Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information for

Pyrene Bridged Double [7]helicene Embedded With a Heptagonal Ring

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S1. Experimental Details

Chromatography. Open-column chromatography and thin-layer chromatography (TLC) were performed on silica gel (Merck silica gel 100-200 mesh). Chiral stationary phase HPLC separations were performed on SHIMADZU 223.

NMR Spectroscopy. The NMR measurements were performed at 298 K on NMR spectrometers operating at 400 MHz ^{1}H and 101 MHz ^{13}C frequencies (151 MHz for (*P*, *M*-**3**)). Standard pulse sequences were used, and the data was processed using 2-fold zero-filling in the indirect dimension for all 2D experiments. Chemical shifts (δ) are reported in parts per million (ppm) relative to the solvent residual peak (^{1}H and ^{13}C NMR, respectively): CD_2Cl_2 (δ = 5.32 and 53.84 ppm) and *J* values are given in Hz.

High-resolution mass spectrometry (HRMS). The matrix-assisted laser desorption ionization-time of flight (MALDI-TOF) - HRMS were measured on Bruker ultrafleXtreme. *Trans*-2-[3-(4-*tert*-butylphenyl)-2-methyl-2-propenylidene]malononitrile (DCTB) dissolved in chloroform (30 mg/mL) was used as a supporting matrix, while Cesium iodide dissolved in acetonitrile (40 mg/mL) used as a reference in the MALDI-TOF–HRMS measurement. The calculated mass was exported from mMass software.[1]

Melting point. Melting points were measured using an OptiMelt Automated Melting Point System.

UV−vis and Fluorescence spectroscopy. UV−vis spectra were measured on the JASCO V-670 spectrometer, while emission spectra were measured Edinburgh FLS 980 photoluminescence spectrometer in DCM (OD = 0.05). The fluorescence lifetimes were measured in DCM (OD = 0.05) using a 418.6 nm pulsed laser diode with a pulse frequency of 1/50 ns. The fluorescence quantum yields were measured in DCM in three different concentrations (OD = 0.2 – 0.5) using the same spectrometer with a 450 W xenon arc lamp as a light source and a calibrated integrating sphere.

CPL and CD spectroscopy. CPL and CD spectra were recorded with a customized JASCO CPL-300/J-1500 hybrid spectrometer.

S2. Photophysical Properties

A. Comparison of UV-vis absorption, emission, and CD plots in DCM.

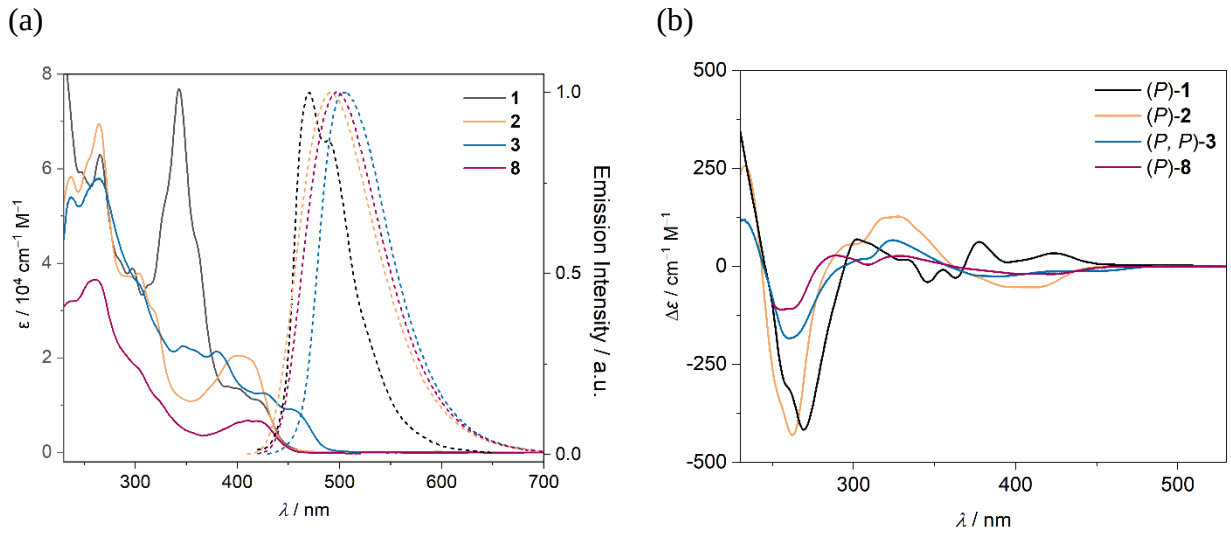


Figure S1. (a) UV–vis absorption and emission spectra of **1**, **2**, **3**, and **8** in dichloromethane. (b) Electronic CD spectra of **1**, **2**, **3**, and **8** in dichloromethane.

B. Solid state emission and CPL spectra.

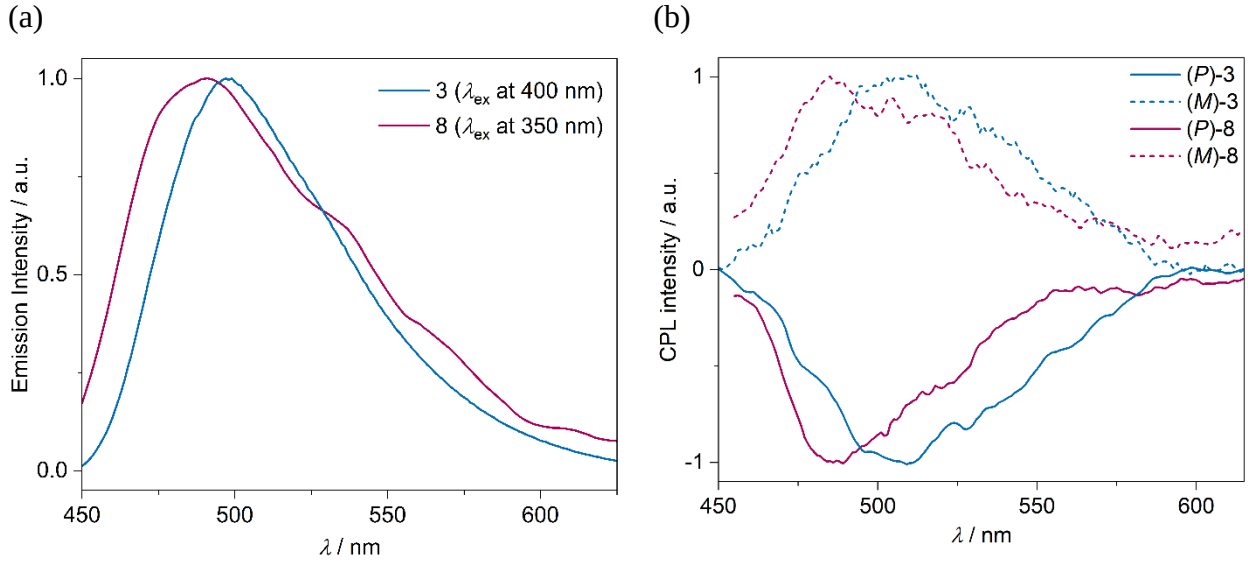


Figure S2. Solid state (a) emission spectra and (b) CPL spectra of **3** and **8** (excited at 380 nm).

S3. Chiral stationary phase HPLC data

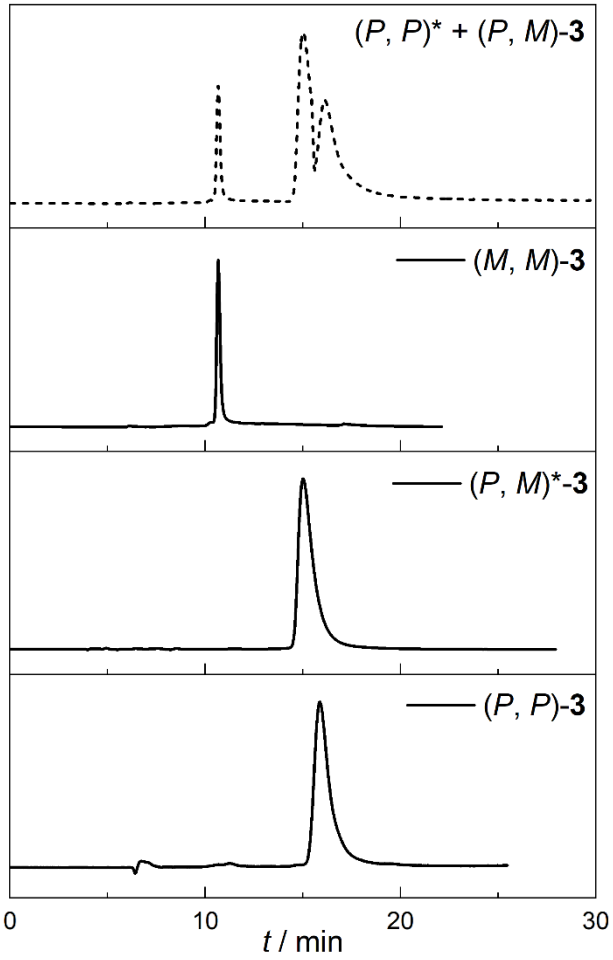


Figure S3. HPLC chromatogram of diastereomeric mixture of **3** using chiral stationary phase column. (The chromatogram detector was set at 375 nm with a bandwidth of 4 nm.)

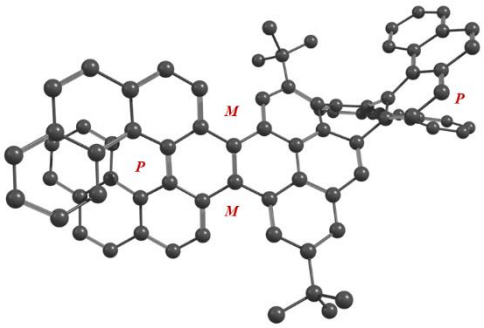
Table S1. Overview of parameters for HPLC separation of stereoisomers of **3**.

Compound	Eluent *n*-hexane/*i*PrOH	First fraction	Second fraction	Third fraction	α^b	Rs^c	*er*
3	94:6	*MM*	*PM**	*PP*	1.36	2.48	98:2

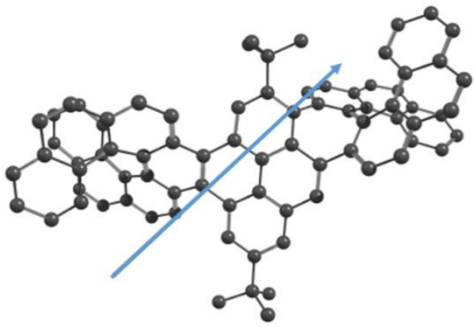
[a]Phenomenex Lux i-Amylose-3, 5 µm (250 x 4.6 mm). Sample injection: 30 µL of a ~1 mg/mL solution in hexane/*i*PrOH. Separation conditions: Eluent, flow rate: 0.5 mL/min, 25 °C. [b]Selectivity parameter: $\alpha = t_{R2}/t_{R1}$, where t_{R1}, and t_{R2} are elution times for first and second fraction, respectively. [c]Resolution parameter: $R_S = 2(t_{R2} - t_{R1})/(w_1 + w_2)$, where w_1 and w_2 are peak widths for first and second fraction, respectively. Note α and *R*s for **3** was calculated only for *PP* and *MM*.

S4. Quantum chemical calculations

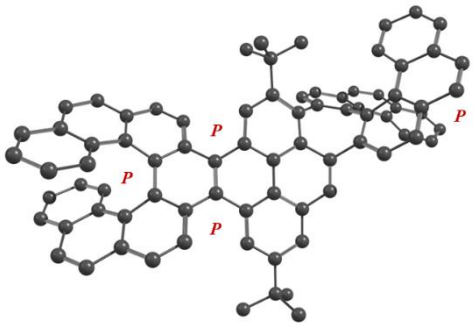
DFT calculations were performed using Gaussian 16 suite.[2] Geometries were optimized using ωB97XD functional and 6-31G(d,p) basis set in the gas phase. Frequency analysis was performed to verify the stationary state geometry. In all cases no imaginary frequency was found. TD-DFT calculations were performed on ωB97XD/6-31G(d,p) optimized geometries at the B3LYP/6-31g(d,p) level. The effect of the solvent was accounted for using PCM (with dichloromethane as the solvent). SpecDis[3] and Avogadro[4] software were used to analyze the TD-DFT calculated spectra and to generate graphical images of frontier molecular orbitals (FMOs), respectively.



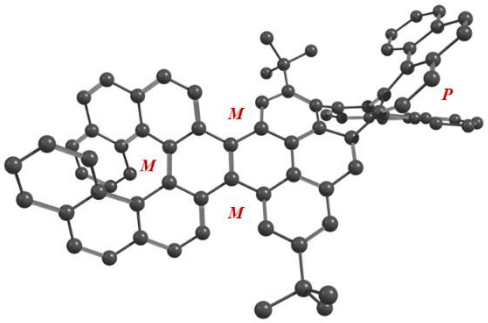
(3A) 1.5 kcal mol^{-1}



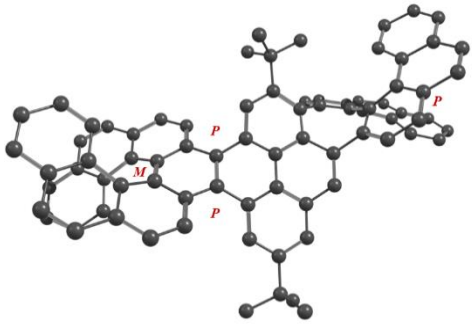
Dipole moment of 3A



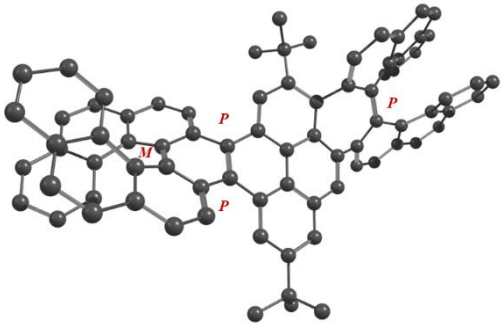
(3B) 4.1 kcal mol^{-1}



(3C) 5.7 kcal mol^{-1}



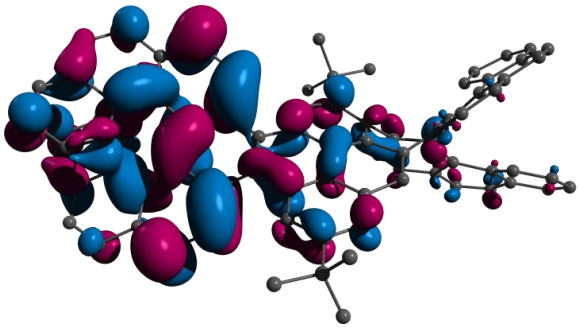
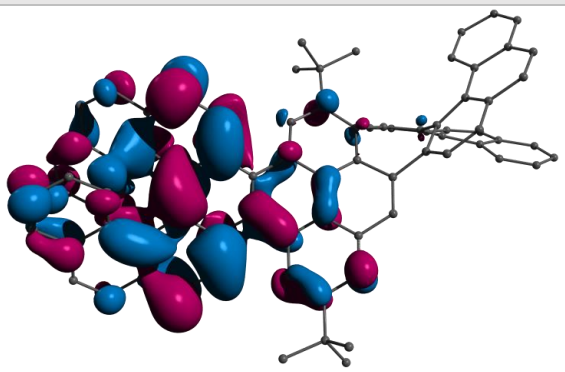
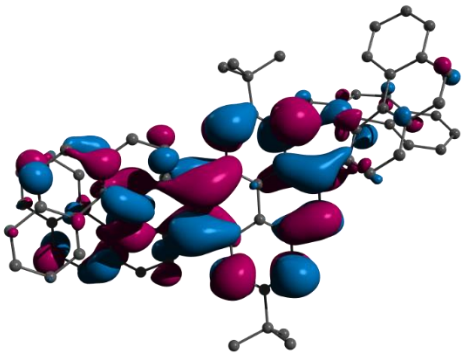
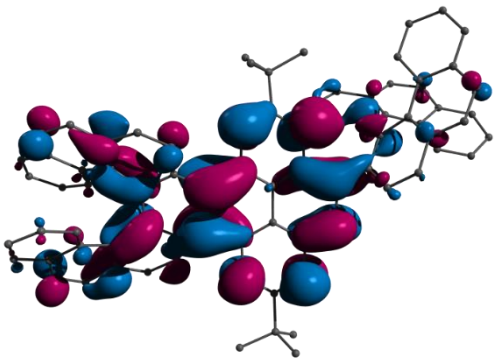
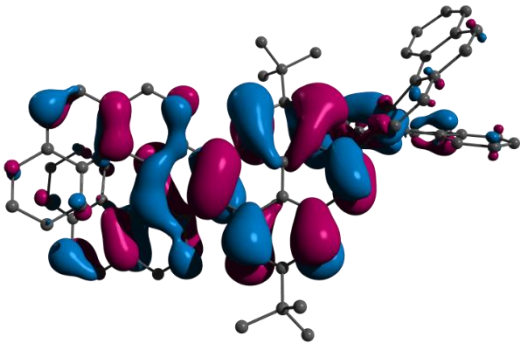
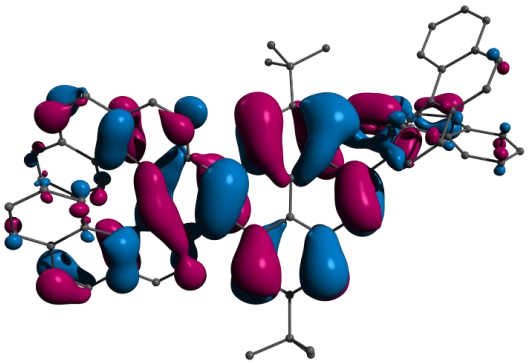
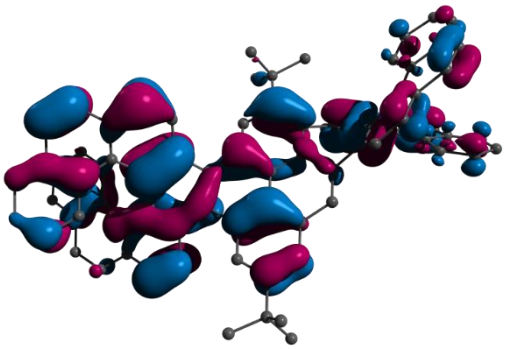
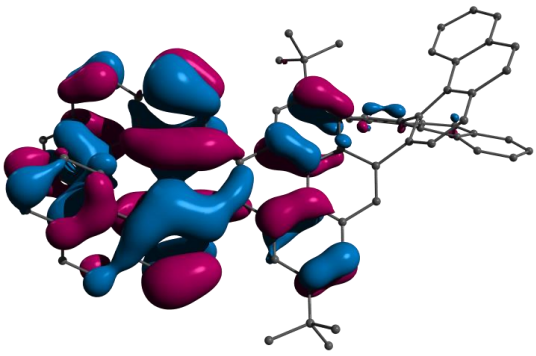
(3D) 0.0 kcal mol^{-1}



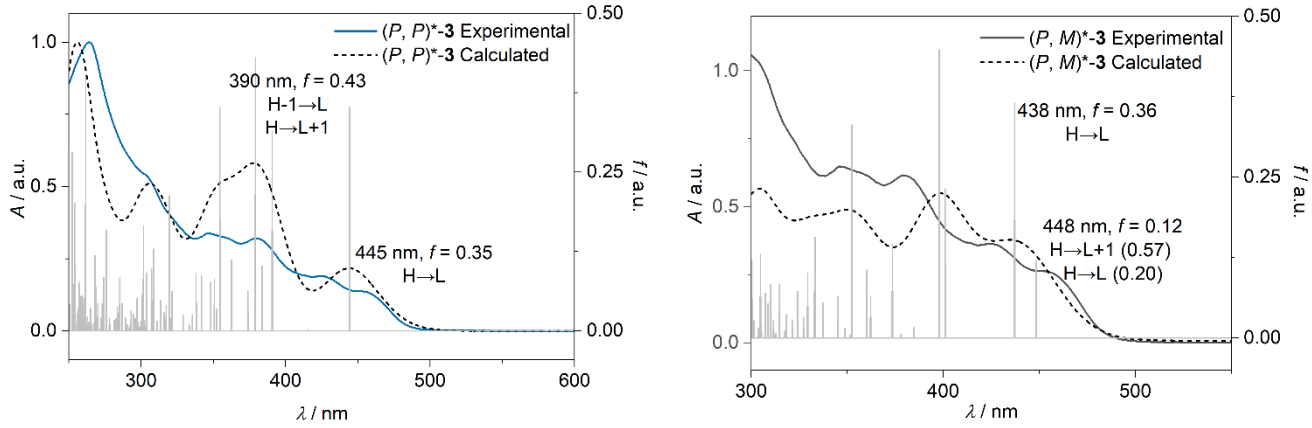
(3E) 28.4 kcal mol^{-1}

Figure S4. Relative Gibbs's free energies and optimized geometries of diastereomers of **3**. Hydrogen atoms are omitted for clarity.

Table S2. Frontier molecular orbitals of (*P*, *P*)-**3** and (*P*, *M*)-**3** (isosurface value 0.02). Hydrogen atoms are omitted for clarity.

FMOs	(*P*, *P*)-**3A**	(*P*, *M*)-**3C**
LUMO+1		
LUMO		
HOMO		
HOMO–1		

(a)



(b)

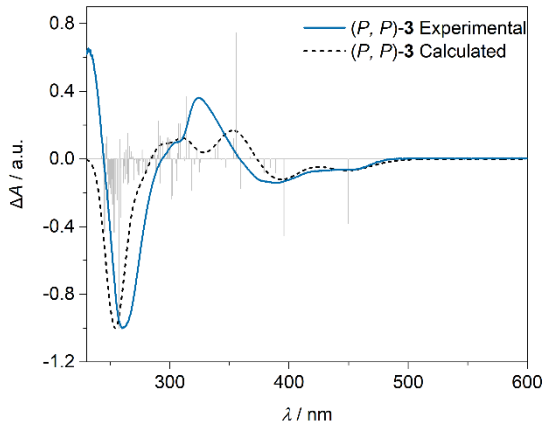


Figure S5. Comparison of experimental (solid) and TD-DFT calculated (dashed) (a) UV–vis absorption (b) ECD spectra of (*P*, *P*)-**3** (shifted by 0.07 eV, 10 nm) and (*P*, *M*)*-**3** (shifted by 0.04 eV, 15 nm) along with assignments of key transitions. H = HOMO, L = LUMO, *f* = oscillator strength.

Table S3a. Summary of TD-DFT calculated key transitions of (*P*, *P*)-**3**.

Excited singlet state	Wavelength / nm	Energy / eV	Major transitions	Contribution	oscillator strength (*f*)
1	445	2.78	HOMO→LUMO	0.69	0.35
3	390	3.18	HOMO→LUMO+2	0.53	0.43
			HOMO–1→LUMO	0.33	
8	359	3.45	HOMO→LUMO+4	0.56	0.35
			HOMO–3→LUMO	0.34	

Table S3b. Summary of TD-DFT calculated key transitions of (*P*, *M*)-**3**.

Excited singlet state	Wavelength / nm	Energy / eV	Major transitions	Contribution	oscillator strength (*f*)
1	448	2.76	HOMO→LUMO+1	0.57	0.12
			HOMO→LUMO	0.20	
2	438	2.83	HOMO→LUMO	0.65	0.36
4	398	3.11	HOMO–1→LUMO+1	0.49	0.45

NICS calculations: The Nucleus Independent Chemical Shift (NICS) calculations were performed on ωB97XD/6-31G(d,p) optimized geometry at GIAO-B3LYP/6-311+G(2d,p) level. Considering the non-planarity of molecule the NICS(1)$_{ZZ}$ values were obtained by placing dummy atom at 1 Å above and below the each ring.

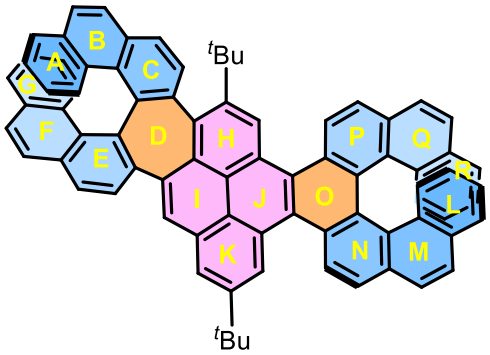


Table S4. The calculated NICS(0) and NICS(1)$_{ZZ}$ values for (*P*, *P*)-**3**.

Ring	NICS(1)$_{ZZ}$ (Up)	NICS(1)$_{ZZ}$ (Down)	NICS(0)$_{ZZ}$	NICS(0)$_{iso}$	**Ring**	NICS(1)$_{ZZ}$ (Up)	NICS(1)$_{ZZ}$ (Down)	NICS(0)$_{ZZ}$	NICS(0)$_{iso}$
A	−12.28	−13.42	−9.75	−9.18	**J**	−4.16	−3.75	18.57	1.15
B	−10.49	−7.59	−7.69	−4.89	**K**	−26.23	−28.82	−10.78	−8.73
C	−3.00	−3.64	−4.81	−6.50	**L**	−30.30	−33.08	−17.14	−9.30
D	11.05	14.45	21.30	8.48	**M**	−21.17	−20.94	−6.54	−5.17
E	−7.50	−6.09	−5.99	−6.67	**N**	−15.95	−9.66	−4.73	−5.03
F	−9.04	−11.82	−6.81	−4.82	**O**	−6.31	−6.50	6.15	−1.10
G	−15.08	−12.88	−9.32	−9.23	**P**	−10.26	−16.67	−4.79	−5.03
H	−28.71	−22.15	−9.52	−7.88	**Q**	−21.39	−21.66	−6.40	−5.23
I	−6.97	−13.54	8.78	−1.63	**R**	−33.42	−30.53	−16.91	−9.32

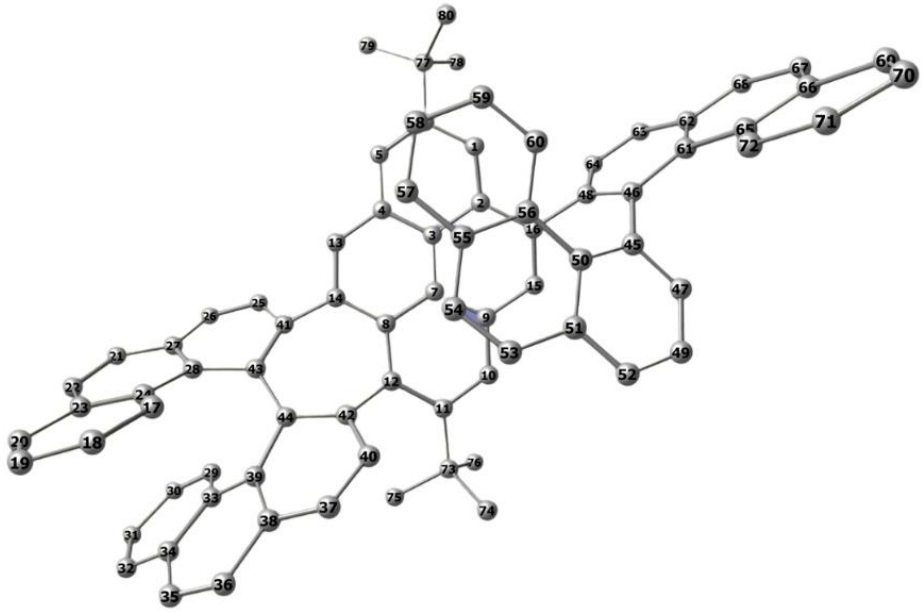


Table S5. Mulliken charges and spin densities for radical cation of **8**.

Atom no.	Mulliken charges	Spin densities	Atom no.	Mulliken charges	Spin densities	Atom no.	Mulliken charges	Spin densities
1	-0.163482	0.264863	26	-0.146228	0.067297	51	0.067740	-0.000944
2	0.108330	-0.104373	27	0.086285	-0.015958	52	-0.167475	0.001073
3	-0.006361	0.044216	28	-0.032250	0.017031	53	-0.150528	0.001419
4	0.106025	-0.057983	29	-0.132121	-0.015118	54	-0.142390	0.000910
5	-0.189932	0.195718	30	-0.125709	0.014679	55	0.075095	0.001266
6	0.138253	-0.115557	31	-0.123569	-0.012248	56	0.026335	-0.001290
7	0.007890	-0.041204	32	-0.156031	0.012179	57	-0.167624	0.002457
8	0.072874	0.007984	33	0.037175	0.027447	58	-0.120807	-0.000823
9	0.107371	0.073733	34	0.079624	-0.015933	59	-0.134576	0.001511
10	-0.167386	0.067456	35	-0.129754	0.041661	60	-0.133960	0.001937
11	0.078877	-0.038924	36	-0.153901	-0.020690	61	0.020046	-0.005642
12	-0.050876	0.190418	37	-0.143256	0.009807	62	0.076593	0.008120
13	-0.202123	0.144692	38	0.084343	0.040544	63	-0.162581	-0.006486
14	0.035401	0.000081	39	-0.042643	-0.050226	64	-0.164339	0.008810
15	-0.167778	-0.042328	40	-0.120786	0.008774	65	0.031451	0.002949
16	0.000808	0.156844	41	0.010749	0.076786	66	0.068010	-0.002468
17	-0.132083	0.003815	42	-0.014392	0.001654	67	-0.141615	0.006084
18	-0.126061	-0.002488	43	0.005813	-0.012079	68	-0.157420	-0.004168
19	-0.124110	0.005056	44	0.025105	0.115327	69	-0.162862	0.001673
20	-0.156758	-0.004181	45	-0.082325	0.000686	70	-0.121489	-0.001602
21	-0.152639	0.008820	46	-0.042610	0.013987	71	-0.140683	0.001625
22	-0.132695	-0.002825	47	-0.113216	0.000334	72	-0.122927	-0.001429
23	0.078908	0.006681	48	0.013668	-0.015999	73	-0.056146	0.002043
24	0.033430	-0.001935	49	-0.133005	0.000600	74	-0.337779	0.000622
25	-0.159308	-0.038487	50	0.029218	0.003147	75	-0.346806	0.000192
76	-0.344055	-0.000681	78	-0.345135	-0.001746	80	-0.339585	-0.001888
77	-0.074939	0.006345	79	-0.360332	-0.000012			

S5. NMR spectroscopy

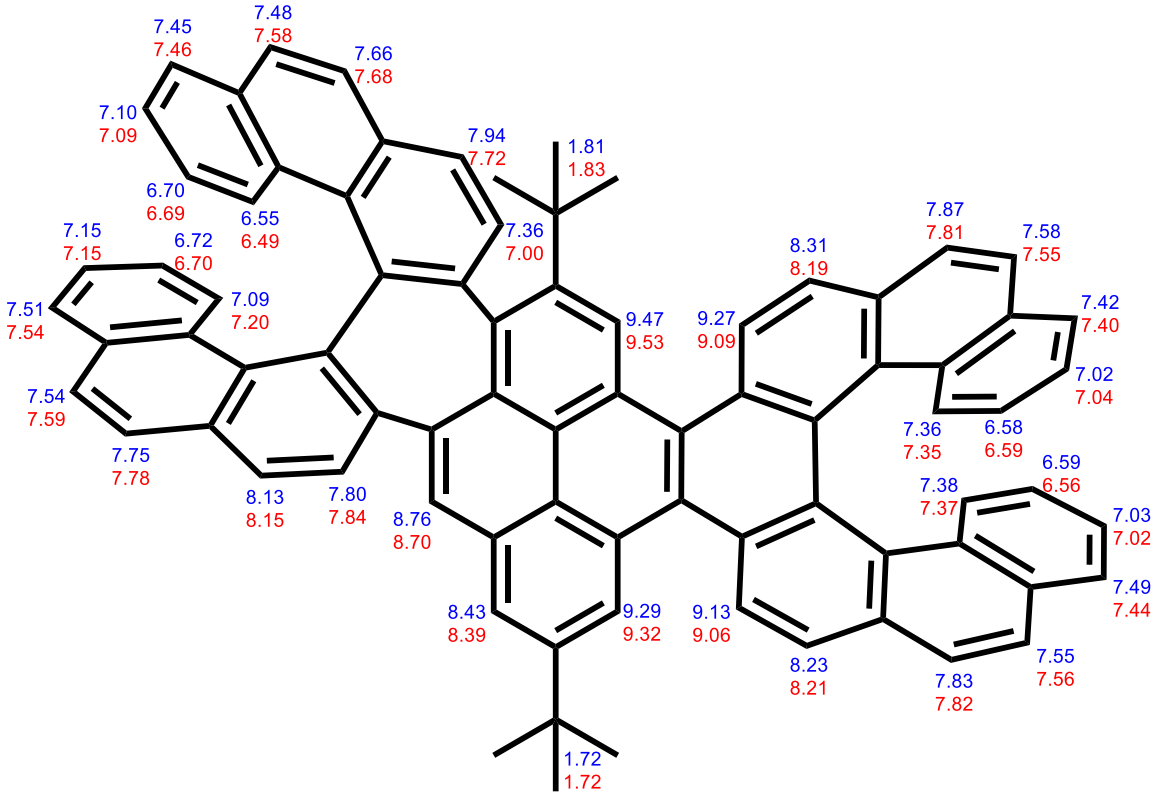


Figure S6. ^{1}H NMR peaks assigned to respective atoms in (*P*, *P*)-**3** (blue), (*P*, *M*)-**3** (red)**.**

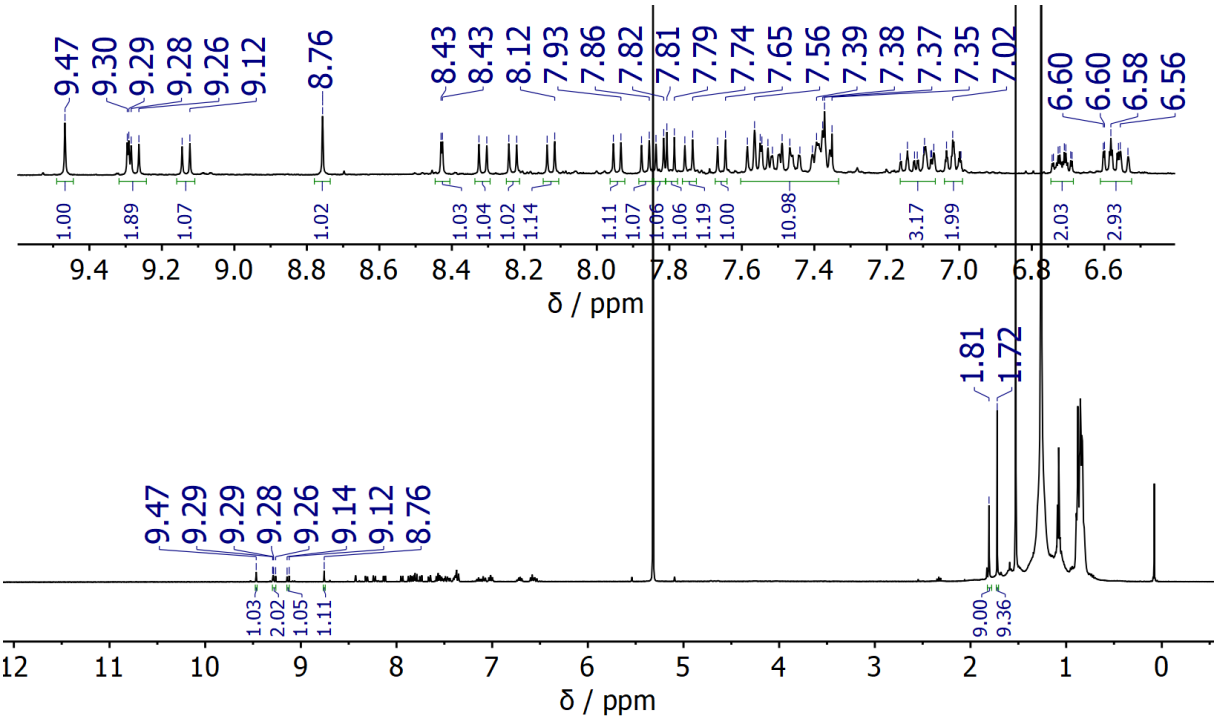


Figure S7. ^{1}H NMR spectrum of (*P*, *P*)-**3** (400 MHz, CD_2Cl_2).

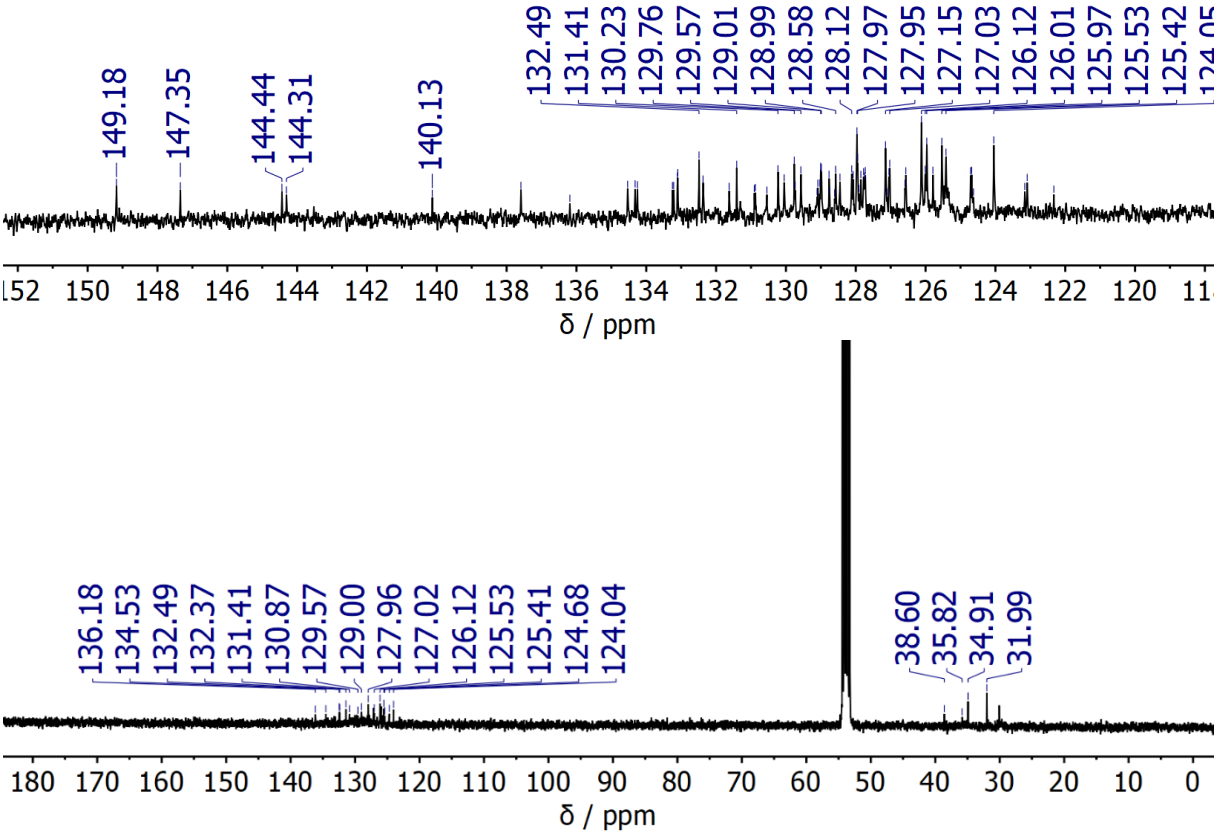


Figure S8. ^{13}C{^{1}H} NMR spectrum of (*P*, *P*)-**3** (101 MHz, CD_2Cl_2).

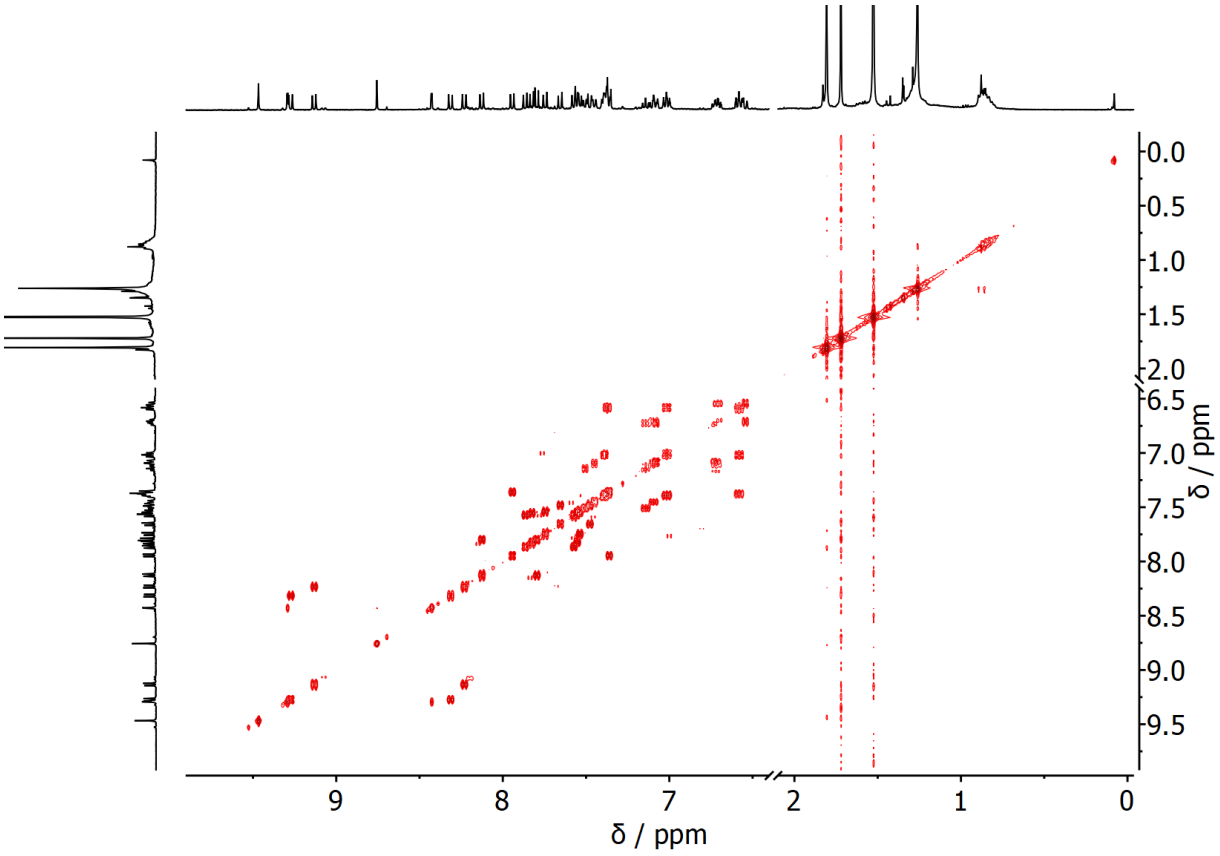


Figure S9. $^{1}H - {}^{1}H$ COSY NMR spectrum of (*P*, *P*)-**3** (400 MHz, CD_2Cl_2).

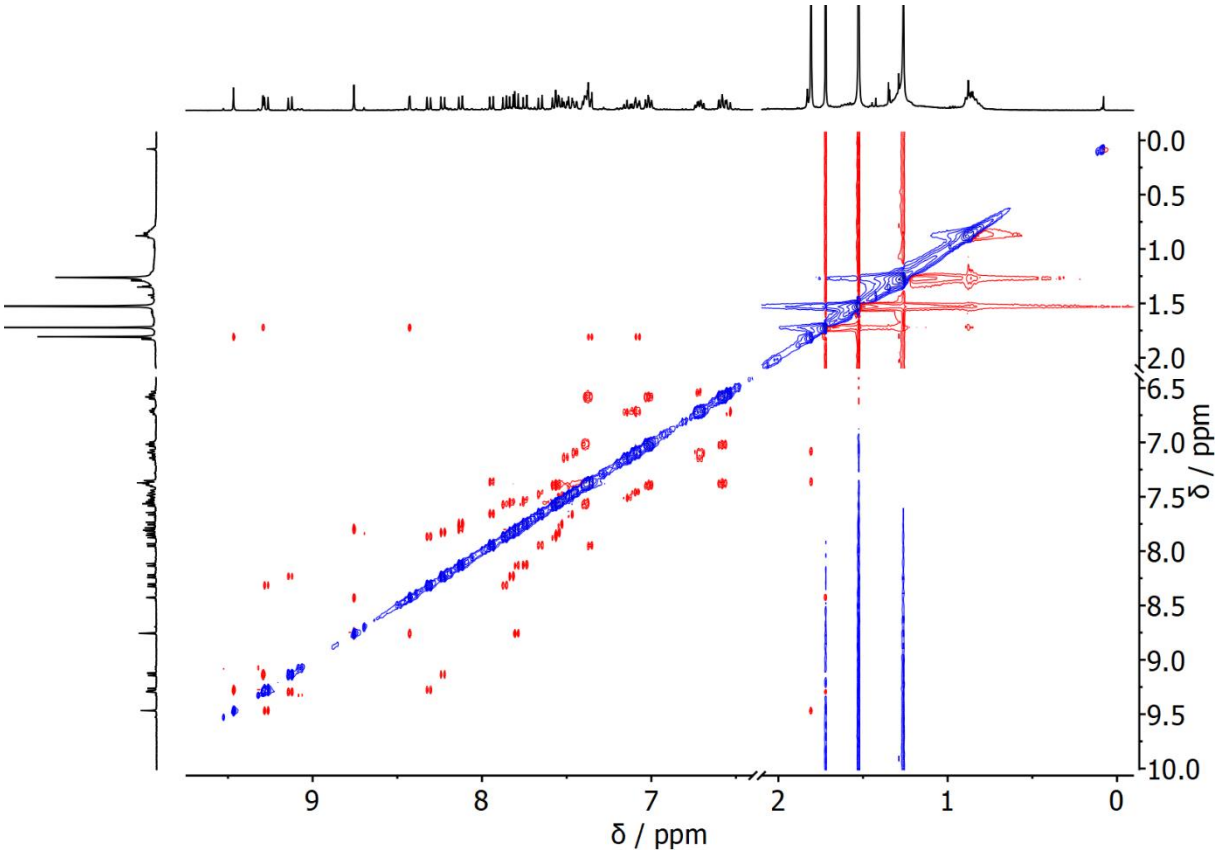


Figure S10. $^{1}H - {}^{1}H$ NOESY NMR spectrum of (*P*, *P*)-**3** (400 MHz, CD_2Cl_2).

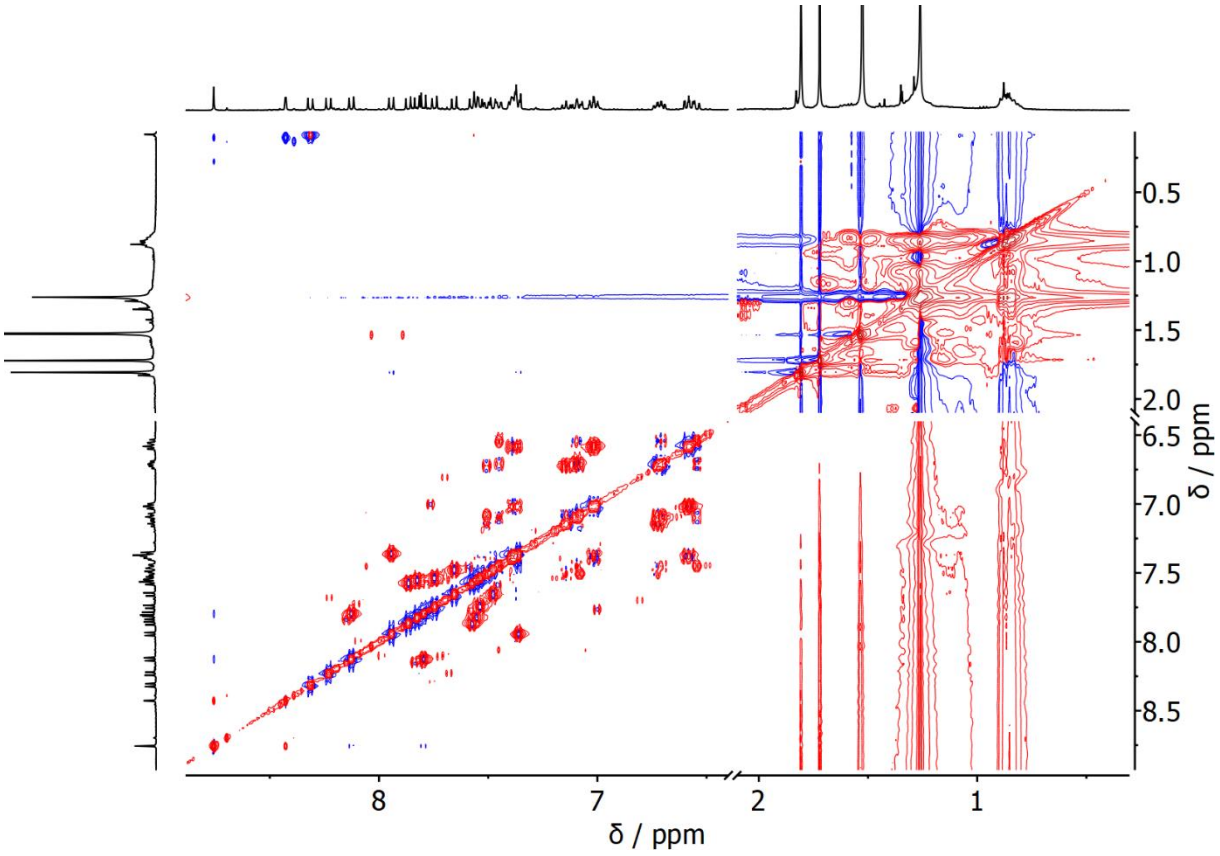


Figure S11. $^{1}H - {}^{1}H$ TOCSY NMR spectrum of (*P*, *P*)-**3** (400 MHz, CD_2Cl_2).

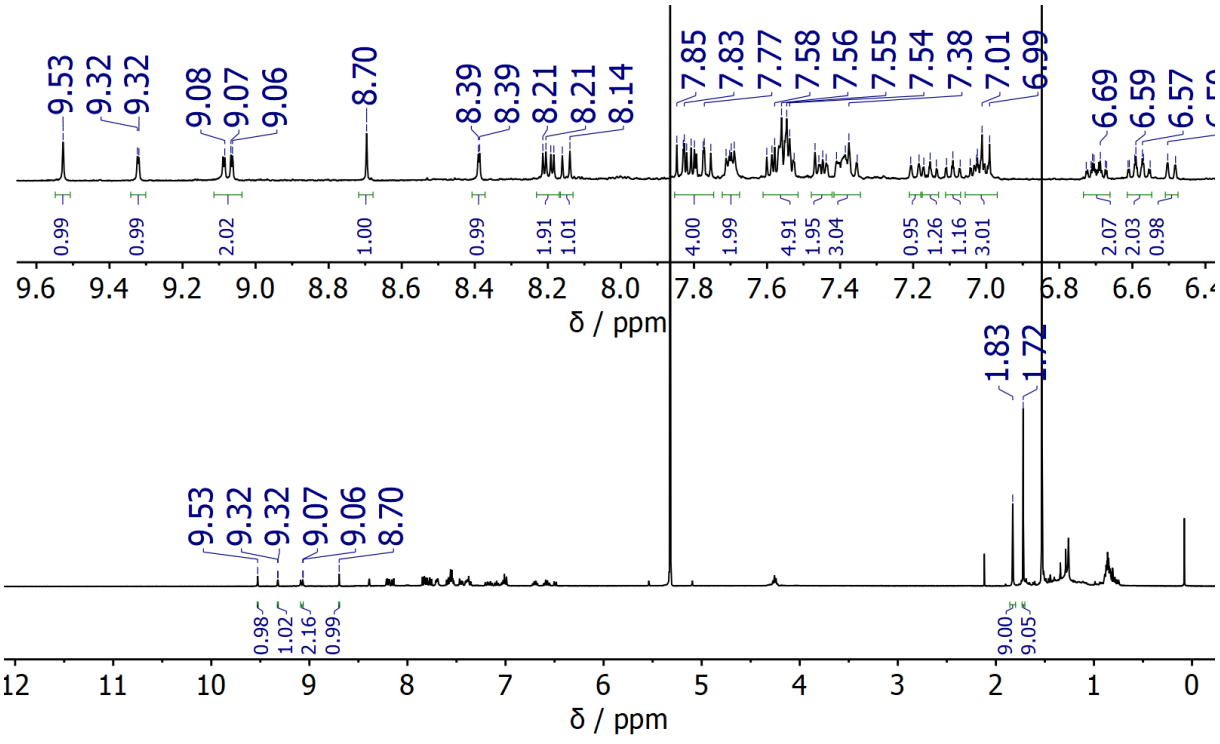


Figure S12. ^{1}H NMR spectrum of (*P*, *M*)-**3** (400 MHz, CD_2Cl_2).

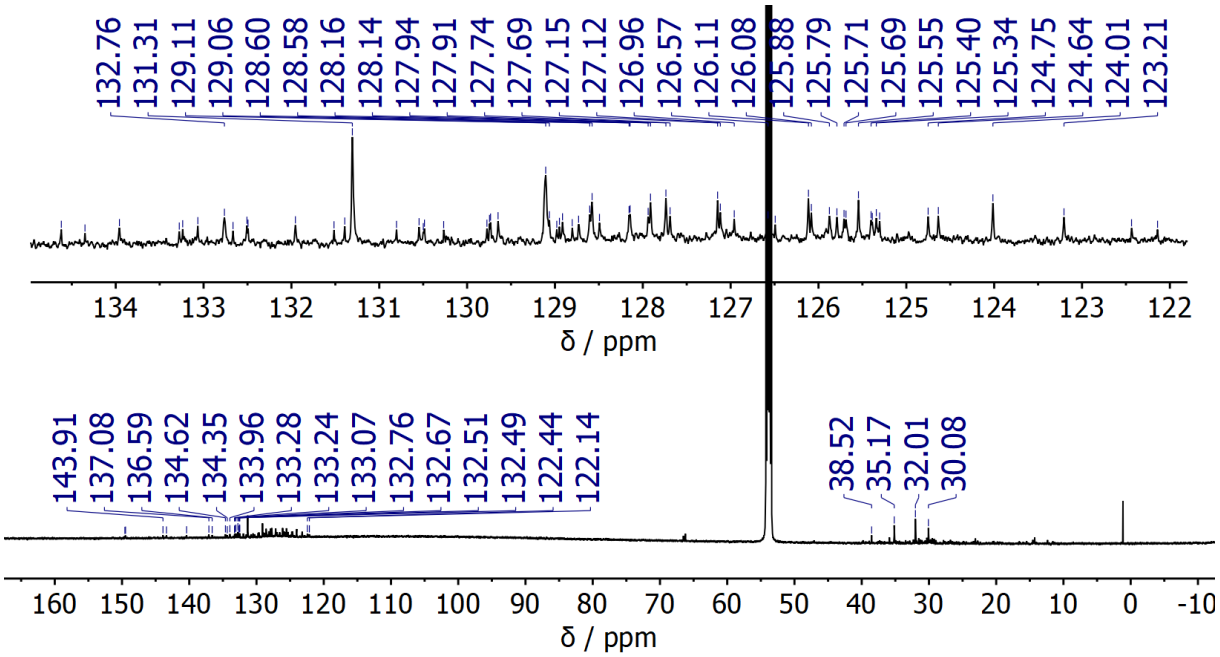


Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum of (*P*, *M*)-**3** (151 MHz, CD_2Cl_2).

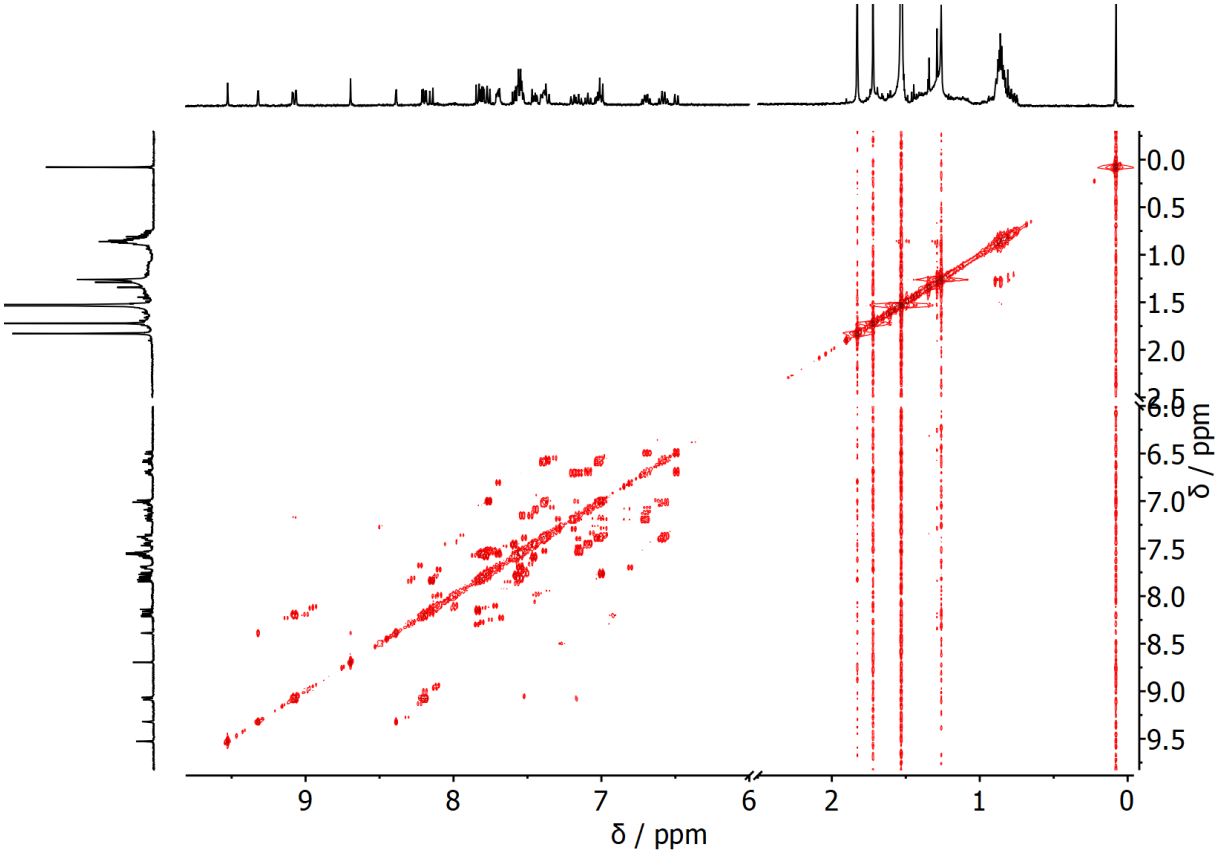


Figure S14. ^{1}H – ^{1}H COSY NMR spectrum of (*P*, *M*)-**3** (400 MHz, CD_2Cl_2).

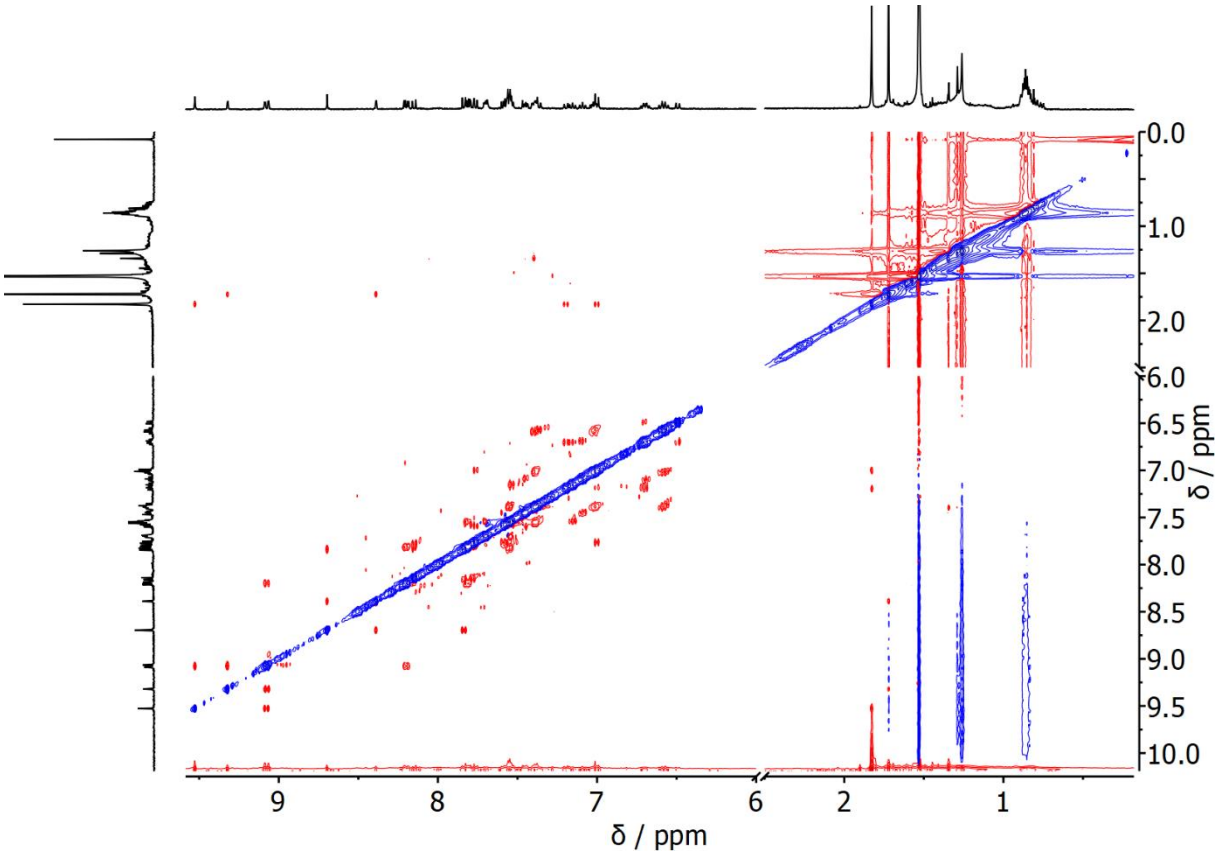


Figure S15. ^{1}H – ^{1}H NOESY NMR spectrum of (*P*, *M*)-**3** (400 MHz, CD_2Cl_2).

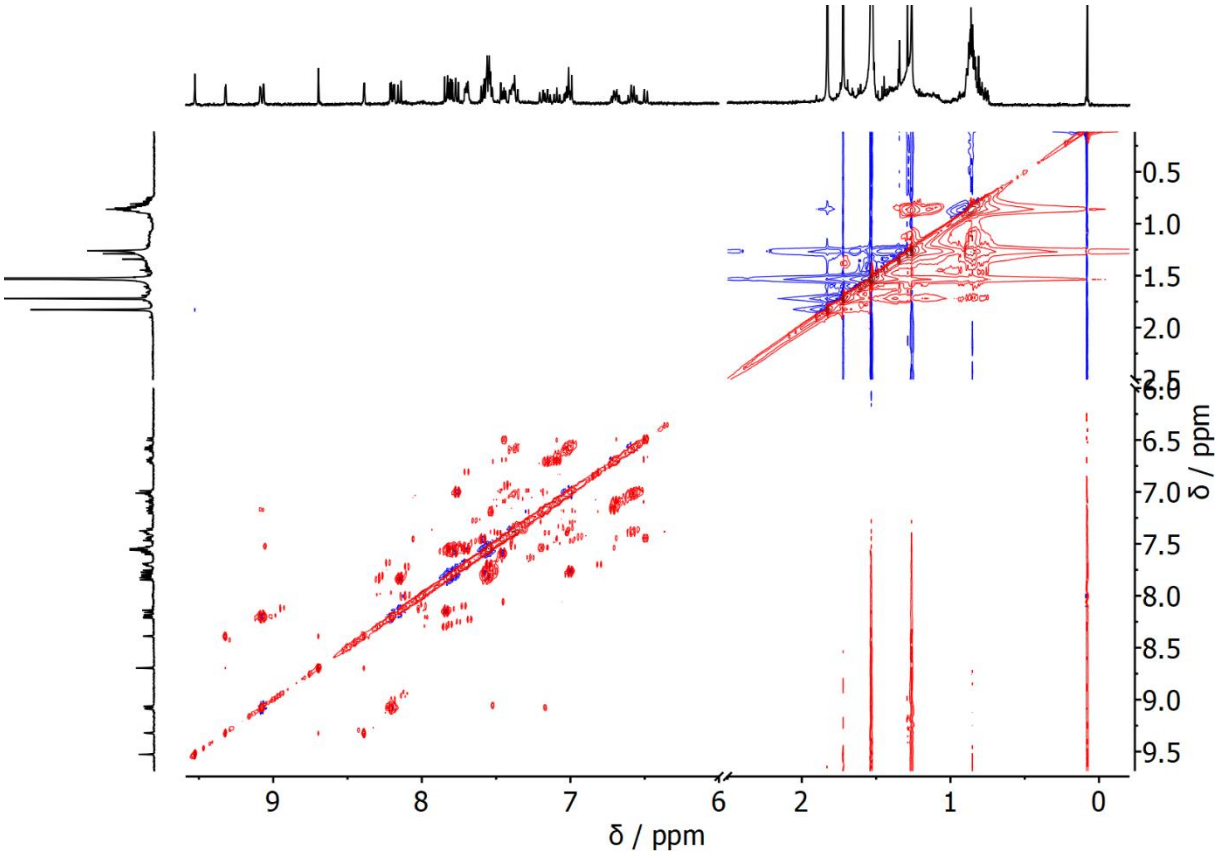


Figure S16. ^{1}H – ^{1}H TOCSY NMR spectrum of (*P*, *M*)-**3** (400 MHz, CD_2Cl_2).

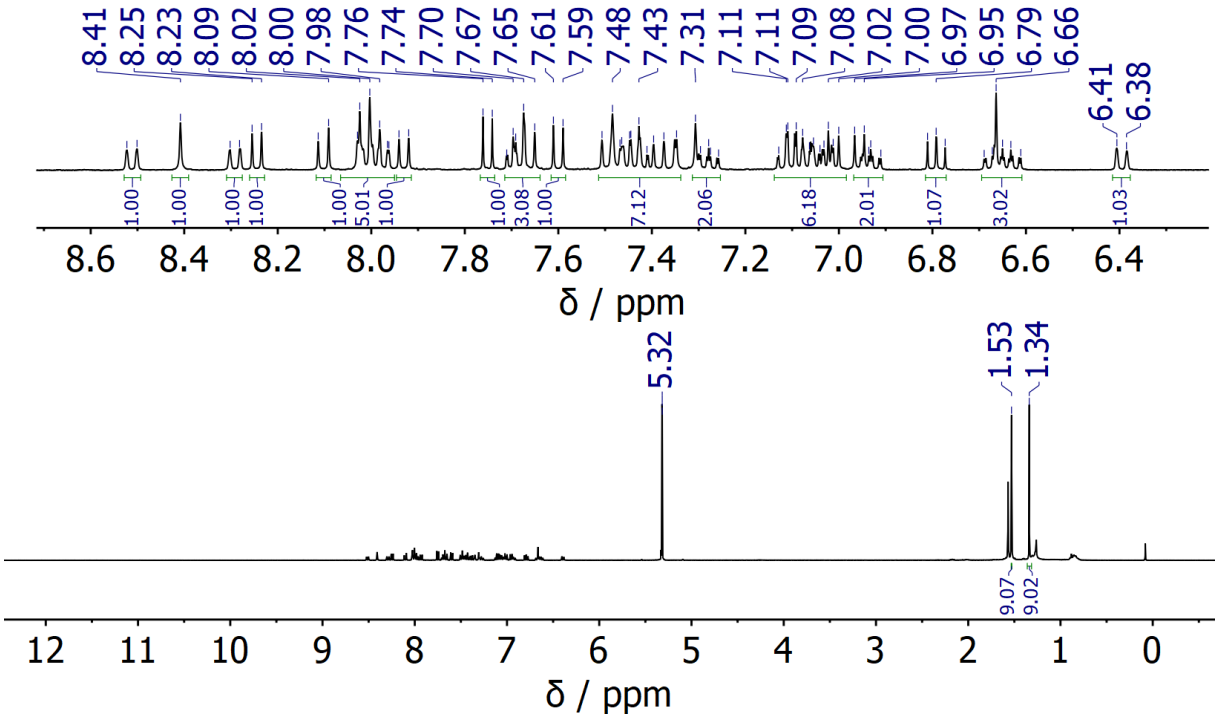


Figure S17. ^{1}H NMR spectrum of **8** (400 MHz, CD_2Cl_2).

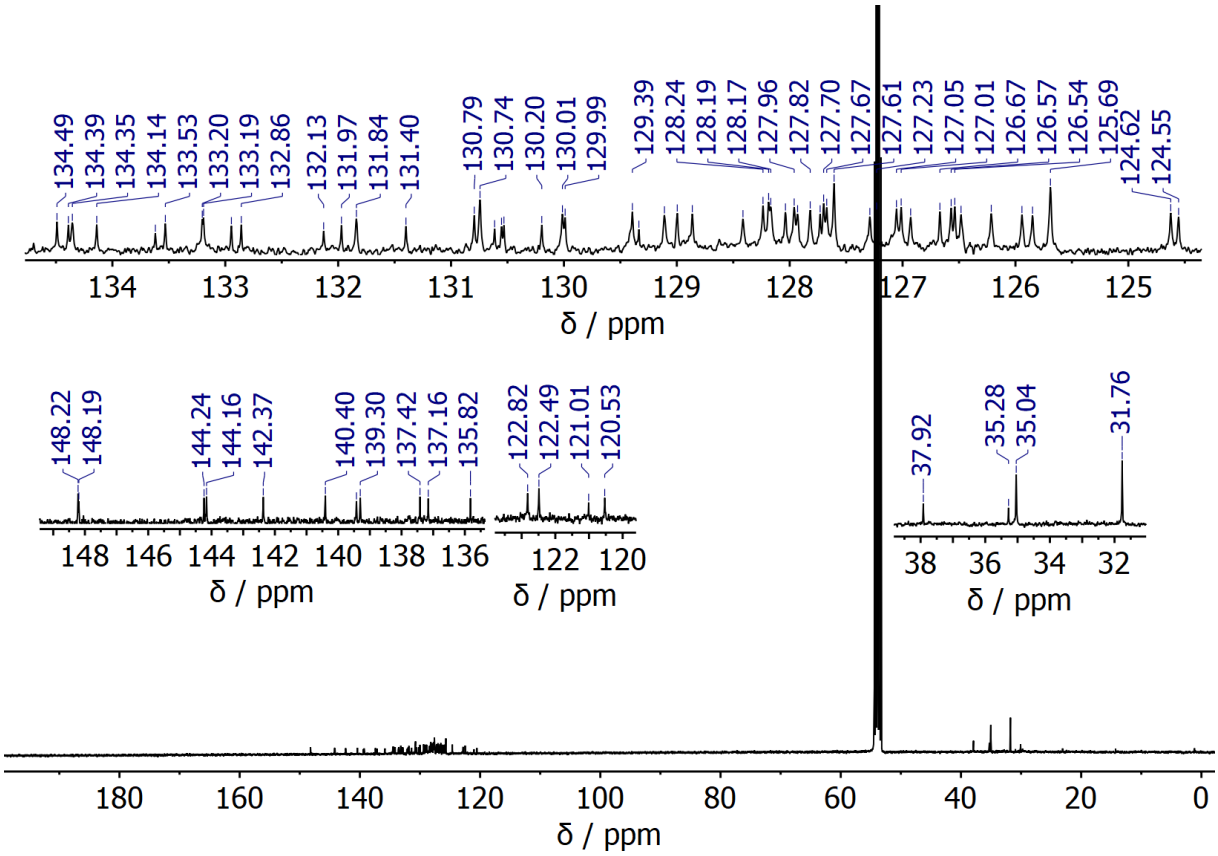


Figure S18. ^{13}C{^{1}H} NMR spectrum of **8** (101 MHz, CD_2Cl_2).

S6. High-resolution mass spectrometry (HRMS)

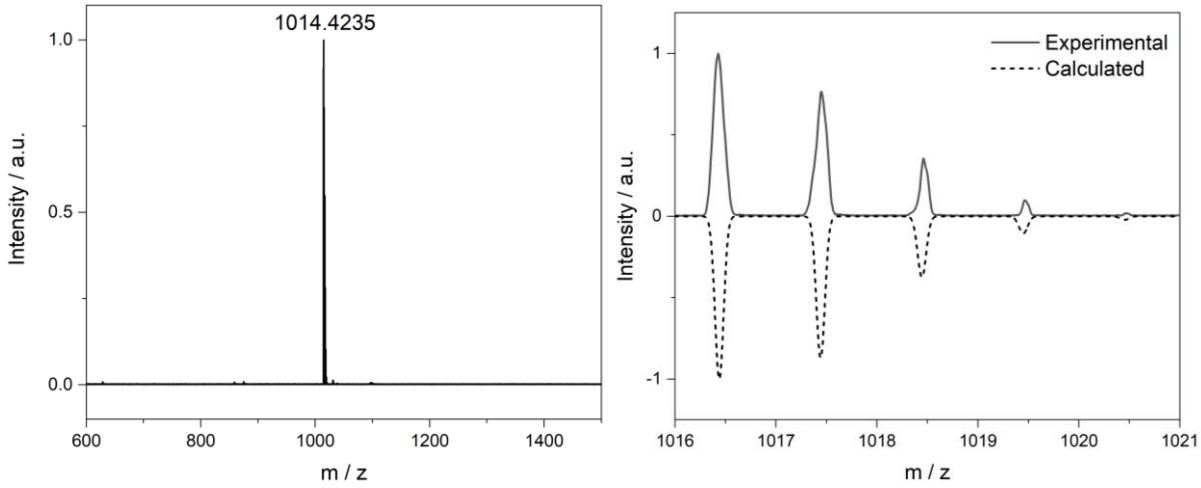


Figure S19. MALDI-TOF HRMS of (*P*, *P*)-**3**.

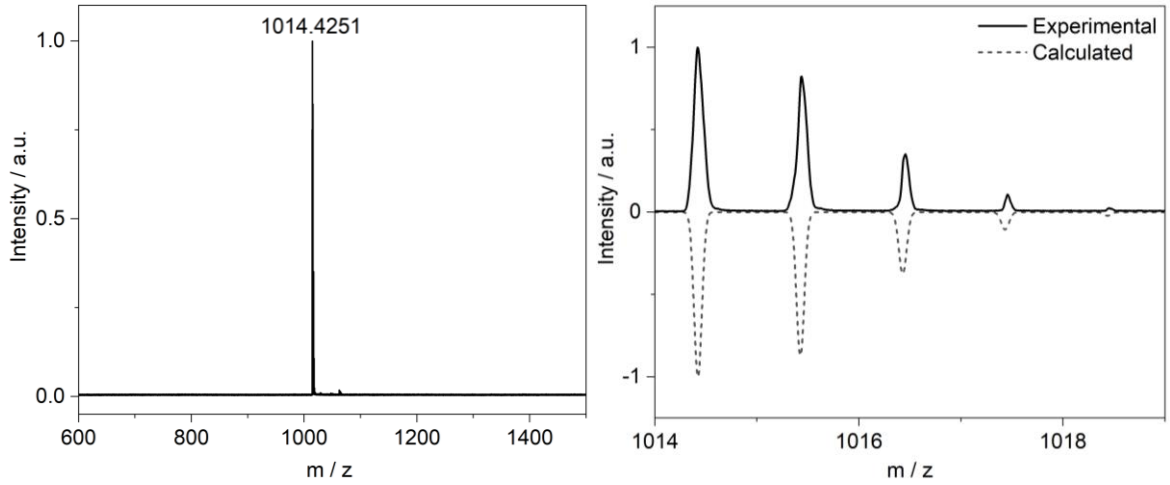


Figure S20. MALDI-TOF HRMS of (*P*, *M*)-**3**.

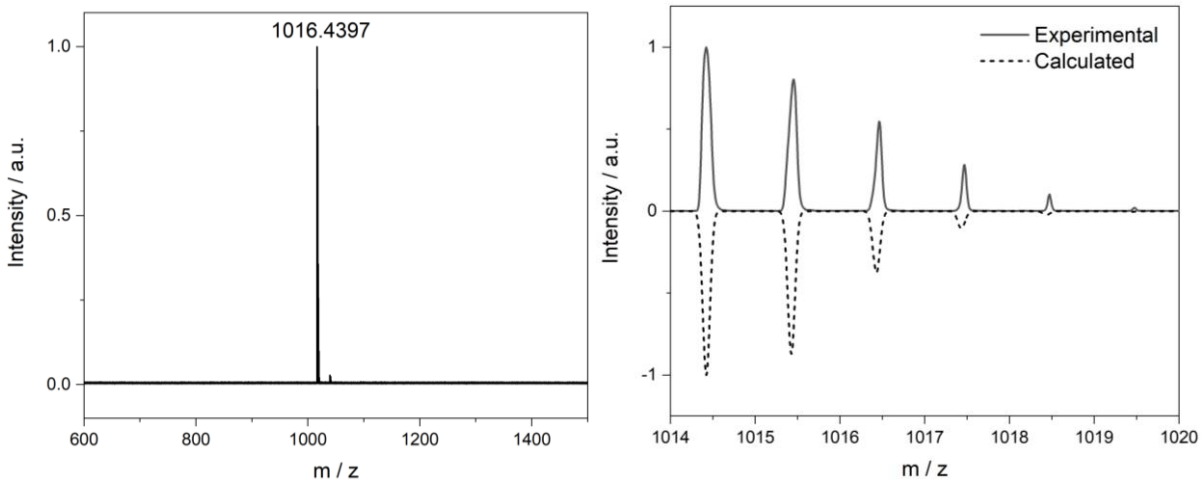


Figure S21. MALDI-TOF HRMS of **6**.

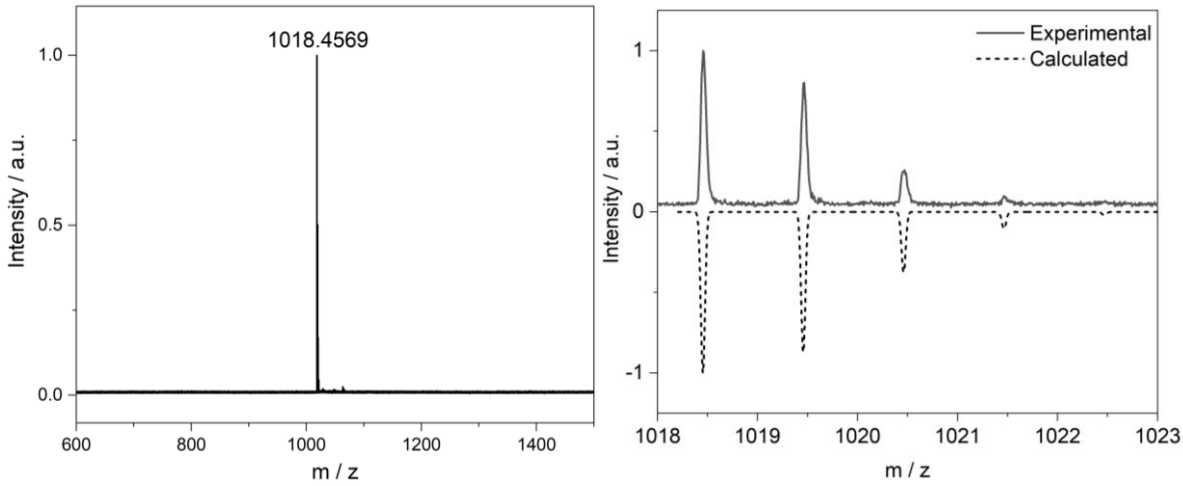


Figure S22. MALDI-TOF HRMS of **7**.

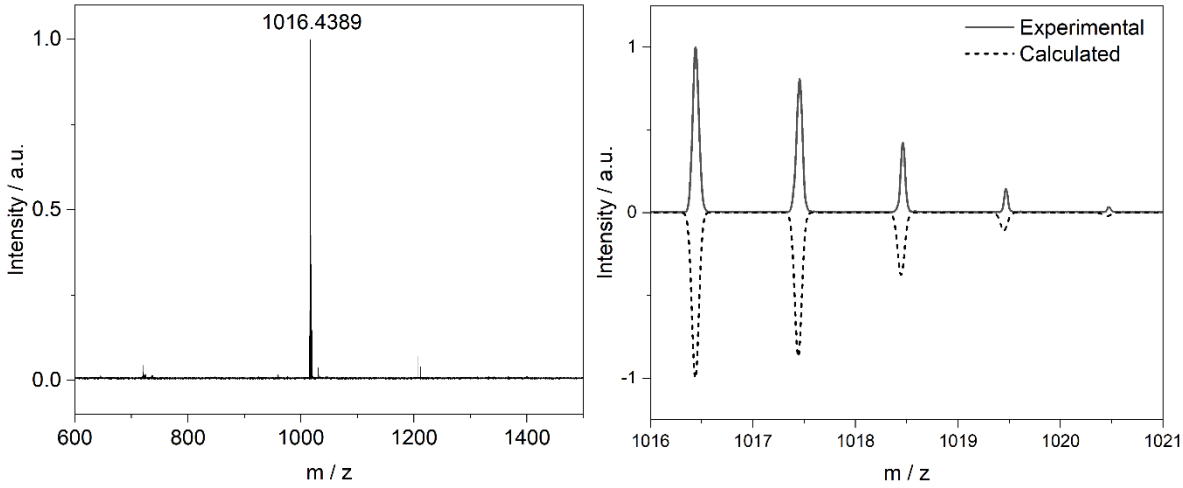
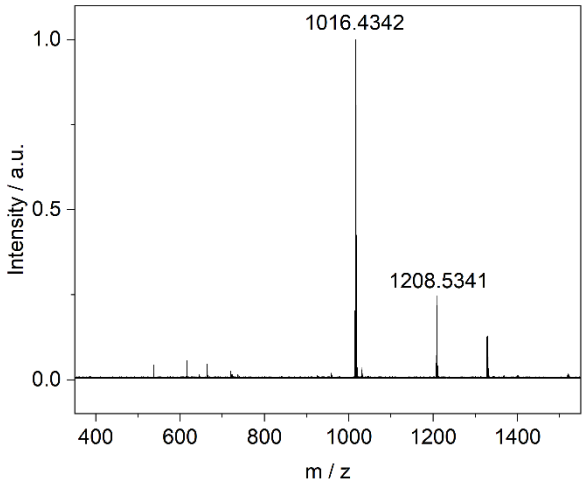


Figure S23. MALDI-TOF HRMS of **8**.

(a)



(b)

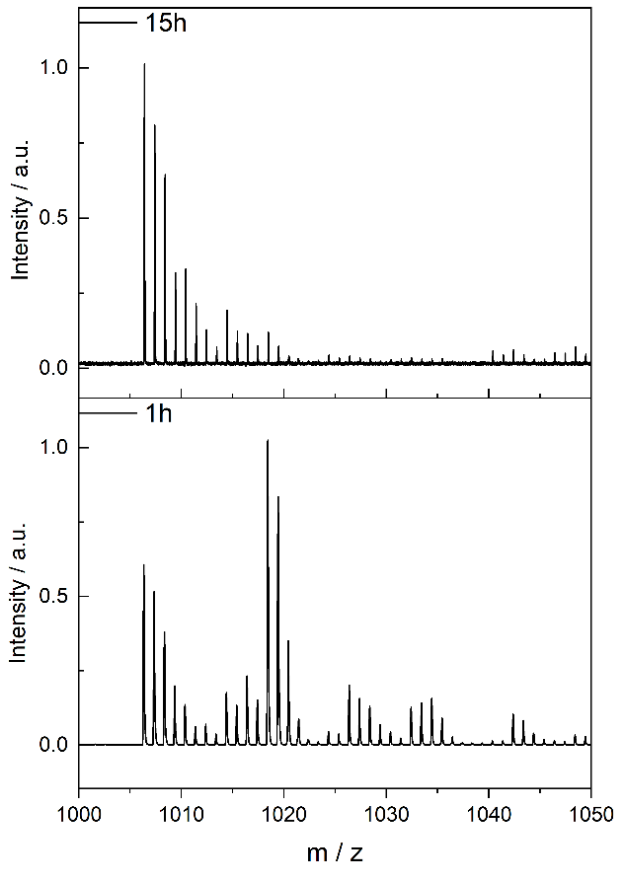


Figure S24. MALDI-TOF HRMS of reaction mixture of (a) Suzuki coupling−C-H activation after heating overnight for 15h (b) Scholl reaction with **7** in presence of triflic acid.

S7. Cartesian coordinates

3A

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- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction = 1.100558 (Hartree/Particle)
Thermal correction to Energy = 1.158745
Thermal correction to Enthalpy = 1.159689
Thermal correction to Gibbs Free Energy = 1.010042
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H	2.264369000	-2.353352000	2.178522000
H	8.615306000	-1.166346000	3.978002000
H	6.459969000	-2.313980000	4.315312000
H	-9.339491000	-4.013248000	-1.081661000
H	-9.804978000	-2.354566000	-2.855546000
H	-8.055772000	-0.685379000	-3.464254000
H	-5.959853000	-0.582169000	-2.215704000
H	-5.864912000	-0.772994000	2.161434000
H	-7.565443000	-1.979835000	3.431712000
H	-9.978351000	-1.742876000	2.849838000
H	-10.653207000	-0.152049000	1.081248000
H	5.485702000	-2.410708000	-0.094478000
H	7.042736000	-4.231925000	0.211406000
H	9.272947000	-4.200171000	-0.912182000
H	9.827000000	-2.329110000	-2.435494000
H	9.916152000	0.548641000	2.916730000
H	10.113027000	2.487916000	1.391047000
H	8.121276000	3.202758000	0.069332000
H	6.054266000	1.946189000	0.174892000

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction = 1.100831 (Hartree/Particle)
Thermal correction to Energy = 1.158871
Thermal correction to Enthalpy = 1.159815
Thermal correction to Gibbs Free Energy = 1.011320
Sum of electronic and zero-point Energies = -3079.173457
Sum of electronic and thermal Energies = -3079.115417
Sum of electronic and thermal Enthalpies = -3079.114473
Sum of electronic and thermal Free Energies = -3079.262969

3C

C	2.105898000	-0.909149000	0.140192000
C	1.203826000	-1.982521000	0.028894000
C	-0.148765000	-1.684405000	-0.179992000
C	0.307496000	4.402041000	-0.281524000
C	-1.049072000	4.704518000	-0.199569000
C	-1.952422000	3.646425000	-0.080300000
C	0.756656000	3.080577000	-0.304121000
C	-0.177549000	2.023470000	-0.201929000
C	-1.549704000	2.305869000	-0.015792000
C	2.134501000	2.750457000	-0.539465000
C	2.587207000	1.468608000	-0.522794000
C	1.660291000	0.392366000	-0.198323000
C	0.279483000	0.671584000	-0.247872000
C	-0.653202000	-0.389796000	-0.283716000
C	-2.086044000	-0.078768000	-0.308134000
C	-2.499827000	1.189214000	0.083186000
C	-1.509038000	6.168140000	-0.245837000
C	-0.890341000	6.926943000	0.943537000
C	-1.041564000	6.810542000	-1.565351000
C	1.578662000	-3.485384000	0.019957000
C	3.090031000	-3.756922000	-0.038497000
C	0.987650000	-4.095348000	-1.274760000
C	0.977693000	-4.226915000	1.227697000
C	-3.035647000	6.305674000	-0.160377000
C	-4.418065000	-0.908490000	-0.217648000
C	-4.856709000	0.424203000	0.152258000
C	-3.081078000	-1.082689000	-0.620893000
C	-3.879563000	1.384309000	0.479281000
C	-2.781723000	-2.191961000	-1.476120000
C	-5.271608000	-2.080632000	-0.206572000
C	-4.974653000	-3.125782000	-1.096138000
C	-3.727934000	-3.120387000	-1.780927000
C	-5.936306000	-4.158560000	-1.334155000
C	-7.119244000	-4.174717000	-0.672410000
C	-7.364395000	-3.250673000	0.392109000
C	-6.403854000	-2.251622000	0.684796000
C	-6.245913000	0.834028000	0.215236000
C	-6.595442000	1.859365000	1.108501000
C	-5.565109000	2.625872000	1.719563000
C	-4.269314000	2.460899000	1.339914000
C	-7.297876000	0.263442000	-0.605485000
C	-8.648876000	0.474451000	-0.235873000
C	-8.955269000	1.375426000	0.832675000
C	-7.971106000	2.095965000	1.424191000
C	4.743501000	0.134516000	-0.727689000
C	4.541817000	-0.326017000	0.670887000
C	3.870800000	1.115185000	-1.195287000
C	3.338502000	-0.947563000	0.986389000
C	4.154744000	1.772769000	-2.410376000
C	5.852928000	-0.297583000	-1.521303000
C	6.161945000	0.456457000	-2.680752000
C	5.300637000	1.486667000	-3.103472000
C	7.375773000	0.221155000	-3.409364000
C	8.256360000	-0.718236000	-3.007171000
C	7.948013000	-1.581763000	-1.904472000
C	6.730908000	-1.424710000	-1.191541000
C	5.571044000	-0.184253000	1.657420000
C	5.431134000	-0.910898000	2.863657000
C	4.210388000	-1.549961000	3.158328000
C	3.168930000	-1.506868000	2.272339000
C	6.788879000	0.611068000	1.484566000
C	7.878633000	0.395769000	2.367755000
C	7.727164000	-0.470925000	3.500607000
C	6.533599000	-1.039483000	3.772965000
C	-8.520087000	-3.364098000	1.197329000
C	-8.690800000	-2.567267000	2.303116000
C	-7.680670000	-1.657622000	2.665350000
C	-6.562023000	-1.512016000	1.879948000
C	-7.042794000	-0.440544000	-1.805337000
C	-8.062297000	-1.021744000	-2.521103000
C	-9.393809000	-0.910605000	-2.081136000
C	-9.679272000	-0.154783000	-0.970206000
C	6.418991000	-2.416577000	-0.234310000
C	7.290104000	-3.441218000	0.063082000
C	8.525469000	-3.539520000	-0.592308000
C	8.835405000	-2.627091000	-1.572877000
C	9.090603000	1.093033000	2.180193000
C	9.222268000	2.032828000	1.185547000
C	8.116310000	2.328977000	0.375654000
C	6.931489000	1.643069000	0.528010000
H	-0.846273000	-2.509148000	-0.169582000
H	1.044200000	5.196655000	-0.365186000
H	-3.008592000	3.867678000	-0.075058000
H	2.811176000	3.556713000	-0.810042000
H	-1.205472000	7.975864000	0.930076000
H	-1.208247000	6.485693000	1.893246000
H	0.202811000	6.906470000	0.913962000
H	-1.365097000	7.855804000	-1.614564000
H	-1.462458000	6.280635000	-2.425301000
H	0.047886000	6.794175000	-1.660903000
H	3.570214000	-3.167453000	-0.825625000
H	3.592836000	-3.545567000	0.905385000
H	3.255316000	-4.814566000	-0.266782000
H	1.366273000	-3.570036000	-2.156890000
H	1.279346000	-5.147660000	-1.352459000
H	-0.104521000	-4.058464000	-1.299534000
H	1.419987000	-3.886560000	2.167822000
H	1.171692000	-5.301317000	1.140108000
H	-0.105372000	-4.087008000	1.292261000
H	-3.536776000	5.814717000	-1.000537000
H	-3.432277000	5.885092000	0.769508000
H	-3.308711000	7.365001000	-0.186589000
H	-1.820258000	-2.224095000	-1.973247000
H	-3.523335000	-3.893666000	-2.515428000
H	-5.706815000	-4.913473000	-2.080733000
H	-7.867672000	-4.931298000	-0.889376000
H	-5.830463000	3.377011000	2.457577000
H	-3.499846000	3.082408000	1.779906000
H	-9.995235000	1.522513000	1.109219000
H	-8.205603000	2.847642000	2.172490000
H	3.457866000	2.513744000	-2.786734000
H	5.544561000	2.035438000	-4.008556000
H	7.582228000	0.844599000	-4.274454000
H	9.192950000	-0.867506000	-3.536546000
H	4.097940000	-2.054665000	4.113579000
H	2.205697000	-1.928237000	2.535647000
H	8.575662000	-0.610281000	4.164180000
H	6.393138000	-1.641333000	4.666195000
H	-9.263539000	-4.112418000	0.937308000
H	-9.581245000	-2.663861000	2.915927000
H	-7.779339000	-1.070295000	3.572284000
H	-5.783830000	-0.824171000	2.186275000
H	-6.027101000	-0.515223000	-2.172965000
H	-7.835979000	-1.563433000	-3.433562000
H	-10.192847000	-1.388199000	-2.638989000
H	-10.707767000	-0.010392000	-0.651329000
H	5.469424000	-2.392803000	0.275031000
H	7.007226000	-4.178028000	0.807894000
H	9.215637000	-4.340252000	-0.346998000
H	9.768276000	-2.707789000	-2.123956000
H	9.916217000	0.887635000	2.855941000
H	10.158823000	2.564295000	1.050935000
H	8.184844000	3.110578000	-0.374019000
H	6.091817000	1.929931000	-0.087929000

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction = 1.100967 (Hartree/Particle)
Thermal correction to Energy = 1.159005
Thermal correction to Enthalpy = 1.159949
Thermal correction to Gibbs Free Energy = 1.011233
Sum of electronic and zero-point Energies = -3079.170683
Sum of electronic and thermal Energies = -3079.112645
Sum of electronic and thermal Enthalpies = -3079.111701
Sum of electronic and thermal Free Energies = -3079.260417

3D

C	2.084508000	-0.930396000	-0.024752000
C	1.175892000	-1.967514000	-0.320289000
C	-0.186243000	-1.657131000	-0.326918000
C	0.261615000	4.375928000	0.442594000
C	-1.095501000	4.652790000	0.599473000
C	-2.004011000	3.609551000	0.410619000
C	0.716255000	3.080509000	0.190649000
C	-0.217471000	2.026391000	0.061479000
C	-1.601568000	2.308297000	0.082824000
C	2.100138000	2.789183000	-0.060576000
C	2.550411000	1.524688000	-0.282944000
C	1.631479000	0.406974000	-0.122732000
C	0.246734000	0.682868000	-0.063664000
C	-0.682234000	-0.383899000	-0.045427000
C	-2.102940000	-0.092018000	0.101872000
C	-2.547188000	1.210051000	-0.098628000
C	-1.546870000	6.076242000	0.953181000
C	-0.901835000	6.499539000	2.286195000
C	-1.101225000	7.039343000	-0.163549000
C	1.561777000	-3.408303000	-0.729479000
C	3.072907000	-3.645531000	-0.867987000
C	0.957766000	-3.653701000	-2.132317000
C	0.981044000	-4.443327000	0.251025000
C	-3.070705000	6.186962000	1.100984000
C	-4.455490000	-0.778628000	0.420939000
C	-4.816417000	0.309288000	-0.477680000
C	-3.083090000	-1.076679000	0.533736000
C	-3.915495000	1.390008000	-0.556504000
C	-2.700443000	-2.262838000	1.223276000
C	-5.416086000	-1.550399000	1.162876000
C	-5.019703000	-2.811086000	1.646188000
C	-3.641200000	-3.138602000	1.678391000
C	-6.002519000	-3.749025000	2.102372000
C	-7.317973000	-3.429329000	2.106277000
C	-7.738884000	-2.089715000	1.820115000
C	-6.779054000	-1.119751000	1.440686000
C	-6.027886000	0.333202000	-1.252407000
C	-6.479281000	1.575459000	-1.735023000
C	-5.595644000	2.683624000	-1.729746000
C	-4.327538000	2.568516000	-1.242430000
C	-6.827681000	-0.842958000	-1.564476000
C	-8.170003000	-0.666428000	-1.980656000
C	-8.656022000	0.650916000	-2.266926000
C	-7.817884000	1.713323000	-2.227601000
C	4.715842000	0.265278000	-0.730997000
C	4.530597000	-0.451640000	0.557610000
C	3.831573000	1.304892000	-1.012138000
C	3.337048000	-1.137121000	0.760396000
C	4.105424000	2.175483000	-2.088057000
C	5.826895000	-0.002927000	-1.593105000
C	6.127203000	0.955276000	-2.592897000
C	5.253351000	2.035187000	-2.821075000
C	7.344272000	0.873050000	-3.348995000
C	8.236086000	-0.113713000	-3.124440000
C	7.935509000	-1.171645000	-2.204056000
C	6.715051000	-1.164459000	-1.479822000
C	5.574717000	-0.500899000	1.537081000
C	5.466659000	-1.463979000	2.568246000
C	4.263852000	-2.178716000	2.735466000
C	3.204425000	-1.967261000	1.895966000
C	6.778000000	0.333376000	1.513020000
C	7.884905000	-0.036715000	2.319835000
C	7.765424000	-1.119371000	3.253165000
C	6.586133000	-1.755487000	3.417144000
C	-9.088460000	-1.709906000	1.987930000
C	-9.473881000	-0.396822000	1.860426000
C	-8.502538000	0.586832000	1.608323000
C	-7.187401000	0.232945000	1.413142000
C	-6.316921000	-2.160423000	-1.534731000
C	-7.128665000	-3.247265000	-1.764148000
C	-8.491916000	-3.068246000	-2.054214000
C	-8.993636000	-1.795268000	-2.183432000
C	6.410265000	-2.324218000	-0.731619000
C	7.291786000	-3.377581000	-0.629477000
C	8.531002000	-3.336374000	-1.283649000
C	8.833733000	-2.251418000	-2.071731000
C	9.082722000	0.706450000	2.262335000
C	9.183932000	1.829939000	1.476599000
C	8.061183000	2.262690000	0.756094000
C	6.889645000	1.538753000	0.781740000
H	-0.895989000	-2.444326000	-0.547352000
H	0.997854000	5.170379000	0.531592000
H	-3.057957000	3.795285000	0.561927000
H	2.781698000	3.628647000	-0.170750000
H	-1.200440000	5.823980000	3.093526000
H	-1.214692000	7.514366000	2.554418000
H	0.190296000	6.491028000	2.228967000
H	-1.416491000	8.062122000	0.069181000
H	-1.544686000	6.753756000	-1.122536000
H	-0.014270000	7.045403000	-0.284922000
H	3.544428000	-2.869704000	-1.478738000
H	3.582457000	-3.683368000	0.095460000
H	3.239731000	-4.606748000	-1.364302000
H	1.352050000	-2.930261000	-2.852085000
H	1.221447000	-4.658820000	-2.477448000
H	-0.132089000	-3.577526000	-2.141082000
H	-0.106919000	-4.359500000	0.335810000
H	1.409742000	-4.328367000	1.250906000
H	1.210033000	-5.457042000	-0.094590000
H	-3.449291000	5.543154000	1.901128000
H	-3.339433000	7.217722000	1.351297000
H	-3.590828000	5.926441000	0.173281000
H	-1.653282000	-2.467843000	1.400581000
H	-3.337651000	-4.073113000	2.141764000
H	-5.668169000	-4.736119000	2.408681000
H	-8.067391000	-4.159321000	2.398039000
H	-5.921049000	3.612083000	-2.190362000
H	-3.625284000	3.377778000	-1.390558000
H	-9.687421000	0.767091000	-2.586891000
H	-8.154501000	2.699977000	-2.532840000
H	3.399006000	2.964392000	-2.322451000
H	5.489589000	2.743312000	-3.610094000
H	7.543744000	1.648428000	-4.082946000
H	9.175378000	-0.150823000	-3.668549000
H	4.179089000	-2.880097000	3.560560000
H	2.253921000	-2.456963000	2.075805000
H	8.626573000	-1.375449000	3.863517000
H	6.470613000	-2.531058000	4.168757000
H	-9.815837000	-2.474979000	2.244696000
H	-10.513601000	-0.115227000	1.992364000
H	-8.786328000	1.633487000	1.572686000
H	-6.451887000	1.009055000	1.246220000
H	-5.265073000	-2.320703000	-1.336669000
H	-6.708536000	-4.246912000	-1.725584000
H	-9.133182000	-3.929167000	-2.213279000
H	-10.030191000	-1.638107000	-2.468431000
H	5.458112000	-2.408234000	-0.233450000
H	7.014180000	-4.245723000	-0.040463000
H	9.229447000	-4.161714000	-1.190620000
H	9.769036000	-2.216496000	-2.623500000
H	9.922217000	0.383975000	2.872026000
H	10.109841000	2.394852000	1.440733000
H	8.106252000	3.179976000	0.178025000
H	6.036208000	1.926481000	0.244710000

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction = 1.100302 (Hartree/Particle)
Thermal correction to Energy = 1.158511
Thermal correction to Enthalpy = 1.159455
Thermal correction to Gibbs Free Energy = 1.009862
Sum of electronic and zero-point Energies = -3079.179128
Sum of electronic and thermal Energies = -3079.120919
Sum of electronic and thermal Enthalpies = -3079.119974
Sum of electronic and thermal Free Energies = -3079.269568

3E

C	-1.966911000	-0.827100000	0.001903000
C	-1.085064000	-1.911953000	-0.209043000
C	0.276571000	-1.621956000	-0.350996000
C	-0.080754000	4.465754000	-0.187137000
C	1.280244000	4.743607000	-0.082663000
C	2.166552000	3.668311000	0.019991000
C	-0.553638000	3.152709000	-0.249341000
C	0.361939000	2.079933000	-0.176779000
C	1.737251000	2.335705000	0.028688000
C	-1.939127000	2.849259000	-0.459890000
C	-2.420687000	1.571998000	-0.482559000
C	-1.506718000	0.479914000	-0.232565000
C	-0.118170000	0.741441000	-0.265978000
C	0.798277000	-0.330579000	-0.349124000
C	2.228173000	-0.037062000	-0.351774000
C	2.654943000	1.201547000	0.114254000
C	1.761124000	6.201328000	-0.080922000
C	1.324263000	6.885257000	-1.390045000
C	1.134628000	6.937382000	1.118608000
C	-1.496380000	-3.395995000	-0.427431000
C	-2.992075000	-3.597084000	-0.740287000
C	-1.095484000	-4.284785000	0.763192000
C	-0.742699000	-3.907121000	-1.681962000
C	3.287785000	6.314562000	0.032398000
C	4.599294000	-0.692142000	-0.587746000
C	4.875833000	0.198873000	0.531152000
C	3.242730000	-0.937042000	-0.878182000
C	3.973456000	1.263837000	0.726334000
C	2.922862000	-1.949971000	-1.826968000
C	5.622962000	-1.323306000	-1.376534000
C	5.269750000	-2.455235000	-2.134448000
C	3.899537000	-2.737642000	-2.360641000
C	6.287884000	-3.305956000	-2.676203000
C	7.598908000	-3.019804000	-2.497907000
C	7.995252000	-1.771732000	-1.915715000
C	7.007300000	-0.875311000	-1.439557000
C	6.007048000	0.052051000	1.406589000
C	6.409541000	1.170843000	2.159523000
C	5.530936000	2.275709000	2.282815000
C	4.316915000	2.280973000	1.662085000
C	6.773819000	-1.176555000	1.561791000
C	8.068528000	-1.107396000	2.132141000
C	8.523961000	0.121802000	2.711208000
C	7.693693000	1.187567000	2.795425000
C	-4.828222000	0.593511000	-0.393312000
C	-4.547449000	-0.663326000	0.341752000
C	-3.820155000	1.395501000	-0.968224000
C	-3.251253000	-1.059501000	0.718091000
C	-4.167993000	2.223135000	-2.067232000
C	-6.175752000	1.095369000	-0.545319000
C	-6.500796000	1.838522000	-1.700872000
C	-5.460023000	2.341328000	-2.504292000
C	-7.876338000	2.051405000	-2.053066000
C	-8.876050000	1.634888000	-1.243497000
C	-8.577597000	1.127664000	0.064915000
C	-7.229722000	0.934776000	0.448351000
C	-5.593105000	-1.575467000	0.743726000
C	-5.442963000	-2.299026000	1.948236000
C	-4.184087000	-2.320402000	2.581300000
C	-3.103812000	-1.813668000	1.909217000
C	-6.786015000	-1.842505000	-0.047359000
C	-7.892180000	-2.479683000	0.561797000
C	-7.769878000	-2.988826000	1.897250000
C	-6.573638000	-2.966602000	2.527543000
C	9.355564000	-1.394527000	-1.884561000
C	9.731594000	-0.140235000	-1.467033000
C	8.744074000	0.794711000	-1.113386000
C	7.415598000	0.436807000	-1.109487000
C	6.269981000	-2.454702000	1.230315000
C	7.055841000	-3.580072000	1.325106000
C	8.383346000	-3.484780000	1.775606000
C	8.868741000	-2.269068000	2.194379000
C	-6.958820000	0.686624000	1.811786000
C	-7.976883000	0.495017000	2.717622000
C	-9.317727000	0.564268000	2.303504000
C	-9.607981000	0.897552000	1.001402000
C	-9.079360000	-2.669493000	-0.177297000
C	-9.152949000	-2.307657000	-1.501863000
C	-8.016947000	-1.782078000	-2.140456000
C	-6.858176000	-1.566761000	-1.430328000
H	0.966650000	-2.451863000	-0.398160000
H	-0.803040000	5.275240000	-0.250630000
H	3.228367000	3.864430000	0.056476000
H	-2.615051000	3.679400000	-0.641888000
H	1.662412000	7.926953000	-1.405782000
H	1.752120000	6.372760000	-2.257085000
H	0.236483000	6.886029000	-1.503552000
H	1.466832000	7.980899000	1.139199000
H	1.429246000	6.465095000	2.060879000
H	0.042038000	6.936133000	1.070501000
H	-3.335843000	-2.897562000	-1.508395000
H	-3.636121000	-3.492319000	0.131209000
H	-3.137661000	-4.611456000	-1.124822000
H	-0.037159000	-4.160792000	1.014314000
H	-1.689159000	-4.055738000	1.650596000
H	-1.260847000	-5.338661000	0.514362000
H	-0.937399000	-3.262208000	-2.544554000
H	0.338987000	-3.967399000	-1.537895000
H	-1.087351000	-4.916453000	-1.926979000
H	3.795309000	5.836501000	-0.811392000
H	3.662236000	5.866971000	0.958921000
H	3.576347000	7.370079000	0.036012000
H	1.898060000	-2.087207000	-2.144681000
H	3.638173000	-3.551393000	-3.031179000
H	5.980368000	-4.205874000	-3.201090000
H	8.370065000	-3.693697000	-2.859661000
H	5.809455000	3.092217000	2.943006000
H	3.603758000	3.059576000	1.896632000
H	9.518904000	0.155426000	3.145506000
H	7.998463000	2.091583000	3.314859000
H	-3.366679000	2.715772000	-2.605728000
H	-5.693621000	2.883094000	-3.415732000
H	-8.090731000	2.538498000	-2.999973000
H	-9.916020000	1.759098000	-1.530466000
H	-4.066305000	-2.814688000	3.540622000
H	-2.100382000	-1.947336000	2.296809000
H	-8.633473000	-3.460988000	2.356111000
H	-6.446137000	-3.436659000	3.498406000
H	10.101079000	-2.109320000	-2.221661000
H	10.779820000	0.140112000	-1.447968000
H	9.026208000	1.807960000	-0.846893000
H	6.670484000	1.180286000	-0.858361000
H	5.242958000	-2.555562000	0.904609000
H	6.642174000	-4.546138000	1.055044000
H	9.006334000	-4.371806000	1.828517000
H	9.871824000	-2.187941000	2.603802000
H	-5.930485000	0.650407000	2.150878000
H	-7.739262000	0.294526000	3.757080000
H	-10.117507000	0.393364000	3.016873000
H	-10.638955000	1.015265000	0.679746000
H	-9.930921000	-3.129927000	0.315730000
H	-10.070391000	-2.459930000	-2.061195000
H	-8.048461000	-1.549369000	-3.199710000
H	-5.984905000	-1.179379000	-1.941343000

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction = 1.099073 (Hartree/Particle)
Thermal correction to Energy = 1.157226
Thermal correction to Enthalpy = 1.158170
Thermal correction to Gibbs Free Energy = 1.009672
Sum of electronic and zero-point Energies = -3079.134833
Sum of electronic and thermal Energies = -3079.076681
Sum of electronic and thermal Enthalpies = -3079.075737
Sum of electronic and thermal Free Energies = -3079.224235

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C	2.030346000	-0.988663000	-0.137674000
C	1.106601000	-2.044705000	-0.356247000
C	-0.229950000	-1.717628000	-0.526254000
C	0.321680000	4.409586000	-0.561011000
C	-1.021287000	4.738086000	-0.477828000
C	-1.950541000	3.691257000	-0.361042000
C	0.758043000	3.065267000	-0.567004000
C	-0.188416000	2.024842000	-0.450081000
C	-1.567309000	2.345458000	-0.290595000
C	2.120230000	2.715562000	-0.760403000
C	2.554608000	1.411959000	-0.737302000
C	1.616582000	0.360513000	-0.448167000
C	0.244633000	0.669777000	-0.440048000
C	-0.723278000	-0.388826000	-0.496476000
C	-2.096565000	-0.059501000	-0.538646000
C	-2.501469000	1.265656000	-0.108235000
C	-1.453926000	6.210640000	-0.523117000
C	-0.813687000	6.958869000	0.661407000
C	-0.983714000	6.842499000	-1.846561000
C	1.486962000	-3.537488000	-0.522980000
C	2.999788000	-3.806616000	-0.523177000
C	0.970037000	-3.971807000	-1.915565000
C	0.821101000	-4.423513000	0.545049000
C	-2.977054000	6.376440000	-0.426883000
C	-4.478459000	-0.637102000	-0.654214000
C	-4.646813000	0.258929000	0.505693000
C	-3.153208000	-0.917469000	-1.039948000
C	-3.741476000	1.356215000	0.588114000
C	-2.918616000	-1.922590000	-2.014635000
C	-5.564139000	-1.231163000	-1.360665000
C	-5.291456000	-2.370268000	-2.158027000
C	-3.953897000	-2.680802000	-2.489550000
C	-6.365216000	-3.215093000	-2.586514000
C	-7.648945000	-2.932435000	-2.258400000
C	-7.982763000	-1.685999000	-1.632205000
C	-6.951165000	-0.784913000	-1.274652000
C	-5.675533000	0.111787000	1.471563000
C	-6.040150000	1.249807000	2.236781000
C	-5.192989000	2.389035000	2.234740000
C	-4.048909000	2.417155000	1.496211000
C	-6.436525000	-1.116306000	1.682825000
C	-7.695763000	-1.040672000	2.328057000
C	-8.108545000	0.189959000	2.929596000
C	-7.272698000	1.261886000	2.951637000
C	4.718878000	0.099966000	-0.725879000
C	4.374698000	-0.398467000	0.631771000
C	3.892358000	1.072002000	-1.285053000
C	3.166361000	-1.091613000	0.789143000
C	4.308170000	1.756099000	-2.446825000
C	5.923872000	-0.299783000	-1.388972000
C	6.361875000	0.485431000	-2.483791000
C	5.537127000	1.505990000	-2.995784000
C	7.665030000	0.290444000	-3.052243000
C	8.506138000	-0.641971000	-2.558706000
C	8.071917000	-1.543643000	-1.531539000
C	6.768019000	-1.427422000	-0.983708000
C	5.301875000	-0.293335000	1.713214000
C	5.098301000	-1.123958000	2.843083000
C	3.905298000	-1.870784000	2.959300000
C	2.943745000	-1.809025000	1.991419000
C	6.487782000	0.566109000	1.708224000
C	7.498088000	0.348440000	2.680948000
C	7.290429000	-0.602106000	3.733007000
C	6.114025000	-1.259138000	3.842665000
C	-9.330411000	-1.314210000	-1.441896000
C	-9.659270000	-0.059299000	-0.983704000
C	-8.642094000	0.879328000	-0.749080000
C	-7.319639000	0.525359000	-0.903303000
C	-5.958285000	-2.390942000	1.315572000
C	-6.744734000	-3.514989000	1.446519000
C	-8.041076000	-3.415298000	1.977064000
C	-8.496123000	-2.199361000	2.431046000
C	6.343723000	-2.461191000	-0.118181000
C	7.184125000	-3.485038000	0.258850000
C	8.500434000	-3.540241000	-0.221071000
C	8.925031000	-2.588250000	-1.117380000
C	8.680556000	1.118363000	2.657637000
C	8.854408000	2.124430000	1.737211000
C	7.819391000	2.411518000	0.835173000
C	6.666146000	1.658065000	0.828001000
H	-0.951206000	-2.521318000	-0.595606000
H	1.074811000	5.187838000	-0.650611000
H	-3.008708000	3.915055000	-0.366809000
H	2.831508000	3.510223000	-0.968808000
H	-1.111511000	8.012914000	0.650470000
H	-1.131371000	6.522786000	1.613586000
H	0.278578000	6.919762000	0.623181000
H	-1.288414000	7.893471000	-1.895383000
H	0.104553000	6.805330000	-1.948695000
H	-1.419570000	6.319025000	-2.702995000
H	3.528971000	-3.122608000	-1.193577000
H	3.440198000	-3.721166000	0.470888000
H	3.181509000	-4.827512000	-0.873545000
H	1.247955000	-5.013461000	-2.107557000
H	1.409514000	-3.349865000	-2.701196000
H	-0.118043000	-3.901555000	-1.996250000
H	-0.265780000	-4.301754000	0.557537000
H	1.197574000	-4.197656000	1.546483000
H	1.036586000	-5.477741000	0.340725000
H	-3.230641000	7.440670000	-0.449759000
H	-3.373849000	5.962290000	0.505867000
H	-3.492843000	5.896372000	-1.264482000
H	-1.916140000	-2.084406000	-2.391250000
H	-3.761291000	-3.502706000	-3.173373000
H	-6.119488000	-4.115190000	-3.142802000
H	-8.453960000	-3.608040000	-2.532571000
H	-5.443425000	3.223224000	2.884284000
H	-3.350408000	3.234760000	1.619207000
H	-9.073066000	0.228837000	3.427361000
H	-7.552073000	2.169318000	3.479607000
H	3.648512000	2.492802000	-2.892522000
H	5.880831000	2.076755000	-3.853664000
H	7.969350000	0.939328000	-3.868376000
H	9.507532000	-0.759166000	-2.962667000
H	3.745882000	-2.468022000	3.852601000
H	1.990698000	-2.305764000	2.131329000
H	8.077221000	-0.742784000	4.468410000
H	5.929734000	-1.935099000	4.672684000
H	-10.108290000	-2.031618000	-1.688018000
H	-10.699151000	0.216476000	-0.840961000
H	-8.894321000	1.890930000	-0.448793000
H	-6.550532000	1.269497000	-0.739498000
H	-4.953750000	-2.491049000	0.924107000
H	-6.354903000	-4.480614000	1.141779000
H	-8.665095000	-4.299319000	2.060555000
H	-9.473796000	-2.116734000	2.897622000
H	5.330556000	-2.471460000	0.250778000
H	6.814414000	-4.255188000	0.928077000
H	9.165055000	-4.340209000	0.088805000
H	9.925353000	-2.636963000	-1.538631000
H	9.447094000	0.912936000	3.399726000
H	9.767352000	2.711129000	1.729140000
H	7.918200000	3.238462000	0.139438000
H	5.878185000	1.934202000	0.142344000

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C	0.670574000	0.106314000	-6.002296000
C	-0.670574000	-0.106314000	-6.002296000
C	1.404992000	0.207014000	-4.775871000
C	0.709563000	0.085182000	-3.557276000
C	-0.709563000	-0.085182000	-3.557276000
C	-1.404992000	-0.207014000	-4.775871000
C	2.802773000	0.413465000	-4.768287000
C	3.510040000	0.521016000	-3.584288000
C	2.803834000	0.368676000	-2.377700000
C	1.435381000	0.096359000	-2.329527000
C	-1.435381000	-0.096359000	-2.329527000
C	-2.803834000	-0.368676000	-2.377700000
C	-3.510040000	-0.521016000	-3.584288000
C	-2.802773000	-0.413465000	-4.768287000
C	-0.529639000	0.518863000	1.296930000
C	0.529639000	-0.518863000	1.296930000
C	-1.294251000	0.630847000	0.096376000
C	1.294251000	-0.630847000	0.096376000
C	0.721793000	-0.122369000	-1.094112000
C	-0.721793000	0.122369000	-1.094112000
C	-2.516608000	1.377432000	0.140171000
C	-0.844414000	1.312175000	2.417785000
C	-2.147925000	1.891143000	2.481916000
C	-2.947721000	1.928681000	1.308531000
C	-2.661991000	2.327345000	3.729547000
C	-1.929323000	2.214652000	4.876356000
C	-0.555461000	1.830005000	4.826240000
C	0.026549000	1.481746000	3.581229000
C	0.251397000	1.855603000	5.985248000
C	1.605960000	1.624781000	5.908569000
C	2.201698000	1.401331000	4.657790000
C	1.425374000	1.347178000	3.517229000
C	0.844414000	-1.312175000	2.417785000
C	2.147925000	-1.891143000	2.481916000
C	2.947721000	-1.928681000	1.308531000
C	2.516608000	-1.377432000	0.140171000
C	-0.026549000	-1.481746000	3.581229000
C	0.555461000	-1.830005000	4.826240000
C	1.929323000	-2.214652000	4.876356000
C	2.661991000	-2.327345000	3.729547000
C	-0.251397000	-1.855603000	5.985248000
C	-1.605960000	-1.624781000	5.908569000
C	-2.201698000	-1.401331000	4.657790000
C	-1.425374000	-1.347178000	3.517229000
C	-5.015770000	-0.805139000	-3.529423000
C	5.015770000	0.805139000	-3.529423000
C	-5.719956000	0.320811000	-2.748063000
C	-5.641921000	-0.883491000	-4.927855000
C	-5.250731000	-2.150448000	-2.816660000
C	5.641921000	0.883491000	-4.927855000
C	5.250731000	2.150448000	-2.816660000
C	5.719956000	-0.320811000	-2.748063000
H	1.213361000	0.193143000	-6.939334000
H	-1.213361000	-0.193143000	-6.939334000
H	3.304479000	0.503993000	-5.725628000
H	3.331870000	0.500156000	-1.440259000
H	-3.331870000	-0.500156000	-1.440259000
H	-3.304479000	-0.503993000	-5.725628000
H	-3.087055000	1.525420000	-0.768126000
H	-3.903217000	2.444636000	1.348663000
H	-3.680724000	2.703421000	3.763838000
H	-2.359164000	2.489397000	5.835127000
H	-0.214917000	2.085057000	6.939272000
H	2.215984000	1.646321000	6.805945000
H	3.276291000	1.273129000	4.581828000
H	1.901855000	1.188149000	2.557282000
H	3.903217000	-2.444636000	1.348663000
H	3.087055000	-1.525420000	-0.768126000
H	2.359164000	-2.489397000	5.835127000
H	3.680724000	-2.703421000	3.763838000
H	0.214917000	-2.085057000	6.939272000
H	-2.215984000	-1.646321000	6.805945000
H	-3.276291000	-1.273129000	4.581828000
H	-1.901855000	-1.188149000	2.557282000
H	-5.361234000	0.387580000	-1.716513000
H	-5.552025000	1.290271000	-3.227558000
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H	-6.715395000	-1.076362000	-4.839371000
H	-5.517007000	0.053642000	-5.479801000
H	-5.208387000	-1.695205000	-5.520541000
H	-6.322473000	-2.371024000	-2.766882000
H	-4.757144000	-2.965500000	-3.354632000
H	-4.864049000	-2.141260000	-1.793594000
H	5.208387000	1.695205000	-5.520541000
H	6.715395000	1.076362000	-4.839371000
H	5.517007000	-0.053642000	-5.479801000
H	4.757144000	2.965500000	-3.354632000
H	4.864049000	2.141260000	-1.793594000
H	6.322473000	2.371024000	-2.766882000
H	5.361234000	-0.387580000	-1.716513000
H	5.552025000	-1.290271000	-3.227558000
H	6.799383000	-0.139185000	-2.711467000

2 Excited State S_1

C	6.117487000	-0.097686000	0.468289000
C	5.886575000	-1.441122000	0.162815000
C	4.598815000	-1.816607000	-0.215147000
C	1.950197000	3.737042000	0.084379000
C	0.651118000	3.371918000	-0.118700000
C	0.333585000	1.954057000	-0.010909000
C	2.993754000	2.777049000	0.290403000
C	2.722408000	1.409482000	0.015552000
C	1.396646000	0.993519000	-0.296215000
C	4.310270000	3.160566000	0.627523000
C	5.326798000	2.241576000	0.710674000
C	5.094471000	0.868145000	0.415678000
C	3.783696000	0.469611000	0.042582000
C	3.538177000	-0.889376000	-0.289825000
C	2.241413000	-1.246195000	-0.717848000
C	1.189237000	-0.333829000	-0.745218000
C	-0.363613000	4.432357000	-0.609827000
C	-0.464063000	5.616169000	0.367976000
C	0.166138000	4.950152000	-1.967125000
C	6.994647000	-2.502405000	0.223356000
C	7.172458000	-3.133197000	-1.170580000
C	6.597643000	-3.593303000	1.235771000
C	8.343681000	-1.913927000	0.658173000
C	-1.775640000	3.882096000	-0.867157000
C	-1.363063000	0.189557000	0.540502000
C	-1.322156000	-0.383993000	-0.826209000
C	-0.775303000	1.478657000	0.743472000
C	-0.086102000	-0.733332000	-1.373265000
C	-1.249866000	2.263573000	1.840561000
C	-2.175758000	-0.399457000	1.549057000
C	-2.635902000	0.427199000	2.606777000
C	-2.165499000	1.766721000	2.712800000
C	-3.624273000	-0.040089000	3.516109000
C	-4.155710000	-1.284520000	3.397894000
C	-3.656474000	-2.196687000	2.419818000
C	-2.626318000	-1.791307000	1.529186000
C	-2.533176000	-0.702893000	-1.528607000
C	-2.447774000	-1.604492000	-2.616219000
C	-1.186565000	-2.001228000	-3.105714000
C	-0.034145000	-1.528943000	-2.537855000
C	-3.858240000	-0.190461000	-1.178342000
C	-5.006212000	-0.804145000	-1.742733000
C	-4.858992000	-1.821916000	-2.741825000
C	-3.634868000	-2.157076000	-3.202559000
C	-4.144434000	-3.522462000	2.378475000
C	-3.603320000	-4.450635000	1.522813000
C	-2.524830000	-4.080981000	0.702944000
C	-2.047051000	-2.789326000	0.713023000
C	-4.071177000	0.943695000	-0.362501000
C	-5.337354000	1.374797000	-0.036595000
C	-6.467176000	0.699159000	-0.521678000
C	-6.295974000	-0.362949000	-1.377510000
H	7.109005000	0.237613000	0.752153000
H	4.384679000	-2.851428000	-0.469037000
H	2.241544000	4.783799000	0.039734000
H	4.511262000	4.209960000	0.825944000
H	6.328272000	2.556342000	0.989400000
H	2.056961000	-2.273854000	-1.018039000
H	0.507208000	6.088369000	0.539931000
H	-0.862772000	5.303399000	1.337667000
H	-1.137386000	6.378915000	-0.037480000
H	1.151896000	5.412261000	-1.868538000
H	0.250343000	4.128694000	-2.685026000
H	-0.519507000	5.698158000	-2.380276000
H	7.447319000	-2.372995000	-1.908249000
H	7.963749000	-3.890329000	-1.146687000
H	6.255748000	-3.619572000	-1.515829000
H	6.460195000	-3.165108000	2.233379000
H	5.665034000	-4.089615000	0.953030000
H	7.379108000	-4.358649000	1.295268000
H	8.697786000	-1.150508000	-0.041925000
H	9.096213000	-2.707828000	0.689895000
H	8.288736000	-1.469647000	1.657093000
H	-1.751504000	2.981010000	-1.487255000
H	-2.363133000	4.640158000	-1.394580000
H	-2.305981000	3.643119000	0.056540000
H	-0.816379000	3.244514000	1.997836000
H	-2.516829000	2.374739000	3.541709000
H	-3.973827000	0.638134000	4.289352000
H	-4.939265000	-1.619364000	4.071303000
H	-1.143105000	-2.669752000	-3.960766000
H	0.930795000	-1.784187000	-2.962390000
H	-5.754289000	-2.274260000	-3.158360000
H	-3.520547000	-2.879554000	-4.005492000
H	-4.948238000	-3.799541000	3.054937000
H	-3.984597000	-5.466470000	1.500678000
H	-2.054660000	-4.817403000	0.059284000
H	-1.196284000	-2.550136000	0.090521000
H	-3.227187000	1.509465000	0.002451000
H	-5.453886000	2.249724000	0.594802000
H	-7.463841000	1.032005000	-0.250401000
H	-7.156923000	-0.868138000	-1.806473000

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