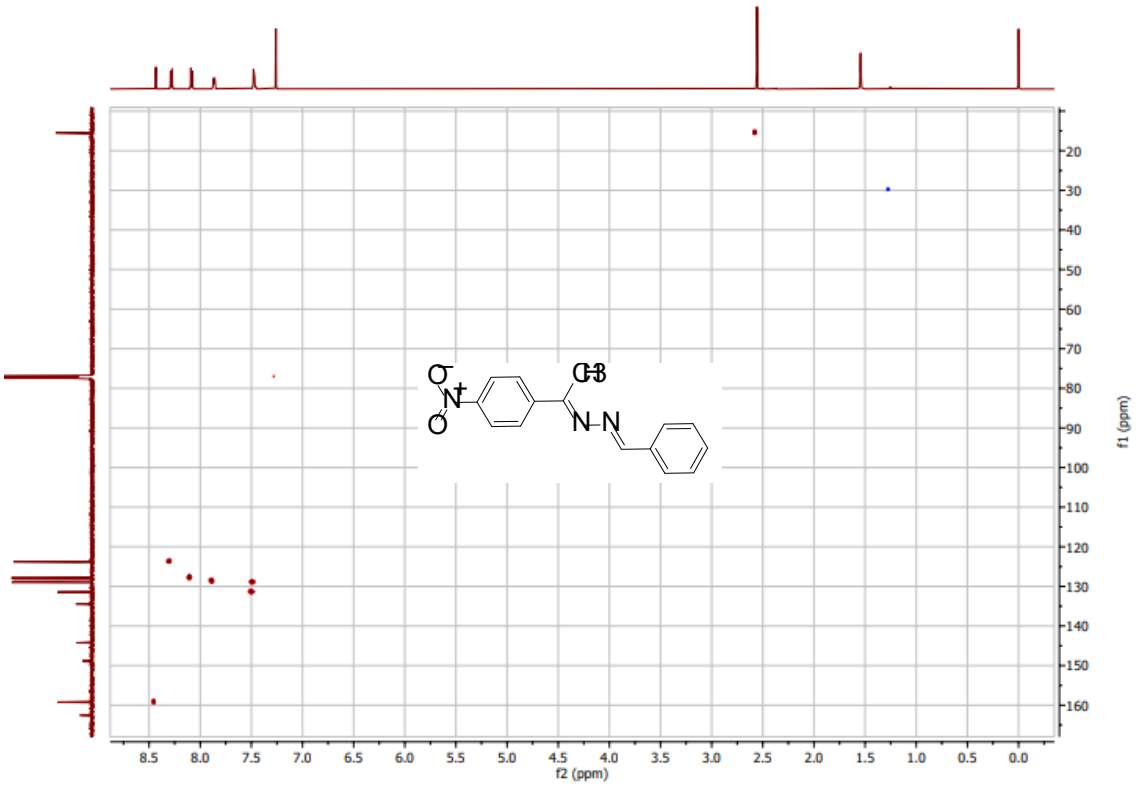


Figure S3. HSQC plot of AZN1.

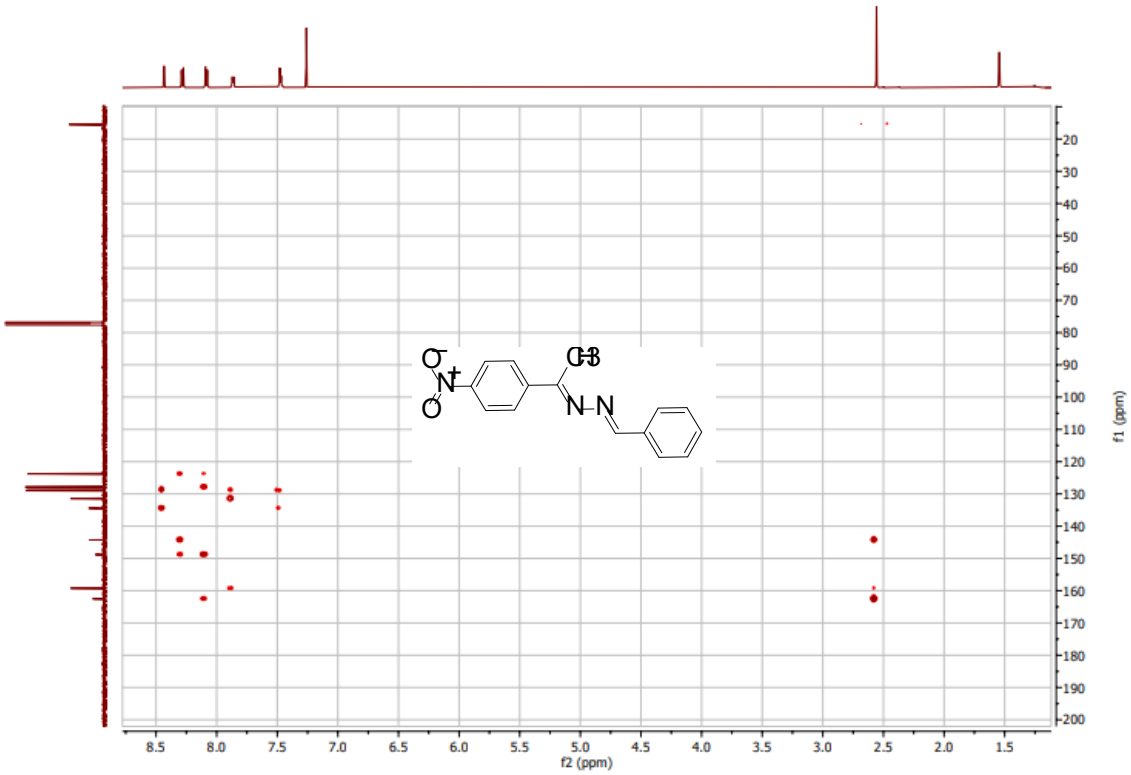


Figure S4. HMBC plot of AZN1.

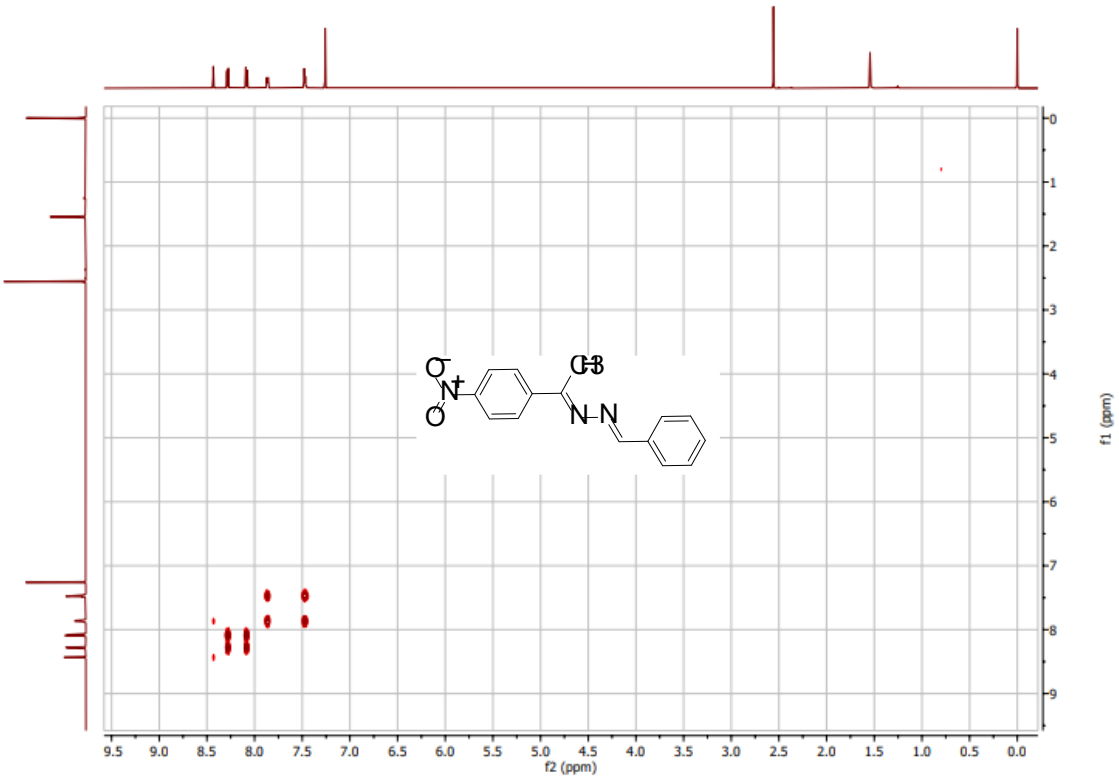


Figure S5. COSY plot of AZN1.

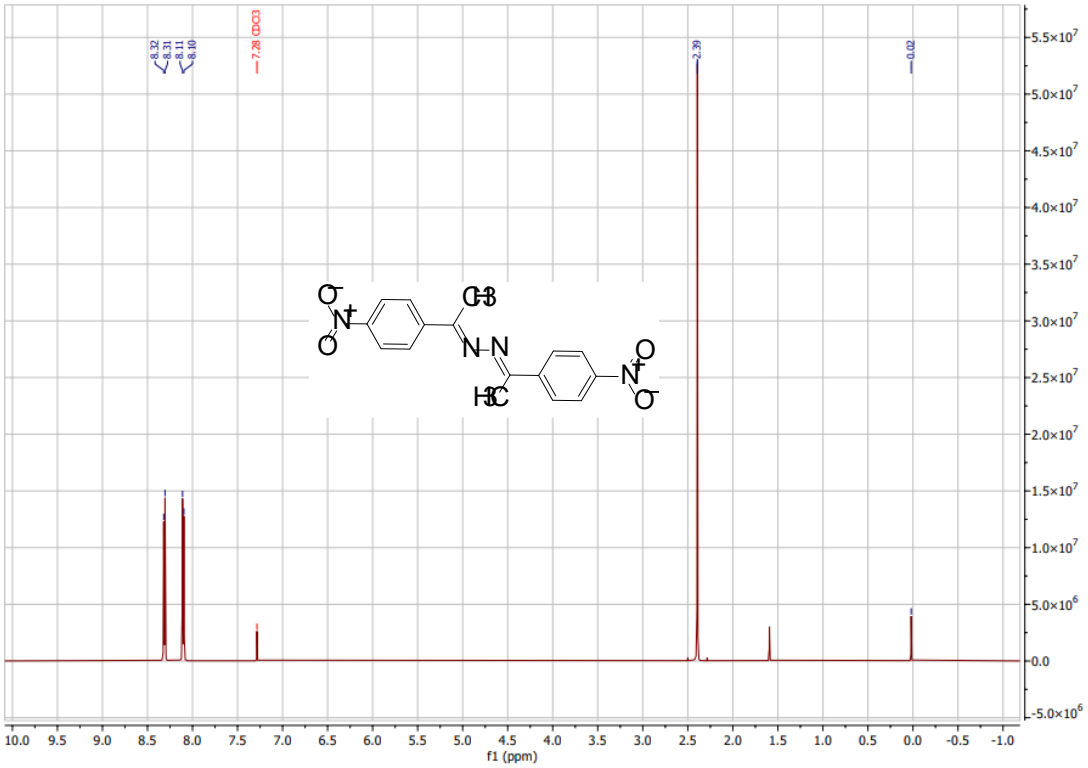


Figure S6. ^{1}H NMR spectrum of AZN2.

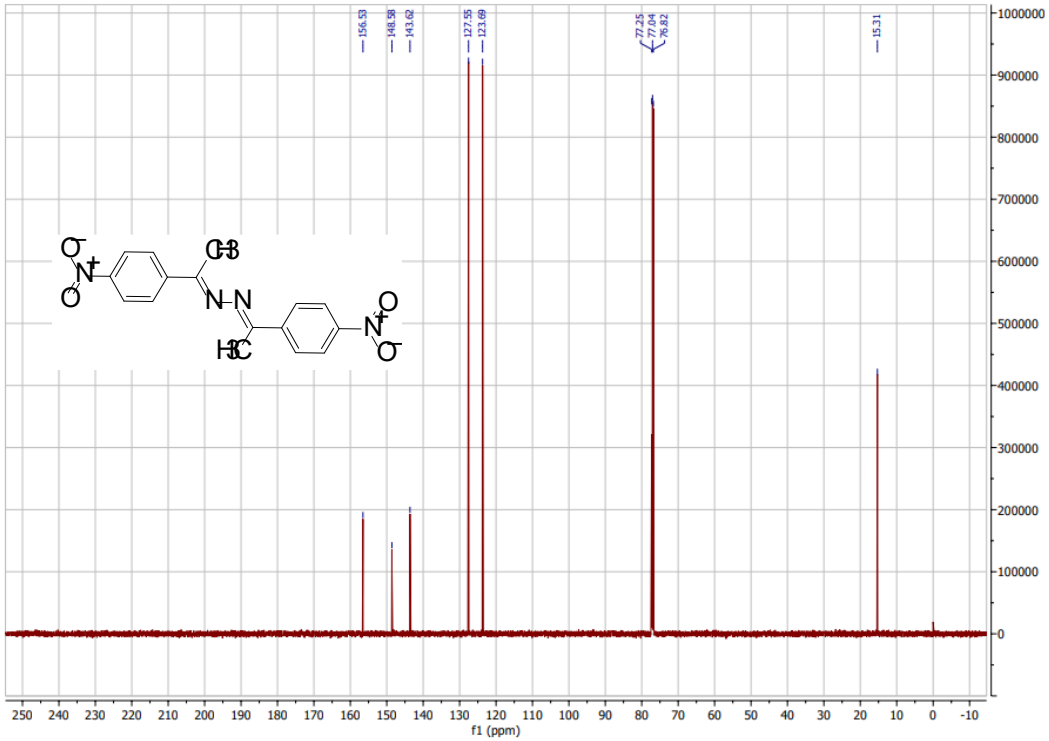


Figure S7. ^{13}C NMR spectrum of AZN2.

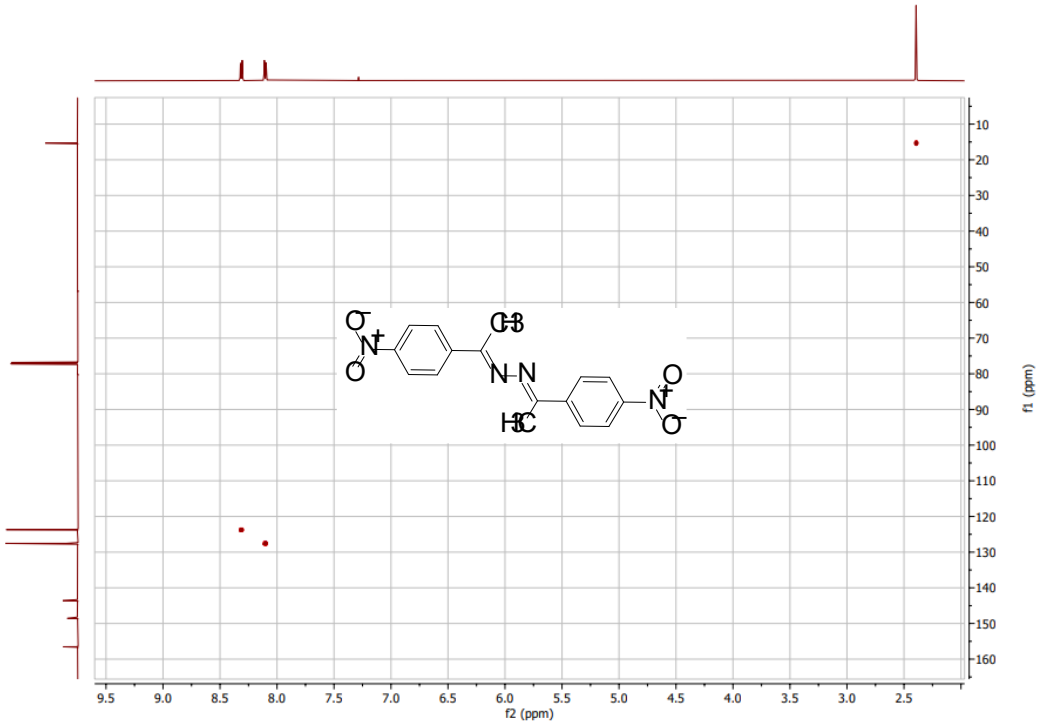


Figure S8. HSQC plot of AZN2.

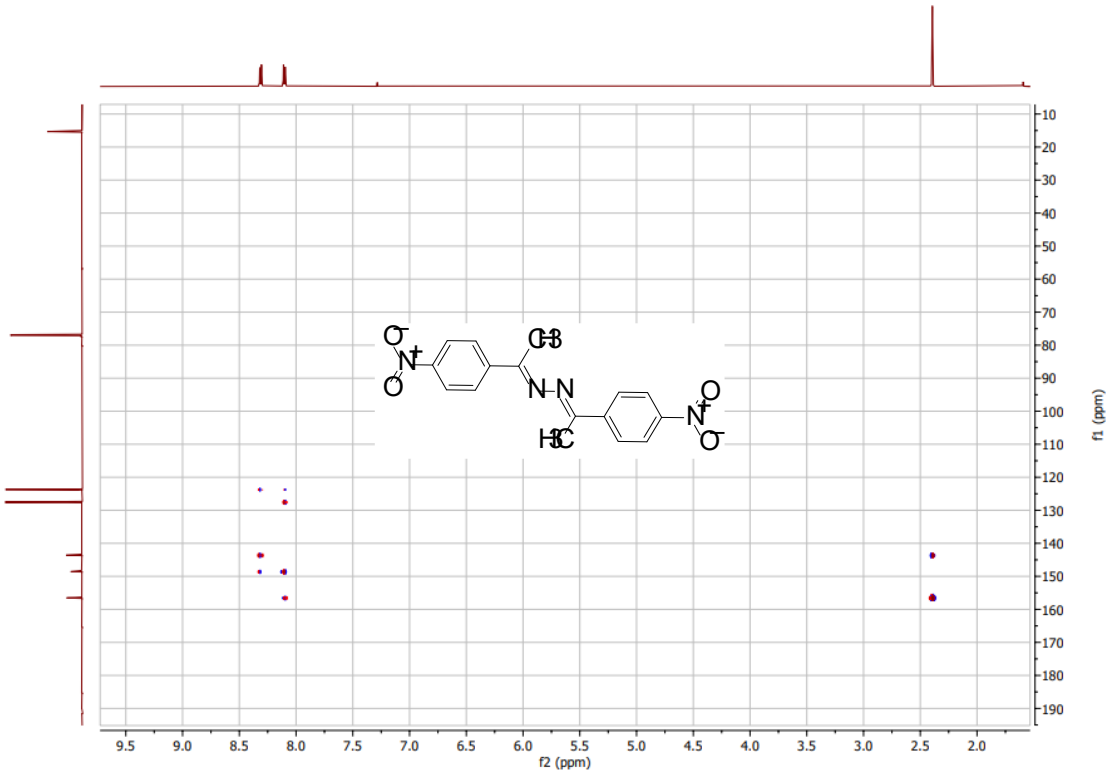


Figure S9. HMBC plot of AZN2.

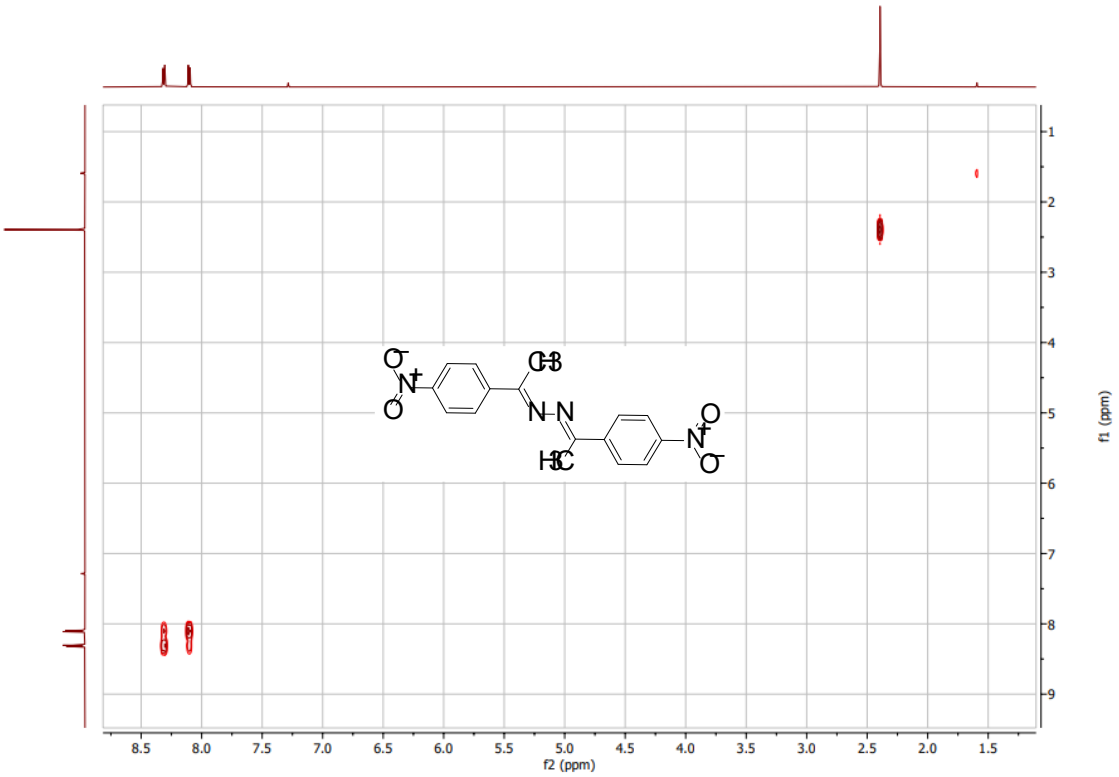
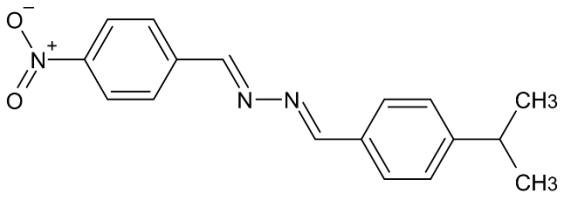
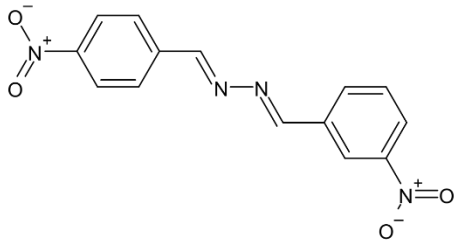


Figure S10. COSY plot of AZN2.

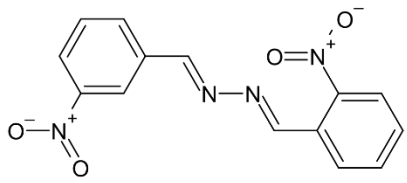
2. Comparison figures



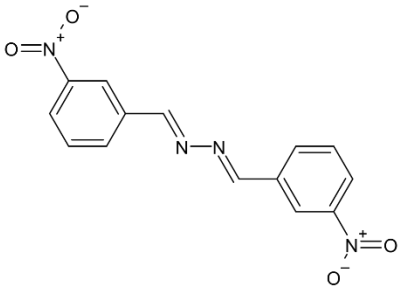
(1E,2E)-1-[(4-nitrophenyl)methylidene]-2-{[4-(propan-2-yl)phenyl]methylidene}hydrazine (AZN3)



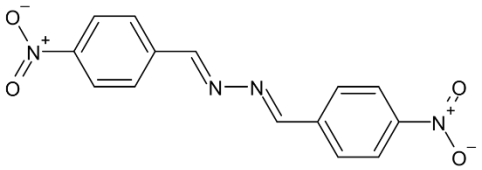
(1E,2E)-1-[(3-nitrophenyl)methylidene]-2-[(4-nitrophenyl)methylidene]hydrazine (AZN4)



(1E,2E)-1-[(2-nitrophenyl)methylidene]-2-[(3-nitrophenyl)methylidene]hydrazine (AZN5)



(1E,2E)-bis[(3-nitrophenyl)methylidene]hydrazine (AZN6)



(1E,2E)-bis[(4-nitrophenyl)methylidene]hydrazine (AZN7)

Figure S11. Nitro-substituted Azines (AZNs 3 to 7).

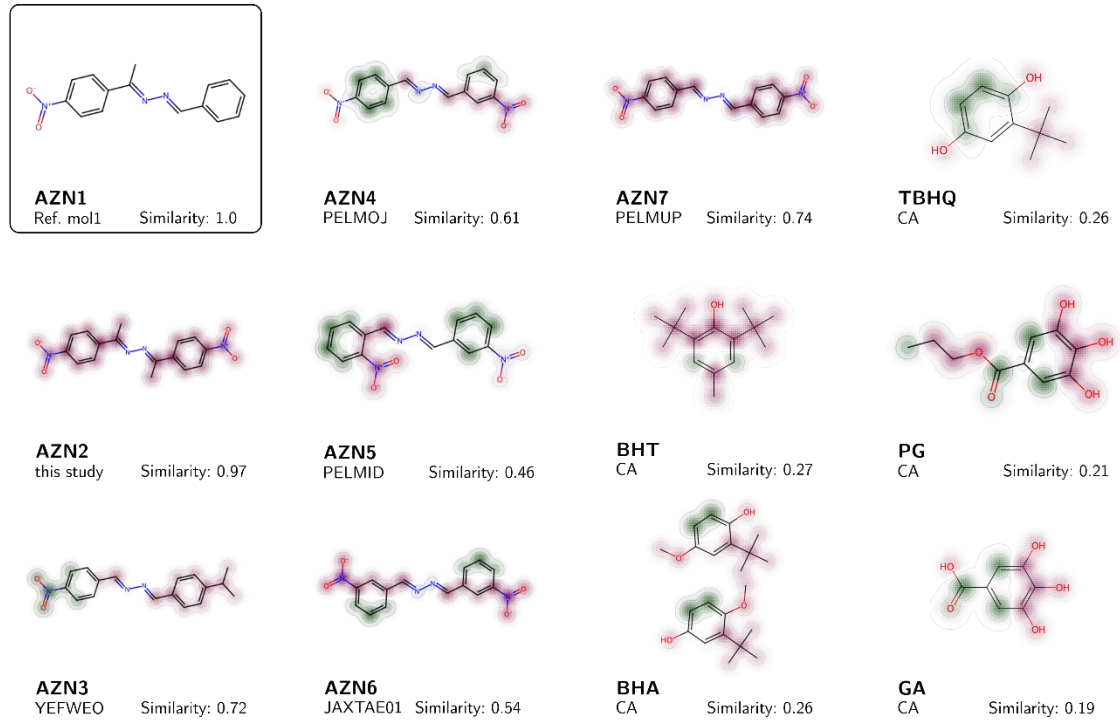


Figure S12. The maps of molecular similarity obtained by using the Tanimoto index comparing nitro-substituted azines (AZNs 3 to 7) and commercial additives (CA) to (a) AZN1 and (b) AZN2 as reference molecules.

3. Supplementary crystallographic tables

Table S1. Final Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for AZN1 at 120(2) K. U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{IJ} tensor.

Atom	x	y	z	U(eq)
O1	1.16580(9)	1.12616(10)	0.16764(9)	0.02776(18)
O2	1.09543(10)	1.31327(10)	0.14584(9)	0.02952(18)
N1	1.06927(9)	1.18240(10)	0.16841(9)	0.02037(17)
N2	0.35374(9)	0.84256(9)	0.26106(8)	0.01976(16)
N3	0.22303(9)	0.76914(9)	0.31321(8)	0.02137(17)
C1	0.91690(9)	1.09084(9)	0.20220(8)	0.01698(15)
C2	0.91562(9)	0.97860(9)	0.27136(8)	0.01823(16)
C3	0.77784(9)	0.89980(9)	0.31321(8)	0.01794(16)
C4	0.64181(9)	0.93073(9)	0.28322(8)	0.01584(15)
C5	0.64485(9)	1.04116(9)	0.20818(8)	0.01783(16)
C6	0.78321(9)	1.12350(9)	0.16875(8)	0.01861(16)
C7	0.49638(9)	0.84754(9)	0.32967(8)	0.01699(15)
C8	0.51905(9)	0.77092(9)	0.44634(8)	0.02216(17)
C9	0.06259(9)	0.67688(9)	0.19983(8)	0.01832(16)
C10	-0.09278(9)	0.59046(9)	0.23126(8)	0.01637(15)
C11	-0.07117(9)	0.60184(9)	0.38541(8)	0.01756(15)
C12	-0.22065(9)	0.51693(9)	0.41110(8)	0.01918(16)
C13	-0.39353(9)	0.42029(9)	0.28400(8)	0.01966(16)
C14	-0.41609(9)	0.40916(9)	0.13107(8)	0.02047(16)
C15	-0.26622(9)	0.49375(9)	0.10442(8)	0.01949(16)

Table S2. Anisotropic displacement parameters ($Å^2$) for AZN1 at 120(2) K. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka^*b^*U_{12}]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	0.0186(3)	0.0351(4)	0.0290(3)	0.0140(3)	0.0122(3)	0.0141(3)
O2	0.0271(3)	0.0298(3)	0.0315(4)	0.0210(3)	0.0145(3)	0.0112(3)
N1	0.0160(3)	0.0227(3)	0.0158(3)	0.0083(3)	0.0056(3)	0.0071(3)
N2	0.0169(3)	0.0231(3)	0.0198(3)	0.0099(3)	0.0098(3)	0.0106(3)
N3	0.0173(3)	0.0251(3)	0.0210(3)	0.0102(3)	0.0108(3)	0.0102(3)
C1	0.0152(3)	0.0171(3)	0.0155(3)	0.0068(3)	0.0067(3)	0.0072(3)
C2	0.0167(3)	0.0186(3)	0.0198(4)	0.0087(3)	0.0077(3)	0.0106(3)
C3	0.0183(3)	0.0177(3)	0.0204(4)	0.0103(3)	0.0091(3)	0.0109(3)
C4	0.0160(3)	0.0146(3)	0.0154(3)	0.0063(3)	0.0066(3)	0.0082(3)
C5	0.0174(3)	0.0181(3)	0.0188(3)	0.0090(3)	0.0071(3)	0.0108(3)
C6	0.0190(3)	0.0185(3)	0.0185(3)	0.0103(3)	0.0077(3)	0.0100(3)
C7	0.0176(3)	0.0156(3)	0.0165(3)	0.0063(3)	0.0078(3)	0.0088(3)
C8	0.0234(4)	0.0249(4)	0.0259(4)	0.0166(3)	0.0142(3)	0.0144(3)
C9	0.0190(4)	0.0203(3)	0.0188(4)	0.0100(3)	0.0090(3)	0.0123(3)
C10	0.0165(3)	0.0162(3)	0.0174(3)	0.0076(3)	0.0070(3)	0.0101(3)
C11	0.0152(3)	0.0176(3)	0.0171(3)	0.0073(3)	0.0052(3)	0.0085(3)
C12	0.0186(4)	0.0198(3)	0.0186(4)	0.0095(3)	0.0082(3)	0.0100(3)
C13	0.0163(3)	0.0173(3)	0.0241(4)	0.0095(3)	0.0087(3)	0.0085(3)
C14	0.0155(3)	0.0192(3)	0.0205(4)	0.0066(3)	0.0038(3)	0.0089(3)
C15	0.0187(4)	0.0208(3)	0.0166(3)	0.0075(3)	0.0055(3)	0.0112(3)

Table S3. Bond Lengths for AZN1 at 120(2) K.

Bonds	Length (Å)	Bonds	Length (Å)
O1-N1	1.2322(2)	C11-C12	1.3869(3)
O2-N1	1.2311(2)	C12-C13	1.3978(3)
N1-C1	1.4675(3)	C13-C14	1.3909(3)
N2-N3	1.3997(3)	C14-C15	1.3948(3)
N2-C7	1.2921(2)	C2-H2	0.9300
N3-C9	1.2786(2)	C3-H3	0.9300
C1-C2	1.3848(3)	C5-H5	1.0000
C1-C6	1.3918(3)	C6-H6	0.9700
C2-C3	1.3903(3)	C8-H8A	0.9600
C3-C4	1.4001(3)	C8-H8B	0.9600
C4-C5	1.4062(3)	C8-H8C	0.9600
C4-C7	1.4823(3)	C9-H9	0.9300
C5-C6	1.3856(3)	C11-H11	0.9300
C7-C8	1.5020(3)	C12-H12	0.9300
C9-C10	1.4662(3)	C13-H13	0.9300
C10-C11	1.4033(3)	C14-H14	0.9300
C10-C15	1.4001(3)	C15-H15	0.9300

Table S4. Bond Angles for AZN1 at 120(2) K.

Bonds	Angle (°)	Bonds	Angle (°)
O1-N1-O2	123.80(1)	C1-C2-H2	121.00
O1-N1-C1	118.12(1)	C3-C2-H2	121.00
O2-N1-C1	118.07(1)	C2-C3-H3	120.00
N3-N2-C7	113.96(1)	C4-C3-H3	120.00
N2-N3-C9	113.04(1)	C4-C5-H5	120.00
N1-C1-C2	117.93(1)	C6-C5-H5	120.00
N1-C1-C6	119.40(1)	C1-C6-H6	123.00
C2-C1-C6	122.64(1)	C5-C6-H6	119.00
C1-C2-C3	118.46(1)	C7-C8-H8A	109.00
C2-C3-C4	120.67(1)	C7-C8-H8B	109.00
C3-C4-C5	119.13(1)	C7-C8-H8C	109.00
C3-C4-C7	120.31(1)	H8A-C8-H8B	109.00
C5-C4-C7	120.56(1)	H8A-C8-H8C	109.00
C4-C5-C6	120.85(1)	H8B-C8-H8C	109.00
C1-C6-C5	118.21(1)	N3-C9-H9	119.00
N2-C7-C4	116.00(1)	C10-C9-H9	119.00
N2-C7-C8	124.28(1)	C10-C11-H11	120.00
C4-C7-C8	119.69(1)	C12-C11-H11	120.00
N3-C9-C10	121.06(1)	C11-C12-H12	120.00
C9-C10-C11	121.38(1)	C13-C12-H12	120.00
C9-C10-C15	119.22(1)	C12-C13-H13	120.00
C11-C10-C15	119.41(1)	C14-C13-H13	120.00
C10-C11-C12	120.11(1)	C13-C14-H14	120.00
C11-C12-C13	120.27(1)	C15-C14-H14	120.00
C12-C13-C14	119.98(1)	C10-C15-H15	120.00
C13-C14-C15	119.99(1)	C14-C15-H15	120.00
C10-C15-C14	120.25(1)		

Table 5. Hydrogen Atom Coordinates and Isotropic Displacement Parameters ($Å^2$) for AZN1 at 120(2) K.

Atom	x	y	z	U(eq)
H2	1.004852	0.956442	0.289397	0.022
H3	0.776007	0.825781	0.361615	0.021
H5	0.5474(18)	1.0620(17)	0.1847(16)	0.028(3)
H6	0.7833(19)	1.2010(19)	0.1196(18)	0.034(3)
H8A	0.443795	0.768908	0.498626	0.033
H8B	0.642331	0.843594	0.526592	0.033
H8C	0.485499	0.651285	0.388385	0.033
H9	0.044144	0.664397	0.095745	0.022
H11	0.043566	0.666417	0.470486	0.021
H12	-0.205798	0.524328	0.513301	0.023
H13	-0.493421	0.363460	0.301689	0.024
H14	-0.531086	0.345320	0.046590	0.025
H15	-0.281551	0.485879	0.002009	0.023

Table S6. Final Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for AZN2 at 120(2) K. U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{IJ} tensor.

Atom	x	y	z	U(eq)
O1	0.36402	-0.33847	-0.08223	0.0343
O2	0.35615	-0.20034	-0.15537	0.0314
O3	0.37610	0.83719	0.31659	0.0407
O4	0.37816	0.69878	0.38949	0.0356
N1	0.36215	-0.23495	-0.09792	0.0250
N2	0.36024	0.20857	0.09119	0.0236
N3	0.35734	0.28926	0.14263	0.0238
N4	0.37325	0.73364	0.33195	0.0279
C1	0.36733	-0.14797	-0.04486	0.0225
C2	0.39759	-0.18381	0.01755	0.0263
C3	0.40381	-0.10134	0.06752	0.0249
C4	0.37902	0.01544	0.05513	0.0201
C5	0.34986	0.04831	-0.00914	0.0232
C6	0.34403	-0.03285	-0.05957	0.0238
C7	0.38369	0.10356	0.10898	0.0210
C8	0.41396	0.06632	0.17759	0.0256
C9	0.37286	0.39576	0.12456	0.0203
C10	0.40021	0.43508	0.05580	0.0256
C11	0.36608	0.48371	0.17832	0.0196
C12	0.36429	0.44854	0.24477	0.0227
C13	0.36487	0.52999	0.29539	0.0241
C14	0.36545	0.64698	0.27884	0.0234
C15	0.36236	0.68517	0.21402	0.0247
C16	0.36365	0.60272	0.16379	0.0225

Table S7. Anisotropic displacement parameters ($Å^2$) for AZN2 at 120(2) K. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka^*b^*U_{12}]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	0.0442(5)	0.0214(3)	0.0372(4)	-0.0045(3)	0.0015(3)	0.0025(2)
O2	0.0377(4)	0.0337(4)	0.0227(3)	-0.0049(2)	0.0003(2)	0.0025(3)
O3	0.0584(5)	0.0253(3)	0.0384(4)	-0.0069(3)	-0.0007(3)	0.0056(3)
O4	0.0441(5)	0.0396(4)	0.0231(3)	-0.0064(3)	0.0024(3)	0.0011(3)
N1	0.0244(4)	0.0243(3)	0.0264(3)	-0.0041(3)	-0.0001(2)	0.0022(2)
N2	0.0317(4)	0.0216(3)	0.0175(3)	-0.0011(2)	-0.0020(2)	0.0012(2)
N3	0.0321(4)	0.0217(3)	0.0176(3)	-0.0013(2)	-0.0024(2)	0.0011(2)
N4	0.0291(4)	0.0287(4)	0.0260(4)	-0.0053(3)	-0.0001(3)	0.0024(3)
C1	0.0235(5)	0.0222(4)	0.0217(4)	-0.0021(3)	-0.0011(3)	0.0031(3)
C2	0.0351(5)	0.0199(3)	0.0239(4)	0.0011(3)	-0.0004(3)	0.0008(3)
C3	0.0328(5)	0.0222(4)	0.0197(3)	0.0022(3)	0.0011(3)	-0.0003(3)
C4	0.0212(4)	0.0211(4)	0.0181(3)	0.0010(2)	-0.0005(2)	0.0016(2)
C5	0.0274(4)	0.0223(3)	0.0200(3)	0.0009(3)	0.0018(3)	-0.0008(3)
C6	0.0271(4)	0.0239(4)	0.0203(3)	-0.0001(3)	0.0025(3)	0.0000(3)
C7	0.0216(4)	0.0234(4)	0.0179(3)	0.0004(3)	-0.0007(2)	0.0019(3)
C8	0.0312(5)	0.0268(4)	0.0188(3)	0.0002(3)	0.0031(3)	-0.0017(3)
C9	0.0212(4)	0.0226(4)	0.0172(3)	0.0016(3)	-0.0009(2)	-0.0013(2)
C10	0.0340(5)	0.0255(4)	0.0174(3)	0.0030(3)	-0.0035(3)	-0.0022(3)
C11	0.0199(4)	0.0213(4)	0.0177(3)	0.0016(2)	-0.0006(2)	-0.0005(2)
C12	0.0269(5)	0.0228(4)	0.0183(3)	0.0021(3)	-0.0012(3)	-0.0009(3)
C13	0.0270(5)	0.0262(4)	0.0190(3)	0.0010(3)	-0.0006(3)	-0.0008(3)
C14	0.0228(5)	0.0247(4)	0.0226(4)	-0.0032(3)	-0.0001(3)	0.0005(3)
C15	0.0272(5)	0.0224(4)	0.0246(4)	0.0004(3)	-0.0004(3)	0.0005(3)
C16	0.0260(5)	0.0218(4)	0.0197(3)	0.0029(3)	-0.0002(2)	0.0001(3)

Table 8. Bond Lengths for AZN2 at 120(2) K.

Bonds	Length (Å)	Bonds	Length (Å)
O1-N1	1.2311(9)	C11-C16	1.3988(10)
O2-N1	1.2303(9)	C12-C13	1.3869(10)
O3-N4	1.2300(9)	C13-C14	1.3851(10)
O4-N4	1.2322(9)	C14-C15	1.3829(10)
N1-C1	1.4677(10)	C15-C16	1.3890(10)
N2-N3	1.3938(10)	C2-H2	0.9300
N2-C7	1.2935(9)	C3-H3	0.9300
N3-C9	1.2920(9)	C5-H5	0.9300
N4-C14	1.4678(10)	C6-H6	0.9300
C1-C2	1.3819(10)	C8-H8A	0.9600
C1-C6	1.3874(10)	C8-H8B	0.9600
C2-C3	1.3875(10)	C8-H8C	0.9600
C3-C4	1.4005(10)	C10-H10A	0.9600
C4-C5	1.4031(10)	C10-H10B	0.9600
C4-C7	1.4880(10)	C10-H10C	0.9600
C5-C6	1.3838(10)	C12-H12	0.9300
C7-C8	1.5018(10)	C13-H13	0.9300
C9-C10	1.5026(10)	C15-H15	0.9300
C9-C11	1.4867(10)	C16-H16	0.9600
C11-C12	1.4034(10)		

Table S9. Bond Angles for AZN2 at 120(2) K.

Bonds	Angle (°)	Bonds	Angle (°)
O1-N1-O2	123.83(1)	C12-C13-C14	118.45(4)
O1-N1-C1	117.93(4)	N4-C14-C13	118.80(4)
O2-N1-C1	118.24(4)	N4-C14-C15	118.71(4)
N3-N2-C7	114.75(4)	C13-C14-C15	122.46(1)
N2-N3-C9	114.50(4)	C14-C15-C16	118.46(4)
O3-N4-O4	123.46(1)	C11-C16-C15	120.88(4)
O3-N4-C14	118.24(4)	C1-C2-H2	121.00
O4-N4-C14	118.29(4)	C3-C2-H2	121.00
N1-C1-C2	118.51(4)	C2-C3-H3	120.00
N1-C1-C6	118.86(4)	C4-C3-H3	120.00
C2-C1-C6	122.61(1)	C4-C5-H5	119.00
C1-C2-C3	118.53(4)	C6-C5-H5	119.00
C2-C3-C4	120.73(3)	C1-C6-H6	121.00
C3-C4-C5	118.86(1)	C5-C6-H6	121.00
C3-C4-C7	120.79(3)	C7-C8-H8A	109.00
C5-C4-C7	120.35(4)	C7-C8-H8B	109.00
C4-C5-C6	121.03(4)	C7-C8-H8C	109.00
C1-C6-C5	118.22(4)	H8A-C8-H8B	109.00
N2-C7-C4	114.95(4)	H8A-C8-H8C	109.00
N2-C7-C8	125.55(1)	H8B-C8-H8C	109.00
C4-C7-C8	119.51(4)	C9-C10-H10A	109.00
N3-C9-C10	125.56(1)	C9-C10-H10B	109.00
N3-C9-C11	115.34(4)	C9-C10-H10C	109.00
C10-C9-C11	119.06(4)	H10A-C10-H10B	109.00
C9-C11-C12	120.37(4)	H10A-C10-H10C	109.00
C9-C11-C16	120.79(4)	H10B-C10-H10C	109.00
C12-C11-C16	118.83(1)	C11-C12-H12	120.00
C11-C12-C13	120.83(4)	C13-C12-H12	120.00

Table 10. Hydrogen Atom Coordinates and Isotropic Displacement Parameters ($Å^2$) for AZN2 at 120(2) K.

Atom	x	y	z	U(eq)
H2	0.41343	-0.26148	0.02588	0.0320
H3	0.42468	-0.12386	0.10971	0.0300
H5	0.33421	0.12586	-0.01798	0.0280
H6	0.32500	-0.01082	-0.10219	0.0290
H8A	0.40994	0.13191	0.20690	0.0380
H8B	0.36658	0.00666	0.19249	0.0380
H8C	0.48472	0.03661	0.17724	0.0380
H10A	0.40155	0.36904	0.02672	0.0380
H10B	0.34825	0.48970	0.04066	0.0380
H10C	0.46829	0.47162	0.05609	0.0380
H12	0.36270	0.36963	0.25498	0.0270
H13	0.36487	0.50660	0.33942	0.0290
H15	0.35947	0.76422	0.20428	0.0300
H16	0.36000	0.62780	0.11860	0.0410

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