Supporting Information for:

Photolysis of α-Azidoacetophenones: Trapping of Triplet Alkyl Nitrenes in Solution

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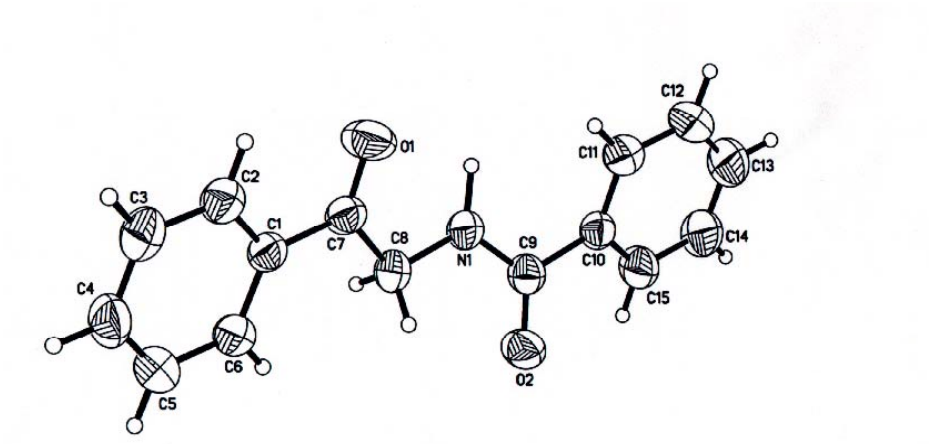
α-azidoacetophenone (1a)
IR (KBr, ν_{max}): 2104, 1695, 1217 cm^{-1}.
^{1}H-NMR (250 MHz, $CDCl_3$) δ 7.9 (s, 7Hz, 2H), 7.6 (t, 7Hz, 1H), 7.5 (t, 7Hz, 2H), 4.5 (s, 2H) ppm.
MS m/z (rel. intensity): 161(M^+, 1) 105 (100), 77 (80).

2-benzoylamino-1-phenylethanone (3a)
MP: 122-124ºC (lit[1]. 123-125ºC).
IR (KBr, ν_{max}): 3358, 1692, 1636, 1523, 1365, 1224 cm^{-1}.
^{1}H-NMR (250 MHz, $CDCl_3$) δ 8.04 (d, 7Hz, 2H), 7.89 (d, 7 Hz, 2H), 7.66 (t, 7Hz, 1H), 7.5 (m, 5H), 7.3 (broad s, 1H), 4.98 (d, 4Hz, 2H) ppm.
MS m/z (rel. intensity): 239 (M^+, 10), 105 (100).

CRYSTAL DATA OF 3a



Chemical formula: $C_{15}H_{13}NO_2$
Crystal system: Monoclinic
Space group: $P2_1/c$

[1] Demeuov, N. B.; Akhmedzhanova, V. I.; Moldagulov, M. A.; Shakirov, R. S.; *Chem. Nat. Compd. (Engl.Transl.),* **1998**, 34, 484.

a = 13.063(2) Å $\alpha = 90^{o}$
b = 5.3745(6) Å $\beta = 99.449(2)^{o}$
c = 17.450(2) Å $\gamma = 90^{o}$
Volume = 1208.5(2) $Å^3$ Z = 4
$\rho_{(calcd)}$ = 1.315 Mg/m^3 μ = 0.088 mm^{-1}

No. of reflections for lattice parameters: 1707
θ range for lattice parameters (º): 2.37 to 28.30

EXPERIMENTAL

Crystallization

Crystallization source: diethyl ether
Crystal size (mm): 0.34 x 0.14 x 0.08
Crystal description: colorless rod

Data Collection

Temperature (K): 296(2)
Mo Kα Radiation: λ=0.71073 Å
θ range for data collection (º): 2.37 to 28.30
No. of reflections collected: 7654
No. of independent reflections: 2984
R_{int} = 0.0629
Absorption correction (Tmin, Tmax): 0.971, 0.993

REFINEMENT

Full-matrix least-squares on F^2
No. of reflections I>2σ(I): 1551
Final R indices [I>2σ(I)]: R1 = 0.0582, wR2 = 0.1213
R indices (all data): R1 = 0.1252, wR2 = 0.1489
Extinction coefficient = 0.002(2)
S = 1.000
Largest residual peak: 0.178 e$Å^{-3}$

Treatment of Hydrogen Atoms

The hydrogen atom on N1 was found directly and held fixed in subsequent refinements. The remaining hydrogen atom positions were calculated based on geometrical criteria and treated with a
riding model. The isotropic temperature factors for the H-atoms were defined as 1.2U_{eq} of the adjacent atom.

Table 1. Atomic coordinates [x10^4] and equivalent isotropic displacement parameters [Å^{2}x10^3]. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	-420(1)	1725(3)	3864(1)	69(1)
O(2)	-1785(1)	8715(3)	2407(1)	60(1)
N(1)	-1352(1)	4783(3)	2770(1)	47(1)
C(1)	988(1)	4299(4)	4390(1)	40(1)
C(2)	1291(2)	2709(4)	5012(1)	48(1)
C(3)	2164(2)	3207(4)	5548(1)	55(1)
C(4)	2747(2)	5288(5)	5466(1)	58(1)
C(5)	2465(2)	6877(4)	4851(1)	58(1)
C(6)	1582(2)	6407(4)	4316(1)	49(1)
C(7)	33(2)	3690(4)	3829(1)	43(1)
C(8)	-357(1)	5551(4)	3210(1)	46(1)
C(9)	-2015(2)	6483(4)	2412(1)	44(1)
C(10)	-3051(1)	5614(4)	2005(1)	43(1)
C(11)	-3542(2)	3498(4)	2221(1)	57(1)
C(12)	-4521(2)	2885(5)	1831(2)	73(1)
C(13)	-4998(2)	4331(5)	1228(2)	75(1)
C(14)	-4511(2)	6404(5)	1006(1)	68(1)
C(15)	-3549(2)	7052(5)	1397(1)	55(1)

Table 2. Bond lengths [Å] and angles [º].

O(1)-C(7)	1.217(2)	O(2)-C(9)	1.237(2)
N(1)-C(9)	1.340(2)	N(1)-C(8)	1.457(2)
C(1)-C(2)	1.388(3)	C(1)-C(6)	1.391(3)
C(1)-C(7)	1.489(3)	C(2)-C(3)	1.376(3)
C(3)-C(4)	1.374(3)	C(4)-C(5)	1.374(3)
C(5)-C(6)	1.383(3)	C(7)-C(8)	1.499(3)
C(9)-C(10)	1.497(3)	C(10)-C(15)	1.386(3)
C(10)-C(11)	1.387(3)	C(11)-C(12)	1.387(3)
C(12)-C(13)	1.373(4)	C(13)-C(14)	1.370(4)
C(14)-C(15)	1.372(3)		

C(9)-N(1)-C(8)	120.3(2)	C(2)-C(1)-C(6)	118.8(2)
C(2)-C(1)-C(7)	118.6(2)	C(6)-C(1)-C(7)	122.5(2)
C(3)-C(2)-C(1)	120.7(2)	C(4)-C(3)-C(2)	119.9(2)
C(3)-C(4)-C(5)	120.3(2)	C(4)-C(5)-C(6)	120.1(2)
C(5)-C(6)-C(1)	120.1(2)	O(1)-C(7)-C(1)	121.3(2)
O(1)-C(7)-C(8)	120.3(2)	C(1)-C(7)-C(8)	118.4(2)
N(1)-C(8)-C(7)	111.1(2)	O(2)-C(9)-N(1)	121.7(2)
O(2)-C(9)-C(10)	120.1(2)	N(1)-C(9)-C(10)	118.2(2)
C(15)-C(10)-C(11)	119.0(2)	C(15)-C(10)-C(9)	117.6(2)
C(11)-C(10)-C(9)	123.3(2)	C(12)-C(11)-C(10)	119.5(2)
C(13)-C(12)-C(11)	120.5(2)	C(14)-C(13)-C(12)	120.3(2)
C(13)-C(14)-C(15)	119.7(2)	C(14)-C(15)-C(10)	121.0(2)

Table 3. Anisotropic displacement parameters [$Å^2x10^3$]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)^2U_{11} + ... + 2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
O(1)	74(1)	45(1)	77(1)	7(1)	-21(1)	-16(1)
O(2)	54(1)	48(1)	69(1)	7(1)	-11(1)	-6(1)
N(1)	39(1)	44(1)	52(1)	0(1)	-6(1)	2(1)
C(1)	39(1)	36(1)	42(1)	-3(1)	1(1)	3(1)
C(2)	47(1)	46(1)	48(1)	3(1)	2(1)	4(1)
C(3)	51(1)	61(2)	50(1)	4(1)	0(1)	11(1)
C(4)	44(1)	65(2)	59(1)	-13(1)	-6(1)	5(1)
C(5)	49(1)	52(1)	69(1)	-5(1)	0(1)	-5(1)
C(6)	46(1)	44(1)	55(1)	3(1)	0(1)	0(1)
C(7)	45(1)	37(1)	46(1)	-3(1)	3(1)	3(1)
C(8)	38(1)	48(1)	49(1)	3(1)	-2(1)	3(1)
C(9)	41(1)	47(1)	42(1)	0(1)	2(1)	0(1)
C(10)	38(1)	43(1)	48(1)	-4(1)	3(1)	2(1)
C(11)	49(1)	47(1)	72(1)	3(1)	2(1)	0(1)
C(12)	55(2)	54(2)	107(2)	-4(2)	4(1)	-14(1)
C(13)	45(1)	75(2)	96(2)	-16(2)	-14(1)	-4(1)
C(14)	52(1)	72(2)	72(2)	0(1)	-16(1)	4(1)
C(15)	47(1)	57(2)	58(1)	6(1)	-4(1)	-1(1)

Table 4. Hydrogen coordinates ($x10^4$) and isotropic displacement parameters ($Å^2x10^3$).

	x	y	z	U(eq)
H(1)	-1589	2920	2787	56
H(2)	901(2)	1292(4)	5068(1)	57
H(3)	2358(2)	2135(4)	5965(1)	66
H(4)	3335(2)	5624(5)	5829(1)	69
H(5)	2868(2)	8270(4)	4794(1)	69
H(6)	1385(2)	7502(4)	3905(1)	59
H(8A)	-434(1)	7156(4)	3448(1)	55
H(8B)	145(1)	5727(4)	2862(1)	55
H(11)	-3216(2)	2498(4)	2623(1)	69
H(12)	-4858(2)	1484(5)	1979(2)	88
H(13)	-5654(2)	3901(5)	969(2)	90
H(14)	-4831(2)	7368(5)	592(1)	82
H(15)	-3226(2)	8478(5)	1251(1)	66

Detailed X-ray crystallographic data (excluding structure factors) are available from the Cambridge Crystallographic Data Centre, as a supplementary publication no. CCDC-1557621. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax (+44)-1223-336-033; e-mail deposit@ccdc.cam.ac.uk).

α-azidoacetophenone (1b)
MP: 78-81ºC (lit. 86-87ºC)[2].
IR (KBr, ν_{max}): 2105, 1690, 1587, 1219, 8181 cm^{-1}.
^{1}H-NMR (250 MHz, $CDCl_3$) δ 7.7 (d, 8Hz, 2H), 7.6 (d, 8Hz, 2H), 4.53 (s, 2H) ppm.
MS m/z (rel. intensity): 240/238 (M^+, 30), 185/183 (100) 157/155 (75),

2-(4-bromobenzoylamino)-1-(4-bromophenyl)ethanone (3b)
MP: 194-196ºC (lit. 193-197ºC)[3].
IR (KBr, ν_{max}): 3333, 1689 1638, 1587, 1520, 12210, 994 cm^{-1}.
^{1}H-NMR (250 MHz, $CDCl_3$) δ 7.90 (d, 7 Hz, 2H), 7.7 (m, 6H), 7.20 (broad s, 1H), 4.91 (d, 4Hz, 2H) ppm.
MS m/z (rel. intensity): 399/397/395 (M^+, 2), 183/185 (100) 155/157 (50).

[2] Boyer, J.H.; Straw, D. J. Am. Chem. Soc. **1952**, *74*, 4506,
[3] Dann,O.; *Justus Liebigs Ann. Chem*. **1975**; 160.