## Supporting Structural Data

# Charge Shift and Triplet State Formation in the 9-Mesityl-10-Methylacridinium Cation

*Andrew C. Benniston, Anthony Harriman, Peiyi Li, James P. Rostron, Hendrik J. van Ramesdonk, Michiel, M. Groenveld, Hong Zhang and Jan W. Verhoeven*

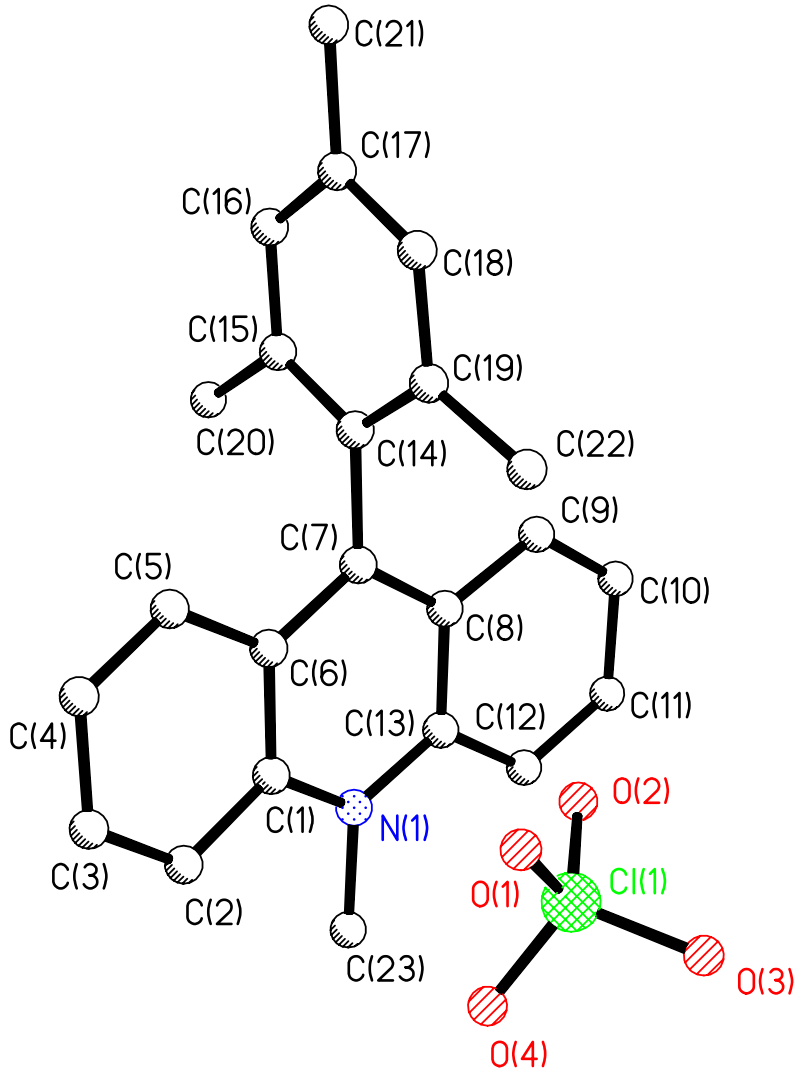


**Fig. S1.** Ball and stick representation of the X-ray molecular structure for Mes-Acr$^{+}$, as the perchlorate salt. Hydrogen atoms are omitted for clarity.

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## A N A L Y T I C A L  R E P O R T

Date 2 August, 2004

Name Dr A C Benniston – Newcastle

Sample ID ACRID

Formula $C_{23}H_{22}ClNO_4$

| ELEMENT | C | H | N | S | Cl | Br | I | | |
|---|---|---|---|---|---|---|---|---|---|
| % Theory | 67.07 | 5.38 | 3.40 | | | | | | |
| % Found 1 | 67.11 | 5.42 | 3.41 | | | | | | |
| % Found 2 | 67.07 | 5.42 | 3.42 | | | | | | |

Comments :

Assay No 100510 Analyst Richard Morris

**Fig. S2.** Elemental analysis report for Mes-Acr$^+$ $ClO_4^-$.

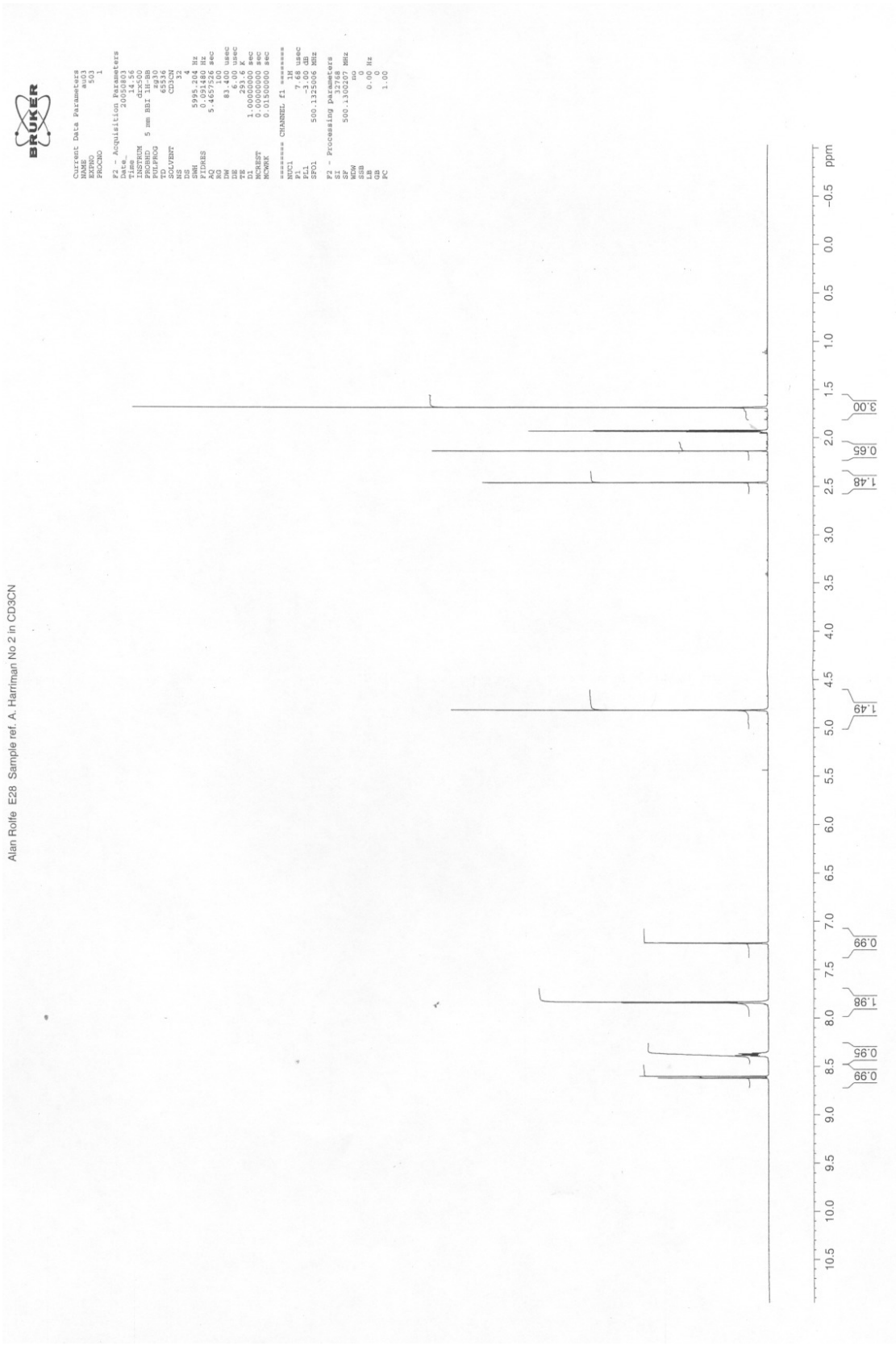


**Fig.S3** 500 MHz $^{1}$H NMR spectrum of $MesAcr^{+}ClO_4^{-}$ in $CD_3CN$ at 20 $^{o}$C.

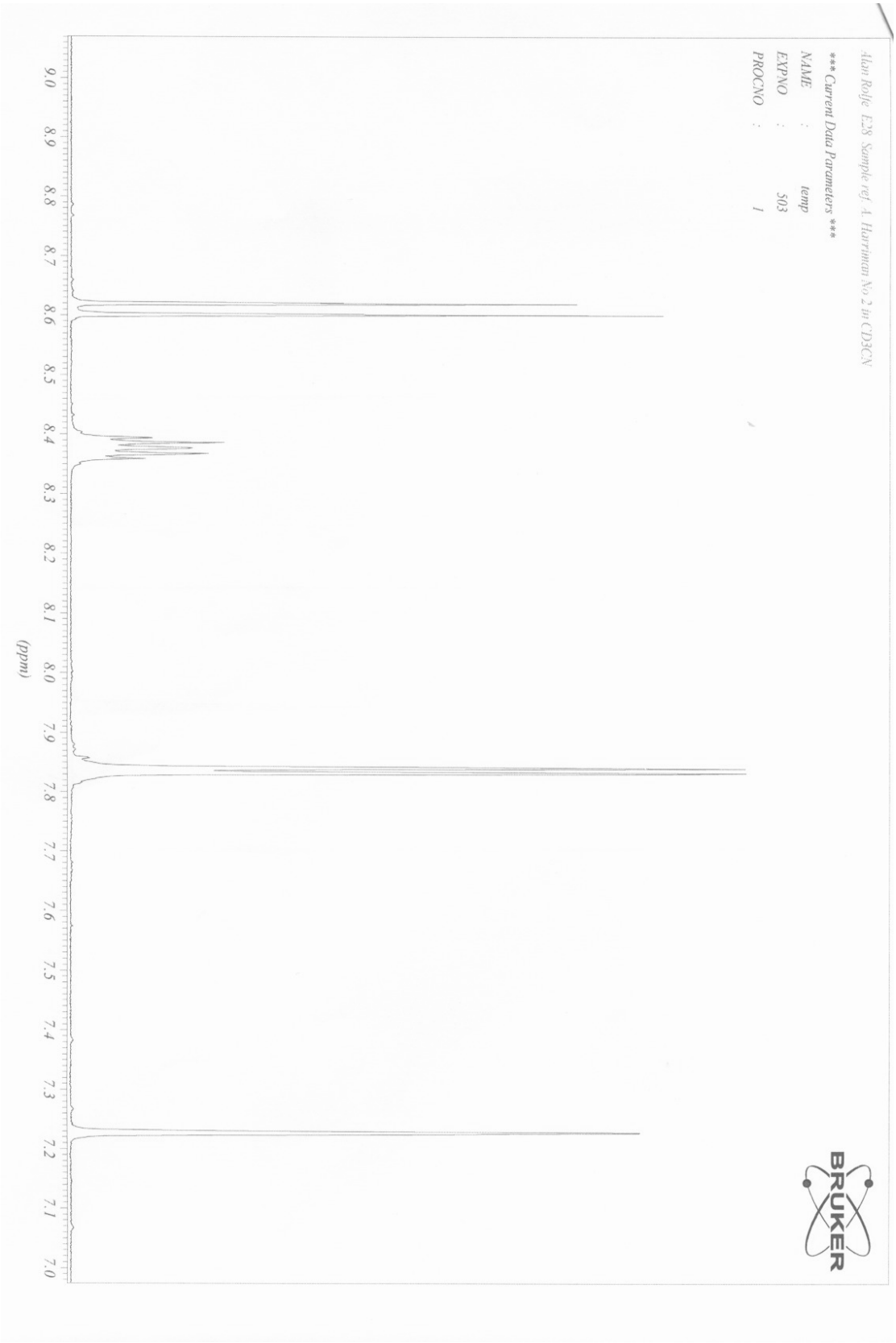


**Fig.S4** Aromatic region of the 500 MHz $^{1}$H NMR spectrum of MesAcr$^{+}$ $ClO_4^{-}$ in $CD_3CN$ at 20 $^{o}$C.

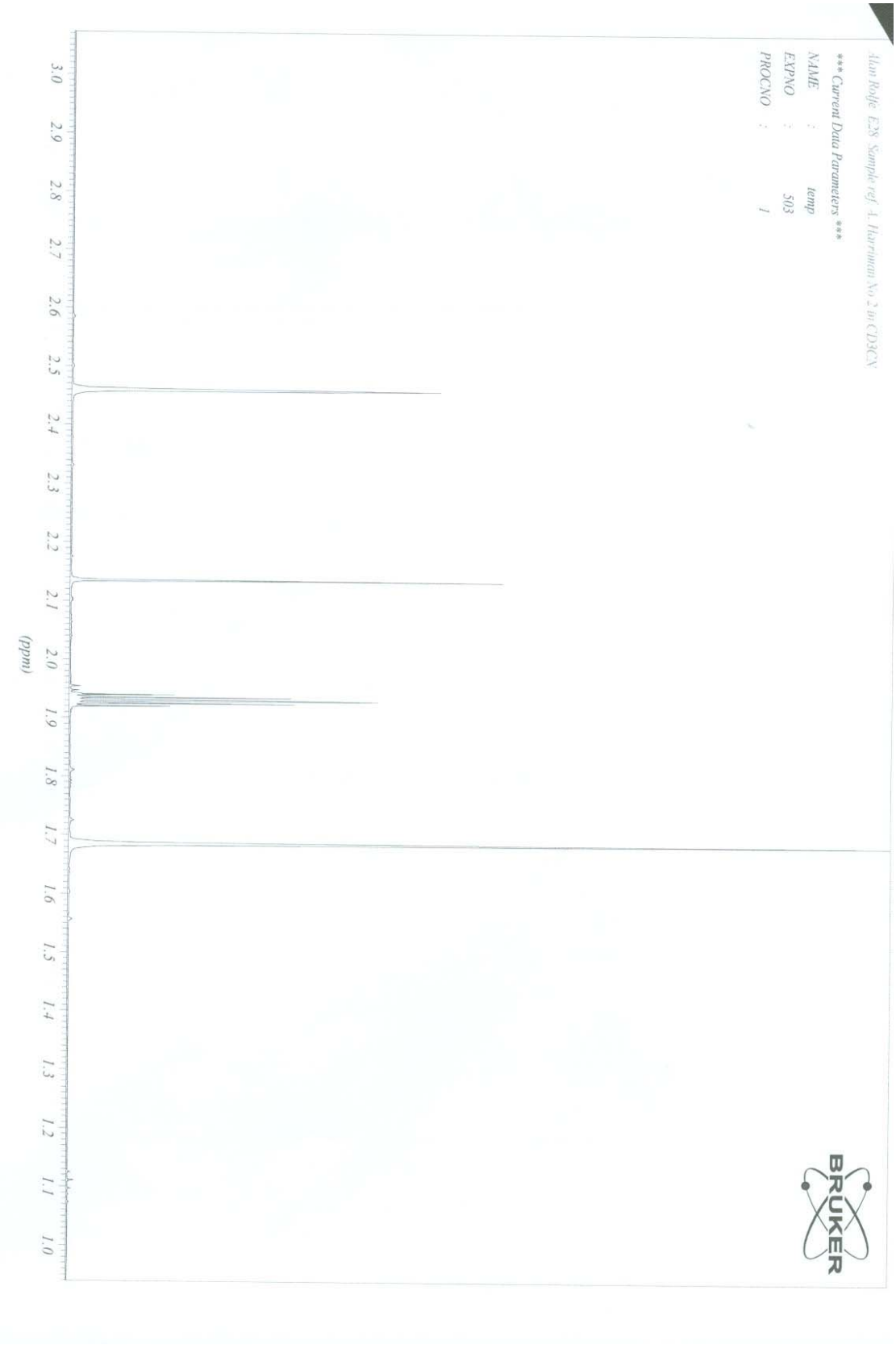


**Fig.S5** Partial 500 MHz $^{1}$H NMR spectrum of MesAcr$^{+}$ $ClO_4^{-}$ in $CD_3CN$ at 20 $^{o}$C showing the mesityl methyl protons and the solvent reference signal at $\delta$ = 1.93.

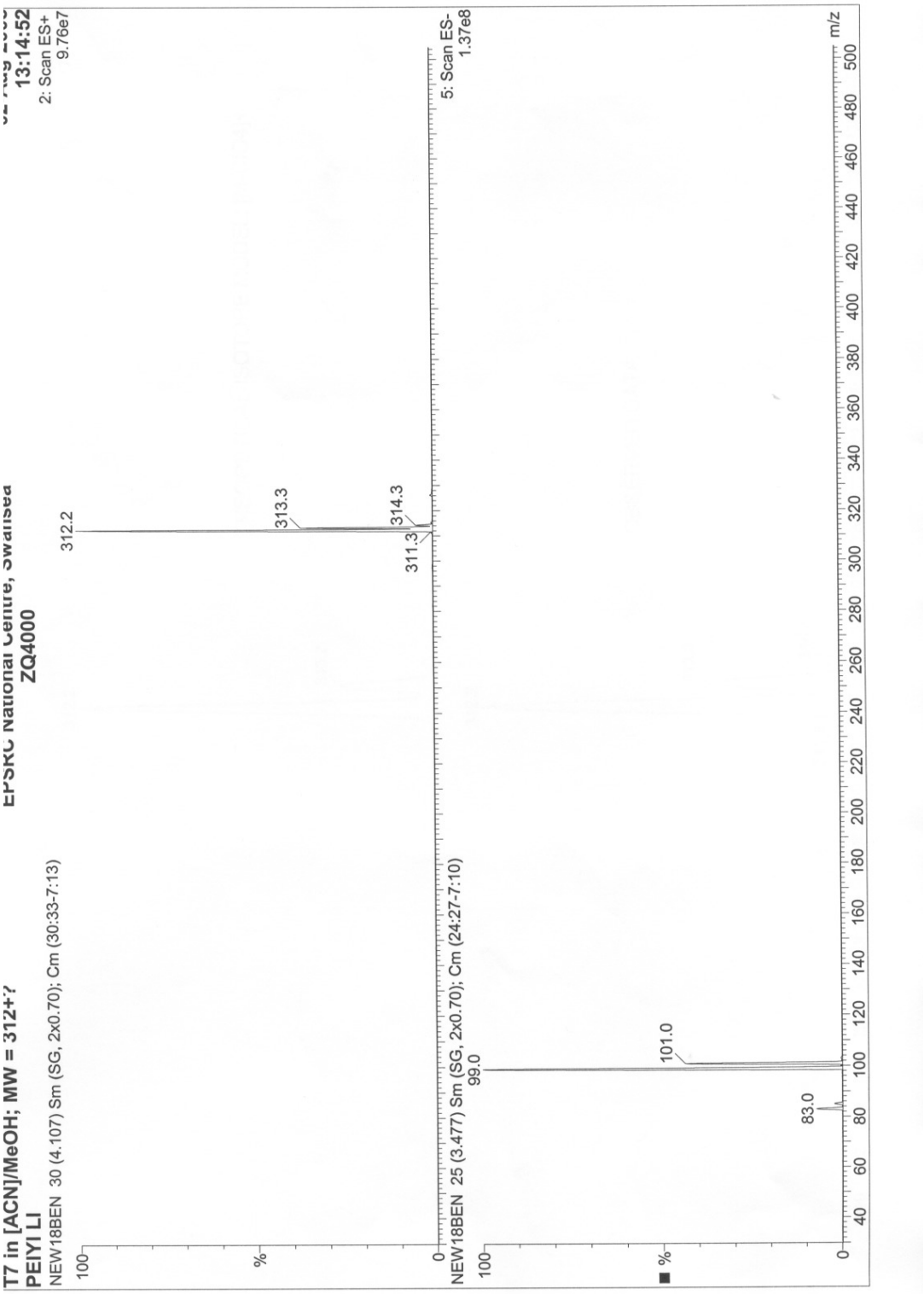


**Fig. S6** Electrospray mass spectrum of $MesAcr^{+}\ ClO_4^{-}$ showing the $[M\text{-}ClO_4]^{+}$ ion and the $ClO_4^{-}$ ion.

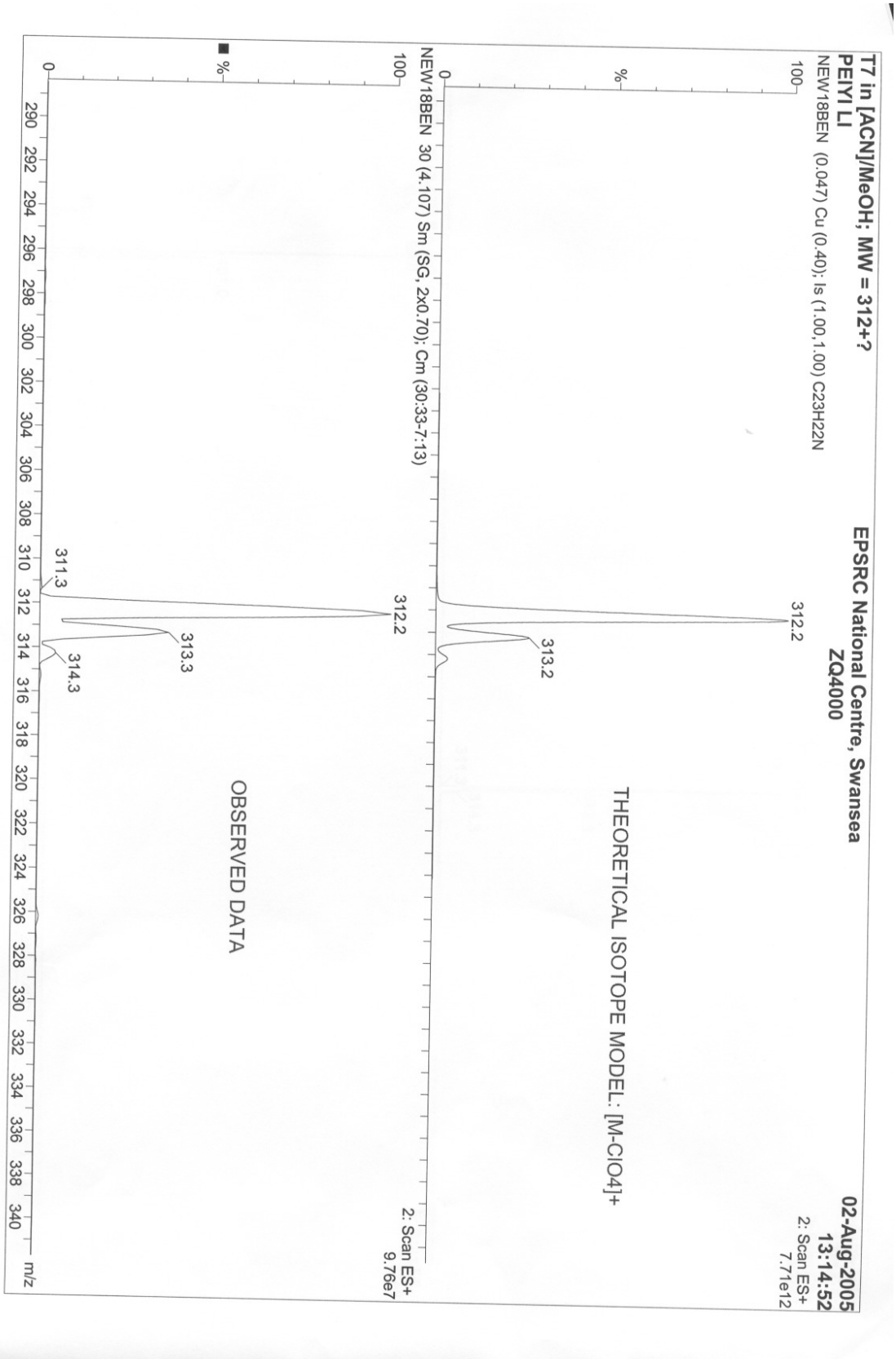


**Fig. S7** Comparison of the theoretical and observed electrospray mass spectral data for $MesAcr^{+}ClO_4^{-}$.

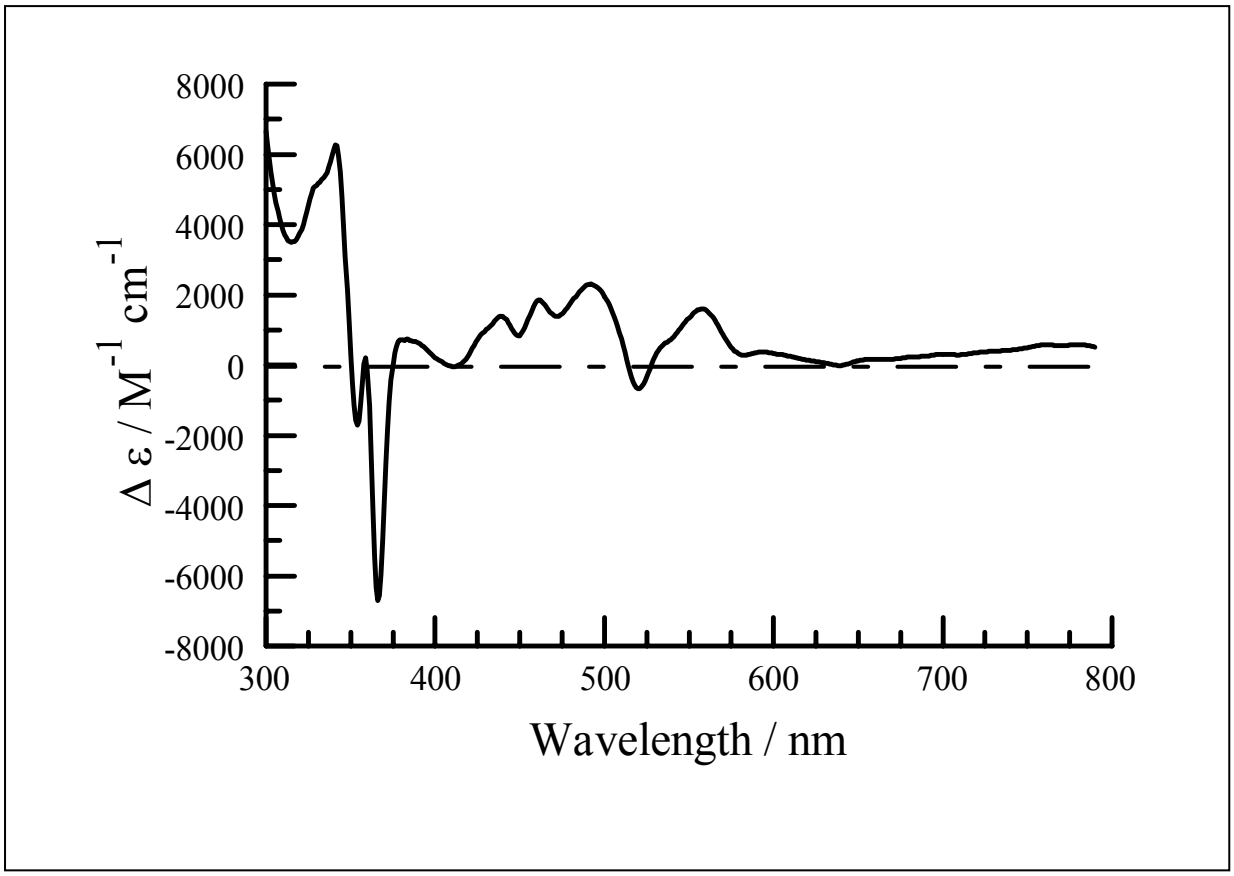


**Fig. S8** Difference between the transient absorption spectra recorded for the triplet state of Mes-Acr+ and the acridinyl radical in deoxygenated acetonitrile solution.

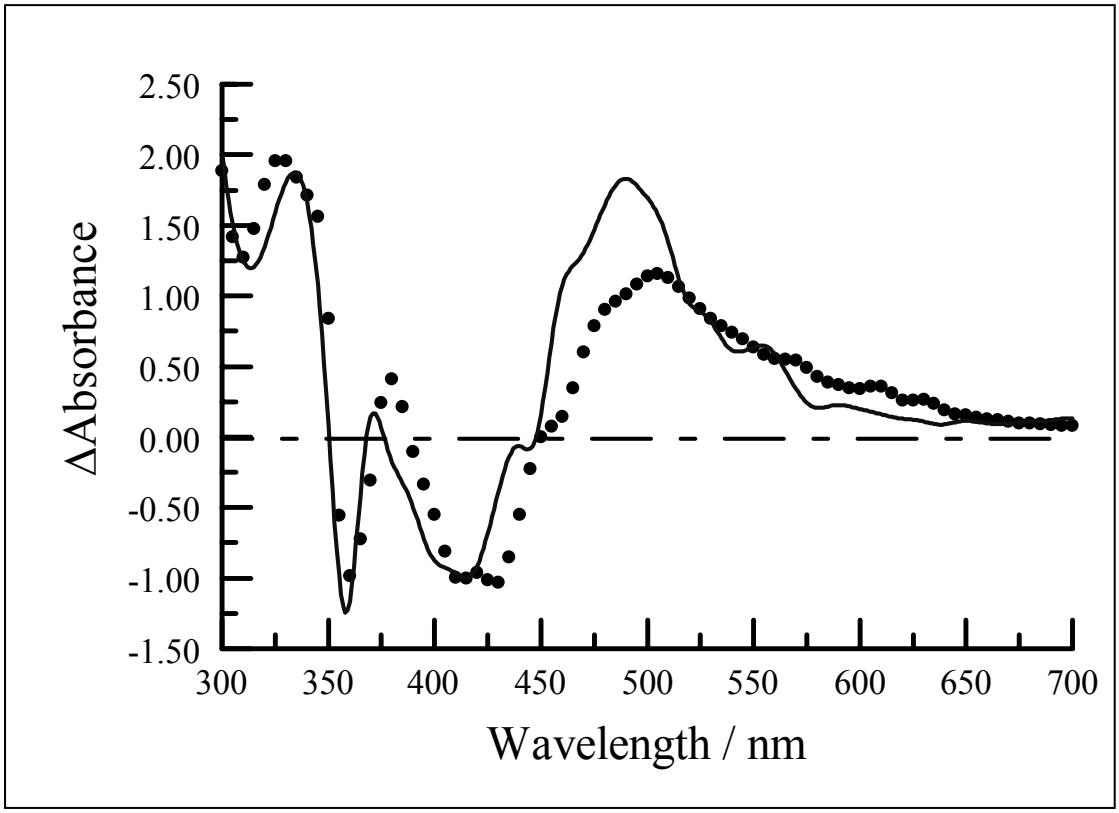


**Fig. S9** Comparison of the transient absorption spectra recorded for the triplet excited states of **Mes-Acr**$^+$ (solid line) and 9-phenyl-10-methylacridiunium perchlorate (solid points) in deoxygenated acetonitrile. The latter sample contained 10% v/v iodoethane.

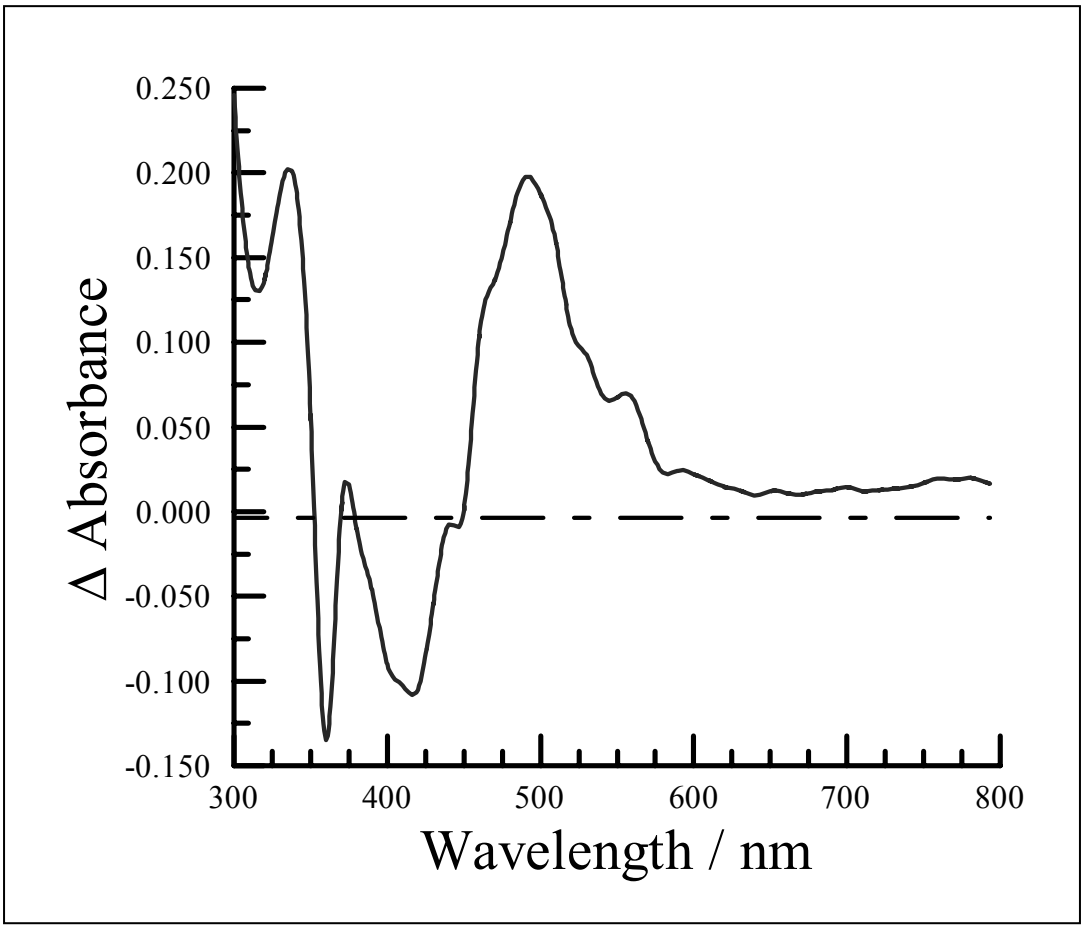


**Fig S10** Transient differential absorption spectrum obtained on laser excitation of **Mes-Acr**$^{+}$ in deoxygenated butyronitrile at 77 K.