

SUPPLEMENTARY INFORMATION FILE

Triply twisted Möbius annulene: A new class of two-photon active material – A computational study

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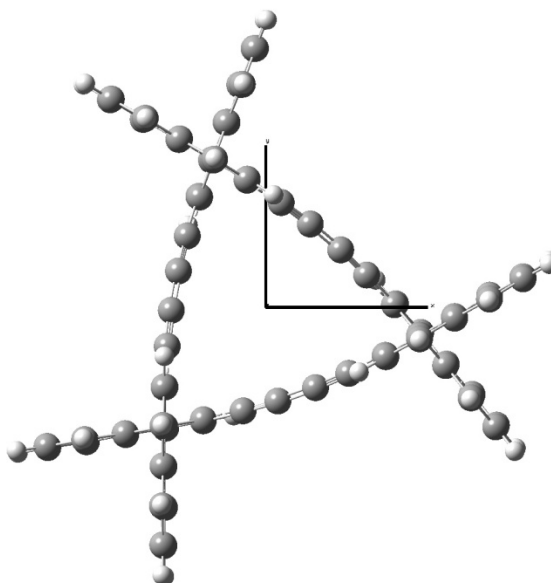
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Contents:

- Optimized geometry and corresponding Cartesian co-ordinates of the systems studied
- 2SM results for the second excited state

1) MA

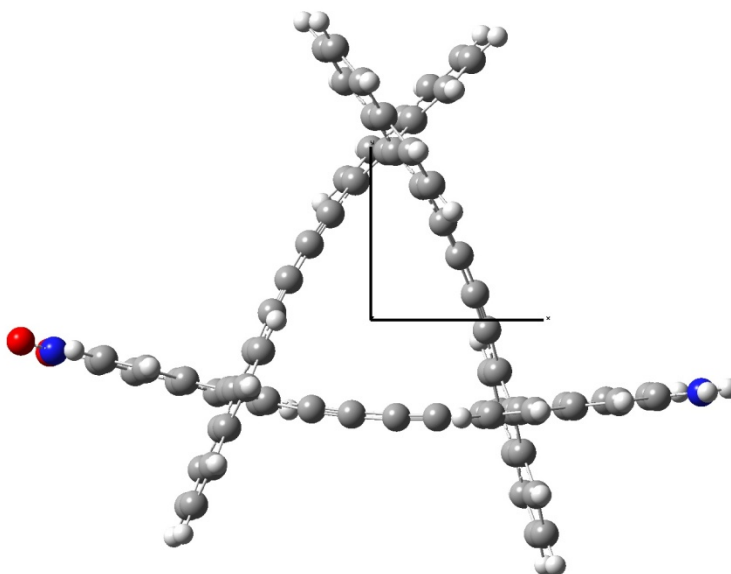


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2) SMA-1



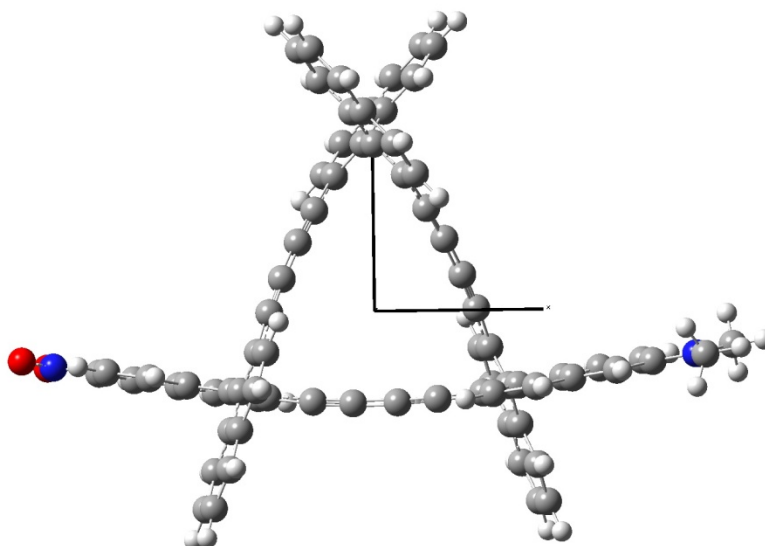
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3) SMA-2

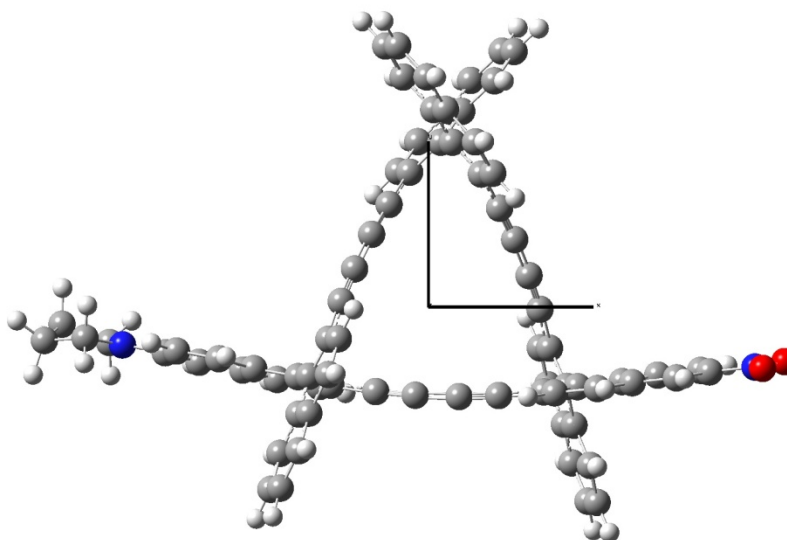


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H	-2.63365700	-2.67389000	-2.96252200
H	2.72355500	-0.21992400	-4.00587500
N	9.50951600	-1.37085700	1.88222200
N	-9.53006000	-1.54360400	-1.98779500
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O	-10.46478200	-1.35517600	-1.15385400
C	10.60015300	-1.10793000	0.94287300
H	11.52886200	-0.98748800	1.50232600
H	10.73890500	-1.93643600	0.23521800
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C	9.78299300	-1.38850200	3.31782200
H	9.21486300	-0.61178400	3.84916000
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4) SMA-3

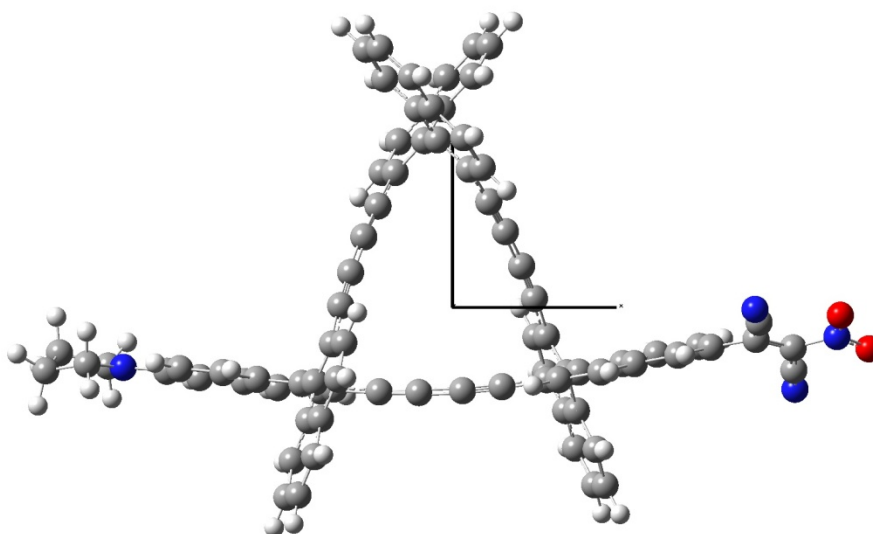


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C	-0.91362200	4.09993100	-2.59618100
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C	1.00771500	5.91293200	-1.58835300
C	0.37443500	4.98097800	-0.69949400
C	1.27856300	6.84954800	-3.85694300
C	2.22982000	7.73417000	-3.38991700
C	2.59329100	7.72323500	-2.01938900
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C	-0.76855600	6.95247600	1.17093100
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C	0.15570300	5.96776400	1.63240900
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C	1.94588700	4.04119800	2.67035600
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5) SMA-4

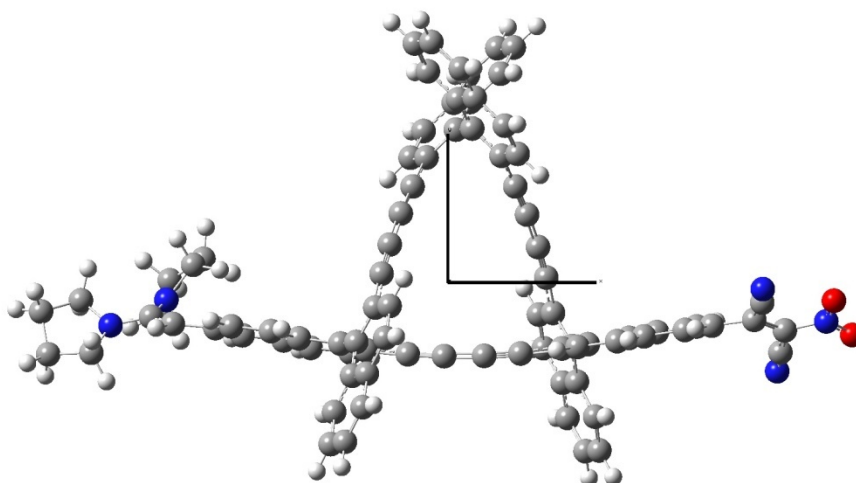


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6) SMA-5



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C	4.18483400	-2.13165900	-1.81106900
C	3.22845900	-2.20483300	-4.48029900
C	3.86235700	-3.36046400	-3.94284200
C	4.34367900	-3.32751100	-2.58747500
C	3.06504400	-1.07285100	-3.72195600
C	3.53878800	-1.01802200	-2.37059100
C	3.31321300	0.17180300	-1.62443900
C	3.03478600	1.19449400	-1.00819500
C	2.66480200	2.28516500	-0.28904000
C	2.27052400	3.23140400	0.38331300
H	-2.01970100	3.46584500	-2.46271100
H	-1.23419100	5.07754700	-4.17033600
H	0.24512600	6.93606000	-4.82689600
H	2.02176300	8.57235500	-4.26720200
H	3.00178200	8.60947700	-1.97506400
H	2.20864500	7.03905600	-0.25340800
H	0.86314000	7.21254900	5.02079900
H	-1.11031600	7.06486600	0.45262400
H	-1.89288000	8.73407300	2.08452600
H	-0.90791600	8.82192300	4.37313100
H	2.33485700	5.31518400	4.46711200
H	3.11068000	3.60718000	2.85194600

H	-1.74085600	-1.80742200	6.26108000
H	-4.19677700	-4.41791000	1.99518000
H	-4.41100700	-6.34276900	3.51529600
H	-3.57095900	-6.20198300	5.85854900
H	-2.49898200	-4.11687500	6.66533500
H	-5.00679300	-2.25235000	-2.48778100
H	-2.58725500	-2.52762800	-2.05425100
H	-5.59767300	-1.56758100	3.00801800
H	-7.27416400	-1.87027300	-1.66218100
H	-7.98125700	-1.28506500	2.54468600
H	6.08299100	-1.92962400	3.27385700
H	6.67741800	-1.65357300	-2.25975900
H	9.04037400	-1.30150400	-1.83711100
H	8.33330300	-1.54938100	2.42047300
H	5.31373800	-4.50081700	-1.03941700
H	3.66165600	-4.55403200	-5.73504800
H	4.75487200	-6.56019700	-4.77164200
H	5.57129000	-6.52183400	-2.41700400
H	2.86901200	-2.23376600	-5.50466200
H	2.57367600	-0.19663000	-4.12906700
H	3.66748800	-2.27562900	2.85066100
H	-1.48032500	0.12480200	4.73531600
C	10.31764400	-1.25068700	0.63458900
C	11.34740500	-1.60635000	-0.21419300
C	10.58590600	-0.67164900	1.92150300
N	10.60397500	-0.21777400	3.00490900
C	11.20008300	-2.34581200	-1.41489300
N	11.08981700	-2.97655500	-2.39947600
N	12.74471400	-1.30351000	0.10306100
O	13.61958200	-1.76015400	-0.68881400
O	13.00077100	-0.60918600	1.12768500
C	-9.26297400	-1.38815600	0.22941800
C	-9.99604100	-1.14830100	-0.91541300
H	-9.83254000	-1.52357200	1.14390700
C	-12.00661900	-2.35564600	0.00177600
H	-11.97483800	-1.96339400	1.03108900
H	-11.49689300	-3.32437900	-0.00075000
N	-11.35986800	-1.43412300	-0.95440700
C	-13.69936000	-0.97012400	-0.99951600
C	-13.46108600	-2.41053000	-0.49321000
H	-14.54116000	-0.89272300	-1.69401600
H	-13.90320000	-0.30569400	-0.15089800
H	-14.15988700	-2.70738300	0.29427000
H	-13.55492900	-3.12634400	-1.31888500
C	-8.57747100	0.59758200	-2.08540100
C	-9.68782700	-1.12219400	-3.44190800
H	-7.67430100	0.43030900	-1.48900900
H	-9.10212200	1.46486100	-1.66299900
H	-10.70344500	-1.50196100	-3.57376200
H	-8.99606300	-1.95765000	-3.64166000
C	-8.23291900	0.79863800	-3.57977900
C	-9.36793700	0.07931400	-4.34501800

H	-7.27070200	0.32402300	-3.80922000
H	-8.14794100	1.85697300	-3.84312800
H	-10.24724100	0.73044500	-4.42531200
C	-12.35743000	-0.59217300	-1.66364100
H	-12.38419900	-0.82122100	-2.73741000
H	-12.11612700	0.47116500	-1.55791400
N	-9.48006800	-0.57975900	-2.08197400
H	-9.07480400	-0.22025700	-5.35578200

- **2SM results for the second excited state**

System	Excited state	$\Delta\mu$ (a.u.)	$\cos\theta$ (degree)	δ_{TPA}^{2SM} (10^4 a.u.)	$\delta_{TPA}^{Resp.}$ (10^4 a.u.)
UMA	2	0.030	-0.360	0.0	0.0
SMA-1	2	0.748	-0.923	0.132	1.100
SMA-2	2	0.695	-0.927	0.112	1.250
SMA-3	2	0.677	-0.929	0.105	1.360
SMA-4	2	9.669	-0.824	0.135	0.242
SMA5	2	9.646	-0.398	0.034	0.384