Electronic Supplementary Material (ESI) for ChemComm.

-ELECTRONIC SUPPORTING INFORMATION-

Electrocatalytic oxidative *Z-E* isomerization of a stilbene favoured by the presence of an electroactive persistent radical

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1. General Details.

All reactions were carried out using solvents which were dried by routine procedures. Starting compounds were purchased from Sigma Aldrich and used without further purification.

Infrared (IR) spectra were obtained in transmission mode with a Jasco 4700 Fourier transform (FTIR) spectrometer in the spectral range from 400-4000 cm^{-1} with a resolution of 4 cm^{-1} and 32 scans.

A JASCO V-780 UV-visible/NIR spectrophotometer was used for the UV-Vis-NIR electronic absorption spectroscopy measurements.

^{1}H and ^{13}C NMR spectra were recorded at 250 or 400 MHz in a Bruker Advance apparatus. The following abbreviations for stating the multiplicity of the signals have been used: s (singlet), bs (broad singlet), d (doublet), t (triplet), bt (broad triplet), st (pseudotriplet), m (multiplet), and q (quaternary carbon atom). Chemical shifts refer to signals of tetramethylsilane in the case of ^{1}H and ^{13}C NMR spectra.

ESR spectra were obtained with a Bruker 300 spectrometer equipped with a TE 102 microwave cavity, a variable temperature unit, and a field frequency lock system, and line positions were determined with a NMR gaussmeter. The modulation amplitude was kept well below the line width, and the microwave power was well below saturation.

The cyclic voltammetric measurements were performed on Autolab electrochemical analyzer (PGSTAT 204 potentiostat/galvanostat) with NOVA 1.9 software and a conventional three-electrode configuration: WE = Au or Pt wire, CE = Pt wire and RE= Ag wire. Ferrocene was used as internal reference. The experiments were carried out with a 10^{-3} M solution of the compounds in dry CH_2Cl_2 containing 0.2 M of $[(n\text{-}Bu)_4N]PF_6$ as supporting electrolyte. Deoxygenation of the solutions was achieved by bubbling nitrogen for at least 10 min.

Time-of-flight secondary ion mass spectrometric (ToF-SIMS) measurements were recorded under the following specific analysis conditions: primary gun energy 25 KV, extractor energy 8.5 KV, emission current 1.05 mA, employing Bi^{3+} with an intensity of the primary ions of 0.25 pA. The experiments were performed in vacuum at $8.3 \cdot 10^{-9}$ mbar. The spot size was $200 \cdot 200$ μm, with a resolution of $128 \cdot 128$ pixels, collecting in excess of $1 \cdot 10^{12}$ of ionic intensity per spectrum.

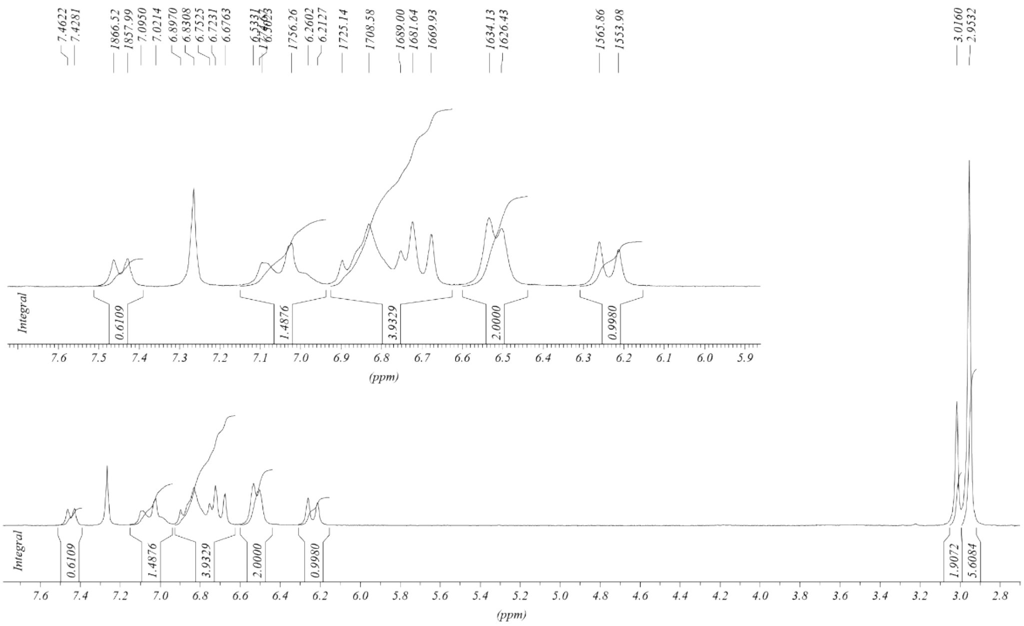
Spectroelectrochemistry measurement were performed with the help of a thin-layer cell from a demountable omni cell from Specac (WE = CE = Pt gauze and RE= silver wire). All the spectra were collected at constant potential electrolysis at r.t. and a 400 nm/min a scan rate..

2. Synthetic procedures

Synthesis of 4-(bis(perchlorophenyl)methyl)-2,3,5,6-tetrachlorostyryl)-*N,N*-dimethylamine (αH-PTM-DMA).

Diethyl (4-(bis(perchlorophenyl)methyl)-2,3,5,6-tetrachlorobenzyl)-phosphonate (450 mg, 0.513 mmol) **1** was placed in a dry 25 mL Schlenk flask under argon atmosphere. Dry THF (10 mL) was added to dissolve the reagent and the flask was cooled at -78° C (acetone/liquid N_2 bath). Afterwards, potassium *tert*-butoxide (62 mg, 0.552 mmol) was added and the mixture stirred for 30 minutes. To the resulting intense yellow-orange solution, 4-dimethylamine-benzaldehyde (75 mg, 0.503 mmol,) dissolved in dry THF (4 mL) was added dropwise and the solution stirred for a further 72 h at ambient temperature. The dark solution was quenched upon addition of aqueous 0.1 M HCl drops until a yellow suspension was obtained. Water (8 mL) was added and neutralized and the crude product was extracted with CH_2Cl_2 (3 x 20 mL). The combined organic layers were washed with water, dried over Na_2SO_4, filtered off and evaporated under reduced pressure. The *E/Z* proportion of compound **αH-PTM-DM** in the crude product was 25/75 based on the CH_3 protons is NMR spectrum. Finally, chromatographic purification (SiO_2, hexane/CH_2Cl_2 90/10), yielded a mixture of E/Z isomers of the compound **αH-PTM-DM** as a yellow powder (290 mg; 66% yield). Only one fraction of the column yielded almost pure *Z* isomer (Fig S2). A small quantity of the pure *E* and *Z* isomers were separated by preparative thin layer chromatography. Anal. Calc. for $C_{29}H_{13}Cl_{14}N$: C, 39,96; H, 1,50; N, 1,61. Found: C, 39,67; H, 1,70; N, 1,85; mp *Z isomer* 160 °C; *E isomer* 168 °C dec. **^{1}H NMR** (250 MHz, $CDCl_3$): *Z isomer*, δ/ppm = 7.04 (m, 1H), 6.82 (m, 2H), 6,73 (d, 1H, ^3J = 11.9 Hz, vinyl-H), 6.52 (d, 2H, ^3J = 7.9 Hz, Ar-H), 6.23 (d, 2H, ^3J = 11.9 Hz, vinyl-H), 2.95 (s, 6H) ppm; *E isomer*, δ/ppm = 7.44 (d, 2H, ^3J = 8.6 Hz, Ar-H), 7,05 (d, 2H; ^3J = 16.5 Hz, vinyl-H), 7.01 (s, 1H αH) 6.86 (d, 1H ^3J = 16.5 Hz, vinyl-H), 6.73 (d, 2H, ^3J = 8.6 Hz, Ar-H), 3.02 (s, 6H). **^{13}C NMR (101 MHz, CD_2Cl_2) δ(ppm) =** 151.53, 151.41, 139.16, 138.75, 137.29, 135.66, 135.41, 135.10, 134.52, 134.25, 133.91, 133.73, 132.89, 132.83, 132.57, 129.79, 128.53, 124.33, 120.41, 118.62, 112.58, 112.10, 102.18, 57.11(**αH-C)**, 54.38, 54.11, 53.84, 53.57, 53.30, 40.53(**-N-(CH_3)$_2$**), 40.34. **EM (m/z) (MALDI-ToF)** calc. for $C_{29}H_{13}Cl_{14}N$, 870,66; found, 869,25 $[M-H]^+$. **UV-Vis.** (λ_{max} / nm (ε / $M^{-1}cm^{-1}$)): *Z isomer* 300 (9942), 365(6666,68); *E isomer*, 289 (11774),379 (21066)

a)



b)

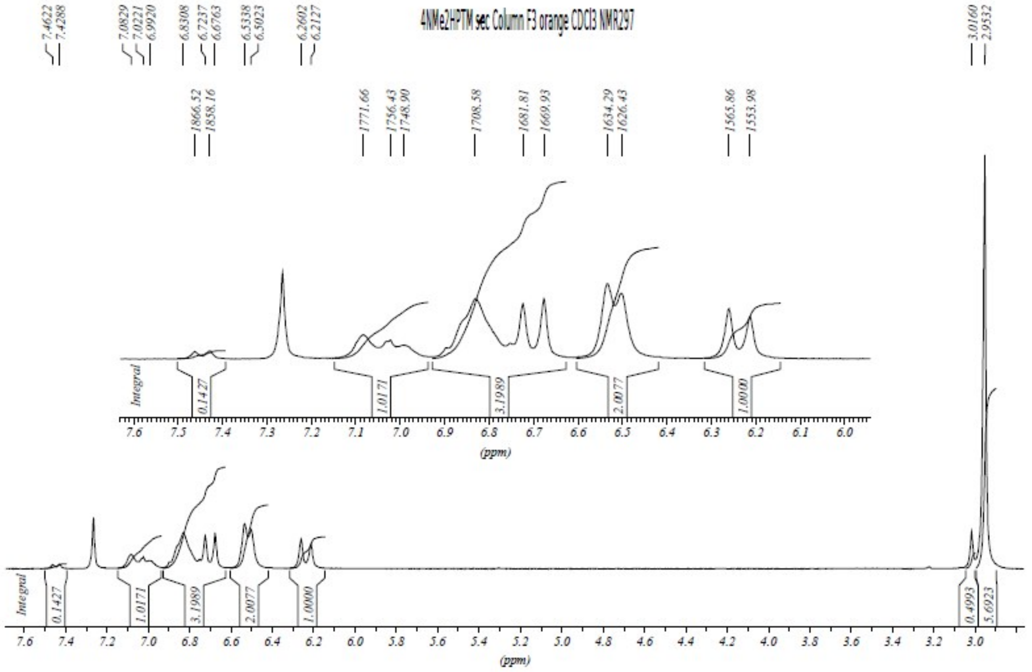


Figure S1- ^{1}H NMR spectrum of a) as synthesized and b) the column fraction containing the most ***Z*-αH-PTM-DMA** enriched fraction (92 %).

When both, the reaction and the purification were performed in a laboratory equipped with red light, the proportion of the *E/Z* isomers was 95/5 (NMR Figure S2). The reason of the large difference in the *E/Z* isomers ratio is that that **-αH-PTM-DMA** undergoes *E-Z* isomerization upon white light illumination as happens with some related αH-PTM stilbenes.[1] Figure S3 shows the changes observed in the NMR spectrum of ***Z*-αH-PTM-DMA** upon exposure to laboratory ambient light for 3 hours. The observed changes in the peaks corresponding to the CH3 protons confirm the increasing of the Z isomer proportion from 15% to 25%.

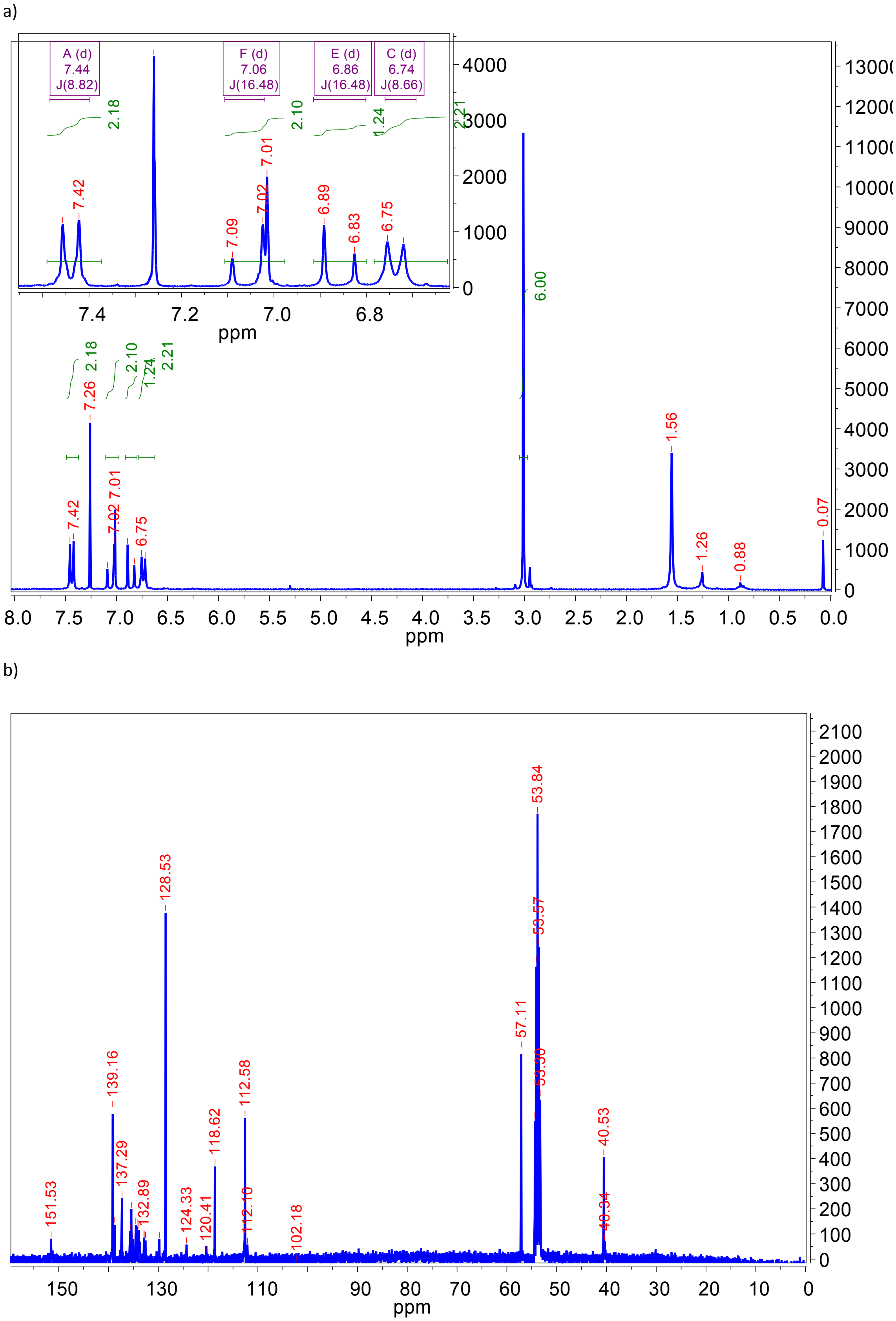


Figure S2: a) ^{1}H-NMR spectrum (250 MHz, $CDCl_3$) and b) ^{13}C-NMR spectrum (400 MHz, CD_2Cl_2) of the ***E*-αH-PTM-DMA** enriched (95 %) compound obtained when the reaction is performed under red light.

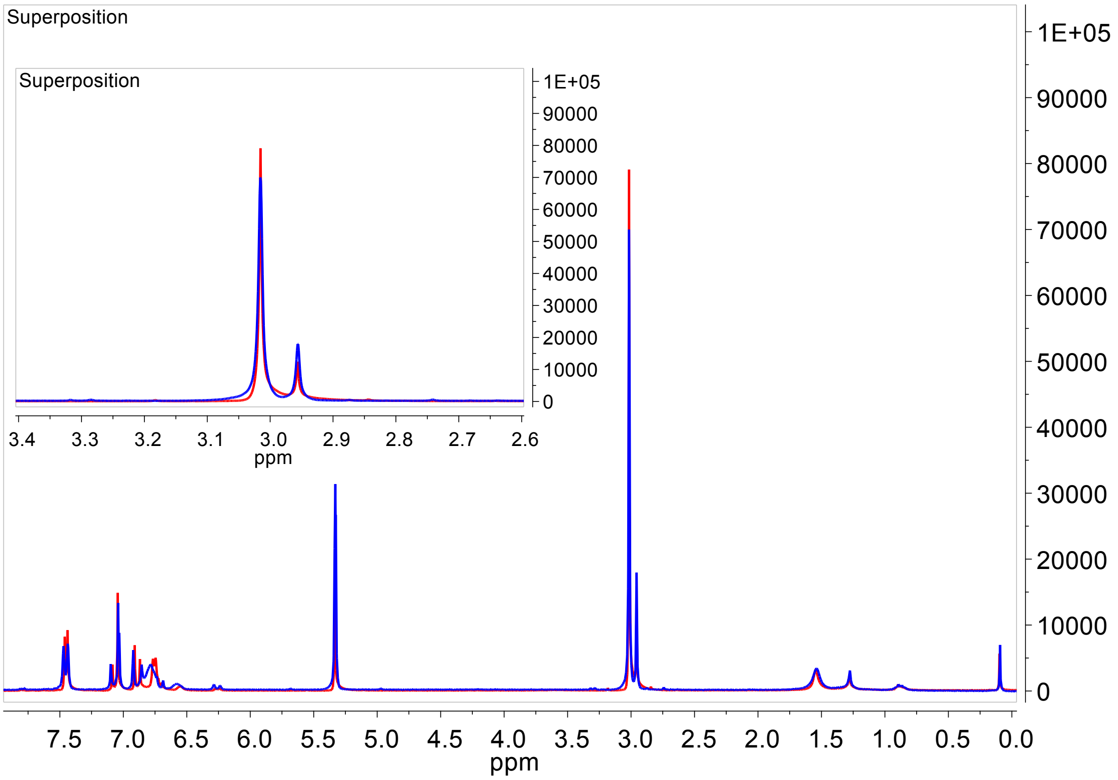


Figure S3- ^{1}H-NMR spectrum (250 MHz, CDCl$_3$) of the ***E*-αH-PTM-DMA** enriched (E/Z 0,85) (red) and upon 3 hours exposure to ambient light (blue). From the peaks corresponding to the CH3 an increase of the ***Z*-αH-PTM-DMA** isomer until (E/Z 0,75) is observed.

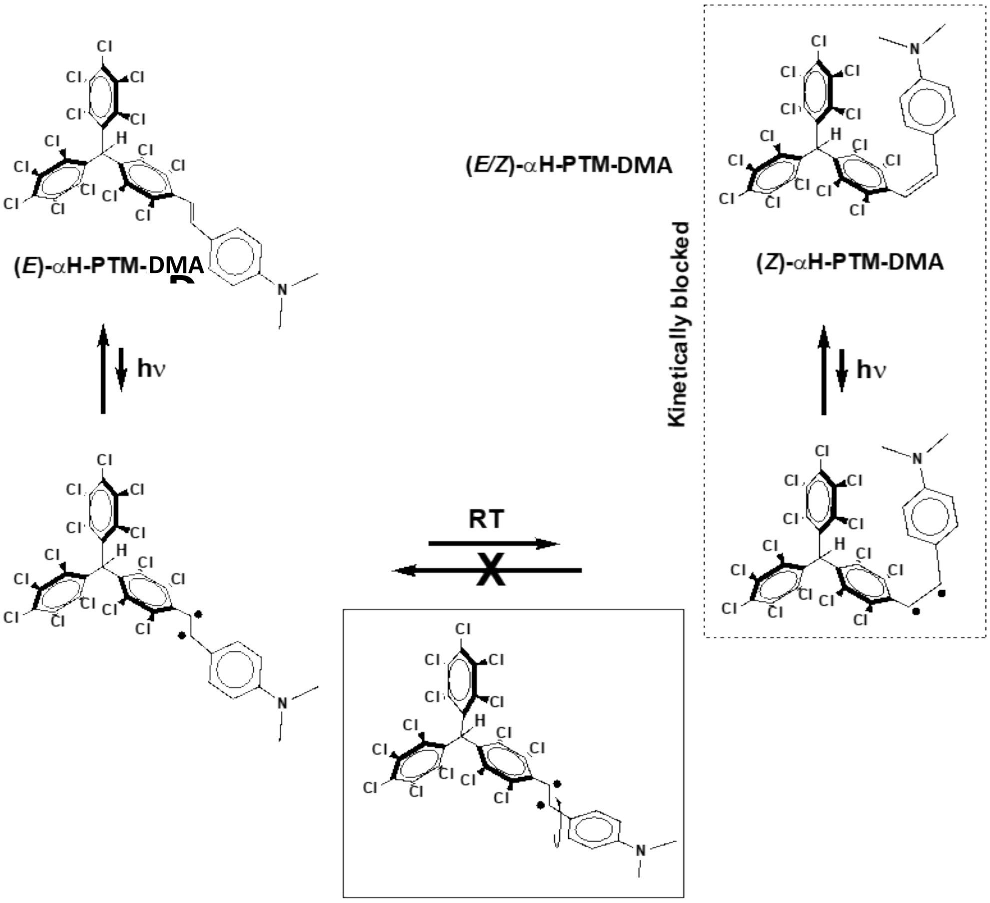


Figure S4- According to Ref. 1, this figure shows the proposed mechanistic scheme for the isomerization process-taking place in **αH-PTM-DMA**, under the effect of light irradiation and temperature. First, light opens the central double-bond, which allows the free rotation of the ethylene unit due to thermal fluctuations (RT). Then, **αH-PTM-DMA** gets kinetically blocked in the Z conformation, shifting the equilibrium towards such a conformation.

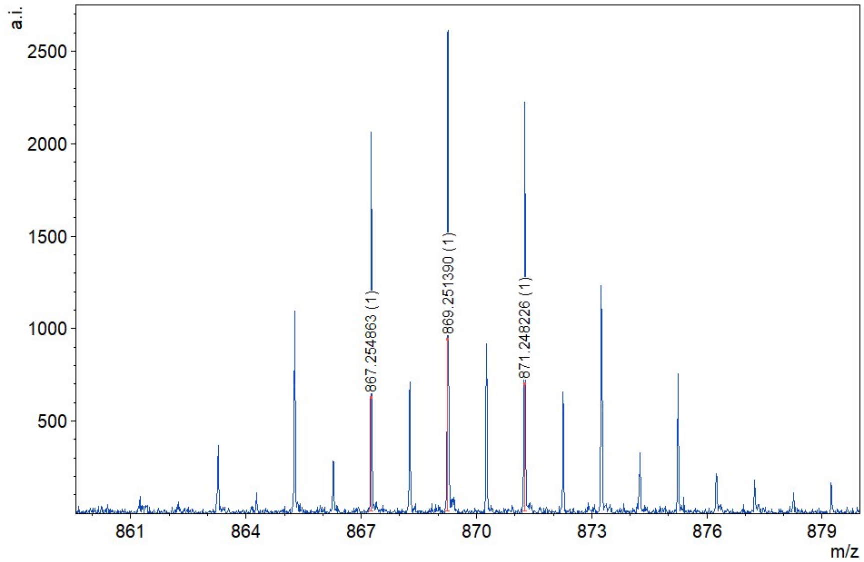
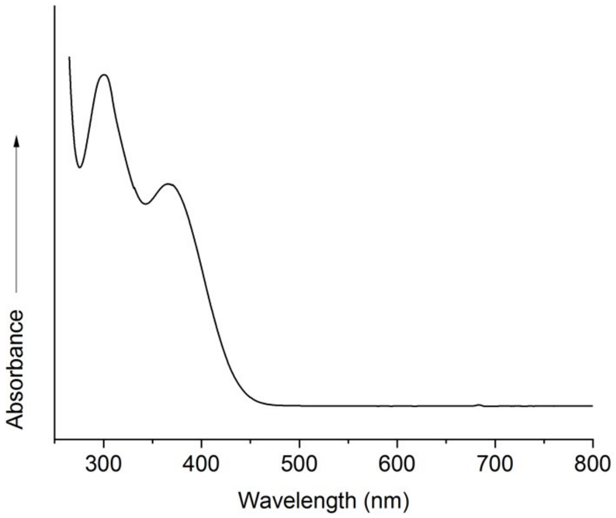


Figure S5- MALDI-MS of ***(Z)*-αH-PTM-DMA**



a)

b)

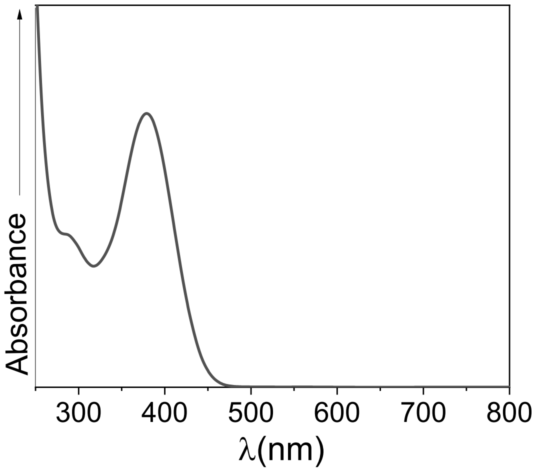


Figure S6 –UV-Vis electronic absorption spectrum of a) ***(Z)*-αH-PTM-DMA** in CH_2Cl_2, and b) ***(E)*-αH-PTM-DMA** in CH_2Cl_2

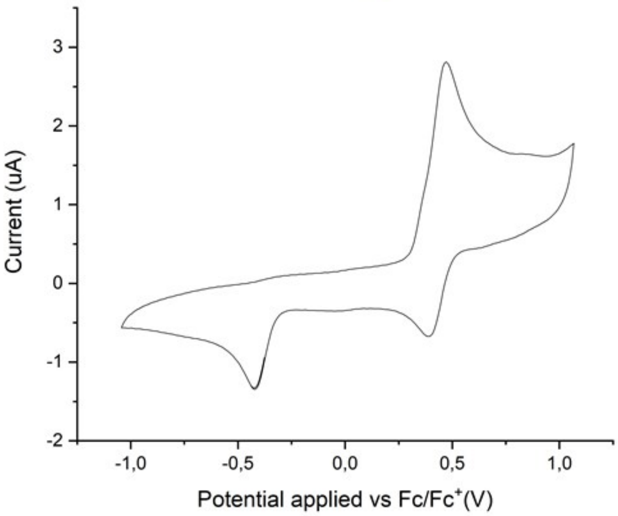


Figure S7 – Cyclic voltammogram of ***(Z)*-αH-PTM-DMA** (0.1 mM), in CH_2Cl_2 using 0,2M $TBAPF_6$ as electrolyte (vs Fc/Fc^+). Using Pt wire as working and counter electrode.

Synthesis of 18-crown-6 K^+[*(Z)*-PTM-DMA]$^-$

Finely grinded potassium hydroxide (202 mg, 3.56 mmol) and 18-crown-6 (50 mg, 0,198 mmol) were added to a solution of **αH-PTM-DM** (*E/Z* isomers proportion 20/80) (150 mg, 0.172 mmol) in 8 ml of dry THF under argon atmosphere and light exclusion. The resulting dark purple mixture was stirred for 48 h. and after filtration, the solvent was evaporated under reduced pressure. The crude product was redissolved in 4 ml of CH_2Cl_2 and reprecipitated by addition of n-hexane giving a violet microcrystalline powder of **18-crown-6 K^+ [PTM-DMzA]$^-$** (153 mg, 75% yield). Crystals suitable for X-ray structure determination were obtained by slow diffusion of hexane into a CH_2Cl_2 solution of **18-crown-6 K^+ [PTM-DMA]$^-$**. The crystal structure shows that the anion is the *Z* isomer. By comparison of the UV-Vis spectrum of the solutions of single crystals and the microcrystalline powder of **18-crown-6 K^+ [PTM-DMA]$^-$** it was determined that all the samples consist on the pure *Z* isomer. Mp 170 °C dec. **LDI-ToF** (negative mode): *m/z.* calc. for $C_{29}H_{12}Cl_{14}N_,$ 869,65; found, 868,24 $[M-H]^+$. **FT- IR.:** 517, 528, 581, 593, 603, 614, 634, 648, 670, 690, 723, 764, 778, 810, 823, 835, 962 (st.), 1106 (st.), 1035, 1106, 1133, 1161, 1226, 1250, 1283, 1362 (st.), 1452, 1474, 1512 (st.), 1608 (st.), 1970, 2433, 2903 (st.), 3013 cm^{-1}. **UV-Vis.** (λ_{max} / nm (ε / $M^{-1}cm^{-1}$)): 284 (14128), 521 (23119).

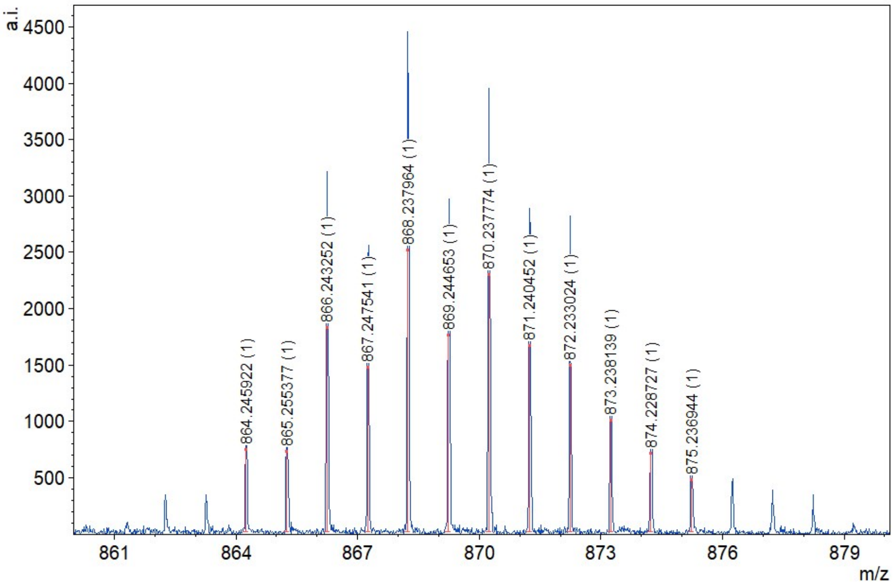


Figure S8. MALDI-MS of **18-crown-6 K$^+$ [*(Z)-PTM-DMA]*$^-$**

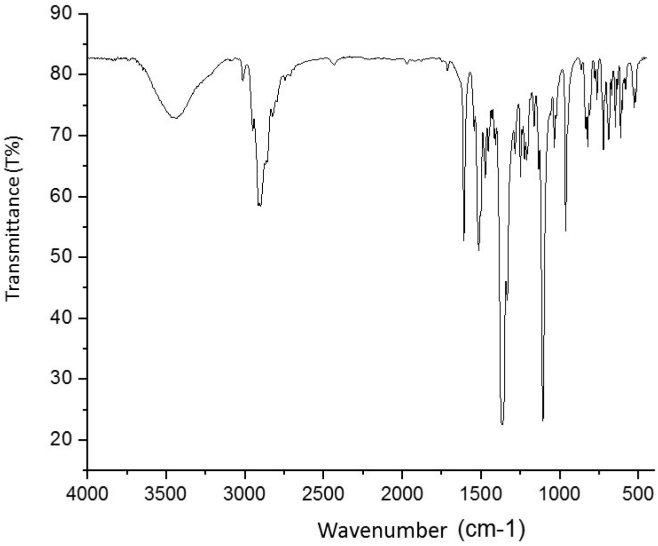


Figure S9. FT-IR of **18-crown-6 K$^+$ [*(Z)*-PTM-DMA]**$^-$ in powder*.*

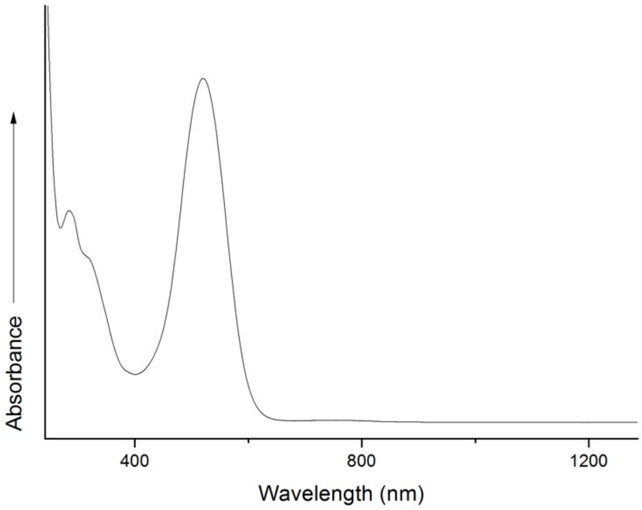


Figure S10 –UV-Vis electronic absorption spectrum of **18-crown-6 K$^+$ [*(Z)*-PTM-DMA]$^-$** in CH_2Cl_2,

Synthesis of PTM$^•$-DMA radical

a) Synthesis from **18-crown-6 K$^+$ [*(Z)*-PTM-DMA]$^-$**

Fe $(ClO_4)_3$ (35 mg, 0,099 mmol) was added to a solution of **18-crown-6 K$^+$[*(Z)*-PTM-DMA]$^-$** (100 mg, 0,085 mmol) in 5 ml of dry THF under argon atmosphere and light exclusion. The mixture was stirred for one hour and then filtered thorough 2 cm of SiO_2. After evaporation of the solvent the crude product was purified by column chromatography (SiO_2, CH_2Cl_2), yielding radical **PTM$^•$-DMA** (*E* isomer) (46 mg , 67%) as a red-brown powder. Anal. Calc. for $C_{29}H_{12}Cl_{14}N$: C, 39,98; H, 1,39; N, 1,61. Found: C, 40,21; H, 1,52; N, 1,87. ; mp 175 ^oC dec. **FT-IR** ν/cm^{-1}: 2924, 2954, 1600, 1524, 1360, 1337, 1321, 1262, 1187, 1169, 966,948, 808. **UV-Vis-NIR** (CH_2Cl_2) (λ_{max} / nm (ε / $M^{-1}cm^{-1}$)): **(*E* isomer):** 392 (30100), 495 (5319), 556 (4840), 811 (2875). **LDI-ToF** (negative mode): *m/z.* calc. for $C_{29}H_{12}Cl_{14}N_,$ 869,65; found, 868,24 $[M-H]^+$. **EPR** (CH_2Cl_2, rt.): *g* = 2.0026, two lines $a(^1H_a)$ = 1.9 G, $a(^{13}C_{Ar})$ = 12.6, 14.3 G, $a(^{13}C_\alpha)$ = 29.4 G.

Intermediate (*Z* isomer): UV-Vis-NIR (CH_2Cl_2) (λ_{max} / nm (ε / $M^{-1}cm^{-1}$)): 387 (25609), 489 (2460), 556 (1969), 780 (1023). $]^+$. **EPR** (THF, rt.): *g* = 2.0022, two lines $a(^1H_a)$ = 2.6 G, $a(^{13}C_{Ar})$ = 13, 10 G, $a(^{13}C_\alpha)$ = 29.3 G.

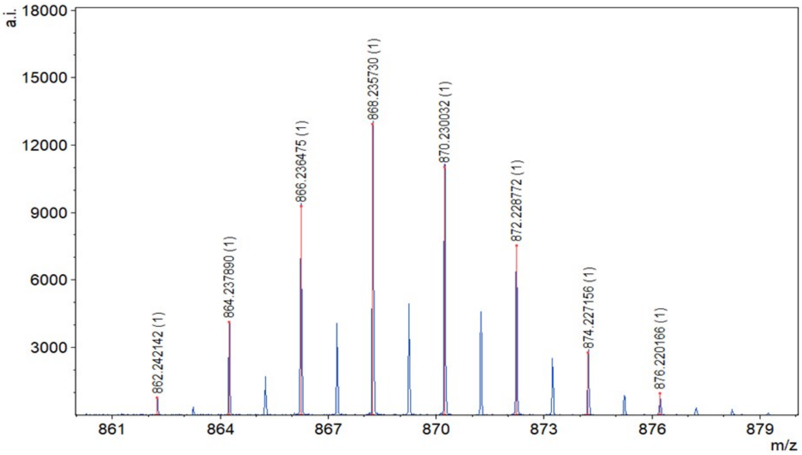


Figure S11-MALDI-MS of ***(E)*-PTM$^•$-DMA** radical

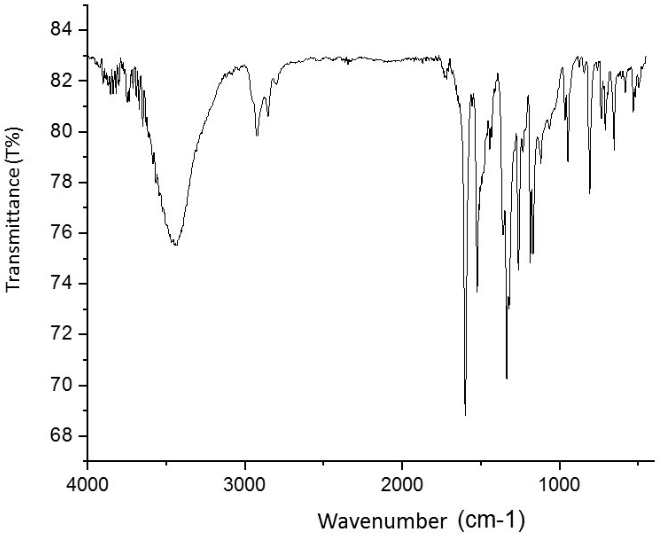


Figure S12. FT-IR of ***(E)*-PTM•-DMA** radical in powder.

b) Synthesis from ***(E)*-αH-PTM-DMA**

A solution of TBAOH in H_2O (54–56%) (8µL, 0.017mmol) was added to a solution of compound ***(E)*-αH-PTM-DMA** (10.2 mg, 0.012 mmol) in dry THF (1 mL), the reaction mixture was stirred for 2 h leading to the corresponding **TBA$^+$ [*(E)*-PTM-DMA]$^-$**. Then $AgNO_3$ (8 mg, 0.047 mmol) was added to oxidize the anion to the radical and the mixture was further stirred for 1 h. The reaction mixture was filtered thorough a small column packed with silica gel. The residue at the top of the column was further washed with CH_2Cl_2, and then combined filtrates were concentrated under reduced pressure yielding 9 mg of radical ***(E)*-PTM$^•$-DMA** (90%). UV-Vis and ESR data are coincident with the ones reported for the radical obtained in procedure a) from the **18-crown-6 K$^+$ [*(Z)*-PTM-DMA]$^-$**.

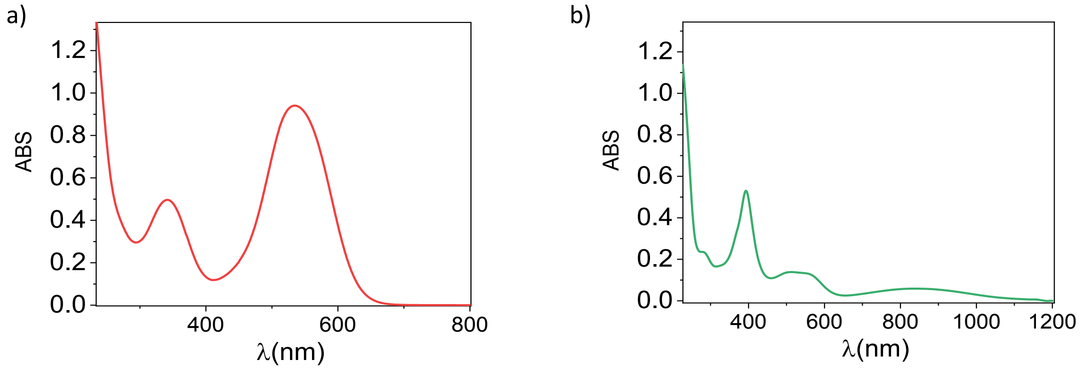


Figure S13. UV-Vis spectra of of a) **TBA$^+$ [*(E)*-PTM-DMA]$^-$** and b) ***(E)*-PTM$^•$-DMA**.

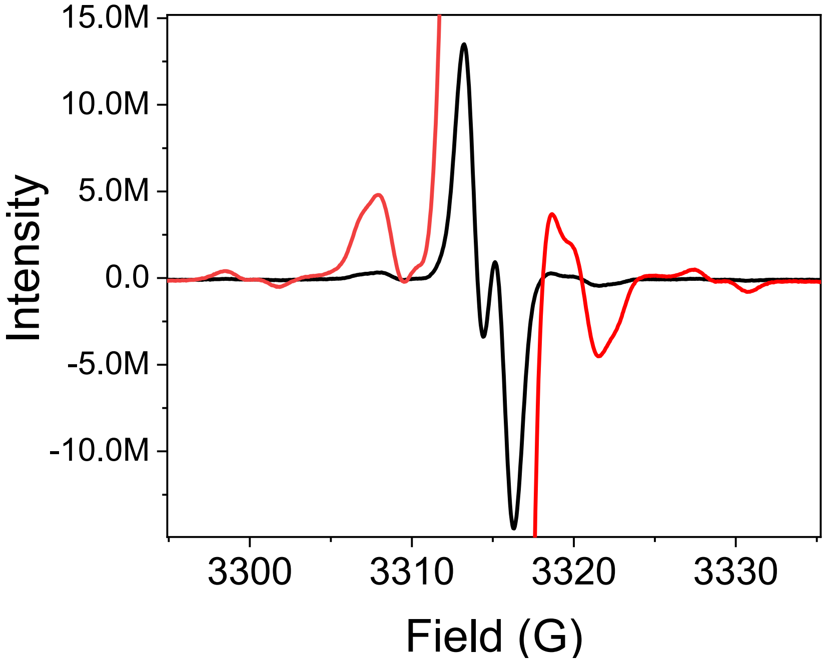


Figure S14. EPR spectra of ***(E)*-PTM$^•$-DMA** in CH_2Cl_2 acquired at r.t.

3. Crystallografic data for 18-crown-6 K$^+$ [*(Z)*-PTM-DMA]$^-$.

Moiety formula= 2(C41 H36 Cl14 K N O6), CH$_2$Cl$_2$, M = 2433.15, triclinic P-1, **a** =11.6030(10) Å **b** =13.398(2) Å **c** = 19.749(3) Å; α = 90.788(6) deg; β =105.517(7) deg; γ= 113.557(7) deg; V = 2686.3(6) Å^3; T = 233(1) K; Z = 2; Mo Kα (⍰ = 0:71073 Å), 5396 reflections collected, 3564 independent reflections with I > 2⍰(I), R1 [I > 2s(I)] = 0:0546; wR2 (all data) = 0.1685, goodness-of-fit: 1.134.

Data were measured with a Nonius Kappa CCD and the structure was solved by direct methods (SHELXS-97) [1a] and refined by full-matrix least-squares methods on F2 (SHELXL-97) [1b].
Crystallographic data for the reported structure have been deposited with the Cambridge Crystallographic Data Centre. Reference number CCDC 1906103

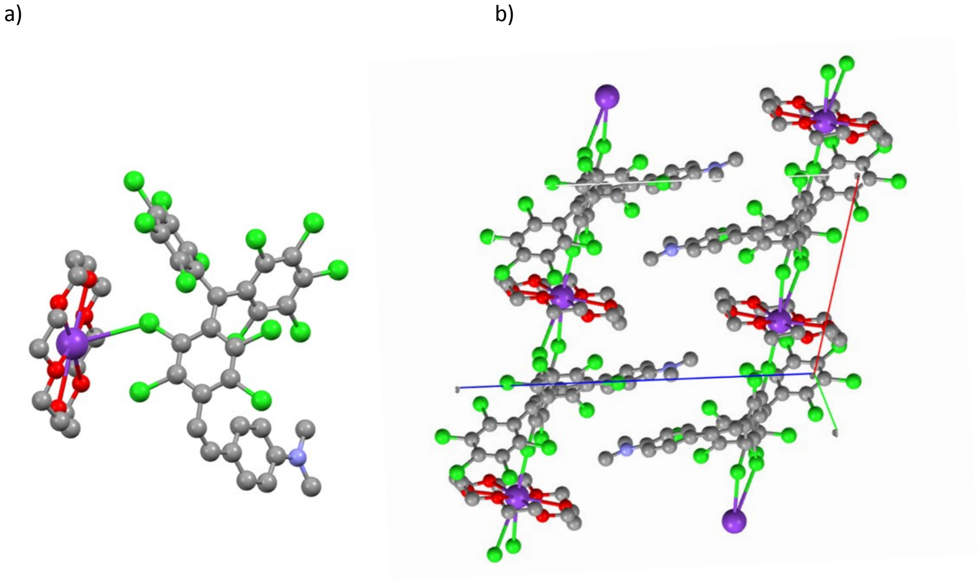


Figure S15- a) asymmetric unit. b) view of the packing of polymeric chains showing the dimerized molecules thorough the aromatic rings of the amine.

4. Spectroelectrochemistry measurements

Spectroelectrochemistry measurements were performed at r.t. with a 10^{-3} M solution of **18-crown-6 K^+ [*(Z)*-PTM-DMA]$^-$** in CH_2Cl_2 using 0,2M $TBAPF_6$ as electrolyte.

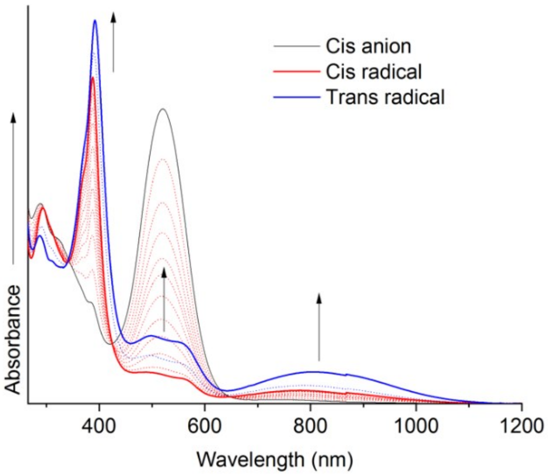


Figure S16- UV-Vis electronic absorption spectra for the electrochemical oxidation of **18-crown-6 K^+ [*(Z)*-PTM-DMA]$^-$** (black line) up to ***(E)*-PTM$^•$-DMA** (blue line), through ***(Z)*-PTM$^•$-DMA** (red line), in CH_2Cl_2 using 0,2M $TBAPF_6$ as electrolyte.

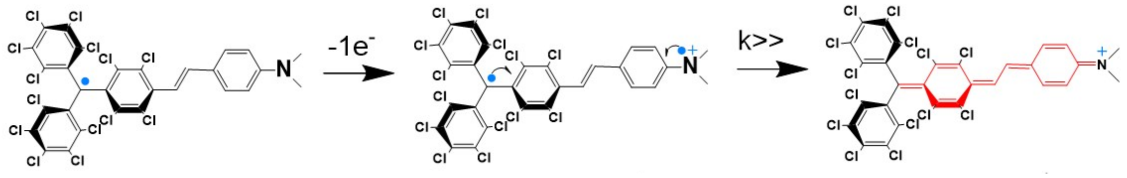


Figure S17 Schematic representation of the generation of the closed-shell quinoidal structure for **[PTM-DMA]$^+$**, resulting from the electron pairing between the lone electron of the PTM$^•$ moiety with the unpaired electron of the newly formed radical cation species.

a)

b

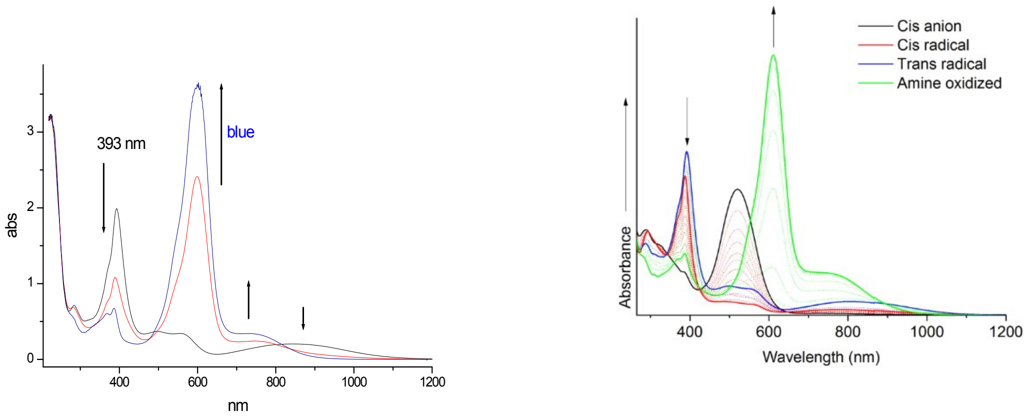


Figure S18- UV-Vis electronic absorption spectra for the a) chemical oxidation with 2,5 to 4 fold excess of Ag^+BF4^- in THF of ***(E)*-PTM$^•$-DMA** (black line) up to **[PTM-DMA]$^+$** (blue line) and b) electrochemical oxidation of ***(E)*-PTM$^•$-DMA** (blue line) up to **[PTM-DMA]$^+$** (green line), in CH_2Cl_2 using 0,2M $TBAPF_6$ as electrolyte.

Table S1 Summarized data of ESR and UV-Vis electronic absorption spectra for the *(E/Z)* isomers of **PTM$^{\bullet}$-DMA**. Additionally, relevant values of ***(E)*-αH-PTM-DMA** and **[PTM-DMA]$^{-}$** have also been included.

	λ_{max} / nm (ε / $M^{-1}cm^{-1}$)	$a(^{1}H_{a})$ / g (G)
(Z)-αH-PTM-DMA	300 (9942), 365 (6666)	-
(E)-αH-PTM-DMA	289 (11774),379 (21066)	-
[*(Z)*-PTM-DMA]$^{-}$	284 (14128), 521 (23119)	-
[*(E)*-PTM-DMA]$^{-}$	342 (14311), 535 (27049)	-
(Z)-PTM$^{\bullet}$-DMA	387 (25609), 489 (2460), 556 (1969), 780 (1023)	2.6 (2.0022)
(E)-PTM$^{\bullet}$-DMA	392 (30100), 495 (5319), 556 (4840), 811 (2875)	1.9 (2.0026)

5. Theoretical data

Quantum chemical calculations were done in the framework of the density functional theory as implemented in the Gaussian 09 package.[3] Simulations were performed in THF solvent, considering the polarizable continuum model (PCM). The (U)B3LYP exchange-correlation functional and the 6-31G(d,p) basis set were used in all calculations. Minimum energy structures were reached and confirmed by vibrational analyses. No negative frequencies were found. Chemcraft 1.8 software[4] was used to analyze the TD-DFT calculated spectra while theoretical Raman spectra were generated by means of GaussSum software.[5]

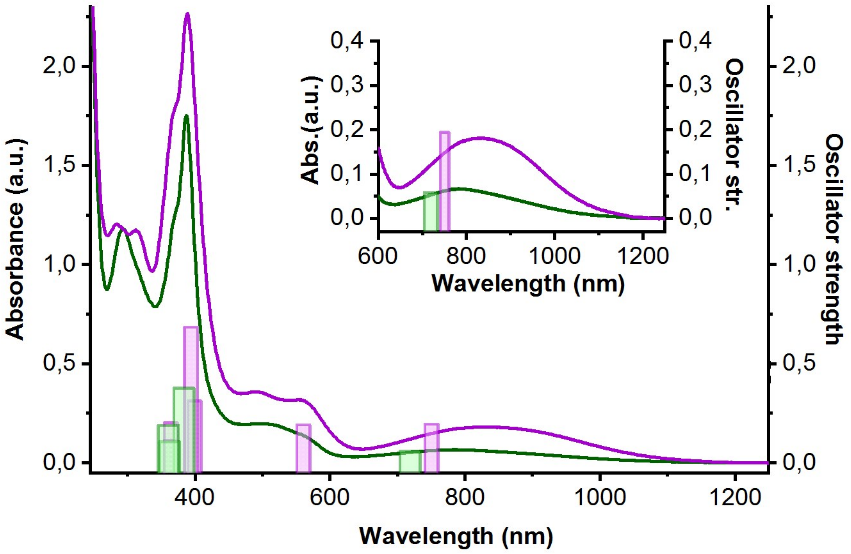


Figure S19- Experimental UV-Vis electronic absorption spectra of **[(*Z*)-PTM-DMA]•** (green) and **[(*E*)-PTM-DMA]•** (purple) radical isomers together with their relative TD-DFT calculated energy transition with oscillator strengths. An UB3LYP/6-31G(d,p) level of theory with the inclusion of solvent effect (i.e., THF) was considered. No further correction to the theoretical data was applied.

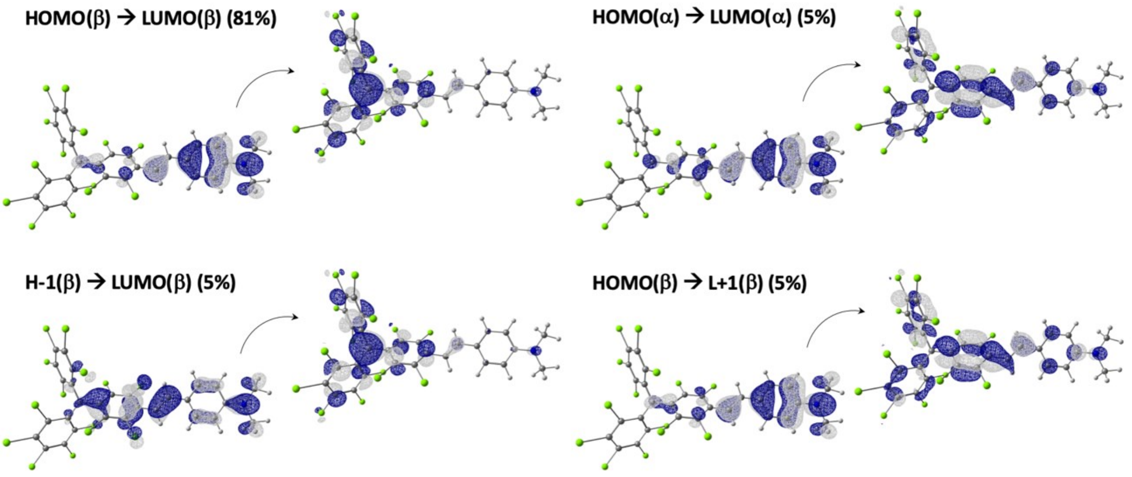


Figure S20- Calculated topologies (UB3LYP/6-31G(d,p)) of the main orbitals of **[(*E*)-PTM-DMA]•** related to the experimental UV/Vis absorption band at lower energies.

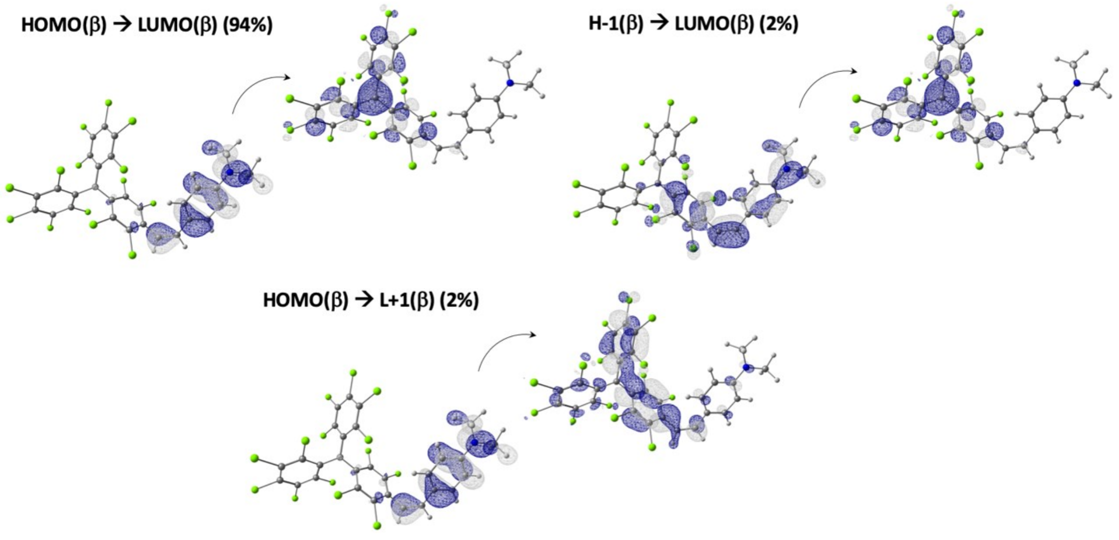


Figure 21- Calculated topologies (UB3LYP/6-31G(d,p)) of the main orbitals of **[*(Z)*-PTM-DMA]•** related to the experimental UV/Vis absorption band at lower energies.

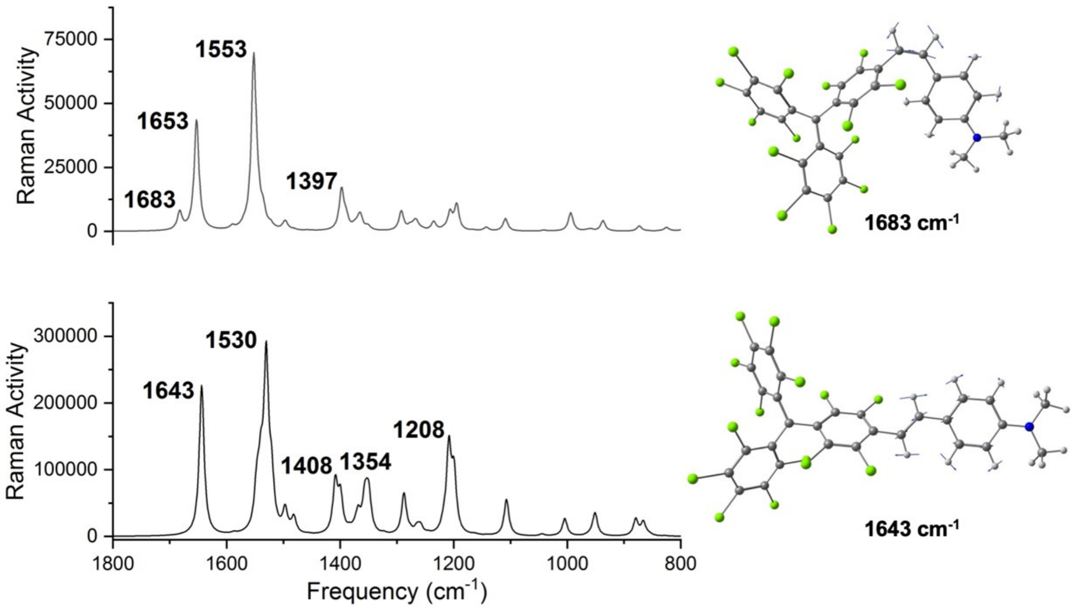


Figure S22. Theoretical UB3LYP/6-31G(d,p) Raman spectra of **[*(Z)*-PTM-DMA]•** (top) and **[*(E)*-PTM-DMA]•** (bottom) radical isomers together with the vibrational eigenvectors mainly associated with the stilbene moiety.

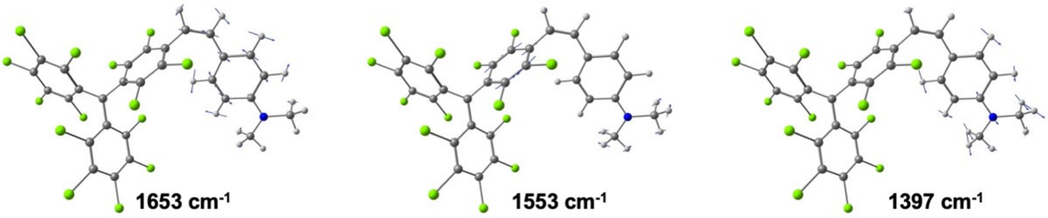


Figure S23. Vibrational eigenvectors related to the 1600-1200cm^{-1} bands of the UB3LYP/6-31G(d,p) Raman spectrum of **[*(Z)*-PTM-DMA]•**.

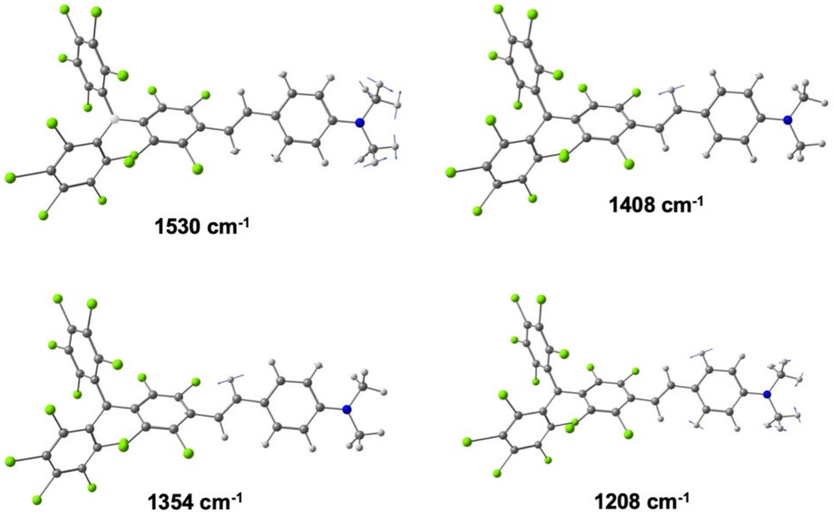
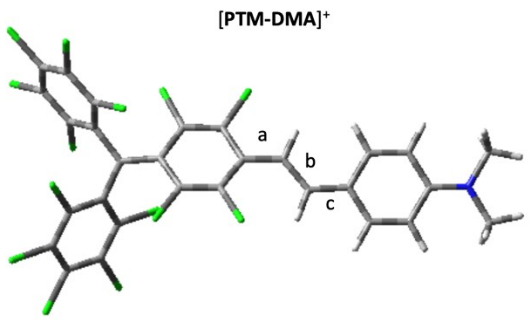


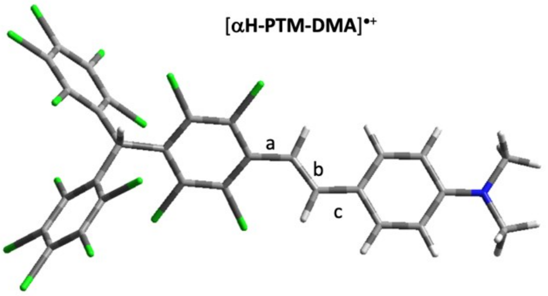
Figure S24. Vibrational eigenvectors related to the 1600-1200cm^{-1} bands of the UB3LYP/6-31G(d,p) Raman spectrum of **[*(E)*-PTM-DMA]**$^{\bullet}$.

To predict the π bond order of the cationic species of **PTM$^{\bullet}$-DMA** and **αH-PTM-DMA** the spin-unrestricted (U) approach was used in the case of [**αH-PTM-DMA]**$^{\bullet+}$.

Table S2.-Selected bond distances (in Å) of the DFT [(U)B3LYP/6-31G(d,p)] optimized structures for [**PTM-DMA]**$^{+}$ and [**αH-PTM-DMA]**$^{\bullet+}$

	a	b	c
[**PTM-DMA]**$^{+}$	1.41530	1.39015	1.41678
[**αH-PTM-DMA]**$^{\bullet+}$	1.45078	1.37384	1.42881





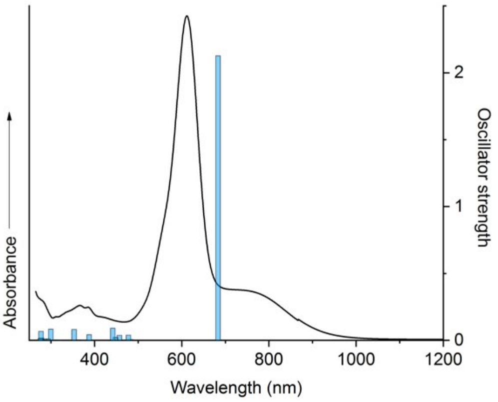


Figure S25- UV-Vis electronic absorption spectrum of **[PTM-DMA]**$^{+}$ (green line) together with the positions and oscillatory strength of the calculated transitions at a TD-DFT\B3LYP\6-31G(d,p) level of theory (blue). No further corrections were applied to the theoretical data.

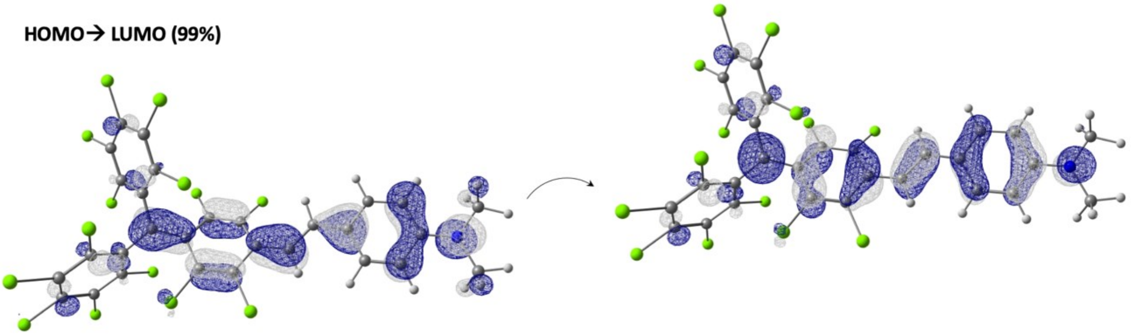


Figure S26. Calculated topologies (B3LYP/6-31G(d,p)) of the main orbitals of **[PTM-DMA]**$^{+}$ related to the experimental UV/Vis absorption band at lower energies.

Cartesian coordinates of the optimized geometries at DFT [(U)B3LYP/6-31G(d,p)] level of theory:

[*(E)*-PTM-DMA]$^{\bullet}$

C	-5.32777900	-1.08209000	0.86199700
H	-5.79644300	-1.82992600	1.49488700
C	-6.12003300	-0.22243100	0.17416300
H	-5.65986600	0.46167900	-0.53032000
C	-7.57975500	-0.17565700	0.19012000
C	-8.38813800	-0.32347900	1.34510100
C	-8.27814200	0.08371700	-1.01685600
C	-9.78244300	-0.25024800	1.28657600
Cl	-7.62560900	-0.49209800	2.91282700
C	-9.66932500	0.14817300	-1.08246200
Cl	-7.34551400	0.25037700	-2.49095400
C	-10.48129600	-0.02443400	0.07022000
Cl	-10.67917600	-0.31051300	2.78623100
Cl	-10.41931600	0.31661500	-2.65180700
C	-11.94950500	0.02858400	0.00932600
C	-12.76046000	-1.02013500	0.67196200
C	-12.62908400	1.12784500	-0.71538200
C	-13.83444100	-0.70001400	1.53880700
C	-12.50541200	-2.39859900	0.46209400

C	-12.29766800	2.48638000	-0.48293600
C	-13.64769200	0.87924900	-1.66837900
C	-14.61623100	-1.68877400	2.15032400
Cl	-14.15486500	0.96331000	1.95086200
C	-13.26511800	-3.39697500	1.08622200
Cl	-11.27919000	-2.89825400	-0.67217500
C	-12.93308300	3.53226200	-1.16529400
Cl	-11.13478800	2.90450200	0.74677600
C	-14.30665300	1.91716700	-2.34015000
Cl	-14.04558200	-0.75955100	-2.11019000
C	-14.32921000	-3.04392700	1.92943400
Cl	-15.92474300	-1.25166200	3.20811700
Cl	-12.91991200	-5.07704000	0.80198000
C	-13.94624900	3.25023400	-2.09376100
Cl	-12.49768000	5.18564900	-0.85019000
Cl	-15.55092000	1.56688600	-3.50259600
Cl	-15.28328200	-4.27459200	2.69420500
Cl	-14.74801300	4.54081000	-2.93115400
C	-3.87847500	-1.15242700	0.82058300
C	-3.22049300	-2.18237200	1.52508900
C	-3.05839500	-0.24337900	0.11605700
C	-1.84183200	-2.31311300	1.53085300
H	-3.81519100	-2.90116800	2.08332900
C	-1.68037800	-0.35542400	0.10978800
H	-3.50690200	0.57736800	-0.43540300
C	-1.02283900	-1.39980400	0.81742800
H	-1.39622900	-3.12500500	2.09124700
H	-1.10248100	0.37317100	-0.44447000
N	0.34409500	-1.51580600	0.81047000
C	1.16102300	-0.55333700	0.08307500
H	2.21086700	-0.82221700	0.19262200
H	0.92300300	-0.54774900	-0.98778900
H	1.02946100	0.46645600	0.46684500
C	0.99206900	-2.58340600	1.56043800
H	2.07062700	-2.51000500	1.42688500
H	0.77658700	-2.51550800	2.63449700
H	0.67369100	-3.57365400	1.21151400

[***(Z)*-PTM-DMA]**$^{\bullet}$

C	-5.62303000	-0.51350100	1.60417600
H	-4.58440700	-0.19090600	1.67068900
C	-6.44628600	0.37258300	1.00091100
H	-5.98171300	1.25551700	0.56736800
C	-7.90584900	0.30954800	0.78602100
C	-8.84785300	0.29872000	1.83572600
C	-8.42410400	0.37156600	-0.52312800
C	-10.22450700	0.30499000	1.58668300
Cl	-8.27134800	0.34875200	3.48282900
C	-9.79688300	0.36610800	-0.78290200
Cl	-7.28482300	0.40053800	-1.84988500
C	-10.74862100	0.32631500	0.26789800
Cl	-11.31284600	0.40853900	2.94926800
Cl	-10.32583700	0.28844500	-2.44520800
C	-12.20159900	0.30717700	0.00508100
C	-13.06438800	-0.68860500	0.68335100
C	-12.80182200	1.27988900	-0.93761200
C	-14.25450200	-0.31177600	1.35363500
C	-12.74174900	-2.06864500	0.69125500
C	-12.53893000	2.66911200	-0.83953500
C	-13.66995100	0.87065500	-1.97995800
C	-15.08031200	-1.25128900	1.98478600
Cl	-14.67923900	1.37257600	1.49567200
C	-13.54775000	-3.01485000	1.33791100

Cl	-11.36092300	-2.64841400	-0.20080400
C	-13.09825500	3.59421400	-1.73090400
Cl	-11.57190800	3.28433800	0.47329800
C	-14.25203600	1.78812700	-2.86439000
Cl	-13.96417000	-0.82535900	-2.25416800
C	-14.72502400	-2.60836900	1.98357100
Cl	-16.53133000	-0.74652900	2.79750400
Cl	-13.11717700	-4.69884900	1.32329100
C	-13.96310600	3.15566500	-2.74473200
Cl	-12.75239100	5.29037400	-1.57508100
Cl	-15.30958400	1.24369800	-4.13167900
Cl	-15.73433200	-3.77576000	2.77519100
Cl	-14.66985500	4.29643500	-3.84341000
C	-5.85506700	-1.84206500	2.15946400
C	-4.85425200	-2.41742200	2.96864200
C	-6.99645100	-2.63306100	1.91368400
C	-4.98709600	-3.67585300	3.53408600
H	-3.94535400	-1.85316500	3.16301900
C	-7.14514200	-3.89650300	2.46189900
H	-7.77880300	-2.26603400	1.25875800
C	-6.15032300	-4.45478400	3.30757700
H	-4.18234300	-4.05905400	4.14852800
H	-8.03714000	-4.46180800	2.22343400
N	-6.30534800	-5.69853200	3.87435700
C	-7.46342600	-6.51557900	3.53963600
H	-7.42595400	-7.43984200	4.11551800
H	-8.39870400	-6.00236600	3.79108200
H	-7.49527000	-6.77777100	2.47292200
C	-5.21779800	-6.29022500	4.64076500
H	-5.53762300	-7.25823300	5.02529300
H	-4.31552700	-6.44419300	4.03274000
H	-4.94624900	-5.66247500	5.49753700

[αH-PTM-DMA]$^{\bullet+}$

C	-5.31384700	-1.15346400	0.91342500
H	-5.77216700	-1.82930000	1.62557100
C	-6.11785100	-0.38792000	0.10413800
H	-5.64123700	0.18510900	-0.68273100
C	-7.56662800	-0.31345500	0.08788500
C	-8.40419100	-0.42213400	1.22775300
C	-8.21471500	-0.06630400	-1.15212700
C	-9.79954600	-0.32444700	1.12918500
Cl	-7.69139300	-0.56796600	2.81220600
C	-9.60559800	-0.00258400	-1.25017400
Cl	-7.25150000	0.08116900	-2.59872300
C	-10.44346300	-0.13990100	-0.11599000
Cl	-10.71503500	-0.35597800	2.60310100
Cl	-10.30978800	0.22790600	-2.82731100
C	-11.96581500	-0.18911900	-0.36761400
C	-12.78794600	-1.11975200	0.55089300
C	-12.63590800	1.12881200	-0.81080100
C	-13.75137600	-0.71475200	1.49492300
C	-12.63481300	-2.51031200	0.35946500
C	-12.23870200	2.42654800	-0.44022000
C	-13.69457600	1.03070200	-1.74060900
C	-14.54382000	-1.64753700	2.18856300
Cl	-13.96029300	0.96395700	1.90413900
C	-13.39705400	-3.45719200	1.05754400
Cl	-11.46070000	-3.10877700	-0.79579400
C	-12.85601700	3.57190200	-0.97182600
Cl	-10.99434900	2.67707000	0.75602600
C	-14.33967700	2.16005000	-2.26596200
Cl	-14.23507800	-0.53987200	-2.28460800

C	-14.36836100	-3.02192700	1.97081600
Cl	-15.73298400	-1.11255800	3.33070000
Cl	-13.16266700	-5.15456900	0.79203100
C	-13.91203600	3.44059300	-1.88523000
Cl	-12.33166900	5.15553600	-0.49622600
Cl	-15.64491200	1.98818000	-3.39200500
Cl	-15.33516200	-4.17377500	2.82686500
Cl	-14.68340800	4.84561600	-2.53692500
H	-11.99082900	-0.75350000	-1.30211600
C	-3.88613600	-1.18291900	0.86568600
C	-3.19369700	-2.12919500	1.67788400
C	-3.08912500	-0.31459200	0.05968100
C	-1.82644500	-2.22078400	1.68670500
H	-3.77227000	-2.79931400	2.30624900
C	-1.72214100	-0.38970500	0.05622400
H	-3.56467900	0.43486200	-0.56263800
C	-1.03391400	-1.35041700	0.87023600
H	-1.35175600	-2.95815200	2.32002800
H	-1.16175100	0.29127900	-0.57026200
N	0.31544800	-1.42913200	0.86740700
C	1.12285100	-0.52892900	0.03256500
H	2.17584000	-0.75529200	0.18319300
H	0.88710100	-0.66565300	-1.02706400
H	0.95038200	0.51569400	0.30810400
C	1.01376500	-2.41785300	1.70051600
H	2.08541100	-2.32089300	1.54280800
H	0.80261200	-2.25081400	2.76103500
H	0.71416700	-3.43454700	1.42959900

[**PTM-DMA**]$^{+}$

C	-5.32071500	-0.96016400	1.07415400
H	-5.78547200	-1.58165100	1.82888300
C	-6.11996600	-0.14259700	0.28340100
H	-5.63089400	0.34772500	-0.54665100
C	-7.52053000	0.05623700	0.32760500
C	-8.37821000	-0.19297900	1.46048500
C	-8.18552600	0.59513400	-0.83700700
C	-9.75054700	-0.10106800	1.37344100
Cl	-7.65944600	-0.47590600	3.02411400
C	-9.55863100	0.70904900	-0.93028000
Cl	-7.21095700	1.02567800	-2.22006300
C	-10.43114100	0.27586600	0.14583500
Cl	-10.67195000	-0.23040800	2.84173500
Cl	-10.22289300	1.18708600	-2.46116900
C	-11.83638400	0.17999300	0.01415500
C	-12.57407500	-0.93518900	0.66103400
C	-12.62809800	1.15874600	-0.76556800
C	-13.72713700	-0.71107500	1.45425200
C	-12.18146300	-2.28358900	0.44985700
C	-12.52995800	2.54956300	-0.49512100
C	-13.56430300	0.74969200	-1.74675800
C	-14.46744400	-1.77098700	1.99386900
Cl	-14.17961400	0.90658500	1.90142500
C	-12.91432500	-3.35137300	0.98519300
Cl	-10.83242100	-2.67273800	-0.58381100
C	-13.35462900	3.47797200	-1.14141800
Cl	-11.43651400	3.14317700	0.72252500
C	-14.38991900	1.67036900	-2.40520800
Cl	-13.61431300	-0.90972800	-2.26327300
C	-14.06291900	-3.09665800	1.75602400
Cl	-15.86219500	-1.46288300	2.97051000
Cl	-12.43261100	-4.98880900	0.69006900

C	-14.29203700	3.03842700	-2.09581700
Cl	-13.24497900	5.16498900	-0.76805600
Cl	-15.51448700	1.13971200	-3.60857600
Cl	-14.97093500	-4.40699100	2.41352700
Cl	-15.31179000	4.17768300	-2.89238800
C	-3.91833900	-1.11629200	0.94678100
C	-3.25894800	-2.07972400	1.76555600
C	-3.09751400	-0.36279200	0.05500000
C	-1.90488600	-2.28799600	1.70694100
H	-3.85288200	-2.66879700	2.45846700
C	-1.74315300	-0.55528800	-0.01547800
H	-3.54222800	0.39288800	-0.58321500
C	-1.09021200	-1.53004600	0.80844000
H	-1.45807300	-3.03294000	2.35140600
H	-1.16458000	0.04411100	-0.70550800
N	0.24674600	-1.72288800	0.73806900
C	1.07092800	-0.93565300	-0.18379700
H	2.10950600	-1.24392200	-0.08232700
H	0.76584400	-1.09670900	-1.22299300
H	1.00737500	0.13354200	0.04359800
C	0.90188300	-2.72393300	1.58493800
H	1.96897600	-2.72563500	1.37219800
H	0.76389500	-2.49430100	2.64670000
H	0.51068500	-3.72685500	1.38497600

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