

Supplementary data for

Influence of Electron-Donating Substituents on the Stability of Sandwich-Type Complexes of Crown-Containing Anthraquinoneimines

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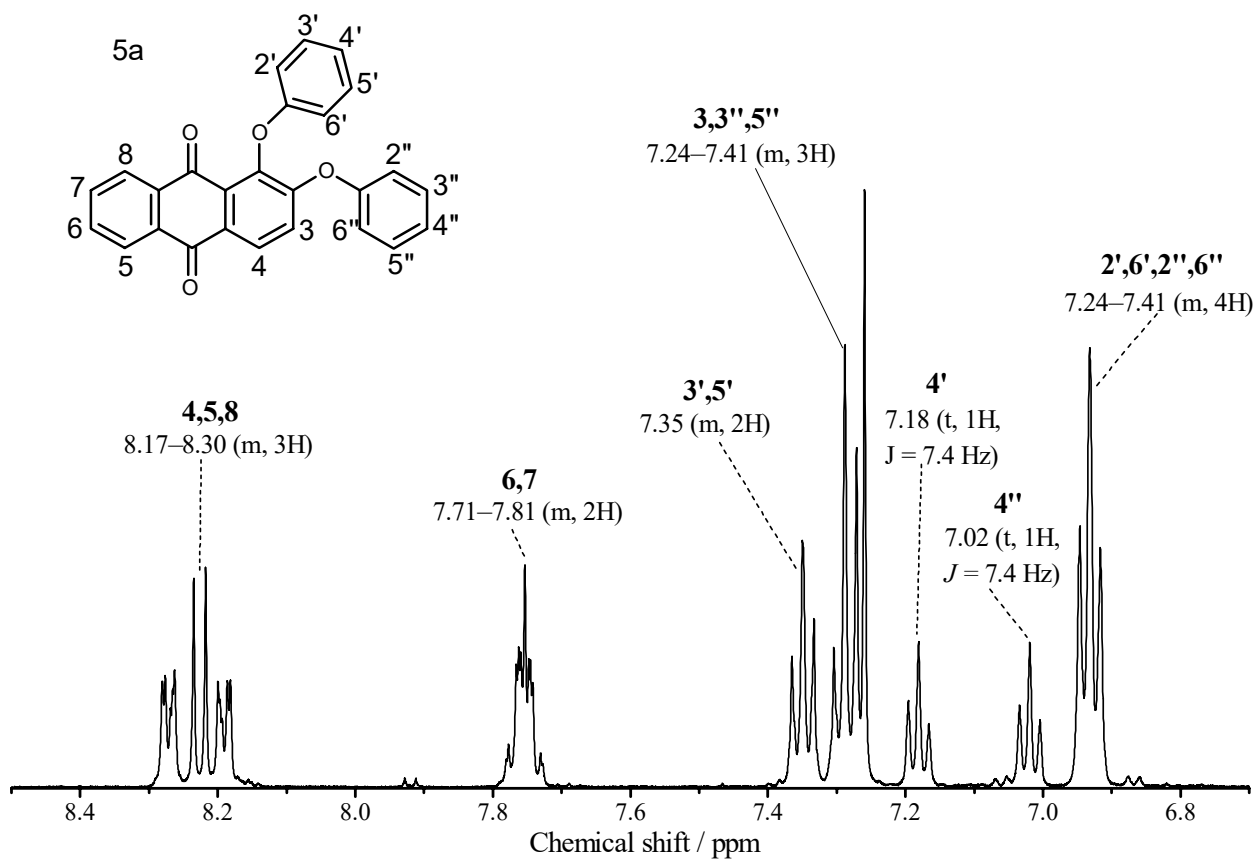
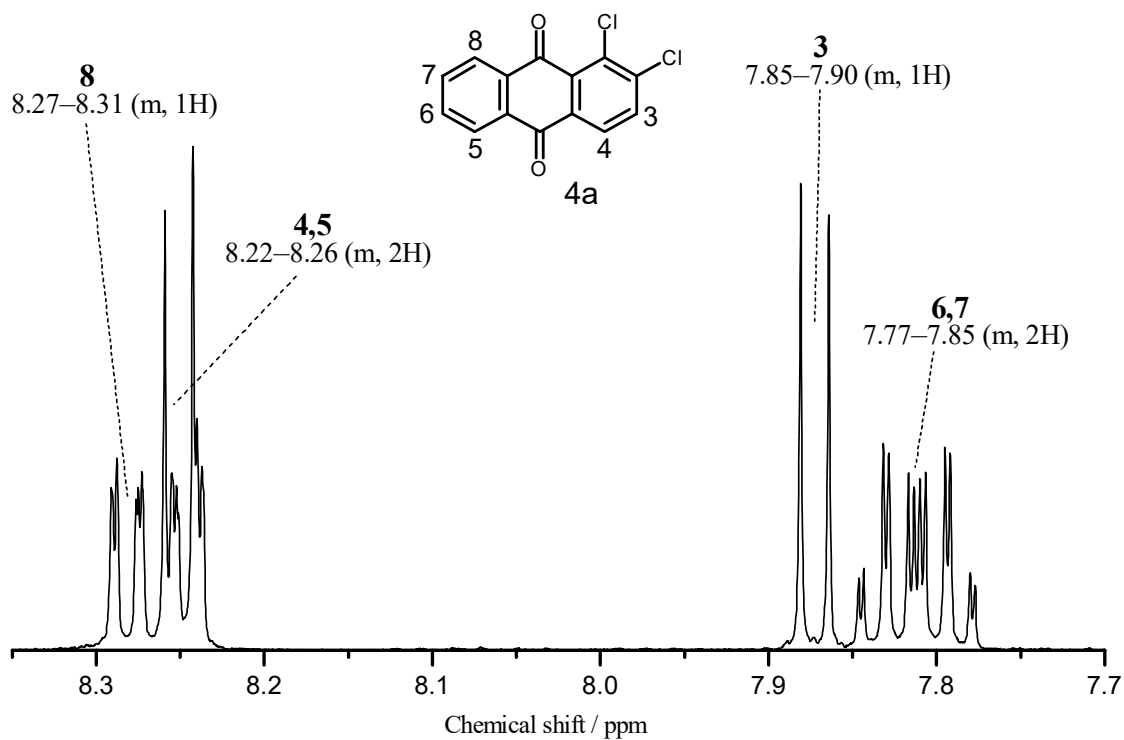
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I Figures S1–S10: NMR spectroscopy data



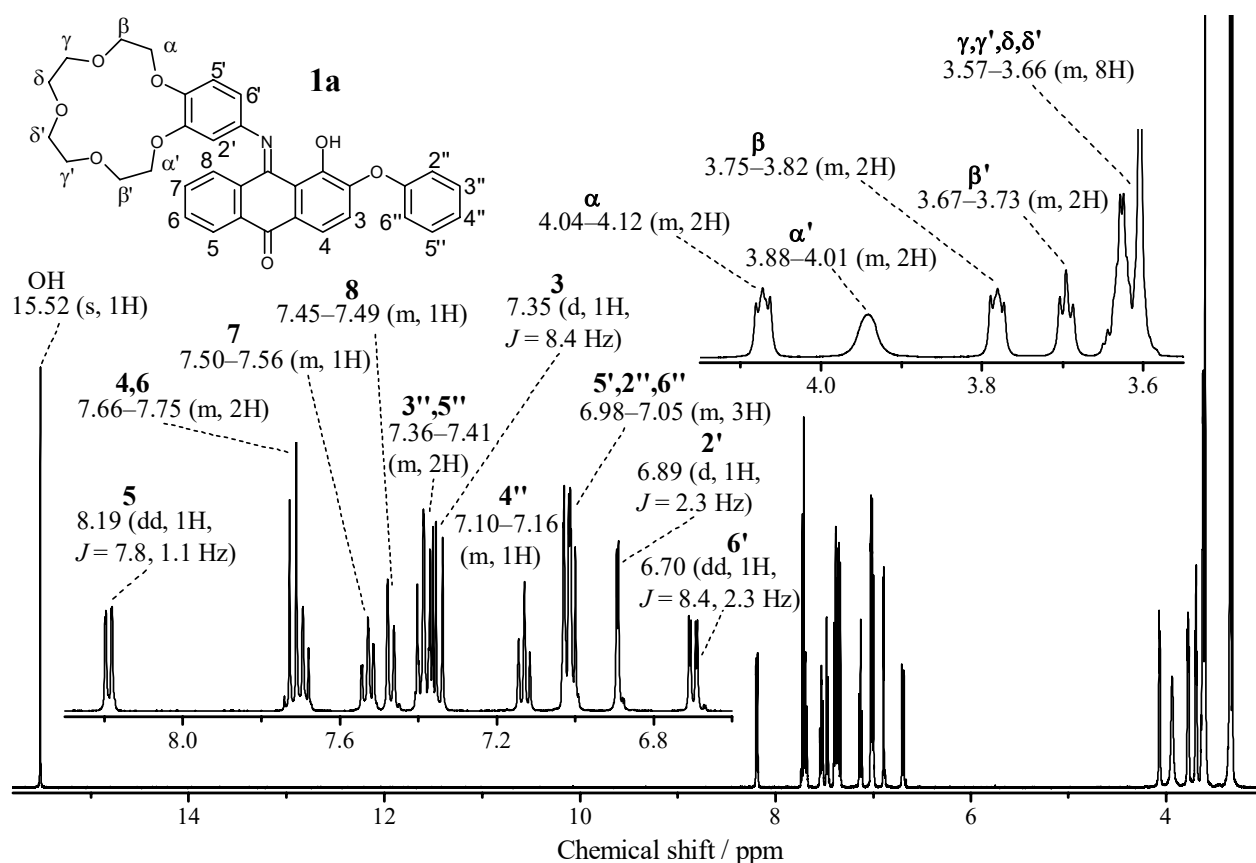


Figure S3. ^1H NMR spectrum of **1a** in $\text{DMSO}-d_6$.

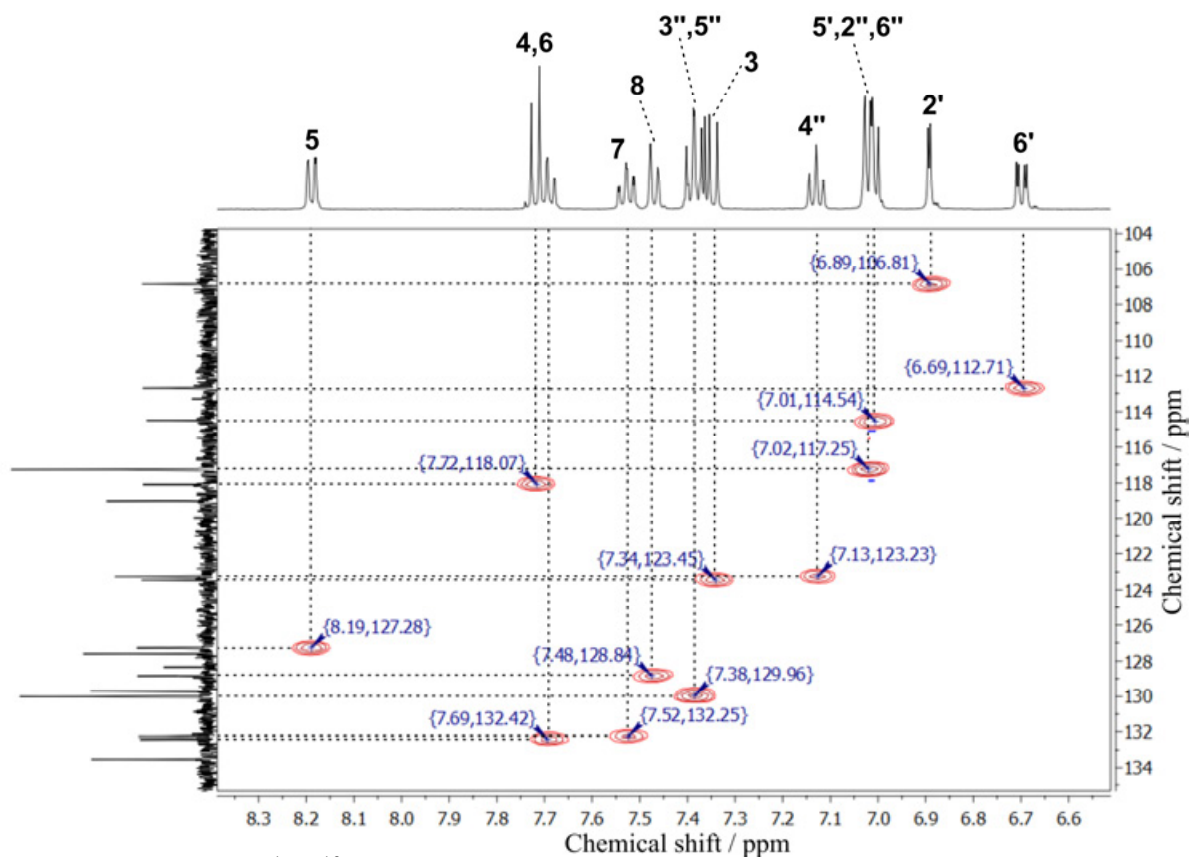


Figure S4. $^1\text{H}-^{13}\text{C}$ HSQC spectrum of **1a** in $\text{DMSO}-d_6$ (aromatic region).

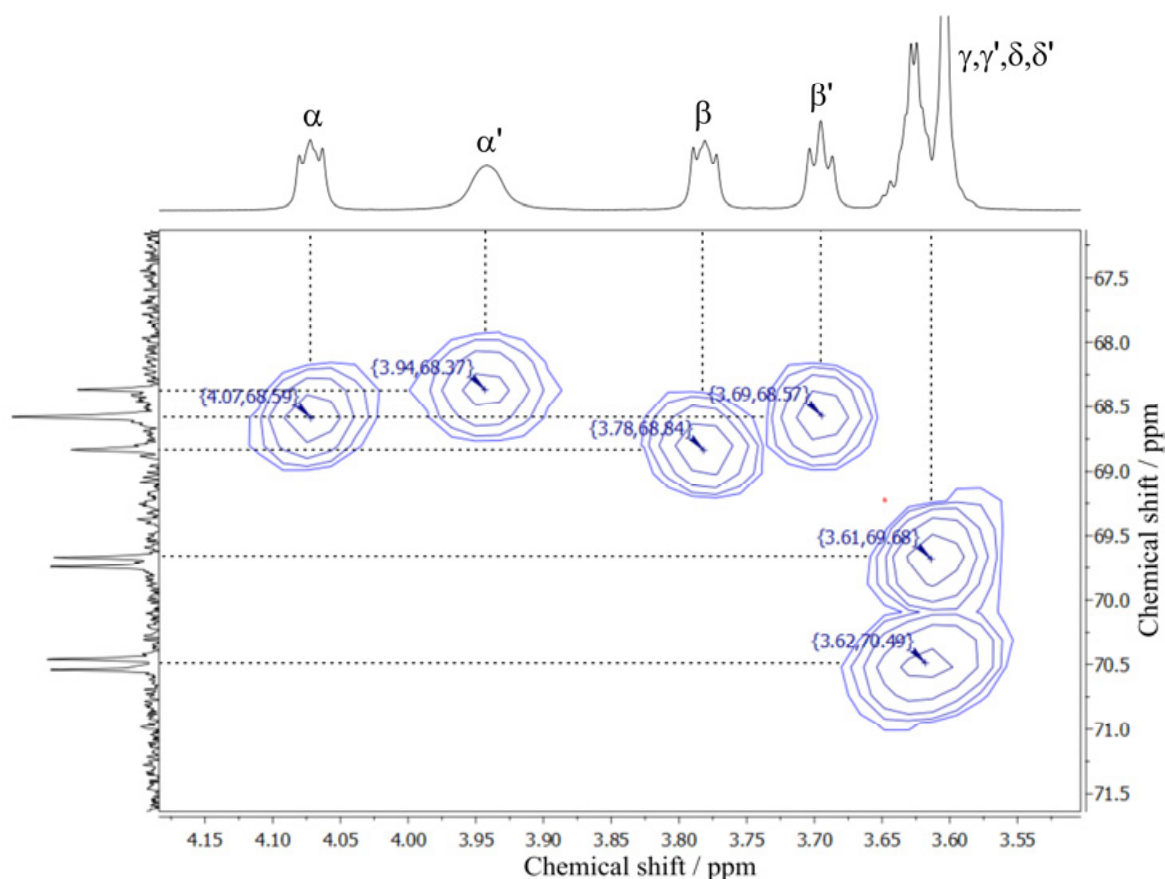


Figure S5. ^1H - ^{13}C HSQC spectrum of **1a** in $\text{DMSO}-d_6$ (aliphatic region).

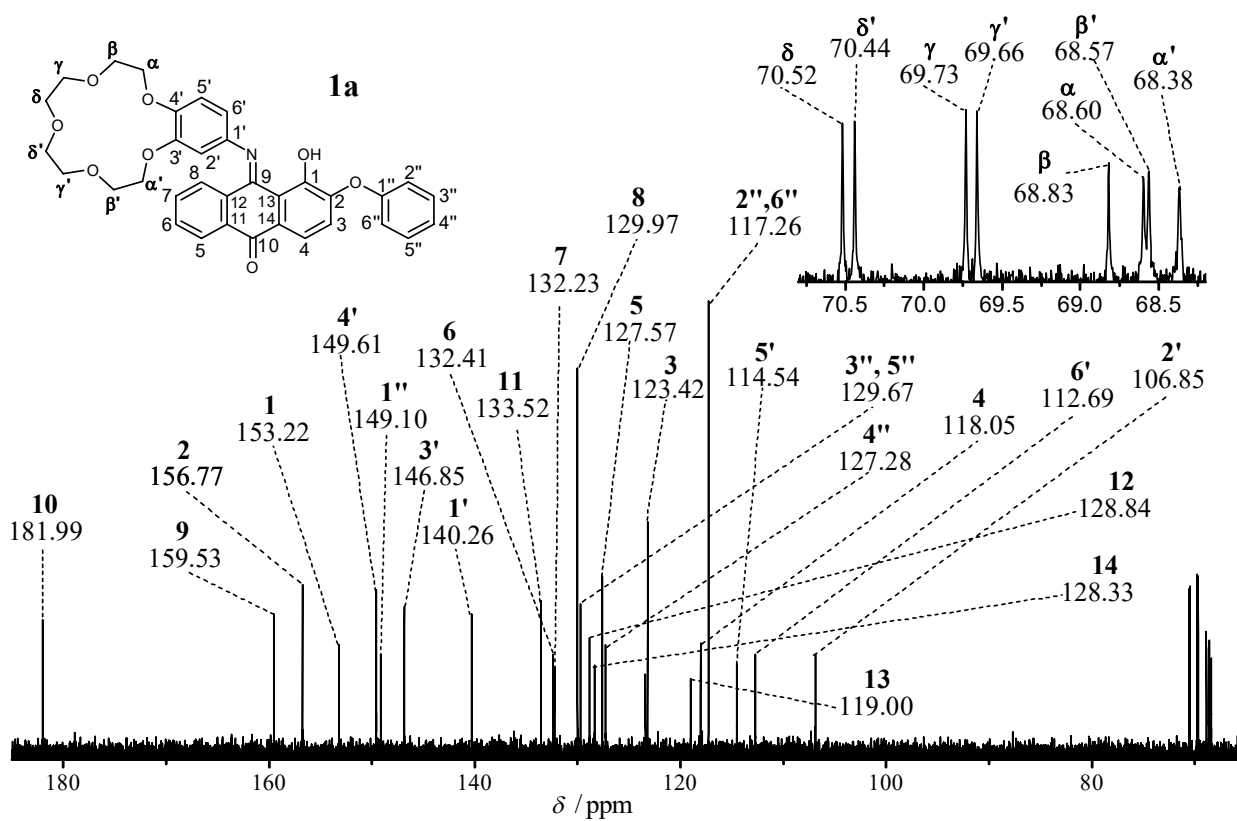


Figure S6. ^{13}C NMR spectrum of **1a** in $\text{DMSO}-d_6$.

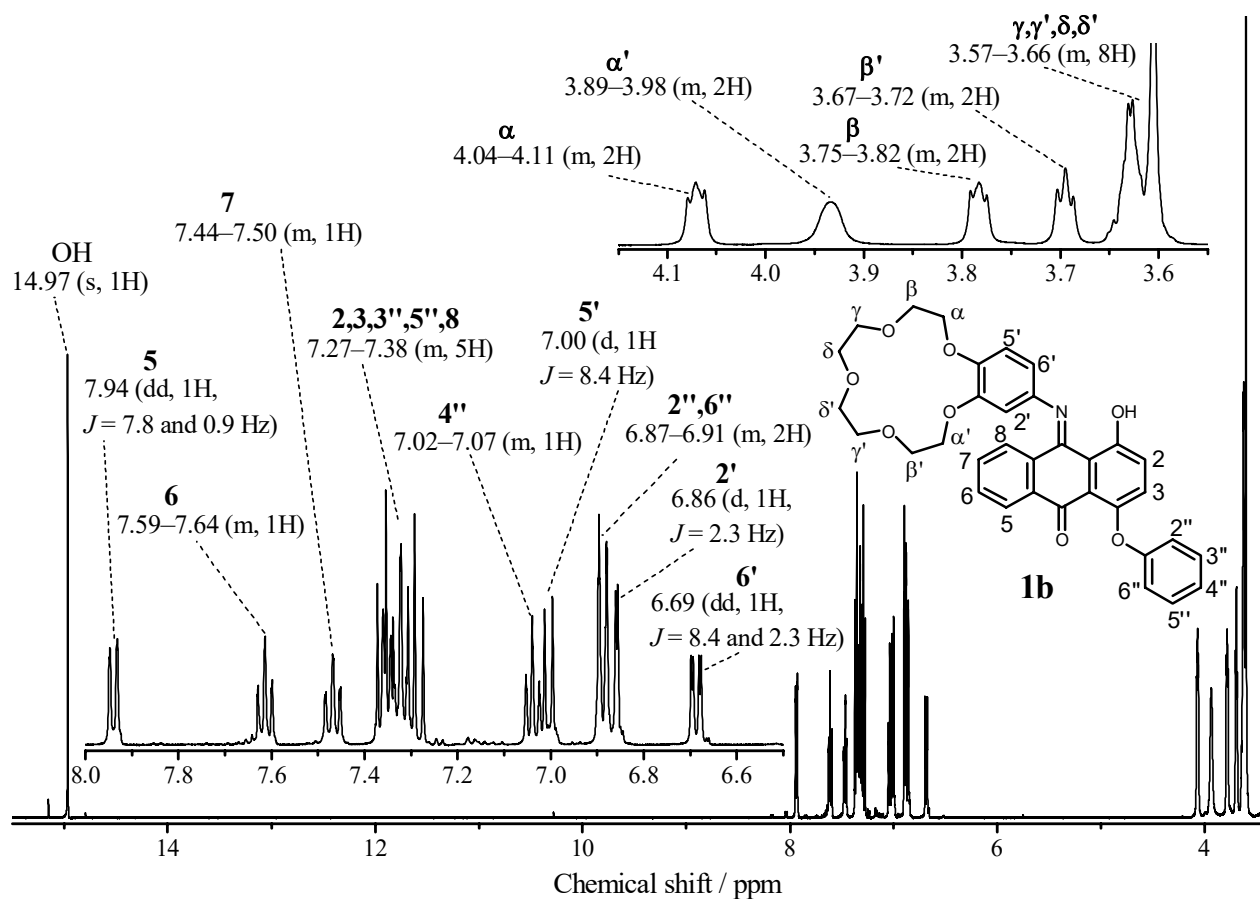


Figure S7. ^1H NMR spectrum of **1b** in $\text{DMSO}-d_6$.

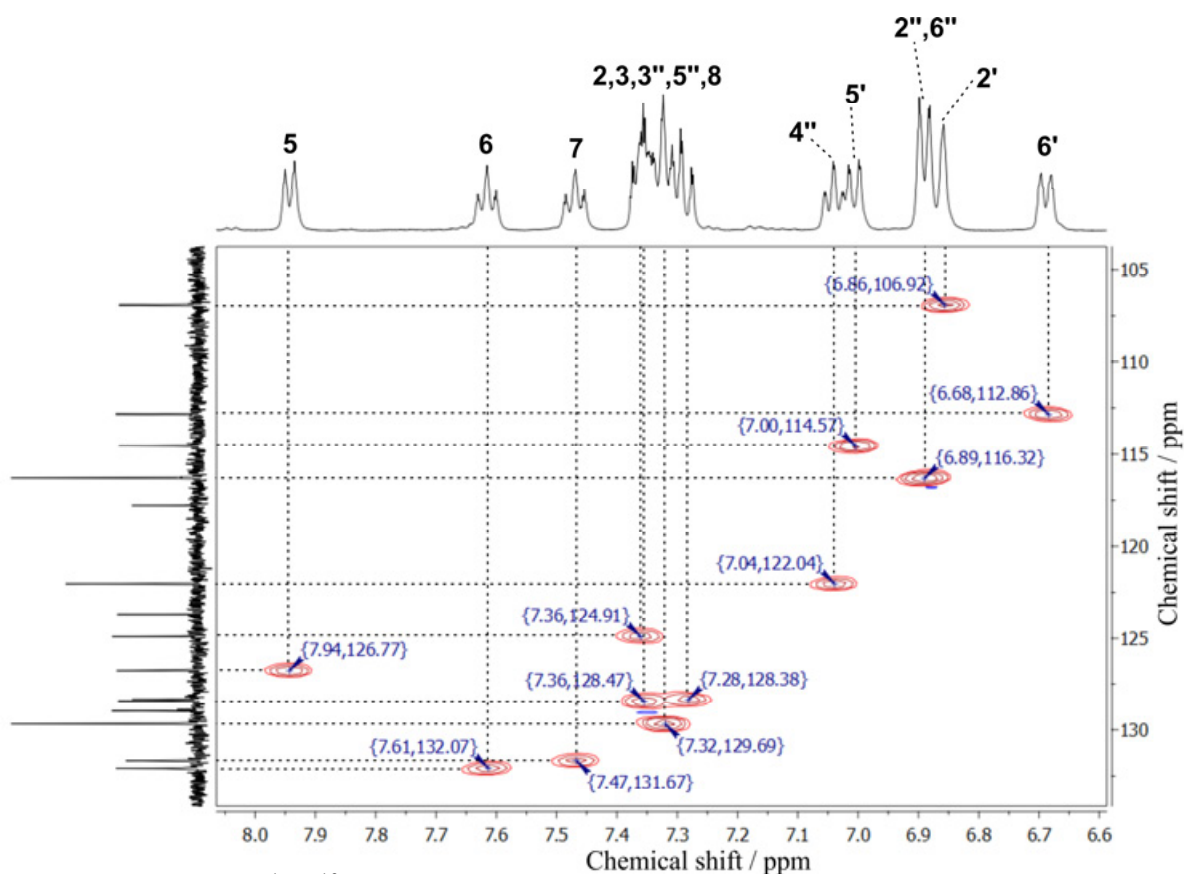


Figure S8. ^1H - ^{13}C HSQC spectrum of **1b** in $\text{DMSO}-d_6$ (aromatic region).

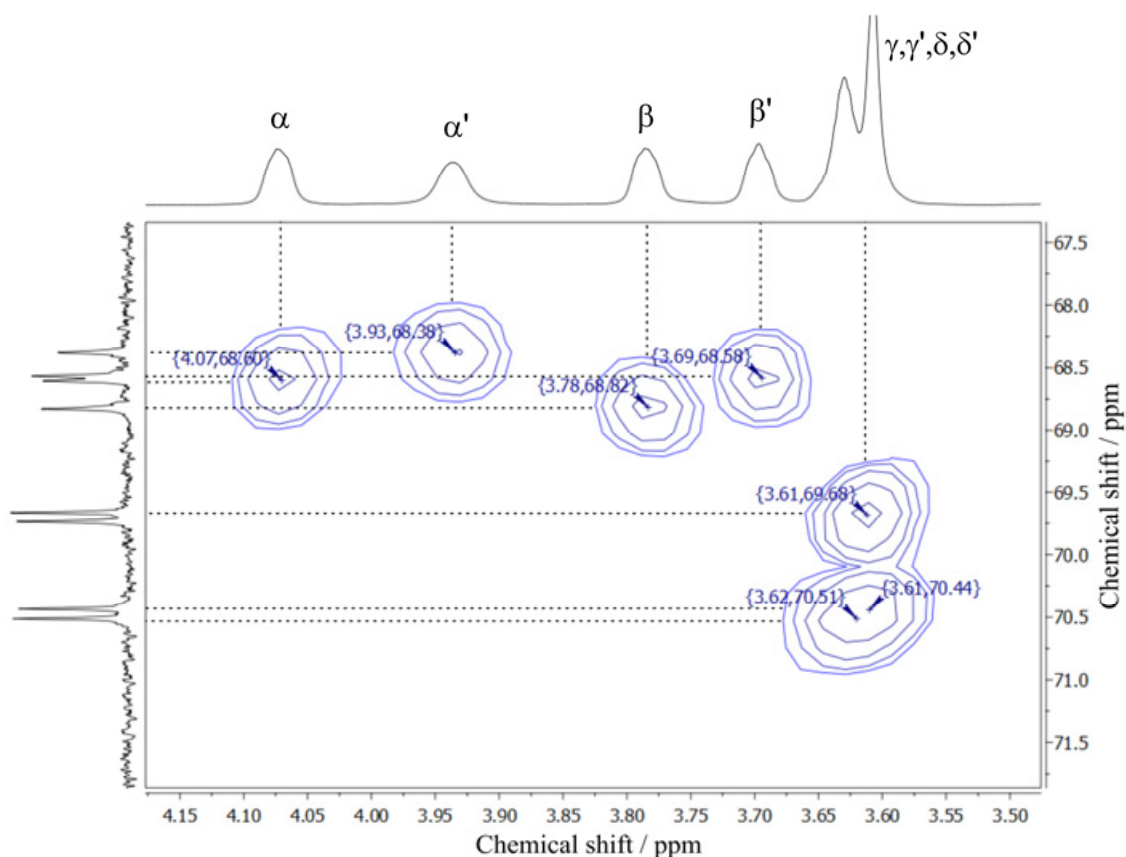


Figure S9. ^1H - ^{13}C HSQC spectrum of **1b** in $\text{DMSO}-d_6$ (aliphatic region).

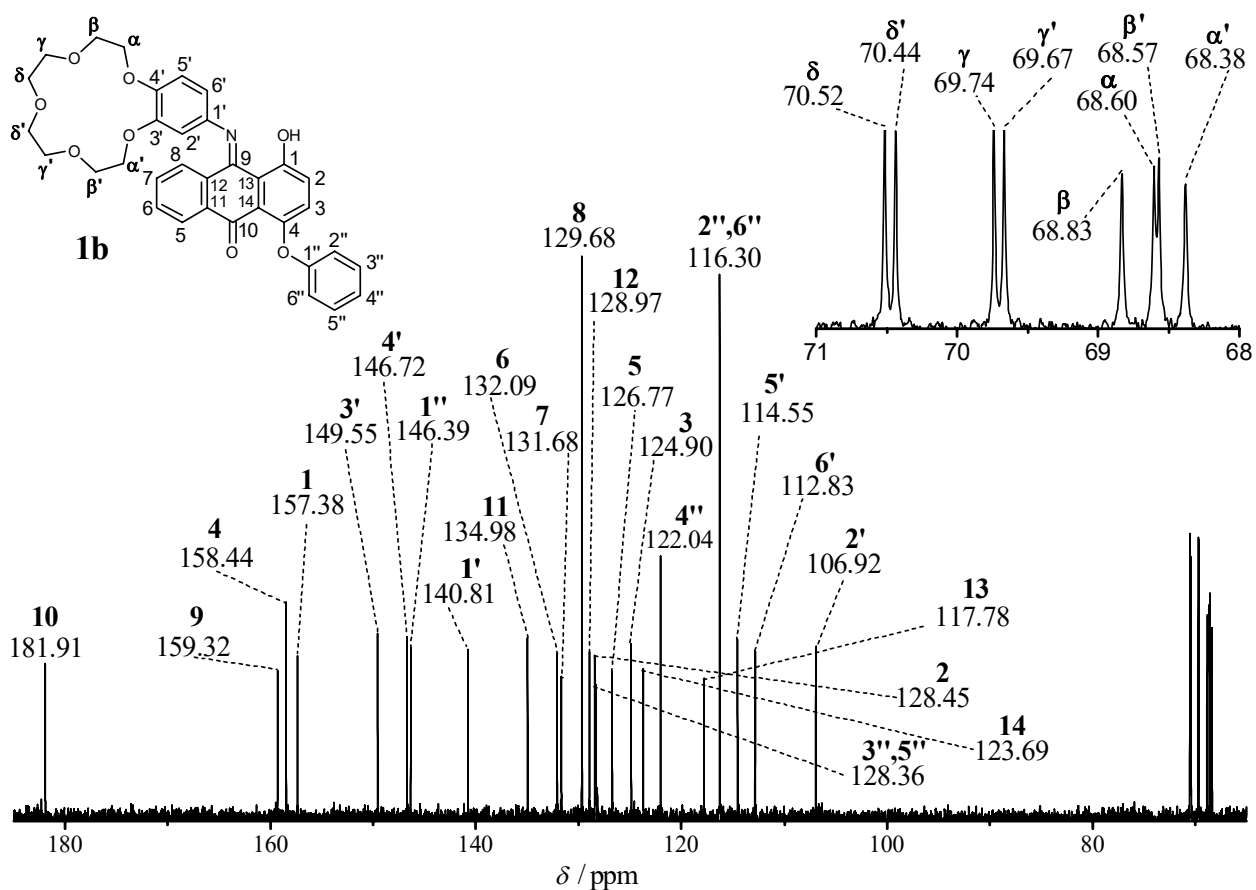


Figure S10. ^{13}C NMR spectrum of **1b** in $\text{DMSO}-d_6$.

II Figures S11–S13: UV-Vis spectroscopy data

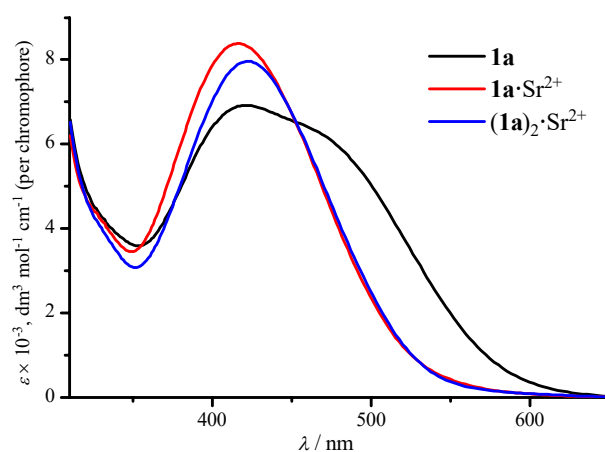


Figure S11. Absorption spectra of dye **1a** and its 1:1 and 2:1 complexes with Sr^{2+} in MeCN.

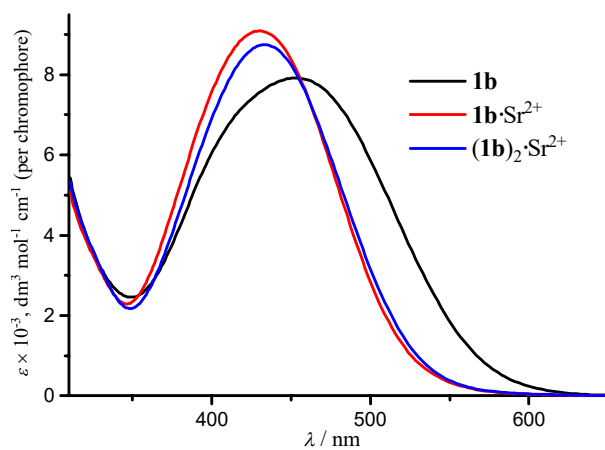


Figure S12. Absorption spectra of dye **1b** and its 1:1 and 2:1 complexes with Sr^{2+} in MeCN.

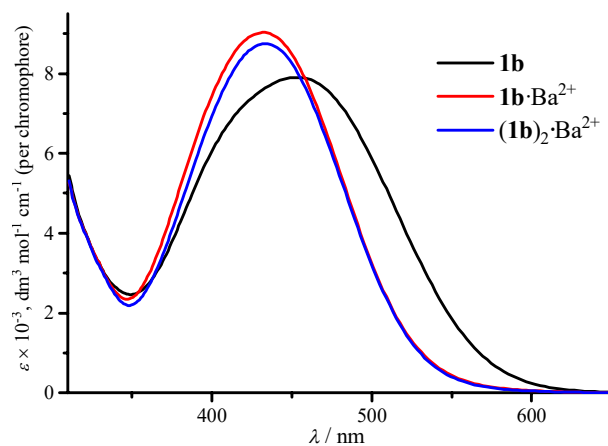
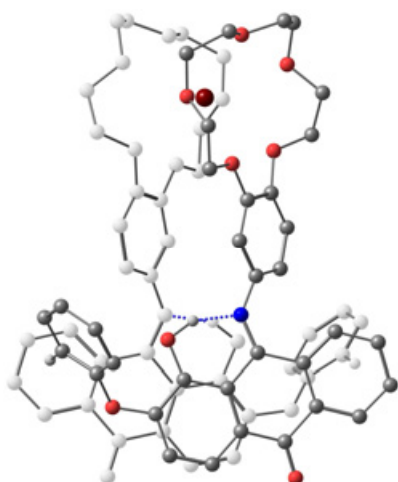


Figure S13. Absorption spectra of dye **1b** and its 1:1 and 2:1 complexes with Ba^{2+} in MeCN.

III Table S1: Cartesian coordinates from DFT calculations in the gas phase

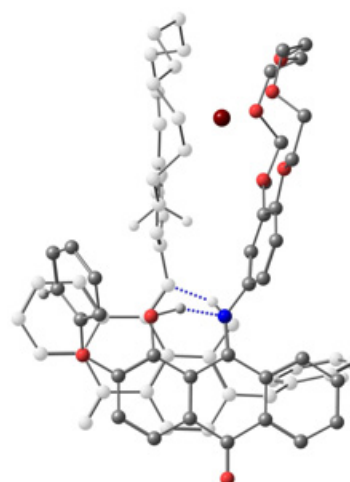


in-[*anti*-(*s-trans*-**1a**)₂]·Ba²⁺

DFT energy (gas phase) = −3967.17553717 a.u.

Cartesian coordinates (Å):

C	2.895243000	-4.806899000	-2.981711000
C	4.213179000	-5.264009000	-2.873727000
C	5.211141000	-4.391183000	-2.451945000
C	4.900547000	-3.068895000	-2.124035000
C	3.564518000	-2.618524000	-2.165758000
C	2.573782000	-3.500225000	-2.627799000
C	6.023935000	-2.144448000	-1.802841000
C	5.708122000	-0.700674000	-1.748644000
C	4.360914000	-0.259439000	-1.713156000
C	3.254473000	-1.225719000	-1.774829000
C	6.756480000	0.208492000	-1.655281000
C	6.501577000	1.573841000	-1.524909000
C	5.193921000	2.031014000	-1.446380000
C	4.109645000	1.124469000	-1.520240000
O	7.161015000	-2.567595000	-1.628861000
N	2.066988000	-0.746105000	-1.521292000
O	2.876532000	1.619857000	-1.364745000
H	2.117858000	-5.470645000	-3.347778000
H	4.459848000	-6.287578000	-3.137841000
H	6.248321000	-4.700330000	-2.385290000
H	1.551530000	-3.162053000	-2.731045000
H	7.771204000	-0.171033000	-1.666231000
H	7.306378000	2.292562000	-1.419994000
H	2.275414000	0.801777000	-1.379932000
C	2.895178000	4.806915000	2.981669000
C	4.213103000	5.264055000	2.873676000
C	5.211086000	4.391246000	2.451907000
C	4.900523000	3.068946000	2.124017000
C	3.564503000	2.618545000	2.165744000
C	2.573747000	3.500229000	2.627776000
C	6.023934000	2.144519000	1.802847000
C	5.708152000	0.700737000	1.748659000
C	4.360951000	0.259475000	1.713158000
C	3.254490000	1.225732000	1.774819000
C	6.756529000	-0.208406000	1.655310000
C	6.501657000	-1.573760000	1.524933000
C	5.194014000	-2.030960000	1.446386000
C	4.109716000	-1.124440000	1.520240000
O	7.161009000	2.567687000	1.628892000
N	2.067014000	0.746095000	1.521276000
O	2.876617000	-1.619856000	1.364736000
H	2.117779000	5.470648000	3.347731000
H	4.459849000	6.287634000	3.13772000
H	6.248259000	4.700417000	2.385248000
H	1.551503000	3.162033000	2.731026000
H	7.771246000	0.171139000	1.666271000
H	7.306476000	-2.292461000	1.420023000
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O	-4.775976000	1.420725000	-2.463272000
O	-2.689548000	-0.277521000	-1.915446000
O	-3.134236000	-2.220890000	-0.241361000
O	-5.857096000	-2.624925000	-0.302381000



out-[*anti*-(*s-trans*-**1a**)₂]·Ba²⁺

DFT energy (gas phase) = −3967.17545335 a.u.

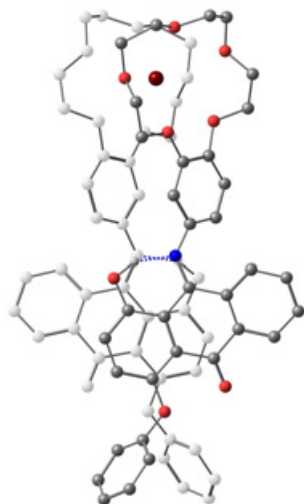
Cartesian coordinates (Å):

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C	3.955014000	-1.929995000	-2.251039000
C	3.293618000	-3.167261000	-2.207875000
C	6.088185000	-0.628047000	-2.695284000
C	5.411718000	0.603122000	-2.223136000
C	4.094356000	0.544099000	-1.711852000
C	3.325920000	-0.704457000	-1.731365000
C	6.095293000	1.814570000	-2.288676000
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H	-3.433475000	-4.020122000	1.484330000
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H	-5.649569000	-4.147156000	0.778427000
H	-8.166608000	-2.979869000	-0.647508000
H	-6.683262000	-3.679684000	-1.329706000
H	-7.579636000	-0.743114000	-1.592099000
H	-7.712056000	-1.971380000	-2.866261000
H	-5.703235000	-2.080103000	-4.298493000
H	-5.287129000	-3.215247000	-2.987404000
H	-3.276508000	-2.501281000	-4.196599000
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H	0.431424000	-1.552497000	0.533885000
H	-2.987042000	-3.474689000	3.124937000
O	-3.704276000	1.517488000	-2.108434000
O	-2.270862000	1.617909000	0.200539000
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C	-7.149208000	2.190011000	0.228078000
C	-5.833494000	2.677275000	-1.713194000
C	-4.897868000	2.026747000	-2.719746000
C	-2.653273000	2.489549000	-1.953351000
C	-1.594278000	1.931752000	-1.030645000
C	-0.142679000	1.187997000	1.328733000
C	0.512626000	0.677036000	2.470555000
C	-0.241695000	0.337883000	3.600715000
C	-1.631474000	0.509533000	3.602575000
H	-4.150529000	1.522170000	4.269828000
H	-4.498358000	-0.145391000	3.727957000
H	-6.587988000	1.242619000	3.820714000
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H	-7.869017000	0.207221000	0.684418000
H	-6.699141000	3.055363000	0.732678000
H	-8.080702000	2.521120000	-0.250675000
H	-6.712573000	3.072311000	-2.239673000
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H	-5.392793000	1.164491000	-3.173769000
H	-3.057630000	3.413770000	-1.525255000
H	-2.209444000	2.717768000	-2.929166000
H	-0.824354000	2.692577000	-0.872996000
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Ba	-4.396696000	-0.315665000	-0.089895000
H	0.260729000	-0.058409000	4.476108000
H	1.124668000	-1.119055000	-3.680292000
O	5.182815000	-3.004192000	0.531914000
O	3.601431000	4.127464000	-0.933092000
C	4.920675000	-3.984149000	1.480556000
C	5.124337000	-3.787899000	2.845078000
C	4.496232000	-5.214765000	0.983235000
C	4.882763000	-4.845630000	3.722653000
C	4.264876000	-6.263792000	1.871119000
C	4.452128000	-6.083802000	3.243841000
H	5.476568000	-2.830657000	3.214461000
H	4.367783000	-5.330992000	-0.086994000
H	5.046284000	-4.699926000	4.786421000
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C	3.645678000	-3.986195000	3.042949000
C	2.223052000	-5.705489000	1.357736000
C	2.602052000	-4.760612000	3.547728000
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H	4.211883000	-3.319857000	3.685821000
H	1.687592000	-6.386563000	0.701761000
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H	1.082750000	-6.230230000	3.114539000



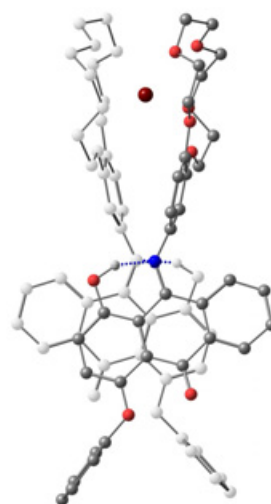
in-[anti-(s-trans-1b)₂]·Ba²⁺

DFT energy (gas phase) = -3967.16668724 a.u.

Cartesian coordinates (Å):

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C	-3.890933000	-3.468991000	0.283976000
C	-2.573634000	-3.122500000	0.637202000
C	-1.597387000	-4.132444000	0.674738000
C	-5.023064000	-2.504884000	0.414268000
C	-4.756812000	-1.268543000	1.180004000
C	-3.403057000	-0.868788000	1.416271000
C	-2.282641000	-1.722323000	1.001630000
C	-5.814206000	-0.470473000	1.658209000
C	-5.534154000	0.710982000	2.374158000
C	-4.234838000	1.124318000	2.556264000
C	-3.158011000	0.368437000	2.065795000
O	-6.113683000	-2.792041000	-0.069280000
N	-1.090194000	-1.183717000	1.056280000
O	-1.925325000	0.869290000	2.263546000
H	-1.147096000	-6.204617000	0.343437000
H	-3.442048000	-6.764111000	-0.442188000
H	-5.212583000	-4.992007000	-0.411809000
H	-0.597040000	-3.907975000	1.019685000
O	-7.082772000	-0.883468000	1.438725000
H	-6.352852000	1.311308000	2.747363000
H	-1.308487000	0.200025000	1.825703000
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C	-3.202733000	5.750992000	0.134204000
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C	-5.534098000	-0.710967000	-2.374255000
C	-4.234775000	-1.124290000	-2.556341000
C	-3.157964000	-0.368412000	-2.065833000
O	-6.113703000	2.791987000	0.069255000
N	-1.090183000	1.183735000	-1.056283000
O	-1.925268000	-0.869251000	-2.263554000
H	-1.147142000	6.204627000	-0.343327000
H	-3.442109000	6.764082000	0.442281000
H	-5.212627000	4.991960000	0.411845000
H	-0.597053000	3.908003000	-1.019611000
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C	1.484861000	5.022824000	-0.362957000
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H	1.873457000	5.185490000	0.634880000
H	0.195055000	4.396486000	-3.969682000
H	-0.446324000	5.877130000	0.023246000
H	-1.288603000	5.487381000	-2.290338000



out-[anti-(s-trans-1b)₂]·Ba²⁺

DFT energy (gas phase) = -3967.16598814 a.u.

Cartesian coordinates (Å):

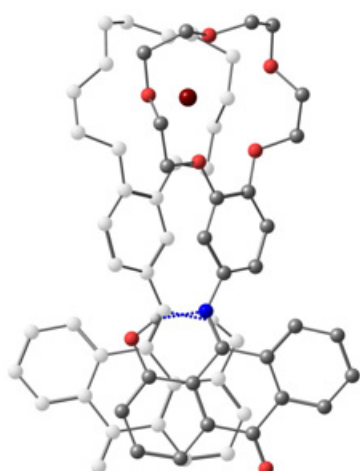
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C	-4.071279000	-3.211253000	0.633111000
C	-2.725053000	-2.812673000	0.538577000
C	-1.809290000	-3.678061000	-0.085257000
C	-5.135584000	-2.319921000	1.184974000
C	-4.760872000	-0.925632000	1.499431000
C	-3.387972000	-0.525332000	1.428257000
C	-2.338467000	-1.474437000	1.024305000
C	-5.742573000	0.011799000	1.883731000
C	-5.367050000	1.330668000	2.206760000
C	-4.046920000	1.714125000	2.154133000
C	-3.045062000	0.806648000	1.776614000
O	-6.269436000	-2.768428000	1.321340000
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O	-1.782227000	1.276552000	1.757685000
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H	-3.873747000	-6.277439000	-0.833356000
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H	-0.779217000	-3.384045000	-0.216444000
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C	-3.200930000	5.507786000	0.134851000
C	-4.144054000	4.533964000	-0.166706000
C	-3.749140000	3.293753000	-0.679669000
C	-2.386399000	3.016754000	-0.900253000
C	-1.444591000	4.019079000	-0.604265000
C	-4.830804000	2.306572000	-0.969082000
C	-4.426469000	0.971958000	-1.455188000
C	-3.046034000	0.695769000	-1.715582000
C	-2.002424000	1.703487000	-1.452858000
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C	-4.992411000	-1.313323000	-2.104348000
C	-3.669571000	-1.580278000	-2.363874000
C	-2.685713000	-0.593774000	-2.189718000
O	-5.997647000	2.637210000	-0.782496000
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O	4.104226000	-2.084117000	-0.717029000
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O	7.738381000	-1.343884000	1.549347000
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C	2.770304000	-2.025752000	-0.322428000
C	4.601840000	-3.195755000	-1.474083000
C	5.924778000	-3.620192000	-0.863375000
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C	4.856565000	-0.564763000	3.633661000
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H	8.483152000	-3.729512000	-0.681610000
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H	-0.454673000	-2.418425000	-1.326641000
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H	6.358886000	-4.439852000	-1.450689000
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C	1.689119000	2.372969000	1.127639000
C	0.380495000	2.174052000	0.683391000
C	0.142388000	1.601296000	-0.580585000
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H	2.805571000	1.141672000	-3.541474000
H	3.116493000	-0.480145000	-2.863643000
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H	8.770396000	1.980970000	0.800775000
H	5.764214000	3.966319000	-0.165416000
H	6.358908000	4.439844000	1.450694000
H	3.894692000	4.029478000	1.434232000
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Ba	5.760435000	-0.000001000	0.000000000
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C	5.939695000	0.447442000	3.597038000
C	3.668374000	1.185940000	3.221973000
C	2.589493000	1.164207000	2.158430000
C	1.107932000	1.690687000	-0.288205000
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H	7.725348000	1.628040000	3.751417000
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H	3.256181000	0.838535000	4.177259000
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H	6.778766000	3.850205000	-0.663189000
Ba	5.408770000	-0.050201000	0.105257000
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H	-3.746229000	2.725686000	2.402010000
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O	-7.029760000	-0.390758000	1.965740000
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C	-8.827879000	0.399002000	3.307679000
C	-8.365650000	1.474229000	1.169759000
C	-9.926305000	1.240722000	3.489605000
C	-9.463101000	2.312513000	1.372101000
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C	-8.569332000	-1.036698000	-1.445300000
C	-8.897322000	0.829303000	-2.977547000
C	-9.719762000	-1.638627000	-1.957868000
C	-10.049060000	0.216586000	-3.473505000
C	-10.460642000	-1.017239000	-2.965635000
H	-7.980878000	-1.507570000	-0.667156000
H	-8.560118000	1.792256000	-3.346604000
H	-10.039553000	-2.596120000	-1.557853000
H	-10.623616000	0.705939000	-4.254086000
H	-11.357920000	-1.490985000	-3.351728000

H	-7.753165000	1.554395000	0.279840000
H	-10.532994000	1.144290000	4.384845000
H	-9.710163000	3.051928000	0.616240000
H	-11.099885000	2.850884000	2.668494000
C	-7.680750000	-0.650803000	-1.839905000
C	-8.265586000	-1.542591000	-0.947090000
C	-8.096783000	-0.547130000	-3.165187000
C	-9.302483000	-2.357194000	-1.408381000
C	-9.132639000	-1.369129000	-3.609855000
C	-9.735909000	-2.274097000	-2.732875000
H	-7.911201000	-1.601434000	0.074519000
H	-7.622596000	0.174498000	-3.822700000
H	-9.770754000	-3.057584000	-0.723593000
H	-9.472184000	-1.295794000	-4.638564000
H	-10.544888000	-2.908774000	-3.081137000

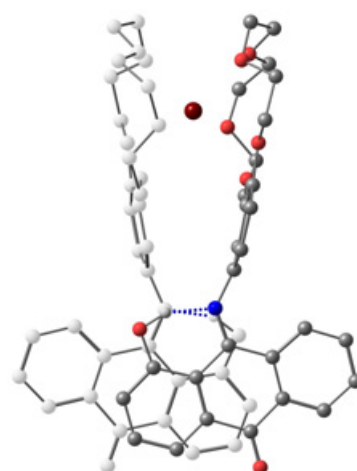


in-[anti-(s-trans-1c)₂]·Ba²⁺

DFT energy (gas phase) = −3354.59666992 a.u.

Cartesian coordinates (Å):

C	3.334933000	5.479276000	0.124850000
C	4.616464000	5.819540000	-0.319038000
C	5.629412000	4.867104000	-0.283895000
C	5.364533000	3.570034000	0.165401000
C	4.055799000	3.195294000	0.535239000
C	3.057018000	4.182107000	0.545090000
C	6.514479000	2.643173000	0.343931000
C	6.257903000	1.396056000	1.105888000
C	4.929724000	0.977380000	1.374140000
C	3.789838000	1.798494000	0.953481000
C	7.350048000	0.631985000	1.498704000
C	7.151543000	-0.569178000	2.186307000
C	5.865945000	-1.021439000	2.440102000
C	4.752014000	-0.278723000	2.020441000
O	7.629806000	2.927592000	-0.076079000
N	2.611638000	1.236763000	1.033136000
O	3.536087000	-0.803065000	2.255620000
H	2.551512000	6.230626000	0.150869000
H	4.827846000	6.828850000	-0.657980000
H	6.647704000	5.107904000	-0.568891000
H	2.063584000	3.945315000	0.901392000
H	8.343382000	0.985874000	1.250477000
H	8.002556000	-1.169137000	2.489592000
H	2.889661000	-0.150666000	1.843739000
C	3.334933000	-5.479276000	-0.124876000
C	4.616470000	-5.819556000	0.318984000
C	5.629421000	-4.867122000	0.283851000
C	5.364539000	-3.570040000	-0.165408000
C	4.055800000	-3.195286000	-0.535213000
C	3.057017000	-4.182096000	-0.545079000
C	6.514484000	-2.643178000	-0.343945000
C	6.257897000	-1.396053000	-1.105884000
C	4.929714000	-0.977365000	-1.374106000
C	3.789836000	-1.798473000	-0.953405000
C	7.350040000	-0.631986000	-1.498715000
C	7.151531000	0.569177000	-2.186316000
C	5.865932000	1.021446000	-2.440091000
C	4.752002000	0.278738000	-2.020412000
O	7.629814000	-2.927598000	0.076056000
N	2.611628000	-1.236763000	-1.033073000
O	3.536080000	0.803095000	-2.255587000



out-[anti-(s-trans-1c)₂]·Ba²⁺

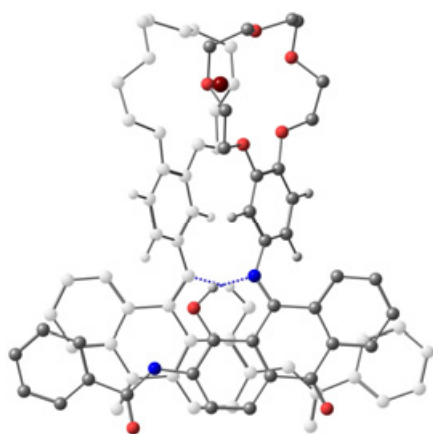
DFT energy (gas phase) = −3354.59560061 a.u.

Cartesian coordinates (Å):

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C	-5.831302000	-4.600686000	-0.546269000
C	-5.476758000	-3.412182000	0.096202000
C	-4.132774000	-2.980063000	0.115154000
C	-3.178061000	-3.754283000	-0.564207000
C	-6.571967000	-2.596457000	0.687434000
C	-6.205153000	-1.297259000	1.301003000
C	-4.858134000	-0.860562000	1.321300000
C	-3.781861000	-1.703174000	0.781936000
C	-7.228518000	-0.520741000	1.835633000
C	-6.938141000	0.721673000	2.402696000
C	-5.629742000	1.180919000	2.440824000
C	-4.586483000	0.407206000	1.913149000
O	-7.735547000	-2.975448000	0.632985000
N	-2.570044000	-1.241386000	0.924332000
O	-3.344882000	0.923552000	1.977817000
H	-2.785288000	-5.511123000	-1.732058000
H	-5.150113000	-6.289418000	-1.694160000
H	-6.876007000	-4.890986000	-0.532951000
H	-2.147889000	-3.436842000	-0.611931000
H	-8.241438000	-0.902207000	1.789384000
H	-7.737074000	1.336983000	2.802668000
H	-2.756084000	0.194538000	1.613395000
C	-3.228520000	5.253228000	0.759581000
C	-4.565195000	5.494210000	1.086930000
C	-5.538088000	4.582323000	0.694623000
C	-5.187307000	3.427157000	-0.010065000
C	-3.837597000	3.165366000	-0.333478000
C	-2.870256000	4.107146000	0.056641000
C	-6.285818000	2.506129000	-0.406032000
C	-5.911065000	1.271453000	-1.135225000
C	-4.558674000	1.003813000	-1.467022000
C	-3.486952000	1.935150000	-1.083084000
C	-6.925898000	0.376184000	-1.450335000
C	-6.623026000	-0.824514000	-2.099960000
C	-5.312431000	-1.120614000	-2.436881000
C	-4.276673000	-0.220842000	-2.138273000
O	-7.451715000	2.759512000	-0.127857000
N	-2.284592000	1.595859000	-1.459236000
O	-3.032085000	-0.579075000	-2.507956000

H	2.551510000	-6.230624000	-0.150902000
H	4.827855000	-6.828876000	0.657895000
H	6.647718000	-5.107933000	0.568823000
H	2.063578000	-3.945291000	-0.901359000
H	8.343376000	-0.985882000	-1.250507000
H	8.002543000	1.169130000	-2.489615000
H	2.889640000	0.150706000	-1.843710000
O	-4.271262000	-0.062184000	2.851966000
O	-2.165587000	1.173175000	1.601879000
O	-2.573776000	2.032597000	-0.818454000
O	-5.286811000	2.458228000	-0.981711000
O	-6.228990000	1.416128000	1.482832000
C	-1.023504000	1.491524000	0.882892000
C	-1.244014000	1.994288000	-0.409367000
C	-3.071084000	3.122356000	-1.608903000
C	-4.387547000	3.576936000	-1.005968000
C	-6.598532000	2.740368000	-0.480787000
C	-6.668315000	2.703601000	1.034969000
C	-6.327860000	1.267682000	2.904407000
C	-5.624381000	-0.017226000	3.311316000
C	-3.358957000	0.743241000	3.601871000
C	-2.003941000	0.682038000	2.937215000
C	0.268024000	1.295631000	1.342450000
C	1.375740000	1.619682000	0.532177000
C	1.147484000	2.125902000	-0.761253000
C	-0.157796000	2.300500000	-1.224241000
H	-3.218288000	2.770125000	-2.634410000
H	-2.358244000	3.952039000	-1.602359000
H	-4.219668000	3.953339000	0.011035000
H	-7.247456000	1.963756000	-0.897471000
H	-6.948058000	3.713463000	-0.846821000
H	-7.705034000	2.882324000	1.350096000
H	-6.035740000	3.480043000	1.486670000
H	-7.382117000	1.223030000	3.208416000
H	-5.873982000	2.141029000	3.390383000
H	-6.107839000	-0.885294000	2.857045000
H	-5.666790000	-0.131400000	4.402119000
H	-3.283964000	0.365800000	4.630123000
H	-3.699612000	1.785298000	3.635236000
H	-1.307468000	1.317102000	3.494476000
H	-1.612478000	-0.340358000	2.904903000
H	0.464310000	0.859293000	2.312769000
H	1.987725000	2.342214000	-1.408236000
H	-0.325432000	2.667852000	-2.232543000
H	-4.816241000	4.381959000	-1.616954000
O	-5.286842000	-2.458214000	0.981699000
O	-2.573804000	-2.032615000	0.818447000
O	-2.165587000	-1.173188000	-1.601876000
O	-4.271244000	0.062187000	-2.851976000
O	-6.228993000	-1.416109000	-1.482853000
C	-1.244037000	-1.994313000	0.409374000
C	-1.023512000	-1.491545000	-0.882880000
C	-2.003928000	-0.682051000	-2.937210000
C	-3.358940000	-0.743242000	-3.601876000
C	-5.624360000	0.017239000	-3.311334000
C	-6.327852000	-1.267664000	-2.904429000
C	-6.668333000	-2.703577000	-1.034992000
C	-6.598562000	-2.740342000	0.480765000
C	-4.387591000	-3.576932000	1.005967000
C	-3.071125000	-3.122363000	1.608902000
C	-0.157829000	-2.300534000	1.224257000
C	1.147457000	-2.125935000	0.761284000
C	1.375727000	-1.619706000	-0.532139000
C	0.268020000	-1.295651000	-1.342424000
H	-1.307454000	-1.317118000	-3.494468000
H	-1.612458000	0.340343000	-2.904893000
H	-3.283937000	-0.365799000	-4.630126000
H	-5.666761000	0.131413000	-4.402138000
H	-6.107814000	0.885311000	-2.857066000
H	-5.873976000	-2.141013000	-3.390401000
H	-7.382107000	-1.223004000	-3.208446000
H	-7.705052000	-2.882291000	-1.350127000
H	-6.035762000	-3.480025000	-1.486686000
H	-6.948101000	-3.713433000	0.846798000
H	-7.247481000	-1.963723000	0.897442000
H	-4.219713000	-3.953345000	-0.011032000
H	-4.816295000	-4.381946000	1.616957000
H	-2.358293000	-3.952054000	1.602366000
H	-3.218327000	-2.770124000	2.634408000
H	-0.325476000	-2.667889000	2.232557000
H	1.987690000	-2.342245000	1.408278000
H	0.464317000	-0.859305000	-2.312737000
H	-3.699602000	-1.785296000	-3.635245000
Ba	-4.250739000	0.000001000	-0.000006000
H	5.684816000	-1.964995000	2.943379000
H	5.684803000	1.965000000	-2.943368000

H	-2.460716000	5.964582000	1.048254000
H	-4.843430000	6.389612000	1.633875000
H	-6.588067000	4.739301000	0.915359000
H	-1.829612000	3.959718000	-0.188811000
H	-7.940208000	0.628221000	-1.166350000
H	-7.413535000	-1.532186000	-2.328164000
H	-2.466016000	0.215167000	-2.263227000
O	5.470981000	-2.263335000	1.102027000
O	2.790101000	-2.641414000	0.696887000
O	1.781432000	-1.282524000	-1.220040000
O	3.633134000	-0.022411000	-2.733032000
O	5.885862000	-1.339739000	-1.544766000
C	1.414461000	-2.475306000	0.763796000
C	0.857386000	-1.729707000	-0.292647000
C	1.349389000	-0.716110000	-2.465123000
C	2.563681000	-0.739836000	-3.371628000
C	4.907034000	-0.148641000	-3.382491000
C	5.658157000	-1.400280000	-2.959189000
C	6.641416000	-2.447233000	-1.044411000
C	6.753941000	-2.308422000	0.465787000
C	4.874688000	-3.552407000	1.307294000
C	3.440030000	-3.360887000	1.744195000
C	0.592972000	-2.926719000	1.791065000
C	-0.766632000	-2.601670000	1.791716000
C	-1.315381000	-1.821146000	0.764352000
C	-0.491300000	-1.413079000	-0.305205000
H	0.983949000	0.302394000	-2.308136000
H	0.550314000	-1.323777000	-2.903271000
H	2.865091000	-1.778159000	-3.552899000
H	5.478757000	0.733543000	-3.084481000
H	4.782693000	-0.139399000	-4.471830000
H	6.617924000	-1.438136000	-3.491568000
H	5.096905000	-2.313557000	-3.198431000
H	7.646989000	-2.448892000	-1.486332000
H	6.145378000	-3.385807000	-1.325227000
H	7.243774000	-1.365459000	0.725315000
H	7.356579000	-3.129676000	0.872459000
H	5.432461000	-4.099504000	2.077720000
H	4.894333000	-4.132360000	0.377451000
H	2.974889000	-4.343219000	1.884577000
H	3.371705000	-2.792969000	2.679911000
H	0.997610000	-3.510183000	2.609966000
H	-0.931724000	-0.822929000	-1.099729000
H	2.322190000	-0.266006000	-4.331140000
O	3.348063000	-0.056660000	2.812563000
O	1.796975000	1.421800000	1.143898000
O	3.109381000	2.608388000	-0.699019000
O	5.766785000	1.991275000	-0.822400000
O	5.815985000	1.056800000	1.855650000
C	1.014502000	1.902649000	0.109128000
C	1.740466000	2.547955000	-0.910856000
C	3.922645000	3.254678000	-1.677339000
C	5.316076000	3.325953000	-1.094167000
C	6.972583000	1.922983000	-0.052745000
C	6.714101000	2.089489000	1.436401000
C	5.447267000	1.151217000	3.238344000
C	4.557495000	-0.031349000	3.585675000
C	2.281615000	0.745570000	3.346580000
C	1.182480000	0.854958000	2.309683000
C	-0.351107000	1.702548000	-0.010569000
C	-1.016823000	2.099604000	-1.191684000
C	-0.294967000	2.765144000	-2.191882000
C	1.076159000	2.999332000	-2.045540000
H	3.559905000	4.270773000	-1.870651000
H	3.902667000	2.681705000	-2.612082000
H	5.997790000	3.809753000	-1.804948000
H	7.691767000	2.677093000	-0.394916000
H	7.392050000	0.933369000	-0.255486000
H	6.274793000	3.070497000	1.660688000
H	7.663455000	2.008866000	1.982856000
H	6.346527000	1.119765000	3.867939000
H	4.938396000	2.108720000	3.413622000
H	4.325202000	-0.020376000	4.657110000
H	5.080164000	-0.961129000	3.347951000
H	2.653067000	1.746996000	3.593096000
H	1.888242000	0.277823000	4.257567000
H	0.391294000	1.513947000	2.683248000
H	0.753825000	-0.123349000	2.071150000
H	-0.915377000	1.191195000	0.756229000
H	1.614597000	3.505511000	-2.838267000
H	5.291990000	3.915055000	-0.170154000
Ba	3.979612000	-0.061537000	0.066017000
H	-0.806502000	3.072427000	-3.097131000
H	-1.400038000	-2.916394000	2.613445000
H	-5.047187000	-2.048345000	-2.931905000
H	-5.376310000	2.144857000	2.867635000

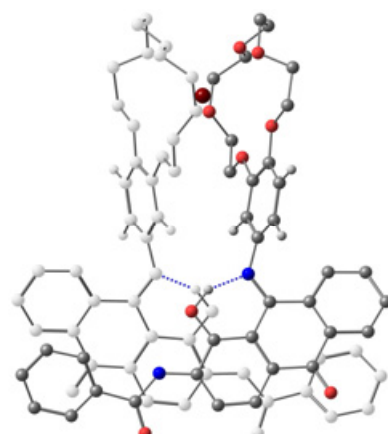


in-[anti-(*s*-trans-1d)₂]·Ba²⁺

DFT energy (gas phase) = −4154.18553602 a.u.

Cartesian coordinates (Å):

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C	2.822810000	6.099954000	1.775989000
C	3.979310000	5.342637000	1.635122000
C	3.911734000	3.948602000	1.579046000
C	2.663615000	3.289051000	1.626750000
C	1.511778000	4.067307000	1.841651000
C	5.196858000	3.193576000	1.561971000
C	5.115588000	1.725579000	1.639626000
C	3.860450000	1.058028000	1.619874000
C	2.610138000	1.812342000	1.502841000
C	6.298624000	0.998693000	1.678626000
C	6.295390000	-0.396045000	1.702406000
C	5.081651000	-1.083277000	1.667862000
C	3.864468000	-0.354238000	1.628160000
O	6.269108000	3.788854000	1.521119000
N	1.519632000	1.109871000	1.316682000
O	2.735307000	-1.093634000	1.587451000
H	0.687530000	6.033817000	2.080256000
H	2.882642000	7.183109000	1.807652000
H	4.956668000	5.804564000	1.571907000
H	0.550046000	3.593058000	1.976818000
H	7.233146000	1.547300000	1.667250000
H	7.216044000	-0.960425000	1.720840000
H	1.990253000	-0.418901000	1.469994000
C	1.591030000	-5.454638000	-1.911722000
C	2.823393000	-6.099955000	-1.775765000
C	3.979800000	-5.342491000	-1.634933000
C	3.912065000	-3.948459000	-1.579015000
C	2.663870000	-3.289051000	-1.626825000
C	1.512136000	-4.067462000	-1.841712000
C	5.197104000	-3.193286000	-1.561968000
C	5.115670000	-1.725298000	-1.639633000
C	3.860454000	-1.057895000	-1.619936000
C	2.610217000	-1.812341000	-1.502989000
C	6.298620000	-0.998269000	-1.678556000
C	6.295221000	0.396470000	-1.702326000
C	5.081397000	1.083557000	-1.667844000
C	3.864301000	0.354367000	-1.628222000
O	6.269419000	-3.788437000	-1.520983000
N	1.519639000	-1.109977000	-1.316847000
O	2.735035000	1.093605000	-1.587610000
H	0.688120000	-6.034089000	-2.080148000
H	2.883351000	-7.183107000	-1.807289000
H	4.957206000	-5.804300000	-1.571615000
H	0.550356000	-3.593340000	-1.976980000
H	7.233205000	-1.546767000	-1.667133000
H	7.215808000	0.960963000	-1.720709000
H	1.990072000	0.418745000	-1.470304000
O	-5.402007000	-0.657329000	2.765306000
O	-3.278404000	0.790850000	1.788401000
O	-3.675659000	2.151835000	-0.397941000
O	-6.390522000	2.620923000	-0.432176000
O	-7.342604000	1.095080000	1.748701000
C	-2.134002000	1.264123000	1.164801000
C	-2.350224000	2.034551000	0.011124000
C	-4.175564000	3.396612000	-0.908902000
C	-5.482086000	3.708098000	-0.203718000
C	-7.703621000	2.802846000	0.109845000
C	-7.783390000	2.447121000	1.583165000



out-[anti-(*s*-trans-1d)₂]·Ba²⁺

DFT energy (gas phase) = −4154.18514772 a.u.

Cartesian coordinates (Å):

C	-1.296070000	6.038683000	-0.000174000
C	-2.378985000	6.817890000	-0.413373000
C	-3.497769000	6.198835000	-0.959965000
C	-3.530500000	4.813545000	-1.128103000
C	-2.405657000	4.025187000	-0.798120000
C	-1.306442000	4.660107000	-0.193544000
C	-4.818706000	4.201499000	-1.564862000
C	-4.895851000	2.731180000	-1.544129000
C	-3.722932000	1.943907000	-1.373664000
C	-2.432322000	2.566988000	-1.073446000
C	-6.128360000	2.119629000	-1.738094000
C	-6.255400000	0.730197000	-1.763816000
C	-5.114899000	-0.066502000	-1.660897000
C	-3.842898000	0.544587000	-1.507100000
O	-5.771149000	4.906983000	-1.879618000
N	-1.390067000	1.773959000	-1.033735000
O	-2.790367000	-0.297914000	-1.452605000
H	-0.437707000	6.505985000	0.473396000
H	-2.361916000	7.894997000	-0.278357000
H	-4.382298000	6.759283000	-1.238481000
H	-0.458128000	4.082931000	0.144798000
H	-6.999968000	2.751221000	-1.861927000
H	-7.221338000	0.256077000	-1.858211000
H	-1.997842000	0.294544000	-1.263092000
C	-1.295818000	-6.038611000	0.000356000
C	-2.378709000	-6.817879000	0.413506000
C	-3.497551000	-6.198889000	0.960051000
C	-3.530372000	-4.813598000	1.128172000
C	-2.405563000	-4.025176000	0.798235000
C	-1.306278000	-4.660035000	0.193719000
C	-4.818624000	-4.201625000	1.564901000
C	-4.895866000	-2.731313000	1.544099000
C	-3.722990000	-1.943968000	1.373664000
C	-2.432320000	-2.566978000	1.073556000
C	-6.128425000	-2.119835000	1.737974000
C	-6.255557000	-0.730411000	1.763631000
C	-5.115105000	0.066362000	1.660723000
C	-3.843055000	-0.544651000	1.507013000
O	-5.771045000	-4.907162000	1.879605000
N	-1.390103000	-1.773901000	1.033870000
O	-2.790570000	0.297907000	1.452503000
H	-0.437403000	-6.505868000	-0.473165000
H	-2.361574000	-7.894985000	0.278486000
H	-4.382053000	-6.759388000	1.238549000
H	-0.457974000	-4.082815000	-0.144572000
H	-6.999996000	-2.751481000	1.861794000
H	-7.221530000	-0.256352000	1.857964000
H	-1.998011000	-0.294527000	1.263057000
O	6.827536000	2.072181000	-1.115375000
O	4.131148000	2.511049000	-0.893425000
O	2.977616000	1.312460000	1.052428000
O	4.736594000	0.175675000	2.772018000
O	7.093669000	1.330822000	1.609295000
C	2.748273000	2.442662000	-0.988551000
C	2.112111000	1.794605000	0.086511000
C	2.487428000	0.901330000	2.336262000
C	3.667733000	0.986378000	3.284408000
C	5.980924000	0.311136000	3.475023000
C	6.796600000	1.503357000	3.001408000

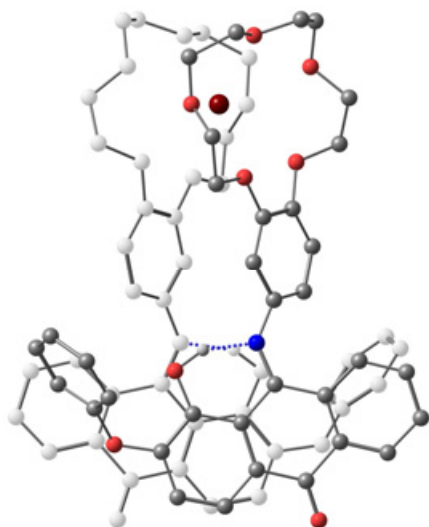
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C	-6.754574000	-0.702439000	3.226085000
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C	-3.127557000	0.037751000	2.997886000
C	-0.843590000	0.992279000	1.591470000
C	0.263216000	1.515651000	0.894524000
C	0.040307000	2.278575000	-0.266652000
C	-1.261084000	2.525897000	-0.704007000
H	-4.336733000	3.289264000	-1.985841000
H	-3.456553000	4.199367000	-0.721836000
H	-5.303261000	3.836508000	0.871447000
H	-8.355799000	2.137499000	-0.464424000
H	-8.042969000	3.834273000	-0.044948000
H	-8.822603000	2.553167000	1.922016000
H	-7.156353000	3.110824000	2.194192000
H	-8.507174000	0.538374000	3.385848000
H	-6.998153000	1.389387000	3.770144000
H	-7.242981000	-1.450366000	2.596850000
H	-6.797648000	-1.047370000	4.267157000
H	-4.413320000	-0.600705000	4.592289000
H	-4.816799000	0.992110000	3.901412000
H	-2.428675000	0.540813000	3.673906000
H	-2.745473000	-0.960532000	2.759913000
H	-0.648243000	0.367788000	2.452894000
H	0.888123000	2.657327000	-0.823676000
H	-1.425446000	3.101522000	-1.610359000
H	-5.908161000	4.636246000	-0.606580000
O	-6.390397000	-2.621204000	0.432053000
O	-3.675502000	-2.152021000	0.398173000
O	-3.278416000	-0.791106000	-1.788323000
O	-5.402046000	0.657186000	-2.765156000
O	-7.342636000	-1.095238000	-1.748632000
C	-2.350108000	-2.034727000	-0.011043000
C	-2.133979000	-1.264350000	-1.164772000
C	-3.127631000	-0.037976000	-2.997797000
C	-4.484362000	0.024592000	-3.660076000
C	-6.754616000	0.702364000	-3.225922000
C	-7.451152000	-0.643731000	-3.103824000
C	-7.783407000	-2.447292000	-1.583181000
C	-7.703526000	-2.803147000	-0.109896000
C	-5.481902000	-3.708288000	0.203409000
C	-4.175467000	-3.396920000	0.908791000
C	-1.260913000	-2.526027000	0.704031000
C	0.040449000	-2.278697000	0.266593000
C	0.263268000	-1.515818000	-0.894630000
C	-0.843596000	-0.992503000	-1.591531000
H	-2.428777000	-0.541017000	-3.673862000
H	-2.745533000	0.960301000	-2.759819000
H	-4.413432000	0.600449000	-4.592175000
H	-6.797681000	1.047335000	-4.266983000
H	-7.242978000	1.450286000	-2.596654000
H	-6.998315000	-1.389416000	-3.770114000
H	-8.507276000	-0.538365000	-3.385674000
H	-8.822646000	-2.553314000	-1.921961000
H	-7.156416000	-3.110942000	-2.194313000
H	-8.042807000	-3.834605000	0.044831000
H	-8.355695000	-2.137883000	0.464478000
H	-5.302981000	-3.836436000	-0.871771000
H	-5.907972000	-4.636550000	0.606015000
H	-3.456417000	-4.199623000	0.721644000
H	-4.336756000	-3.289798000	1.985734000
H	-1.425213000	-3.101612000	1.610421000
H	0.888304000	-2.657403000	0.823589000
H	-0.648309000	-0.368037000	-2.452986000
H	-4.816930000	-0.992323000	-3.901212000
N	4.941442000	2.466611000	-1.636073000
H	3.986591000	2.780546000	-1.539868000
C	5.944594000	3.424019000	-1.597693000
C	5.453374000	4.834947000	-1.510017000
C	4.666468000	7.506372000	-1.236888000
C	6.346597000	5.784452000	-0.997277000
C	4.169473000	5.237505000	-1.902876000
C	3.778289000	6.568212000	-1.765832000
C	5.952861000	7.112572000	-0.857321000
H	7.334886000	5.453804000	-0.700880000
H	3.479299000	4.530095000	-2.355836000
H	2.785982000	6.875360000	-2.082996000
H	6.648938000	7.841990000	-0.454480000
O	7.132581000	3.139804000	-1.603008000
N	4.941855000	-2.466347000	1.636063000
H	3.987050000	-2.780374000	1.539685000
C	5.945105000	-3.423652000	1.597748000
C	5.454024000	-4.834620000	1.509940000
C	4.667393000	-7.506094000	1.236468000
C	4.169990000	-5.237262000	1.902274000
C	6.347506000	-5.784065000	0.997539000
C	5.953914000	-7.112212000	0.857420000
C	3.778942000	-6.567987000	1.765055000

C	7.906235000	2.377034000	1.067687000
C	8.080419000	2.126354000	-0.422157000
C	6.269234000	3.356213000	-1.427214000
C	4.857316000	3.164960000	-1.934869000
C	1.986571000	2.910716000	-2.054788000
C	0.600138000	2.743288000	-2.049717000
C	-0.040727000	2.100369000	-0.979838000
C	0.737059000	1.614917000	0.093681000
H	2.087623000	-0.115342000	2.273857000
H	1.699551000	1.580890000	2.677329000
H	3.994375000	2.029791000	3.366833000
H	6.533277000	-0.609686000	3.272654000
H	5.802703000	0.387588000	4.554268000
H	7.728399000	1.551431000	3.580495000
H	6.256215000	2.449115000	3.142961000
H	8.891351000	2.380606000	1.553406000
H	7.429986000	3.347752000	1.259313000
H	8.547922000	1.151571000	-0.589478000
H	8.728302000	2.896762000	-0.857770000
H	6.879529000	3.848931000	-2.194630000
H	6.247738000	3.989385000	-0.532712000
H	4.422718000	4.147507000	-2.149772000
H	4.829823000	2.551396000	-2.843167000
H	2.456405000	3.403219000	-2.898202000
H	0.242719000	1.092003000	0.902831000
H	3.373431000	0.626030000	4.278167000
O	4.736521000	-0.175552000	-2.771986000
O	2.977562000	-1.312293000	-1.052335000
O	4.131133000	-2.510889000	0.893481000
O	6.827539000	-2.072113000	1.115332000
O	7.093615000	-1.330725000	-1.609330000
C	2.112074000	-1.794453000	-0.086411000
C	2.748255000	-2.442518000	0.988633000
C	4.857323000	-3.164875000	1.934864000
C	6.269217000	-3.356143000	1.427144000
C	8.080409000	-2.126287000	0.422090000
C	7.906197000	-2.376941000	-1.067755000
C	6.796513000	-1.503249000	-3.001438000
C	5.980830000	-0.311023000	-3.475027000
C	3.667643000	-0.986261000	-3.284334000
C	2.487354000	-0.901184000	-2.336169000
C	0.737018000	-1.614777000	-0.093559000
C	-0.040752000	-2.100259000	0.979957000
C	0.600136000	-2.743192000	2.049818000
C	1.986572000	-2.910596000	2.054873000
H	4.422702000	-4.147419000	2.049734000
H	4.829885000	-2.551356000	2.843195000
H	6.879529000	-3.848906000	2.194517000
H	8.728293000	-2.896707000	0.857680000
H	8.547922000	-1.151510000	0.589418000
H	7.429950000	-3.347659000	-1.259390000
H	8.891304000	-2.380502000	-1.553493000
H	7.728298000	-1.551320000	-3.580547000
H	6.256124000	-2.449006000	-3.142984000
H	5.802575000	-0.387475000	-4.554267000
H	6.533195000	0.609795000	-3.272675000
H	3.994275000	-2.029678000	-3.366739000
H	3.373325000	-0.625936000	-4.278097000
H	1.699467000	-1.580746000	-2.677207000
H	2.087558000	0.115492000	-2.273775000
H	0.242666000	-1.091860000	-0.902700000
H	2.456424000	-3.403116000	2.898269000
H	6.247670000	-3.989281000	0.532619000
N	-5.095534000	1.454149000	1.703967000
H	-4.171585000	1.851700000	1.612071000
C	-6.173014000	2.322064000	1.624097000
C	-5.804323000	3.769244000	1.696536000
C	-5.263421000	6.509590000	1.817815000
C	-6.728170000	4.693060000	1.194408000
C	-4.607913000	4.229684000	2.268975000
C	-4.342950000	5.594896000	2.333722000
C	-6.454101000	6.056962000	1.245224000
H	-7.650203000	4.321394000	0.762562000
H	-3.900933000	3.532698000	2.710508000
H	-3.420854000	5.945790000	2.786741000
H	-7.168954000	6.765567000	0.839585000
O	-7.327450000	1.940229000	1.496985000
N	-5.095224000	-1.454283000	-1.704204000
H	-4.171249000	-1.851767000	-1.612287000
C	-6.172642000	-2.322284000	-1.624387000
C	-5.803828000	-3.769437000	-1.696719000
C	-5.262694000	-6.509747000	-1.817773000
C	-4.607466000	-4.229832000	-2.269295000
C	-6.727510000	-4.693281000	-1.194337000
C	-6.453323000	-6.057162000	-1.245039000
C	-4.342392000	-5.595029000	-2.333934000
H	-3.900627000	-3.532832000	-2.711029000
H	-7.649509000	-4.321648000	-0.762389000

H	3.479569000	-4.529899000	2.354934000
H	7.335886000	-5.453346000	0.701525000
H	6.650198000	-7.841579000	0.454847000
H	2.786517000	-6.875193000	2.081793000
O	7.133067000	-3.139335000	1.603325000
Ba	-5.372901000	-0.000141000	0.000085000
H	4.362908000	8.544144000	-1.133451000
H	4.363934000	-8.543882000	1.132904000

H	-7.168046000	-6.765788000	-0.839208000
H	-3.420337000	-5.945890000	-2.787064000
O	-7.327089000	-1.940537000	-1.497113000
Ba	5.224994000	0.000046000	0.000020000
H	0.006186000	-3.105196000	2.881127000
H	0.006178000	3.105256000	-2.881033000
H	-5.054823000	7.574360000	1.866274000
H	-5.054005000	-7.574503000	-1.866142000

IV Table S2: Cartesian coordinates from DFT calculations in solution

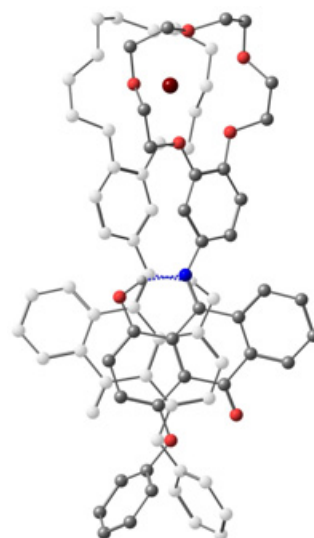


in-[*anti*-(*s*-*trans*-**1a**)₂]·Ba²⁺

DFT/CPCM energy = −3967.40431489 a.u.

Cartesian coordinates (Å):

C	2.661354000	-4.679869000	-3.126590000
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C	4.999659000	-4.387180000	-2.627549000
C	4.755759000	-3.063341000	-2.242413000
C	3.439504000	-2.552115000	-2.242780000
C	2.406494000	-3.371549000	-2.725865000
C	5.919496000	-2.205061000	-1.910006000
C	5.678116000	-0.753036000	-1.800503000
C	4.356869000	-0.244893000	-1.740495000
C	3.195638000	-1.155310000	-1.806223000
C	6.777007000	0.098577000	-1.694271000
C	6.594017000	1.467434000	-1.518873000
C	5.310527000	1.983946000	-1.412323000
C	4.177213000	1.143553000	-1.512384000
O	7.048232000	-2.685814000	-1.774645000
N	2.046774000	-0.624364000	-1.508238000
O	2.972448000	1.699536000	-1.349768000
H	1.845522000	-5.292476000	-3.497550000
H	4.152874000	-6.226812000	-3.356211000
H	6.020668000	-4.750915000	-2.600364000
H	1.399185000	-2.987424000	-2.801788000
H	7.772858000	-0.325689000	-1.731953000
H	7.436708000	2.141820000	-1.412022000
H	2.324391000	0.906098000	-1.361651000
C	2.662175000	4.679838000	3.126293000
C	3.958576000	5.201605000	3.056481000
C	5.000509000	4.386794000	2.627588000
C	4.756463000	3.062997000	2.242405000
C	3.440127000	2.551977000	2.242570000
C	2.407172000	3.371562000	2.725512000
C	5.920120000	2.204534000	1.910182000
C	5.678533000	0.752544000	1.800652000
C	4.357214000	0.244629000	1.740344000
C	3.196110000	1.155227000	1.805929000
C	6.777306000	-0.099256000	1.694686000
C	6.594126000	-1.468090000	1.519275000
C	5.310573000	-1.984378000	1.412414000
C	4.177382000	-1.143785000	1.512173000
O	7.048946000	2.685115000	1.774965000
N	2.047201000	0.624448000	1.507827000
O	2.972565000	-1.699558000	1.349245000
H	1.846383000	5.292567000	3.497140000
H	4.153901000	6.226547000	3.356149000
H	6.021577000	4.750375000	2.600560000
H	1.399792000	2.987594000	2.801278000
H	7.773220000	0.324841000	1.732604000
H	7.436730000	-2.142623000	1.412666000
H	2.324674000	-0.905982000	1.361081000
O	-4.897453000	1.403415000	-2.477125000



in-[*anti*-(*s*-*trans*-**1b**)₂]·Ba²⁺

DFT/CPCM energy = −3967.39075286 a.u.

Cartesian coordinates (Å):

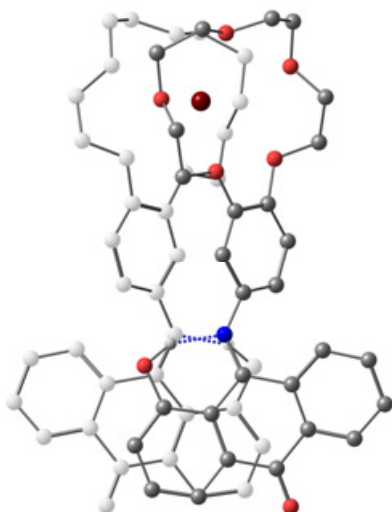
C	-1.826678000	5.442766000	-0.036146000
C	-3.110449000	5.764289000	0.419347000
C	-4.113963000	4.803330000	0.374496000
C	-3.840089000	3.513567000	-0.099785000
C	-2.529609000	3.159748000	-0.475148000
C	-1.538162000	4.154070000	-0.474689000
C	-4.983720000	2.583016000	-0.288764000
C	-4.752623000	1.413970000	-1.168633000
C	-3.413373000	0.979427000	-1.400536000
C	-2.264533000	1.770903000	-0.913550000
C	-5.823959000	0.717672000	-1.761730000
C	-5.579085000	-0.421143000	-2.542143000
C	-4.291889000	-0.894946000	-2.692984000
C	-3.199937000	-0.220078000	-2.125923000
O	-6.069359000	2.833992000	0.239104000
N	-1.101204000	1.192920000	-0.982480000
O	-1.981003000	-0.745492000	-2.337086000
H	-1.047298000	6.198423000	-0.049598000
H	-3.329003000	6.765352000	0.778149000
H	-5.129295000	5.038480000	0.673304000
H	-0.541184000	3.927126000	-0.825815000
O	-7.076242000	1.255032000	-1.655299000
H	-6.402194000	-0.932793000	-3.024141000
H	-1.344295000	-0.132295000	-1.834003000
C	-1.826547000	-5.442762000	0.036327000
C	-3.110298000	-5.764321000	-0.419195000
C	-4.113832000	-4.803379000	-0.374399000
C	-3.839994000	-3.513596000	0.099847000
C	-2.529529000	-3.159743000	0.475233000
C	-1.538065000	-4.154046000	0.474835000
C	-4.983648000	-2.583063000	0.288781000
C	-4.752586000	-1.413972000	1.168594000
C	-3.413346000	-0.979389000	1.400496000
C	-2.264482000	-1.770871000	0.913566000
C	-5.823943000	-0.717672000	1.761650000
C	-5.579097000	0.421167000	2.542041000
C	-4.291917000	0.895018000	2.692857000
C	-3.199946000	0.220160000	2.125815000
O	-6.069277000	-2.834086000	-0.239088000
N	-1.101160000	-1.192869000	0.982454000
O	-1.981028000	0.745622000	2.336946000
H	-1.047154000	-6.198406000	0.049828000
H	-3.328823000	-6.765397000	-0.777978000
H	-5.129152000	-5.038557000	-0.673223000
H	-0.541103000	-3.927071000	0.825988000
O	-7.076219000	-1.255058000	1.655222000
H	-6.402220000	0.932803000	3.024030000
H	-1.344320000	0.132409000	1.833890000
O	5.869625000	0.108816000	-2.850687000

O	-2.719556000	-0.136543000	-1.896658000
O	-3.173436000	-2.195859000	-0.453664000
O	-5.872267000	-2.658332000	-0.211103000
O	-6.820026000	-0.617480000	-1.966024000
C	-1.596447000	-0.807318000	-1.482089000
C	-1.844023000	-1.951475000	-0.694674000
C	-3.633134000	-3.504943000	-0.070494000
C	-5.001650000	-3.689384000	-0.691866000
C	-7.185540000	-2.672814000	-0.788202000
C	-7.238132000	-1.976700000	-2.135060000
C	-6.870559000	0.130075000	-3.185909000
C	-6.248306000	1.494155000	-2.946888000
C	-3.938377000	1.111102000	-3.494905000
C	-2.585833000	0.933858000	-2.847573000
C	-0.298214000	-0.412981000	-1.750783000
C	0.785286000	-1.178858000	-1.277538000
C	0.539756000	-2.311064000	-0.488209000
C	-0.774673000	-2.685855000	-0.190698000
H	-3.674029000	-3.559886000	1.020930000
H	-2.955639000	-4.271482000	-0.455914000
H	-4.917888000	-3.639973000	-1.783851000
H	-7.826572000	-2.148874000	-0.073381000
H	-7.542816000	-3.704242000	-0.890004000
H	-8.268672000	-2.007186000	-2.512955000
H	-6.585429000	-2.467060000	-2.868635000
H	-7.913651000	0.258708000	-3.503917000
H	-6.338741000	-0.422225000	-3.970691000
H	-6.789884000	2.027273000	-2.162128000
H	-6.290855000	2.085271000	-3.869757000
H	-3.893931000	1.937612000	-4.215520000
H	-4.208584000	0.191609000	-4.026522000
H	-1.856220000	0.665096000	-3.616934000
H	-2.252311000	1.838645000	-2.330068000
H	-0.090790000	0.490930000	-2.308605000
H	1.365726000	-2.879917000	-0.081260000
H	-0.955392000	-3.547668000	0.442352000
H	-5.400630000	-4.671850000	-0.409200000
O	-5.871889000	2.658694000	0.211805000
O	-3.172909000	2.195813000	0.452651000
O	-2.719101000	0.136642000	1.896105000
O	-4.896980000	-1.403134000	2.477170000
O	-6.819665000	0.617685000	1.966498000
C	-1.843536000	1.951542000	0.694047000
C	-1.596001000	0.807438000	1.481533000
C	-2.585334000	-0.933494000	2.847325000
C	-3.937826000	-1.110582000	3.494802000
C	-6.247766000	-1.494027000	2.947092000
C	-6.870122000	-0.130025000	3.186290000
C	-7.237749000	1.976883000	2.135736000
C	-7.185121000	2.673211000	0.788989000
C	-5.000965000	3.689288000	0.692994000
C	-3.632780000	3.505232000	0.070781000
C	-0.774162000	2.685987000	0.190212000
C	0.540251000	2.311264000	0.487854000
C	0.785745000	1.179015000	1.277140000
C	-0.297774000	0.413127000	1.750309000
H	-1.855684000	-0.664503000	3.616567000
H	-2.251818000	-1.838415000	2.330051000
H	-3.893314000	-1.936925000	4.215606000
H	-6.290149000	-2.085212000	3.869926000
H	-6.789366000	-2.027141000	2.162349000
H	-6.338339000	0.422225000	3.971130000
H	-7.913198000	-0.258782000	3.504303000
H	-8.268298000	2.007338000	2.513612000
H	-6.585059000	2.467112000	2.869410000
H	-7.542281000	3.704663000	0.890983000
H	-7.826237000	2.149462000	0.074104000
H	-4.916657000	3.638969000	1.784895000
H	-5.400007000	4.672016000	0.411328000
H	-2.955028000	4.271425000	0.456426000
H	-3.674238000	3.561015000	-1.020578000
H	-0.954872000	3.547786000	-0.442865000
H	1.366236000	2.880150000	0.080989000
H	-0.090366000	-0.490787000	2.308131000
H	-4.207984000	-0.190966000	4.026232000
Ba	-4.919149000	0.000151000	0.000047000
O	5.177584000	-3.301664000	1.045794000
O	5.177727000	3.301247000	-1.045699000
C	4.242803000	4.116954000	-1.667686000
C	4.014460000	4.058371000	-3.041969000
C	3.581846000	5.041718000	-0.860288000
C	3.088026000	4.934220000	-3.610306000
C	2.662209000	5.915311000	-1.442891000
C	2.407867000	5.862769000	-2.816723000
H	4.544925000	3.332205000	-3.649971000
H	3.785735000	5.061063000	0.204454000
H	2.900616000	4.889910000	-4.679451000
H	2.140351000	6.633697000	-0.817065000

O	3.673783000	1.113943000	-1.570412000
O	4.099716000	2.093790000	0.744196000
O	6.788852000	2.390686000	1.215579000
O	7.772240000	1.573280000	-1.329493000
C	2.538988000	1.437441000	-0.869690000
C	2.772777000	1.989775000	0.406763000
C	4.540202000	3.014648000	1.758842000
C	5.905667000	3.512101000	1.334059000
C	8.106158000	2.715010000	0.750488000
C	8.180061000	2.822677000	-0.760554000
C	7.836630000	1.574050000	-2.759817000
C	7.226162000	0.283967000	-3.277877000
C	4.919366000	0.898715000	-3.568481000
C	3.559192000	0.702066000	-2.942842000
C	1.245576000	1.217225000	-1.309175000
C	0.152208000	1.577438000	-0.496605000
C	0.387562000	2.120107000	0.774369000
C	1.696451000	2.317188000	1.224517000
H	4.581282000	2.492614000	2.718995000
H	3.851034000	3.860787000	1.825814000
H	5.821721000	4.035409000	0.374430000
H	8.748614000	1.899861000	1.096040000
H	8.449958000	3.650717000	1.206548000
H	9.214860000	3.046979000	-1.051752000
H	7.532769000	3.622645000	-1.142150000
H	8.882680000	1.636058000	-3.087964000
H	7.304299000	2.452659000	-3.145067000
H	7.765520000	-0.578381000	-2.879413000
H	7.286200000	0.262197000	-4.372920000
H	4.888573000	0.583589000	-4.619225000
H	5.188831000	1.960039000	-3.524352000
H	2.831344000	1.329794000	-3.465346000
H	3.235379000	-0.342515000	-2.983248000
H	1.050895000	0.746434000	-2.264000000
H	-0.443718000	2.356069000	1.424969000
H	1.869615000	2.711711000	2.219746000
H	6.291834000	4.209389000	2.088409000
O	6.788892000	-2.390669000	-1.215592000
O	4.099763000	-2.093787000	-0.744204000
O	3.673824000	-1.113986000	1.570429000
O	5.869647000	-0.108814000	2.850688000
O	7.772278000	-1.573255000	1.329475000
C	2.772821000	-1.989780000	-0.406769000
C	2.539032000	-1.437450000	0.869688000
C	3.559222000	-0.702100000	2.942855000
C	4.919400000	-0.898714000	3.568495000
C	7.226188000	-0.283957000	3.277864000
C	7.836664000	-1.574033000	2.759798000
C	8.180122000	-2.822639000	0.760528000
C	8.106209000	-2.714963000	-0.750514000
C	5.905722000	-3.512098000	-1.334045000
C	4.540250000	-3.014669000	-1.758828000
C	1.696494000	-2.317187000	-1.224522000
C	0.387604000	-2.120097000	-0.774378000
C	0.152249000	-1.577411000	0.496587000
C	1.245620000	-1.217211000	1.309162000
H	2.831387000	-1.329841000	3.465361000
H	3.235383000	0.342473000	2.983252000
H	4.888600000	-0.583570000	4.619233000
H	7.286236000	-0.262186000	4.372907000
H	7.765538000	0.578393000	2.879396000
H	7.304341000	-2.452650000	3.145042000
H	8.882713000	-1.636034000	3.087948000
H	9.214925000	-3.046925000	1.051724000
H	7.532844000	-3.622623000	1.142116000
H	8.450031000	-3.650658000	-1.206582000
H	8.748640000	-1.899793000	-1.096063000
H	5.821794000	-4.035393000	-0.374407000
H	6.291892000	-4.209394000	-2.088388000
H	3.851086000	-3.860814000	-1.825772000
H	4.581320000	-2.492659000	-2.718995000
H	1.869656000	-2.711718000	-2.219749000
H	-0.443672000	-2.356057000	-1.424984000
H	1.050940000	-0.746420000	2.263987000
H	5.188883000	-1.960034000	3.524388000
Ba	5.863124000	0.000013000	0.000003000
H	-4.094419000	1.789957000	3.273579000
H	-4.094368000	-1.789865000	-3.273731000
C	-8.233273000	0.520122000	-1.858736000
C	-9.284983000	1.209734000	-2.462286000
C	-8.399428000	-0.782132000	-1.384811000
C	-10.527518000	0.586820000	-2.589981000
C	-9.645740000	-1.393887000	-1.526482000
C	-10.712889000	-0.717398000	-2.123468000
H	-9.122260000	2.225265000	-2.808988000
H	-7.586526000	-1.302151000	-0.892084000
H	-11.349224000	1.124416000	-3.054290000
H	-9.782493000	-2.403153000	-1.148515000

H	1.687994000	6.540532000	-3.265591000
C	4.242423000	-4.117152000	1.667708000
C	3.581400000	-5.041852000	0.860289000
C	4.013879000	-4.058407000	3.041952000
C	2.661505000	-5.915215000	1.442828000
C	3.087186000	-4.934025000	3.610223000
C	2.406964000	-5.862507000	2.816618000
H	3.785435000	-5.061315000	-0.204424000
H	4.544392000	-3.332293000	3.649976000
H	2.139596000	-6.633548000	0.816983000
H	2.899623000	-4.889586000	4.679336000
H	1.686889000	-6.540090000	3.265434000

H	-11.680394000	-1.200604000	-2.221477000
C	-8.233263000	-0.520168000	1.858706000
C	-8.399453000	0.782080000	1.384781000
C	-9.284935000	-1.209793000	2.462308000
C	-9.645774000	1.393810000	1.526486000
C	-10.527478000	-0.586901000	2.590041000
C	-10.712891000	0.717305000	2.123511000
H	-7.586564000	1.302114000	0.892049000
H	-9.122180000	-2.225316000	2.809019000
H	-9.782556000	2.403072000	1.148520000
H	-11.349157000	-1.124504000	3.054391000
H	-11.680402000	1.200493000	2.221547000

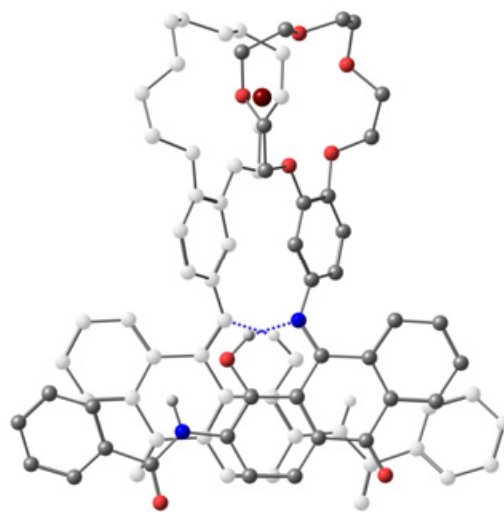


in-[*anti*-(*s*-*trans*-**1c**)₂]·Ba²⁺

DFT/CPCM energy = −3354.82017718 a.u.

Cartesian coordinates (Å):

C	3.310498000	5.465792000	0.145795000
C	4.587359000	5.819912000	-0.303761000
C	5.607761000	4.876565000	-0.273082000
C	5.357115000	3.571737000	0.171381000
C	4.050351000	3.183746000	0.539630000
C	3.045377000	4.163877000	0.560912000
C	6.513129000	2.661897000	0.358422000
C	6.273603000	1.408344000	1.109903000
C	4.954156000	0.979970000	1.390976000
C	3.794709000	1.783493000	0.962573000
C	7.379546000	0.656083000	1.504489000
C	7.197684000	-0.538245000	2.201390000
C	5.915248000	-0.999155000	2.467488000
C	4.791099000	-0.268215000	2.053664000
O	7.639604000	2.972246000	-0.036272000
N	2.636870000	1.195642000	1.039064000
O	3.581290000	-0.792147000	2.317664000
H	2.517305000	6.206521000	0.174832000
H	4.787409000	6.831145000	-0.644242000
H	6.620609000	5.136221000	-0.560316000
H	2.053223000	3.916061000	0.911464000
H	8.369956000	1.015540000	1.253116000
H	8.055911000	-1.125035000	2.512304000
H	2.920863000	-0.163596000	1.873519000
C	3.310576000	-5.465807000	-0.145782000
C	4.587437000	-5.819894000	0.303798000
C	5.607819000	-4.876524000	0.273128000
C	5.357148000	-3.571705000	-0.171346000
C	4.050380000	-3.183744000	-0.539612000
C	3.045430000	-4.163900000	-0.560908000
C	6.513147000	-2.661846000	-0.358390000
C	6.273606000	-1.408326000	-1.109922000
C	4.954153000	-0.979967000	-1.390985000
C	3.794718000	-1.783498000	-0.962572000
C	7.379537000	-0.656077000	-1.504563000
C	7.197654000	0.538222000	-2.201509000
C	5.915210000	0.999124000	-2.467583000
C	4.791075000	0.268203000	-2.053691000
O	7.639624000	-2.972164000	0.036320000
N	2.636878000	-1.195648000	-1.039073000
O	3.581254000	0.792149000	-2.317613000
H	2.517402000	-6.206556000	-0.174830000



in-[*anti*-(*s*-*trans*-**1d**)₂]·Ba²⁺

DFT/CPCM energy = −4154.43277579 a.u.

Cartesian coordinates (Å):

C	1.724702000	5.499200000	1.976470000
C	2.976174000	6.118223000	1.903307000
C	4.114975000	5.337257000	1.750168000
C	4.016353000	3.946779000	1.629435000
C	2.748992000	3.318400000	1.632902000
C	1.613198000	4.117514000	1.846923000
C	5.277067000	3.164724000	1.576762000
C	5.169811000	1.698761000	1.649653000
C	3.902574000	1.062947000	1.627077000
C	2.659199000	1.843541000	1.492269000
C	6.338656000	0.941785000	1.700406000
C	6.301346000	-0.450790000	1.719095000
C	5.069820000	-1.104054000	1.677586000
C	3.868604000	-0.346852000	1.646441000
O	6.373387000	3.732334000	1.514156000
N	1.579438000	1.146838000	1.285927000
O	2.727688000	-1.053837000	1.617092000
H	0.829739000	6.092435000	2.137171000
H	3.061484000	7.197208000	1.983650000
H	5.100307000	5.785128000	1.724997000
H	0.635409000	3.664927000	1.924981000
H	7.290107000	1.460171000	1.703685000
H	7.210464000	-1.032836000	1.738278000
H	1.995255000	-0.350588000	1.464201000
C	1.724741000	-5.499276000	-1.976188000
C	2.976244000	-6.118244000	-1.903110000
C	4.115025000	-5.337222000	-1.750098000
C	4.016356000	-3.946745000	-1.629406000
C	2.748968000	-3.318417000	-1.632793000
C	1.613191000	-4.117590000	-1.846687000
C	5.277046000	-3.164641000	-1.576856000
C	5.169728000	-1.698683000	-1.649755000
C	3.902469000	-1.062918000	-1.627094000
C	2.659129000	-1.843555000	-1.492205000
C	6.338540000	-0.941664000	-1.700603000
C	6.301174000	0.450910000	-1.719304000
C	5.069628000	1.104126000	-1.677713000
C	3.868440000	0.346879000	-1.646469000
O	6.373392000	-3.732209000	-1.514333000
N	1.579358000	-1.146873000	-1.285853000
O	2.727500000	1.053821000	-1.617018000
H	0.829788000	-6.092555000	-2.136788000

H	4.787506000	-6.831121000	0.644286000
H	6.620668000	-5.136157000	0.560376000
H	2.053277000	-3.916112000	-0.911481000
H	8.369956000	-1.015519000	-1.253199000
H	8.055871000	1.125000000	-2.512471000
H	2.920848000	0.163636000	-1.873386000
O	-4.339793000	0.043601000	2.852711000
O	-2.142843000	1.086062000	1.600232000
O	-2.558551000	2.096552000	-0.704724000
O	-5.246898000	2.423085000	-1.154013000
O	-6.239174000	1.542017000	1.366008000
C	-1.005347000	1.420508000	0.909034000
C	-1.233425000	1.989383000	-0.361131000
C	-2.998473000	3.049954000	-1.689557000
C	-4.358974000	3.543321000	-1.244057000
C	-6.564394000	2.739106000	-0.684161000
C	-6.641979000	2.807118000	0.828941000
C	-6.310299000	1.504926000	2.795580000
C	-5.697284000	0.203937000	3.282599000
C	-3.393172000	0.819728000	3.589999000
C	-2.031137000	0.642089000	2.962965000
C	0.286610000	1.197663000	1.352263000
C	1.382632000	1.572007000	0.550361000
C	1.152814000	2.124166000	-0.717910000
C	-0.153874000	2.325330000	-1.171499000
H	-3.048041000	2.555711000	-2.663824000
H	-2.303571000	3.892751000	-1.735786000
H	-4.268170000	4.038915000	-0.270317000
H	-7.208300000	1.935256000	-1.052699000
H	-6.904151000	3.687619000	-1.116199000
H	-7.676824000	3.026873000	1.123358000
H	-5.993086000	3.594749000	1.232722000
H	-7.358024000	1.554971000	3.120407000
H	-5.782625000	2.374739000	3.206339000
H	-6.233864000	-0.650020000	2.863062000
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H	-1.306778000	1.259337000	3.502486000
H	-1.704284000	-0.402209000	2.979241000
H	0.478500000	0.717097000	2.302725000
H	1.987480000	2.366230000	-1.362211000
H	-0.323827000	2.729330000	-2.163544000
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C	-1.005340000	-1.420505000	-0.909020000
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C	-6.641976000	-2.807134000	-0.828951000
C	-6.564383000	-2.739129000	0.684151000
C	-4.358951000	-3.543329000	1.244028000
C	-2.998464000	-3.049957000	1.689561000
C	-0.153856000	-2.325300000	1.171521000
C	1.152829000	-2.124137000	0.717924000
C	1.382640000	-1.572004000	-0.550359000
C	0.286615000	-1.197670000	-1.352260000
H	-1.306779000	-1.259370000	-3.502469000
H	-1.704283000	0.402186000	-2.979252000
H	-3.363052000	-0.480566000	-4.633234000
H	-5.758399000	-0.155151000	-4.376721000
H	-6.233862000	0.650008000	-2.863076000
H	-5.782631000	-2.374753000	-3.206345000
H	-7.358028000	-1.554981000	-3.120417000
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H	-2.303552000	-3.892746000	1.735781000
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H	5.747951000	-1.940010000	2.981775000
H	5.747897000	1.939967000	-2.981888000

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H	0.635375000	-3.665051000	-1.924681000
H	7.290010000	-1.460013000	-1.703947000
H	7.210269000	1.032992000	-1.738564000
H	1.995096000	0.350556000	-1.464050000
O	-5.382266000	-0.597510000	2.778600000
O	-3.203496000	0.723258000	1.765624000
O	-3.646117000	2.204904000	-0.273638000
O	-6.349640000	2.612236000	-0.587658000
O	-7.298658000	1.194223000	1.693615000
C	-2.077655000	1.232957000	1.169389000
C	-2.319409000	2.062054000	0.053804000
C	-4.110466000	3.353811000	-1.007268000
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C	-7.656503000	2.814626000	-0.032206000
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C	-7.353277000	0.833794000	3.077769000
C	-6.734901000	-0.542277000	3.248789000
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C	-3.073783000	-0.016499000	2.992289000
C	-0.779451000	0.959343000	1.566920000
C	0.301316000	1.547850000	0.884784000
C	0.062917000	2.356136000	-0.233975000
C	-1.248882000	2.603578000	-0.650551000
H	-4.178178000	3.089510000	-2.066211000
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H	-5.355628000	3.989239000	0.621258000
H	-8.310224000	2.110217000	-0.554721000
H	-8.001597000	3.834564000	-0.238372000
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H	-7.036646000	3.224632000	2.012328000
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H	-4.707865000	1.034576000	3.886494000
H	-2.349165000	0.470062000	3.651548000
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O	-6.349735000	-2.612184000	0.587749000
O	-3.646177000	-2.204846000	0.273816000
O	-3.203586000	-0.723580000	-1.765753000
O	-5.382285000	0.597369000	-2.778664000
O	-7.298674000	-1.194322000	-1.693614000
C	-2.319480000	-2.062069000	-0.053695000
C	-2.077737000	-1.233125000	-1.169397000
C	-3.073814000	0.016313000	-2.992333000
C	-4.428362000	0.000255000	-3.659469000
C	-6.734928000	0.542128000	-3.248840000
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C	-7.656586000	-2.814611000	0.032288000
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C	-4.110568000	-3.353748000	1.007430000
C	-1.248947000	-2.603500000	0.650721000
C	0.062851000	-2.356080000	0.234130000
C	0.301238000	-1.547899000	-0.884705000
C	-0.779533000	-0.959513000	-1.566934000
H	-2.349185000	-0.470187000	-3.651625000
H	-2.736724000	1.032610000	-2.766826000
H	-4.379881000	0.567793000	-4.597521000
H	-6.783198000	0.838332000	-4.303858000
H	-7.275806000	1.279761000	-2.651471000
H	-6.821551000	-1.589792000	-3.668713000
H	-8.397077000	-0.805315000	-3.417509000
H	-8.728150000	-2.701137000	-1.819374000
H	-7.036731000	-3.224755000	-2.012225000
H	-8.001682000	-3.834538000	0.238509000
H	-8.310317000	-2.110171000	0.554749000
H	-5.355671000	-3.989174000	-0.621142000
H	-5.862131000	-4.592450000	0.981302000
H	-3.419807000	-4.190888000	0.876693000
H	-4.178332000	-3.089433000	2.066363000
H	-1.429270000	-3.211515000	1.530367000
H	0.895938000	-2.774344000	0.786052000
H	-0.572560000	-0.291527000	-2.392678000
H	-4.707904000	-1.034618000	-3.886710000
N	4.876638000	2.483809000	-1.625533000
H	3.907890000	2.742029000	-1.483341000
C	5.809398000	3.488433000	-1.653388000
C	5.249819000	4.871810000	-1.537163000
C	4.333663000	7.500939000	-1.222485000
C	6.124389000	5.881659000	-1.113217000

C	3.914047000	5.195111000	-1.821662000
C	3.460636000	6.503752000	-1.663784000
C	5.668648000	7.187651000	-0.951356000
H	7.154881000	5.622829000	-0.898164000
H	3.221396000	4.445666000	-2.192343000
H	2.425498000	6.743430000	-1.887263000
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O	7.021453000	3.278548000	-1.743463000
N	4.876871000	-2.483743000	1.625399000
H	3.908124000	-2.741985000	1.483251000
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C	3.914335000	-5.195055000	1.821679000
C	6.124646000	-5.881593000	1.113131000
C	5.668916000	-7.187596000	0.951337000
C	3.460933000	-6.503707000	1.663864000
H	3.221696000	-4.445609000	2.192382000
H	7.155124000	-5.622757000	0.898011000
H	6.352054000	-7.959947000	0.610501000
H	2.425811000	-6.743393000	1.887410000
O	7.021703000	-3.278456000	1.743295000
Ba	-5.407062000	0.000035000	-0.000072000
H	3.976183000	8.518509000	-1.094335000
H	3.976478000	-8.518474000	1.094449000

V Tables S3–S6: DFT calculated free energies in solution

Table S3. Gibbs free energies (G_{soln}) for different conformers of complex $(\mathbf{1a})_2 \cdot \text{Ba}^{2+}$.

<i>in</i> -[<i>anti</i> -(<i>s-trans</i> - 1a) ₂] · Ba ²⁺	<i>out</i> -[<i>anti</i> -(<i>s-trans</i> - 1a) ₂] · Ba ²⁺
$E_{\text{gas}} = -3967.175537 \text{ a.u.}$ $\Delta G_{\text{corr_gas}} = 1.056956 \text{ a.u.}$ $\Delta G_{\text{solv}} = -0.224020 \text{ a.u.}$ $G_{\text{soln}} = E_{\text{gas}} + \Delta G_{\text{corr_gas}} + \Delta G_{\text{sol}} =$ $-3967.884455 \text{ a.u.}$	$E_{\text{gas}} = -3967.175453 \text{ a.u.}$ $\Delta G_{\text{corr_gas}} = 1.056112 \text{ a.u.}$ $\Delta G_{\text{solv}} = -0.222030 \text{ a.u.}$ $G_{\text{soln}} = E_{\text{gas}} + \Delta G_{\text{corr_gas}} + \Delta G_{\text{sol}} =$ $-3967.883482 \text{ a.u.}$
$G_{\text{soln}}(\text{in}) - G_{\text{soln}}(\text{out}) = -0.61 \text{ kcal/mol}$	

Table S4. Gibbs free energies (G_{soln}) for different conformers of complex $(\mathbf{1b})_2 \cdot \text{Ba}^{2+}$.

<i>in</i> -[<i>anti</i> -(<i>s-trans</i> - 1b) ₂] · Ba ²⁺	<i>out</i> -[<i>anti</i> -(<i>s-trans</i> - 1b) ₂] · Ba ²⁺
$E_{\text{gas}} = -3967.166687 \text{ a.u.}$ $\Delta G_{\text{corr_gas}} = 1.055549 \text{ a.u.}$ $\Delta G_{\text{solv}} = -0.218570 \text{ a.u.}$ $G_{\text{soln}} = E_{\text{gas}} + \Delta G_{\text{corr_gas}} + \Delta G_{\text{sol}} =$ $-3967.870660 \text{ a.u.}$	$E_{\text{gas}} = -3967.165988 \text{ a.u.}$ $\Delta G_{\text{corr_gas}} = 1.057089 \text{ a.u.}$ $\Delta G_{\text{solv}} = -0.219006 \text{ a.u.}$ $G_{\text{soln}} = E_{\text{gas}} + \Delta G_{\text{corr_gas}} + \Delta G_{\text{sol}} =$ $-3967.868838 \text{ a.u.}$
$G_{\text{soln}}(\text{in}) - G_{\text{soln}}(\text{out}) = -1.14 \text{ kcal/mol}$	

Table S5. Gibbs free energies (G_{soln}) for different conformers of complex $(\mathbf{1c})_2 \cdot \text{Ba}^{2+}$.

<i>in</i> -[<i>anti</i> -(<i>s-trans</i> - 1c) ₂] · Ba ²⁺	<i>out</i> -[<i>anti</i> -(<i>s-trans</i> - 1c) ₂] · Ba ²⁺
$E_{\text{gas}} = -3354.596670 \text{ a.u.}$ $\Delta G_{\text{corr_gas}} = 0.904978 \text{ a.u.}$ $\Delta G_{\text{solv}} = -0.219450 \text{ a.u.}$ $G_{\text{soln}} = E_{\text{gas}} + \Delta G_{\text{corr_gas}} + \Delta G_{\text{sol}} =$ $-3355.216704 \text{ a.u.}$	$E_{\text{gas}} = -3354.595601 \text{ a.u.}$ $\Delta G_{\text{corr_gas}} = 0.906023 \text{ a.u.}$ $\Delta G_{\text{solv}} = -0.219436 \text{ a.u.}$ $G_{\text{soln}} = E_{\text{gas}} + \Delta G_{\text{corr_gas}} + \Delta G_{\text{sol}} =$ $-3355.215037 \text{ a.u.}$
$G_{\text{soln}}(\text{in}) - G_{\text{soln}}(\text{out}) = -1.05 \text{ kcal/mol}$	

Table S6. Gibbs free energies (G_{soln}) for different conformers of complex $(\mathbf{1d})_2 \cdot \text{Ba}^{2+}$.

<i>in</i> -[<i>anti</i> -(<i>s-trans</i> - 1d) ₂] · Ba ²⁺	<i>out</i> -[<i>anti</i> -(<i>s-trans</i> - 1d) ₂] · Ba ²⁺
$E_{\text{gas}} = -4154.185536 \text{ a.u.}$ $\Delta G_{\text{corr_gas}} = 1.100208 \text{ a.u.}$ $\Delta G_{\text{solv}} = -0.241799 \text{ a.u.}$ $G_{\text{soln}} = E_{\text{gas}} + \Delta G_{\text{corr_gas}} + \Delta G_{\text{sol}} =$ $-4154.945691 \text{ a.u.}$	$E_{\text{gas}} = -4154.185148 \text{ a.u.}$ $\Delta G_{\text{corr_gas}} = 1.101881 \text{ a.u.}$ $\Delta G_{\text{solv}} = -0.242185 \text{ a.u.}$ $G_{\text{soln}} = E_{\text{gas}} + \Delta G_{\text{corr_gas}} + \Delta G_{\text{sol}} =$ $-4154.944866 \text{ a.u.}$
$G_{\text{soln}}(\text{in}) - G_{\text{soln}}(\text{out}) = -0.52 \text{ kcal/mol}$	

VI Table S7, Figure S14: DFT calculated stacking parameters in solution

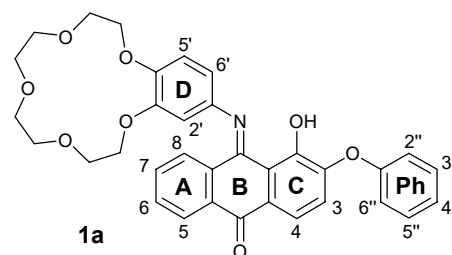
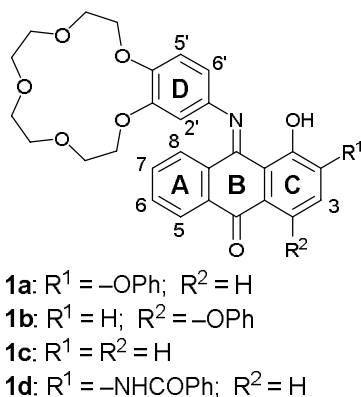


Table S7. Stacking parameters h , r , and θ (see Figure S14) for the most stable conformers of complexes $(\mathbf{1a-d})_2 \cdot \text{Ba}^{2+}$, as derived from DFT calculations; the symbols **A–D** and **Ph** denote different rings in the dye.

Stacking parameters h (Å), r (Å), and θ (deg)	$(\mathbf{1a})_2 \cdot \text{Ba}^{2+}$	$(\mathbf{1b})_2 \cdot \text{Ba}^{2+}$	$(\mathbf{1c})_2 \cdot \text{Ba}^{2+}$	$(\mathbf{1d})_2 \cdot \text{Ba}^{2+}$
h (D,D)	3.378	3.298	3.314	3.429
r (D,D)	1.465	1.324	1.267	1.406
θ (D,D)	1.78	1.07	0.68	3.50
h (C,C)	3.367	3.514	3.322	3.346
r (C,C)	0.770	1.764	1.387	0.569
θ (C,C)	1.30	9.19	1.47	3.37
h (Ph,Ph)	—	3.622	—	—
r (Ph,Ph)	—	1.667	—	—
θ (Ph,Ph)	—	31.85	—	—
h (H(2'')–A)	2.669	—	—	—
θ (Ph,A)	75.96	—	—	—
h (H(6')–Ph)	3.201	—	—	—
θ (Ph,D)	76.39	—	—	—

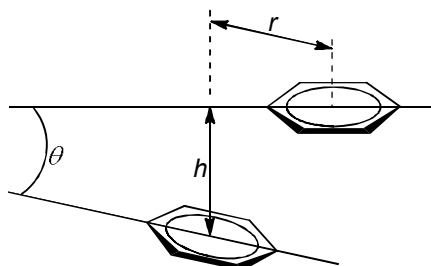


Figure S14. Definition of stacking parameters h , r , and θ : h (stacking distance) is the distance between the center of one ring and the plane defined by the neighboring ring; r (displacement) is the distance between the centers of two rings projected on the plane defined by one of the rings; θ (inclination) is the angle between the planes of two rings.