UV Photolysis Study of *Para*-Aminobenzoic Acid Using Parahydrogen Matrix Isolation Spectroscopy

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Electronic Supplementary Information Table of Contents:

Table S1: The observed wavenumbers and their absorption cross sections used in this work.

Species	Mode	Frequency	Absorption Coefficient
PABA	ν_{37} NH_2 Scissor	1624.2 cm^{-1}	271.97 km mol^{-1}
PABA Radical Conformer (I)	ν_{23} H-C-C Rock	1079.5 cm^{-1}	70.4 km mol^{-1}
PABA Radical Conformer (II)	ν_{23} H-C-C Rock	1077.2 cm^{-1}	49.8 km mol^{-1}
trans-HOCO	ν_{2} C=O Stretch	1845.1 cm^{-1}	203.6 km mol^{-1}

Table S2: Geometry of the two Conformers of PABA

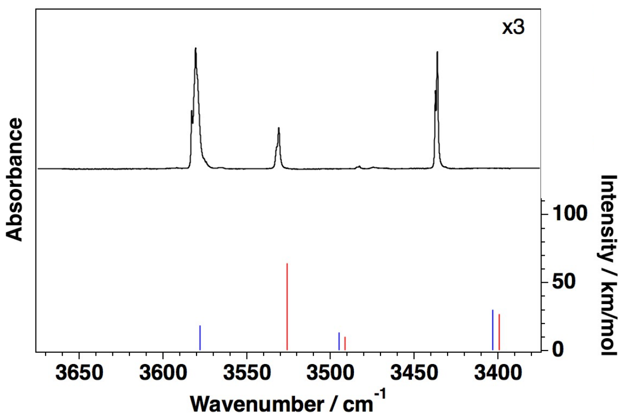
Parameter	Conformer (I)	Conformer (II)
$r(H_{11} - N_9)$	1.014	1.014
$r(H_{10} - N_9)$	1.014	1.014
$r(N_9 - C_4)$	1.386	1.385
$r(C_4 - C_3)$	1.412	1.410
$r(C_4 - C_5)$	1.412	1.412
$r(C_3 - C_2)$	1.390	1.391
$r(C_5 - C_6)$	1.388	1.387
$r(C_6 - C_1)$	1.405	1.406
$r(C_1 - C_2)$	1.406	1.405
$r(C_5 - H_8)$	1.093	1.093
$r(C_3 - H_{12})$	1.093	1.093
$r(C_2 - H_{13})$	1.090	1.094
$r(C_6 - H_7)$	1.091	1.091
$r(C_1 - C_{14})$	1.478	1.492
$r(C_{14} - O_{15})$	1.216	1.209
$r(C_{14} - O_{16})$	1.362	1.364
$r(H_{17} - O_{16})$	0.974	0.969
$\angle(H_{11} - N_9 - C_4)$	116.131	116.105
$\angle(H_{10} - N_9 - C_4)$	116.097	116.239
$\angle(H_{10} - N_9 - H_{11})$	112.622	112.630
$\angle(N_9 - C_4 - C_3)$	120.730	120.858
$\angle(N_9 - C_4 - C_5)$	120.690	120.790
$\angle(C_4 - C_3 - H_{12})$	119.399	119.581
$\angle(C_4 - C_5 - H_8)$	119.425	119.384
$\angle(C_6 - C_5 - H_8)$	120.084	119.973
$\angle(C_2 - C_3 - H_{12})$	119.970	119.923
$\angle(C_5 - C_6 - H_7)$	120.711	120.722
$\angle(C_3 - C_2 - H_{13})$	119.880	117.792
$\angle(C_5 - C_4 - C_3)$	118.524	118.307
$\angle(C_2 - C_3 - C_4)$	120.631	120.494
$\angle(C_6 - C_5 - C_4)$	120.491	120.643
$\angle(C_1 - C_6 - C_5)$	120.918	121.250
$\angle(C_1 - C_2 - C_3)$	120.706	121.290
$\angle(C_1 - C_6 - H_7)$	118.372	118.028
$\angle(C_1 - C_2 - H_{13})$	119.414	120.885
$\angle(C_{14} - C_1 - C_2)$	122.733	124.112
$\angle(C_{14} - C_1 - C_6)$	118.535	117.857
$\angle(O_{16} - C_{14} - C_1)$	113.089	117.026
$\angle(O_{15} - C_{14} - C_1)$	125.360	123.600
$\angle(H_{17} - O_{16} - C_{14})$	105.041	109.511
$\Theta(C_3 - C_4 - N_9 - H_{11})$	-159.333	-159.218
$\Theta(C_5 - C_4 - N_9 - H_{10})$	159.288	159.259

$\Theta(C_3 - C_4 - N_9 - H_{10})$	-23.495	-23.227
$\Theta(C_5 - C_4 - N_9 - H_{11})$	23.450	23.268
$\Theta(C_2 - C_3 - C_4 - C_5)$	0.035	0.650
$\Theta(C_6 - C_5 - C_4 - C_3)$	-0.019	-0.237
$\Theta(H_{12} - C_3 - C_2 - H_{13})$	0.278	1.651
$\Theta(H_8 - C_5 - C_6 - H_7)$	-0.276	-0.673
$\Theta(C_2 - C_3 - C_4 - N_9)$	-177.242	-176.925
$\Theta(C_6 - C_5 - C_4 - N_9)$	177.259	177.340
$\Theta(C_3 - C_4 - C_5 - H_8)$	-179.885	179.606
$\Theta(N_9 - C_4 - C_3 - H_{12})$	2.602	3.528
$\Theta(N_9 - C_4 - C_5 - H_8)$	-2.607	-2.818
$\Theta(C_5 - C_4 - C_3 - H_{12})$	179.879	-178.987
$\Theta(C_4 - C_5 - C_6 - H_7)$	179.859	179.168
$\Theta(C_4 - C_3 - C_2 - H_{13})$	-179.879	-177.894
$\Theta(C_2 - C_1 - C_6 - H_7)$	-179.863	-178.509
$\Theta(C_6 - C_1 - C_2 - H_{13})$	179.864	176.753
$\Theta(C_1 - C_2 - C_3 - C_4)$	-0.036	0.034
$\Theta(C_1 - C_6 - C_5 - C_4)$	0.004	-0.0871
$\Theta(C_1 - C_2 - C_3 - H_{12})$	-179.879	179.580
$\Theta(C_1 - C_6 - C_5 - H_8)$	179.869	179.287
$\Theta(C_{14} - C_1 - C_2 - C_3)$	-179.870	-179.026
$\Theta(C_{14} - C_1 - C_6 - C_5)$	179.891	179.576
$\Theta(C_{14} - C_1 - C_2 - H_{13})$	-0.026	-1.161
$\Theta(C_{14} - C_1 - C_6 - H_7)$	0.032	-0.462
$\Theta(O_{15} - C_{14} - C_1 - C_2)$	179.871	165.206
$\Theta(O_{15} - C_{14} - C_1 - C_6)$	-0.019	-12.712
$\Theta(O_{16} - C_{14} - C_1 - C_2)$	-0.116	-14.895
$\Theta(O_{16} - C_{14} - C_1 - C_6)$	179.994	167.187
$\Theta(H_{17} - O_{16} - C_{14} - C_1)$	-179.963	-10.030
$\Theta(H_{17} - O_{16} - C_{14} - O_{15})$	0.049	169.873

r = distance (Å)
∠ = angle (°)
Θ = dihedral angle (°)

Figure S1 a) through j) : The entire spectrum of PABA in a solid pH_2 matrix with the theoretical intensities of Conformer **(I)** (red) and Conformer **(II)** (blue). Some spectra are enlarged for clarity, as identified in the top right corner.

a)



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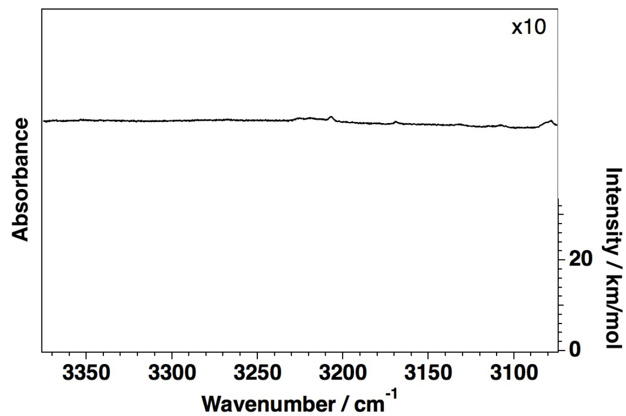

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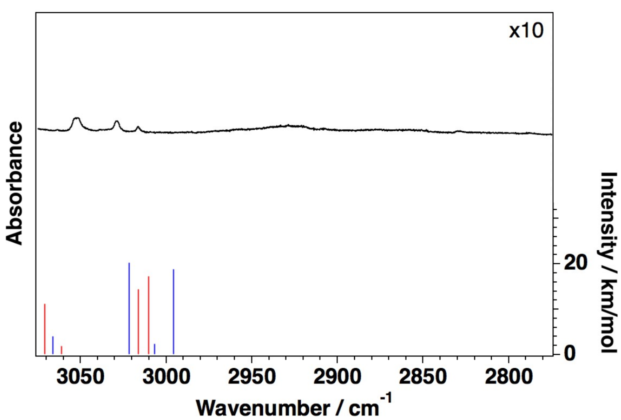

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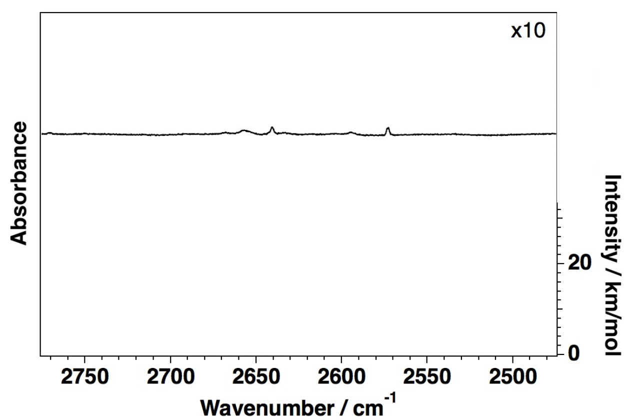

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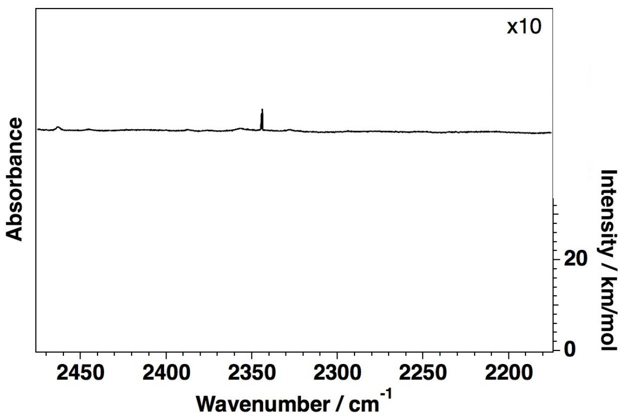
x10
Absorbance
Intensity / km/mol
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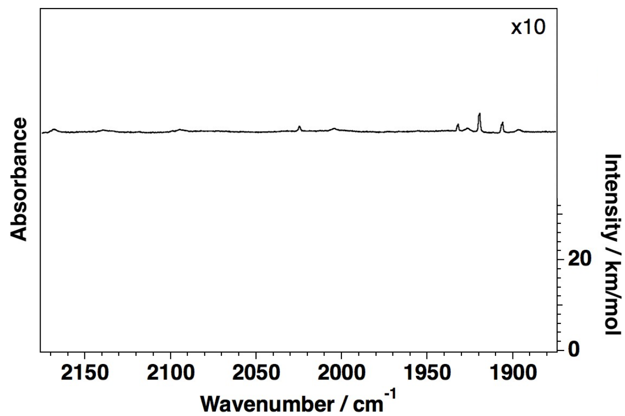
20
2450
2400
2350
2300
2250
2200
Wavenumber / cm-1

f)


x10
Absorbance
Intensity / km/mol
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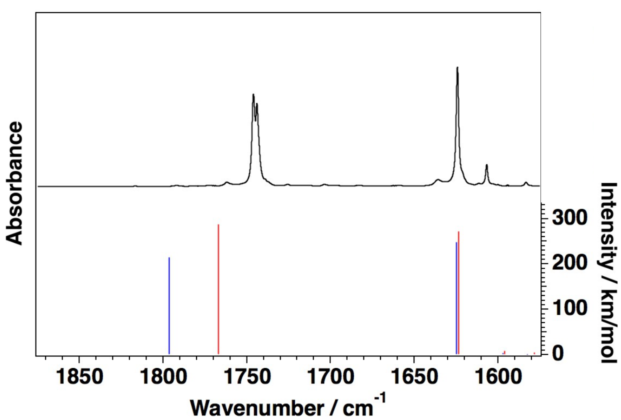
20
2150
2100
2050
2000
1950
1900
Wavenumber / cm-1

g)


Absorbance
Intensity / km/mol
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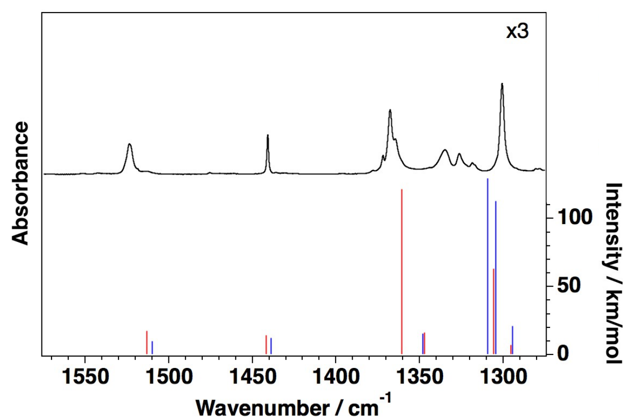
200
300
1850
1800
1750
1700
1650
1600
Wavenumber / cm-1

h)


x3
Absorbance
Intensity / km/mol
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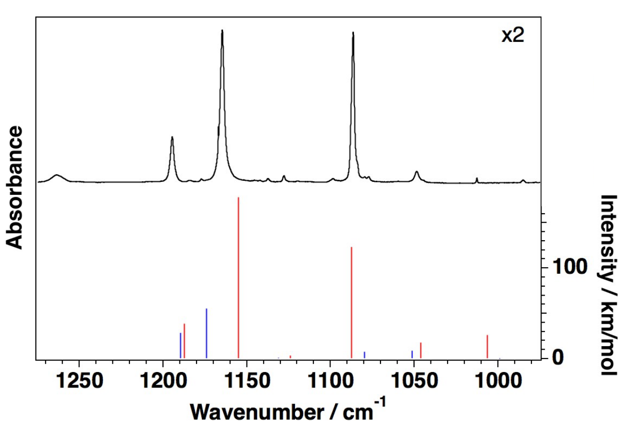
50
100
1550
1500
1450
1400
1350
1300
Wavenumber / cm-1

i)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Absorbance
Intensity / km/mol
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100
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1200
1150
1100
1050
1000
Wavenumber / cm-1

j)

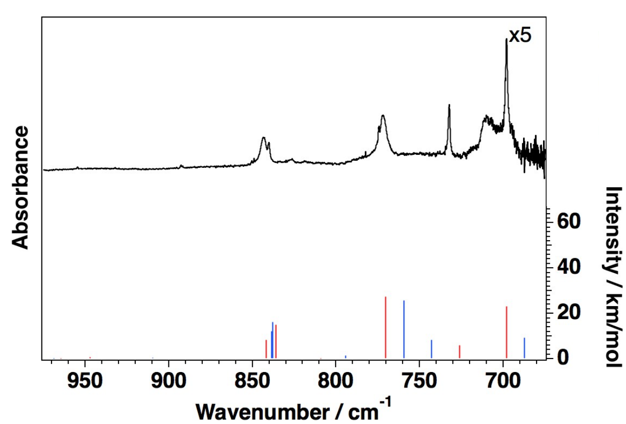

x5
Absorbance
Intensity / km/mol
0
20
40
60
950
900
850
800
750
700
Wavenumber / cm-1

Table S3: The frequencies and intensities of the calculated PABA Conformer **(I)** compared to the calculated Conformer **(II)** and the experimental *p*H_2 matrix. Intensities are in parentheses beside frequencies.

Mode	**Sym**	**Assignment**	**Conformer (I) (cm^{-1})**	**Conformer (II) (cm^{-1})**	***p*H_2 Matrix (cm^{-1})**
ν_1	A	O-C-O Wag	77.40 (0.69)	50.01 (7.12)	n. o.
ν_2		C-C Bend	101.16 (2.23)	105.56 (1.54)	n. o.
ν_3		C-C-C Scissor	189.34 (1.72)	195.31 (6.33)	n. o.
ν_4		C=C Wag	275.32 (1.46)	277.03 (12.21)	n. o.
ν_5		C=C-C Scissor	348.94 (30.76)	351.56 (13.00)	n. o.
ν_6		NH_2 Rock	366.85 (2.15)	345.16 (1.66)	n. o.
ν_7		C-N Rock	383.66 (1.89)	380.70 (7.94)	n. o.
ν_8		NH_2 Wag	388.06 (1086.14)	391.74 (39.58)	n. o.
ν_9		C=C Twist	415.24 (1.08)	404.83 (27.69)	n. o.
ν_{10}		NH_2 Wag	439.60 (663.93)	445.02 (1298.84)	n. o.
ν_{11}		O-C-C Scissor	500.11 (14.08)	404.02 (2641.23)	n. o.
ν_{12}		O-H Bend	563.52 (56.18)	475.95 (730.65)	n. o.
ν_{13}		O-C-O Scissor	589.67 (158.76)	599.92 (36.20)	n. o.
ν_{14}		C=C-C Scissor	641.76 (1.41)	642.30 (1.24)	n. o.
ν_{15}		C=C-C Wag	697.92 (23.09)	687.23 (9.28)	698.0 (20.62)
ν_{16}		O-C-O Scissor	725.94 (7.59)	742.73 (8.27)	732.3 (4.13)
ν_{17}		C-C-C Bend	770.40 (27.35)	759.42 (25.75)	771.6 (10.92)
ν_{18}		C-C-C Bend	809.04 (0.29)	794.16 (1.32)	n. o.
ν_{19}		C-C-C Bend	836.13 (14.97)	838.04 (16.22)	840*
ν_{20}		C=C-C Scissor	841.92 (8.41)	838.50 (12.08)	843*
ν_{21}		C-H Bend	947.20 (0.74)	909.67 (0.47)	954.6 (0.18)
ν_{22}		H-C-C Scissor	964.63 (0.21)	968.89 (0.28)	967.4 (0.12)
ν_{23}		H-C-C Rock	1006.49 (26.28)	999.06 (0.84)	1012.6 (0.68)
ν_{24}		NH_2 Rock	1046.07 (17.85)	1051.34 (9.14)	1048.5 (6.52)
ν_{25}		NH_2 Rock	1087.64 (123.18)	1079.82 (7.83)	1086.6 (54.61)
ν_{26}		C-O Stretch	1124.00 (3.82)	1131.30 (1.14)	1127.9 (1.74)
ν_{27}		H-C-C Bend	1154.98 (178.25)	1173.98 (55.47)	1164.8 (81.01)
ν_{28}		C-O-H Scissor	1187.34 (38.55)	1189.72 (28.34)	1194.7 (19.26)
ν_{29}		C-H Bend	1295.27 (7.09)	1294.46 (21.24)	1274.6 (1.23)
ν_{30}		C-O Stretch	1305.85 (63.39)	1304.45 (112.93)	1300.6 (32.48)
ν_{31}		C-O Stretch	1347.04 (16.10)	1309.13 (129.43)	1335*
ν_{32}		H-C-O Bend	1360.55 (121.57)	1348.09 (15.36)	1364.2, 1367.8 (41.33)
ν_{33}		C=C Stretch	1441.77 (14.14)	1438.93 (12.28)	1440.9 (6.18)
ν_{34}		C=C Asym. Str.	1513.15 (17.55)	1510.00 (10.02)	1523.8 (13.82)
ν_{35}		C=C Asym. Str.	1578.09 (5.01)	1582.56 (1.29)	1583.3 (2.96)

ν_{36}		NH_2 Scissor	1596.06 (8.61)	1596.88 (4.23)	1606.7 (12.26)
ν_{37}		NH_2 Scissor	1623.35 (271.97)	1624.82 (247.70)	1624.2 (100.00)
ν_{38}		C=O Stretch	1767.10 (287.04)	1796.53 (214.92)	1743.9, 1746.3 (109.75)
ν_{39}		C-H Asym. Str.	3010.33 (17.31)	2995.80 (18.87)	3016.2 (0.70)
ν_{40}		C-H Asym. Str.	3016.28 (14.37)	3006.91 (2.38)	3028.9 (2.57)
ν_{41}		C-H Sym. Str.	3061.17 (1.94)	3021.66 (20.25)	3052.3 (3.25)
ν_{42}		C-H Sym. Str.	3070.83 (11.15)	3066.25 (4.01)	3079.3 (3.01)
ν_{43}		N-H Asym. Str.	3399.32 (26.90)	3403.04 (30.16)	3436.2, 3437.3 (19.59)
ν_{44}		N-H Sym. Str.	3491.38 (10.41)	3494.92 (13.52)	3531.0, 3532.3 (8.59)
ν_{45}		O-H Stretch	3525.95 (64.46)	3577.95 (18.67)	3580.4, 3583.0 (19.32)

Theoretical calculated with B3LYP / cc-pVDZ Anharmonic
Intensities in km/mol
Experimental intensities are relative to 1624.2 cm^{-1} peak
*Two PABA peaks overlap
Two values are given for doublet peaks; their combined intensity is written beside in parentheses.
n. o. = not observed

Table S4: The frequencies and intensities of the aromatic-centred anilino radical.

Frequency (cm^{-1})	Intensity (km/mol)
654.25	26.03
766.81	0.14
781.50	48.97
799.32	21.15
888.18	0.16
909.37	0.014
970.12	2.70
1029.70	4.083
1070.07	4.65
1112.82	5.73
1152.66	5.57
1268.79	0.07
1276.33	21.52
1320.04	4.55
1398.45	2.35
1450.24	22.54
1568.73	24.14
1592.14	0.51
1606.46	66.34
3014.25	7.51
3017.48	16.87
3035.87	4.00
3043.28	25.95
3367.01	5.51
3448.78	6.10

Calculated with B3LYP / cc-pVDZ Anharmonic

Table S5: The frequencies and intensities of the aromatic-centred benzoic acid radical.

Frequency (cm^{-1})	**Intensity (km/mol)**
729.32	50.76
763.07	6.82
795.10	0.20
822.77	7.76
920.97	0.05
967.78	175.71
972.57	47.14
1029.06	9.86
1074.37	23.88
1090.68	1.79
1156.65	5.53
1182.37	16.73
1270.52	0.40
1298.86	343.65
1324.29	4.65
1370.52	39.41
1442.56	4.02
1558.92	12.17
1588.92	0.82
1801.96	15.81
3013.32	10.77
3049.73	2.91
3056.14	3.16
3065.65	2.76
3581.69	25.29

Calculated with B3LYP / cc-pVDZ Anharmonic

Figure S2 a) through j) : The PABA radical peaks from > 280 nm, 266 nm, and 213 nm irradiation compared to the calculated anharmonic B3LYP / cc-pVDZ intensities.

Conformer (I) = Black   Conformer (II) = Pink

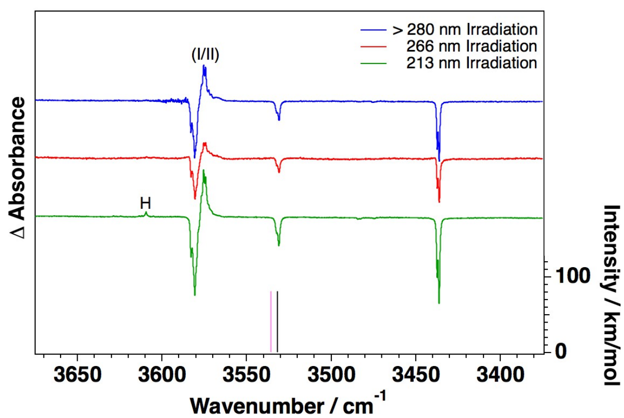
266 nm data is scaled by a factor of 2.

(I) = Conformer **(I)**   (II) = Conformer **(II)**

H = *trans*-HOCO Radical   * = Unidentified Peak

C = CO_2 O = CO   K = Unknown Ketene

a)



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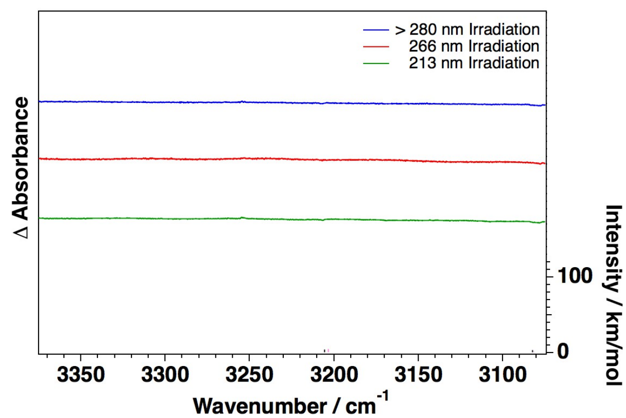

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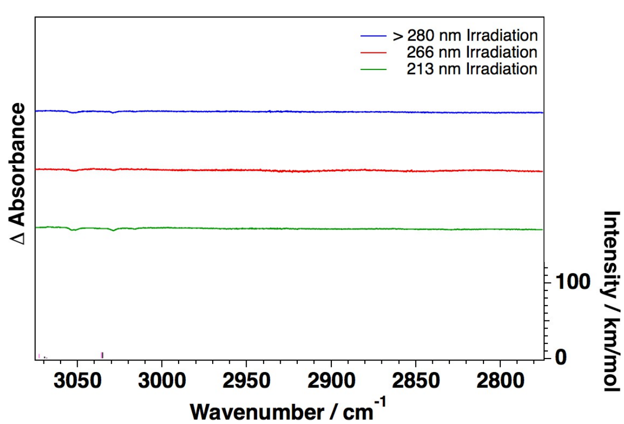

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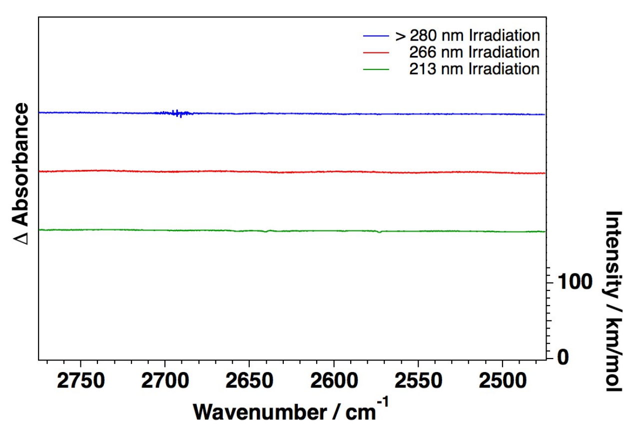

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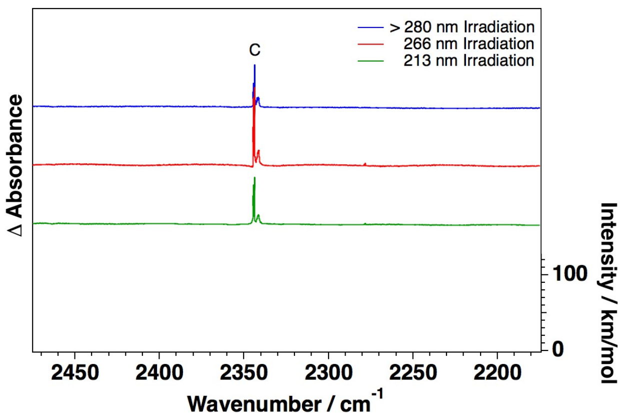
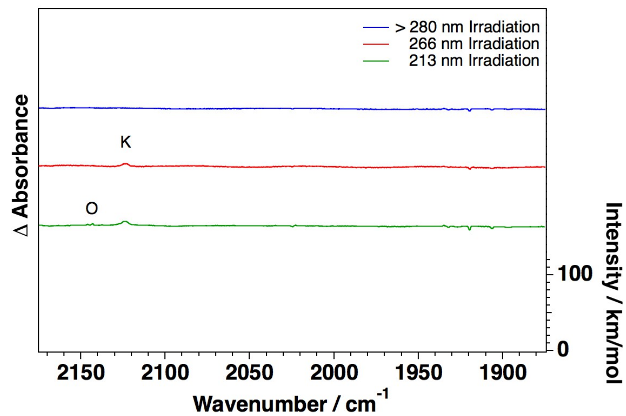

> 280 nm Irradiation
266 nm Irradiation
213 nm Irradiation
C
Δ Absorbance
Intensity / km/mol
100
0
2450 2400 2350 2300 2250 2200
Wavenumber / cm-1

f)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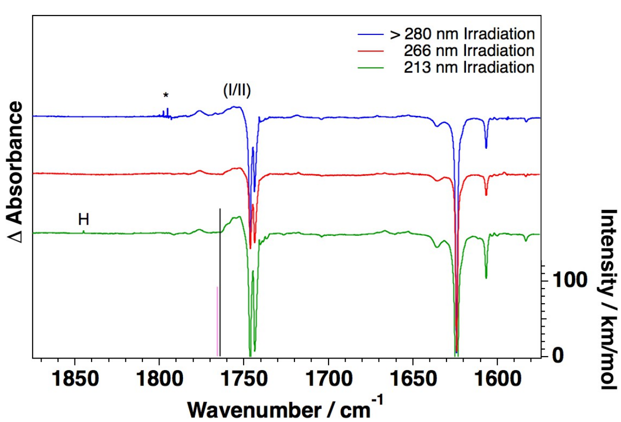
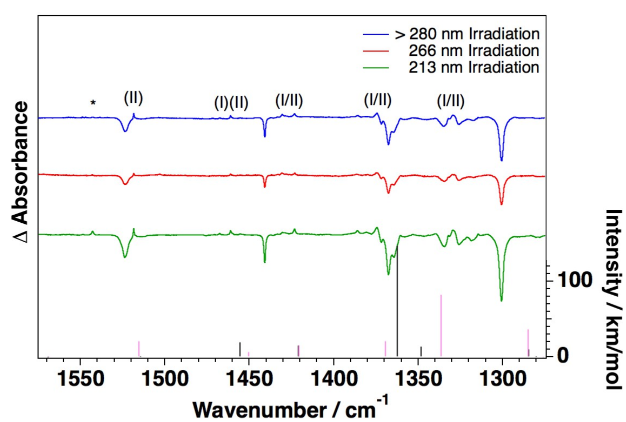
266 nm Irradiation
213 nm Irradiation
K
O
Δ Absorbance
Intensity / km/mol
100
0
2150 2100 2050 2000 1950 1900
Wavenumber / cm-1

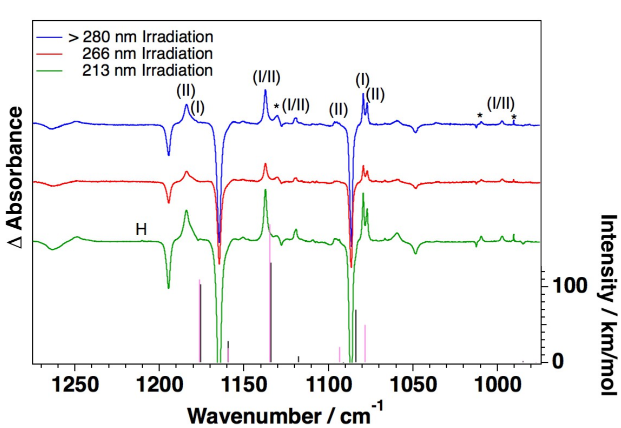
g)


> 280 nm Irradiation
266 nm Irradiation
213 nm Irradiation
*
(I/II)
H
Δ Absorbance
Intensity / km/mol
100
0
1850 1800 1750 1700 1650 1600
Wavenumber / cm-1

h)


> 280 nm Irradiation
266 nm Irradiation
213 nm Irradiation
*
(II)
(I)(II)
(I/II)
(I/II)
(I/II)
Δ Absorbance
Intensity / km/mol
100
0
1550 1500 1450 1400 1350 1300
Wavenumber / cm-1

i)


> 280 nm Irradiation
266 nm Irradiation
213 nm Irradiation
(II)
(I)
(I/II)
*
(I/II)
(II)
(I)
(II)
*
(I/II)
*
H
Δ Absorbance
Intensity / km/mol
100
0
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Wavenumber / cm-1

j)

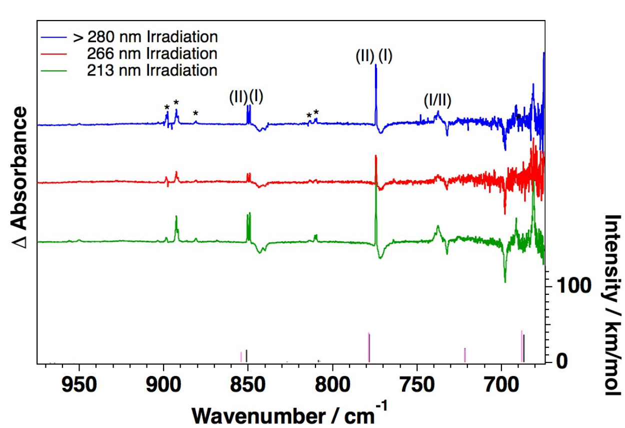
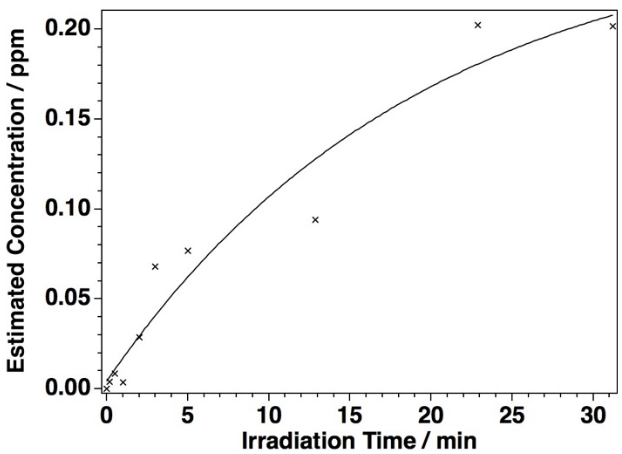

> 280 nm Irradiation
266 nm Irradiation
213 nm Irradiation
* *
*
(II)(I)
**
(II) (I)
(I/II)
Δ Absorbance
Intensity / km/mol
100
0
950 900 850 800 750 700
Wavenumber / cm-1

Figure S3 a) and b): The temporal behaviour of the unknown ketene following 266 nm and 213 nm photolysis. Concentrations estimated with intensities from methyl ketene.

a)



b)

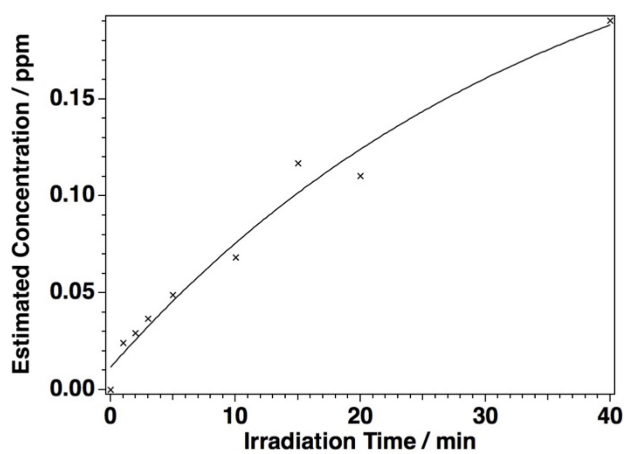


Table S6: The frequencies and intensities of the PABA radical Conformer **(II)** compared to the calculated Conformer **(I)** and the experimental pH_2 matrix. Intensities are in parentheses beside frequencies.

Mode	**Sym**	**Assignment**	**Conformer (I) (cm^{-1})**	**Conformer (II) (cm^{-1})**	**pH_2 Matrix (cm^{-1}) Conformer (I)**	**pH_2 Matrix (cm^{-1}) Conformer (I)**
ν_1	A’	O-C-O Wag	75.47 (2.21)	76.21 (0.23)	n. o.	n. o.
ν_2		C-C Bend	98.94 (0.26)	98.49 (0.28)	n. o.	n. o.
ν_3		C=C Wag	259.69 (2.27)	260.28 (1.96)	n. o.	n. o.
ν_4		C=C Wag	385.85 (5.85)	386.13 (2.74)	n. o.	n. o.
ν_5		C=C-C Wag	476.26 (15.10)	473.99 (24.95)	n. o.	n. o.
ν_6		O-H OOP Bend	567.44 (45.00)	570.77 (47.71)	n. o.	n. o.
ν_7		H-N-C Bend	663.64 (50.01)	660.53 (48.21)	n. o.	n. o.
ν_8		C-H Bend	686.98 (37.37)	688.05 (42.63)	n. o.	n. o.
ν_9		C-C-C Bend	778.48 (38.00)	778.74 (39.86)	774.3 (16.5)	774.6 (19.0)
ν_{10}		C-H OOP Bend	808.67 (3.56)	807.51 (2.60)	n. o.	n. o.
ν_{11}		C-C-C Bend	851.22 (16.97)	854.31 (14.04)	849.1 (13.0)	850.5 (11.7)
ν_{12}		H-C-C Wag	967.18 (0.18)	977.21 (0.42)	n. o.	n. o.
ν_{13}		H-C-C Rock	964.65 (0.33)	953.12 (0.04)	n. o.	n. o.
$2\nu_6$		O-H Bend	1117.83 (8.28)	1124.85 (6.87)	1119.5 (22.5)	1119.5 (22.5)
ν_{14}	A”	C-C-C Scissor	197.25 (2.81)	197.19 (0.44)	n. o.	n. o.
ν_{15}		C=C-C Scissor	348.48 (3.05)	348.30 (2.32)	n. o.	n. o.
ν_{16}		N-C-C Scissor	402.69 (6.98)	402.32 (9.71)	n. o.	n. o.
ν_{17}		O-C-C Scissor	502.77 (3.58)	501.98 (8.03)	n. o.	n. o.
ν_{18}		O-C-O Scissor	591.16 (41.27)	591.67 (37.82)	n. o.	n. o.
ν_{19}		C=C-C Scissor	626.22 (0.17)	625.73 (1.04)	n. o.	n. o.
ν_{20}		O-C-O Scissor	721.73 (19.67)	721.77 (18.91)	737.6 (36.4)	737.6 (36.4)
ν_{21}		C=C-C Scissor	826.94 (1.29)	826.89 (1.36)	n. o.	n. o.
ν_{22}		H-C-C Wag	984.84 (1.99)	984.84 (1.43)	997.3 (8.3)	997.3 (8.3)
ν_{23}		H-C-C Rock	1083.84 (70.35)	1078.48 (49.80)	1079.5 (49.0)	1077.2 (35.3)
ν_{24}		O-C-C Stretch	1091.25 (0.75)	1093.57 (20.98)	n. o.	1095.3 (25.6)
ν_{25}		H-C-C Bend	1134.02 (132.18)	1134.69 (183.40)	1137.4 (92.3)	1137.4 (92.3)
ν_{26}		H-N-C Bend	1159.28 (28.95)	1159.38 (19.03)	n. o.	n. o.
ν_{27}		H-O-C Scissor	1175.83 (103.46)	1176.46 (109.87)	1180.8 (24.0)	1184.2 (100.00)
ν_{28}		C-H Rock	1284.48 (9.83)	1284.88 (36.69)	n. o.	n. o.
ν_{29}		C-N Stretch	1280.07 (0.57)	1276.05 (0.19)	n. o.	n. o.
ν_{30}		H-N-C Stretch	1348.41 (13.87)	1336.48 (82.29)	1329.3*	1329.3*

					1332.0*	1332.0*
ν_{31}		C-C-O Bend	1362.56 (147.40)	1369.37 (20.75)	1374.6 (13.5)	1374.6 (13.5)
ν_{32}		C=C Asym. Str.	1420.91 (15.27)	1420.76 (14.69)	1423.3 (5.8) 1429.5 (5.9)	1423.3 (5.8) 1429.5 (5.9)
ν_{33}		C=C Sym. Str.	1455.42 (19.56)	1450.59 (6.26)	1461.1 (3.3)	1460.0 (1.1)
ν_{34}		C=C-C Asym. Str.	1514.64 (0.74)	1515.47 (20.46)	n. o.	1518.5 (4.5)
ν_{35}		C=C-C Asym. Str.	1569.31 (0.10)	1569.07 (0.67)	n. o.	n. o.
ν_{36}		C=O Stretch	1764.16 (196.99)	1765.90 (92.99)	1744 – 1746*	1744 – 1746*
ν_{37}		C-H Asym. Str.	3035.31 (8.71)	3036.04 (8.42)	n. o.	n. o.
ν_{38}		C-H Sym. Str.	3069.40 (2.87)	3072.62 (6.48)	n. o.	n. o.
ν_{39}		C-H Asym. Str.	3068.19 (1.31)	3068.53 (1.28)	n. o.	n. o.
ν_{40}		C-H Sym. Str.	3082.43 (3.25)	3081.33 (1.33)	n. o.	n. o.
ν_{41}		N-H Stretch	3205.58 (4.48)	3203.48 (5.36)	n. o.	n. o.
ν_{42}		O-H Stretch	3531.75 (81.52)	3535.61 (81.74)	3570.9 (2.3); 3572.7 (15.5); 3574.3 (29.0); 3575.5 (41.3)	3570.9 (2.3); 3572.7 (15.5); 3574.3 (29.0); 3575.5 (41.3)

Theoretical calculated with B3LYP / cc-pVDZ Anharmonic
Intensities in km/mol
Experimental intensities are relative to 1184.2 cm^{-1} peak
*PABA radical peak overlaps with a PABA peak
Two values are given for doublet peaks
n. o. = not observed

Table S7: Other photoproducts observed following PABA irradiation.

Photoproduct	**Previously Recorded (cm^{-1})**	**$p$$H_2$ Matrix (cm^{-1})**
trans-HOCO ν_3	1210.3	1210.3
trans-HOCO ν_2	1845.1	1845.1
Unknown Ketene	---	2124.6
CO	2142.1	2142.1
CO_2	2343.1	2343.1
trans-HOCO ν_1	3612.2	3612.2

Table S8: The frequencies and intensities of the PABA radical Conformer **(III)** and Conformer **(IV).**

Mode	Sym	Assignment	Conformer (III) Frequency (cm^{-1})	Conformer (III) Intensity (km mol^{-1})	Conformer (IV) Frequency (cm^{-1})	Conformer (IV) Intensity (km mol^{-1})
ν_1	A	O-C-O Wag	50.35	8.54	52.03	4.73
ν_2		C-C Bend	100.20	4.20	98.80	4.74
ν_3		C=C Wag	258.80	1.77	258.26	2.73
ν_4		C=C Wag	379.28	1.49	381.25	15.90
ν_5		C=C-C Wag	405.00	79.67	391.25	114.27
ν_6		O-H OOP Bend	509.65	8.51	510.81	2.76
ν_7		H-N-C Bend	668.55	704.74	666.55	117.31
ν_8		C-H Bend	674.44	4007.59	675.15	2636.93
ν_9		C-C-C Bend	768.73	12.77	768.66	14.93
ν_{10}		C-H OOP Bend	800.30	1.04	796.04	8.28
ν_{11}		C-C-C Bend	843.44	26.68	855.48	15.55
ν_{12}		H-C-C Wag	973.58	0.37	980.51	1.67
ν_{13}		H-C-C Rock	940.55	0.34	925.39	0.20
$2\nu_6$		O-H Bend	1017.75	0.11	1020.12	0.13
ν_{14}		C-C-C Scissor	205.20	14.65	202.67	9.33
ν_{15}		C=C-C Scissor	344.15	0.92	342.54	2.53
ν_{16}		N-C-C Scissor	403.47	2.43	404.16	13.94
ν_{17}		O-C-C Scissor	471.98	8.82	463.85	5.49
ν_{18}		O-C-O Scissor	599.12	7.65	598.81	6.27
ν_{19}		C=C-C Scissor	626.86	0.03	626.38	1.22
ν_{20}		O-C-O Scissor	743.55	4.65	742.49	8.52
ν_{21}		C=C-C Scissor	829.34	1.22	829.36	1.67
ν_{22}		H-C-C Wag	980.24	2.25	982.84	0.52
ν_{23}		H-C-C Rock	1074.20	13.00	1072.39	20.04
ν_{24}		O-C-C Stretch	1093.04	12.75	1095.89	11.30
ν_{25}		H-C-C Bend	1141.25	20.32	1140.62	32.83
ν_{26}		H-N-C Bend	1157.40	8.66	1161.26	22.20
ν_{27}		H-O-C Scissor	1187.86	10.31	1168.25	19.65
ν_{28}		C-H Rock	1289.31	58.66	1285.18	10.55
ν_{29}		C-N Stretch	1279.82	59.88	1282.74	33.72
ν_{30}		H-N-C Stretch	1300.79	219.58	1297.00	483.88
ν_{31}		C-C-O Bend	1361.58	19.62	1352.31	2.05

ν_{32}		C=C Asym. Str.	1420.55	19.97	1423.90	12.21
ν_{33}		C=C Sym. Str.	1449.77	11.39	1448.29	2.44
ν_{34}		C=C-C Asym. Str.	1512.18	0.02	1512.75	3.00
ν_{35}		C=C-C Asym. Str.	1563.76	0.05	1564.64	0.98
ν_{36}		C=O Stretch	1786.44	196.76	1787.89	182.16
ν_{37}		C-H Asym. Str.	3003.48	7.95	3005.98	14.59
ν_{38}		C-H Sym. Str.	3061.01	3.30	3062.16	1.31
ν_{39}		C-H Asym. Str.	3026.31	19.40	3030.24	8.02
ν_{40}		C-H Sym. Str.	3064.70	2.32	3068.65	2.58
ν_{41}		N-H Stretch	3229.16	3.08	3225.34	4.03
ν_{42}		O-H Stretch	3577.19	26.02	3576.12	23.71

Theoretical calculated with B3LYP / cc-pVDZ Anharmonic