

Electronic Supporting Information (ESI)

2-Diazo-1-(4-hydroxyphenyl)ethanone: A Versatile Photochemical and Synthetic Reagent^a

Sanjeewa N. Senadheera,^b Anthony S. Evans,^c John P. Toscano,^c and Richard S. Givens^{b*}

^b Department of Chemistry, University of Kansas, Lawrence, Kansas 66045, U.S.A.

^c Department of Chemistry, Johns Hopkins University, Baltimore, Maryland 21218, U.S.A.

*corresponding author: givensr@ku.edu

Contents:

Figures:

Pg 2; Figure SI1 X-ray crystal structure of 2-diazo-1-(4-hydroxyphenyl)ethanone (**1a**)

Pg 2; Figure SI2 Crystal packing of **1a** in the crystalline lattice cell

Pg 3; Figure SI3 The UV-vis Spectrum of diazo pHp **1a** in 50 % aqueous CH₃CN

Pg 3; Figure SI4 The UV-vis spectra of diazo pHp **1a** at different pH Values

Pg 4; Figure SI5 Stern-Volmer plot for the photolysis of diazo pHp **1a** in 50% aq. CH₃CN

Pg 5; Figure SI6. Plots of observed rate of (a) decay of ketene **3a** and (b) growth intermediate **22** or **23** at 1685 cm⁻¹ as a function of diethylamine concentration in acetonitrile.

Tables:

Pg 6; Table SI1 Measured structural parameters of **1a** in the crystalline ground state

Pg 6; Table SI2 Observed pseudo-first order kinetics (k_{obs}) for the decay of the ketene **3a**

Figures:

Figure SI1. X-ray Crystal Structure of **1a**

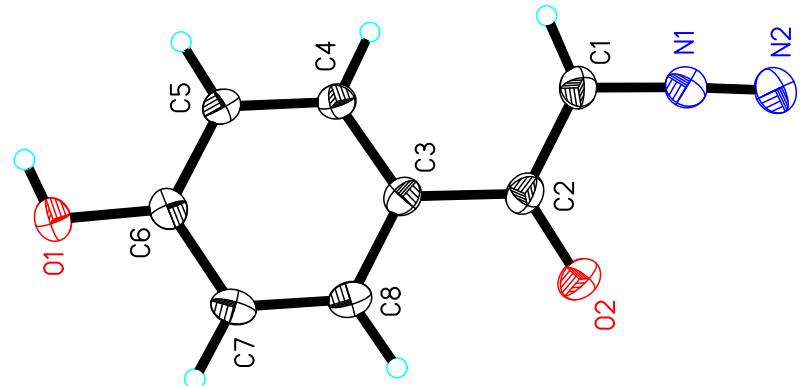


Figure SI2. Crystal packing of **1a** in the crystalline lattice cell

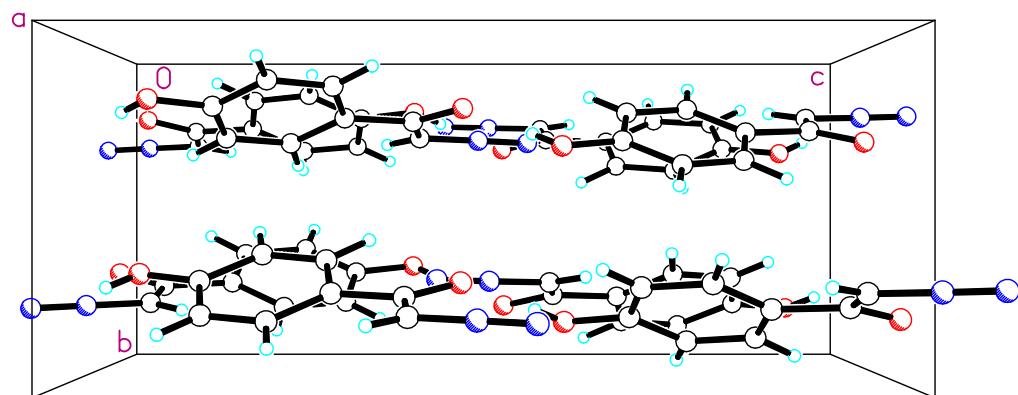


Figure SI3. The UV-vis Spectrum of diazo pHp **1a** in 50 % aqueous CH₃CN

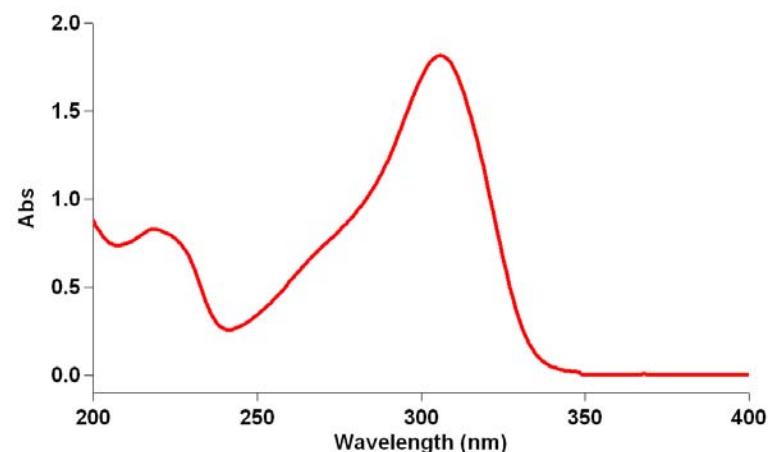


Figure SI4. The UV-vis spectra of diazo *p*HP **1a** at different pH Values

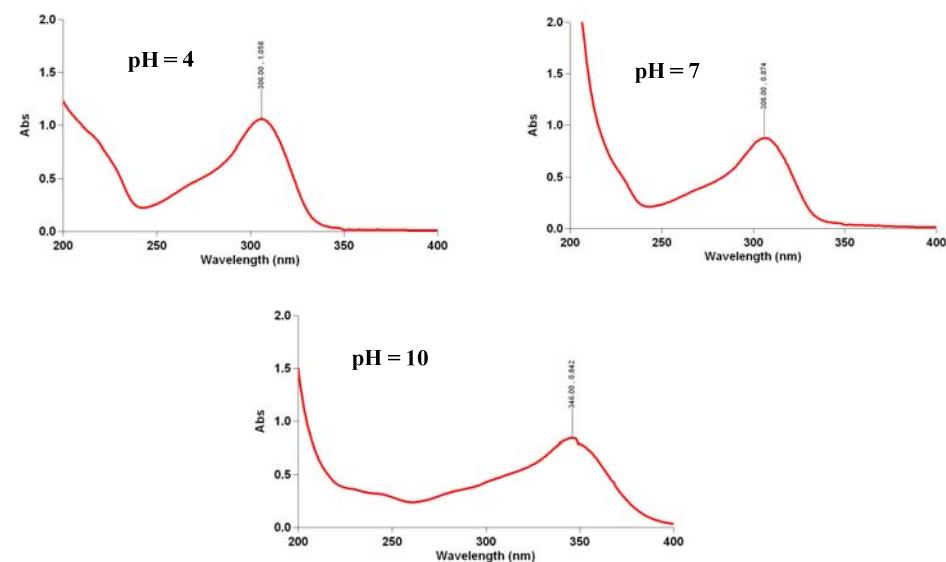


Figure SI5. Stern-Volmer plot for the photolysis of diazo *p*HP **1a** in 50% aqueous CH₃CN at 300 nm

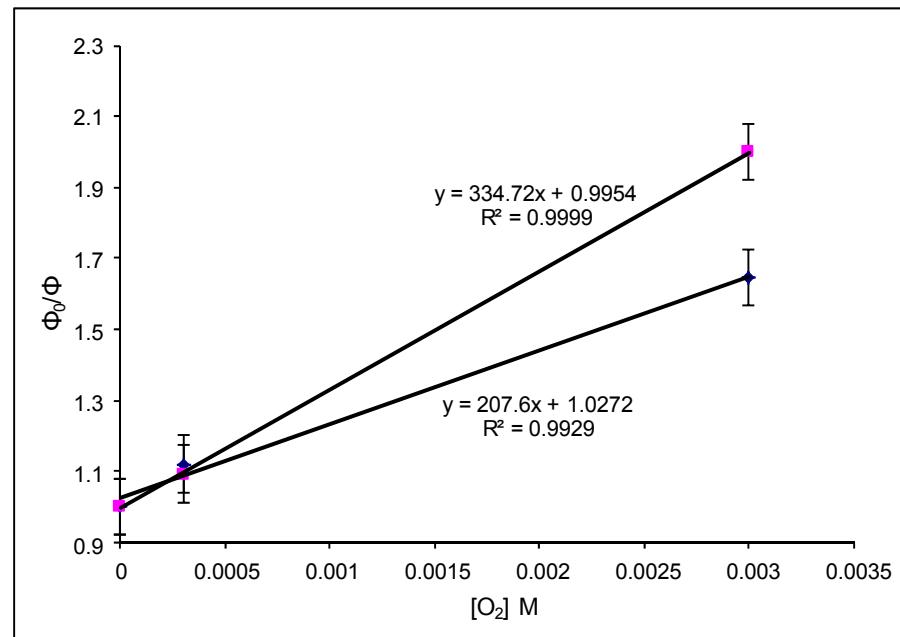
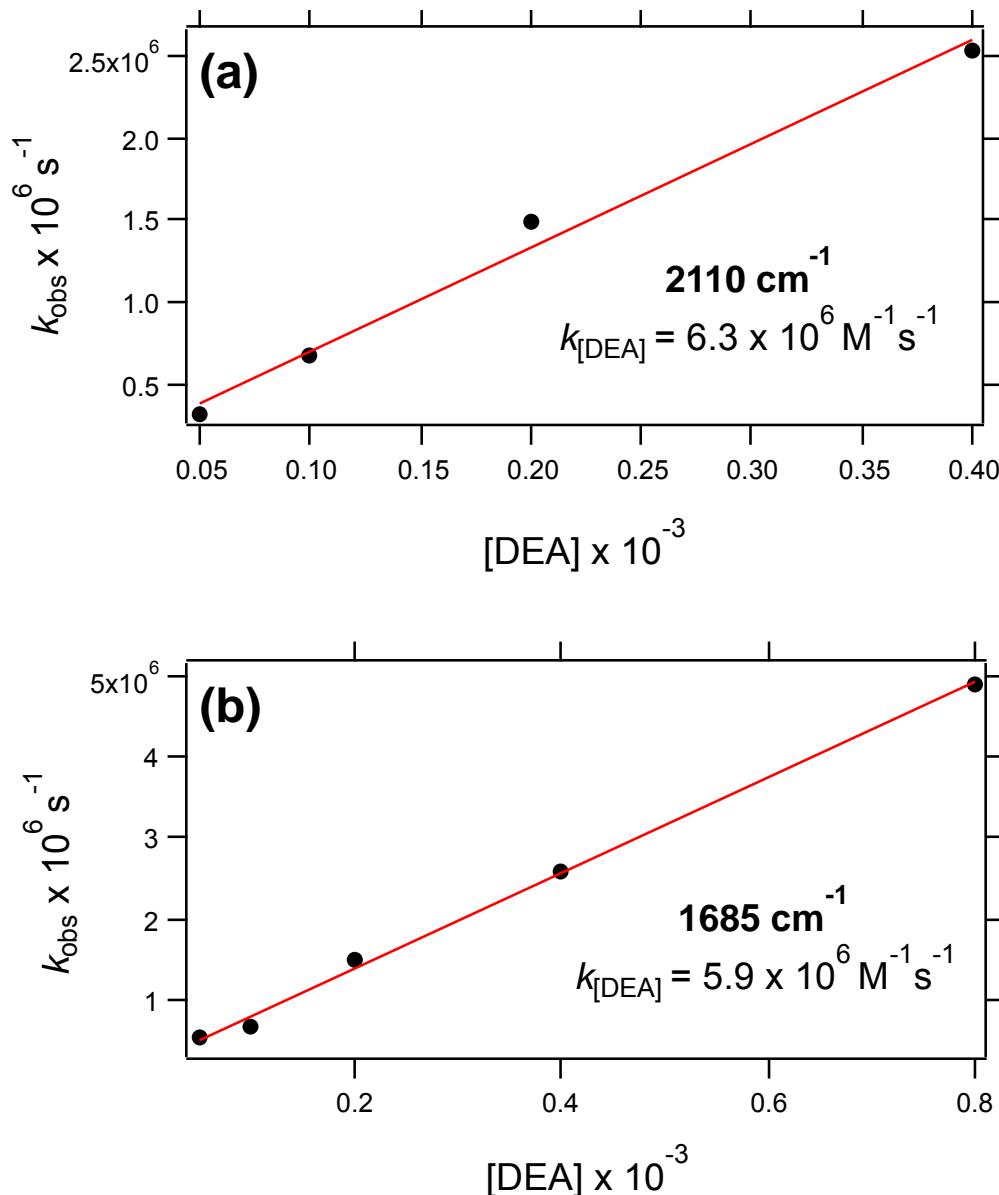


Figure SI6. Plots of observed rate of (a) decay of ketene **3a** at 2110 cm^{-1} and (b) growth of intermediate **22** or **23** at 1685 cm^{-1} as a function of diethylamine concentration in acetonitrile. Black markers are experimental values; red lines represent least-square fits of the data to a linear function.



Tables:

Table SI1. Measured structural parameters of **1a** in the crystalline ground state

	Bond length / Å		Bond angle / (°)		Dihedral angle / (°)
N1-N2	1.110	N2-N1-C1	177.5	N2-N1-C1-C2	22
N1-C1	1.321	N1-C1-C2	116.8	N1-C1-C2-O2	2
C1-H1	0.950	C2-C1-H1	129	N1-C1-C2-C3	179.7
C1-C2	1.431	O2-C2-C1	120.7	O2-C2-C3-C4	-168.5
O2-C2	1.241	O2-C2-C3	121.7	C1-C2-C3-C4	13.8
C2-C3	1.480	C1-C2-C3	117.6	O2-C2-C3-C8	12.3
C3-C4	1.399	C2-C3-C4	122.7	C1-C2-C3-C8	-165.4

Table SI2. Observed pseudo-first order kinetics (k_{obs}) for the decay of the ketene intermediate **3a**

[DEA] / mM	v/cm ⁻¹	$k_{\text{obs}}/ 10^6 \text{ s}^{-1}$
0.05	2110	0.324
0.10	2110	0.678
0.20	2110	1.490
0.40	2110	2.539