Supplementary Material

Synthesis, Structural Studies and Computational Evaluation of Cyclophanes Incorporating Imidazole-2-Selones

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^{1}H and ^{13}C NMR spectra of selone compounds

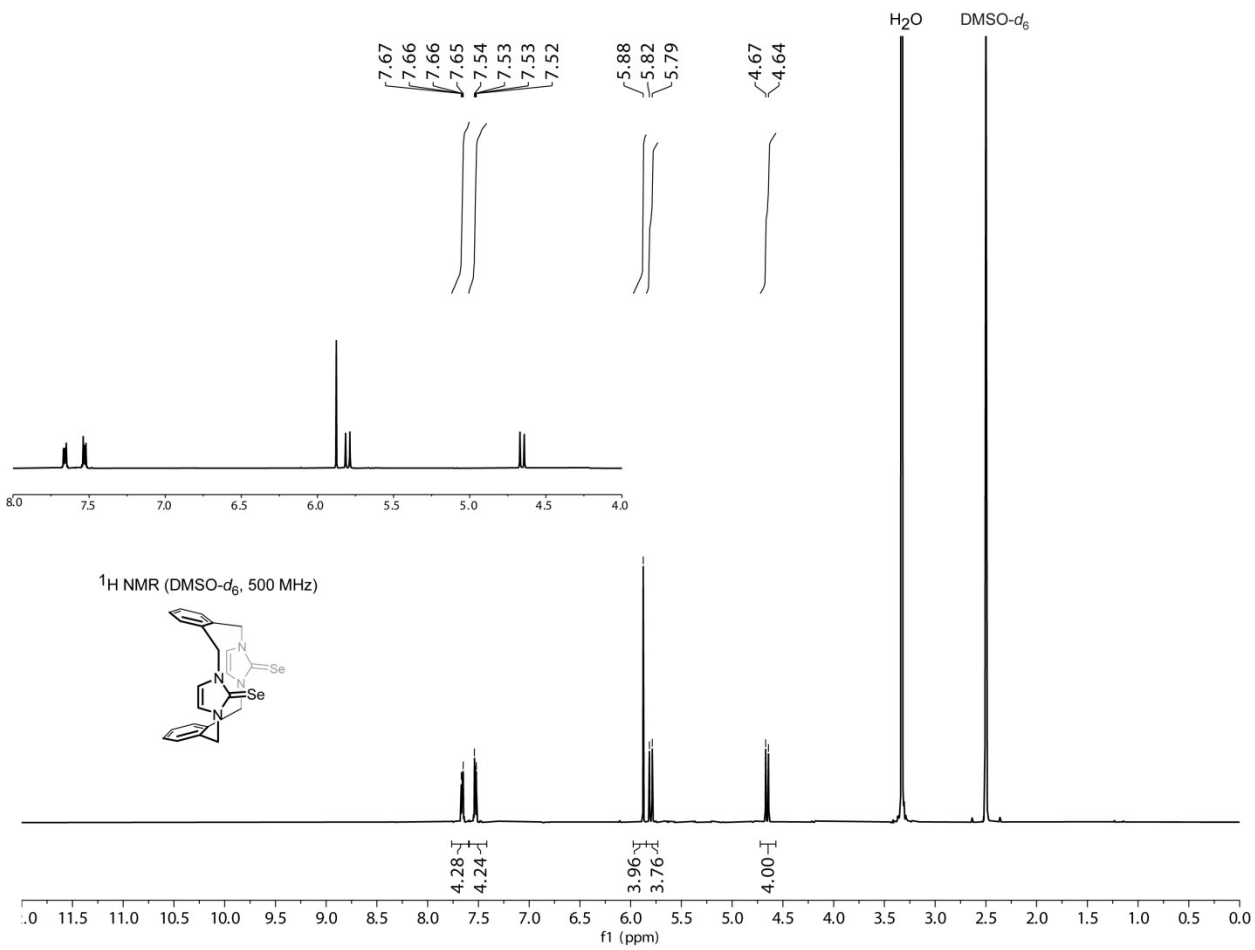

Figure S1. ^{1}H NMR of **8** in DMSO-d_6 at 500.10 MHz.

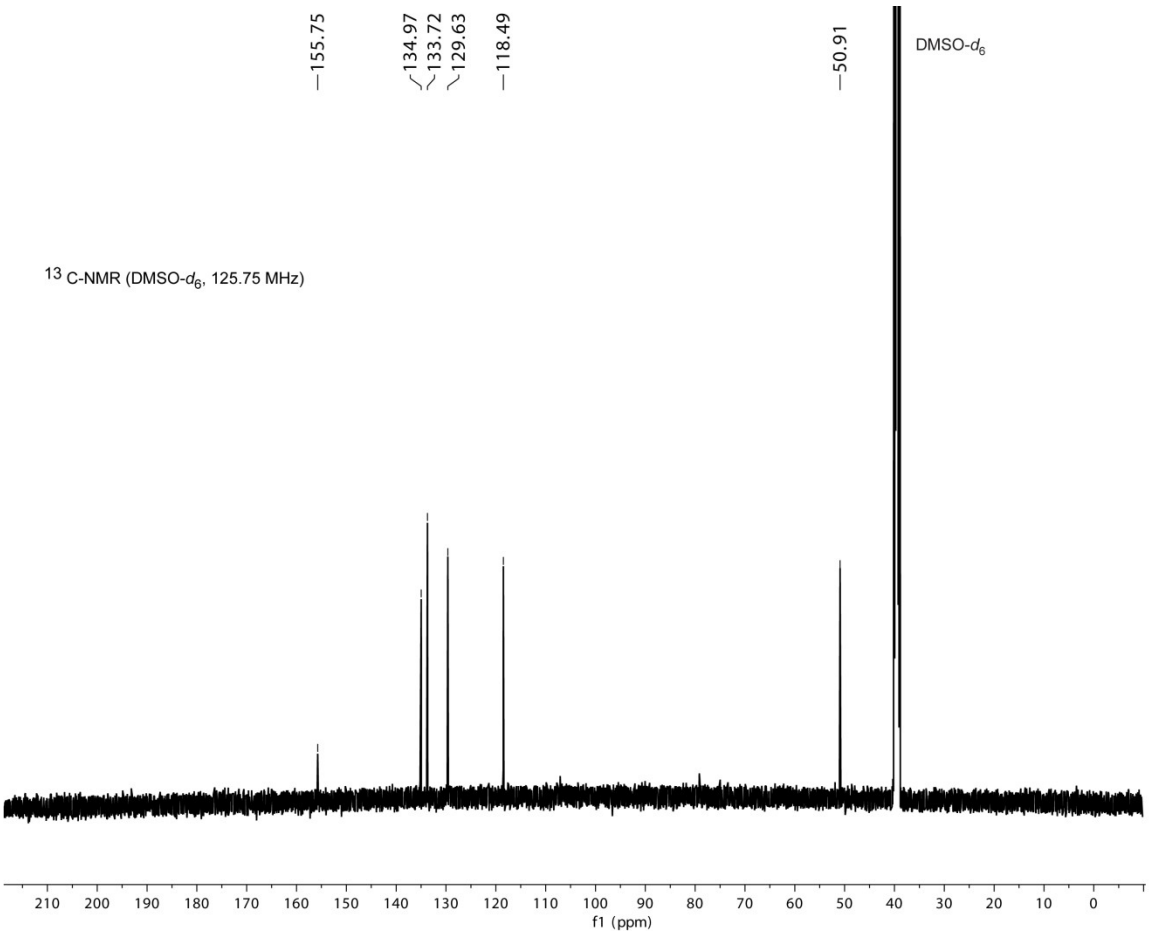

Figure S2. ^{13}C NMR of **8** in DMSO-d_6 at 125.75 MHz.

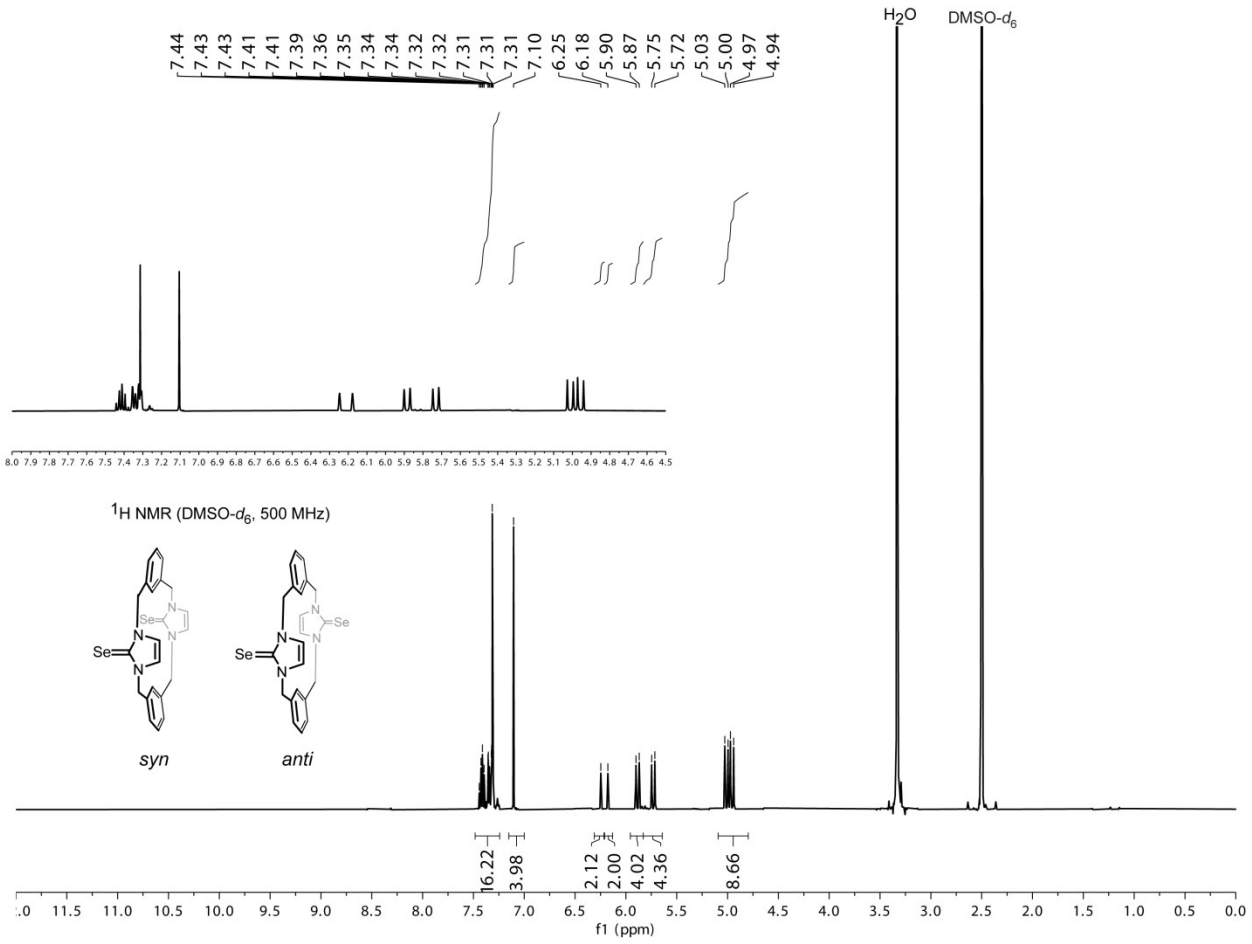

Figure S3. ^{1}H NMR of **9** in DMSO-d_6 at 500.10 MHz.

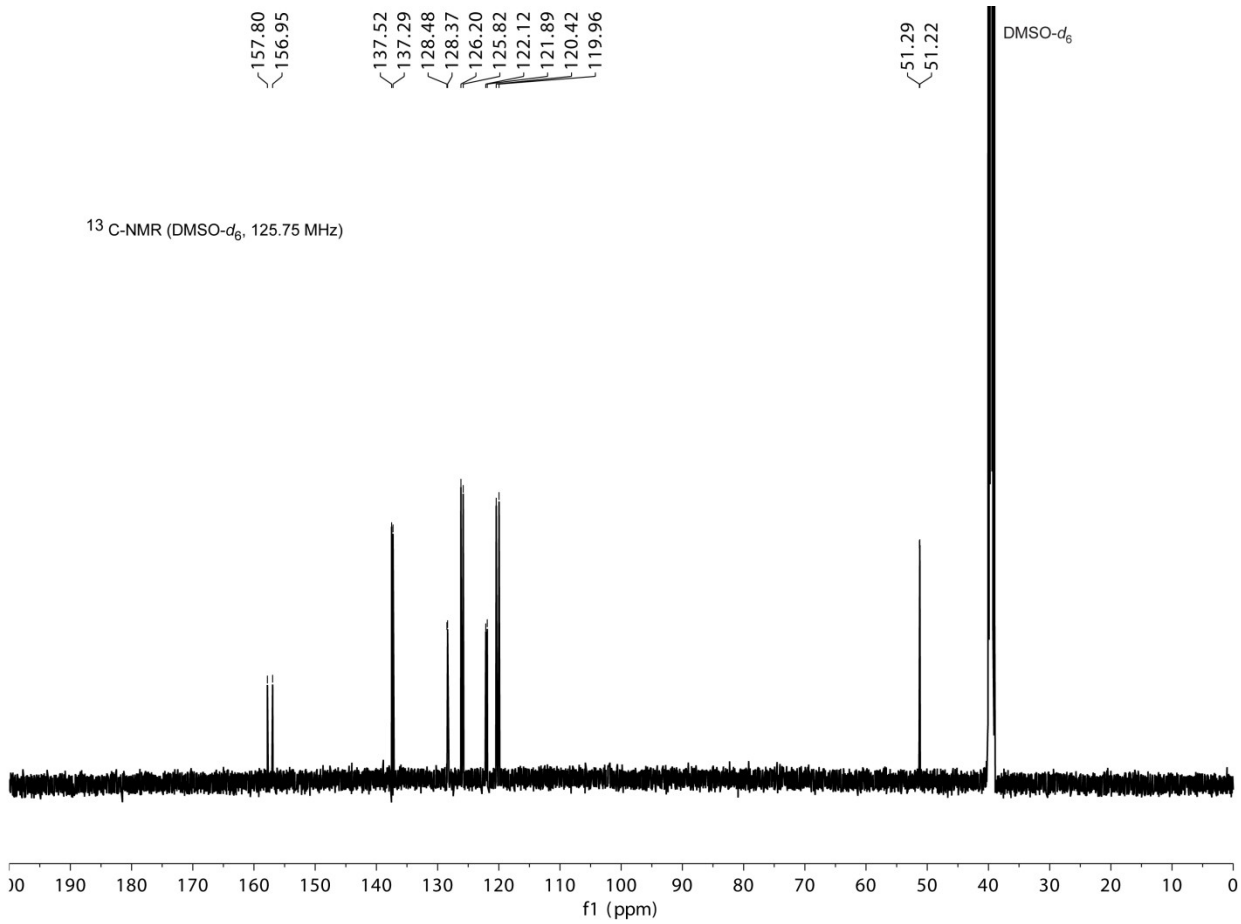

Figure S4. ^{13}C NMR of **9** in DMSO-d_6 at 125.75 MHz.

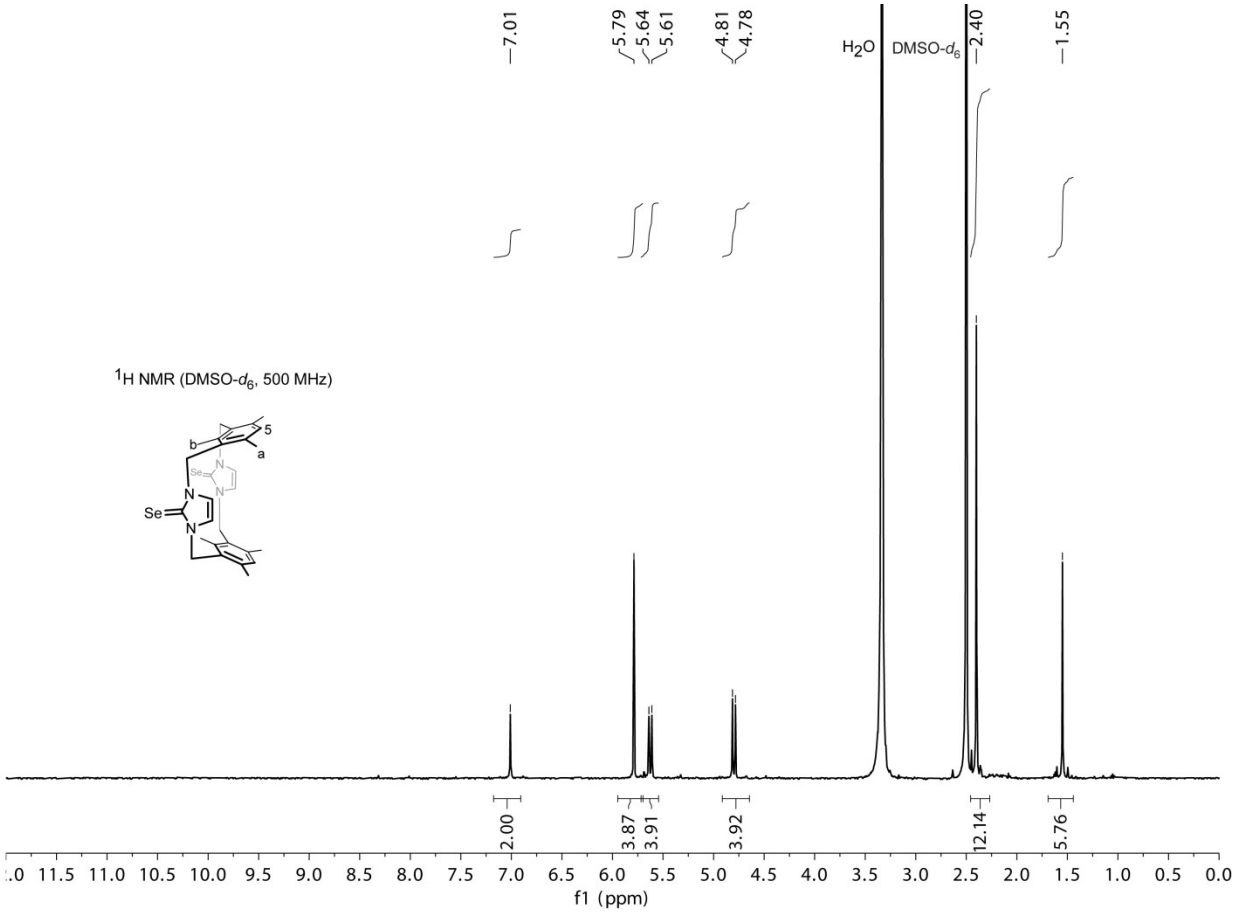

Figure S5. ^{1}H NMR of **10** in DMSO-d_6 at 500.10 MHz.

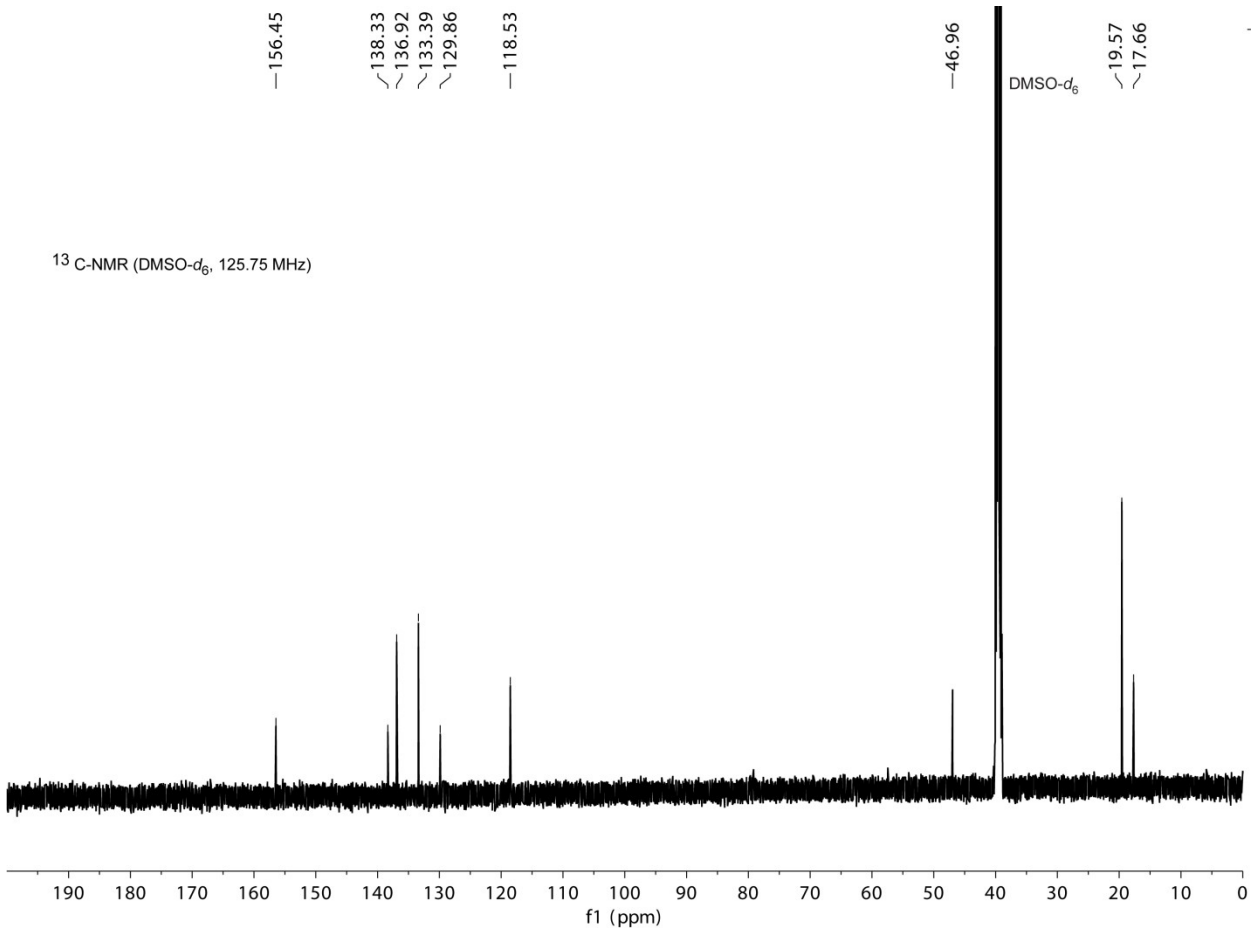

Figure S6. ^{13}C NMR of **10** in DMSO-d_6 at 125.75 MHz.

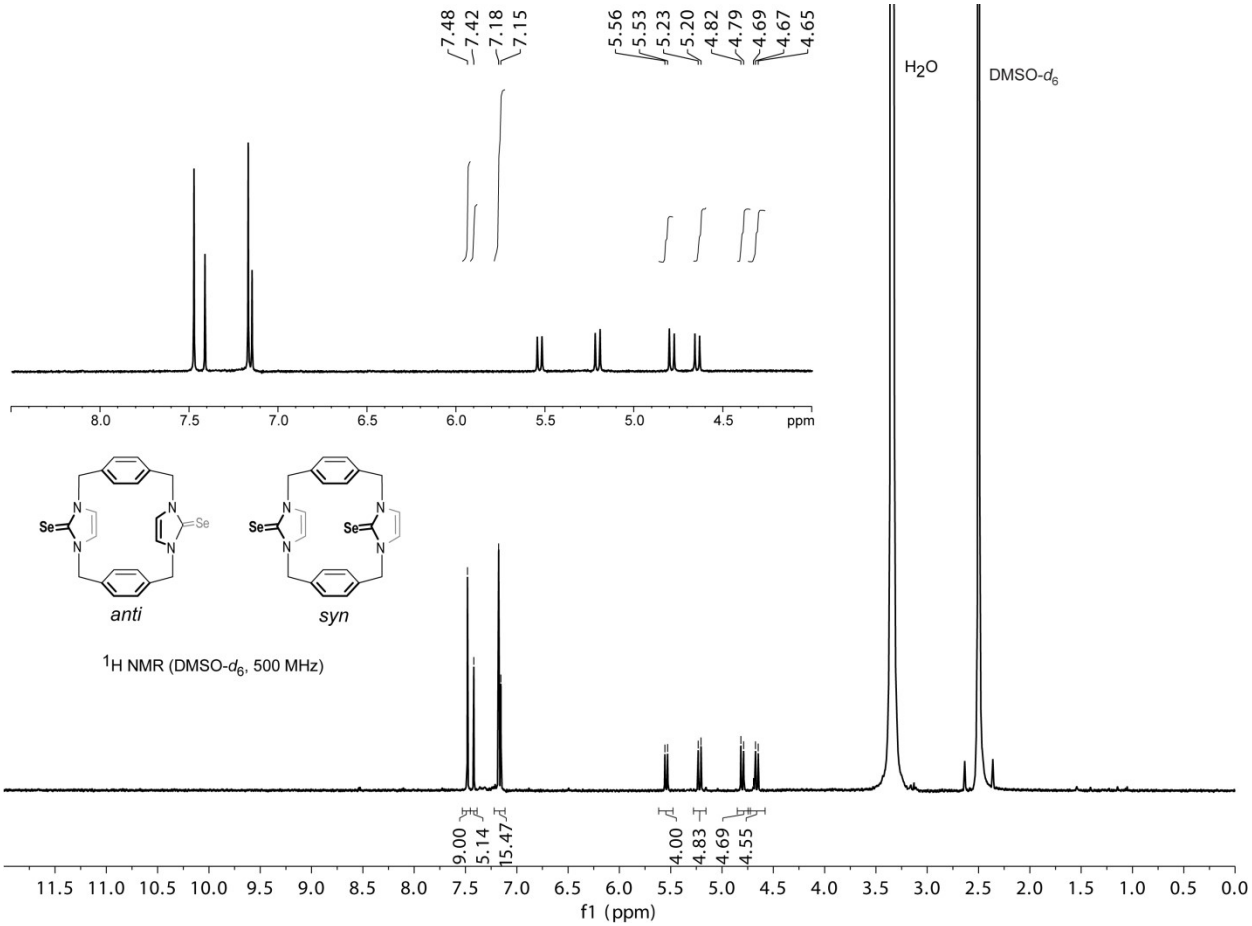

Figure S7. ^{1}H NMR of **11** in DMSO-d_6 at 500.10 MHz.

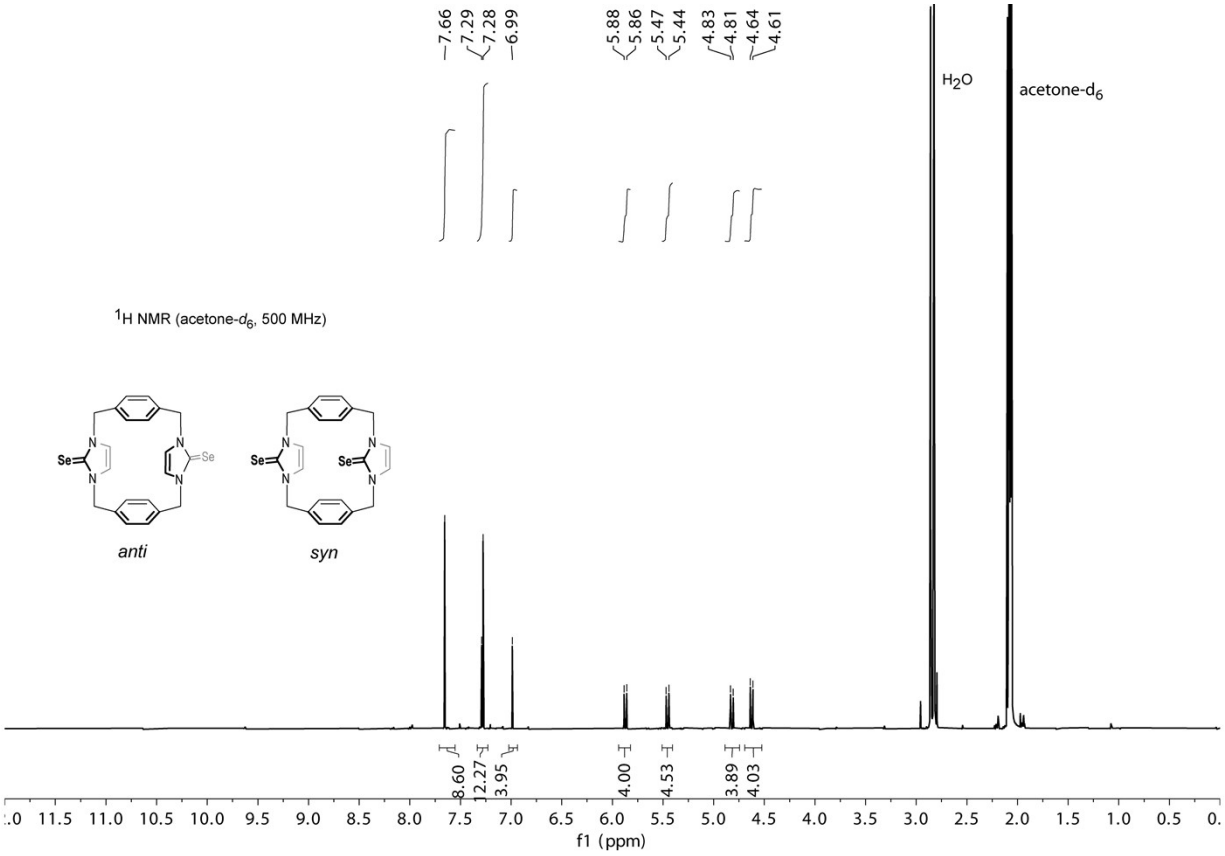

Figure S8. ^{1}H NMR of **11** in acetone-d_6 at 500.10 MHz.

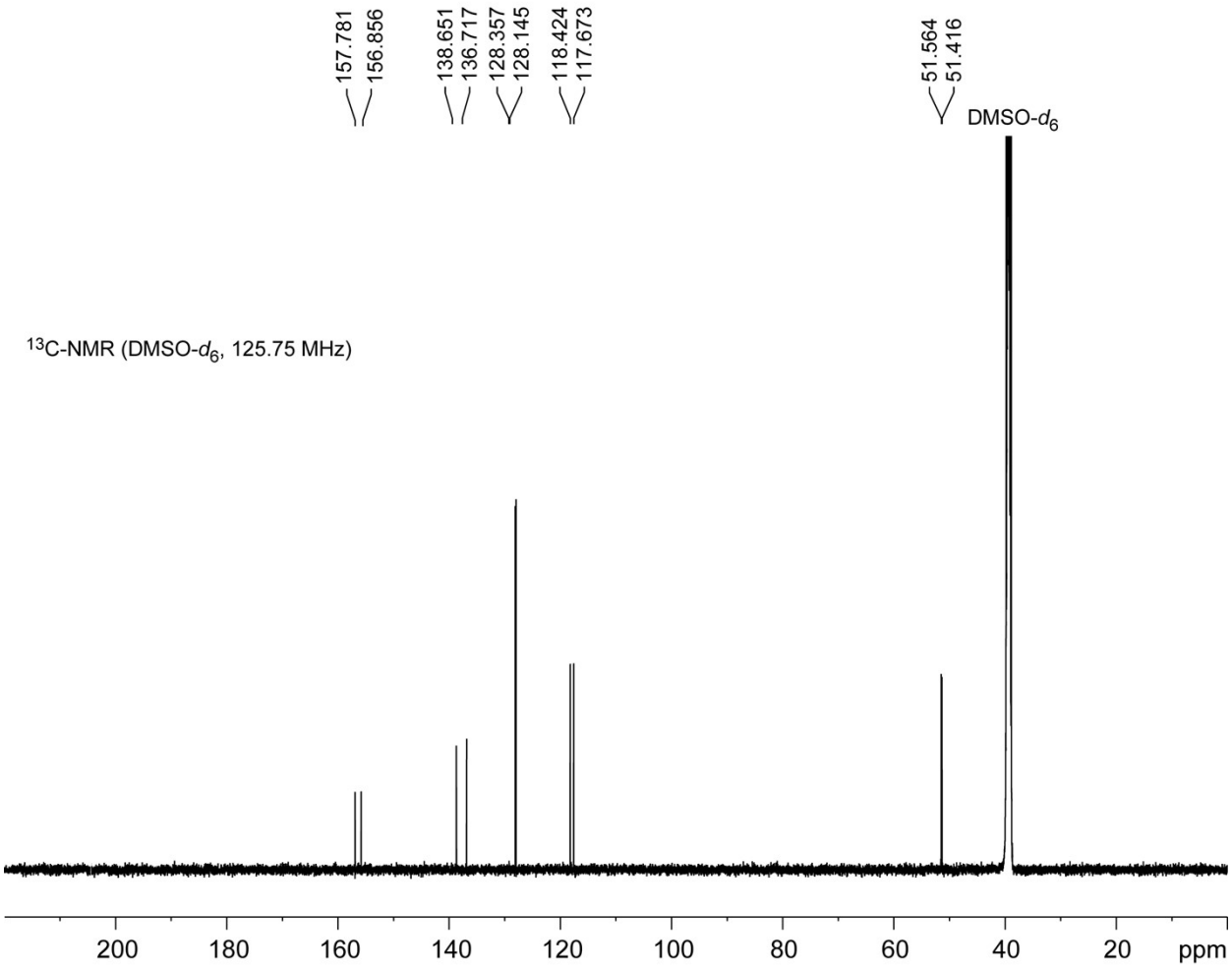

Figure S9. ^{13}C NMR of **11** in DMSO-d_6 at 125.75 MHz.

Table S1: The Cartesian coordinates in (Angstroms) of **8** geometry

Se	10.201300000	11.267500000	2.132400000
Se	13.262400000	8.992700000	3.036300000
C	8.138300000	8.694900000	1.705500000
H	8.788900000	9.070400000	1.061700000
H	7.234100000	8.995300000	1.436200000
C	10.562100000	10.870800000	5.413400000
H	10.346400000	11.837200000	5.403600000
H	11.421600000	10.748500000	4.937900000
C	12.654500000	8.814700000	6.285600000
H	13.161700000	9.502600000	5.785800000
H	13.303800000	8.257900000	6.785400000
C	10.723900000	7.121100000	2.055600000
H	11.433100000	6.594100000	1.611100000
H	10.713200000	8.024500000	1.651000000
N	8.437500000	9.207900000	3.056800000
C	9.385400000	10.125700000	3.337300000
N	9.504400000	10.136300000	4.688600000
C	8.557400000	9.287400000	5.243400000
H	8.403300000	9.144000000	6.170100000
C	7.893600000	8.704500000	4.227900000
H	7.190200000	8.071400000	4.298600000
C	10.722900000	10.417200000	6.848600000
C	11.710700000	9.489800000	7.262200000
C	11.806900000	9.180300000	8.611400000
H	12.486300000	8.580200000	8.896200000
C	10.953400000	9.714500000	9.553300000
H	11.049100000	9.486900000	10.470400000
C	9.954400000	10.584600000	9.152000000
H	9.334100000	10.932200000	9.780800000
C	9.878100000	10.939700000	7.810900000
H	9.216900000	11.566800000	7.543900000
N	11.908300000	7.970000000	5.339700000
C	12.021600000	8.056900000	3.996600000
N	11.029100000	7.234500000	3.501100000
C	10.401600000	6.615500000	4.553500000
H	9.705300000	5.972800000	4.481100000
C	10.929800000	7.063800000	5.695900000
H	10.682300000	6.809400000	6.577400000
C	9.384800000	6.453400000	1.826300000
C	8.198400000	7.177200000	1.650200000
C	7.014600000	6.474600000	1.410700000
H	6.205600000	6.955900000	1.285300000
C	6.994400000	5.107400000	1.355400000
H	6.177500000	4.651100000	1.194600000
C	8.171500000	4.383500000	1.533500000
H	8.166400000	3.434000000	1.497800000
C	9.346800000	5.076600000	1.760800000
H	10.154300000	4.588400000	1.874500000

Table S2: The Cartesian coordinates in (Angstroms) of **9** geometry

Se	1.774200000	9.565000000	1.647200000
C	3.060700000	8.787200000	2.710800000
N	2.918300000	7.686000000	3.490800000
C	1.733500000	6.842800000	3.535500000
H	2.012400000	5.897200000	3.444900000
H	1.157700000	7.061600000	2.760700000
C	4.103300000	7.423700000	4.164900000
H	4.259500000	6.712200000	4.774400000
C	4.981200000	8.357200000	3.795300000
H	5.879000000	8.433300000	4.095500000
N	4.343500000	9.199800000	2.890000000
C	4.966900000	10.334500000	2.225800000
H	4.542700000	10.457500000	1.340000000
H	5.923500000	10.128400000	2.074700000
C	0.922900000	6.991500000	4.800900000
C	0.904000000	8.197300000	5.508200000
H	1.453000000	8.918100000	5.223000000
C	0.089100000	8.353800000	6.626400000
C	-0.691900000	7.271000000	7.050800000
H	-1.238900000	7.357200000	7.822100000
C	-0.671300000	6.073300000	6.351200000
H	-1.208200000	5.345900000	6.641700000
C	0.130900000	5.933600000	5.228200000
H	0.138800000	5.112700000	4.750700000
Se	3.180400000	10.416300000	7.975900000
C	1.893900000	11.194100000	6.912200000
N	2.036300000	12.295300000	6.132300000
C	3.221100000	13.138500000	6.087500000
H	2.942200000	14.084100000	6.178100000
H	3.796900000	12.919700000	6.862400000
C	0.851300000	12.557600000	5.458200000
H	0.695100000	13.269100000	4.848700000
C	-0.026600000	11.624100000	5.827700000
H	-0.924400000	11.548000000	5.527500000
N	0.611100000	10.781500000	6.733100000
C	-0.012300000	9.646800000	7.397200000
H	0.411900000	9.523800000	8.283100000
H	-0.968900000	9.852900000	7.548300000
C	4.031700000	12.989800000	4.822100000
C	4.050600000	11.784000000	4.114800000
H	3.501600000	11.063200000	4.400100000
C	4.865500000	11.627500000	2.996600000
C	5.646500000	12.710300000	2.572200000
H	6.193500000	12.624100000	1.800900000
C	5.625900000	13.908000000	3.271800000
H	6.162800000	14.635400000	2.981300000
C	4.823700000	14.047700000	4.394800000
H	4.815800000	14.868600000	4.872300000

Table S3: The Cartesian coordinates in (Angstroms) of **10** geometry

Se	8.181600000	5.865400000	1.021800000
N	8.257600000	3.079000000	1.757300000
C	7.496500000	4.208000000	1.515600000
N	6.215100000	3.888600000	1.769400000
C	6.135600000	2.551300000	2.121600000
H	5.340900000	2.068100000	2.314700000
C	7.383400000	2.062200000	2.138800000
H	7.629600000	1.174300000	2.370300000
C	9.709600000	2.995400000	1.816000000
H	10.097300000	3.905000000	1.758900000
H	10.043300000	2.470400000	1.045200000
C	10.144400000	2.337900000	3.103800000
C	10.766100000	1.081600000	3.098600000
C	11.068200000	0.359300000	1.812600000
H	11.708800000	0.881900000	1.286700000
H	10.240700000	0.245000000	1.299700000
H	11.451200000	-0.520100000	2.014100000
C	5.072200000	4.804400000	1.809100000
H	4.478700000	4.629900000	1.035300000
H	5.391400000	5.739200000	1.748000000
C	4.297200000	4.611000000	3.100300000
C	3.102400000	3.886100000	3.103800000
H	6.361700000	6.140500000	5.239500000
H	6.833600000	5.519400000	3.842100000
H	5.865500000	6.793500000	3.865300000
C	2.432300000	3.388400000	1.821200000
H	2.276400000	4.146700000	1.218800000
H	1.576100000	2.966200000	2.041500000
H	3.014600000	2.735900000	1.379200000
Se	8.181600000	5.865400000	7.609500000
N	8.257600000	3.079000000	6.873900000
C	7.496500000	4.208000000	7.115600000
N	6.215100000	3.888600000	6.861800000
C	6.135600000	2.551300000	6.509700000
H	5.340900000	2.068100000	6.316600000
C	7.383400000	2.062200000	6.492400000
H	7.629600000	1.174300000	6.261000000
C	9.709600000	2.995400000	6.815200000
H	10.097300000	3.905000000	6.872400000
H	10.043300000	2.470400000	7.586000000
C	9.843400000	2.964200000	4.315600000
C	10.144400000	2.337900000	5.527500000
C	10.766100000	1.081600000	5.532600000
C	11.056700000	0.489000000	4.315600000
H	11.474300000	-0.364000000	4.315600000
C	9.157200000	4.305300000	4.315600000
H	9.019000000	4.601700000	5.239500000
H	8.290200000	4.228800000	3.864500000
H	9.714700000	4.957600000	3.842900000
C	11.068200000	0.359300000	6.818700000

H	11.708800000	0.881900000	7.344500000
H	10.240700000	0.245000000	7.331500000
H	11.451200000	-0.520100000	6.617200000
C	5.072200000	4.804400000	6.822100000
H	4.478700000	4.629900000	7.595900000
H	5.391400000	5.739200000	6.883300000
C	4.881900000	5.032700000	4.315600000
C	4.297200000	4.611000000	5.530900000
C	3.102400000	3.886100000	5.527500000
C	2.495700000	3.549300000	4.315600000
H	1.664600000	3.089700000	4.315600000
C	6.094000000	5.953400000	4.315600000
C	2.432300000	3.388400000	6.810100000
H	2.276400000	4.146700000	7.412500000
H	1.576100000	2.966200000	6.589700000
H	3.014600000	2.735900000	7.252000000

Table S4: The cartisian coordinates in (Angstroms) optimized geometry of **11** using BP86/def2-TZVP of **syn** conformers

Se	-3.272923000	-0.003275000	-1.848414000
C	-3.205111000	0.000999000	-0.013078000
N	-3.192341000	-1.091099000	0.832825000
C	-3.161746000	-0.674371000	2.156601000
H	-3.160507000	-1.378570000	2.978487000
C	-3.161368000	0.683946000	2.154088000
H	-3.158946000	1.390989000	2.973527000
N	-3.191054000	1.096000000	0.829021000
C	-2.908820000	-2.467204000	0.397451000
H	-3.396549000	-3.145451000	1.111417000
H	-3.370399000	-2.592862000	-0.590868000
C	-1.410994000	-2.682271000	0.347953000
C	-0.699814000	-2.458519000	-0.838075000
H	-1.246347000	-2.228705000	-1.752926000
C	-0.698541000	-2.974364000	1.519849000
H	-1.238429000	-3.182843000	2.446257000
C	-2.906773000	2.470169000	0.388925000
H	-3.367370000	2.592569000	-0.600092000
H	-3.394774000	3.151178000	1.099889000
C	-1.408843000	2.685258000	0.340285000
C	-0.696270000	2.452518000	-0.843167000
H	-1.241857000	2.214594000	-1.756379000
C	-0.697494000	2.983692000	1.510997000
H	-1.238053000	3.197757000	2.436071000
Se	3.279692000	-0.002787000	-1.845066000
C	3.205928000	-0.000293000	-0.009965000
N	3.188875000	-1.093437000	0.834548000

C	3.152379000	-0.678328000	2.158680000
H	3.147107000	-1.383528000	2.979675000
C	3.152572000	0.679935000	2.157871000
H	3.146156000	1.385917000	2.978186000
N	3.189236000	1.093686000	0.833465000
C	2.905446000	-2.468695000	0.396459000
H	3.393569000	-3.148582000	1.108623000
H	3.366592000	-2.591903000	-0.592364000
C	1.407579000	-2.683396000	0.347218000
C	0.696019000	-2.458650000	-0.838366000
H	1.242219000	-2.228632000	-1.753405000
C	0.695441000	-2.975279000	1.519379000
H	1.235631000	-3.184716000	2.445387000
C	2.907668000	2.468713000	0.394149000
H	3.370577000	2.591404000	-0.593749000
H	3.394979000	3.148412000	1.106838000
C	1.410063000	2.685418000	0.342628000
C	0.699482000	2.452276000	-0.841944000
H	1.246600000	2.213551000	-1.754041000
C	0.696695000	2.983758000	1.512159000
H	1.235682000	3.197623000	2.438199000

Table S5: The optimized geometry of **11** using BP86/def2-TZVP of **anti** conformers

Se	2.949967500	3.028510200	-0.340492700
C	1.154172200	3.390503100	-0.172808200
N	0.229687600	3.560399100	-1.183406100
C	-1.020842100	3.840216900	-0.649739700
H	-1.886499000	4.008811300	-1.276477300
C	-0.890052600	3.856813200	0.701514000
H	-1.619607600	4.045521300	1.478293400
N	0.440404000	3.586715200	0.992220700
C	0.452269700	3.162674800	-2.581967500
H	-0.188906300	3.796121400	-3.210437300
H	1.504285300	3.374293700	-2.812973700
C	0.124316100	1.693509000	-2.743939000
C	1.123731100	0.724099000	-2.577920000
H	2.157538900	1.040656900	-2.439625100
C	-1.202925800	1.276500900	-2.904426100
H	-1.992626000	2.018914600	-3.040646800
C	0.926702400	3.212675100	2.329131800
H	2.003727800	3.424702400	2.351108800
H	0.417411800	3.858760500	3.057652600
C	0.635831700	1.747442000	2.575479800
C	1.596091300	0.772352400	2.270127700
H	2.592413500	1.083550200	1.955758400
C	-0.645673400	1.337341700	2.963476300
H	-1.402992900	2.084231100	3.211365400
Se	-2.744524000	-1.623054200	0.241722600
C	-1.139721000	-2.496919900	0.098905600

N	-0.511033700	-2.921019400	-1.055182400
C	0.683122800	-3.558170400	-0.748804000
H	1.320587800	-3.980542600	-1.514938600
C	0.814630600	-3.541724700	0.604814500
H	1.588216200	-3.948216400	1.243861000
N	-0.299834900	-2.894791900	1.120163600
C	-0.916442900	-2.492523500	-2.396645900
H	-2.002330300	-2.635203800	-2.481871500
H	-0.414564100	-3.158876600	-3.112562300
C	-0.548129800	-1.039319900	-2.623570100
C	0.786444100	-0.626993900	-2.522009300
H	1.571646100	-1.366086400	-2.349329700
C	-1.539737500	-0.076004400	-2.834998000
H	-2.583934000	-0.384154200	-2.894297900
C	-0.443364300	-2.442036400	2.506412900
H	0.187198500	-3.096336200	3.124993500
H	-1.492889100	-2.582528600	2.798838200
C	-0.042014500	-0.985777300	2.634377900
C	1.256931200	-0.579545500	2.304264200
H	2.004558200	-1.324798100	2.024240900
C	-0.986763100	-0.015186600	2.983611300
H	-2.005577600	-0.320204900	3.223734300

The optimized geometry of 11

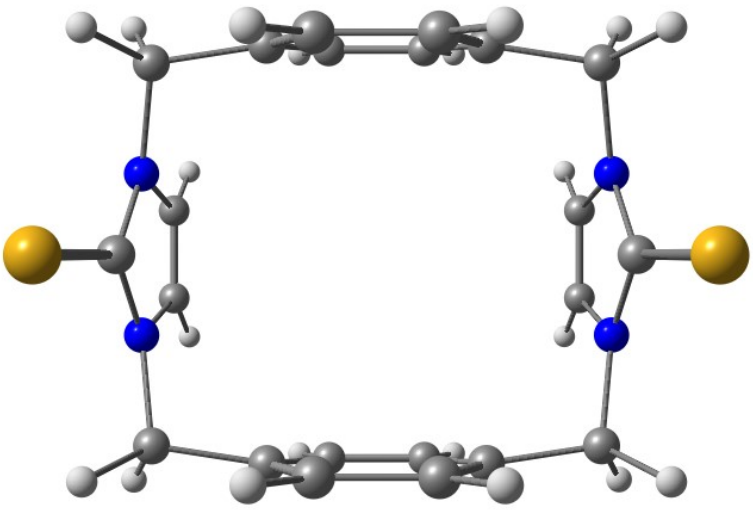

Figure S10: The optimized geometry of **11** using BP86/def2-TZVP of **syn** conformers

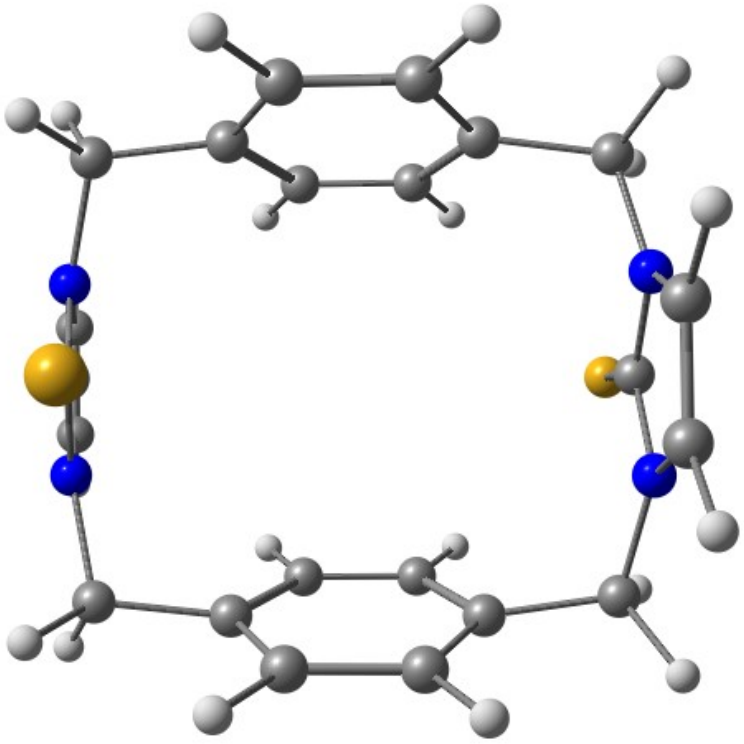

Figure S11: The optimized geometry of **11** using BP86/def2-TZVP of **anti** conformers