Photo and collision induced isomerisation of a substituted pyridinium: an ion mobility study[†]

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A cationic degradation product, formed in solution from retinal Schiff base, is examined in the gas phase using ion mobility spectrometry, photoisomerisation action spectroscopy, and collision induced dissociation (CID). The degradation product is found to be *N*-*n*-butyl-2-(β -ionylidene)-4-methylpyridinium (BIP) produced through 6π electrocyclicisation of RSB followed by protonation and loss of dihydrogen. Ion mobility measurements show that BIP exists as *trans* and *cis* isomers that can be interconverted through buffer gas collisions and by exposure to light, with a maximum response at $\lambda = 420$ nm. The BIP molecule, which is easily generated from RSB, has possible applications as a photoactivated molecular switch.

1 Introduction

Fig. 1 Retinal protonated Schiff base (RPSB), and *trans* and *cis* isomers of *N*-*n*-butyl-2-(β -ionylidene)-4-methylpyridinium (BIP), which can be interconverted with UV/visible light or buffer gas collisions. Note that the displayed 9-*cis* BIP isomer is a representative *cis* isomer.

One of the more remarkable aspects of biology is that a single molecule can perform different functions according to its environment and context. One prominent example is retinal protonated Schiff base (RPSB, Fig. 1), which serves as the key photoactive molecule in the visual receptors of animals, and also as the primary light-activated molecule in proton and

chloride ion pumps in microbes.^{1,2} In these examples the primary photoresponse is the structural rearrangement of the retinal molecule.³ *In vivo*, the opsin-hosted RPSB chromophore is photo-stable, and is recycled for many visual phototransduction events. However, as light sensitive structures (e.g. the eyes of vertebrates) age, the concentration of fluorescent lipofuscin granules associated with lysosomal digestion of the cell increases. The lipofuscin granules are known to contain several bisretinoid species including A2E and all-*trans* retinal dimer, which are formed from retinal through dimerisation and condensation pathways. These pigments are associated with age-related macular degeneration and vision loss.^{4–6}

Degradation of RPSB outside the cellular environment has been examined in several studies. For example, it was recently shown that photofragmentation of RPSB in the gas phase produces the protonated Schiff base of β -ionone, through elimination of toluene following intramolecular cyclisation of the polyene chain.^{7,8} Other degradation mechanisms are important in solution. Okamura and coworkers investigated the 6π electrocyclicisation of retinal Schiff base (RSB) in C_6D_6 to form a dihydropyridine (DHP, Fig. 2), in a process that occurs more rapidly for 13-*cis* RSB than *trans* RSB.⁹ As shown in Fig. 2, protonation of DHP might reasonably be expected to be followed by dihydrogen loss and formation of the BIP cation [*N*-*n*-butyl-2-(β -ionylidene)-4-methylpyridinium (m/z 338)].

Our interest in the BIP cation was prompted by a recognition that although an acidified, fresh solution of RSB, when electrosprayed, produced mainly RPSB ($m/z=340$), as the solution aged over several days, the main electrosprayed ion became one with $m/z=338$ (corresponding to loss of H_2).⁷ In the current study we have used ion mobility spectrometry (IMS), collision induced dissociation (CID) mass spectrometry and density functional theory (DFT) calculations to investigate the

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$m/z=338$ cation and confirm that it is indeed BIP. Furthermore, using ion mobility mass spectrometry, we demonstrate that BIP has two geometrical isomers that are interconvertible in the gas phase with visible/UV light or by collisions with N_2 buffer gas. Because it is easy to generate from RPSB and can be reversibly photoisomerised, BIP may be appropriate as the core molecular unit for light-activated molecular machines.

Fig. 2 Successive transformation of RSB to dihydropyridine (DHP), protonated dihydropyridine (PDHP), and *N*-*n*-butyl-2-(β -ionylidene)-4-methylpyridinium (BIP).

2 Experimental Details

Fig. 3 Tandem ion mobility spectrometer. Electrosprayed ions accumulate in the first ion funnel (IF1) and are periodically launched through an ion gate (IG1) into the first drift region (IMS 1) where they travel through N_2 buffer gas ($P \approx 6.2$ Torr) propelled by an electric field ($E \approx 44$ V cm^{-1}). The ions encounter a second ion gate (IG2) that can be opened to pass mobility-selected isomers. Immediately after IG2, ions can be irradiated with light from a tunable OPO. Alternatively, the ions can be energised in the collisional excitation region (slammer), where an adjustable potential difference is applied between grid electrodes separated by 3 mm. After travelling through the second drift region (IMS 2), the ions are collected by an ion funnel (IF2), and pass through an octopole and quadrupole mass filter before striking a detector.

The $m/z=338$ degradation product of RPSB was examined using a custom-built tandem ion mobility apparatus in which different isomers are separated and are characterised by their drift mobility and by their isomerisation behaviour following exposure to light [photoisomerisation action (PISA) spectroscopy] or collisions with buffer gas molecules [collisional induced isomerisation (CII)]. The tandem ion mobility spectrometer and photoisomerisation action spectroscopy approach have been described previously and further details are given below.^{10–13} High resolution CID mass spectra and MS^n spectra for BIP cations and fragment ions were collected using a Thermo Scientific XL Hybrid Ion Trap-Orbitrap mass spectrometer and a modified Thermo Scientific LTQ XL mass spectrometer, respectively. Details of the supporting CID measurements are given in the ESI.

Arrangements for the ion mobility experiments are illustrated in Fig. 3 and can be described as follows. Briefly, electrosprayed cations, produced from a degraded 10^{-4} M solution of acidified RSB in methanol/water (electrospray voltage ≈ 3 kV, flow rate ≈ 10 $\mu L/min$), were accumulated in an ion funnel before being launched in 100 μs pulses at 20 Hz into a 0.9 m drift tube filled with N_2 buffer gas ($P \approx 6.2$ Torr, $E=44$ V/cm). At the end of the drift tube, the ions were gathered radially by a second ion funnel before passing through a 0.3 mm orifice into an octopole ion guide from where they exit through a second 3 mm orifice into a quadrupole mass filter. Mass-selected ions were sensed by a channeltron detector connected to a discriminator and a multichannel scaler. The ions' arrival time distribution (ATD) was built up as a histogram of ion counts versus time. The mobility resolution for the BIP cations is typically $t_d/\Delta t_d = 70$ –80.¹² Under the prevailing operating conditions the effective temperature of the ions is predicted to be ≈ 310 K.¹⁴

When operated in tandem IMS-photo-IMS mode, alternate ion packets were irradiated 7.5 mm after IG2 with light from a pulsed, tunable optical parametric oscillator (OPO, 10 Hz, $\lambda = 320$ –710 nm, 10 ns pulse width, 5 cm^{-1} bandwidth). The photo-induced change is reflected in the difference between laser-on and laser-off ATDs. Care was taken to avoid saturating the electronic transitions. Typically, the pulse energy was 5–10 mJ/pulse and beam cross section 5 cm^2 , corresponding to a fluence of 1–2 mJ/ cm^2 /pulse. At these light levels, photodissociation of the BIP ions was negligible. Note that we were unable to measure the photoisomerisation response below 320 nm due to interference by a background produced from photoionisation of impurities in the drift gas.

The collisional excitation region (slammer) consists of two copper mesh electrodes separated by 3 mm between which an adjustable potential difference can be applied, and which are situated 15 mm after IG2. For sufficiently high electric fields, collisions with N_2 buffer gas cause the BIP ions to isomerise. Parent and daughter isomer ions are separated in the second

drift region. As demonstrated by Clemmer and coworkers,¹⁶ by monitoring CII as a function of the electric field strength, one can derive information on barrier heights for molecular rearrangements.

Normally, the potential difference between the slammer electrodes is 20 V, corresponding to an electric field in the slammer region of 60 Vcm⁻¹. The electric field between the two electrodes was increased by raising the voltages on all upstream electrodes such that the electric fields throughout the rest of the instrument remained constant. Under normal operating conditions, the highest potential difference between the grids attainable before electrical breakdown was 320 V.

RPSB was synthesised under exclusion of light in an Ar atmosphere according to previous methods.¹⁷ *Trans* retinal (Sigma Aldrich) was dissolved in excess *n*-butylamine (Sigma Aldrich) and allowed to react at 10° C until ¹H NMR showed no evidence of the aldehyde carbonyl signal at ≈ 10 ppm. 2,4-lutidine cations were electrosprayed from a 10⁻⁴ M solution of 2,4-lutidine (Sigma Aldrich, 99%) in 1:1 mixture of methanol and H₂O with 0.2% acetic acid.

3 Results and discussion

3.1 Formation of the *m/z*=338 cation

Fig. 4 Ion mobility spectra of RPSB (*m/z*=340) and BIP (*m/z* 338) showing evidence for *trans* and *cis* BIP isomers. Peak assignments are discussed in the text and given in Table 1.

The *m/z*=338 cation was observed whenever acidified RSB samples were electrosprayed, becoming more abundant as the solution ages, and eventually becoming the predominant ion. As shown in Fig. 4, the ATD for the *m/z*=338 cation exhibits two distinct peaks, labelled X and Y, with a ≈3:1 intensity ratio. The measured collision cross sections (Ω_m) for the two *m/z*=338 isomers with N₂ are 8-12% less than *trans* RPSB (isomer A), indicating that they have more compact structures. Indeed, their collision cross sections are similar to those of the RPSB isomers C' and D, which have been assigned to cyclic

or triple-*cis* forms.^{17,18} Okamura *et al.* found that under relatively mild conditions, RSB in solution undergoes facile 6 π electrocycloislation from the 12,13,14-*cis* form to give the cyclic DHP structure, according to the scheme shown in Fig. 2.^{9,19} Upon preparing the neutral *n*-butylamine Schiff base of 13-*cis* retinal, they found that the initial mixture contained 7% DHP, along with 8% all-*trans* and 85% 13-*cis* RSB.⁹ Heating at 78°C in C₆D₆ for 30 minutes produced a 2:5:3 ratio of 13-*cis* RSB, *trans* RSB, and the DHP form. The efficiency of the 6 π electrocycloislation process was explained by Tanaka *et al.* as due to favourable HOMO-LUMO overlap for the 12,13,14-*cis* RSB form.²⁰ Similar 6 π electrocycloislation of the polyene chain in retinal and carotene systems has been noted in other studies.^{7,9,19,21–23}

Based on the considerations outlined above it seems most likely that the *m/z*=338 ion is the *N*-*n*-butyl-2-(β -ionylidene)-4-methylpyridinium cation (BIP, Fig.1), the dehydrogenated form of the DHP structure observed by Okamura *et al.*,⁹ formed following sequential RSB cyclisation, protonation, and H₂ loss in solution. Attempts to create the *m/z*=338 ion through collisional excitation of RPSB in the first ion funnel or in the slammer region were unsuccessful.

Table 1 Data for BIP and RPSB isomers, including M06-2X/cc-pVDZ energies relative to *trans* RPSB (corrected for vibrational zero point energy), calculated collision cross sections with N₂, and measured collision cross sections with N₂. Calculated energies and collision cross sections are averages over the 6*s-trans*, 6*s-cis*(-) and 6*s-cis*(+) configurations as explained in the ESI. A complete data compilation is given in the ESI.

Structure (calculated)	ΔE^* (kJ/mol)	$\overline{\Omega}_{calc}$ (Å ²)	ATD peak	$\Omega_m^\dagger$ (Å ²)
BIP				
<i>trans</i>	-37	204.5	X	212.4
7- <i>cis</i>	-25	201.6	} Y	203.8
9- <i>cis</i>	-39	201.1		
7,9- <i>cis</i>	-27	200.6		
RPSB[‡]				
<i>trans</i>	0	219.9	A	231.9
single- <i>cis</i>	3-24	215.7-220.3	B	226.9
double- <i>cis</i>	5-44	211.7-222.7	B,C'	226.9, 214.6
triple- <i>cis</i>	23-46	197.9-209.2	} C',D	214.6, 207.9
cyclic	1-63	192.1-210.1		

*relative energies for BIP structures correspond to [BIP+H₂]

[†] estimated absolute errors of ±5 Å² and relative errors of ±0.3 Å².

[‡] RPSB data from refs. 17 and 18

To link the measured collision cross sections for the *m/z*=338 ion with molecular structures we carried out density functional theory (DFT) calculations for different BIP iso-

mers employing the M06-2X functional with a cc-pVDZ basis set. A similar computational approach was used previously for RPSB and its isomers.^{7,18} Cyclisation of *trans* RPSB to form *trans* BIP and H₂ is predicted to be exothermic by 25 kJ/mol. The *trans* and 9-*cis* BIP isomers are calculated to be almost isoenergetic. Collision cross sections ($\bar{\Omega}_{calc}$) for the various BIP isomers with N₂ were determined using MOBCAL calculated with the trajectory method,^{24,25} with appropriate parameters for N₂ buffer gas.²⁶ The *trans* BIP isomer is calculated to have the largest collision cross section with N₂, whereas the *cis* isomers are predicted to have $\approx 2\%$ smaller cross sections. Energies and collision cross sections for the various BIP isomers are provided in Table 1.

Based on the calculated isomer collision cross sections and energies, we assign the observed ATD peaks in Fig. 4 as X = *trans* BIP, and Y = 7-*cis*, 9-*cis*, or 7,9-*cis* BIP. Note that although calculated cross sections overestimate the experimental values by 3-6%, the relative cross sections for the *trans* BIP and RPSB isomers are predicted reasonably well. At this stage we are unable to ascertain if peak Y is due to a single *cis* isomer, or if it contains contributions from all three *cis* isomers. Properties of higher energy cyclic $m/z=338$ isomers were also characterised using DFT. Structural and energetic data for these isomers are presented in the ESI.

3.2 Collision-induced dissociation of the $m/z=338$ cation

Further support for the $m/z=338$ cation's assignment to the BIP structure was obtained through MSⁿ CID mass spectra (recorded using the Orbitrap as outlined in Section 2). Masses of the main fragment ions, their molecular formulae, the corresponding neutral fragment, and MSⁿ fragmentation mass spectra are summarised in Section 4 of the ESI. The main fragmentation pathways are shown in Fig. 5. High resolution mass spectra show that all observed charged fragments contain an N atom, consistent with the proposed cyclic BIP structure. The $m/z=282$ fragment ($-C_4H_8$) can be produced either through loss of the butyl chain or through cyclisation of the polyene chain onto the ionone ring, causing ring opening and loss of C₄H₈. The smallest observed charged fragment at $m/z=108$ has the molecular formula C₇H₁₀N⁺, and is assigned as protonated 2,4-lutidine. This assignment is supported by the close match between the ATD of the $m/z=108$ fragment and a reference ATD of protonated 2,4-lutidine (shown in Fig. 6). Overall, the CID data are consistent with the proposed fragmentation cascade and BIP structure for the $m/z=338$ cation.

3.3 Photoisomerisation of BIP

Having confirmed that the $m/z=338$ cation is indeed BIP, we turn to considering the photoisomerisation of the *trans* and *cis* isomers. The target isomer was selected in the first stage

Fig. 5 Proposed collision induced dissociation pathways for the $m/z=338$ BIP cation.

of the IMS and irradiated with tunable light from an OPO. The laser-on/laser-off ATDs (Fig. 7) show that *trans* BIP is photoconverted to the more compact *cis* BIP, and vice versa. PISA spectra of the *trans* and *cis* BIP isomers (shown in Fig. 8) are very similar and exhibit a broad band with maximum response at ≈ 420 nm. The absorption maximum is shifted by ≈ 200 nm to shorter wavelength compared to RPSB, consistent with a shorter conjugated chain. The photoisomerisation response for the *trans* isomer is around twice that of the *cis* isomer. Currently, it is unclear whether this difference reflects the oscillator strengths for the electronic transitions of the two isomers or is related to the relative photoisomerisation efficiencies.

3.4 Collisional induced isomerisation of BIP

Having established the photoisomerisation behaviour of the *trans* and *cis* BIP isomers, we explored their interconversion through buffer gas collisions in the slammer region. The threshold for collision induced isomerisation of a mobility-selected BIP isomer was ascertained by scanning the potential difference between the slammer electrodes (from 20 to 320 V) while measuring the arrival time distribution of the resulting ions. As explained in the ESI, relative abundances of the parent and daughter ions were determined at each slammer

Fig. 6 Arrival time distributions ($P=6.2$ Torr, N_2 buffer gas) for: a) electrosprayed reference protonated 2,4-lutidine; and b) $m/z=108$ ions formed through collisional activation of electrosprayed ions in IF1.

potential difference, by fitting the ATD with a sum of Gaussian functions, each of which corresponds to a different isomer. The data can be analysed in terms of three isomers, the *trans* (X) and *cis* (Y) isomers, and a more compact isomer, Z, produced in minor quantities at slammer voltages exceeding 210 V. Resulting plots of isomer intensity against slammer voltage are shown in Fig. 9. As explained in the ESI, the breakdown curves were fitted with a sigmoidal function, where the threshold voltage (V_T) is defined as the voltage at which 3.5% of the parent ion population has undergone collision induced isomerisation, or at which the relative abundance of the daughter ion population reaches 3.5%.

Threshold voltages for *trans*→*cis* isomerisation (185 ± 3 V), and reverse *cis*→*trans* isomerisation (190 ± 3 V) are similar, consistent with the DFT predictions of relatively small energy differences between the *trans* and 9-*cis* geometric isomers. Although *trans* BIP (X) is formed preferentially through electrospray ionisation, at high slammer voltages (above 270 V) the *cis* forms of BIP (peak Y) begin to dominate. Possibly, this is because the higher energy 7-*cis* and 7,9-*cis* BIP isomers are also generated at elevated collision energy. It is interesting to note that no matter if the *trans* or *cis* BIP isomer was initially selected, the relative abundance of X:Y:Z at the highest attainable slammer voltage (320 V) was 0.38:0.57:0.05, suggesting that a pseudo-equilibrium between the different isomers is

Fig. 7 Arrival time distributions for mobility-selected $m/z=338$ cations. Laser off data are shown in black, and laser on/laser off difference data are represented by blue dotted lines. Estimated collision cross sections ($\text{\AA}^2$) for photoisomers are indicated by Ω . (a) IG2 opened to transmit isomer X, with alternate ion packets irradiated by 420 nm light. (b) IG2 opened to transmit isomer Y, with alternate ion packets irradiated by 420 nm light.

reached at higher collision energies. The structure of isomer Z is uncertain, but it may correspond to the retro- γ -retinylidene cation resulting from a 1-5 sigmatropic shift.

4 Conclusions

In summary, we have studied one of the main degradation products of retinal Schiff base, showing that RSB undergoes 6π electrocyclication to form the neutral DHP molecule, which, following protonation in solution, loses H_2 to form the BIP cation. Assignment of the cation to BIP is consistent with previous observations of the DHP structure in solution,⁹ and is supported by the DFT calculations, high resolution CID mass spectra, ion mobility ATDs, and PISA spectra. Significantly, BIP can be reversibly converted between *trans* and *cis* forms in the gas phase using either light ($\lambda_{\max} \approx 420$ nm) or buffer gas collisions. The reversible *cis/trans* photoisomerisation properties BIP discovered in this study may be exploited as the core unit in new light-activated molecular machines.

Another notable aspect of the work is the use of ion mobility mass spectrometry to identify the structure of a $m/z=108$ CID fragment from BIP as protonated 2,4-lutidine. Previously, we

Fig. 8 Photoisomerisation action spectra of *trans* BIP (X) and *cis* BIP (Y). The photoisomerisation response is measured as a function of wavelength, and is normalised at each wavelength by photon number.

used a similar approach to identify the main photofragment from RPSB as the protonated Schiff base of β -ionone.⁷ Using tandem IMS in this way, with either collisional or photo excitation, provides a potentially powerful route towards structural elucidation of charged molecular fragments that is less cumbersome than alternative approaches such as isotopic labelling.

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Fig. 9 Breakdown diagrams for collisional isomerisation of *trans* BIP (X, upper) and *cis* BIP (Y, lower). Selected *trans* or *cis* BIP isomers transmitted by IG2 are subjected to energetic collisions with N₂ buffer gas causing *cis/trans* isomerisation. A more compact isomer, Z, is formed in minor quantities at higher voltages.

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