

Supporting Information

Induction and Rationalization of Supramolecular Chirality in Highly-Flexible Zn(II)porphyrin Dimer: Structural, Spectroscopic and Theoretical Investigations

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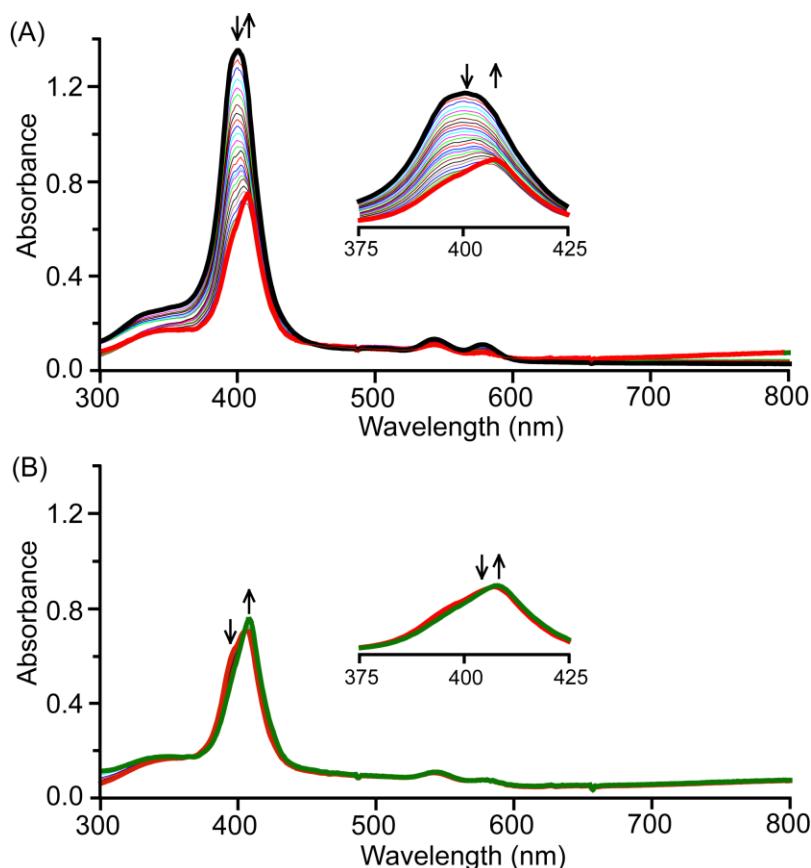


Fig. S1. UV-visible spectral changes of **1** (5×10^{-6} M) in dichloromethane at 295 K upon gradual addition of (R,R)-**G7** as the host–guest molar ratio changes from (A) 1:0 to 1:100 and (B) 1:100 to 1:5000.

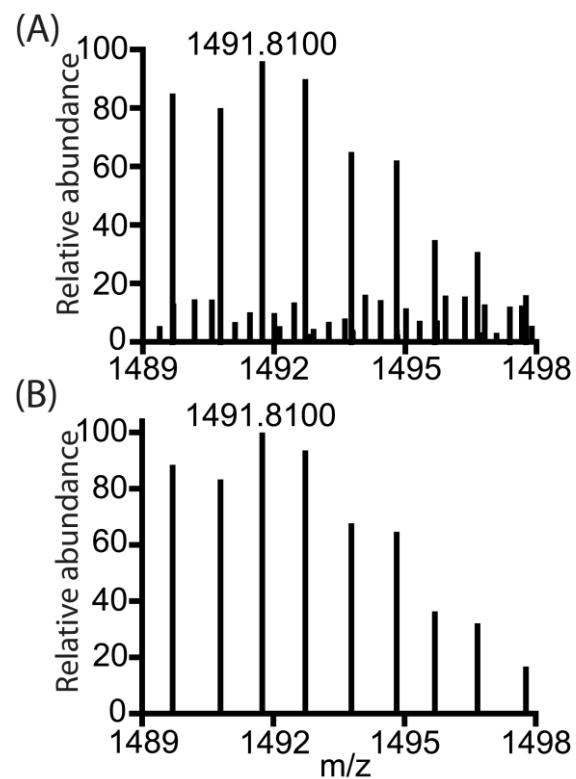


Fig. S2. Isotopic distribution pattern, (A) experimental and (B) theoretical, of ESI-MS of $[1\bullet((S)\text{-G1})_2]^+$

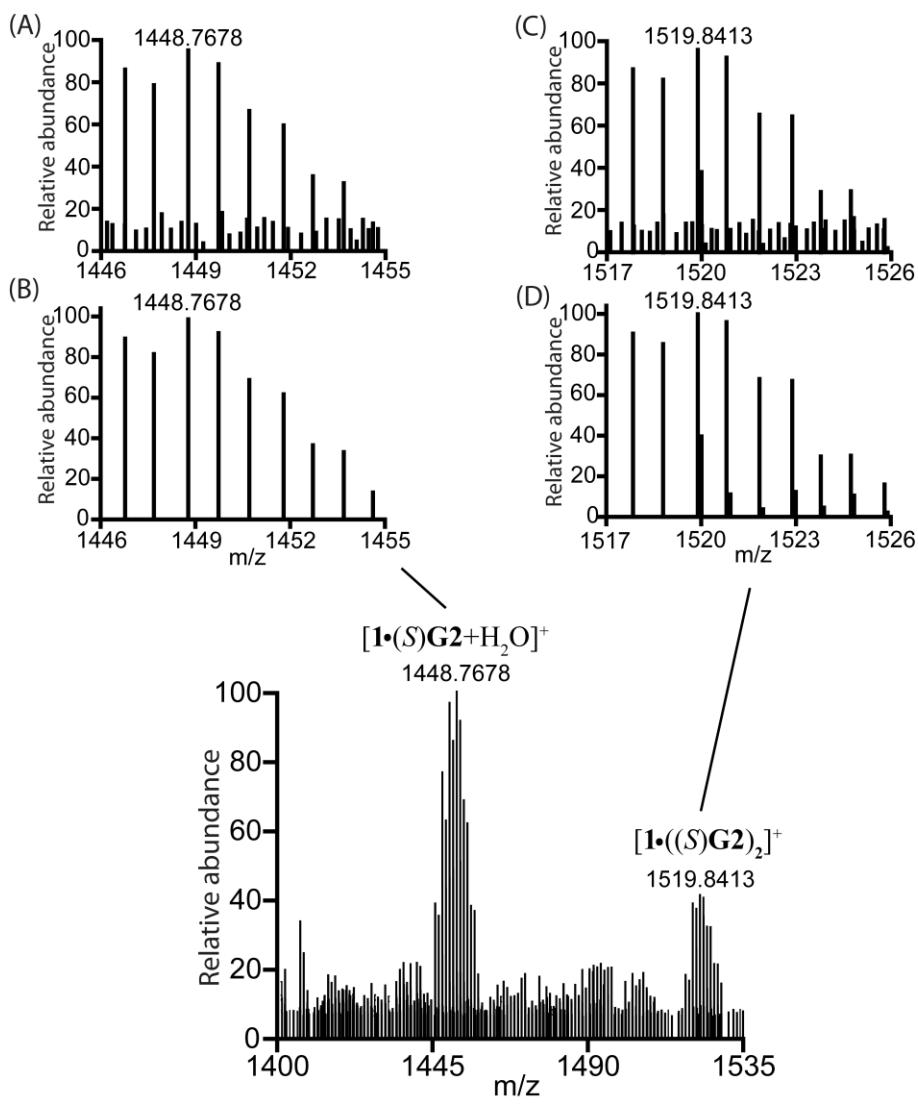


Fig. S3 ESI-MS of **1** in the presence of excess (*S*)-**G2**. Insets show isotopic distribution patterns for $[1\bullet(S)\text{-G2}+\text{H}_2\text{O}]^+$. [(A) experimental and (B) theoretical] and $[(1\bullet((S)\text{-G2}))_2]^+$ [(C) experimental and (D) theoretical].

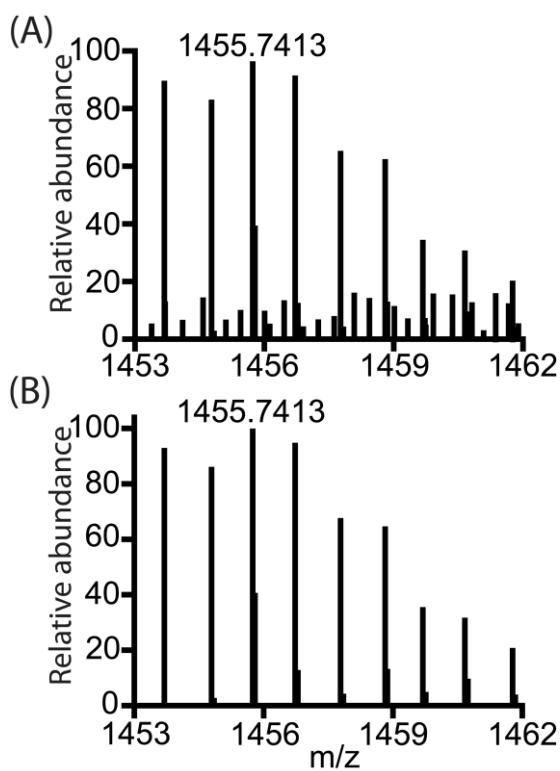


Fig. S4. Isotopic distribution pattern, (A) experimental and (B) theoretical, of ESI-MS of $[1\bullet(S)\text{-G6}+2\text{H}]^+$.

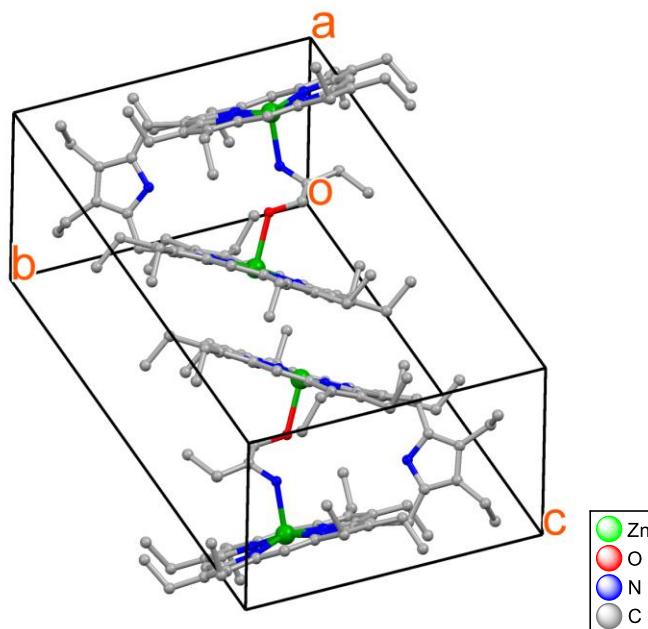


Fig. S5. Diagram illustrating the molecular packing of $\mathbf{1}\bullet(S)\text{-G3}$ in the unit cell (solvent molecules and H atoms have been omitted for clarity).

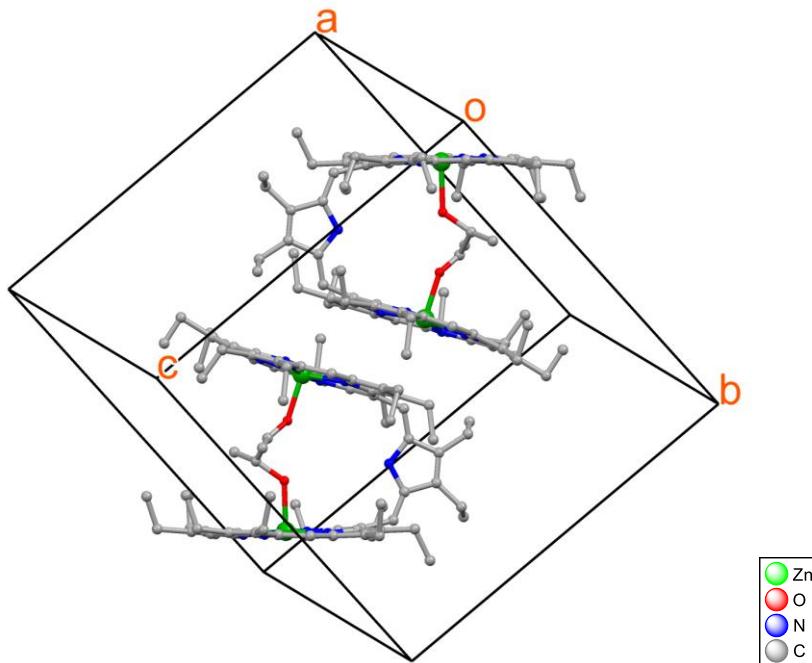


Fig. S6. Diagram illustrating the molecular packing of **1•(R,R)-G7** in the unit cell (solvent molecules and H atoms have been omitted for clarity).

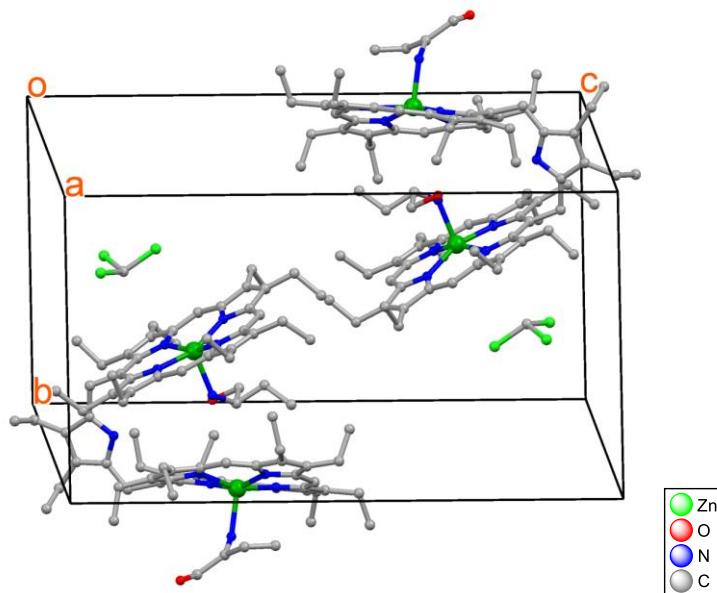


Fig. S7. Diagram illustrating the molecular packing of **1•((S)-G2)2** in the unit cell (solvent molecules and H atoms have been omitted for clarity).

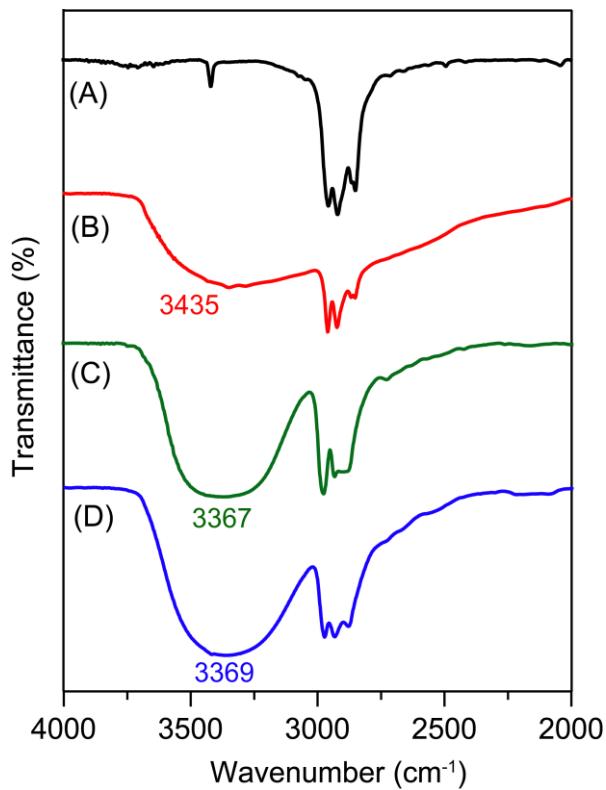


Fig. S8. IR spectra of a solid pure crystalline sample of (A) **1**, (B) **1**•(*(S)*-**G2**)₂, (C) **1**•(*(S)*-**G6**)₂ and (D) **1**•(*(R,R)*-**G7**)₂

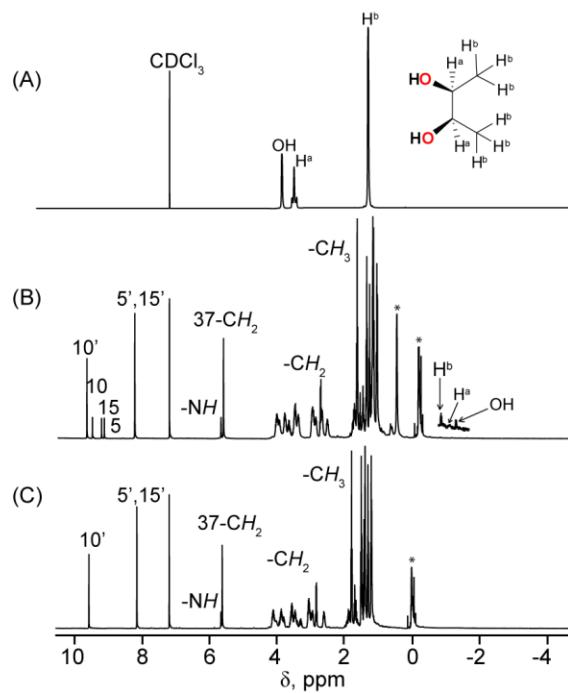


Fig. S9. ^1H NMR spectra of (A) (*R,R*)-**G7**, (B) **1**•(*R,R*)-**G7**, and (C) **1** at 295 K in CDCl_3 . Inset shows the proton numbering scheme for (*R,R*)-**G7**. (Asterisk represents the trace or solvent impurities).

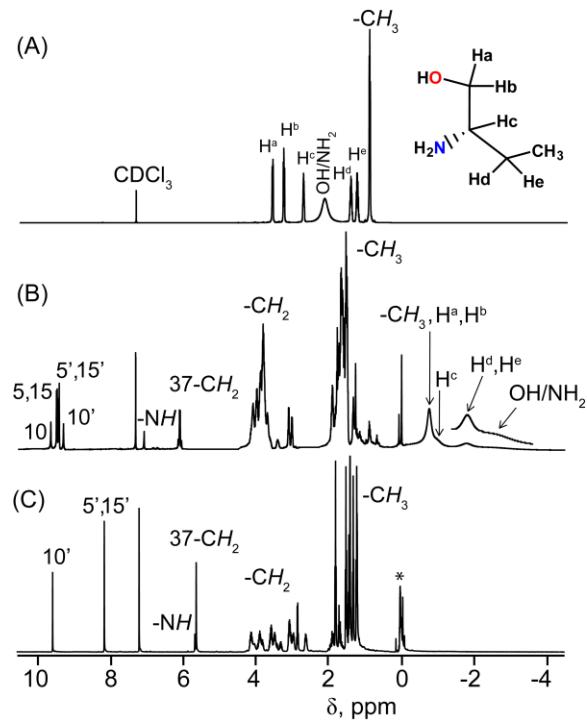


Fig. S10. ^1H NMR spectra of (A) (*S*)-**G2**, (B) **1**•(*(S)*-**G2**)₂, and (C) **1** at 295 K in CDCl_3 . Inset shows the proton numbering scheme for (*S*)-**G2**. (Asterisk represents the trace or solvent impurities).

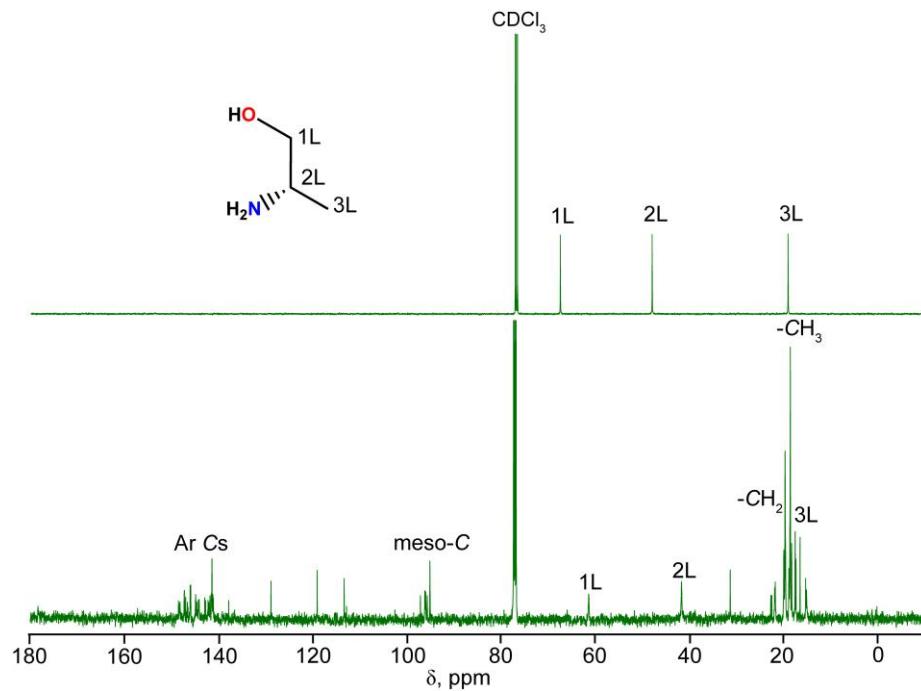


Fig. S11 ^{13}C NMR spectrum of $\mathbf{1}\bullet(S)\text{-G1}$ in CDCl_3 at 295 K. Inset shows expanded regions of the spectrum along with atom numbering scheme used here to assign the peaks.

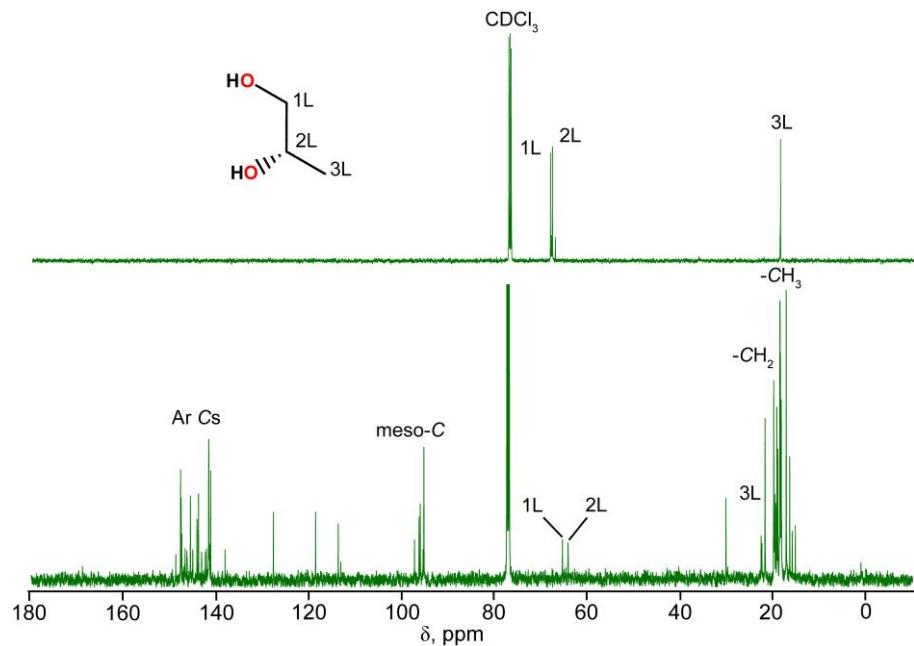


Fig. S12 ^{13}C NMR spectrum of $\mathbf{1}\bullet(S)\text{-G6}$ in CDCl_3 at 295 K. Inset shows expanded regions of the spectrum along with atom numbering scheme used here to assign the peaks.

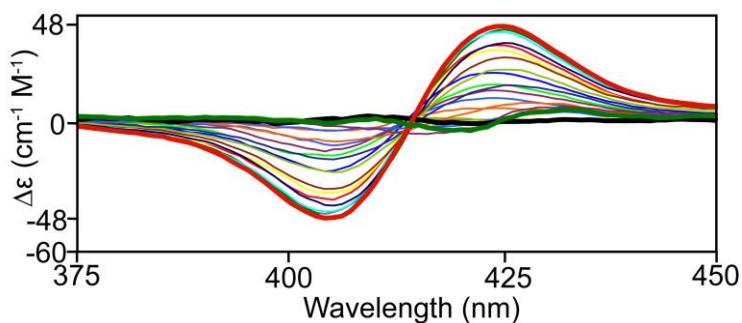


Fig. S13. CD spectral changes of **1** (5×10^{-6} M) in dichloromethane at 295 K upon gradual addition of (S)-**G1** as the host–guest molar ratio changes from 1:0 to 1:5000.

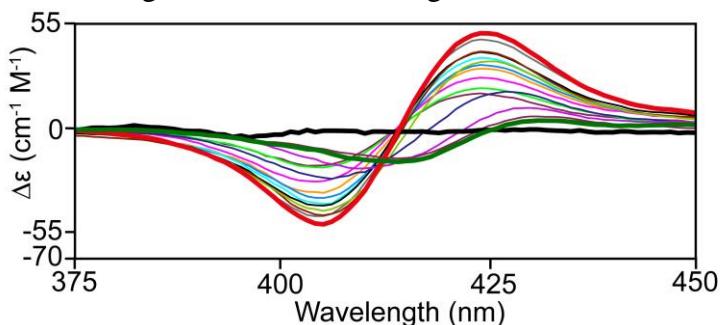


Fig. S14. CD spectral changes of **1** (5×10^{-6} M) in dichloromethane at 295 K upon gradual addition of (S)-**G2** as the host–guest molar ratio changes from 1:0 to 1:5000.

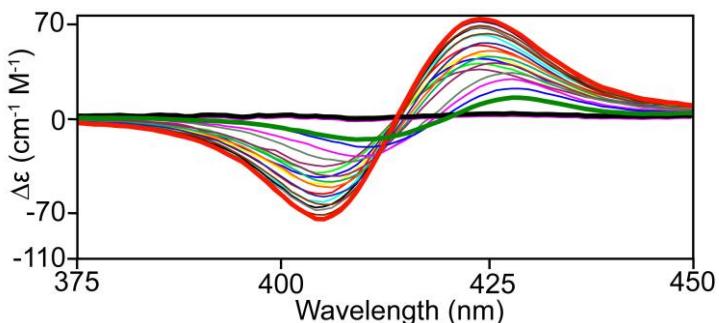


Fig. S15. CD spectral changes of **1** (5×10^{-6} M) in dichloromethane at 295 K upon gradual addition of (S)-**G3** as the host–guest molar ratio changes from 1:0 to 1:5000.

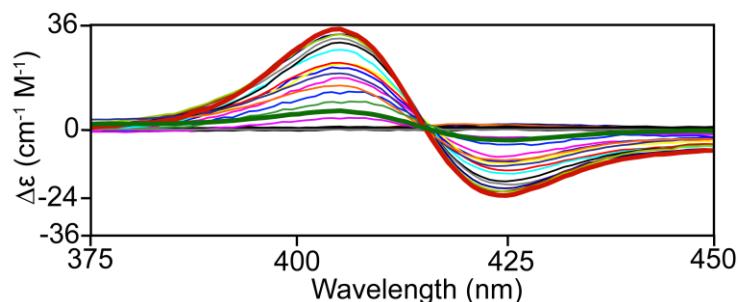


Fig. S16. CD spectral changes of **1** (5×10^{-6} M) in dichloromethane at 295 K upon gradual addition of (R)-**G4** as the host–guest molar ratio changes from 1:0 to 1:5000.

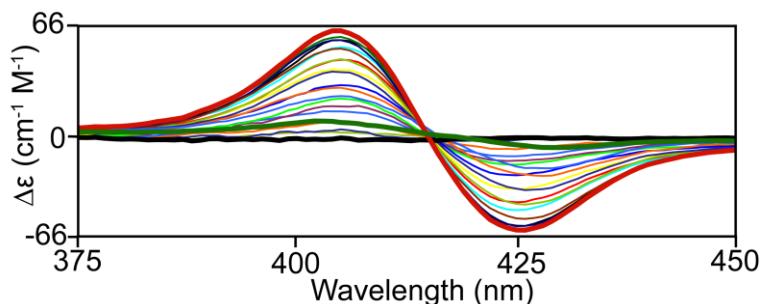


Fig. S17. CD spectral changes of **1** (5×10^{-6} M) in dichloromethane at 295 K upon gradual addition of (*R*)-**G5** as the host–guest molar ratio changes from 1:0 to 1:5000.

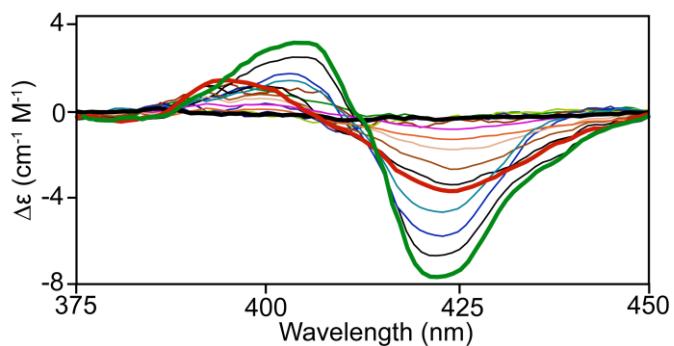


Fig. S18. CD spectral changes of **1** (5×10^{-6} M) in dichloromethane at 295 K upon gradual addition of (*R,R*)-**G7** as the host–guest molar ratio changes from 1:0 to 1:5000.

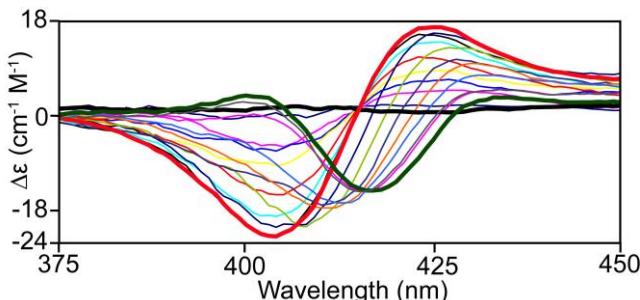


Fig. S19. CD spectral changes of **1** (5×10^{-6} M) in dichloromethane at 295 K upon gradual addition of (*S*)-**G8** as the host–guest molar ratio changes from 1:0 to 1:5000.

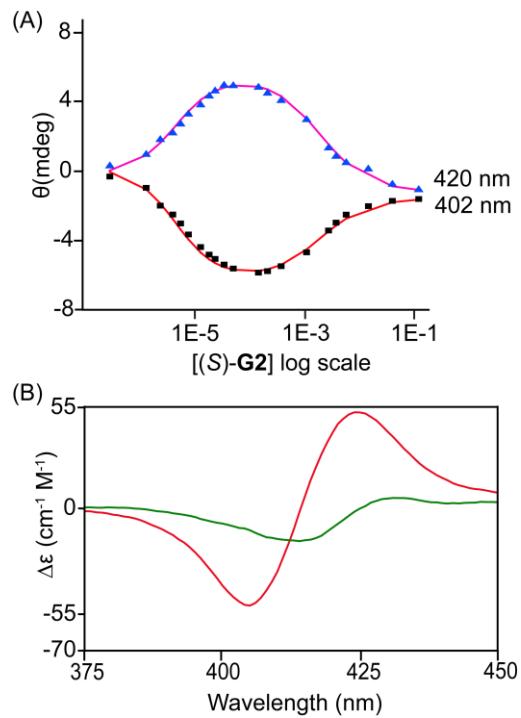


Fig. S20. (A) Fits of the titration data at selected wavelengths of 402 and 420 nm. (B) Calculated CD spectra of $\mathbf{1}\cdot(S)\text{-G2}$ (red line) and $\mathbf{1}\cdot((S)\text{-G2})_2$ (green line).

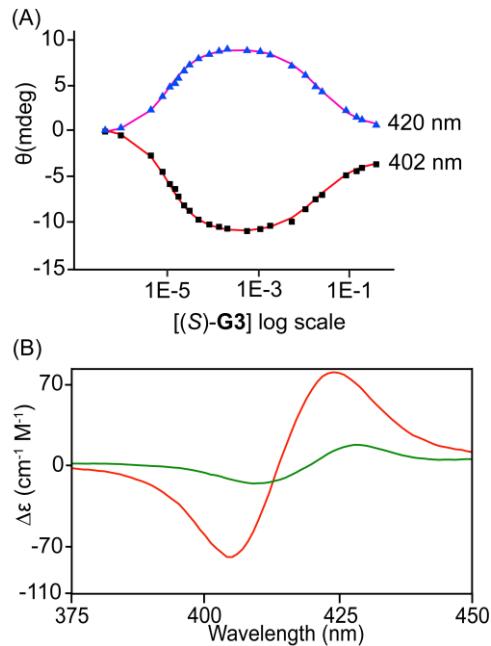


Fig. S21. (A) Fits of the titration data at selected wavelengths of 402 and 420 nm. (B) Calculated CD spectra of $\mathbf{1}\cdot(S)\text{-G3}$ (red line) and $\mathbf{1}\cdot((S)\text{-G3})_2$ (green line).

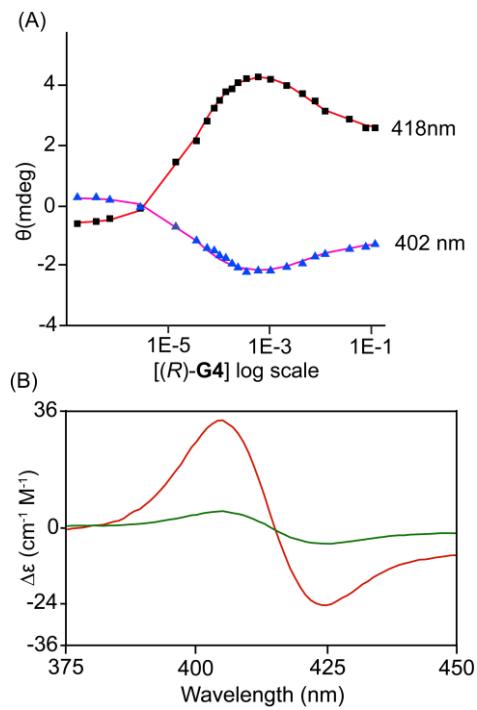


Fig. S22. (A) Fits of the titration data at selected wavelengths of 402 and 418 nm. (B) Calculated CD spectra of $\mathbf{1}\bullet(R)\text{-G4}$ (red line) and $\mathbf{1}\bullet((R)\text{-G4})_2$ (green line).

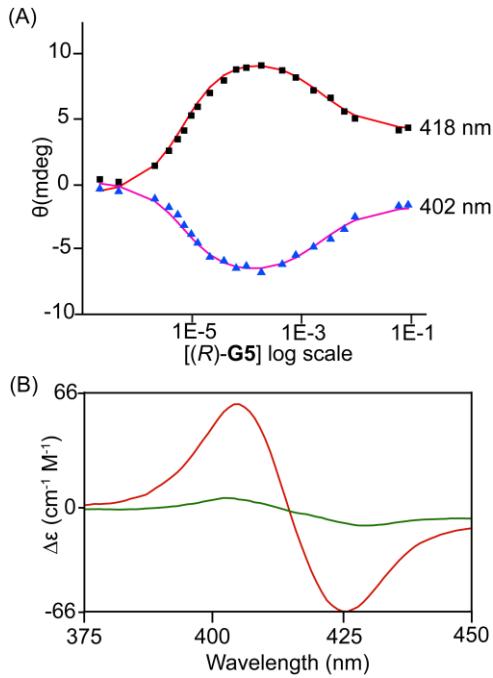


Fig. S23. (A) Fits of the titration data at selected wavelengths of 402 and 418 nm. (B) Calculated CD spectra of $\mathbf{1}\bullet(R)\text{-G5}$ (red line) and $\mathbf{1}\bullet((R)\text{-G5})_2$ (green line).

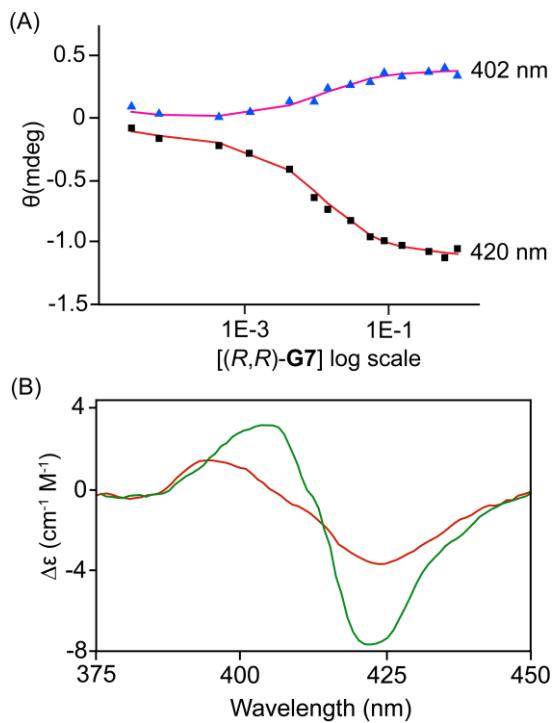


Fig. S24. (A) Fits of the titration data at selected wavelengths of 402 and 420 nm. (B) Calculated CD spectra of $\mathbf{1}\bullet(R,R)\text{-G7}$ (red line) and $\mathbf{1}\bullet((R,R)\text{-G7})_2$ (green line).

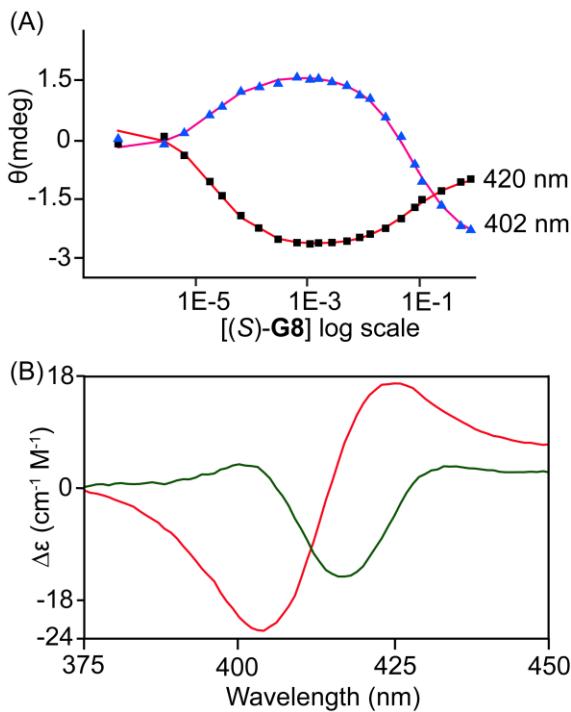


Fig. S25. (A) Fits of the titration data at selected wavelengths of 402 and 420 nm. (B) Calculated CD spectra of $\mathbf{1}\bullet(S)\text{-G8}$ (red line) and $\mathbf{1}\bullet((S)\text{-G8})_2$ (green line).

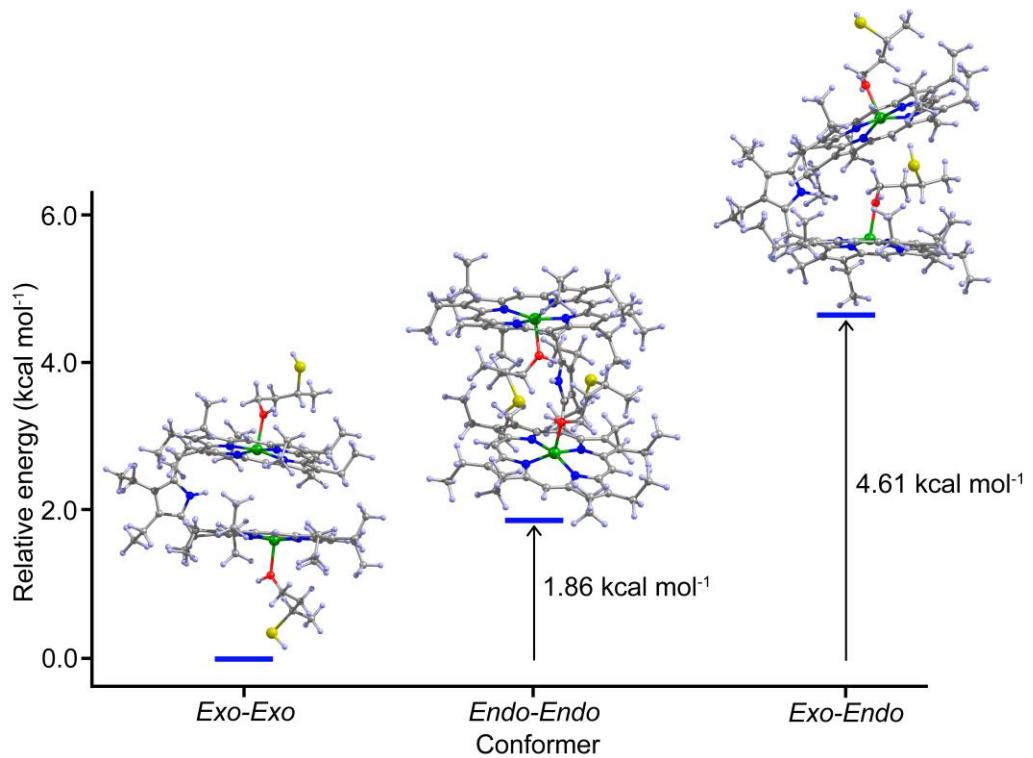


Fig. S26. Relative energy of B3LYP/6-31G+(d,p)-optimized geometries of *exo-exo*, *endo-endo* and *exo-endo* conformers, the unbound –OH of (*R,R*)-G7 replaced by –SH.

Table S1. Selected bond lengths (Å) and bond angles (°) for **1•(S)-G1**, **1•((S)-G2)2**, **1•(S)-G3** and **1•(R,R)-G7**.

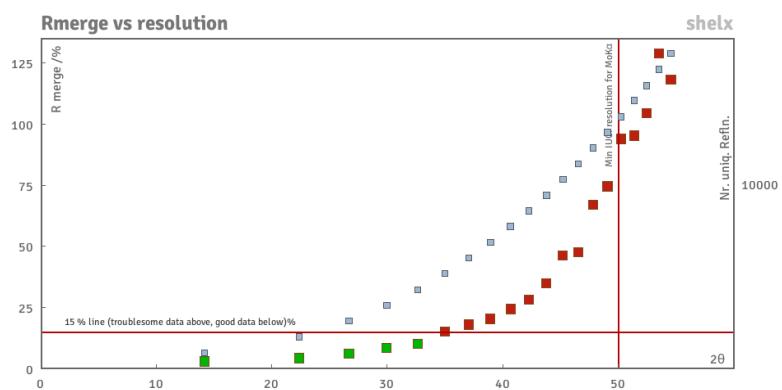
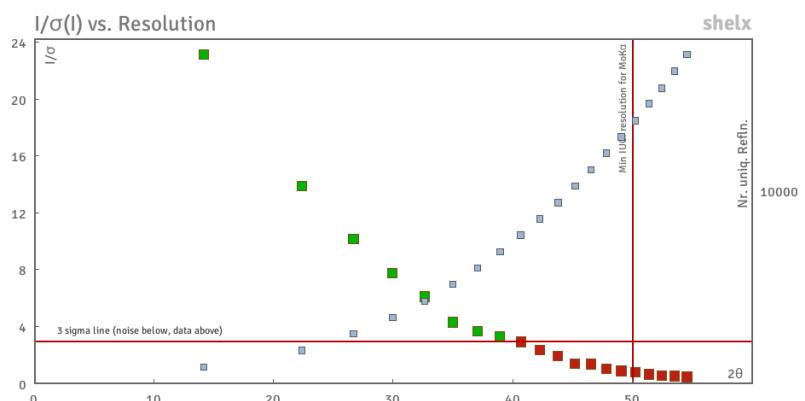
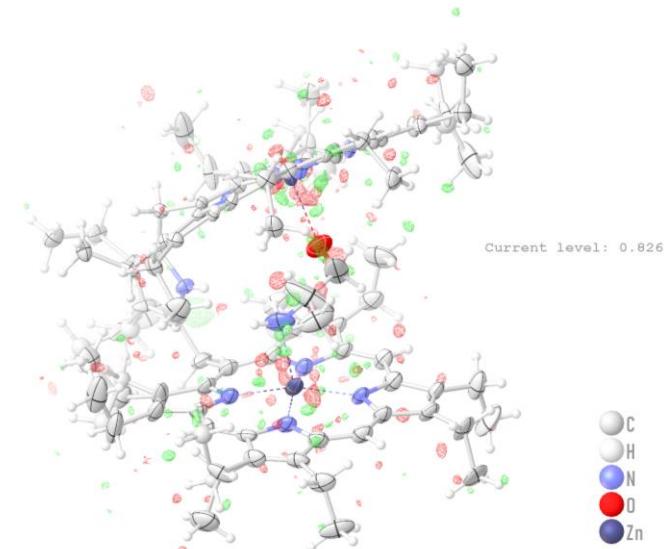
Bond distance (Å)	1•(S)-G1	1•((S)-G2)2	1•(S)-G3	1•(R,R)-G7
Zn(1)-N(1)	2.052(5)	2.081(4)	2.080(6)	2.046(7)
Zn(1)-N(2)	2.036(5)	2.076(4)	2.060(7)	2.059(7)
Zn(1)-N(3)	2.044(5)	2.095(4)	2.072(6)	2.050(8)
Zn(1)-N(4)	2.043(5)	2.080(4)	2.063(7)	2.060(7)
Zn(1)-O(1)/N(11)	2.348(6)	2.158(5)	2.208(9)	2.125(9)
Zn(2)-N(6)	2.069(6)	2.098(4)	2.052(6)	2.016(8)
Zn(2)-N(7)	2.066(6)	2.091(4)	2.039(7)	2.040(7)
Zn(2)-N(8)	2.062(6)	2.081(4)	2.051(6)	2.044(8)
Zn(2)-N(9)	2.072(6)	2.081(4)	2.070(6)	2.045(7)
Zn(2)-N(10)/O(2)	2.189(7)	2.162(5)	2.321(9)	2.190(9)
Bond angles (°)				
N(1)-Zn(1)-N(2)	92.1 (2)	89.92(17)	90.9(3)	91.5(3)
N(1)-Zn(1)-N(3)	173.4(2)	159.76(17)	165.7(3)	169.1(4)
N(1)-Zn(1)-N(4)	88.04(19)	86.08(17)	86.3(3)	88.8(3)
N(2)-Zn(1)-N(3)	88.2(2)	86.26(17)	87.5(3)	87.6(3)
N(2)-Zn(1)-N(4)	177.5(2)	156.17(18)	161.9(3)	171.6(3)
N(3)-Zn(1)-N(4)	91.4(2)	89.42(17)	90.8(3)	90.5(3)
N(7)-Zn(2)-N(9)	163.1(2)	161.12(18)	171.4(3)	175.5(3)
N(7)-Zn(2)-N(8)	87.3(2)	86.76(16)	88.5(3)	88.6(3)
N(9)-Zn(2)-N(8)	89.7(2)	90.01(16)	91.3(3)	91.2(3)
N(7)-Zn(2)-N(6)	90.8(2)	89.97(16)	91.5(3)	91.7(3)
N(9)-Zn(2)-N(6)	87.1(2)	86.69(16)	87.5(3)	87.9(3)
N(8)-Zn(2)-N(6)	162.4(2)	159.83(18)	171.9(3)	173.4(3)

X-ray Structure Solution and Refinement

Slow evaporation of acetonitrile into the dichloromethane solution of **1•(S)-G1**, **1•((S)-G2)2**, **1•(S)-G3** and **1•(R,R)-G7** in air at room temperature gave dark red crystals suitable for X-ray diffraction study. Crystals were coated with light hydrocarbon oil and mounted in the 100 K dinitrogen stream and intensity data were collected using graphite-monochromated Mo K α radiation ($\lambda = 0.71073 \text{ \AA}$). CCDC 2169150, 2169151, 2169152 and 2169153 contain the supplementary crystallographic data of **1•(S)-G1**, **1•(S)-G3**, **1•(R,R)-G7** and **1•((S)-G2)2**, respectively. **1•(S)-G1**, **1•(S)-G3** and **1•(R,R)-G7** contain several severely disordered solvent molecules which could not be modelled properly and thus, the SQUEEZE routine of PLATON were used to remove such unbound and highly disordered solvent molecules (one CHCl₃, two CHCl₃ and two CH₂Cl₂ molecules per unit cell, respectively, in **1•(S)-G1**, **1•(S)-G3** and **1•(R,R)-G7**) but the reported formula includes the solvent molecules. In the refinement, hydrogens were treated as riding atoms using SHELXL default parameters. The crystals were weakly diffracting and the qualities of data are relatively poor. Also, the bound substrates have several orientation disorders. Several crystals per samples were tested with different exposure time and crystals also have solvent-loss problem with long exposure. The reported samples, however, were the best out of several crystals tested. Some images related to the molecular structure and resolution are displayed below:

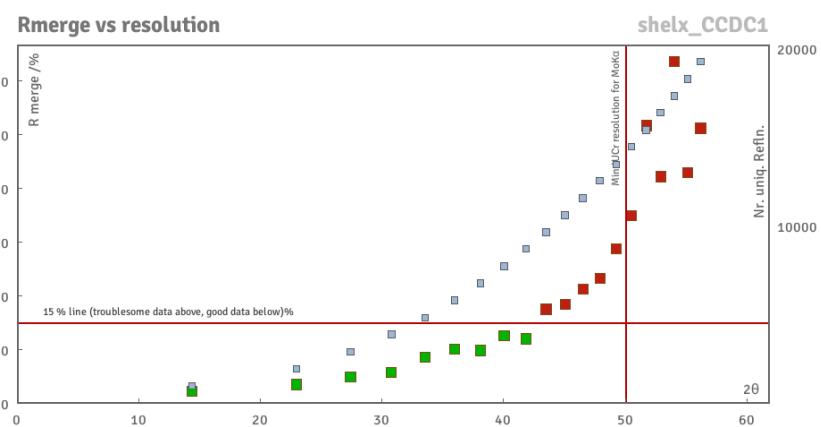
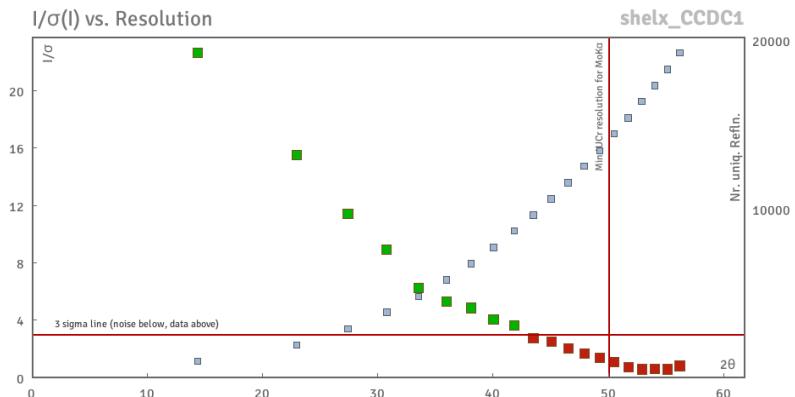
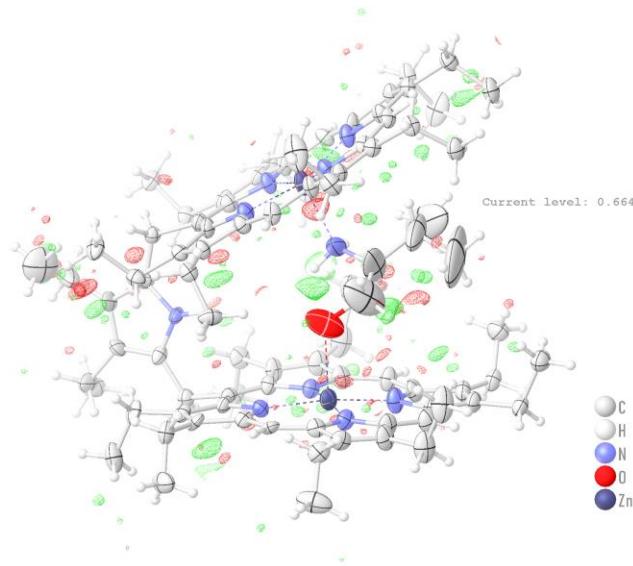
1•(S)-G1 (CCDC 2169150):

An exposure time of 12s at a scan width of 0.5° have been used for this data collection.



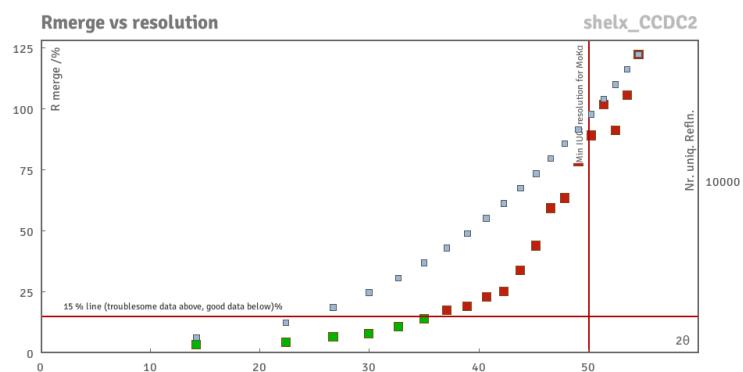
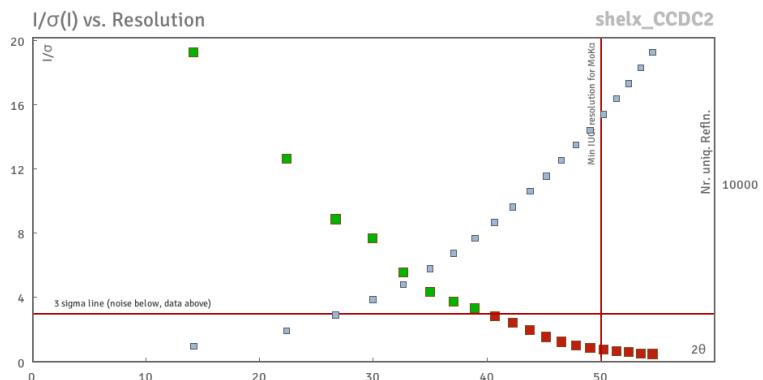
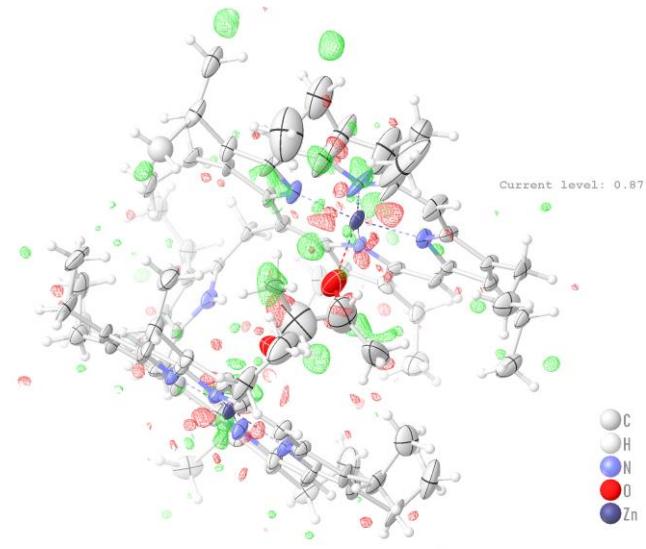
1•(S)-G3 (CCDC 2169151)

An exposure time of 18s at a scan width of 0.5° have been used for this data collection.



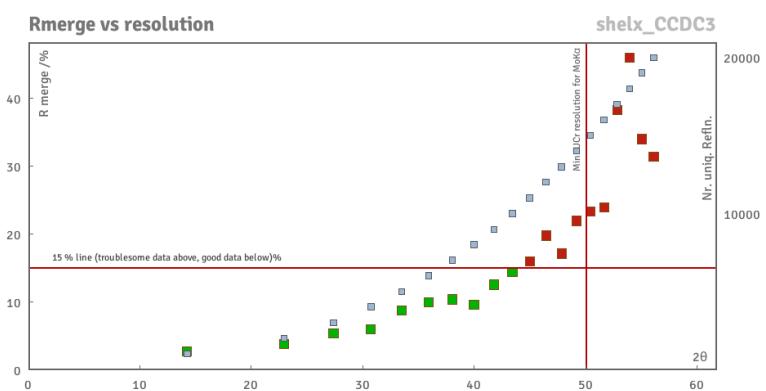
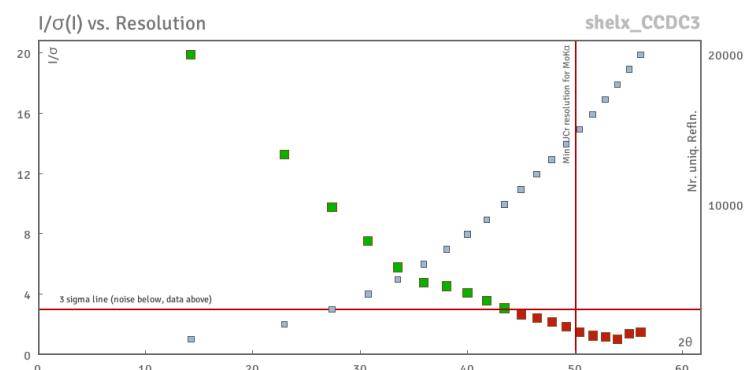
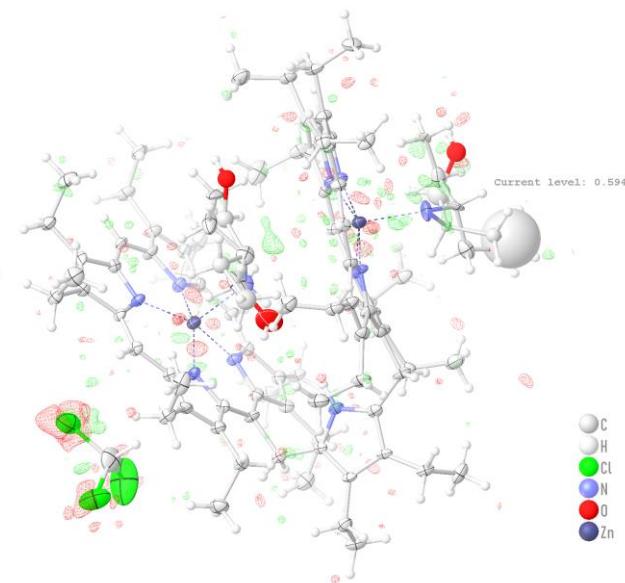
1•(R,R)-G7 (CCDC 2169152)

An exposure time of 15s at a scan width of 0.5° have been used for this data collection.



1•(S)-G2)₂(CCDC 2169153)

An exposure time of 15s at a scan width of 0.5° have been used for this data collection.



Cartesian coordinates

1•((S)-G2)2 (*endo–endo*) B3LYP functional

30	3.802850000	0.642146000	-0.932743000	1	9.175446000	-1.735819000	0.108735000	6	-1.773955000	-3.184019000	4.736631000
30	-3.222867000	-1.426777000	0.958588000	6	8.341895000	-3.007177000	1.653424000	6	-2.140406000	-2.078696000	3.847579000
7	2.470407000	1.489633000	-2.360015000	1	9.227300000	-3.652013000	1.699382000	6	-2.053796000	-0.719695000	4.155480000
7	4.632994000	-0.601664000	-2.434880000	1	7.593428000	-3.498902000	1.021864000	1	-1.654058000	-0.485765000	5.136110000
7	5.600215000	0.299635000	0.143536000	1	7.925781000	-2.925389000	2.663977000	6	-2.481108000	0.381452000	3.401465000
7	3.443420000	2.401480000	0.211458000	6	7.822297000	0.713037000	3.165280000	6	-2.501354000	1.741045000	3.915122000
7	-4.489208000	-0.240818000	-0.279121000	1	7.807447000	1.806045000	3.272615000	6	-2.994868000	2.552899000	2.912467000
7	-4.231600000	-3.181471000	0.296700000	1	8.881095000	0.426902000	3.135688000	6	-3.295800000	1.673471000	1.758837000
7	-2.684425000	-2.579667000	2.677011000	6	7.170687000	0.078894000	4.417263000	6	-3.904409000	2.047107000	0.525902000
7	-2.981647000	0.361192000	2.110417000	1	7.686518000	0.402327000	5.328869000	6	-6.382332000	2.783639000	-1.628446000
7	-1.408941000	3.854168000	-0.477474000	1	7.216377000	-1.014895000	4.367944000	1	-6.348846000	3.456890000	-0.767768000
1	-1.148592000	2.881262000	-0.520413000	1	6.116529000	0.367008000	4.501139000	1	-7.446495000	2.545067000	-1.756870000
6	1.581048000	2.553898000	-2.204345000	6	3.982700000	4.365823000	3.370506000	6	-5.922026000	3.532251000	-2.901310000
6	0.721186000	2.617333000	-3.423704000	1	5.077562000	4.460895000	3.360153000	1	-6.520836000	4.438430000	-3.050280000
6	1.183545000	1.637391000	-4.284000000	1	3.598429000	5.382812000	3.504765000	1	-6.041025000	2.898129000	-3.786236000
6	2.268830000	0.944526000	-3.611806000	6	3.575196000	3.517681000	4.599415000	1	-4.868179000	3.828714000	-2.850169000
6	2.996936000	-0.105817000	-4.198832000	1	3.957941000	3.969814000	5.521825000	6	-7.110290000	0.072099000	-2.960650000
1	2.704665000	-0.365959000	-5.209852000	1	3.972742000	2.499283000	4.529240000	1	-7.777054000	0.940453000	-3.012215000
6	4.081492000	-0.817682000	-3.681272000	1	2.485994000	3.443640000	4.683997000	1	-7.748618000	-0.780861000	-2.694501000
6	4.829356000	-1.863602000	-4.383700000	1	1.127860000	5.932768000	0.885734000	6	-6.510504000	-0.173989000	-4.366697000
6	5.846485000	-2.255703000	-3.538430000	1	2.171753000	6.102606000	2.266027000	1	-7.306377000	-0.328205000	-5.104561000
6	5.720738000	-1.449475000	-2.321080000	6	0.418728000	4.895980000	2.623255000	1	-5.864354000	-1.059094000	-4.372206000
6	6.595074000	-1.484909000	-1.231930000	1	-0.213522000	5.741248000	2.919213000	1	-5.905787000	0.681009000	-4.688662000
1	7.414342000	-2.193272000	-1.291150000	1	0.815438000	4.431905000	3.531564000	6	-6.301718000	-5.113018000	-2.197831000
6	6.554436000	-0.669754000	-0.095349000	1	-0.212851000	4.163574000	2.111793000	1	-7.157682000	-4.433564000	-2.308972000
6	7.536579000	-0.674712000	0.991820000	6	1.567063000	5.376300000	1.707594000	1	-6.725128000	-6.094038000	-1.949039000
6	7.158549000	0.317114000	1.874245000	6	0.858479000	4.779722000	-1.290199000	6	-5.568424000	-5.217604000	-3.556222000
6	5.944322000	0.925200000	1.325650000	1	1.463096000	5.573908000	-0.848008000	1	-6.254655000	-5.552489000	-4.342857000
6	5.247858000	1.998161000	1.879568000	1	0.883846000	5.014653000	-2.358276000	1	-4.740495000	-5.933081000	-3.497233000
1	5.651667000	2.389251000	2.806927000	6	-0.553318000	4.914878000	-0.772159000	1	-5.153904000	-4.248012000	-3.855223000
6	4.119353000	2.669403000	1.385740000	6	-1.264011000	6.091912000	-0.557074000	6	-4.831439000	-6.900421000	0.066516000
6	3.517755000	3.812333000	2.047496000	6	-2.585938000	5.727891000	-0.113069000	1	-5.728493000	-7.302359000	-0.420803000
6	2.478261000	4.255868000	1.250477000	6	-2.650433000	4.333633000	-0.071525000	1	-4.928860000	-7.150238000	1.131789000
6	2.444566000	3.360371000	0.057881000	6	-3.918598000	3.517188000	0.084561000	6	-3.588945000	-7.624400000	-0.504199000
6	1.613637000	3.460566000	-1.101581000	1	-4.372674000	3.532382000	-0.900145000	1	-3.664157000	-8.706491000	-0.345192000
6	-0.497426000	3.454432000	-3.774983000	1	-4.590563000	4.102860000	0.723857000	1	-2.670879000	-7.271294000	-0.021087000
1	-0.642393000	4.296741000	-3.106746000	6	-0.741991000	7.489271000	-0.781646000	1	-3.492268000	-7.442370000	-1.580370000
1	-0.350189000	3.884577000	-4.776273000	1	0.304859000	7.558805000	-0.451030000	6	-1.958657000	-5.766959000	4.561382000
6	-1.820005000	2.650879000	-3.781999000	1	-1.300184000	8.195483000	-0.153356000	1	-2.858386000	-6.351503000	4.326340000
1	-2.659656000	3.311396000	-4.028642000	6	-0.816018000	7.965587000	-2.251107000	1	-1.867515000	-5.780029000	5.654505000
1	-2.017992000	2.212229000	-2.797997000	1	-0.425890000	8.985743000	-2.352808000	6	-0.727327000	-6.476897000	3.949602000
1	-1.802072000	1.840991000	-4.515974000	1	-1.849645000	7.958525000	-2.614819000	1	-0.649134000	-7.505466000	4.320575000
6	0.735580000	1.360904000	-5.699613000	1	-0.228290000	7.312196000	-2.906435000	1	0.196703000	-5.948203000	4.209973000
1	0.127404000	2.199347000	-6.056648000	6	-3.703234000	6.686533000	0.217653000	1	-0.795921000	-6.512108000	2.856484000
1	1.622204000	1.339386000	-6.349972000	1	-4.345109000	6.259794000	1.001010000	6	-1.145055000	-3.035057000	6.095900000
6	-0.056784000	0.050659000	-5.923042000	1	-3.278892000	7.602648000	0.650607000	1	-1.344384000	-3.935706000	6.689333000
1	-0.338299000	-0.045145000	-6.978099000	6	-4.593838000	7.078866000	-0.983835000	1	-1.621812000	-2.205987000	6.636407000
1	-0.973888000	0.030383000	-5.325593000	1	-5.375829000	7.784231000	-0.676633000	6	0.382277000	-2.793279000	6.060039000
1	0.534336000	-0.830940000	-5.653570000	1	-5.082461000	6.198946000	-1.417692000	1	0.784461000	-2.704190000	7.075856000
6	4.501193000	-2.395826000	-5.752098000	1	-4.001151000	7.553091000	-1.774033000	1	0.623212000	-1.871313000	5.518418000
1	4.200069000	-1.571054000	-6.412044000	6	-4.614257000	1.144048000	-0.327037000	1	0.896343000	-3.622666000	5.560963000
6	3.384350000	-3.466951000	-5.747086000	6	-5.656540000	1.481525000	-1.336769000	6	-2.122803000	2.126633000	5.323296000
1	3.172043000	-3.811143000	-6.765964000	6	-6.068666000	0.285929000	1.893396000	1	-2.539257000	1.392326000	6.026021000
1	2.456793000	-3.067471000	-5.321087000	6	-5.342345000	-0.779536000	-1.226173000	1	-2.589351000	3.083001000	5.583573000
1	3.680310000	-4.334704000	-5.147000000	6	-5.555329000	-2.139426000	-1.489154000	6	-0.599110000	2.238079000	5.563617000
6	6.892824000	-3.310799000	-3.773174000	1	-6.234900000	-2.355206000	-2.306276000	1	-0.390800000	2.492348000	6.609456000
1	7.865721000	-2.958476000	-3.404327000	6	-5.067719000	-3.249582000	-0.799387000	1	-0.163967000	3.016596000	4.929304000
1	7.017733000	-3.468672000	-4.851586000	6	-5.422446000	-4.644770000	-1.070283000	1	-0.087980000	1.296379000	5.333712000
6	6.566177000	-4.668048000	-3.105705000	6	-4.794698000	-5.405915000	-0.105299000	6	-3.343463000	4.006152000	3.127928000
1	7.361618000	-5.396689000	-3.300850000	6	-4.058611000	-4.474931000	0.754025000	1	-2.714238000	4.397963000	3.935843000
1	5.625732000	-5.076255000	-3.492765000	6	-3.337359000	-4.826888000	1.898829000	1	-3.097306000	4.608933000	2.253646000
1	6.461769000	-4.558794000	-2.020294000	1	-3.299745000	-5.8833418000	2.141600000	6	-4.824989000	4.218415000	3.523048000
6	8.709480000	-1.611542000	1.095669000	6	-2.725419000	-3.957324000	2.807519000	1	-5.041023000	5.284788000	3.660435000
1	9.478428000	-1.165643000	1.738775000	6	-2.131269000	-4.349763000	4.086361000	1	-5.054393000	3.700136000	4.461500000

1	-5.505874000	3.828389000	2.757731000	1	-2.360730000	-2.270390000	-1.912997000	1	-0.586240000	-1.645396000	0.365562000
6	2.745517000	-1.390460000	1.335243000	6	-0.968157000	-3.714106000	-1.109478000	1	1.340332000	-0.563924000	2.759692000
1	3.574095000	-0.863403000	1.826675000	1	0.059611000	-3.717118000	-0.730484000	1	-0.713502000	-0.645771000	-2.780142000
6	1.653189000	-1.552784000	2.395627000	1	-1.617274000	-4.023594000	-0.284672000	6	3.920940000	-3.632011000	1.841762000
1	2.038543000	-2.121793000	3.249257000	6	3.275766000	-2.726689000	0.780980000	1	4.722087000	-3.108155000	2.378409000
6	-1.345489000	-2.270890000	-1.494651000	1	2.450704000	-3.258081000	0.291197000	1	3.190559000	-3.982852000	2.579925000
6	-0.433989000	-1.688567000	-2.576485000	1	4.013990000	-2.493338000	0.005047000	1	4.361245000	-4.518340000	1.371107000
1	-0.5511517000	-2.256976000	-3.506601000	1	-0.188567000	-2.409842000	2.464147000	6	-1.101221000	-4.718136000	-2.265420000
1	5.4028464000	-2.828959000	-6.202779000	7	2.289130000	-0.536361000	0.196684000	1	-0.385803000	-4.514351000	-3.070582000
8	0.953448000	-1.756307000	-2.120826000	1	1.730366000	-1.067105000	-0.486038000	1	-0.911325000	-5.736944000	-1.909333000
8	0.514021000	-2.248882000	1.800614000	7	-1.368353000	-1.413911000	-0.264534000	1	-2.110943000	4.699878000	-2.694080000
1	1.558652000	-1.385165000	-2.797941000	1	1.731858000	0.251293000	0.532790000	1	-1.311670000	-0.424336000	-0.511438000

1•((S)-G2)₂ (*exo–endo*) B3LYP functional

30	3.527184000	-0.149284000	-0.365407000	1	2.040671000	-4.949584000	-4.444046000	6	-2.672997000	7.238971000	0.525615000
30	-3.400638000	-0.985216000	0.401481000	1	1.532532000	-3.327084000	-4.873894000	1	-2.170962000	8.014377000	1.120672000
7	1.995896000	0.804630000	-1.457078000	6	0.075589000	-4.422327000	-3.702003000	1	-3.501321000	6.873137000	1.148184000
7	3.077805000	-1.982525000	-1.304075000	1	-0.448156000	-4.810172000	-4.583783000	6	-3.266781000	7.897908000	-0.741030000
7	-1.155347000	-1.050642000	0.185406000	1	-0.474673000	-3.547841000	-3.336722000	1	-3.960789000	8.704789000	-0.474840000
1	-1.028274000	-1.198854000	-0.817267000	1	0.042552000	-5.189240000	-2.919929000	1	-3.814234000	7.164525000	-1.344436000
1	-0.912998000	-0.080872000	0.401642000	6	3.627792000	-5.620787000	-2.142071000	1	-2.476510000	8.323843000	-1.369629000
7	4.567332000	-1.285969000	1.085605000	1	4.701198000	-5.705829000	-1.924716000	6	-2.047516000	4.761323000	0.144305000
7	3.352392000	1.454821000	1.010159000	1	3.498358000	-5.984687000	-3.169236000	6	-3.409670000	4.110027000	0.240861000
7	-0.875061000	4.063498000	-0.113692000	6	2.849551000	-6.553168000	-1.183903000	1	-4.030911000	4.442287000	-0.589550000
1	-0.815348000	3.063031000	-0.228200000	1	3.201747000	-7.587041000	-1.279342000	1	-3.923803000	4.499702000	1.116633000
7	-3.602106000	0.518730000	-1.097998000	1	1.777146000	-6.534958000	-1.408343000	6	-3.518768000	1.904484000	-0.969262000
7	-3.980581000	-2.461700000	-1.008911000	1	2.979018000	-6.243154000	-0.141096000	6	-3.542960000	2.497979000	-2.337185000
7	-4.046324000	-2.359601000	1.885206000	6	6.554460000	-4.253453000	2.290292000	6	-3.649857000	1.442556000	-3.223073000
7	-3.616488000	0.607202000	1.787802000	1	5.863215000	-5.070170000	2.041223000	6	-3.685746000	0.217951000	-2.443010000
7	5.371420000	0.753556000	-1.308303000	1	6.805904000	-4.382839000	3.350418000	6	-3.806844000	-1.057810000	-3.014587000
6	1.691703000	2.165582000	-1.442067000	6	7.842805000	-4.416332000	1.448764000	1	-3.824131000	-1.082776000	-4.098631000
6	0.967179000	2.487710000	-2.704417000	1	8.296081000	-5.400025000	1.618665000	6	-3.963483000	-2.288852000	-2.378671000
6	0.802511000	1.291629000	-3.380115000	1	8.579930000	-3.649660000	1.713095000	6	-4.192936000	-3.573443000	-0.346680000
6	1.456420000	0.254636000	-2.600099000	1	7.627915000	-4.319318000	0.378541000	6	-4.373663000	-4.508038000	-2.045352000
6	1.529990000	-1.092041000	-2.992058000	6	6.728093000	-1.612390000	4.158142000	6	-4.242147000	-3.797851000	-0.771213000
1	0.978090000	-1.351033000	-3.889315000	1	6.932159000	-2.588982000	4.614563000	6	-4.400205000	-4.365876000	0.496570000
6	2.254574000	-2.129548000	-2.403620000	1	6.125843000	-1.056149000	4.889536000	1	-4.627215000	-5.426174000	0.527970000
6	2.320909000	-3.509615000	-2.889734000	6	8.069414000	-0.869797000	3.948673000	6	-4.327898000	-3.704819000	1.726597000
6	3.207015000	-4.177463000	-2.068429000	1	8.597723000	-0.745730000	4.901269000	6	-4.552846000	-4.319012000	3.037265000
6	3.673581000	-3.209389000	-1.071536000	1	7.904271000	0.123980000	3.517222000	6	-4.406535000	-3.319072000	3.977208000
6	4.579675000	-3.475822000	-0.039536000	1	8.720730000	-1.427604000	3.266257000	6	-4.094760000	-2.093286000	3.239859000
1	4.981439000	-4.482708000	0.003433000	6	4.050008000	3.008802000	4.359978000	6	-3.891296000	-0.832889000	3.800488000
6	4.990819000	-2.594625000	0.968480000	1	3.940254000	4.083965000	4.543014000	1	-3.941210000	-0.783897000	4.882796000
6	5.870253000	-2.928138000	2.092028000	1	5.125437000	2.800759000	4.451328000	6	-3.667593000	0.390276000	3.151282000
6	5.942616000	-1.803044000	2.889470000	6	3.304599000	2.236498000	5.474695000	6	-3.502428000	1.649812000	3.852763000
6	5.107919000	-0.781777000	2.252094000	1	3.698933000	2.507907000	6.461123000	6	-3.372187000	2.642609000	2.901895000
6	4.820258000	0.483023000	2.767244000	1	3.417448000	1.154345000	5.347281000	6	-3.462521000	1.976351000	1.574209000
1	5.280029000	0.720152000	3.720983000	1	2.233449000	2.464081000	5.462118000	6	-3.440507000	2.583006000	0.283758000
6	3.968334000	1.469741000	2.246489000	6	1.982601000	4.605119000	2.644395000	6	-3.473781000	3.933826000	-2.818163000
6	3.596977000	2.678755000	2.960814000	1	1.800115000	5.347892000	1.870164000	1	-2.836160000	4.546160000	-2.178140000
6	2.743008000	3.397555000	2.142619000	1	2.592715000	5.108779000	3.404715000	1	-2.977091000	3.935269000	-3.796819000
6	2.620280000	2.630729000	0.875899000	6	0.620521000	4.233810000	3.277519000	6	-4.851600000	4.616765000	-2.999867000
6	1.967097000	3.018667000	-0.334721000	1	0.102158000	5.134718000	3.626225000	1	-4.725237000	5.650029000	-3.345009000
6	0.515041000	3.808000000	-3.292422000	1	0.755798000	3.563003000	4.133131000	1	-5.426743000	4.639308000	-2.066998000
1	-0.321718000	3.608685000	-3.972517000	1	-0.022951000	3.731594000	2.549355000	1	-5.455237000	4.083297000	-3.741584000
1	0.112052000	4.482167000	-2.536042000	6	1.617114000	4.500506000	-0.492930000	6	-3.763213000	1.493950000	-4.725013000
6	1.614867000	4.534926000	-4.105365000	1	2.309613000	5.088778000	0.112042000	1	-3.142133000	0.704978000	-5.170135000
1	1.233749000	5.482536000	-4.504416000	1	1.861834000	4.786091000	-1.519114000	1	-3.355463000	2.440062000	-5.099212000
1	1.947820000	3.919649000	-4.948348000	6	0.204871000	4.934039000	-0.175879000	6	-5.210990000	1.337803000	-5.250376000
1	2.497194000	4.756632000	-3.493281000	6	-0.286054000	6.219947000	0.044110000	1	-5.230171000	1.373646000	-6.346003000
6	0.124444000	1.050056000	-4.703280000	6	0.531951000	7.486844000	0.049752000	1	-5.854741000	2.138509000	-4.871095000
1	-0.602452000	1.845331000	-4.901938000	1	1.504230000	7.301845000	0.530154000	1	-5.645226000	0.383765000	-4.931876000
1	-0.460788000	0.122176000	-4.646602000	1	0.031377000	8.242965000	0.668996000	6	-4.280102000	-3.785086000	-4.531922000
6	1.094558000	0.952679000	-5.904898000	6	0.789942000	8.086730000	-1.352126000	1	-3.992984000	-4.816312000	-4.772298000
1	0.542933000	0.752826000	-6.831119000	1	1.385790000	9.005256000	-1.282456000	1	-3.551232000	-3.142983000	-5.044053000
1	1.822290000	0.146501000	-5.760191000	1	-0.1530690						

1	-6.431666000	-4.175643000	-4.660376000	6	-3.437641000	1.797806000	5.351384000	6	6.533263000	-1.275214000	-3.315845000
6	-4.624463000	-5.984506000	-2.198095000	1	-4.182732000	1.143707000	5.823211000	1	6.426784000	-2.116429000	-4.011043000
1	-5.070232000	-6.181160000	-3.180781000	1	-3.715211000	2.817043000	5.640249000	1	7.544150000	-0.870679000	-3.406547000
1	-5.366457000	-6.315746000	-1.459054000	6	-2.043799000	1.473727000	5.940014000	1	6.418118000	-1.679930000	-2.303260000
6	-3.347149000	-6.844534000	-2.046502000	1	-2.043734000	1.588928000	7.030265000	6	-0.233505000	-1.937724000	0.966491000
1	-3.579683000	-7.909761000	-2.161639000	1	-1.280984000	2.143842000	5.526322000	6	-0.604061000	-3.416504000	0.768363000
1	-2.889399000	-6.699040000	-1.061434000	1	-1.749796000	0.443465000	5.707403000	1	-1.613359000	-3.591307000	1.156896000
1	-2.603561000	-6.572004000	-2.804167000	6	-3.182747000	4.091313000	3.308788000	1	-0.647175000	-3.609824000	-0.312326000
6	-4.858968000	-5.773820000	3.269542000	1	-2.581854000	4.644860000	2.585584000	6	0.392203000	-4.396960000	1.411530000
1	-5.559961000	-6.133311000	2.504113000	1	-2.593214000	4.103300000	4.234200000	1	0.138632000	-5.4292211000	1.145312000
1	-5.374445000	-5.891515000	4.230959000	6	-4.507951000	4.841883000	3.590631000	1	0.385887000	-4.329945000	2.505497000
6	-3.604002000	-6.679251000	3.263010000	1	-4.307637000	5.875795000	3.896171000	1	1.415858000	-4.204508000	1.068400000
1	-3.881283000	-7.728516000	3.418108000	1	-5.068040000	4.351035000	4.394648000	6	-0.287313000	-1.492244000	2.423203000
1	-2.909330000	-6.387846000	4.058916000	1	-5.161011000	4.869461000	2.710605000	1	0.411413000	-2.079903000	3.028488000
1	-3.070609000	-6.603622000	2.308692000	8	7.894273000	1.374150000	-2.457297000	1	-1.301506000	-1.615240000	2.818925000
6	-4.516169000	-3.427376000	5.474143000	1	8.661221000	1.971681000	-2.556524000	8	0.100174000	-0.078957000	2.438005000
1	-5.143176000	-4.289293000	5.734895000	6	6.698755000	1.991033000	-3.025642000	1	-0.139560000	0.338185000	3.287531000
1	-5.033031000	-2.544957000	5.874870000	1	6.521666000	2.967982000	-2.552409000	1	4.605038000	1.657402000	-3.026526000
6	-3.149959000	-3.572179000	6.186506000	6	5.495803000	1.073404000	-2.761868000	1	6.178852000	0.210635000	-0.999792000
1	-3.283121000	-3.635590000	7.272838000	6	5.466585000	-0.208418000	-3.622277000	1	5.349362000	1.612988000	-0.754570000
1	-2.501509000	-2.715165000	5.971360000	1	4.472333000	-0.656697000	-3.514183000	1	6.815380000	2.151397000	-4.106015000
1	-2.630538000	-4.477212000	5.852028000	1	5.558278000	0.105098000	-4.671631000	1	0.795901000	-1.785682000	0.608946000

1•((S)-G2)2 (*exo-exo*) B3LYP functional

30	-3.507902000	-0.791175000	-0.427427000	1	-0.313797000	-3.666274000	-5.395086000	6	-0.214753000	-4.858801000	2.194659000
30	2.811411000	1.714144000	0.738742000	1	-0.576684000	-4.776056000	-4.046811000	1	0.154734000	-5.407075000	1.332330000
7	-1.836040000	-1.088894000	-1.675676000	6	-0.112955000	-0.462020000	-4.955390000	1	-0.634027000	-5.612408000	2.874546000
7	-3.931222000	1.039419000	-1.383961000	1	0.865502000	-0.897089000	-5.187894000	6	0.996893000	-4.195065000	2.889771000
7	4.886210000	2.574298000	1.313092000	1	0.055183000	0.620112000	-4.868058000	1	1.759778000	-4.946266000	3.126230000
1	4.869144000	2.394753000	2.318018000	6	-1.065483000	-0.720431000	-6.148034000	1	0.697667000	-3.704209000	3.821197000
1	5.469443000	1.862496000	0.870241000	1	-0.653935000	-0.292255000	-7.069766000	1	1.453594000	-3.441326000	2.241825000
7	-4.754984000	-0.112647000	1.145992000	1	-2.049356000	-0.271356000	-5.973291000	6	-0.098615000	-4.426043000	-0.934739000
7	-2.583817000	-2.172074000	0.889969000	1	-1.213545000	-1.793869000	-6.308468000	1	-0.598045000	-5.245863000	-0.410061000
7	2.216671000	-3.415501000	-0.445799000	6	-3.659419000	3.463560000	-4.260798000	1	-0.256491000	-4.659173000	-1.990769000
1	1.915514000	-2.452220000	-0.443626000	1	-4.547776000	3.986810000	-4.637795000	6	1.378721000	-4.508963000	-0.629773000
7	3.292028000	0.023531000	1.915021000	1	-3.355449000	2.771757000	-5.057800000	6	2.166079000	-5.655100000	-0.539937000
7	1.627546000	2.482056000	2.293147000	6	-2.530135000	4.496587000	-4.037914000	6	1.674401000	-7.074336000	-0.681247000
7	1.873994000	3.082037000	-0.542480000	1	-2.283677000	5.010531000	-4.974826000	1	0.712243000	-7.190783000	-0.159307000
7	3.523083000	0.607594000	-0.914921000	1	-1.623114000	4.011646000	-3.660964000	1	2.371955000	-7.754089000	-0.174351000
7	-4.996232000	-2.329440000	-1.174236000	1	-2.834071000	5.250505000	-3.303314000	6	1.492251000	-7.549261000	-2.141743000
6	-0.989508000	-2.195818000	-1.705323000	6	-5.979613000	4.121723000	-2.108080000	1	1.146280000	-8.589866000	-2.175476000
6	-0.224581000	-2.154102000	-2.984241000	1	-6.970348000	3.776830000	-1.781595000	1	2.435568000	-7.485917000	-2.695780000
6	-0.608585000	-0.9966856000	-3.636430000	1	-6.109799000	4.487961000	-3.134448000	1	0.755834000	-6.931211000	-2.668535000
6	-1.623827000	-0.351131000	-2.822336000	6	-5.543142000	5.303573000	-1.209550000	6	3.522099000	-5.232745000	-0.285126000
6	-2.292041000	0.824240000	-3.199077000	1	-6.286152000	6.109278000	-1.241007000	6	4.724620000	-6.129225000	-0.119628000
1	-1.953173000	1.276167000	-4.124681000	1	-4.581605000	5.711111000	-1.541241000	1	4.438903000	-7.027663000	0.445750000
6	-3.345004000	1.475390000	-2.555106000	1	-5.428891000	4.983671000	-0.167845000	1	5.482074000	-5.621782000	0.492619000
6	-4.020888000	2.688076000	-3.023432000	6	-7.615061000	1.864318000	2.603893000	6	5.385704000	-6.574305000	-1.444431000
6	-5.012753000	2.968513000	-2.105866000	1	-7.332058000	2.880883000	2.298222000	1	6.249047000	-7.223495000	-1.251827000
6	-4.943824000	1.929545000	-1.075869000	1	-7.785131000	1.910627000	3.686858000	1	5.732260000	-5.709092000	-2.020658000
6	-5.762492000	1.850874000	0.055192000	6	-8.943369000	1.484953000	1.906971000	1	4.678303000	-7.129404000	-2.070620000
1	-6.523891000	2.617355000	0.155333000	1	-9.728427000	2.212547000	2.144456000	6	3.522238000	-3.838811000	-0.231930000
6	-5.673773000	0.917563000	1.094154000	1	-9.284604000	0.495365000	2.231825000	6	4.708942000	-2.912557000	-0.034065000
6	-6.487917000	0.911545000	2.311632000	1	-8.822127000	1.456532000	0.818144000	1	5.357109000	-2.999815000	-0.901131000
6	-6.025481000	-0.127191000	3.095300000	6	-6.529168000	-0.570942000	4.441932000	1	5.292193000	-3.310427000	0.791038000
6	-4.931044000	-0.756972000	2.353879000	1	-7.045269000	0.263029000	4.933995000	6	4.069866000	-1.072886000	1.564658000
6	-4.140123000	-1.815662000	2.800931000	1	-5.680251000	-0.826101000	5.090873000	6	4.525014000	-1.734803000	2.814829000
1	-4.384189000	-2.204303000	3.783744000	6	-7.489970000	-1.782080000	4.377339000	6	3.939664000	-1.047342000	3.863030000
6	-3.051368000	-2.430772000	2.165328000	1	-7.819136000	-2.070982000	5.382476000	6	3.158867000	0.035775000	3.291196000
6	-2.255686000	-3.482221000	2.771360000	1	-7.000733000	-2.647596000	3.916220000	6	2.383992000	0.933084000	4.042213000
6	-1.308936000	-3.875327000	1.842497000	1	-8.378712000	-1.543112000	3.782090000	1	2.345101000	0.737814000	5.108534000
6	-1.533892000	-3.048576000	0.626869000	6	-2.450837000	-3.988148000	4.178065000	6	1.643712000	2.030134000	3.597773000
6	-0.875030000	-3.136610000	-0.639165000	1	-1.953140000	-4.957374000	4.297162000	6	0.792369000	2.887442000	4.425219000
6	0.788538000	-3.108019000	-3.582091000	1	-3.519876000	-4.178279000	4.352094000	6	0.265040000	3.848987000	3.587885000
1	1.517321000	-2.516980000	-4.151284000	6	-1.939287000	-3.029167000	5.280287000	6	0.803673000	3.588817000	2.250681000
1	1.373491000	-3.618147000	-2.818280000	1	-2.123713000						

6	0.764712000	4.953671000	-1.363252000	1	-1.225528000	4.723127000	4.847980000	1	4.309115000	-2.732112000	-4.343046000
6	1.438155000	4.379916000	-2.423316000	1	-1.392789000	5.137132000	3.154444000	1	4.362550000	-3.622320000	-2.816761000
6	2.123530000	3.198022000	-1.895001000	6	0.091490000	6.319207000	4.205474000	8	-7.164611000	-3.860669000	-2.190173000
6	2.910426000	2.309071000	-2.629230000	1	-0.617096000	7.117895000	4.454341000	1	-7.709319000	-4.672129000	-2.190361000
1	3.021822000	2.537058000	-3.683677000	1	0.658041000	6.628952000	3.319889000	6	-5.816459000	-4.159793000	-2.666361000
6	3.552301000	1.136823000	-2.193275000	1	0.798720000	6.217875000	5.036743000	1	-5.370636000	-4.953688000	-2.049457000
6	4.331638000	0.267262000	-3.057192000	6	-0.068648000	6.206274000	-1.360836000	6	-4.958799000	-2.890324000	-2.557684000
6	4.742825000	-0.814336000	-2.301367000	1	-0.955034000	6.061990000	-0.728874000	6	-5.281373000	-1.806813000	-3.609794000
6	4.200065000	-0.611795000	-0.932204000	1	-0.446944000	6.397088000	-2.372542000	1	-4.478939000	-1.061468000	-3.573707000
6	4.347239000	-1.450420000	0.213837000	6	0.697663000	7.458188000	-0.870718000	1	-5.219619000	-2.286888000	-4.596560000
6	5.575415000	-2.803785000	3.040105000	1	0.046582000	8.340159000	-0.880672000	6	-6.638404000	-1.092772000	-3.477090000
1	6.307396000	-2.806412000	2.226168000	1	1.561085000	7.663060000	-1.513839000	1	-6.761856000	-0.373943000	-4.295857000
1	6.151773000	-2.521029000	3.931420000	1	1.067032000	7.318235000	0.151583000	1	-7.468937000	-1.802114000	-3.504142000
6	5.030539000	-4.232236000	3.267549000	6	1.510850000	4.857936000	-3.848448000	1	-6.705245000	-0.526361000	-2.540629000
1	5.855615000	-4.945182000	3.384167000	1	0.639602000	5.486773000	-4.069231000	6	5.447179000	3.928413000	1.025074000
1	4.401605000	-4.562728000	2.435542000	1	1.445320000	4.000342000	-4.531872000	6	4.636855000	5.004436000	1.769143000
1	4.421260000	-4.270550000	4.177090000	6	2.796328000	5.657211000	-4.169953000	1	3.610678000	5.011350000	1.380760000
6	4.084990000	-1.309750000	5.339369000	1	2.804660000	5.972455000	-5.219928000	1	4.567147000	4.710216000	2.825974000
1	4.182337000	-0.357068000	5.877165000	1	3.692211000	5.052663000	-3.988231000	6	5.249715000	6.412807000	1.683222000
1	5.015111000	-1.858627000	5.529693000	1	2.864348000	6.553885000	-5.3453585000	1	4.681982000	7.116345000	2.301881000
6	2.907927000	-2.107395000	5.951649000	6	4.691389000	0.580809000	-4.487082000	1	5.246078000	6.800269000	0.658178000
1	3.065118000	-2.263391000	7.025442000	1	3.835212000	1.048694000	-4.989721000	1	6.287188000	6.415691000	2.040143000
1	2.809289000	-3.087332000	5.472698000	1	4.887341000	-0.345435000	-5.038866000	6	5.456526000	4.146231000	-0.491355000
1	1.958756000	-1.576599000	5.818557000	6	5.920603000	1.513438000	-4.613484000	1	6.018515000	5.051008000	-0.733893000
6	0.515305000	2.686757000	5.891118000	1	6.104921000	1.776632000	-5.661448000	1	4.432289000	4.254043000	-0.862004000
1	0.217483000	3.641186000	6.342419000	1	6.821038000	1.026828000	-4.220956000	8	6.133638000	3.043785000	-1.179561000
1	1.435991000	2.383054000	6.407957000	1	5.773385000	2.439010000	-4.045610000	1	5.468677000	2.402560000	-1.504869000
6	-0.585863000	1.635554000	6.168420000	6	5.677725000	-1.857769000	-2.882514000	1	-3.922865000	-3.207304000	-2.732734000
1	-0.746732000	1.516789000	7.246494000	1	6.404820000	-2.201052000	-2.139373000	1	-5.938080000	-2.004982000	-0.952767000
1	-0.311242000	0.659889000	5.752172000	1	6.282224000	-1.365481000	-3.654210000	1	-4.749877000	-3.049331000	-0.491134000
1	-1.534409000	1.937533000	5.710476000	6	4.971431000	-3.067368000	-3.536456000	1	-5.836304000	-4.508321000	-3.707907000
6	-0.652124000	4.986303000	3.950915000	1	5.708111000	-3.756250000	-3.967159000	1	6.491544000	3.971727000	1.376618000

1•((R,R)-G7)₂ (*endo–endo*) B3LYP functional

30	3.872251000	0.530306000	-0.879712000	6	2.569774000	3.934063000	1.538227000	1	8.996025000	-4.165478000	1.677101000
30	-3.370078000	-1.569863000	0.898009000	6	2.572068000	3.179809000	0.252302000	1	7.346896000	-3.899809000	1.075591000
8	2.543745000	-0.822954000	0.167115000	6	1.802899000	3.444541000	-0.923939000	1	7.806262000	-3.311298000	2.681004000
8	-1.499491000	-1.654416000	-0.122554000	6	0.701460000	4.351207000	-4.049007000	6	7.987955000	0.310095000	3.100885000
7	2.542460000	1.488559000	-2.281016000	1	1.126224000	5.265756000	-3.623257000	1	8.042014000	1.402752000	3.198508000
7	4.532035000	-0.782093000	-2.385938000	1	0.941741000	4.416654000	-5.116289000	1	9.026033000	-0.038034000	3.027748000
7	5.633531000	0.037327000	0.166959000	6	-0.838589000	4.376336000	-3.918541000	6	7.356363000	-0.276650000	4.385884000
7	3.607666000	2.247730000	0.304321000	1	-1.242348000	5.295384000	-4.359652000	1	7.929400000	0.022091000	5.271453000
7	-4.505897000	-0.375400000	-0.408395000	1	-1.161944000	4.328732000	-2.876085000	1	7.335862000	-1.371500000	3.435029000
7	-4.173503000	-3.320256000	0.024642000	1	-1.280627000	3.525268000	-4.449072000	1	6.325320000	0.072855000	4.512964000
7	-2.836272000	-2.791532000	2.549525000	6	1.447254000	1.952987000	-5.847836000	6	4.137087000	3.944487000	3.615924000
7	-3.214373000	0.144125000	2.119920000	1	1.323822000	2.946277000	-6.292929000	1	5.233223000	4.017687000	3.604559000
7	-1.336434000	3.698369000	-0.299318000	1	2.319659000	1.513393000	-6.347444000	1	3.770704400	4.960565000	3.811946000
1	-1.091260000	2.730786000	-0.443470000	6	0.197943000	1.104995000	-6.186272000	6	3.716252000	3.034538000	4.794321000
6	1.892866000	2.729236000	-2.159698000	1	0.060351000	1.037416000	-7.271758000	1	4.123482000	3.413932000	5.738993000
6	1.383445000	3.105960000	-3.509137000	1	-0.705940000	1.549097000	-5.755393000	1	4.081880000	2.011270000	4.652638000
6	1.723858000	2.071883000	-4.369642000	1	0.291069000	0.086712000	-5.791426000	1	2.626100000	2.990547000	4.888094000
6	2.456374000	1.085803000	-3.609020000	6	4.123187000	-2.616393000	-5.655353000	1	1.152866000	5.593710000	1.419681000
6	3.009686000	-0.074552000	-4.172098000	1	3.956560000	-1.771970000	-6.338329000	1	2.098133000	5.517141000	2.879017000
1	2.721551000	-0.278330000	-5.197340000	6	2.847070000	-3.490815000	-5.622295000	6	0.401432000	4.185212000	2.857587000
6	3.944516000	-0.949021000	-3.622759000	1	2.580675000	-3.827714000	-6.631008000	1	-0.282217000	4.922278000	3.295273000
6	4.536585000	-2.104051000	-4.302925000	1	1.998671000	-2.930890000	-5.212549000	1	0.771482000	3.539032000	3.660343000
6	5.501043000	-2.608221000	-3.456179000	1	2.998090000	-4.375879000	-4.994199000	1	-0.171635000	3.567577000	2.160653000
6	5.503408000	-1.757167000	-2.262427000	6	6.389365000	-3.803530000	-3.667504000	6	1.572188000	4.898220000	2.141566000
6	6.405257000	-1.858549000	-1.198994000	1	7.410362000	-3.573770000	-3.333387000	6	0.974397000	4.729737000	-0.924784000
1	7.142423000	-2.651761000	-1.263393000	1	6.464481000	-4.019805000	-4.740349000	1	1.536344000	5.492492000	-0.380486000
6	6.492288000	-1.012971000	-0.088097000	6	5.897619000	-5.074663000	-2.934951000	1	0.957434000	5.105788000	-1.941005000
6	7.511686000	-1.081309000	0.962482000	1	6.581834000	-5.913109000	-3.110479000	6	-0.451653000	4.769601000	-0.414663000
6	7.246457000	-0.051960000	1.842526000	1	4.901561000	-5.365508000	-3.287158000	6	-1.156686000	5.926233000	-0.093055000
6	6.061046000	0.640641000	1.332043000	1	5.833140000	-4.905522000	-1.854196000	6	-2.506060000	5.540128000	0.231219000
6	5.426921000	1.730702000	1.925136000	6	8.610547000	-2.106480000	1.037593000	6	-2.592397000	4.152922000	0.106724000
1	5.860754000	2.079475000	2.855780000	1	9.4445670						

6	-0.609545000	7.332392000	-0.118435000	1	-5.489595000	2.843078000	-4.035661000	1	-0.842416000	2.902981000	5.288715000
1	0.419229000	7.344984000	0.270384000	1	-4.402089000	3.687924000	-2.930598000	1	-0.624352000	1.182012000	5.638150000
1	-1.191770000	7.962878000	0.566129000	6	-6.790837000	0.030489000	-3.365795000	6	-3.696225000	3.745948000	3.215095000
6	-0.605149000	7.994539000	-1.516075000	1	-7.436190000	0.910003000	-3.473132000	1	-3.181938000	4.101670000	4.115862000
1	-0.205932000	9.015073000	-1.464815000	1	-7.465861000	-0.817554000	-3.189303000	1	-3.330130000	4.377682000	2.406416000
1	-1.618176000	8.045732000	-1.930079000	6	-6.042939000	-0.198291000	-4.701957000	6	-5.217421000	3.953003000	3.412431000
1	0.012717000	7.426426000	-2.221191000	1	-6.753912000	-0.320256000	-5.527517000	1	-5.450332000	5.014287000	3.561940000
6	-3.632566000	6.484208000	0.574992000	1	-5.416734000	-1.096366000	-4.655940000	1	-5.572984000	3.399274000	4.289225000
1	-4.327403000	6.008600000	1.280231000	1	-5.390153000	0.650181000	-4.934713000	1	-5.787357000	3.596437000	2.546834000
1	-3.227556000	7.356813000	1.104894000	6	-5.865892000	-5.197067000	-2.774507000	6	2.694230000	-1.467104000	1.471883000
6	-4.443568000	6.981399000	-0.644317000	1	-6.761515000	-4.576305000	-2.912798000	1	3.536313000	-0.942778000	1.933098000
1	-5.236770000	7.671723000	-0.331437000	1	-6.228760000	-6.223258000	-2.635437000	6	1.465329000	-1.220600000	2.359793000
1	-4.912344000	6.143807000	-1.174046000	6	-5.014539000	-5.140752000	-4.065414000	1	1.677288000	-1.676712000	3.336069000
1	-3.799250000	7.505914000	-1.358442000	1	-5.601384000	-5.464871000	-4.932902000	6	-1.242792000	-2.106969000	-1.489449000
6	-4.591094000	1.011325000	-0.446816000	1	-4.138012000	-5.793106000	-3.981902000	6	-0.567526000	-0.974912000	-2.276584000
6	-5.497204000	1.386907000	-1.568883000	1	-4.656876000	-4.122318000	-4.255778000	1	-0.249597000	-1.373892000	-3.251100000
6	-5.874501000	0.207869000	-2.183344000	6	-4.389614000	-7.039592000	-0.558752000	1	4.941832000	-3.200784000	-6.093432000
6	-5.247466000	-0.883464000	-1.458290000	1	-5.210442000	-7.479416000	-1.138938000	1	1.695861000	-1.026091000	-0.321080000
6	-5.406750000	-2.234547000	-1.796588000	1	-4.524701000	-7.394030000	0.472177000	8	0.623049000	-0.604636000	-1.509819000
1	-6.003154000	-2.427407000	-2.681588000	6	-3.047155000	-7.584294000	-1.102413000	8	0.328754000	-1.956097000	1.763775000
6	-4.915481000	-3.362397000	-1.137142000	1	-3.018844000	-8.678650000	-1.042171000	6	-1.4671183000	0.240863000	-2.479540000
6	-5.123233000	-4.754460000	-1.543096000	1	-2.200986000	-7.188561000	-0.529167000	1	-1.834841000	0.600385000	-1.515408000
6	-4.492857000	-5.539222000	-0.599153000	1	-2.905651000	-7.295711000	-2.150133000	1	-0.921936000	1.045738000	-2.984430000
6	-3.907455000	-4.626790000	0.387500000	6	-1.964204000	-6.049736000	4.235938000	1	-2.333606000	-0.019829000	-3.097720000
6	-3.237879000	-5.010874000	1.5533597000	1	-2.785659000	-6.684943000	3.878031000	1	1.102253000	0.175095000	-1.880115000
1	-3.122843000	-6.077445000	1.715473000	1	-1.962987000	-6.146114000	5.328902000	1	-2.232643000	-2.282635000	-1.918986000
6	-2.768355000	-4.173076000	2.571348000	6	-0.628244000	-6.601686000	3.684306000	6	-0.442339000	-3.410455000	-1.482437000
6	-2.225171000	-4.617573000	3.855678000	1	-0.487899000	-7.647614000	3.981467000	1	-0.326202000	-3.791799000	-2.503391000
6	-2.005345000	-3.482687000	4.612763000	1	0.219528000	-6.021514000	4.066075000	1	0.555833000	-3.257076000	-1.061743000
6	-2.404261000	-2.342481000	3.785548000	1	-0.602943000	-6.550220000	2.589881000	1	-0.962945000	-4.166189000	-0.887403000
6	-2.432383000	-1.003729000	4.185472000	6	-1.452671000	-3.390733000	6.009195000	6	3.036954000	-2.947275000	1.301614000
1	-2.123442000	-0.808673000	5.206878000	1	-1.607130000	-4.345248000	6.527447000	6	1.103204000	0.250490000	2.527877000
6	-2.843752000	0.118420000	3.453613000	1	-2.013547000	-2.640836000	6.583741000	1	0.876139000	0.696556000	1.556922000
6	-2.938965000	1.456644000	4.012059000	6	0.052204000	-3.035403000	6.061917000	1	0.228091000	0.359457000	3.175923000
6	-3.323766000	2.301851000	2.989982000	1	0.403943000	-2.985060000	7.098957000	1	1.936470000	0.805422000	2.971685000
6	-3.494675000	1.646505000	1.780949000	1	0.243134000	-2.063412000	5.591776000	1	3.927278000	-3.050965000	0.675244000
6	-3.959406000	1.879398000	0.498044000	1	0.649135000	-3.788574000	5.534914000	1	3.241087000	-3.408221000	2.275598000
6	-6.125669000	2.716883000	-1.945870000	6	-2.724679000	1.798959000	5.465434000	1	2.206932000	-3.486170000	0.836370000
1	-6.192267000	3.381978000	-1.080592000	1	-3.118621000	0.987940000	6.092031000	1	-0.672111000	-1.633478000	0.436923000
1	-7.167838000	2.521378000	-2.231344000	1	-3.314389000	2.685600000	5.725680000	1	-0.351775000	-2.166432000	2.437208000
6	-5.454833000	3.455729000	-3.128560000	6	-1.249671000	2.056682000	5.851278000				
1	-5.974910000	4.398368000	-3.336404000	1	-1.164025000	2.282677000	6.920900000				

1•((R,R)-G7)₂ (*exo–endo*) B3LYP functional

30	-3.636770000	-1.067988000	-0.395856000	1	-7.122624000	1.926244000	-0.317448000	1	1.284068000	0.271331000	-4.635943000
30	3.029455000	2.137897000	0.362893000	6	-6.073462000	0.500353000	0.847327000	1	-0.257009000	1.106392000	-4.852576000
7	-1.934118000	-1.319127000	-1.607962000	6	-6.902832000	0.553237000	2.051514000	6	-4.365405000	2.459610000	-4.849124000
7	-4.312161000	0.514784000	-1.617443000	6	-6.340300000	-0.319082000	2.962782000	1	-5.301125000	2.860986000	-5.258582000
1	1.097661000	0.727321000	-0.875570000	6	-5.166157000	-0.902888000	2.314385000	1	-4.033645000	1.686423000	-5.555649000
7	-5.042790000	-0.402773000	1.032698000	6	-4.265201000	-1.794089000	2.897972000	6	-3.310342000	3.591252000	-4.816819000
7	-2.594347000	-2.118131000	1.083732000	1	-4.495752000	-2.104276000	3.911344000	1	-3.148783000	4.000552000	-5.821067000
7	2.395960000	-3.125423000	-0.167649000	6	-3.079666000	-2.315107000	2.363373000	1	-2.349998000	3.222848000	-4.438494000
1	2.038081000	-2.186732000	-0.253600000	6	-2.171232000	-3.172338000	3.104187000	1	-3.635673000	4.407564000	-4.162249000
7	3.977712000	1.041442000	-1.161749000	6	-1.135272000	-3.508031000	2.254684000	6	-6.751768000	3.147931000	-2.775610000
7	2.780586000	3.760100000	-0.955188000	6	-1.431269000	-2.868374000	0.945020000	1	-7.690973000	2.737248000	-2.380087000
7	2.691252000	3.483752000	1.935732000	6	-0.736572000	-3.050306000	-0.290145000	1	-6.928970000	3.332774000	-3.842679000
7	3.822206000	0.733129000	1.721293000	6	0.965074000	-3.218680000	-3.240291000	6	-6.464609000	4.498786000	-2.077530000
6	-0.937957000	-2.289881000	-1.480700000	1	1.203094000	-4.010690000	-2.537743000	1	-7.300730000	5.193973000	-2.218047000
6	-0.191257000	-2.352367000	-2.770386000	1	0.654383000	-3.723322000	-4.168004000	1	-5.560408000	4.963375000	-2.486074000
6	-0.765749000	-1.408760000	-3.604342000	6	2.277207000	-2.452899000	-3.525987000	1	-6.311722000	4.360828000	-1.001164000
6	-1.850446000	-0.778834000	-2.877401000	1	3.069030000	-3.161038000	-3.796658000	6	-8.104084000	1.440830000	2.236144000
6	-2.690129000	0.198324000	-3.431512000	1	2.613178000	-1.899452000	-2.644895000	1	-8.762592000	1.010638000	3.001447000
1	-2.451132000	0.498086000	-4.445610000	1	2.171798000	-1.740892000	-4.348376000	1	-8.693761000	1.466384000	1.309429000
6	-3.802909000	0.818070000	-2.864034000	6	-0.402698000	-1.078401000	-5.030405000	6	-7.750810000	2.891551000	2.642142000
6	-4.630647000	1.843200000	-3.502639000	1	-1.318111000	-1.044607000	-5.638235000	1	-8.658994000	3.495810000	2.752785000
6	-5.646980000	2.138576000	-2.617077000	1	0.204789000	-1.885412000	-5.454408000	1	-7.113367000	3.366718000	

1	-6.651094000	-1.671116000	4.595944000	6	2.044426000	5.758952000	-1.888815000	1	3.276801000	3.948612000	5.975209000
1	-7.863695000	-0.411749000	4.460059000	6	2.206961000	4.980967000	-0.659049000	6	1.132328000	3.739657000	6.216194000
6	-6.042796000	0.229346000	5.441901000	6	1.908267000	5.427023000	0.633709000	1	1.180676000	3.799047000	7.309930000
1	-6.395279000	-0.027427000	6.447844000	1	1.486332000	6.4223108000	0.714756000	1	1.072449000	2.683118000	5.932324000
1	-6.207440000	1.301137000	5.284874000	6	2.156741000	4.756587000	1.835091000	1	0.207213000	4.226587000	5.887866000
1	-4.962866000	0.048335000	5.400995000	6	1.945442000	5.306239000	3.175486000	6	4.456413000	-0.508369000	5.215142000
6	-2.353861000	-3.551111000	4.551211000	6	2.379236000	4.351386000	4.072700000	1	4.779764000	0.431677000	5.680968000
1	-1.784797000	-4.461774000	4.771840000	6	2.845631000	3.210974000	3.281903000	1	5.252210000	-1.232080000	5.426423000
1	-3.407213000	-3.809708000	4.729698000	6	3.367000000	2.022679000	3.794357000	6	3.149334000	-0.982457000	5.893812000
6	-1.938717000	-2.449798000	5.555486000	1	3.427125000	1.959745000	4.875200000	1	3.274841000	-1.041630000	6.981536000
1	-2.112365000	-2.782316000	6.586021000	6	3.811002000	0.892202000	3.096017000	1	2.857408000	-1.972495000	5.527660000
1	-2.511768000	-1.530770000	5.390626000	6	4.318927000	-0.312858000	3.727467000	1	2.324795000	-0.294972000	5.675741000
1	-0.878047000	-2.201325000	5.448918000	6	4.613967000	-1.215617000	2.724166000	6	5.232389000	-2.565948000	2.999091000
6	0.102832000	-4.222755000	2.744612000	6	4.323125000	-0.539730000	1.440194000	1	4.834352000	-3.326917000	2.325116000
1	0.533055000	-4.891279000	2.001353000	6	4.605054000	-0.999756000	0.126546000	1	4.927792000	-2.883342000	4.003759000
1	-0.179281000	-4.858553000	3.593477000	6	6.583284000	-1.360025000	-2.520153000	6	6.779454000	-2.555924000	2.951983000
6	1.210585000	-3.249400000	3.210759000	1	7.408358000	-0.784492000	-2.963175000	1	7.180954000	-3.555862000	3.155962000
1	2.084090000	-3.809743000	3.565283000	1	6.979721000	-1.738882000	-1.572976000	1	7.182930000	-1.866341000	3.702430000
1	0.855290000	-2.604191000	4.019447000	6	6.283292000	-2.542183000	-3.470216000	1	7.154201000	-2.230493000	1.974859000
1	1.530087000	-2.599558000	2.393020000	1	7.176957000	-3.164823000	-3.596885000	6	4.842216000	-3.521905000	-2.347898000
6	0.120242000	-4.319646000	-0.398823000	1	5.980681000	-2.181938000	-4.459168000	6	-5.885197000	-3.073192000	-3.370910000
1	-0.305828000	-5.059795000	0.283333000	1	5.476812000	-3.180704000	-3.093019000	1	-6.902592000	-3.291205000	-0.022310000
1	-0.079676000	-4.743037000	-1.389572000	6	5.703396000	0.898003000	-4.502655000	6	-0.310039000	1.213172000	0.547415000
6	1.611701000	-4.273657000	-0.163485000	1	6.658942000	0.370342000	-4.609645000	6	-1.009188000	2.398394000	-0.108805000
6	2.462969000	-5.355288000	0.050188000	1	5.933389000	1.965102000	-4.621315000	1	-0.519945000	3.339793000	0.163219000
6	2.044120000	-6.802439000	0.120170000	6	4.765523000	0.459735000	-5.653219000	6	-0.171837000	1.313021000	2.069491000
1	1.092772000	-6.890840000	0.666022000	1	5.227116000	0.662381000	-6.626823000	1	0.373328000	2.235504000	2.308971000
1	2.778557000	-7.368223000	0.708325000	1	3.810150000	0.994785000	-5.611682000	1	-3.829325000	-3.335626000	-2.711481000
6	1.879626000	-7.486016000	-1.257230000	1	4.547591000	-0.612178000	-5.593127000	1	-5.761840000	-2.808177000	-0.651419000
1	1.580986000	-8.535457000	-1.142327000	6	2.619986000	5.325244000	-4.381680000	1	-0.811711000	0.272645000	0.297921000
1	2.818050000	-7.458771000	-1.822376000	1	3.587091000	5.008877000	-4.796424000	8	-4.935280000	-2.661429000	-1.150747000
1	1.114878000	-6.980980000	-1.858839000	1	2.576880000	6.413627000	-4.512886000	8	1.087180000	1.103971000	0.025169000
6	3.803054000	-4.837095000	0.179737000	6	1.485508000	4.676961000	-5.210417000	6	-4.952984000	-4.996730000	-1.945781000
6	5.058261000	-5.649679000	0.378456000	1	1.578410000	4.941108000	-6.270463000	1	-5.894417000	-5.137282000	-1.388922000
1	4.830642000	-6.531292000	0.993377000	1	0.504349000	5.014621000	-4.857736000	1	-2.094662000	0.413571000	2.508174000
1	5.793216000	-5.068792000	0.952753000	1	1.513122000	3.584592000	-5.125850000	1	1.451180000	0.140722000	2.124022000
6	5.726768000	-6.123142000	-0.932884000	6	1.423378000	7.126696000	-1.971438000	1	-0.987176000	2.298483000	-1.198966000
1	6.629241000	-6.711030000	-0.723765000	1	1.774896000	7.635667000	-2.877642000	1	-2.060058000	2.443721000	0.193823000
1	6.014701000	-5.269618000	-1.557558000	1	1.765184000	7.742029000	-1.127915000	6	-1.514573000	1.297429000	2.790616000
1	5.043016000	-6.747611000	-1.518769000	6	-0.123731000	7.105040000	-1.979420000	8	0.579455000	0.165234000	2.572545000
6	3.732332000	-3.451685000	0.041685000	1	-0.526357000	8.123487000	-2.031388000	1	-1.339090000	1.262968000	3.869843000
6	4.889427000	-2.484029000	-0.112656000	1	-0.514963000	6.628329000	-1.073573000	1	-2.099087000	2.194761000	2.565303000
1	5.230942000	-2.592844000	-1.137601000	1	-0.500630000	6.543101000	-2.841434000	1	-5.799197000	-1.995056000	-3.529237000
1	5.714410000	-2.843037000	0.508424000	6	1.351590000	6.656687000	-3.471733000	1	-5.739250000	-3.572862000	-4.333114000
6	4.655088000	-1.636484000	-1.032950000	1	1.758512000	7.402935000	-2.775719000	8	-3.817063000	-5.256345000	-1.063696000
6	5.440127000	-0.393250000	-2.268216000	1	1.658392000	6.980133000	-4.474317000	6	-4.918507000	-5.954130000	-3.141479000
6	5.138387000	0.647143000	-3.129035000	6	-0.193195000	6.686868000	3.389525000	1	-5.798442000	-5.839221000	-3.781416000
6	4.223065000	1.533446000	-2.434504000	1	-0.573647000	7.691704000	3.607525000	1	-4.018207000	-5.783287000	-3.741595000
6	3.712659000	2.722207000	-2.973527000	1	-0.635117000	5.989728000	4.110074000	1	-4.899874000	-6.990775000	-2.786802000
1	3.921745000	2.891129000	-4.024622000	1	-0.540279000	6.399026000	2.390698000	1	-3.907143000	-6.140949000	-0.656321000
6	3.028044000	3.744012000	-2.314278000	6	2.367312000	4.417224000	5.575794000				
6	2.558545000	4.992616000	-2.915889000	1	2.401845000	5.465962000	5.896975000				

1•((R,R)-G7)₂ (*exo-exo*) B3LYP functional

30	-3.565698000	-1.033349000	0.029884000	6	-2.929313000	1.610299000	-1.585503000	6	-3.684380000	-3.089582000	3.890297000
30	3.824832000	-0.359120000	0.230521000	6	-2.664061000	2.034029000	-2.989228000	6	-3.602417000	-1.918789000	3.015221000
8	-5.726346000	-0.859461000	-0.277550000	6	-2.626787000	0.880821000	-3.750129000	6	-3.555491000	-0.589330000	3.431765000
8	5.810169000	0.377934000	-0.321030000	6	-2.857610000	-0.240788000	-2.858599000	1	-3.607753000	-0.429629000	4.503288000
7	-3.041146000	0.221636000	-1.570410000	6	-2.861359000	-1.577844000	-3.280849000	6	-3.437107000	0.571798000	2.654520000
7	-3.236653000	-2.746739000	-1.157285000	1	-2.690998000	-1.731617000	-4.340677000	6	-3.434661000	1.912151000	3.212360000
7	-3.555053000	-2.324197000	1.696015000	6	-3.029159000	-2.734339000	-2.520907000	6	-3.315208000	2.801236000	2.160463000
7	-3.310026000	0.639750000	1.281989000	6	-2.988783000	-4.107850000	-3.028640000	6	-3.223069000	1.981450000	0.918096000
7	2.724416000	0.624445000	-1.274939000	6	-3.170940000	-4.936310000	-1.940719000	6	-3.048501000	2.431707000	-0.424775000
7	3.788582000	-2.149155000	-0.874538000	6	-3.320760000	-4.069265000	-0.769099000	6	-2.431758000	3.398555000	-3.605260000
7	4.405735000	-1.518096000	1.892261000	6	-3.488681000	-4.504964000	0.548973000	1	-1.930843000	4.076670000	-2.913379000
7	3.309527000	1.237627000	1.490205000	1	-3.516568000	-5.578206000	0.704439000	1	-1.728764000	3.275023000	

1	-4.473408000	4.212765000	-3.401938000	1	-1.851934000	7.720404000	-1.856863000	1	6.385444000	-5.585795000	-2.779493000
1	-4.150083000	3.457646000	-4.964361000	6	-2.668602000	7.912308000	0.135390000	6	5.899808000	-4.528694000	3.599705000
6	-2.400511000	0.750637000	-5.234094000	1	-3.375024000	8.703012000	-0.146802000	1	5.312549000	-5.331969000	3.134123000
1	-1.898593000	1.646975000	-5.616153000	1	-1.787250000	8.388320000	0.579448000	1	5.806668000	-4.675816000	4.683110000
1	-1.711724000	-0.082567000	-5.429512000	1	-3.139253000	7.295885000	0.909698000	6	7.384657000	-4.699455000	3.199526000
6	-3.695971000	0.524496000	-6.050706000	6	0.957449000	7.281303000	-0.920408000	1	7.753812000	-5.691457000	3.485482000
1	-3.468415000	0.428093000	-7.118994000	1	1.862053000	7.034386000	-1.495666000	1	8.009372000	-3.945925000	3.692859000
1	-4.390621000	1.361971000	-5.924015000	1	0.397516000	7.997332000	-1.536908000	1	7.515582000	-4.584254000	2.117398000
1	-4.212523000	-0.386400000	-5.728364000	6	1.389090000	7.987096000	0.386007000	6	5.536878000	-1.908822000	5.467953000
6	-2.806297000	-4.495368000	-4.470901000	1	1.971972000	8.890998000	0.169447000	1	5.567773000	-2.892201000	5.953822000
1	-2.052833000	-3.846814000	-4.938024000	1	2.007499000	7.327720000	1.005882000	1	4.754420000	-1.338732000	5.987582000
6	-4.109661000	-4.426661000	-5.301849000	1	0.516571000	8.278444000	0.981400000	6	6.896263000	-1.202324000	5.685503000
1	-3.921887000	-4.708698000	-6.344644000	6	2.375638000	1.972853000	-1.320805000	1	7.112634000	-1.096339000	6.755159000
1	-4.529494000	-3.414488000	-5.291362000	6	1.991814000	2.301788000	-2.722528000	1	6.895888000	-0.202909000	5.235755000
1	-4.867041000	-5.105854000	-4.894649000	6	2.079596000	1.124817000	-3.441781000	1	7.710367000	-1.774667000	5.226623000
6	-3.232917000	-6.439339000	-1.918245000	6	2.549869000	0.091726000	-2.534875000	6	3.219035000	2.877962000	4.873793000
1	-2.692713000	-6.820946000	-1.041122000	6	2.800276000	-1.231779000	-2.926435000	1	3.071591000	1.999183000	5.515057000
1	-2.708186000	-6.841184000	-2.794131000	1	2.534688000	-1.474255000	-3.949596000	1	2.428689000	3.583800000	5.149959000
6	-4.674689000	-7.000422000	-1.900500000	6	3.352872000	-2.271668000	-2.179167000	6	4.590607000	3.516314000	5.201361000
1	-4.665373000	-8.096587000	-1.873885000	6	3.570413000	-3.642390000	-2.646092000	1	4.654908000	3.777298000	6.264427000
1	-5.226475000	-6.684196000	-2.792936000	6	4.137825000	-4.333504000	-1.595131000	1	4.743389000	4.429504000	4.614726000
1	-5.224853000	-6.641751000	-1.023291000	6	4.265320000	-3.387276000	-0.484511000	1	5.411385000	2.828656000	4.967950000
6	-3.754162000	-5.647755000	-3.466058000	6	4.765600000	-3.688238000	0.786014000	6	1.650472000	4.440470000	2.715521000
1	-3.408786000	-5.764416000	-4.501044000	1	5.110426000	-4.705064000	0.941642000	1	2.183331000	5.055977000	3.453022000
1	-3.066066000	-6.241499000	-2.849294000	6	4.833916000	-2.830532000	1.889069000	1	1.487759000	5.078517000	1.851054000
6	-5.176296000	-6.245315000	-3.345064000	6	5.323986000	-3.191114000	3.221876000	6	0.260698000	4.069036000	3.286323000
1	-5.179614000	-7.303087000	-3.633456000	6	5.169255000	-2.074520000	4.018630000	1	-0.316316000	4.974649000	3.508380000
1	-5.547877000	-6.170240000	-2.316727000	6	4.583754000	-1.033296000	3.171960000	1	0.349613000	3.482762000	4.207349000
1	-5.879597000	-5.711604000	-3.994505000	6	4.202926000	0.241725000	3.588753000	1	-0.305559000	3.472908000	2.564873000
6	-3.7779792000	-3.046475000	-5.391304000	1	4.370588000	0.466258000	4.636563000	6	-6.859563000	-1.262565000	0.572197000
1	-3.117963000	-2.262715000	-5.783733000	6	3.581947000	1.255956000	2.845722000	1	-6.447243000	-1.340358000	1.580806000
1	-3.409498000	-3.990963000	-5.809618000	6	3.082121000	2.488326000	3.424127000	6	-7.896387000	-0.125239000	0.519310000
6	-5.214474000	-2.798970000	-5.915359000	6	2.486003000	3.212977000	2.409376000	1	-8.848182000	-0.493326000	0.924742000
1	-5.228311000	-2.767126000	-7.011255000	6	2.668892000	2.429918000	1.161114000	6	6.720062000	-0.017586000	-1.409752000
1	-5.891791000	-3.595943000	-5.587827000	6	2.347263000	2.819075000	-0.174850000	6	7.322513000	1.274959000	-1.991841000
1	-5.611122000	-1.848150000	-5.541157000	6	1.594700000	3.609332000	-3.372530000	1	8.187628000	1.014177000	-2.615993000
6	-3.563459000	2.215605000	4.682896000	1	1.015293000	4.241933000	-2.700250000	1	-2.404263000	-5.514786000	-4.528624000
1	-2.944342000	1.512999000	5.256807000	1	0.918480000	3.382372000	-4.206367000	1	-6.096590000	-0.419112000	-1.074444000
1	-3.157820000	3.210755000	4.897621000	6	2.786450000	4.415492000	-3.945909000	8	7.789839000	2.004810000	-0.799375000
6	-5.014045000	2.147945000	5.217878000	1	2.436049000	5.353088000	-4.394153000	8	-8.052276000	0.131398000	-0.923928000
1	-5.040608000	2.362772000	6.292758000	1	3.309027000	3.842498000	-4.719603000	6	6.328990000	2.113844000	-2.791136000
1	-5.447456000	1.154293000	5.057764000	1	3.521888000	4.665869000	-3.172181000	1	5.449742000	2.351961000	-2.185755000
1	-5.654388000	2.876443000	4.708805000	6	1.782983000	0.898200000	-4.901552000	1	6.792137000	3.049616000	-3.126998000
1	-2.638071000	4.815127000	1.702542000	1	1.106815000	1.678172000	-5.270285000	1	5.996329000	1.568848000	-3.681327000
1	-2.907750000	4.490243000	3.384586000	1	1.237146000	-0.047920000	-5.019499000	1	8.035130000	2.922321000	-1.027183000
6	-4.723161000	4.944873000	2.331845000	6	3.037010000	0.862212000	-5.807914000	1	6.082905000	-0.497319000	-2.156265000
1	-4.658551000	6.026361000	2.502473000	1	2.755530000	0.677856000	-6.851599000	6	7.769990000	-0.993468000	-0.885552000
1	-5.372959000	4.518191000	3.103618000	1	3.726037000	0.069423000	-5.495637000	1	8.397435000	-1.357292000	-1.707983000
1	-5.215227000	4.783689000	1.365444000	1	3.580304000	1.812497000	-5.764722000	1	8.413860000	-0.503067000	-0.148811000
6	-3.316405000	4.299465000	2.384995000	6	3.243091000	-4.152422000	-4.023370000	1	7.281961000	-1.851308000	-0.414990000
6	-3.012395000	3.942828000	-0.646276000	1	2.291500000	-3.721893000	-4.362594000	6	-7.410119000	-2.608015000	0.106610000
1	-3.471293000	4.164743000	-1.609768000	1	3.086334000	-5.237931000	-3.984818000	6	-7.464146000	1.139999000	1.255846000
1	-3.676305000	4.418664000	0.071903000	6	4.335701000	-3.845387000	-5.075328000	1	-6.508234000	1.503878000	0.868929000
6	-1.649345000	4.600120000	-0.589875000	1	4.045171000	-4.227318000	-6.061213000	1	-8.215169000	1.931330000	1.143627000
6	-1.310835000	5.937319000	-0.797827000	1	5.287774000	-4.310616000	-4.795566000	1	-7.349133000	0.939945000	2.326803000
6	0.126465000	6.038002000	-0.721029000	1	4.504385000	-2.765919000	-5.163577000	1	-6.611532000	-3.354843000	0.093429000
6	0.622981000	4.759372000	-0.468775000	6	4.574736000	-5.772969000	-1.559242000	1	-8.198926000	-2.953835000	0.785350000
6	2.064568000	4.307072000	-0.404897000	1	4.023221000	-6.342397000	-2.317967000	1	-7.832104000	-2.521314000	-0.899541000
1	2.597377000	4.874873000	0.360887000	1	4.305794000	-6.218993000	-0.592113000	1	6.235503000	1.120523000	0.162917000
1	2.557821000	4.599369000	-1.336049000	6	6.091620000	-5.968059000	-1.795219000	1	-8.563084000	0.949214000	-1.078834000
6	-2.278605000	7.056330000	-1.091398000	1	6.359389000	-7.030186000	-1.746698000				
1	-3.194589000	6.641015000	-1.533682000	1	6.678456000	-5.432588000	-1.040210000				