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SUPPLEMENTARY INFORMATION

On the mechanism of mechanochemical molecular encapsulation in peptidic capsules

M. P. Szymański, H. Jędrzejewska, M. Wierzbicki and A. Szumna*

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Experimental procedures

***Soln*-(L-1)$_2$**: was synthesized according to a previously published procedure[1] in chloroform and vacuum dried (12 h, 1.5 mbar).

***Mill*-(L-1)$_2$**: Tetraformylresorcin[4]arene **2** (103 mg) and L-**3** (86.5 mg) were placed in a milling jar (12 ml volume) with 11 hardened steel balls (Ø 4 mm). The milling process using a Retsch PM100 planetary ball mill lasted for 1 hour at a rotation speed of 500 rpm.

Mechanochemical complexation experiments: In a typical experiment a solid sample of *soln*-(L-**1**)$_2$ (10 mg) and solid C_{60} (typically 1 equivalent, 2.5 mg) were placed in a milling jar (12 ml volume) with 11 hardened steel balls (Ø 4 mm). The milling process using a Retsch PM100 planetary ball mill lasted for 1 hour at a rotation speed of 500 rpm. Then the sample was dissolved in chlobenzene-d_5 and the ratio between complexed and uncomplexed species was analyzed by NMR. All mechanochemical experiments were performed under analogous conditions (using the same vial and the same number of balls of the same size) and repeated at least twice using different batches of (L-**1**)$_2$ (from different synthetic runs).

Solid State Electronic Circular Dichroism measurements (ssECD): Solid-state samples were prepared using the pellet technique. The solid compounds were mixed with dried KCl, ground in a ball mill (Specac Ltd.) for 1 min and pressed at 10 tons under vacuum for 5 min to make a 13-mm diameter transparent disc. Several samples (min. 3, max. 5 depending on a specific case) were prepared for each compound to guarantee proper data quality. Absorption spectra were collected as HT voltage in an ECD spectrometer, and by using a Jasco V-670 UV-Vis-NIR spectrometer equipped with a 60 mm Integrating Sphere (Model ISN-723) coated with barium sulfate. Diffuse transmission UV (DTUV) spectra were obtained in the range of 200–500 nm using 100 nm/min scanning speed, step size of 0.2 nm, bandwidth of 5 nm, fast response, and accumulation of three scans. The spectra were background-corrected using a KCl pellet containing no sample. Absorption spectra obtained by conversion of HT voltage using data-processing software were in line with DTUV, therefore only these spectra are given in the article. All ECD spectra (both in DTCD and transmission mode) were obtained using measurements taken at four different spots (by rotation of the pellet) for each pellet at 100 nm/min scanning speed, 0.2 nm step size, 1 nm bandwidth and 0.5 sec response time. For each spectrum 10 scans were accumulated with continuous scanning mode. DTCD spectra were recorded using the integrating sphere compartment (model DRCD-466 L) coated with barium sulfate in the range of 200–500 nm, while transmission spectra were recorded in the range of 180–500 nm. After measurements for each sample the CD and UV/Vis spectra were averaged over the number of scans and spots. Then the intensities of ssUV/Vis spectra were normalized and the same scaling factors were used for scaling the intensities of the ssECD spectra.

Comparison of ^{1}H and ^{13}C NMR spectra of (L-1)$_2$⊃C_{60} and (L-1)$_2$

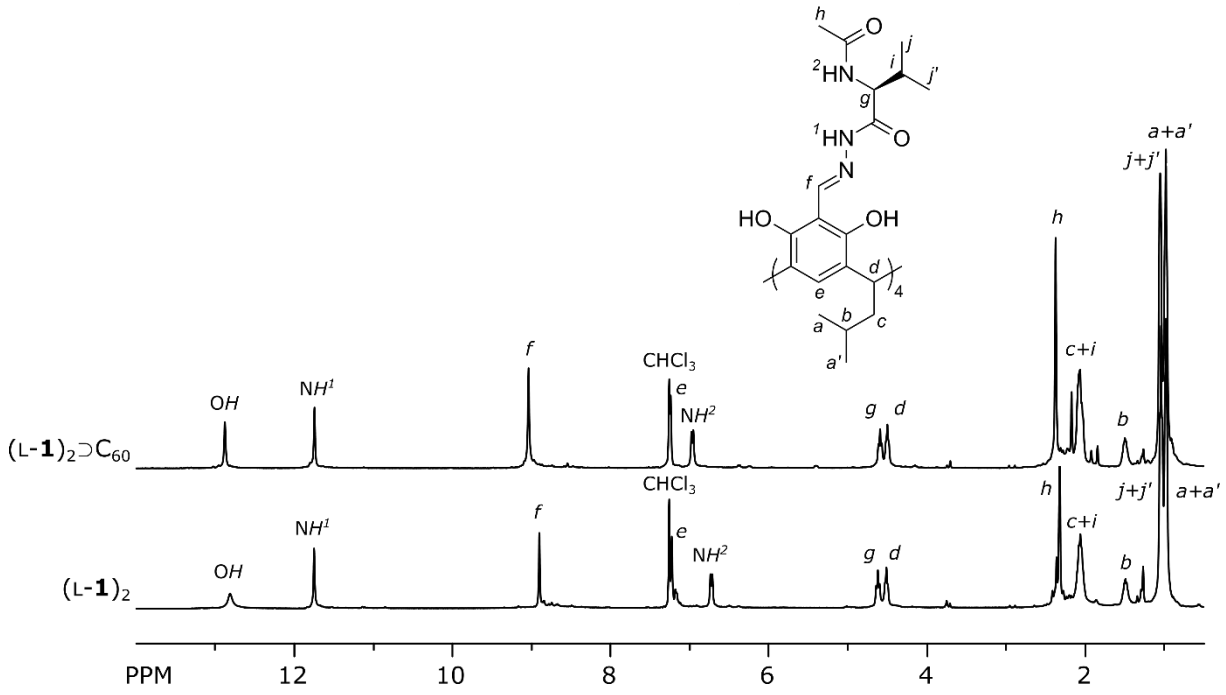


Figure S1. ^{1}H NMR spectra of (L-**1**)$_2$⊃C_{60} and (L-**1**)$_2$ ($CDCl_3$, 298 K, 600 MHz).

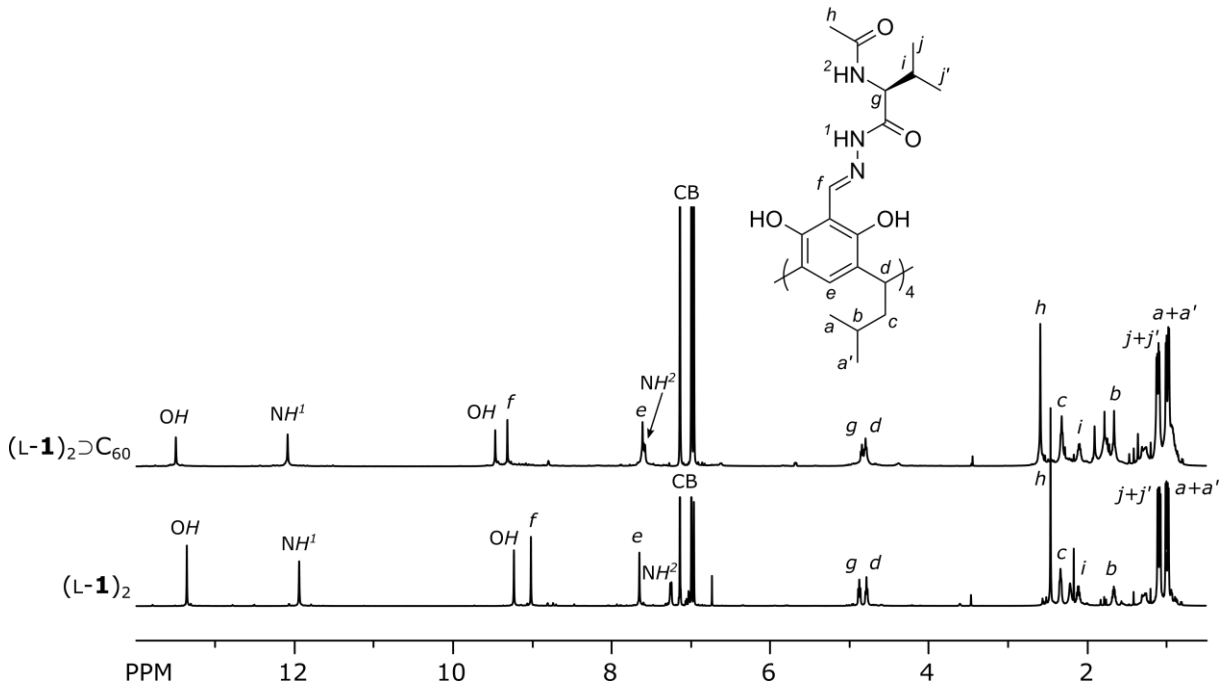


Figure S2. ^{1}H NMR spectra of (L-**1**)$_2$⊃C_{60} and (L-**1**)$_2$ (chlorobenzene-d_5, 298 K, 600 MHz).

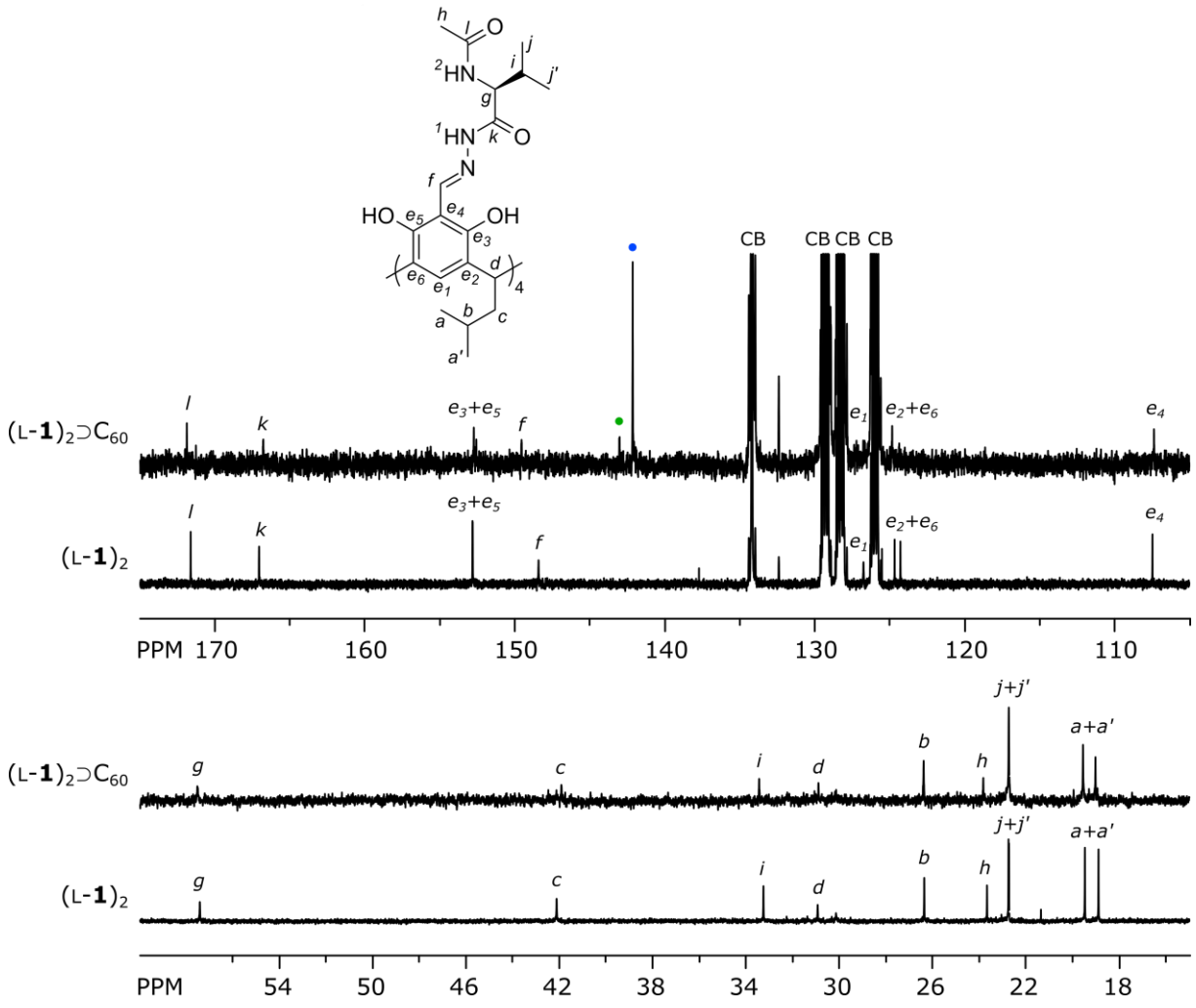


Figure S3. ^{13}C NMR spectra of (L-**1**)$_2$⊃C_{60} and (L-**1**)$_2$ (chlorobenzene-d_5, 298 K, 150 MHz), ● - free C_{60}, ● - encapsulated C_{60}.

^{1}H-^{1}H ROESY spectra of (L-1)$_2$ and (L-1)$_2$⊃C$_{60}$

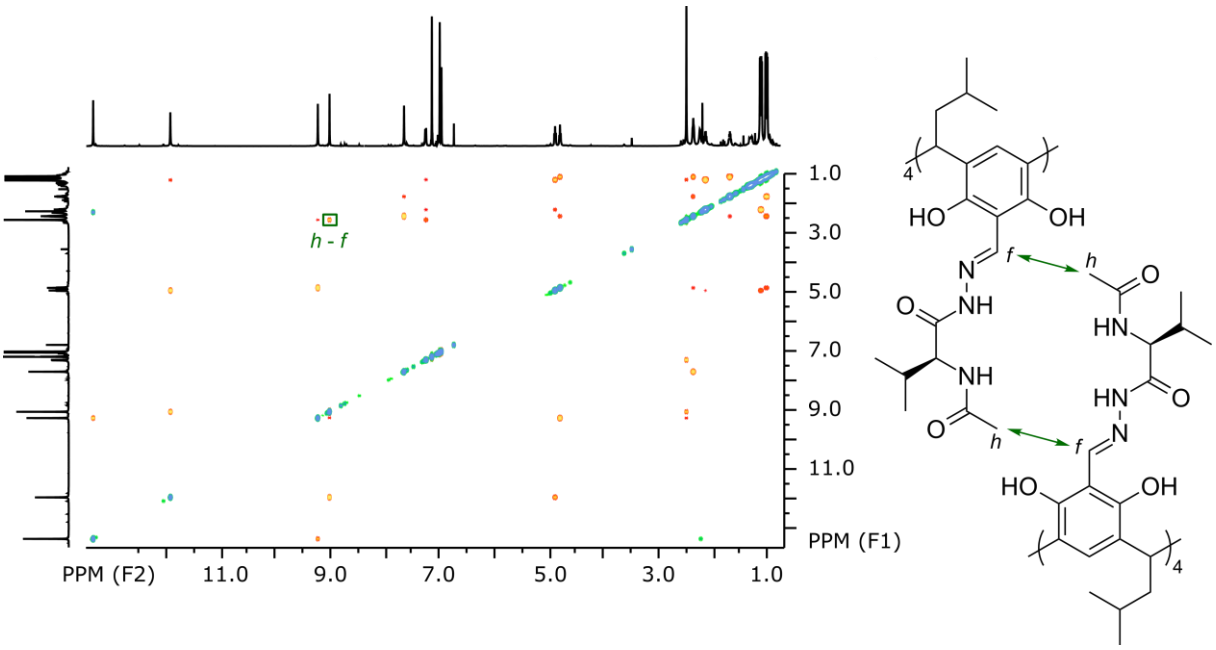


Figure S4. ^{1}H-^{1}H ROESY spectrum of (L-**1**)$_2$ (chlorobenzene-d$_5$, 298 K, 600 MHz).

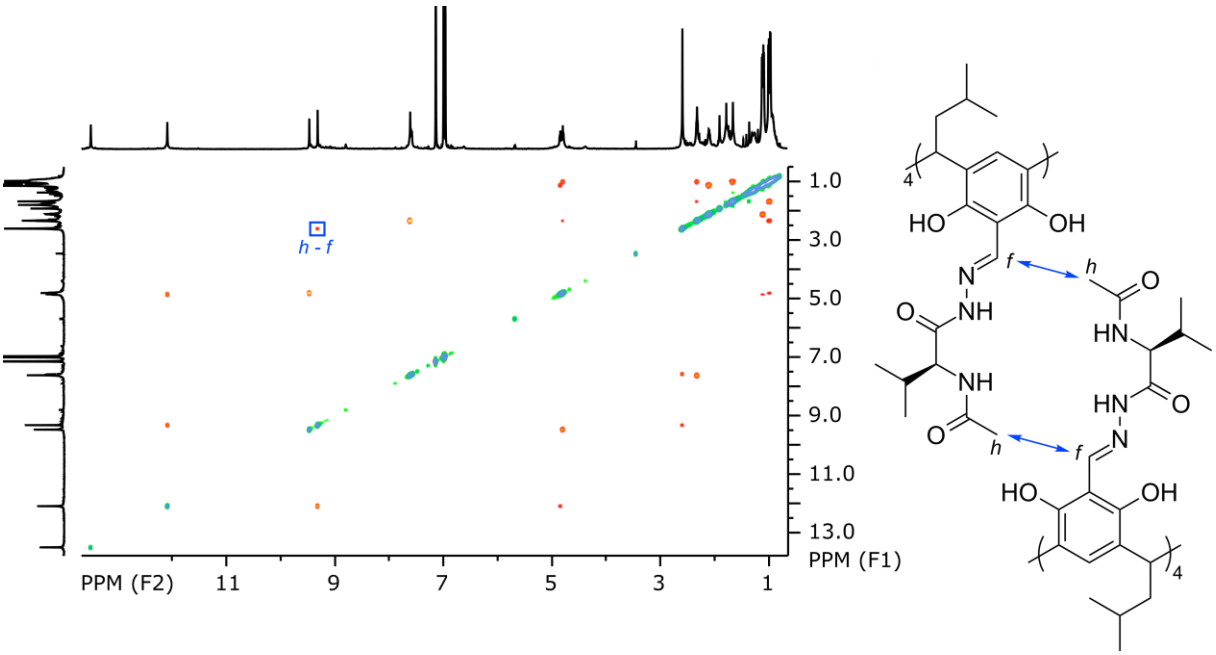


Figure S5. ^{1}H-^{1}H ROESY spectrum of (L-**1**)$_2$⊃C$_{60}$ (chlorobenzene-d$_5$, 298 K, 600 MHz).

^{1}H NMR spectra of the products of the synthesis in solution and in a planetary ball-mill

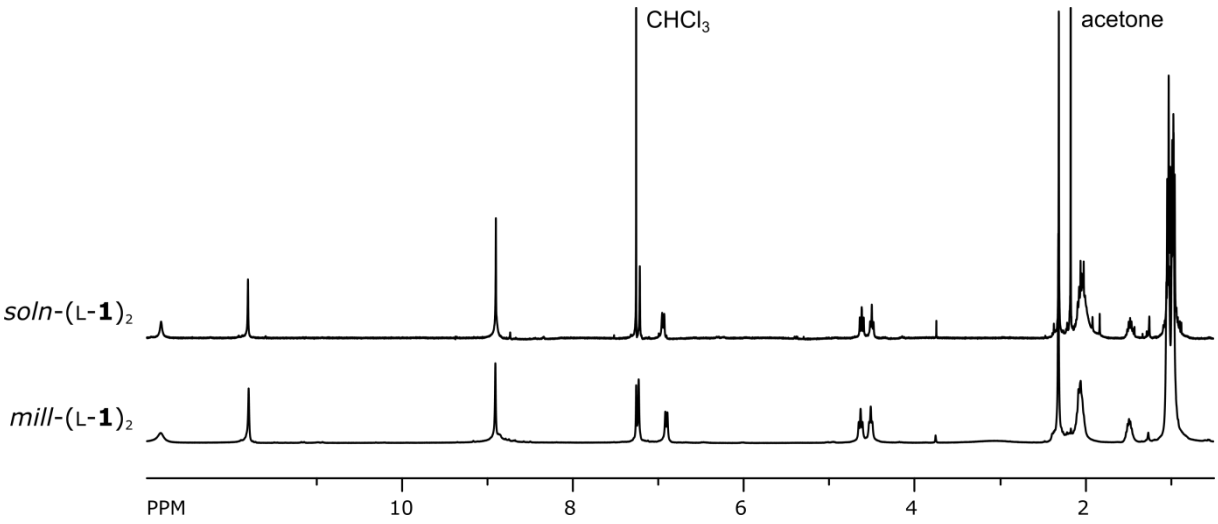


Figure S6. ^{1}H NMR spectra of *soln*-(L-**1**)$_2$ and *mill*-(L-**1**)$_2$ ($CDCl_3$, 298 K, 400 MHz).

C_{60} complexation experiments

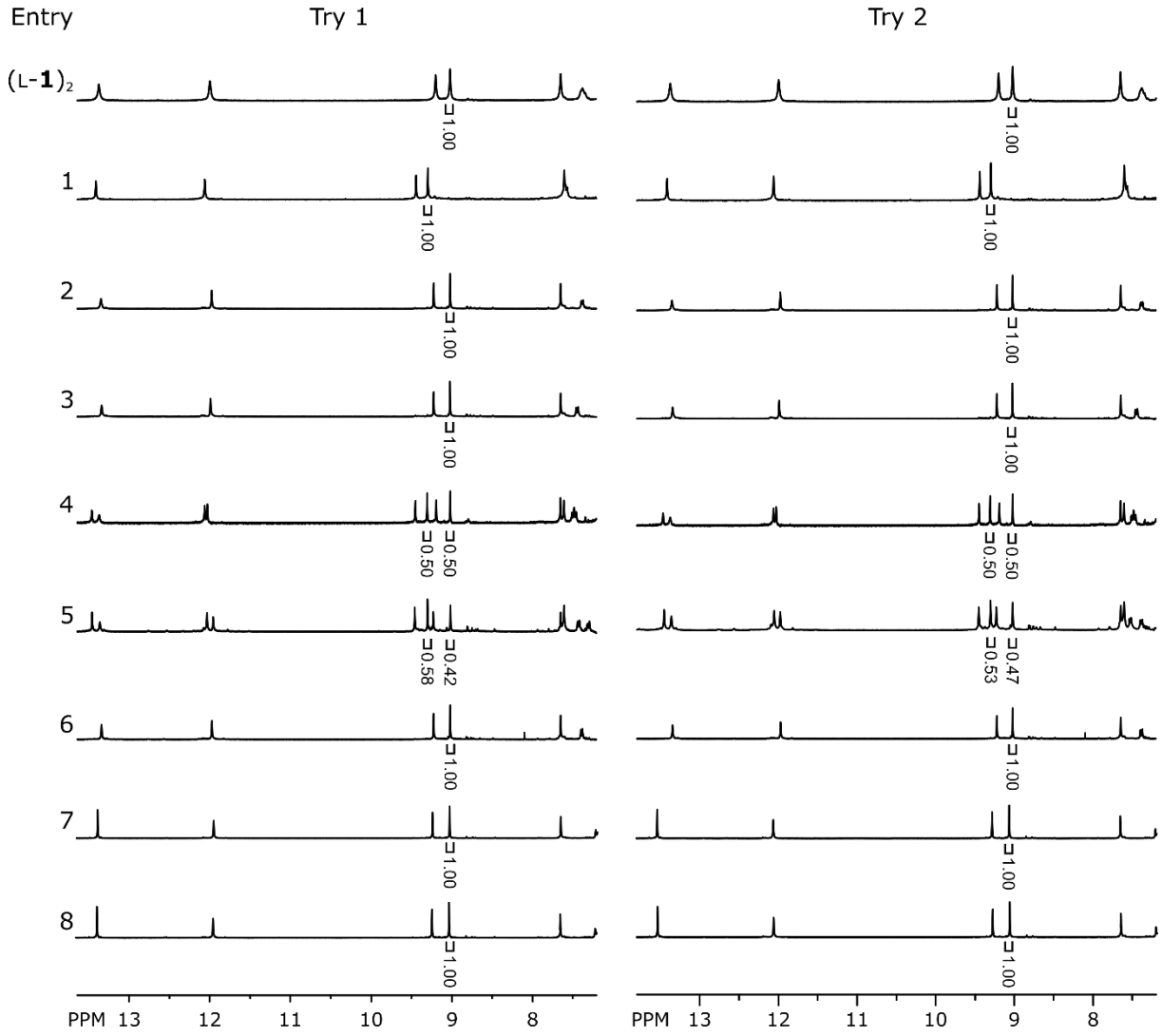


Figure S7. C_{60} complexation studies: ^{1}H NMR spectra (chlorobenzene-d_5, 298 K, 400 MHz). For detailed conditions of specific experiments see Table 1.

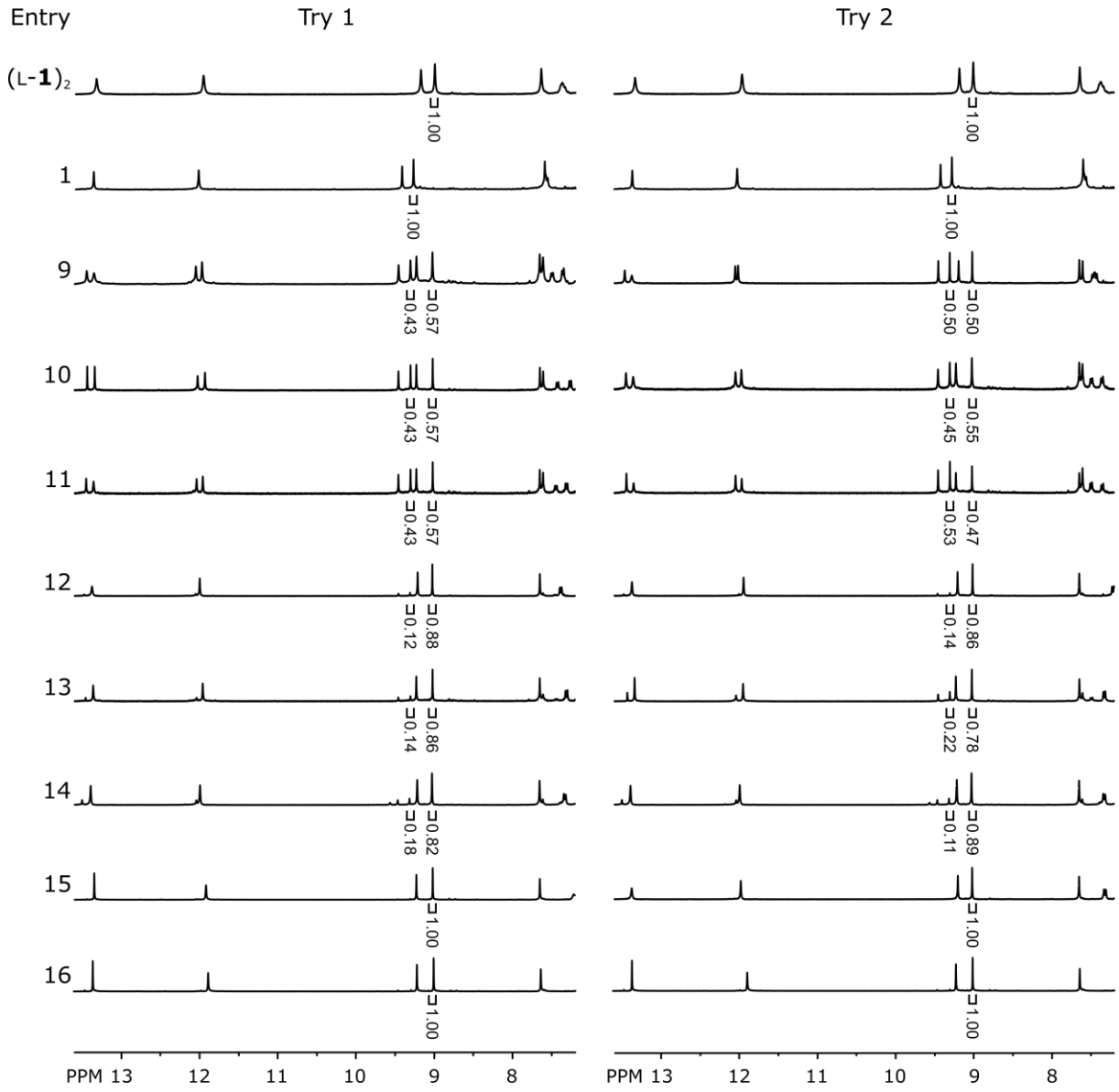


Figure S8. C_{60} complexation studies: ^{1}H NMR spectra (chlorobenzene-d_5, 298 K, 400 MHz). For detailed conditions of specific experiments see Table 1.

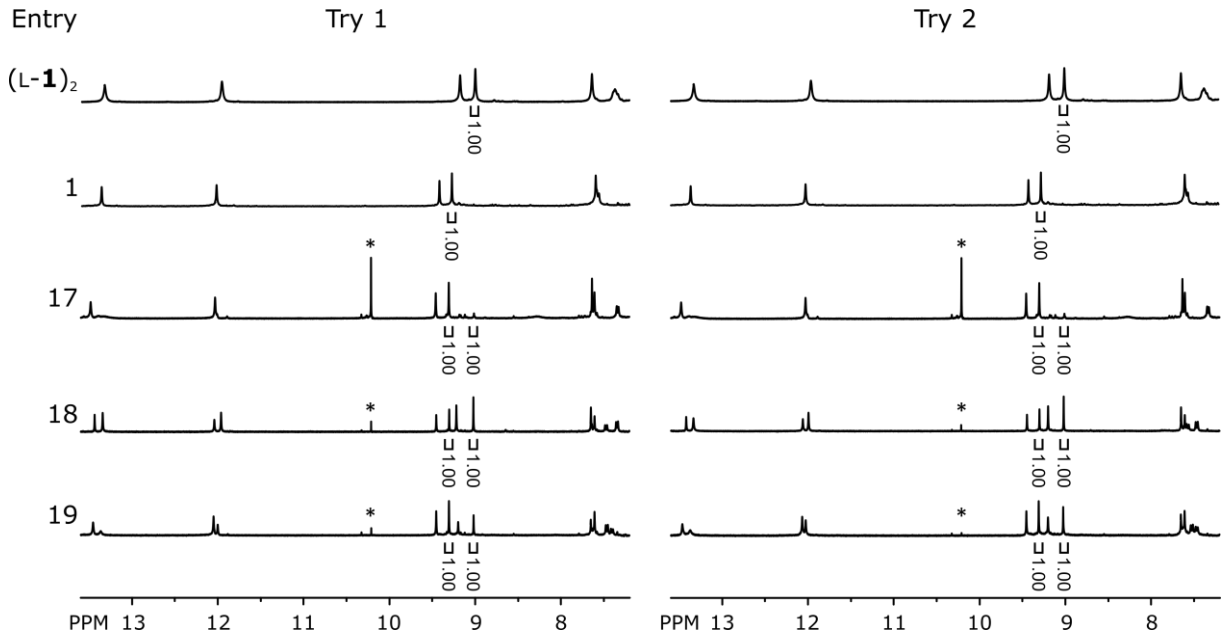


Figure S9. C_{60} complexation studies: ^{1}H NMR spectra (chlorobenzene-d_5, 298 K, 400 MHz). For detailed conditions of specific experiments see Table 1. * - tetraformylresorcin[4]arene.

Solid-state NMR experiments

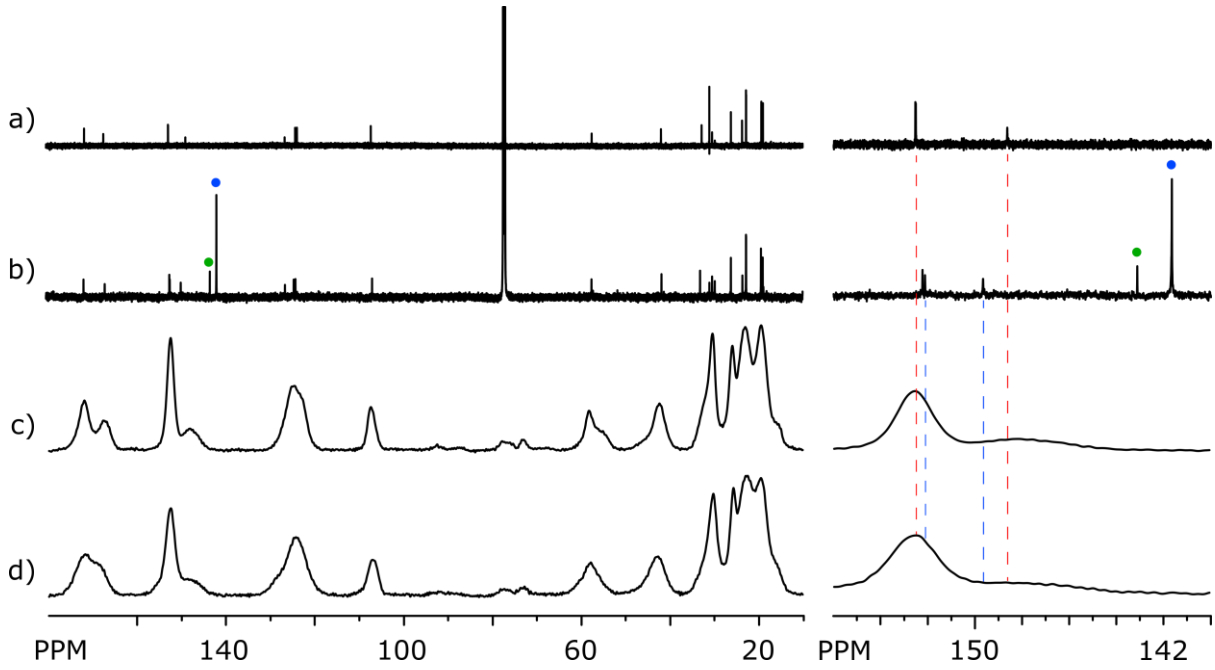


Figure S10. a) ^{13}C NMR spectrum of (L-**1**)$_2$ and b) ^{13}C NMR spectrum of (L-**1**)$_2\supset$C$_{60}$, (both in $CDCl_3$, 298K, 150 MHz); c) CP/MAS ^{13}C NMR spectrum of *soln*-(L-**1**)$_2$ and d) CP/MAS ^{13}C NMR spectrum of *mill*-(L-**1**)$_2$ (both in 298K, 125 MHz). The symbols denote: ● - free C$_{60}$ and ● - encapsulated C$_{60}$.

IR spectra

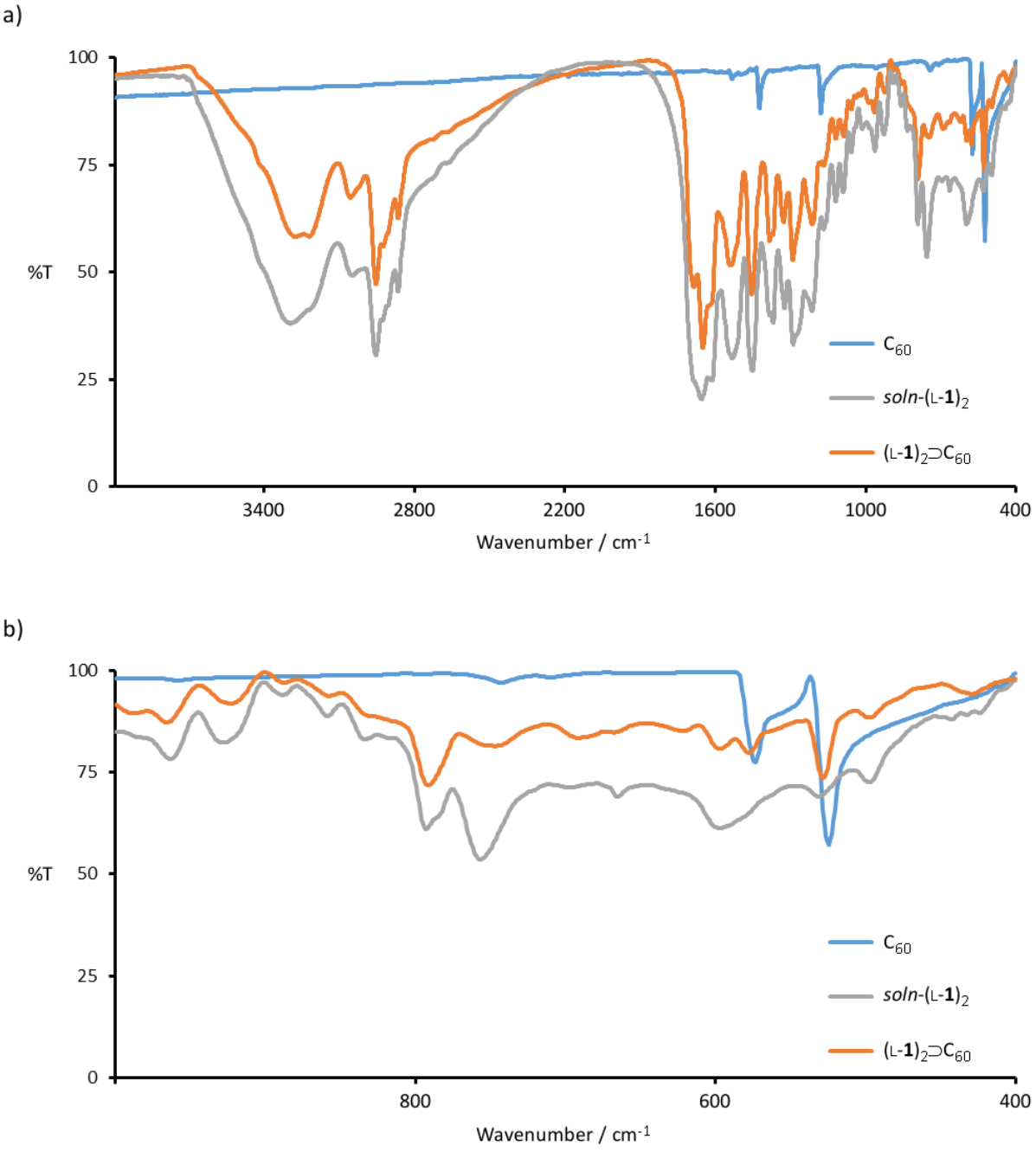
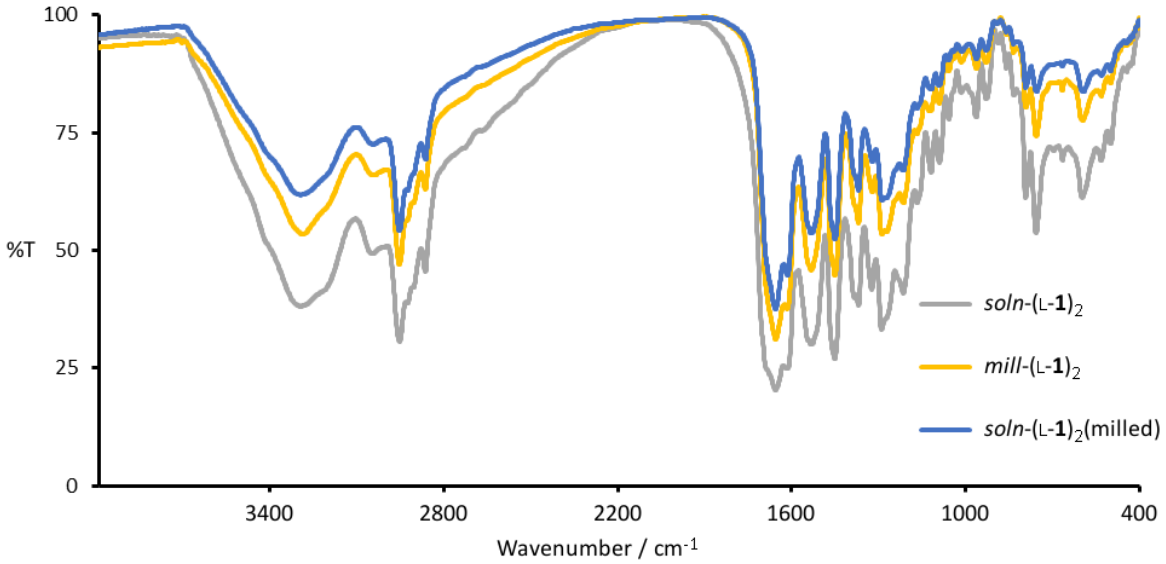


Figure S11. a) IR spectra (KBr pellet) of C_{60}, *soln*-(L-**1**)$_2$ and (L-**1**)$_2$⊃C_{60} b) the spectra expanded in the 400 – 1000 cm^{-1} range.

a)



b)

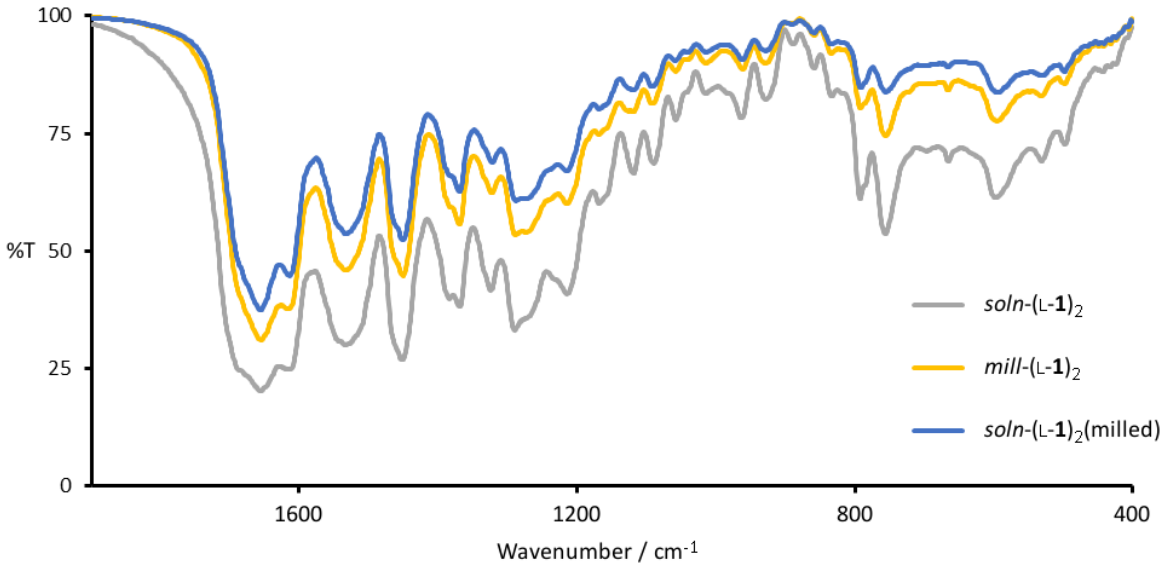


Figure S12. a) IR spectra (KBr pellet) of *soln*-(L-**1**)$_2$, *mill*-(L-**1**)$_2$ and *soln*-(L-**1**)$_2$(milled) b) the spectra expanded in the 400 – 2000 cm^{-1} range.

SEM images

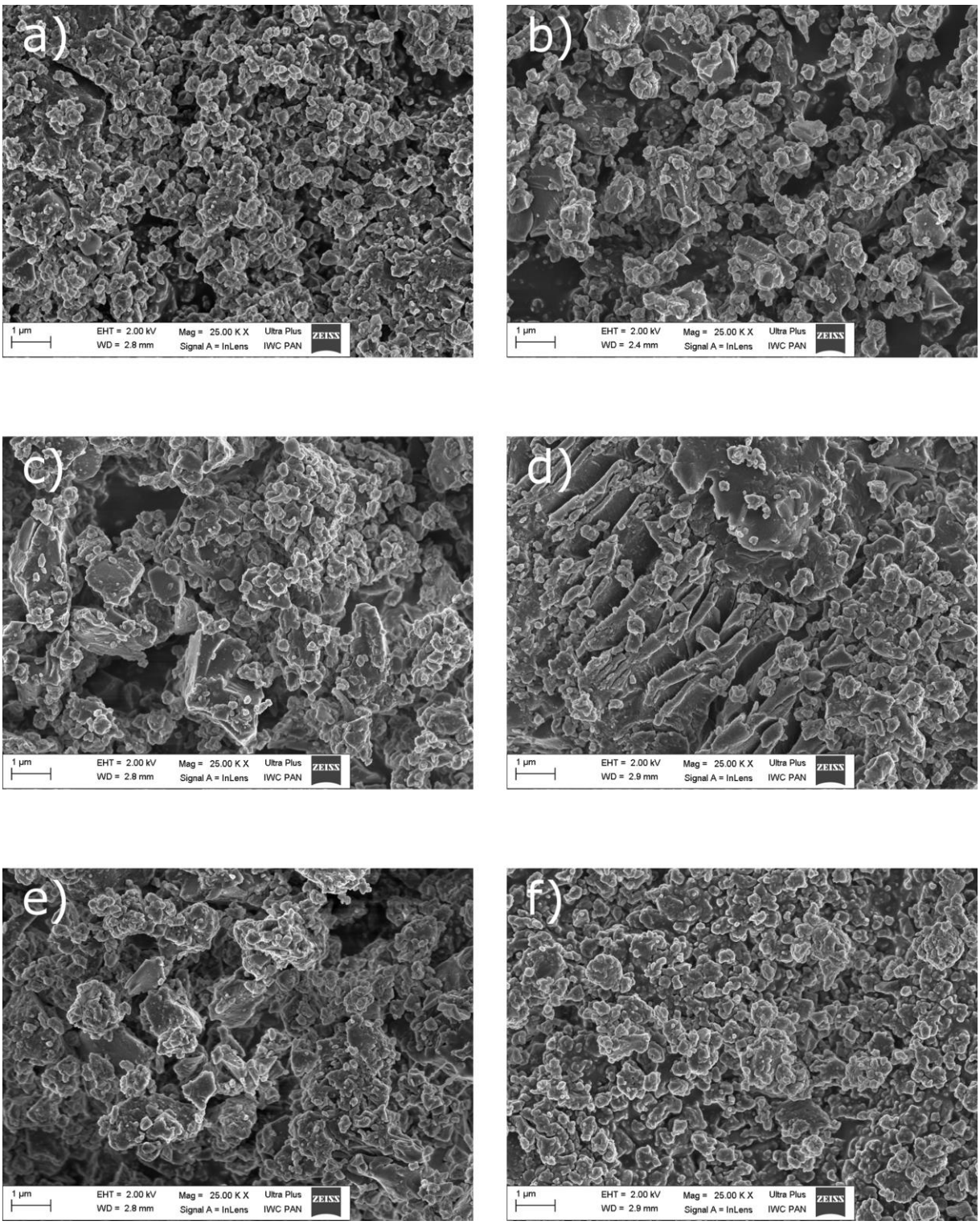


Figure S13. SEM images of: a) *soln*-(L-**1**)$_2$ milled for 1h; b) *soln*-(L-**1**)$_2$ milled for 2h; c) *soln*-(L-**1**)$_2$ + C_{60} milled for 1h; d) *soln*-(L-**1**)$_2$ + C_{60} milled for 2h; e) **2** + L-**3** + C_{60} milled for 1h; f) **2** + L-**3** + C_{60} milled for 2h.

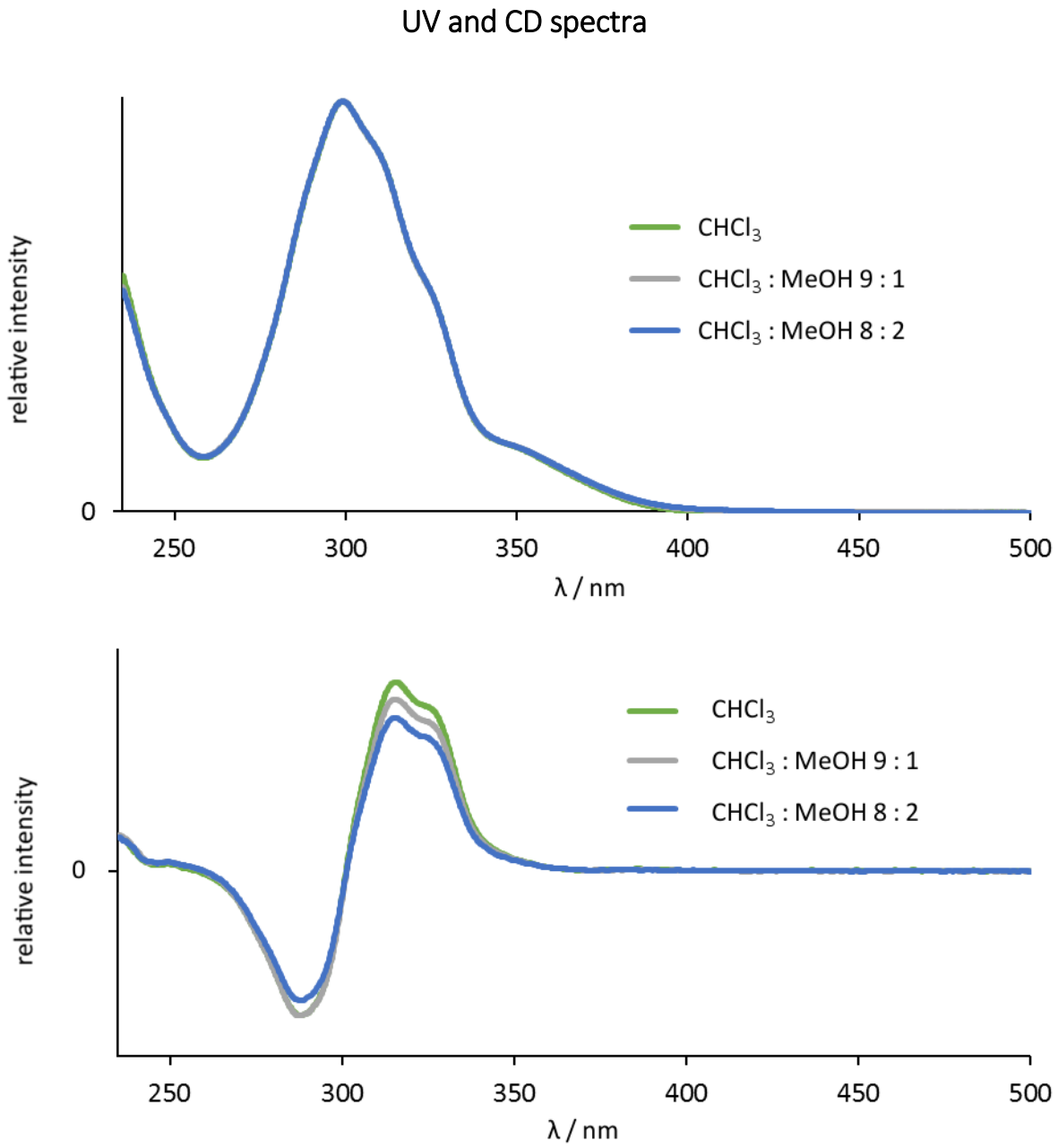


Figure S15. UV and CD spectra of (L-**1**)$_2$ in different solvent systems with increasing polarity (CD spectra were normalized using UV intensities).

Powder XRD spectrum

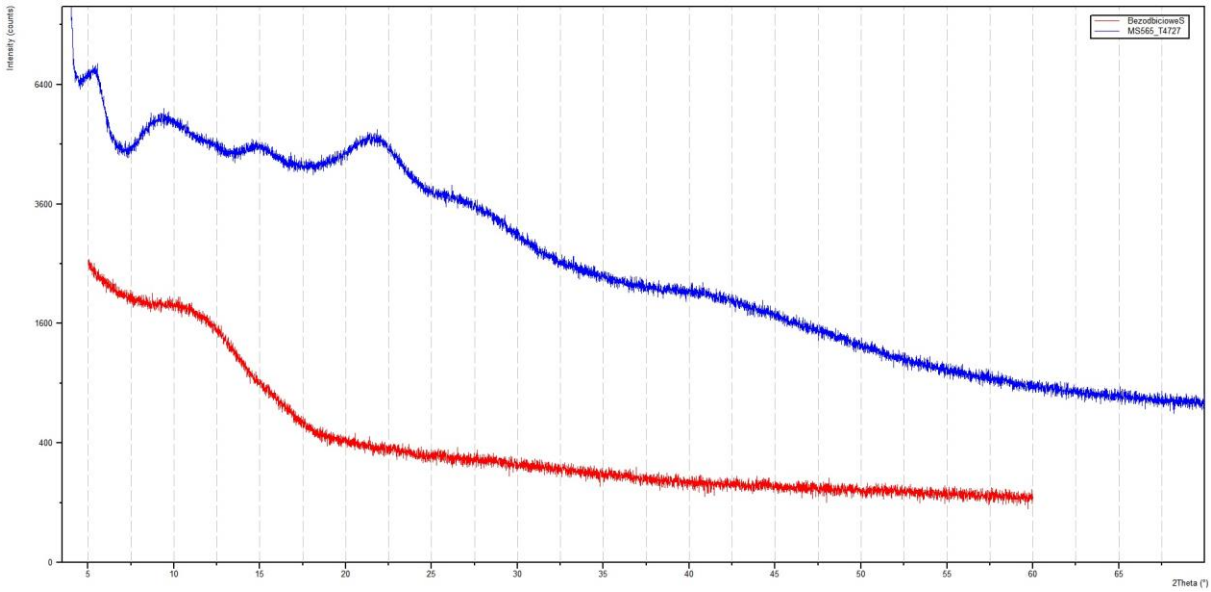


Figure S16. Powder XRD spectrum of *soln*-(L-**1**)$_2$ (blue line), background line (red) (measured using Empyrean Panalitycal Co. diffractometer with Cu radiation).

Crystallographic data

CCDC 1527848 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Crystal data for (L-1)$_2$⊃C$_{60}$	
Moiety formula	$2(C_{76}H_{108}N_{12}O_{16}) \times C_{60} \times 10.21CH_3OH \times 2.91CHCl_3$
Empirical formula	$C_{225.11}H_{259.71}Cl_{8.74}N_{24}O_{42.20}$
Formula weight	4286.62
Temperature (K)	100
Wavelength (Å)	0.7085
Crystal system	Triclinic
Space group	P1
Unit cell dimensions a/b/c (Å), α,β,γ (°)	17.77 (4) 18.09 (5) 19.19 (2) 112.63 96.40 99.29
Unit cell volume (Å^3)	5516.0(7)
Z	1
Calculated density (g/cm^3)	1.290
Absorption coefficient (mm^{-1})	0.191
F(000)	2265
θ range for data collection (°)	24.944 – 1.167
Index ranges	-21 < h < 21 -21 < k < 21 -22 < l < 22
Reflections collected	92673
Independent reflections	34215 (R_{int} = 0.0548)
Completeness to θ_{max}	0.900
Refinement statistics	
Final R indices [>2σ(I)]	0.0633
R indices [all data]	0.0640
Goodness-of-fit	1.025
Largest diff. peak and hole (e Å^{-3})	0.768 / -0.411

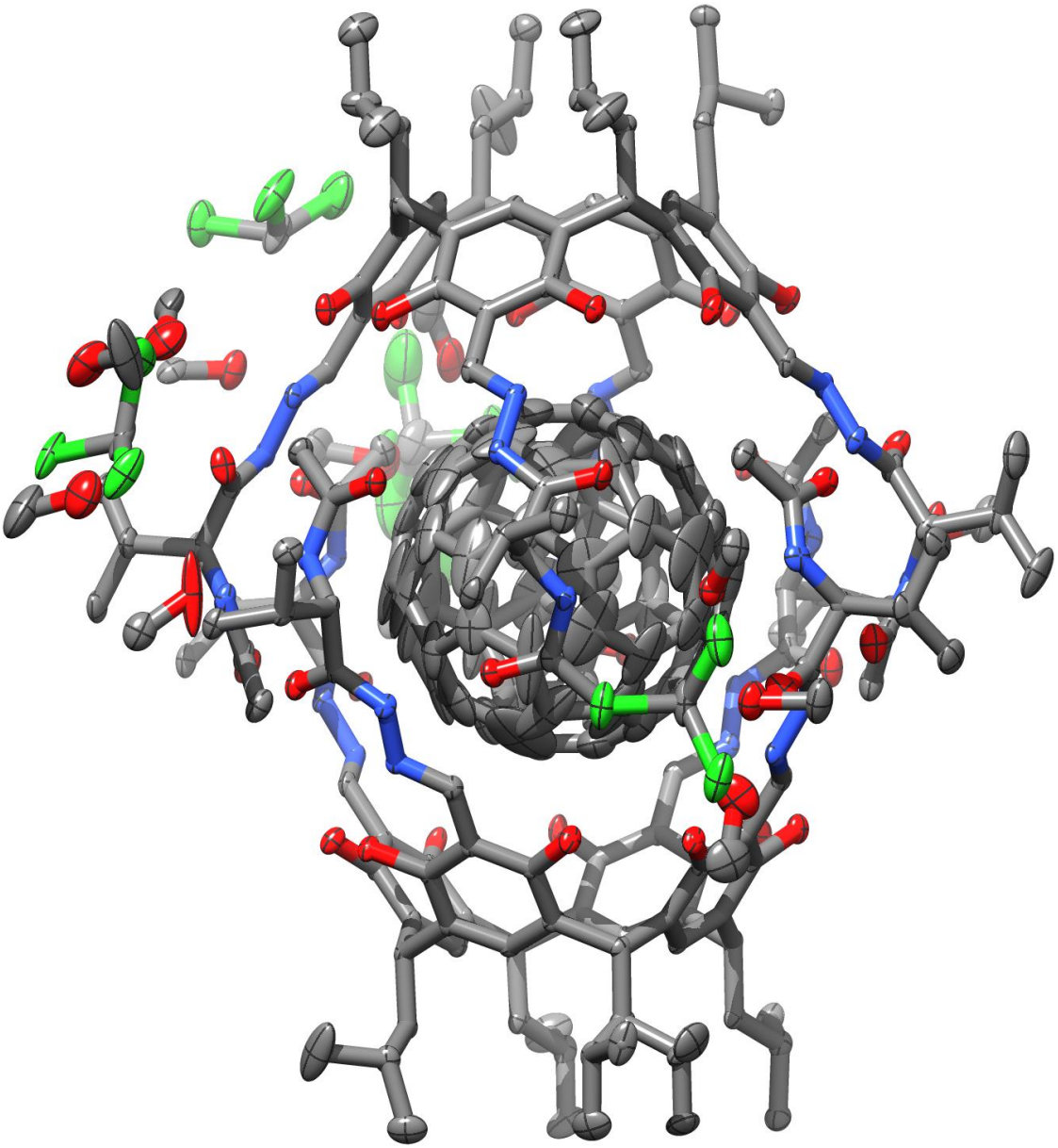


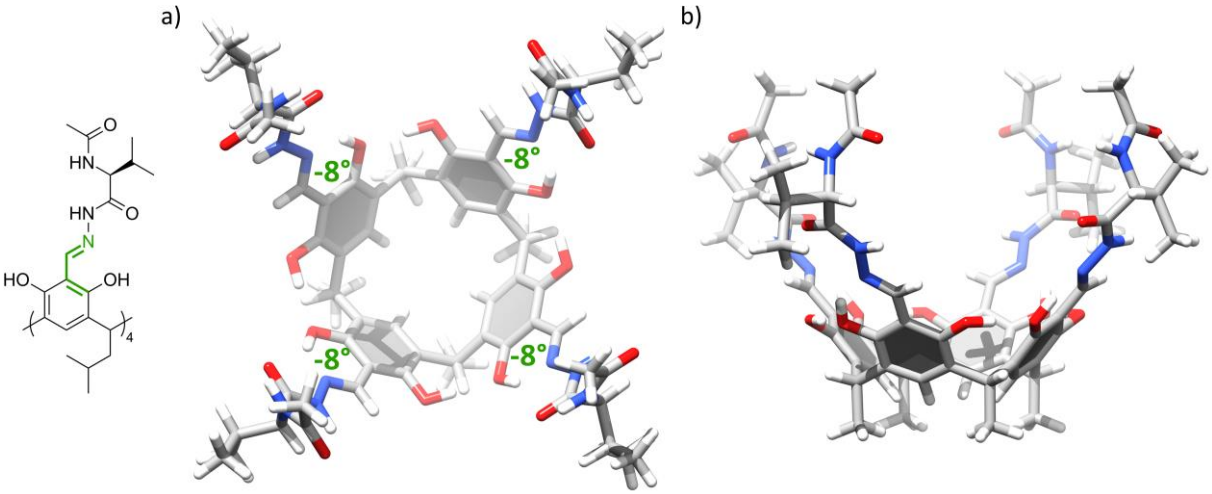
Figure S17. ORTEP representation of the asymmetric unit of the crystal structure of (L-**1**)$_2$⊃C_{60} (50% probability). Hydrogen atoms removed for clarity.

Ab initio calculations

All calculations were performed within the density functional theory (DFT) using Gaussian 09 program suite.[2]
The geometry of the initial structure of L-**1** (conformation 1) was taken from the crystal structure. Conformations 2-5 were obtained by changing positions of peptide arms.
Excited electronic states were determined at the B3LYP/6-31G(d) level by means of the time-dependent DFT (TD DFT) approach (100 excited states). The ECD and UV spectra were simulated by overlapping Gaussian functions for each transition where the width of the band at 1/e height is fixed at 0.16 eV and the resulting intensities of the spectra were scaled to the experimental values (using the lowest energy bands in UV-VIS spectrum as reference). Presentation of molecular orbitals was performed by using the GaussView program.

Atomic Cartesian coordinates for all calculated geometries:

Conformation 1
conf-1



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C	-5.63200000	5.72900000	2.50000000
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C	-5.79700000	4.81900000	4.79500000
O	-6.87600000	4.24100000	4.52500000
C	-5.23400000	4.82600000	6.23600000

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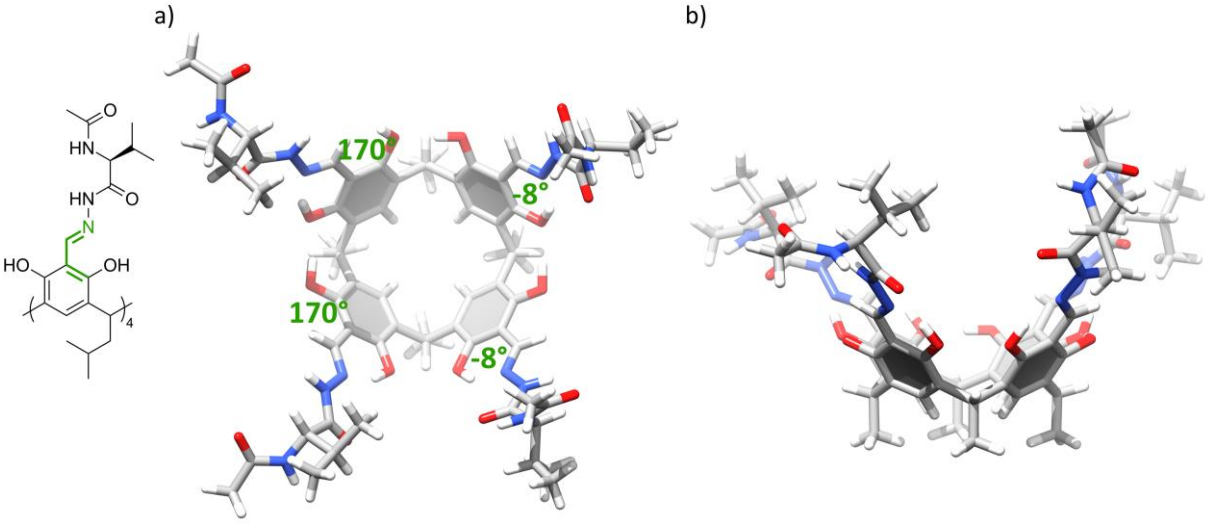
H	-8.70000000	-6.57500000	0.70900000
H	-7.09100000	-7.33600000	0.68200000
H	-7.29100000	-5.65600000	0.12800000
H	-0.08200000	4.34700000	-6.27100000
H	-1.69900000	3.60300000	-6.25300000
H	-0.24600000	2.57500000	-6.22700000
H	0.08200000	-4.34700000	-6.27100000
H	1.69900000	-3.60300000	-6.25300000
H	0.24600000	-2.57500000	-6.22700000
H	-5.86200000	4.20400000	6.87400000
H	-4.21800000	4.43300000	6.23100000
H	-5.22700000	5.84800000	6.61800000
H	-7.17700000	8.74900000	3.25100000
H	-7.34600000	7.07900000	3.84300000
H	-5.95200000	8.06600000	4.34600000
H	6.57500000	-8.70000000	0.70900000
H	5.65600000	-7.29100000	0.12800000
H	7.33600000	-7.09100000	0.68200000
H	8.74900000	7.17700000	3.25100000
H	8.06600000	5.95200000	4.34600000
H	7.07900000	7.34600000	3.84300000
H	7.17700000	-8.74900000	3.25100000

H	7.34600000	-7.07900000	3.84300000
H	5.95200000	-8.06600000	4.34600000

Conformation 2
conf-2



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C	-3.59100000	2.46900000	-2.09900000
C	-3.91800000	1.20700000	-2.67000000
C	-3.19800000	0.70400000	-3.72900000
C	-2.15600000	1.46700000	-4.22100000
C	-1.79300000	2.72100000	-3.74500000
C	-4.38300000	2.98000000	-1.03000000
N	-4.07500000	4.06700000	-0.40900000
N	-4.94100000	4.45500000	0.59500000
C	-4.56000000	5.46400000	1.45200000
O	-3.52900000	6.02400000	1.41900000
C	-5.63200000	5.72900000	2.50000000
N	-5.13200000	5.54700000	3.86600000
C	-5.79700000	4.81900000	4.79500000
O	-6.87600000	4.24100000	4.52500000
C	-5.23400000	4.82600000	6.23600000
C	-5.87000000	7.35400000	2.36500000
C	-6.63700000	7.84400000	3.52800000
C	-6.40400000	7.63300000	0.84400000
C	-3.55600000	-0.67700000	-4.33900000
C	-3.51700000	-0.67600000	-5.88700000
O	-4.40900000	-2.15200000	-2.15000000
O	-0.54600000	-4.96200000	-2.11300000
C	-3.20500000	-2.51000000	-2.66800000
C	-2.46900000	-3.59100000	-2.09900000
C	-1.20700000	-3.91800000	-2.67000000
C	-0.70400000	-3.19800000	-3.72900000
C	-1.46700000	-2.15600000	-4.22100000
C	-2.72100000	-1.79300000	-3.74500000
C	-2.98000000	-4.38300000	-1.03000000

N	-4.06700000	-4.07500000	-0.40900000
N	-4.45500000	-4.94100000	0.59500000
C	-5.46400000	-4.56000000	1.45200000
O	-6.02400000	-3.52900000	1.41900000
C	-5.72900000	-5.63200000	2.50000000
N	-5.54700000	-5.13200000	3.86600000
C	-4.81900000	-5.79700000	4.79500000
O	-4.24100000	-6.87600000	4.52500000
C	-4.82600000	-5.23400000	6.23600000
C	-7.35400000	-5.87000000	2.36500000
C	-7.84400000	-6.63700000	3.52800000
C	-7.63300000	-6.40400000	0.84400000
C	0.67700000	-3.55600000	-4.33900000
C	0.67600000	-3.51700000	-5.88700000
O	4.40900000	2.15200000	-2.15000000
O	0.54600000	4.96200000	-2.11300000
C	3.20500000	2.51000000	-2.66800000
C	2.46900000	3.59100000	-2.09900000
C	1.20700000	3.91800000	-2.67000000
C	0.70400000	3.19800000	-3.72900000
C	1.46700000	2.15600000	-4.22100000
C	2.72100000	1.79300000	-3.74500000
C	2.98000000	4.38300000	-1.03000000
N	2.39501435	5.46292572	-0.63804818
N	2.99013339	6.12211904	0.42016423
C	2.56449795	7.39283916	0.73921883
O	1.73453302	7.99086032	0.16373738
C	3.35421803	7.95888088	1.91124783
N	4.04666441	9.20410151	1.56624986
C	5.35233042	9.41731989	1.85783892
O	6.04789425	8.54303311	2.42620376
C	5.92134778	10.82666125	1.56891822
C	2.16464426	8.42727708	2.95096570
C	2.73320212	9.29787044	3.99966355
C	1.32818932	7.08097579	3.35624830
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C	-0.67600000	3.51700000	-5.88700000
O	2.15200000	-4.40900000	-2.15000000
O	4.96200000	-0.54600000	-2.11300000
C	2.51000000	-3.20500000	-2.66800000
C	3.59100000	-2.46900000	-2.09900000
C	3.91800000	-1.20700000	-2.67000000
C	3.19800000	-0.70400000	-3.72900000
C	2.15600000	-1.46700000	-4.22100000
C	1.79300000	-2.72100000	-3.74500000
C	4.38300000	-2.98000000	-1.03000000
N	5.46292572	-2.39501435	-0.63804818
N	6.12211904	-2.99013339	0.42016423
C	7.39283916	-2.56449795	0.73921883
O	7.99086032	-1.73453302	0.16373738
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C	8.42727708	-2.16464426	2.95096570
C	9.29787044	-2.73320212	3.99966355
C	7.08097579	-1.32818932	3.35624830
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C	3.51700000	0.67600000	-5.88700000
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H	-6.54300000	5.16000000	2.31300000
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H	-4.88400000	7.81400000	2.43300000
H	-4.58900000	-0.88100000	-4.05600000
H	-1.05800000	-1.58000000	-5.03800000
H	-2.44000000	-5.26800000	-0.73100000
H	-4.00500000	-5.84000000	0.69900000
H	-5.16000000	-6.54300000	2.31300000
H	-5.98200000	-4.25700000	4.12400000
H	-7.81400000	-4.88400000	2.43300000
H	0.88100000	-4.58900000	-4.05600000
H	1.05800000	1.58000000	-5.03800000
H	3.88494973	4.06894102	-0.53335230
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H	4.02410735	7.22113941	2.35355634
H	3.52907046	9.93144853	1.09246002
H	1.48163429	9.05030313	2.37324958
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H	1.58000000	-1.05800000	-5.03800000
H	4.06894102	-3.88494973	-0.53335230
H	5.67866608	-3.72665184	0.95158407
H	7.22113941	-4.02410735	2.35355634
H	9.93144853	-3.52907046	1.09246002
H	9.05030313	-1.48163429	2.37324958
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H	-2.72300000	4.62100000	-1.40700000
H	-4.78200000	-0.39700000	-2.11600000
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H	-4.62100000	-2.72300000	-1.40700000
H	2.72300000	-4.62100000	-1.40700000
H	1.06746880	5.32314308	-1.39237252
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H	11.56711957	-5.36913536	2.14964184
H	11.04859876	-5.82031590	0.50719023
H	-4.34700000	-0.08200000	-6.27100000
H	-3.60300000	-1.69900000	-6.25300000
H	-2.57500000	-0.24600000	-6.22700000
H	-6.57500000	8.70000000	0.70900000
H	-7.33600000	7.09100000	0.68200000

H	-5.65600000	7.29100000	0.12800000
H	4.34700000	0.08200000	-6.27100000
H	3.60300000	1.69900000	-6.25300000
H	2.57500000	0.24600000	-6.22700000
H	6.97445460	10.85722363	1.84881813
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H	-4.43300000	-4.21800000	6.23100000
H	-5.84800000	-5.22700000	6.61800000
H	-8.74900000	-7.17700000	3.25100000
H	-7.07900000	-7.34600000	3.84300000
H	-8.06600000	-5.95200000	4.34600000
H	-8.70000000	-6.57500000	0.70900000
H	-7.09100000	-7.33600000	0.68200000
H	-7.29100000	-5.65600000	0.12800000
H	-0.08200000	4.34700000	-6.27100000
H	-1.69900000	3.60300000	-6.25300000
H	-0.24600000	2.57500000	-6.22700000
H	0.08200000	-4.34700000	-6.27100000
H	1.69900000	-3.60300000	-6.25300000
H	0.24600000	-2.57500000	-6.22700000
H	-5.86200000	4.20400000	6.87400000
H	-4.21800000	4.43300000	6.23100000
H	-5.22700000	5.84800000	6.61800000
H	-7.17700000	8.74900000	3.25100000
H	-7.34600000	7.07900000	3.84300000
H	-5.95200000	8.06600000	4.34600000
H	7.34458074	-0.52732396	4.04551030
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H	6.36702317	-1.99980306	3.83357276
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H	2.75394966	10.32759116	3.64346448
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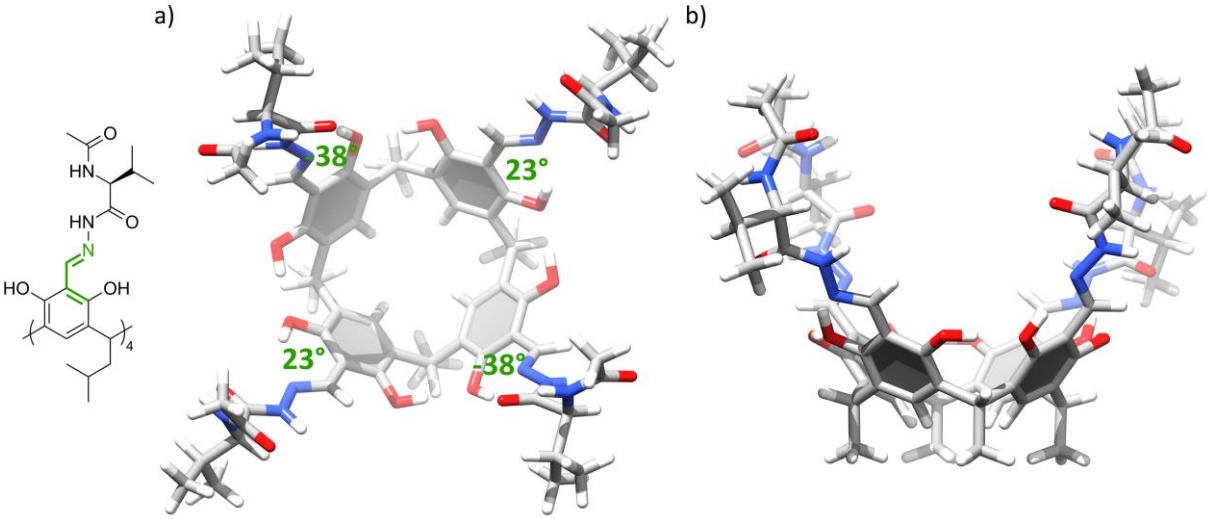
Conformation 3
conf-3



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C	-3.59100000	2.46900000	-2.09900000
C	-3.91800000	1.20700000	-2.67000000
C	-3.19800000	0.70400000	-3.72900000
C	-2.15600000	1.46700000	-4.22100000
C	-1.79300000	2.72100000	-3.74500000
C	-4.38300000	2.98000000	-1.03000000
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N	-5.32267973	4.35623466	4.29393521
C	-6.40042717	3.75747534	4.85535995
O	-7.51667575	3.74980494	4.28513609
C	-6.22925476	3.18574215	6.28270720
C	-5.00279462	6.61272700	3.36183551
C	-5.80177028	7.07225481	4.51571162
C	-5.02854937	7.44434419	1.95322359
C	-3.55600000	-0.67700000	-4.33900000
C	-3.51700000	-0.67600000	-5.88700000
O	-4.40900000	-2.15200000	-2.15000000
O	-0.54600000	-4.96200000	-2.11300000
C	-3.20500000	-2.51000000	-2.66800000
C	-2.46900000	-3.59100000	-2.09900000
C	-1.20700000	-3.91800000	-2.67000000
C	-0.70400000	-3.19800000	-3.72900000
C	-1.46700000	-2.15600000	-4.22100000
C	-2.72100000	-1.79300000	-3.74500000
C	-2.98000000	-4.38300000	-1.03000000
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O	-4.99383498	-6.45825008	4.47463448
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C	0.67600000	-3.51700000	-5.88700000
O	4.40900000	2.15200000	-2.15000000
O	0.54600000	4.96200000	-2.11300000
C	3.20500000	2.51000000	-2.66800000
C	2.46900000	3.59100000	-2.09900000
C	1.20700000	3.91800000	-2.67000000
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C	1.46700000	2.15600000	-4.22100000
C	2.72100000	1.79300000	-3.74500000
C	2.98000000	4.38300000	-1.03000000
N	4.24346051	4.47777286	-0.79175718
N	4.59921065	5.29368598	0.26476713
C	5.89691427	5.26083195	0.72582779
O	6.74518833	4.56729660	0.30500735
C	6.08556570	6.20604013	1.90426113
N	6.54749705	5.50906228	3.10838791
C	5.97322083	5.69100295	4.32179403
O	4.99383498	6.45825008	4.47463448
C	6.64752388	5.00610936	5.53412038
C	7.38017071	7.11040483	1.43349967
C	7.91217202	7.85941458	2.58975093
C	6.94082548	7.89758617	0.06830396
C	-0.67700000	3.55600000	-4.33900000
C	-0.67600000	3.51700000	-5.88700000
O	2.15200000	-4.40900000	-2.15000000
O	4.96200000	-0.54600000	-2.11300000
C	2.51000000	-3.20500000	-2.66800000
C	3.59100000	-2.46900000	-2.09900000
C	3.91800000	-1.20700000	-2.67000000
C	3.19800000	-0.70400000	-3.72900000
C	2.15600000	-1.46700000	-4.22100000
C	1.79300000	-2.72100000	-3.74500000
C	4.38300000	-2.98000000	-1.03000000
N	3.87028710	-3.66292587	-0.06417820
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C	4.26140771	-4.63847205	2.06783711
O	3.12316260	-4.72332680	2.34142023
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N	5.32267973	-4.35623466	4.29393521
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O	7.51667575	-3.74980494	4.28513609
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C	5.80177028	-7.07225481	4.51571162
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H	-3.96428867	6.60306053	3.69324456
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H	-1.05800000	-1.58000000	-5.03800000
H	-2.28762075	-4.91992117	-0.40027575
H	-3.91747061	-5.90488167	0.69277103
H	-5.20099754	-6.81516587	2.09176042
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H	1.05800000	1.58000000	-5.03800000
H	2.28762075	4.91992117	-0.40027575
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H	5.20099754	6.81516587	2.09176042
H	7.32483249	4.86802762	3.02940573
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H	-2.57500000	-0.24600000	-6.22700000
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H	2.57500000	0.24600000	-6.22700000
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H	-0.24600000	2.57500000	-6.22700000
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H	1.69900000	-3.60300000	-6.25300000
H	0.24600000	-2.57500000	-6.22700000
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H	-5.44506046	2.42959442	6.27955787
H	-5.95543596	3.99116610	6.96591472
H	-5.90845718	8.15588828	4.47435454
H	-6.78685827	6.60789895	4.48245078
H	-5.29710871	6.79217397	5.44010571
H	4.77775969	-8.48708265	2.14231627
H	4.30086840	-7.01434769	1.26423345
H	6.02457150	-7.38272114	1.51416264
H	8.42215817	8.75567283	2.23762983
H	8.61650886	7.23145800	3.13492351
H	7.09078660	8.14248164	3.24726903
H	5.90845718	-8.15588828	4.47435454
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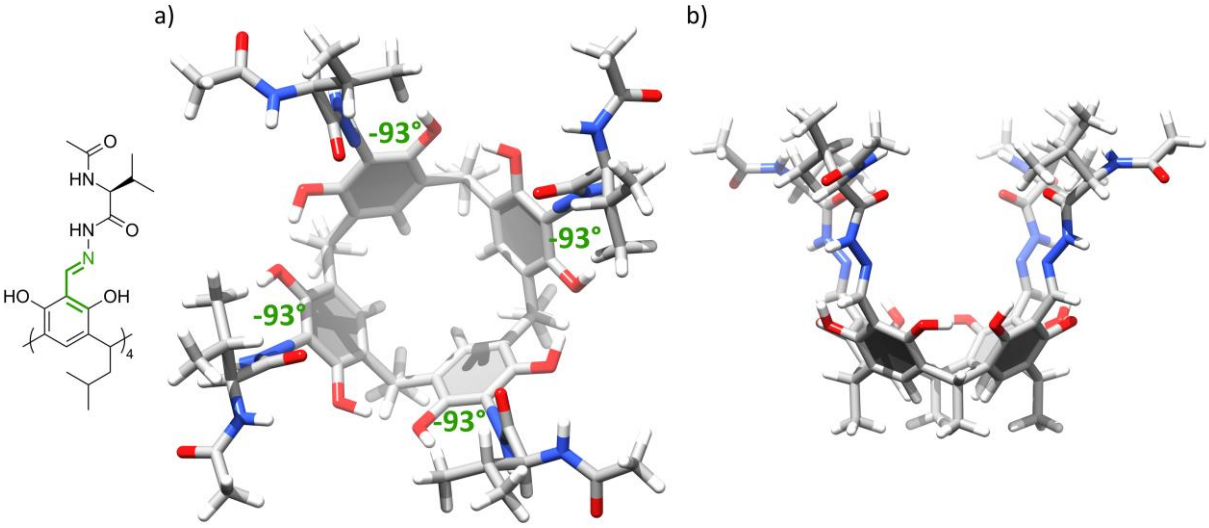
H	5.29710871	-6.79217397	5.44010571

Conformation 4
conf-4



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C	-3.91800000	1.20700000	-2.67000000
C	-3.19800000	0.70400000	-3.72900000
C	-2.15600000	1.46700000	-4.22100000
C	-1.79300000	2.72100000	-3.74500000
C	-4.38300000	2.98000000	-1.03000000
N	-4.10952006	2.72957745	0.20473530
N	-4.95093311	3.30360157	1.13802860
C	-4.86792170	2.89615515	2.45134026
O	-4.14236386	2.06704888	2.85606066
C	-5.88809806	3.62194745	3.31746884
N	-6.80914620	2.69757232	3.98551146
C	-8.15219047	2.87489905	3.97940106
O	-8.68303641	3.83847838	3.37861619
C	-8.99792006	1.90841650	4.84204348
C	-4.95773304	4.22438096	4.53689033
C	-5.82141828	4.67872488	5.64530244
C	-3.88048264	5.24852339	3.85344181
C	-3.55600000	-0.67700000	-4.33900000
C	-3.51700000	-0.67600000	-5.88700000
O	-4.40900000	-2.15200000	-2.15000000
O	-0.54600000	-4.96200000	-2.11300000
C	-3.20500000	-2.51000000	-2.66800000
C	-2.46900000	-3.59100000	-2.09900000
C	-1.20700000	-3.91800000	-2.67000000
C	-0.70400000	-3.19800000	-3.72900000
C	-1.46700000	-2.15600000	-4.22100000
C	-2.72100000	-1.79300000	-3.74500000
C	-2.98000000	-4.38300000	-1.03000000
N	-2.72957745	-4.10952006	0.20473530
N	-3.30360157	-4.95093311	1.13802860
C	-2.89615515	-4.86792170	2.45134026

O	-2.06704888	-4.14236386	2.85606066
C	-3.62194745	-5.88809806	3.31746884
N	-2.69757232	-6.80914620	3.98551146
C	-2.87489905	-8.15219047	3.97940106
O	-3.83847838	-8.68303641	3.37861619
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C	-4.67872488	-5.82141828	5.64530244
C	-5.24852339	-3.88048264	3.85344181
C	0.67700000	-3.55600000	-4.33900000
C	0.67600000	-3.51700000	-5.88700000
O	4.40900000	2.15200000	-2.15000000
O	0.54600000	4.96200000	-2.11300000
C	3.20500000	2.51000000	-2.66800000
C	2.46900000	3.59100000	-2.09900000
C	1.20700000	3.91800000	-2.67000000
C	0.70400000	3.19800000	-3.72900000
C	1.46700000	2.15600000	-4.22100000
C	2.72100000	1.79300000	-3.74500000
C	2.98000000	4.38300000	-1.03000000
N	2.72957745	4.10952006	0.20473530
N	3.30360157	4.95093311	1.13802860
C	2.89615515	4.86792170	2.45134026
O	2.06704888	4.14236386	2.85606066
C	3.62194745	5.88809806	3.31746884
N	2.69757232	6.80914620	3.98551146
C	2.87489905	8.15219047	3.97940106
O	3.83847838	8.68303641	3.37861619
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C	4.67872488	5.82141828	5.64530244
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C	-0.67700000	3.55600000	-4.33900000
C	-0.67600000	3.51700000	-5.88700000
O	2.15200000	-4.40900000	-2.15000000
O	4.96200000	-0.54600000	-2.11300000
C	2.51000000	-3.20500000	-2.66800000
C	3.59100000	-2.46900000	-2.09900000
C	3.91800000	-1.20700000	-2.67000000
C	3.19800000	-0.70400000	-3.72900000
C	2.15600000	-1.46700000	-4.22100000
C	1.79300000	-2.72100000	-3.74500000
C	4.38300000	-2.98000000	-1.03000000
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N	4.95093311	-3.30360157	1.13802860
C	4.86792170	-2.89615515	2.45134026
O	4.14236386	-2.06704888	2.85606066
C	5.88809806	-3.62194745	3.31746884
N	6.80914620	-2.69757232	3.98551146
C	8.15219047	-2.87489905	3.97940106
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C	8.99792006	-1.90841650	4.84204348

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C	5.82141828	-4.67872488	5.64530244
C	3.88048264	-5.24852339	3.85344181
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C	3.51700000	0.67600000	-5.88700000
H	-1.58000000	1.05800000	-5.03800000
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H	-6.42646264	1.89704167	4.46936884
H	-4.37981755	3.38486774	4.92373815
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H	-3.38486774	-4.37981755	4.92373815
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H	1.05800000	1.58000000	-5.03800000
H	3.59558132	5.23840194	-1.26145874
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H	3.38486774	4.37981755	4.92373815
H	-0.88100000	4.58900000	-4.05600000
H	1.58000000	-1.05800000	-5.03800000
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H	5.61722839	-4.01130315	0.86103387
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H	-4.78200000	-0.39700000	-2.11600000
H	0.39700000	-4.78200000	-2.11600000
H	4.78200000	0.39700000	-2.11600000
H	4.62100000	2.72300000	-1.40700000
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H	2.72300000	-4.62100000	-1.40700000
H	-0.39700000	4.78200000	-2.11600000
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H	8.83797869	-0.88523198	4.50404615
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H	-3.26878031	4.70451778	3.13302377
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H	3.60300000	1.69900000	-6.25300000

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H	1.99754753	8.69769770	5.88721294
H	5.67208803	3.24099388	4.62648911
H	4.70451778	3.26878031	3.13302377
H	6.04986152	4.41556745	3.34336982
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H	-0.88523198	-8.83797869	4.50404615
H	-1.99754753	-8.69769770	5.88721294
H	-5.45463751	-5.30676355	6.21138026
H	-5.07902305	-6.75033921	5.24033542
H	-3.83671081	-6.04188729	6.30107581
H	-5.67208803	-3.24099388	4.62648911
H	-6.04986152	-4.41556745	3.34336982
H	-4.70451778	-3.26878031	3.13302377
H	-0.08200000	4.34700000	-6.27100000
H	-1.69900000	3.60300000	-6.25300000
H	-0.24600000	2.57500000	-6.22700000
H	0.08200000	-4.34700000	-6.27100000
H	1.69900000	-3.60300000	-6.25300000
H	0.24600000	-2.57500000	-6.22700000
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H	-8.83797869	0.88523198	4.50404615
H	-8.69769770	1.99754753	5.88721294
H	-5.30676355	5.45463751	6.21138026
H	-6.75033921	5.07902305	5.24033542
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H	3.26878031	-4.70451778	3.13302377
H	4.41556745	-6.04986152	3.34336982
H	5.45463751	5.30676355	6.21138026
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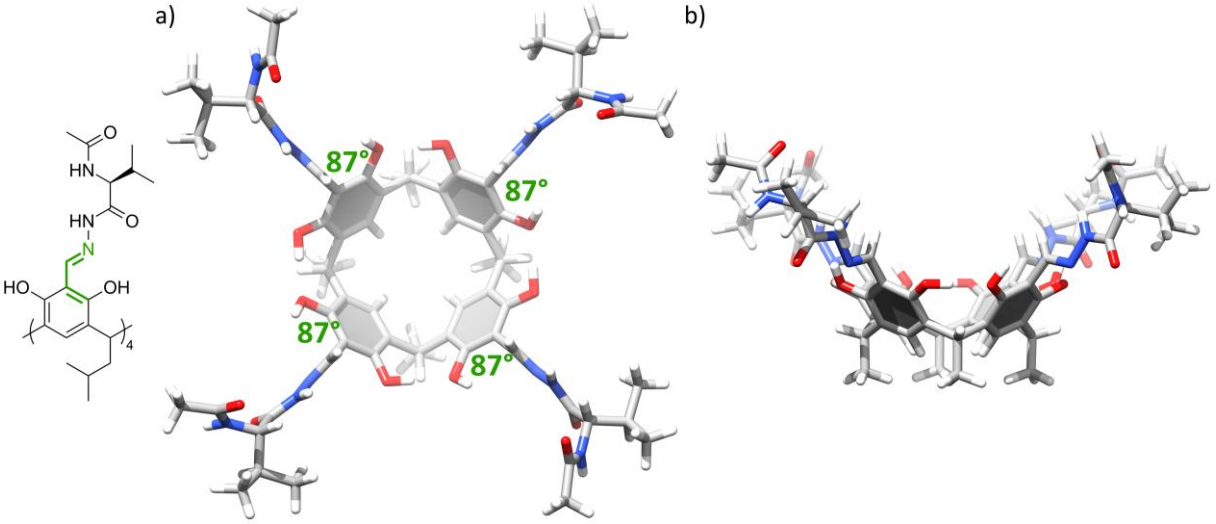
Conformation 5
conf-5



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C	-3.59100000	2.46900000	-2.09900000
C	-3.91800000	1.20700000	-2.67000000
C	-3.19800000	0.70400000	-3.72900000
C	-2.15600000	1.46700000	-4.22100000
C	-1.79300000	2.72100000	-3.74500000
C	-4.38300000	2.98000000	-1.03000000
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C	-7.68767284	5.44132646	1.11450729
N	-7.52406073	6.85440084	1.46881204
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C	-9.55031628	3.72121430	0.38285874
C	-3.55600000	-0.67700000	-4.33900000
C	-3.51700000	-0.67600000	-5.88700000
O	-4.40900000	-2.15200000	-2.15000000
O	-0.54600000	-4.96200000	-2.11300000
C	-3.20500000	-2.51000000	-2.66800000
C	-2.46900000	-3.59100000	-2.09900000
C	-1.20700000	-3.91800000	-2.67000000
C	-0.70400000	-3.19800000	-3.72900000
C	-1.46700000	-2.15600000	-4.22100000
C	-2.72100000	-1.79300000	-3.74500000
C	-2.98000000	-4.38300000	-1.03000000
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N	-4.13207142	-6.10221563	-0.11095536
C	-5.10808336	-7.06644795	-0.23484132

O	-5.65256522	-7.35086581	-1.23498929
C	-5.44132646	-7.68767284	1.11450729
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C	-8.77360464	-7.08675066	2.97631385
C	-5.27893824	-9.30006500	0.81565021
C	-5.88179317	-10.07493454	1.91887328
C	-3.72121430	-9.55031628	0.38285874
C	0.67700000	-3.55600000	-4.33900000
C	0.67600000	-3.51700000	-5.88700000
O	4.40900000	2.15200000	-2.15000000
O	0.54600000	4.96200000	-2.11300000
C	3.20500000	2.51000000	-2.66800000
C	2.46900000	3.59100000	-2.09900000
C	1.20700000	3.91800000	-2.67000000
C	0.70400000	3.19800000	-3.72900000
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C	2.72100000	1.79300000	-3.74500000
C	2.98000000	4.38300000	-1.03000000
N	3.72119384	5.41712742	-1.23805329
N	4.13207142	6.10221563	-0.11095536
C	5.10808336	7.06644795	-0.23484132
O	5.65256522	7.35086581	-1.23498929
C	5.44132646	7.68767284	1.11450729
N	6.85440084	7.52406073	1.46881204
C	7.25459242	7.07611333	2.68307719
O	6.42715926	6.75628064	3.56867666
C	8.77360464	7.08675066	2.97631385
C	5.27893824	9.30006500	0.81565021
C	5.88179317	10.07493454	1.91887328
C	3.72121430	9.55031628	0.38285874
C	-0.67700000	3.55600000	-4.33900000
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O	2.15200000	-4.40900000	-2.15000000
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C	2.51000000	-3.20500000	-2.66800000
C	3.59100000	-2.46900000	-2.09900000
C	3.91800000	-1.20700000	-2.67000000
C	3.19800000	-0.70400000	-3.72900000
C	2.15600000	-1.46700000	-4.22100000
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C	4.38300000	-2.98000000	-1.03000000
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O	7.35086581	-5.65256522	-1.23498929
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N	7.52406073	-6.85440084	1.46881204
C	7.07611333	-7.25459242	2.68307719
O	6.75628064	-6.42715926	3.56867666
C	7.08675066	-8.77360464	2.97631385

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H	-9.50898415	5.88037428	-0.06924949
H	-4.58900000	-0.88100000	-4.05600000
H	-1.05800000	-1.58000000	-5.03800000
H	-2.73908029	-4.10828690	-0.01475796
H	-3.72286397	-5.89855704	0.79048207
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H	5.88037428	9.50898415	-0.06924949
H	-0.88100000	4.58900000	-4.05600000
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H	9.50898415	-5.88037428	-0.06924949
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H	-4.78200000	-0.39700000	-2.11600000
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H	-3.60300000	-1.69900000	-6.25300000
H	-2.57500000	-0.24600000	-6.22700000
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H	3.60300000	1.69900000	-6.25300000

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H	-5.40477116	-11.05284048	1.97806761
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H	-3.06478948	-9.23983292	1.19608597
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H	-0.08200000	4.34700000	-6.27100000
H	-1.69900000	3.60300000	-6.25300000
H	-0.24600000	2.57500000	-6.22700000
H	0.08200000	-4.34700000	-6.27100000
H	1.69900000	-3.60300000	-6.25300000
H	0.24600000	-2.57500000	-6.22700000
H	-6.70335709	8.95193716	3.98106201
H	-6.45838308	9.28817063	2.25029318
H	-8.10838285	9.14992869	2.90486550
H	-11.05284048	5.40477116	1.97806761
H	-9.54167164	5.73677436	2.85787872
H	-10.20178501	6.94789847	1.73189350
H	10.60808355	-3.56752381	0.17438181
H	8.96682639	-3.49407948	-0.50993089
H	9.23983292	-3.06478948	1.19608597
H	5.40477116	11.05284048	1.97806761
H	6.94789847	10.20178501	1.73189350
H	5.73677436	9.54167164	2.85787872
H	11.05284048	-5.40477116	1.97806761
H	9.54167164	-5.73677436	2.85787872
H	10.20178501	-6.94789847	1.73189350

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