Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supporting Information

Ring–Chain Equilibria of Dynamic Macrocycles with a Bis(hindered amino)disulfide Linker

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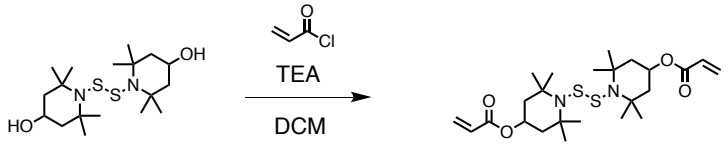
1. Synthesis

BiTEMPS-diacrylate-S



BiTEMPS-diol **BiTEMPS-diacrylate-S**

Triethylamine (8.50 mL, 61.0 mmol) was added to a solution of **BiTEMPS-diol** (3.00 g, 7.97 mmol) in 500 mL of dry CH_2Cl_2 at 0 °C before acryloyl chloride (1.6 mL, 15.8 mmol) was carefully added. The reaction mixture was stirred for 2 hours at 0 °C, and for 18 hours at room temperature under an inert atmosphere. After the solvent was evaporated under reduced pressure, the residue was extracted with CH_2Cl_2. The organic layer was concentrated and purified by column chromatography on silica gel eluting with $CHCl_3$/hexane (7/6, v/v). The obtained eluate was evaporated under reduced pressure to afford **BiTEMPS-diacrylate-S** as a white solid (2.85 g, 74%). ^{1}H NMR ($CDCl_3$), δ (ppm): 6.41-6.37 (d, 2H, -CH_2=$\underline{CH}$-CO-), 6.06–6.13 (m, 2H, -$\underline{CH_2}$=CH-CO-), 5.82–5.80 (d, 2H, -$\underline{CH_2}$=CH-CO-), 5.14–5.21 (m, 2H, -O-$\underline{CH}$-$(CH_2)_2$-), 2.01–1.97 (m, 4H, -O-CH-$\underline{(CH_2)_2}$-), 1.60–1.55 (m, 4H, -O-CH-$\underline{(CH_2)_2}$-), 1.46 (s, 6H, -C-$\underline{CH_3}$), 1.25 (s, 6H, -C-$\underline{CH_3}$), ^{13}C{^{1}H} NMR ($CDCl_3$), δ (ppm): 165.76, 130.69, 128.97, 67.32, 59.65, 45.78, 35.00, 26.84. FT-IR (KBr, cm^{-1}): 2980, 1723, 1634, 1463, 1407, 1381, 1300, 1202, 986, 813, MS (ESI): 507.2309 $[M+Na]^+$, calculated for $C_{24}H_{40}N_2O_4$ S $_2$Na $[M+Na]^+$: 507.2322.

2. Characterization of LPs for cyclization reaction

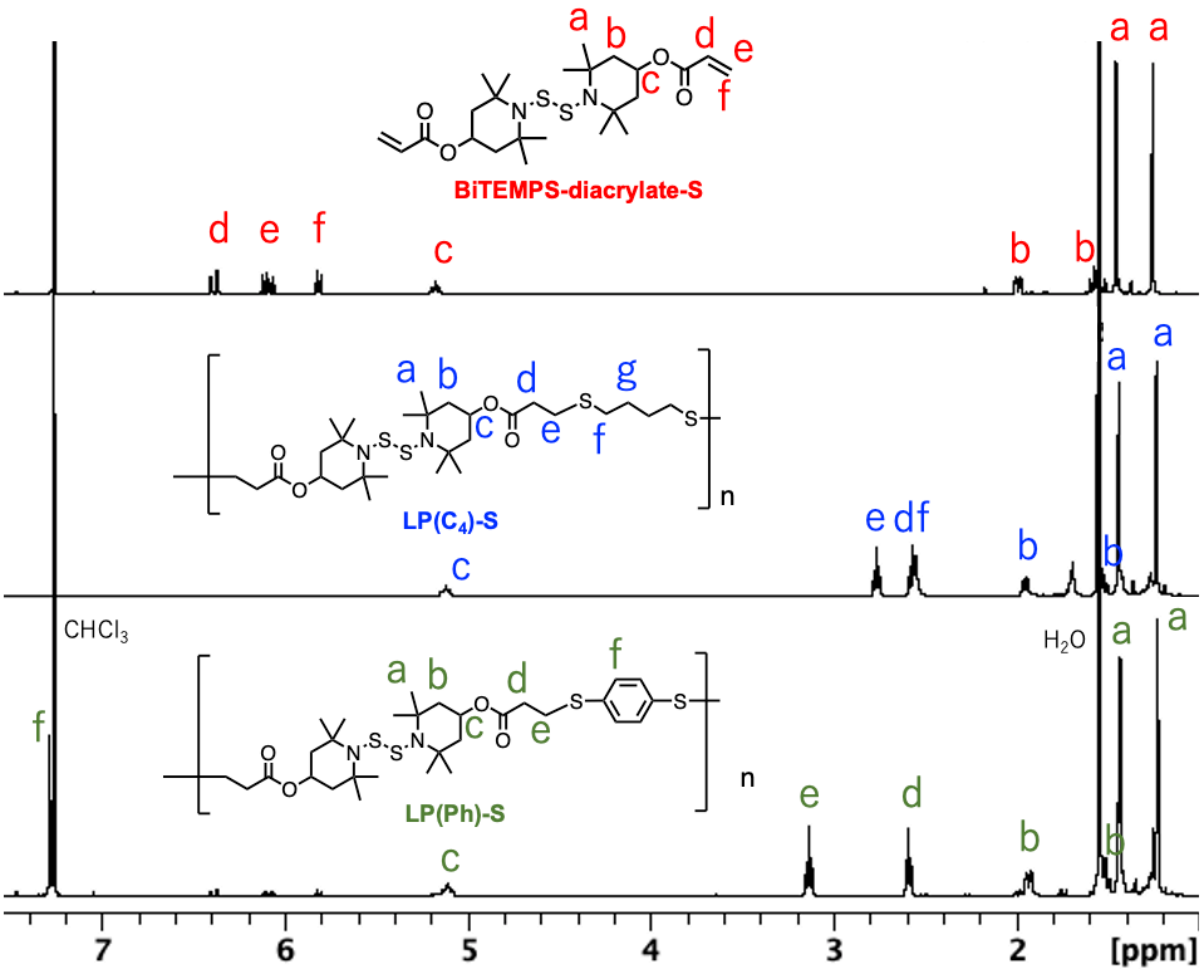


Figure S1. ^{1}H NMR spectra of **BiTEMPS-diacrylate-S** (red), **LP(C$_4$)-S** (blue), and **LP(Ph)-S** (green) (500 MHz, 25 °C, $CDCl_3$).

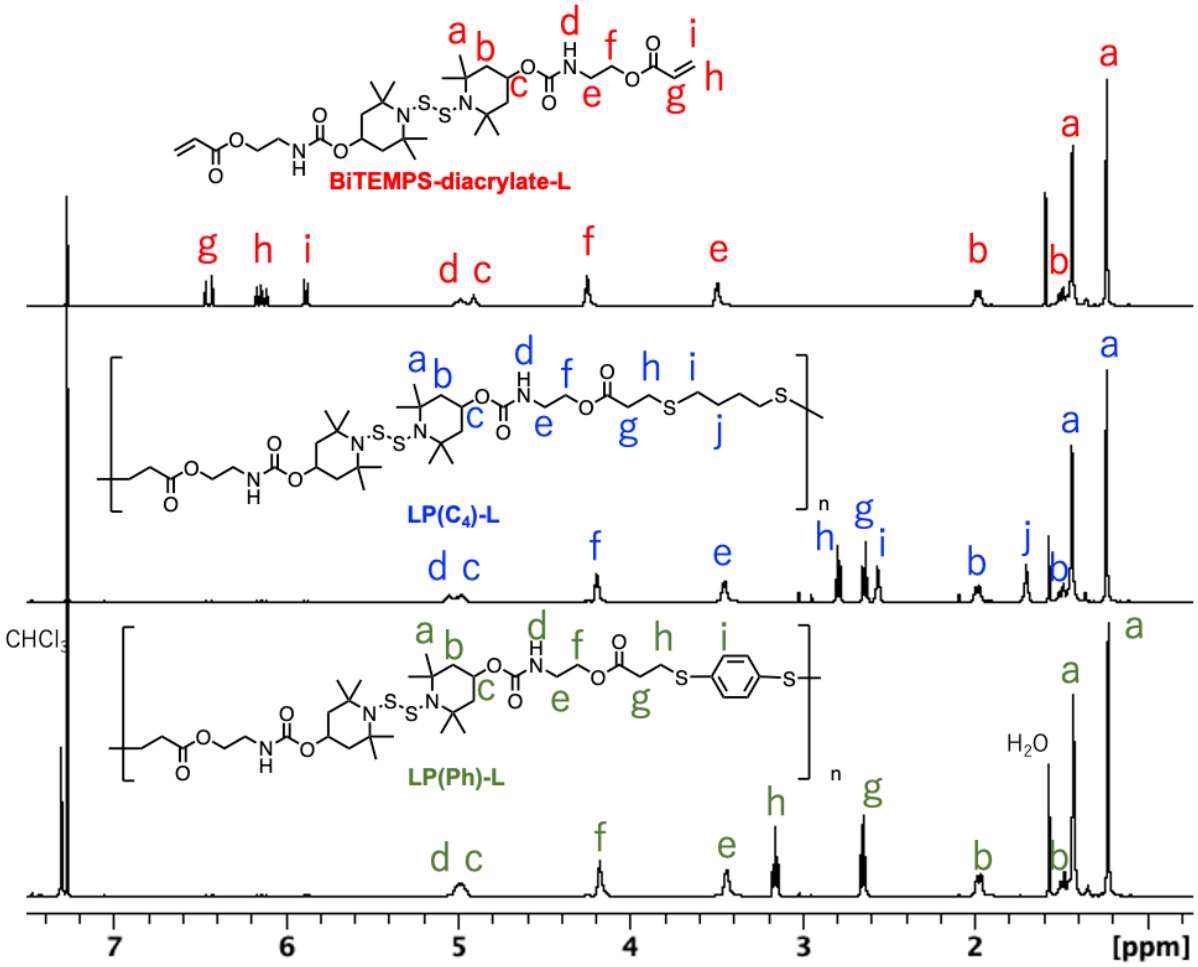


Figure S2. ^{1}H NMR spectra of **BiTEMPS-diacrylate-L** (red), **LP(C$_4$)-L** (blue), and **LP(Ph)-L** (green) (500 MHz, 25 °C, $CDCl_3$).

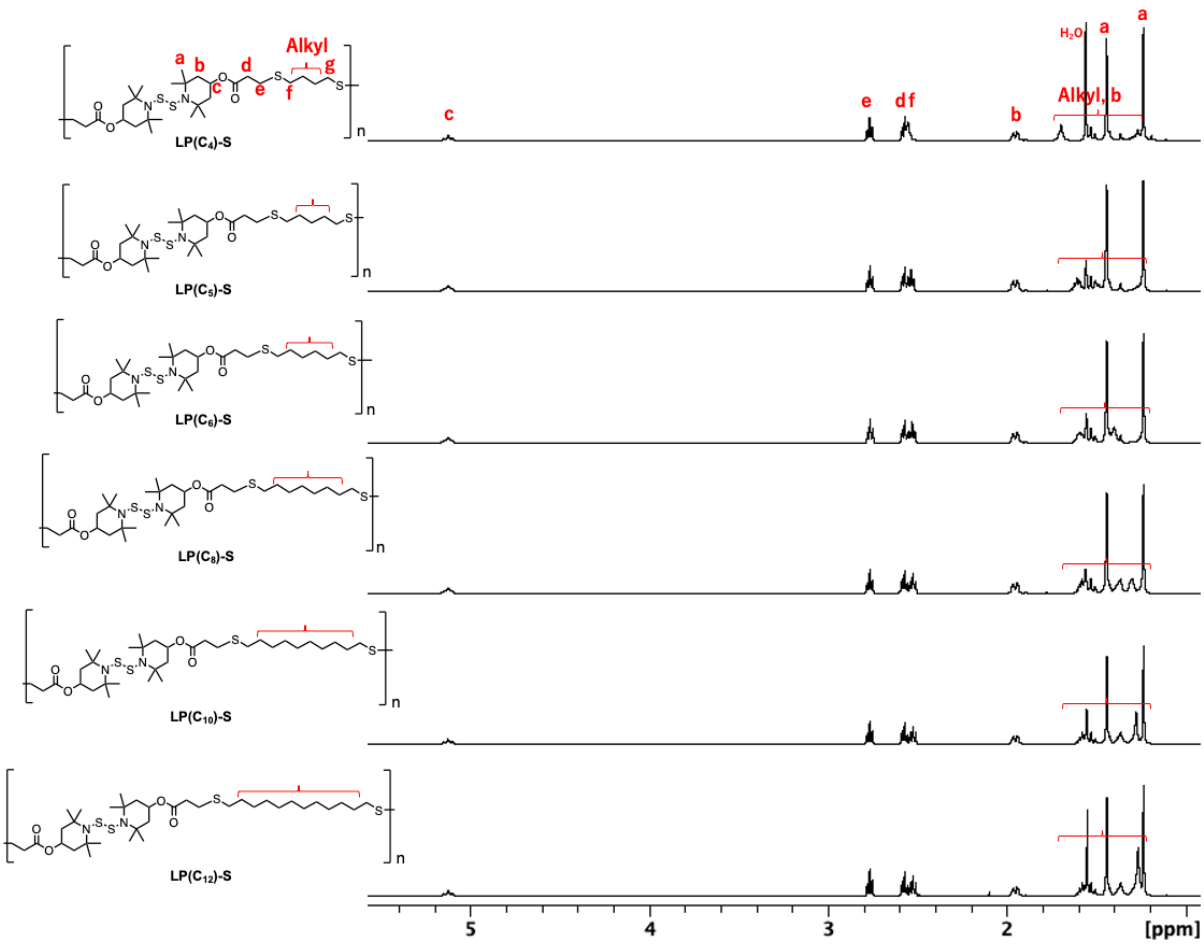


Figure S3. ^{1}H NMR spectra of **LP(C$_x$)-S** (500 MHz, 25 °C, $CDCl_3$).

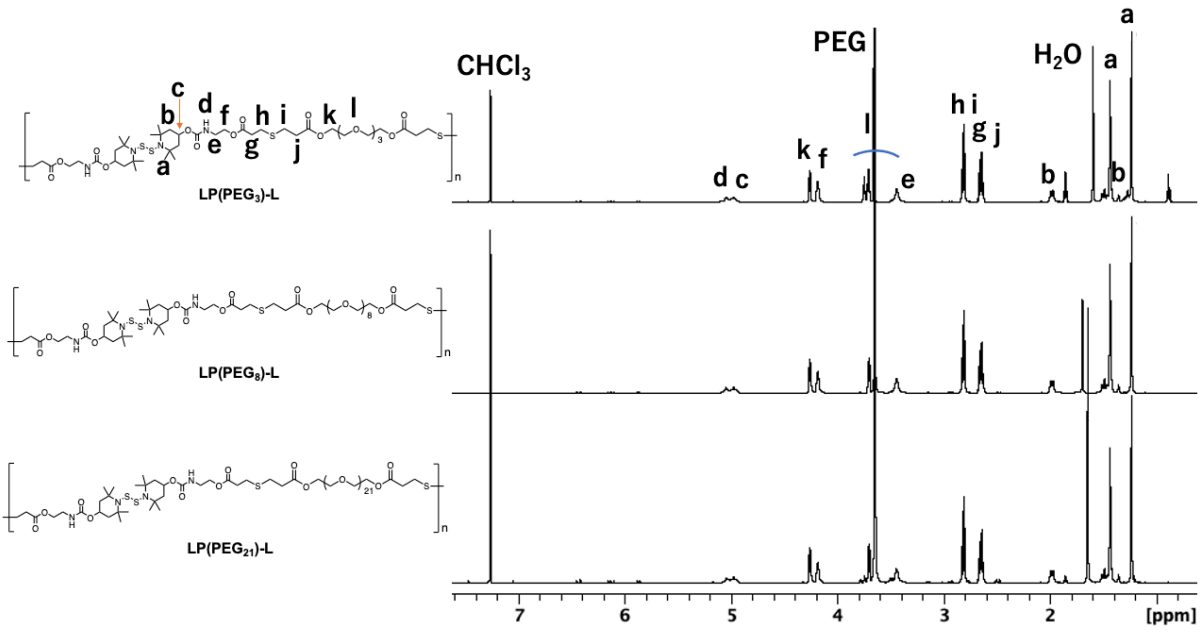


Figure S4. ^{1}H NMR spectra of **LP(PEG$_k$)-L** (500 MHz, 25 °C, $CDCl_3$).

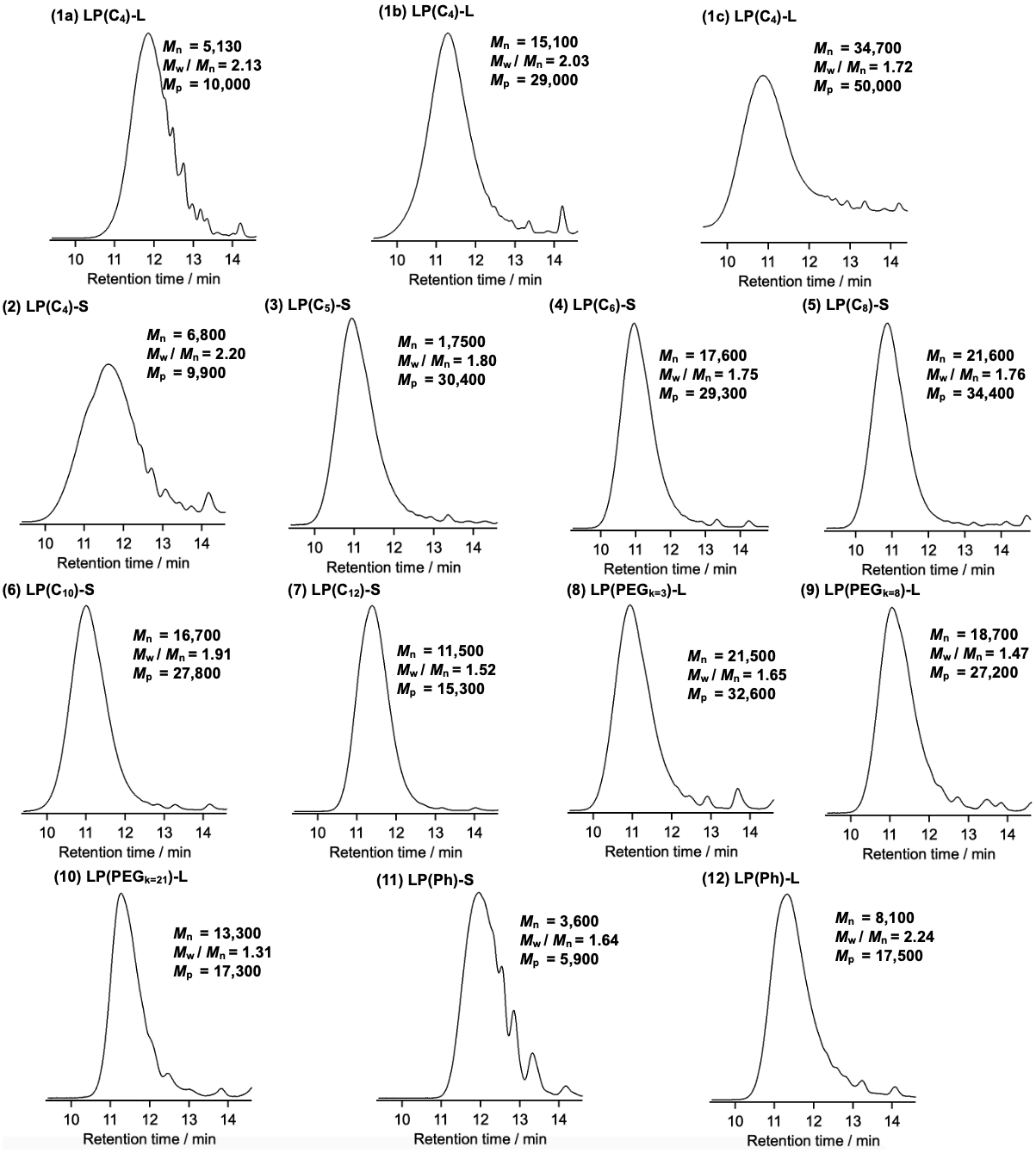


Figure S5. (a) GPC profiles of **LP**s (PS standard, eluent, THF; flow rate, 0.6 mL/min, detected by UV).

3. Reaction tracking of cyclization behaviour

The experiments on solvent dependence were performed using sample 1b at a concentration of 10 g/L. (Note that the other experiments were performed with concentrations in mol of repeating units)

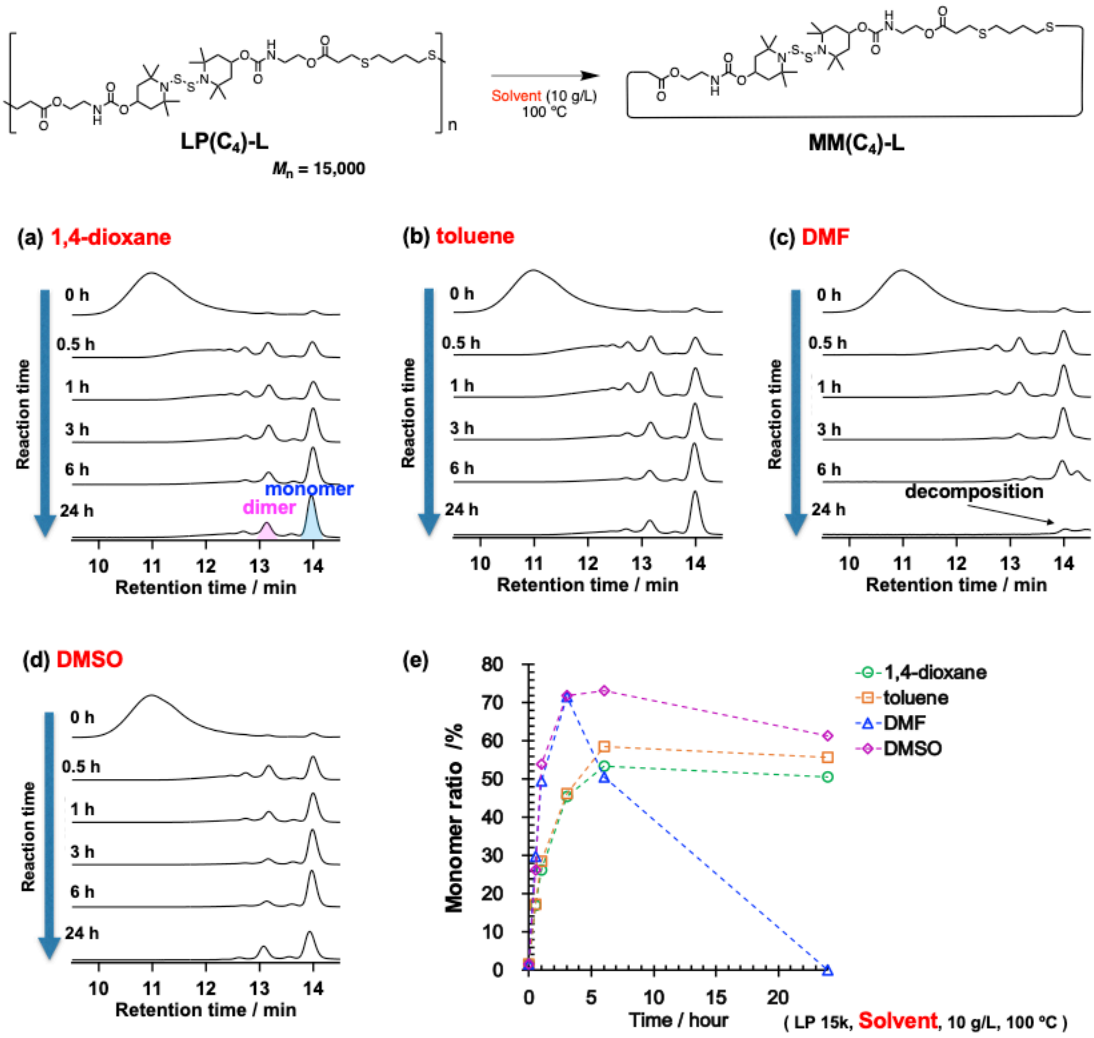


Figure S6. Solvent dependences of producing ratio of **MM(C4)-L** at cyclodepolymerization at 100 ºC at 10 g/L and changes in GPC profile at cyclodepolymerization (PS standard, eluent, THF; flow rate, 0.6 mL/min, detected by UV). (a) 1,4-dioxane, (b) toluene, (c) DMF, and (d) DMSO. (e) Monomer ratio during the cyclodepolymerization.

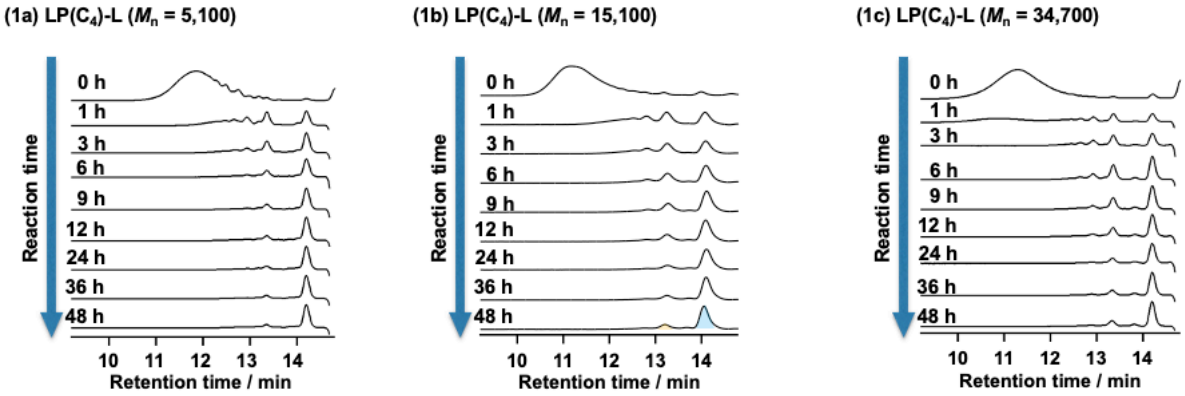


Figure S7. LP's molar weight dependences of producing ratio of **MM(C4)-L** at cyclodepolymerization in toluene at 10 mM at 100 ºC and changes in GPC profiles at cyclodepolymerization (PS standard, eluent, THF; flow rate, 0.6 mL/min, detected by UV). (a) M_n = 5100, (b) M_n = 15100, and (c) M_n = 34700.

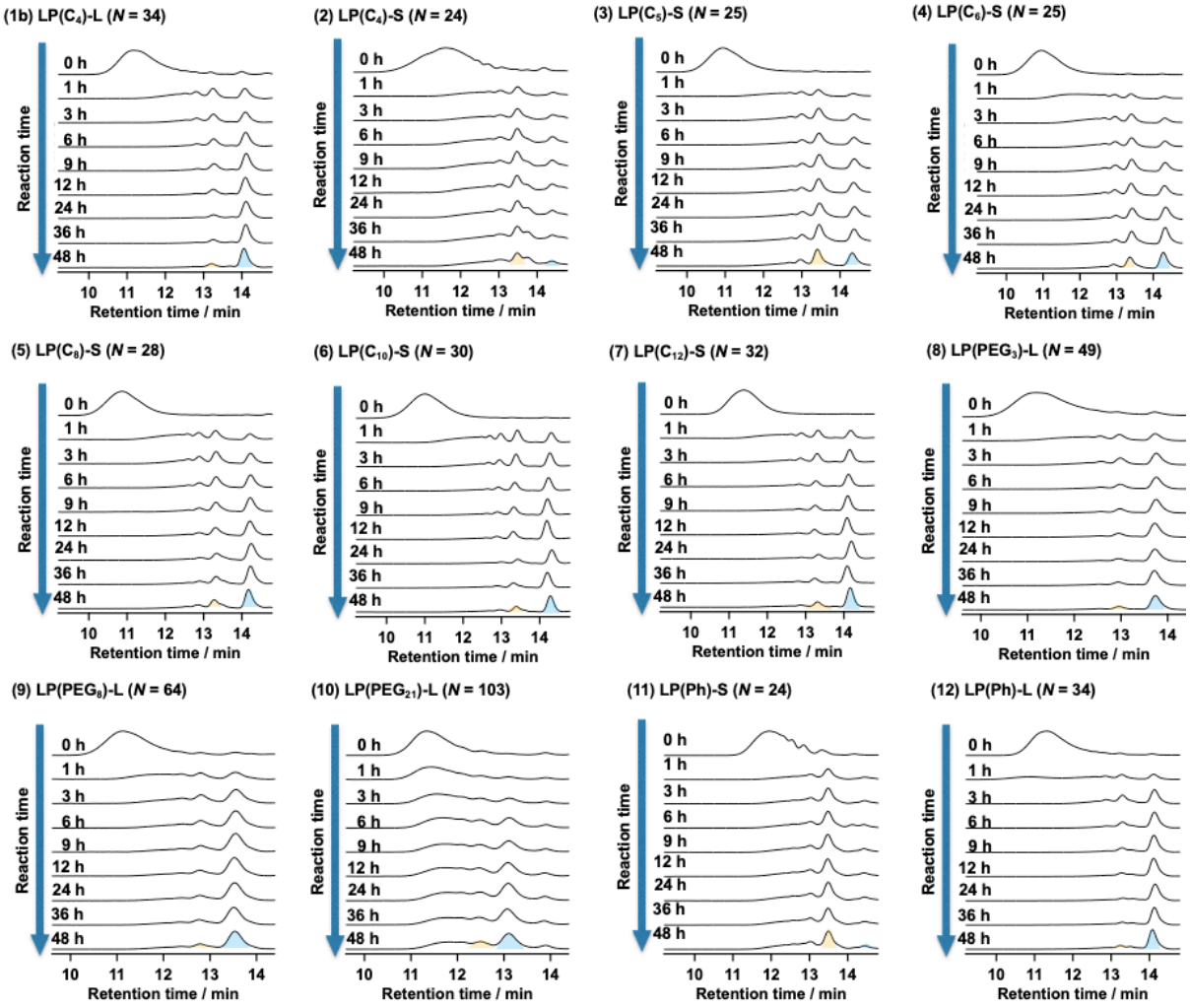


Figure S8. Changes in GPC profile at cyclodepolymerization of LPs (10 mM) (PS standard, eluent, THF; flow rate, 0.6 mL/min, detected by UV).

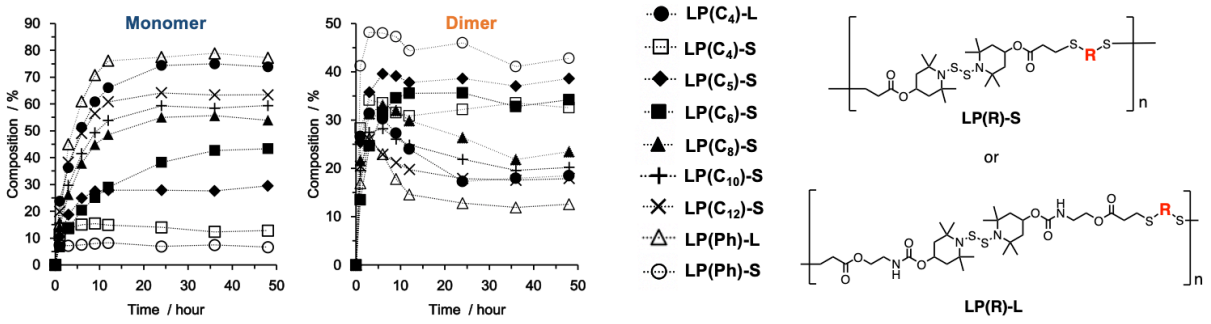


Figure S9. Changes in composition ratio of macrocyclic monomers and dimers during depolymerization reactions of samples 1b to 7, 11, and 12.

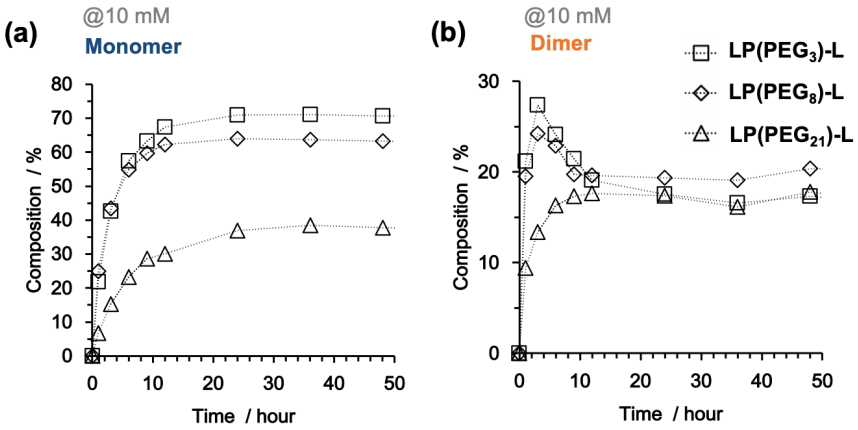


Figure S10. Changes in composition ratio of macrocyclic monomer and dimer during cyclodepolymerization of samples 8 to 10.

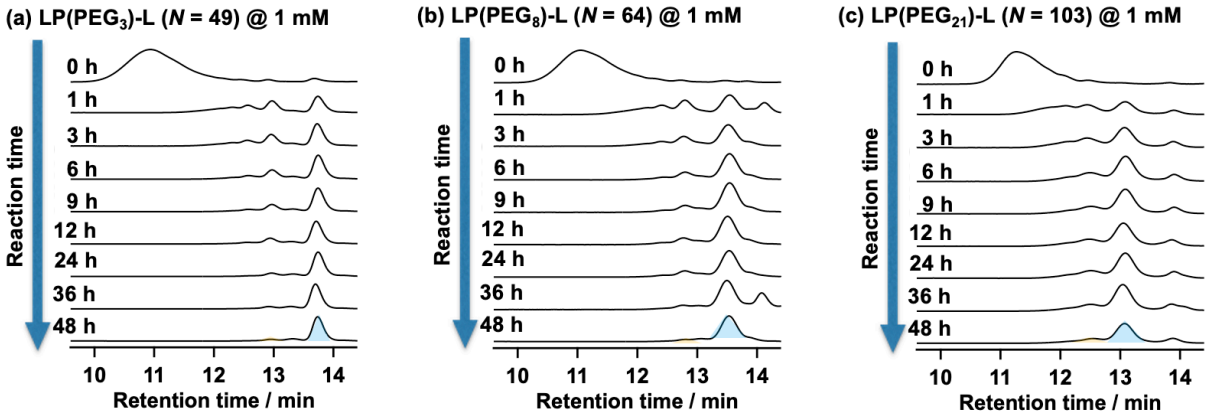


Figure S11. Changes in GPC profile at cyclodepolymerization of LP(PEG$_k$) (1 mM) (PS standard, eluent, THF; flow rate, 0.6 mL/min, detected by UV).

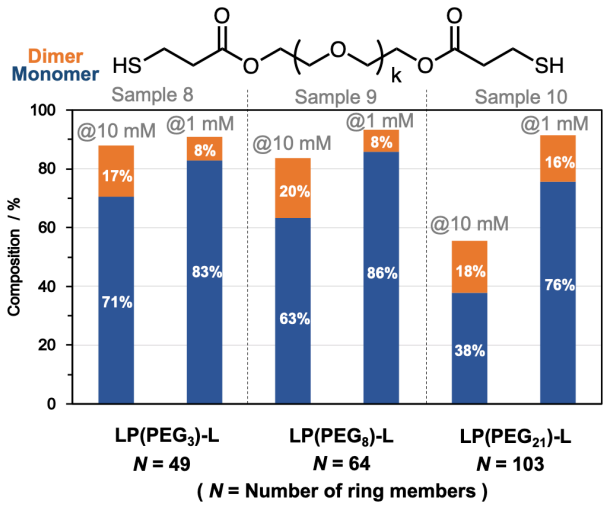
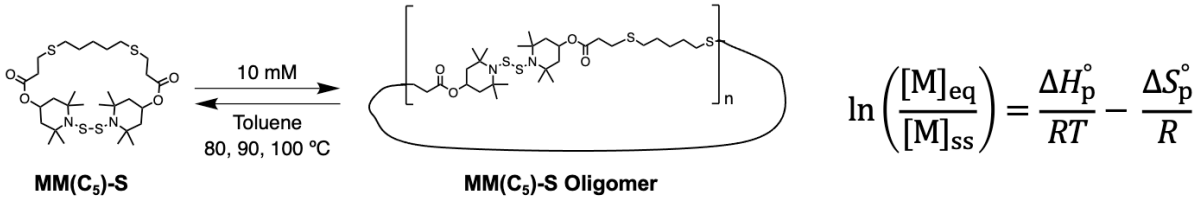


Figure S12. Productivities of macrocyclic monomers and dimers at samples 1 to 12 at 1 mM and 10 mM.

4. Estimation for enthalpy of ring–chain equilibria

Oligomerization behavior

In a test tube, **MM(C$_5$)-S** (in toluene, 10.0 mM of BiTEMPS unit concentration) was added and stirred at 80, 90, or 100 °C for 18 days. The reaction was tracked by gel permeation chromatography (GPC). The ratio of monomer and dimer was calculated from area ratio of peaks. The upper-side of the test tube was kept under 10 °C to prevent the solvent removing outside during this experiment.



$$\ln\left(\frac{[\mathrm{M}]_{\mathrm{eq}}}{[\mathrm{M}]_{\mathrm{ss}}}\right) = \frac{\Delta H_{\mathrm{p}}^{\circ}}{RT} - \frac{\Delta S_{\mathrm{p}}^{\circ}}{R}$$

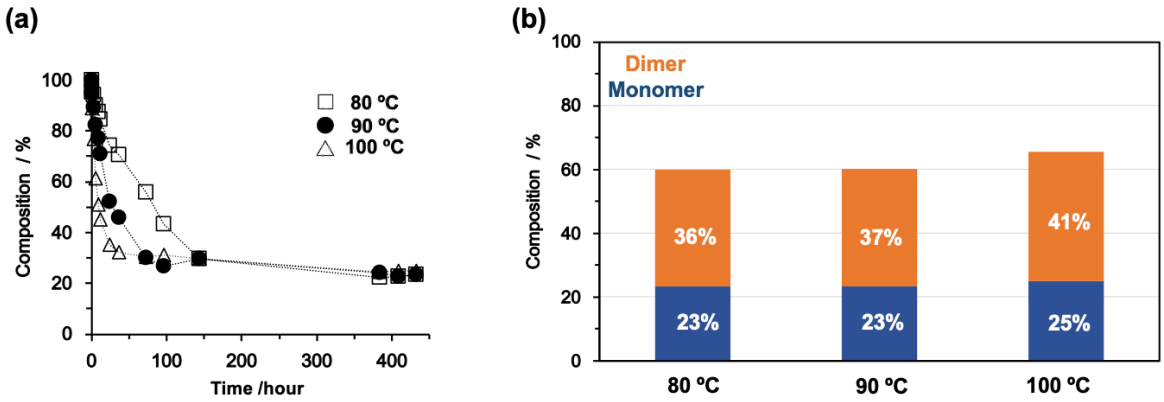


Figure S13. (a) Changes in composition ratio of macrocyclic monomer during oligomerization reactions of **MM(C$_5$)-S** at 10 mM. (a) Productivities of cyclic monomers and dimers after 18 days.

DFT calculation

The calculations of *Δ*H were conducted by using DFT at the UB3LYP/6-31G(d,p) level. **L(C_x)-S** was adducts of **MM(C_x)-S** and **BiTEMPS-OMe** (BiTEMPS derivative with simple structure) and used as linear counterparts *Δ*H value was estimated from the equation below.

$$\Delta H = H(\text{Cyclic}) + H(\text{End}) - H(\text{Linear})$$

As typical strained cyclic monomers, we calculated *Δ*H of δ-valerolactone, ε-caprolactone, 1,2-dithiolane, cyclopentene, and cyclooctene. The calculated *Δ*H values of cyclopentene, and cyclooctene were referred to the article Wang reported[1] (Calculations level was B3LYP/6-31G(d,p)). Optimized geometries from DFT calculations at UB3LYP/6-31g(d,p) level was summarized at the end the document.

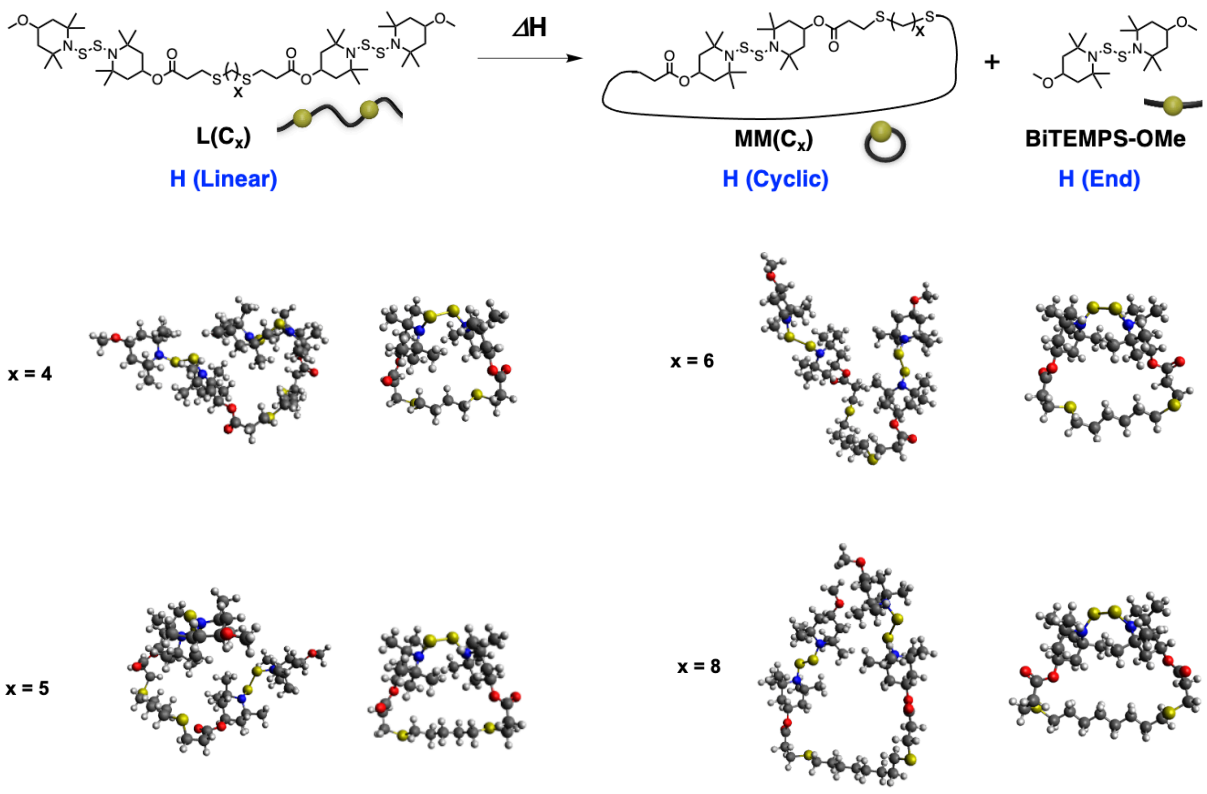


Figure S14. Schematic image of calculations of *Δ*H and optimized structures of **MM(C_x)-S** and its linear counter parts **L(C_x)-S**.

5. Characterization of isolated macrocycles

Spectra

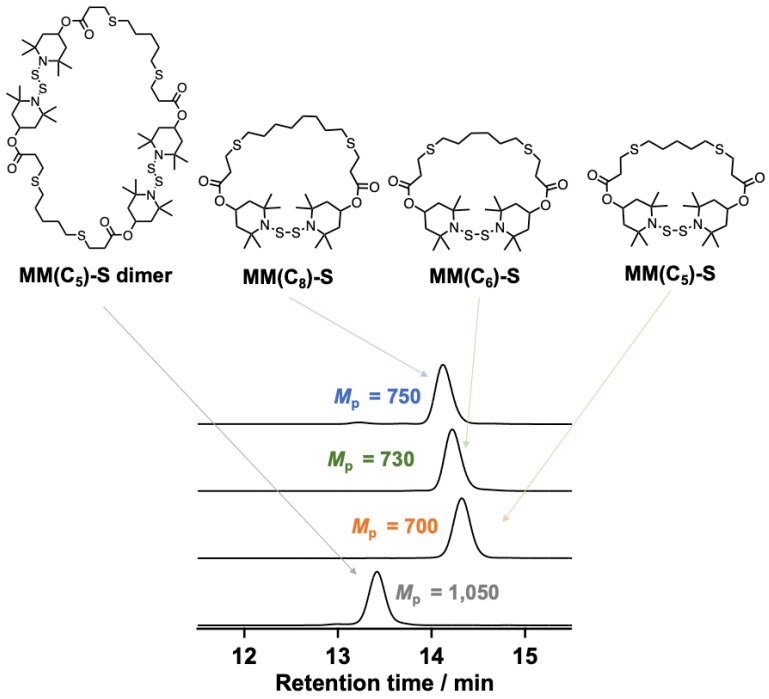


Figure S15. (a) GPC profiles of **MM(C$_5$)-S dimer**, **MM(C$_8$)-S**, **MM(C$_6$)-S**, and **MM(C$_5$)-S** (PS standard, eluent, THF; flow rate, 0.6 mL/min, detected by RI).

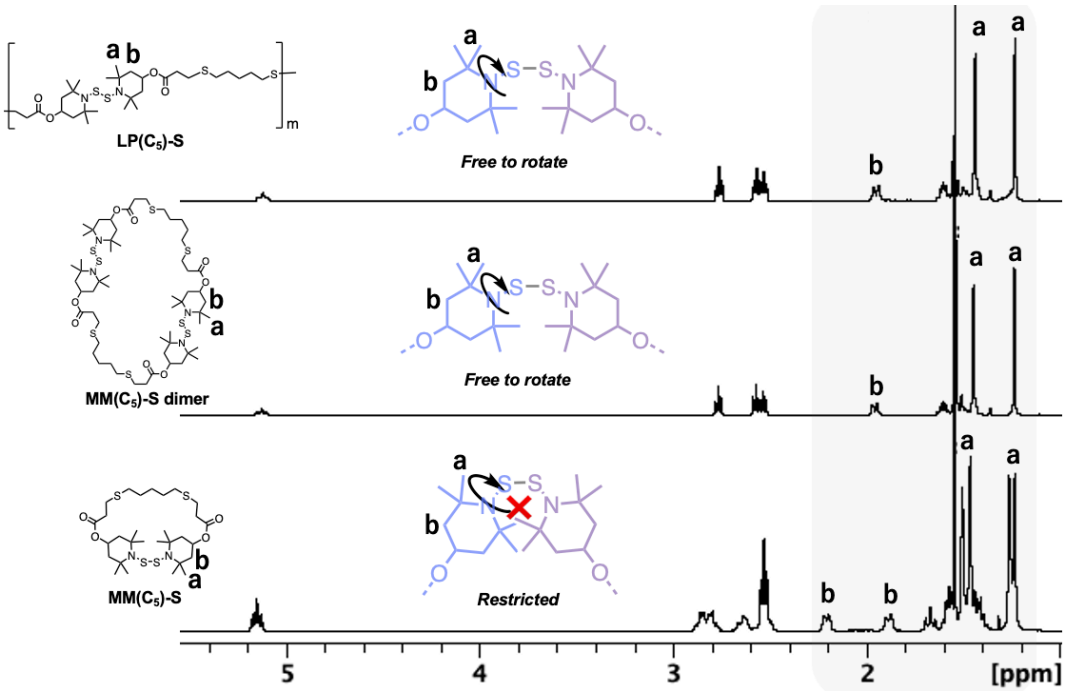


Figure S16. ^{1}H NMR spectra of **MM(C$_5$)-S dimer**, **MM(C$_8$)-S**, **MM(C$_6$)-S**, and **MM(C$_5$)-S** (500 MHz, 25 °C, $CDCl_3$).

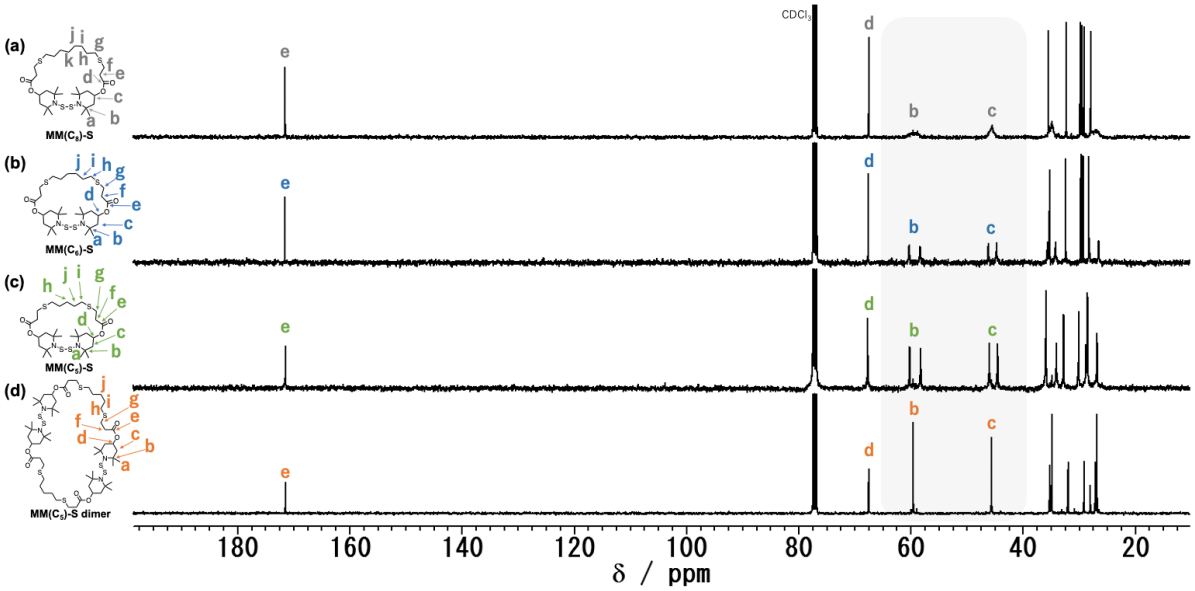


Figure S17. $^{13}C\{^{1}H\}$ NMR spectra of **MM(C$_5$)-S dimer**, **MM(C$_8$)-S**, **MM(C$_6$)-S**, and **MM(C$_5$)-S** (100 MHz, 25 °C, $CDCl_3$).

X-ray crystallography

Single crystals of **MM(C$_5$)-S** and **MM(C$_8$)-S** were obtained by vapor diffusion of heptane into ethyl acetate solutions and mounted on a fiber loop. Diffraction experiments were performed on a Rigaku Saturn CCD area detector with graphite monochromated Mo-Kα radiation (λ = 0.710 73 Å). Intensity data (6° < 2θ < 55°) were corrected for Lorentz–polarization effects and for absorption. Structure solution and refinements were carried out by using the CrystalStructure program package.[2] The structures were solved by SHELXT[3] and refined by full-matrix least-squares techniques against F^2 using the SHELXL-2014/7 program.[4] The crystals of **MM(C$_5$)-S** and **MM(C$_8$)-S** contain nine and two crystallographically independent molecules (Figures S18 and S19). Some of the carbon atoms were partially disordered and refined with restraint geometries and thermal displacement parameters. The CH hydrogen atoms were included in the refinements with a riding model.

CCDC-2261420 and CCDC-2261421 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via http://www.ccdc.cam.ac.uk/data_request/cif.

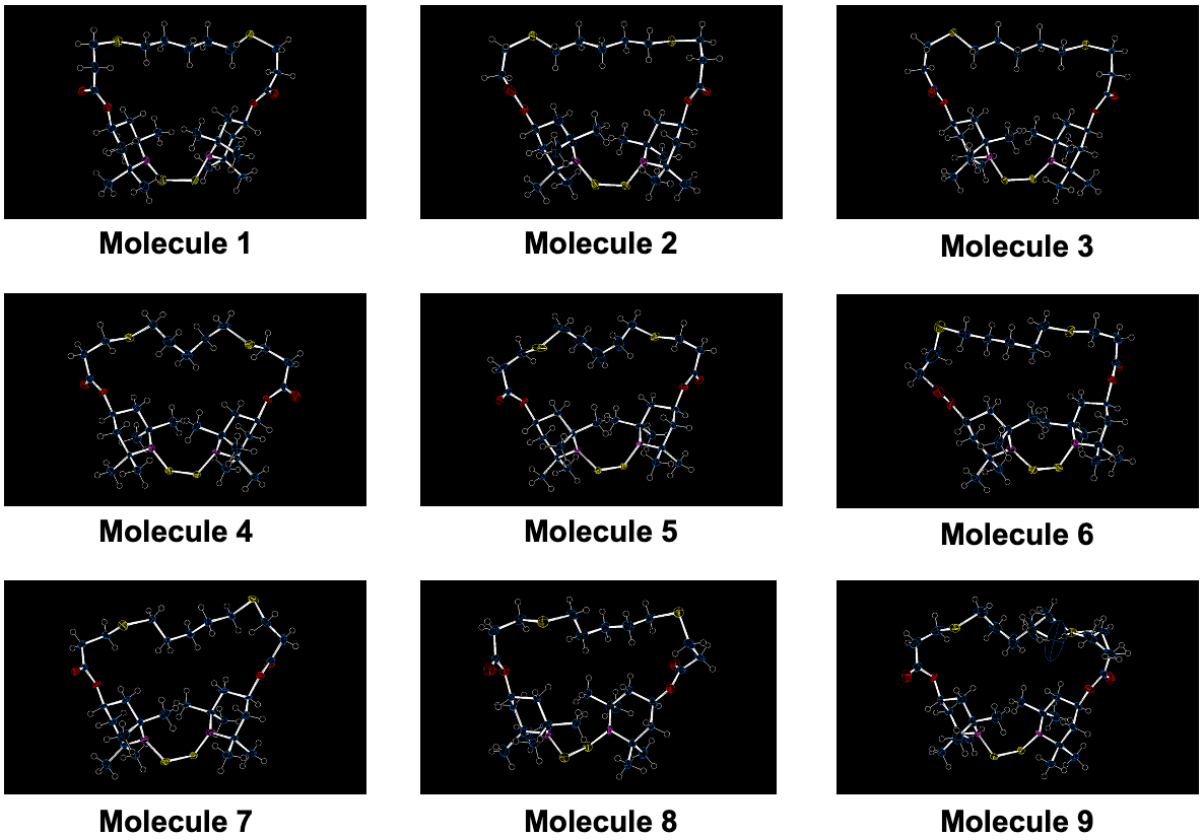


Figure S18. X-ray structures of **MM(C_5)-S**.

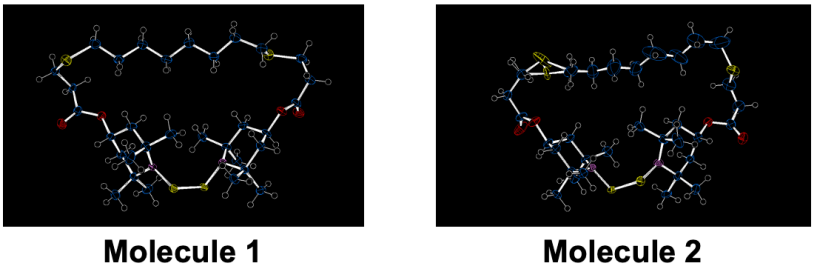


Figure S19. X-ray structures of **MM(C_8)-S**.

6. Polymerization of isolated macrocycles

We conducted polymerization of isolated macrocycles shown in **Figure 4** in a concentrated solution in order to investigate their polymerization behavior. Polymerization was conducted in 1,4-dioxane (256 mM BiTEMPS unit concentration). The polymerization was performed at 80 °C to ensure that early polymerization behavior could be observed. **Figure S21** shows the monomer (m = 1) ratio, dimer (m = 2) ratio, and M_p of the polymer during the polymerization, respectively. These results indicate that the polymerization of MMs with a smaller ring occurred more rapidly. This result suggests that the polymerization behavior of MMs can be controlled by changing the chain length of MMs.

(Experimental detail)

In a 20 mL test tube, **MM(R)-S or L** (in 1,4-dioxane, 256 mM of BiTEMPS unit concentration) and stirred at 80 °C for 9 hours. The reactions were tracked by GPC measurements.

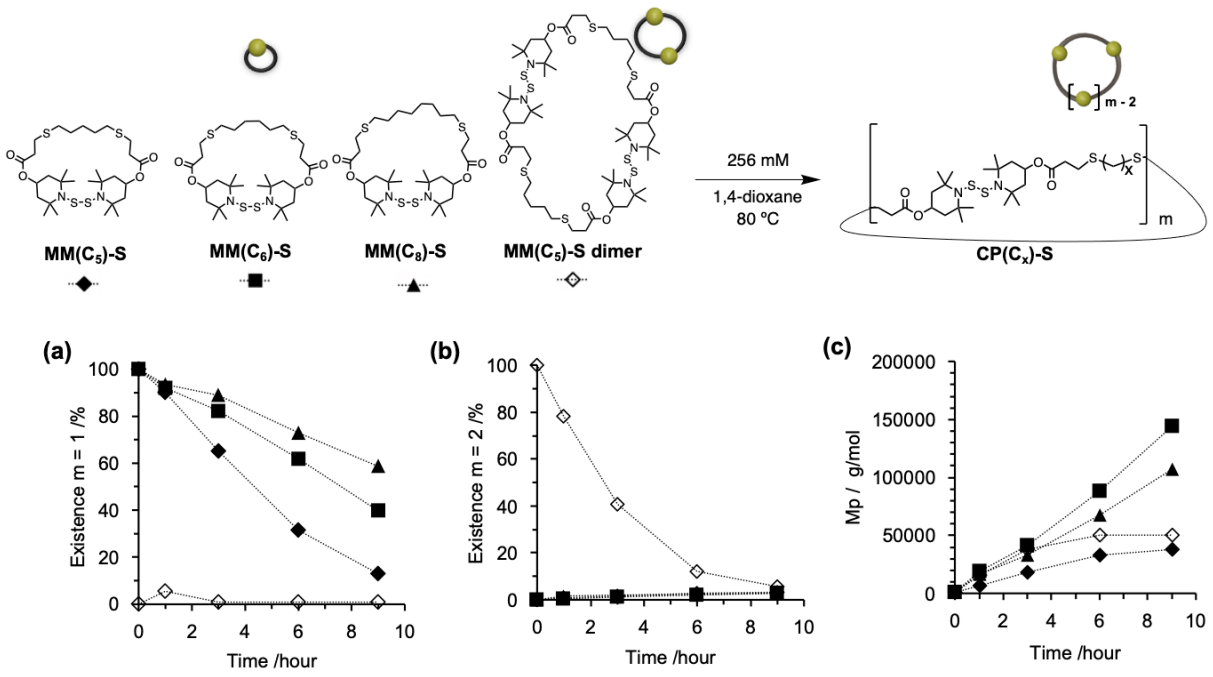


Figure S20. Polymerization behavior of **MM(C$_5$)-S**, **MM(C$_6$)-S**, **MM(C$_8$)-S**, and **MM(C$_5$)-S dimer** in 1,4-dioxane (256 mM) at 80ºC. Composition ratio of (a) monomers (m = 1) and (b) dimers (m = 2). (c) Peak top molecular weight of polymers.

7.Optimized geometries from DFT calculations at UB3LYP/6-31g(d,p) level

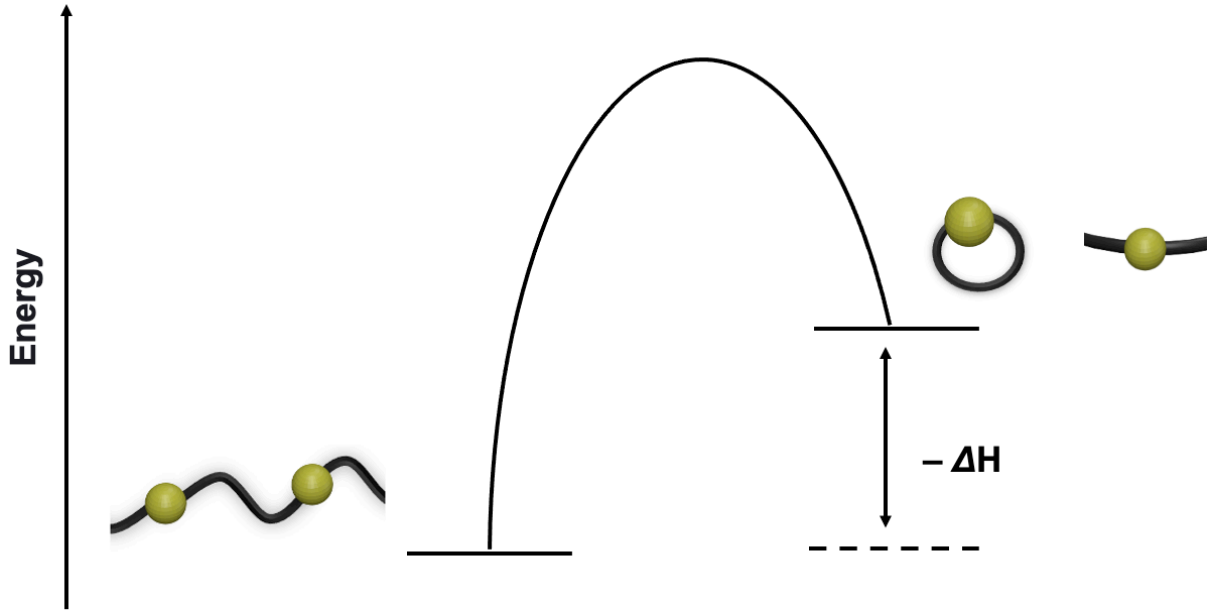
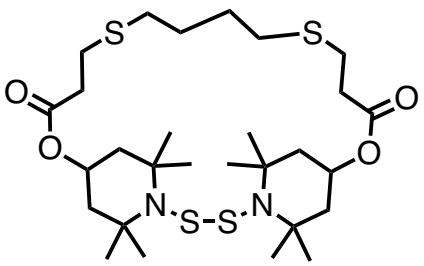


Figure S21. Ring-strain energy (ΔH)

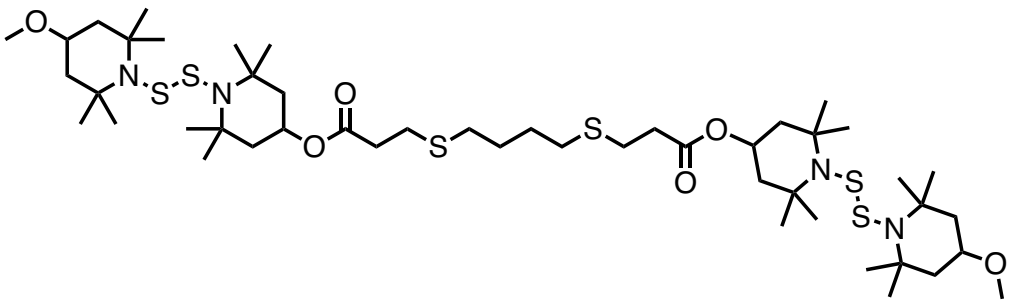


MM(C_4)-S

atom	X	Y	Z
S	-0.69246	-3.95777	0.69506
S	4.54571	3.42211	-0.43046
S	-1.1019	4.77704	-0.83181
S	-2.32574	-3.37351	-0.61868
O	4.07161	-0.84498	-0.90313
O	5.18881	-0.23258	0.97256
O	-4.4276	3.36003	-0.91895
O	-3.53792	2.19771	0.81566
N	0.74304	-3.1246	0.28586
N	-2.82765	-1.78011	-0.28445
C	1.24948	-2.16099	1.33056
C	2.2234	-1.17141	0.65447
H	1.65457	-0.51899	-0.01901
H	2.67815	-0.54728	1.42788
C	3.31153	-1.84814	-0.164
H	4.01386	-2.38101	0.48267
C	2.68805	-2.75171	-1.21379
H	3.47095	-3.26525	-1.78222
H	2.14361	-2.11293	-1.91837
C	1.70974	-3.81017	-0.64562
C	0.08595	-1.32282	1.89379
H	-0.51518	-1.8932	2.60349
H	-0.57324	-0.97105	1.0982
H	0.49775	-0.45699	2.42283

C	1.92784	-2.86539	2.53092
H	2.88105	-3.33219	2.27925
H	1.26583	-3.63584	2.93718
H	2.12353	-2.13709	3.32501
C	0.9483	-4.39177	-1.85195
H	0.31109	-3.63764	-2.31752
H	0.32528	-5.2409	-1.56557
H	1.67321	-4.7405	-2.59457
C	2.47672	-4.97322	0.02675
H	1.77251	-5.65856	0.50755
H	3.19436	-4.63971	0.77802
H	3.03204	-5.53928	-0.72872
C	4.96527	-0.10603	-0.21493
C	5.67916	0.88256	-1.11964
H	5.1256	1.00516	-2.05258
H	6.6444	0.41964	-1.36966
C	5.94772	2.23371	-0.44243
H	6.73285	2.76368	-0.98816
H	6.30085	2.07502	0.58029
C	3.50537	2.79317	0.95676
H	3.09829	1.8128	0.6953
H	4.14769	2.66906	1.83345
C	2.35659	3.76008	1.26974
H	1.8673	3.39519	2.18324
H	2.76217	4.75094	1.50906
C	1.31037	3.87355	0.14997
H	1.76085	4.33442	-0.73632
H	0.9923	2.86782	-0.15219
C	0.07716	4.67666	0.57771
H	0.3597	5.68965	0.88565
H	-0.41164	4.1859	1.42611
C	-2.59358	5.50426	-0.043
H	-2.31809	6.42306	0.48325
H	-3.23514	5.77663	-0.88465

C	-3.36165	4.55931	0.89062
H	-4.24432	5.08776	1.27454
H	-2.76052	4.25776	1.75097
C	-3.84585	3.32763	0.14454
C	-3.7761	0.92953	0.13717
H	-4.69625	1.02912	-0.44333
C	-2.58162	0.64148	-0.76009
H	-1.67726	0.75999	-0.15234
H	-2.53525	1.38427	-1.56165
C	-2.58374	-0.77103	-1.38232
C	-3.95377	-1.57724	0.69725
C	-3.88932	-0.12269	1.22605
H	-3.01301	-0.02595	1.87692
H	-4.77388	0.06779	1.84374
C	-1.19129	-0.98296	-2.00745
H	-0.92498	-0.0905	-2.58287
H	-1.1791	-1.83662	-2.68722
H	-0.43092	-1.14966	-1.24167
C	-3.6186	-0.8655	-2.52957
H	-3.69497	-1.89742	-2.88518
H	-3.29435	-0.24275	-3.36986
H	-4.61533	-0.5267	-2.24394
C	-3.76323	-2.4957	1.91921
H	-2.76262	-2.39204	2.34248
H	-3.92306	-3.54524	1.66599
H	-4.4942	-2.21843	2.68556
C	-5.34315	-1.89265	0.09456
H	-5.33498	-2.88424	-0.36767
H	-5.66293	-1.16906	-0.65648
H	-6.09966	-1.8982	0.88658



L(C_4)-S

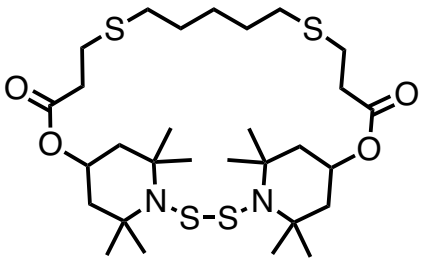
atom	X	Y	Z
S	-3.0362	5.01361	0.92771
S	-5.79011	2.30362	-3.41579
C	1.4835	-2.84146	2.09674
C	1.36745	-2.2094	3.47233
C	0.45432	-0.99365	3.36526
C	-0.96465	-1.30977	2.8385
N	-0.85488	-2.12758	1.5756
C	0.13461	-3.26672	1.46983
S	-2.1548	-2.12636	0.50009
S	-3.83648	-3.60637	1.18492
N	-5.19686	-3.10804	0.33871
C	-1.62368	0.04585	2.52
C	0.42231	-3.57349	-0.01248
C	-0.3965	-4.55872	2.13209
O	2.68853	-1.84414	3.87791
C	-5.41796	-3.6444	-1.05406
C	-6.90381	-3.4604	-1.43911
C	-7.46038	-2.04518	-1.30347
C	-6.7594	-1.25134	-0.19545
C	-6.15158	-2.10879	0.93554
C	-4.49162	-2.93822	-2.06729
C	-5.42882	-1.12791	1.87394
C	-7.23392	-2.84228	1.76007
O	-7.27046	-1.39019	-2.59669
C	-1.80641	-2.01204	3.9296
C	-5.13656	-5.15892	-1.09565

C	-7.90718	-0.2211	-2.79284
O	-8.61357	0.31819	-1.96255
C	-7.65921	0.32626	-4.18652
C	-7.40362	1.83682	-4.17899
C	-2.05583	5.12742	2.47853
C	-0.8548	6.06449	2.29519
C	0.20847	5.53402	1.34813
O	0.68342	4.34211	1.78168
O	0.60238	6.10943	0.35789
C	1.70187	3.69407	0.96696
C	2.60016	2.91705	1.90958
C	3.7031	2.11541	1.17434
N	3.06362	1.28837	0.09051
C	2.03438	1.89373	-0.83602
C	1.03572	2.73627	-0.0042
S	3.80882	-0.15608	-0.41141
C	1.20066	0.78304	-1.5051
C	2.66803	2.75473	-1.95332
C	4.34491	1.18969	2.22586
C	4.7871	3.07787	0.63721
S	5.21351	-0.00523	-2.16882
N	6.81065	-0.52266	-1.90613
C	7.8554	0.47377	-1.48058
C	9.24783	-0.01973	-1.94461
C	9.55619	-1.46471	-1.56494
C	8.4807	-2.35478	-2.16248
C	7.03862	-2.00423	-1.72479
C	6.10122	-2.80408	-2.65145
C	6.78206	-2.46961	-0.27241
C	7.60928	1.81509	-2.19737
C	7.8589	0.72056	0.04512
O	10.80201	-1.90723	-2.10259
C	11.94087	-1.45657	-1.39824
C	2.83922	-1.63601	5.26812

C	-4.32693	3.82822	1.49381
C	-5.48633	3.72572	0.49632
C	-5.10115	3.14195	-0.8711
C	-6.32285	2.95847	-1.77512
H	2.1366	-3.71875	2.14637
H	1.9731	-2.11452	1.43833
H	0.96579	-2.93402	4.19825
H	0.9378	-0.28421	2.68313
H	0.34679	-0.49432	4.33466
H	-1.14349	0.51663	1.65809
H	-2.68795	-0.05425	2.30744
H	-1.50921	0.70671	3.38577
H	0.69447	-2.66307	-0.55277
H	1.26509	-4.27015	-0.06853
H	-0.43245	-4.03019	-0.51243
H	0.30384	-5.38136	1.95164
H	-0.5232	-4.4645	3.21231
H	-1.35984	-4.84377	1.69938
H	-7.03772	-3.79202	-2.47312
H	-7.50728	-4.13129	-0.82027
H	-8.53919	-2.07892	-1.12691
H	-5.94763	-0.67632	-0.65229
H	-7.45549	-0.52827	0.23506
H	-4.67432	-1.86352	-2.11711
H	-3.44455	-3.09857	-1.79654
H	-4.64659	-3.34875	-3.07107
H	-4.60957	-0.62543	1.3554
H	-6.14411	-0.37205	2.21392
H	-5.02499	-1.63197	2.75306
H	-6.75604	-3.42955	2.54988
H	-7.91167	-2.12255	2.23245
H	-7.83642	-3.5248	1.15682
H	-1.31715	-2.89904	4.3369
H	-1.98228	-1.3221	4.76249

H	-2.77552	-2.31594	3.52766
H	-4.083	-5.37703	-0.91808
H	-5.72703	-5.68521	-0.33933
H	-5.40625	-5.55243	-2.08136
H	-6.83216	-0.21304	-4.65256
H	-8.56389	0.11855	-4.77578
H	-7.38827	2.21208	-5.20516
H	-8.20436	2.3528	-3.64408
H	-2.70031	5.51268	3.27531
H	-1.70707	4.13109	2.76362
H	-1.16935	7.04069	1.92002
H	-0.3847	6.21036	3.27535
H	2.24161	4.48201	0.43842
H	1.97837	2.22331	2.48748
H	3.08117	3.59606	2.62212
H	0.39775	2.06026	0.57702
H	0.38872	3.28889	-0.69211
H	0.82528	0.07294	-0.76333
H	0.34311	1.24551	-2.00417
H	1.76873	0.22953	-2.25378
H	1.89327	3.06018	-2.66433
H	3.14112	3.66368	-1.57764
H	3.42223	2.18194	-2.49873
H	3.64758	0.41966	2.56666
H	5.23453	0.68738	1.84461
H	4.6439	1.79468	3.08852
H	5.48002	2.5436	-0.01348
H	4.37314	3.91317	0.06993
H	5.3598	3.49849	1.47087
H	9.30996	0.05084	-3.03699
H	9.99689	0.66528	-1.53192
H	9.58554	-1.57874	-0.46945
H	8.55492	-2.27267	-3.25332
H	8.68085	-3.39972	-1.90405

H	6.15095	-2.42813	-3.67668
H	6.42264	-3.8508	-2.65022
H	5.06112	-2.76863	-2.32517
H	7.50389	-2.06448	0.43922
H	5.78351	-2.17192	0.0574
H	6.84492	-3.562	-0.21924
H	7.51438	1.66425	-3.27617
H	6.70769	2.31775	-1.84609
H	8.46162	2.47723	-2.01406
H	6.84774	0.92295	0.39927
H	8.24705	-0.12839	0.6109
H	8.48311	1.58867	0.28367
H	12.07205	-0.36584	-1.45007
H	11.90561	-1.74832	-0.33658
H	12.80987	-1.92944	-1.86241
H	2.5593	-2.53137	5.84479
H	3.89571	-1.42082	5.445
H	2.24558	-0.78826	5.64008
H	-3.86629	2.84552	1.64711
H	-4.70454	4.17977	2.4601
H	-6.25622	3.08981	0.95394
H	-5.93903	4.71628	0.36492
H	-4.37179	3.79621	-1.36299
H	-4.60441	2.17388	-0.72993
H	-7.03441	2.25563	-1.33389
H	-6.83355	3.91537	-1.92751



MM(C_5)-S

atom	X	Y	Z
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S	3.29231	4.54642	0.69566
S	1.39877	-3.80979	0.78234
O	-4.54067	-0.08408	0.59519
O	-5.29616	0.65641	-1.41079
O	5.83538	1.86996	0.42336
O	4.09139	1.14708	-0.84613
N	-1.48886	-2.87868	-0.25032
N	2.32277	-2.42958	0.40502
C	-1.74042	-1.86292	-1.33925
C	-2.58127	-0.70738	-0.74978
H	-1.9705	-0.15785	-0.02281
H	-2.84917	-0.02208	-1.55739
C	-3.83705	-1.19085	-0.04303
H	-4.53098	-1.64402	-0.75628
C	-3.45819	-2.1411	1.07861
H	-4.35778	-2.50394	1.58704
H	-2.87906	-1.57106	1.81415
C	-2.62249	-3.36089	0.62002
C	-0.40813	-1.25083	-1.8113
H	0.15283	-1.94193	-2.44213
H	0.22503	-0.97626	-0.96637
H	-0.61955	-0.35292	-2.40115
C	-2.43549	-2.46405	-2.58518
H	-3.46242	-2.78095	-2.39847

H	-1.87266	-3.32887	-2.94864
H	-2.46586	-1.72053	-3.3885
C	-2.05077	-4.00273	1.89868
H	-1.33465	-3.33666	2.38466
H	-1.55294	-4.95092	1.68788
H	-2.87071	-4.2011	2.59661
C	-3.51843	-4.4119	-0.0766
H	-2.90518	-5.22685	-0.47175
H	-4.10603	-3.99863	-0.89833
H	-4.2203	-4.84152	0.64611
C	-5.25926	0.737	-0.19949
C	-6.05511	1.74213	0.6127
H	-5.7189	1.74652	1.65112
H	-7.08775	1.36675	0.60299
C	-6.04372	3.15631	0.00967
H	-6.95202	3.68901	0.30351
H	-6.03627	3.09637	-1.08223
C	-3.20501	3.60602	-0.25273
H	-3.12406	2.52953	-0.07527
H	-3.30282	3.76936	-1.33127
C	-1.96932	4.31866	0.30694
H	-1.87159	4.06821	1.37058
H	-2.11711	5.40508	0.25891
C	-0.6697	3.95457	-0.4276
H	-0.59508	2.86334	-0.53254
H	-0.69765	4.36084	-1.44777
C	0.57073	4.47369	0.31491
H	0.4627	5.54504	0.52286
H	0.62568	3.97595	1.29192
C	1.88089	4.23973	-0.44641
H	1.95196	4.91393	-1.30736
H	1.93483	3.20898	-0.81119
C	4.73939	4.56151	-0.43522
H	4.69493	5.44718	-1.07647

H	5.59407	4.6728	0.23729
C	4.9265	3.30751	-1.29896
H	5.86661	3.411	-1.85533
H	4.12069	3.20269	-2.02802
C	5.0269	2.04493	-0.46134
C	3.9731	-0.10096	-0.10526
H	4.87268	-0.21191	0.50338
C	2.72016	-0.0062	0.7523
H	1.89647	0.31165	0.10243
H	2.85244	0.7686	1.51489
C	2.3268	-1.33198	1.44209
C	3.48943	-2.59386	-0.53505
C	3.83085	-1.2088	-1.13503
H	3.03078	-0.92117	-1.82673
H	4.75192	-1.29509	-1.72195
C	0.91269	-1.13535	2.02372
H	0.88018	-0.17614	2.55069
H	0.65815	-1.91914	2.73922
H	0.15063	-1.13492	1.24178
C	3.27042	-1.6301	2.6327
H	3.06143	-2.62371	3.04023
H	3.10197	-0.8977	3.42927
H	4.32803	-1.58339	2.37007
C	3.09554	-3.49583	-1.72046
H	2.17126	-3.15453	-2.19047
H	2.963	-4.535	-1.4142
H	3.89589	-3.46425	-2.4667
C	4.72539	-3.23281	0.14098
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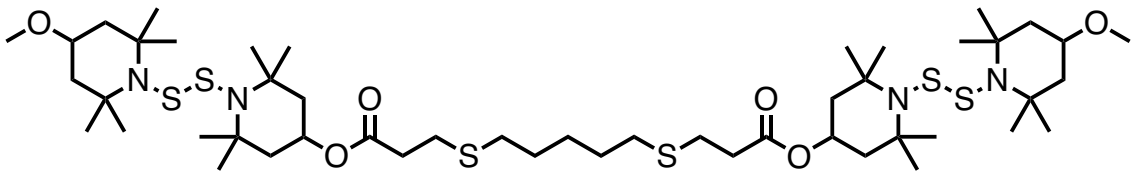
H	5.2084	-2.57757	0.86711
H	5.47368	-3.48779	-0.61701



L(C_5)-S

atom	X	Y	Z
S	-4.34345	-7.00441	-2.00285
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C	9.206	2.20873	-1.33793
C	7.96195	2.663	-0.59195
C	7.07549	1.50034	-0.09001
N	6.78105	0.58495	-1.25231
C	7.89271	0.13259	-2.16841
S	5.29483	-0.21204	-1.35206
S	5.14188	-2.23403	-0.48367
N	4.04201	-2.20415	0.85307
C	5.7665	2.11999	0.43113
C	7.31719	-0.38589	-3.50143
C	8.73425	-1.00676	-1.54762
O	9.89257	3.38973	-1.75001
C	2.59965	-2.4387	0.45736
C	1.6937	-2.22004	1.69199
C	2.15308	-2.99151	2.91607
C	3.56042	-2.5605	3.27461
C	4.58085	-2.79157	2.13437
C	2.18131	-1.37635	-0.57735
C	5.8567	-2.03982	2.54172
C	4.92679	-4.29622	2.01865
O	1.31024	-2.66119	4.05826
C	7.7622	0.77566	1.08889
C	2.34465	-3.83462	-0.1581
C	0.17498	-3.37094	4.20963

O	-0.1824	-4.25817	3.46113
C	-0.56392	-2.95857	5.47106
C	-2.07154	-3.18208	5.36303
C	-3.91117	-5.70574	-3.22579
C	-5.08286	-4.87514	-3.80863
C	-5.31385	-3.56871	-3.07247
O	-4.52691	-2.59405	-3.58191
O	-6.08019	-3.40373	-2.1441
C	-4.61763	-1.26973	-2.98171
C	-3.58829	-1.13431	-1.87348
C	-3.53477	0.28562	-1.25536
N	-3.42761	1.30172	-2.36141
C	-4.29637	1.19857	-3.59064
C	-4.3082	-0.27131	-4.07917
S	-2.69412	2.80579	-2.05132
C	-3.69281	2.02662	-4.74258
C	-5.73889	1.70048	-3.34742
C	-2.26072	0.3307	-0.39072
C	-4.76311	0.51334	-0.34566
S	-4.07553	4.47516	-1.42006
N	-3.72938	5.21356	0.06904
C	-4.39268	4.70802	1.32412
C	-4.47431	5.85748	2.35589
C	-3.16131	6.58478	2.58704
C	-2.68034	7.14103	1.2509
C	-2.49153	6.07472	0.14351
C	-2.30266	6.85045	-1.17556
C	-1.20929	5.24792	0.39718
C	-5.84622	4.3053	1.01074
C	-3.66128	3.49274	1.93661
O	-3.42532	7.61826	3.53507
C	-2.27477	8.16134	4.14999
C	11.23925	3.18799	-2.12831
C	-4.96223	-6.05937	-0.55084

C	-3.90295	-5.25268	0.20235
C	-4.49764	-4.50164	1.40288
C	-3.45382	-3.67318	2.16593
C	-4.06569	-2.90678	3.34101
H	9.6512	0.98051	-3.07526
H	8.22202	2.00584	-3.20962
H	9.86618	1.63414	-0.6687
H	7.37833	3.29807	-1.26872
H	8.25221	3.28136	0.26411
H	5.1957	2.57829	-0.38094
H	5.12891	1.382	0.92156
H	6.0145	2.89802	1.16007
H	6.61191	0.32915	-3.93242
H	8.14574	-0.52083	-4.20446
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H	9.4254	-1.40642	-2.29765
H	1.68515	-1.15423	1.94867
H	0.67195	-2.50729	1.42786
H	2.07689	-4.06904	2.75554
H	3.53533	-1.49286	3.52191
H	3.90828	-3.09355	4.16601
H	2.43568	-0.37267	-0.22823
H	2.65875	-1.54034	-1.5459
H	1.09787	-1.42816	-0.72845
H	5.66413	-0.96566	2.59212
H	6.1809	-2.37833	3.53117
H	6.67148	-2.2218	1.83907
H	5.62158	-4.46377	1.19074
H	5.41227	-4.64152	2.93789
H	4.04897	-4.92342	1.85387
H	8.79725	0.50091	0.88028
H	7.77083	1.42864	1.96836

H	7.21692	-0.13107	1.34454
H	3.03559	-4.0148	-0.98575
H	2.45343	-4.64696	0.56303
H	1.32461	-3.88552	-0.55283
H	-0.16431	-3.57735	6.28699
H	-0.3165	-1.92265	5.71772
H	-2.25689	-4.15955	4.91324
H	-2.52797	-3.15992	6.35592
H	-3.13087	-5.04941	-2.82939
H	-3.45075	-6.2825	-4.03257
H	-4.85451	-4.63326	-4.85098
H	-6.00708	-5.45584	-3.77721
H	-5.63245	-1.15844	-2.59512
H	-2.60535	-1.38113	-2.29194
H	-3.8005	-1.84936	-1.0721
H	-3.32438	-0.51603	-4.49637
H	-5.03815	-0.36273	-4.89023
H	-2.63209	1.79832	-4.87495
H	-4.22116	1.77276	-5.66749
H	-3.79271	3.10023	-4.57989
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H	-6.29937	1.07217	-2.65279
H	-5.72804	2.71678	-2.94587
H	-1.36675	0.25954	-1.01679
H	-2.18858	1.24568	0.1973
H	-2.26931	-0.51623	0.30288
H	-5.70596	0.25414	-0.83058
H	-4.67981	-0.10188	0.55654
H	-4.81937	1.55803	-0.03891
H	-5.20635	6.59892	2.01468
H	-4.84416	5.45102	3.30311
H	-2.41001	5.90034	3.01234
H	-3.42339	7.87555	0.91816
H	-1.72909	7.672	1.36536

H	-3.22663	7.35657	-1.46719
H	-1.52556	7.60717	-1.02554
H	-1.99201	6.2059	-1.99876
H	-1.19344	4.77594	1.38123
H	-1.10447	4.4606	-0.35362
H	-0.33088	5.89906	0.32859
H	-6.36794	5.11501	0.4932
H	-5.90861	3.41119	0.38987
H	-6.36802	4.10319	1.95149
H	-4.27932	3.03717	2.71753
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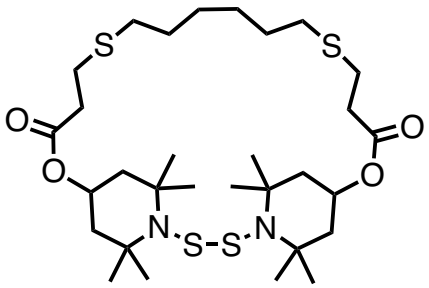
H	-2.70481	3.75847	2.39052
H	-1.67548	7.3848	4.65116
H	-1.62318	8.69446	3.44244
H	-2.62239	8.87458	4.90139
H	11.82215	2.71397	-1.32278
H	11.34137	2.57268	-3.03397
H	11.663	4.17413	-2.33334
H	-5.78705	-5.41863	-0.87163
H	-5.38089	-6.8377	0.09672
H	-3.0993	-5.92047	0.53485
H	-3.43923	-4.52572	-0.47696
H	-5.30592	-3.8461	1.0506
H	-4.96443	-5.2235	2.08821
H	-2.64543	-4.32139	2.52291
H	-2.98241	-2.95311	1.48481
H	-4.81185	-2.18743	2.98627
H	-4.58469	-3.58086	4.03133



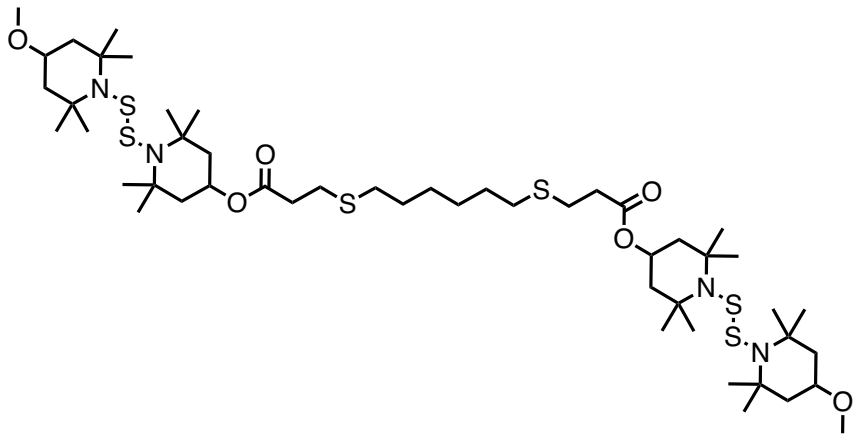
MM(C_6)-S

atom	X	Y	Z
S	-0.89141	-4.05891	-0.86657
S	6.19543	1.68934	-0.8232
S	-1.65867	4.97611	0.79543
S	-2.54835	-3.57619	0.45387
O	3.69947	-0.79601	0.8748
O	5.737	-1.73647	0.52313
O	-4.7462	2.98013	1.28837
O	-4.06976	2.02002	-0.65057
N	0.51397	-3.20736	-0.40388
N	-3.08785	-1.97908	0.18444
C	1.47967	-3.89568	0.52827
C	2.40046	-2.82366	1.16378
H	1.81261	-2.23012	1.87341
H	3.18854	-3.33014	1.73135
C	3.0198	-1.8666	0.15764
H	3.76402	-2.36772	-0.46415
C	1.93813	-1.19549	-0.66882
H	2.39706	-0.52776	-1.40562
H	1.33428	-0.57357	0.00217
C	1.011	-2.18894	-1.40203
C	0.71042	-4.55589	1.68798
H	0.0339	-3.8475	2.16928
H	1.43069	-4.90876	2.43307
H	0.12776	-5.41501	1.35065
C	2.30824	-5.00035	-0.16852

H	3.03525	-4.61035	-0.88218
H	1.64369	-5.68994	-0.69762
H	2.86327	-5.57658	0.5792
C	-0.16687	-1.36878	-1.96259
H	-0.85555	-1.06718	-1.17106
H	-0.73259	-1.93153	-2.7068
H	0.22843	-0.47114	-2.44949
C	1.73914	-2.82906	-2.60908
H	1.92257	-2.06865	-3.3758
H	1.11592	-3.61017	-3.0544
H	2.70381	-3.26794	-2.35069
C	5.0458	-0.83763	0.95271
C	5.59249	0.39527	1.65042
H	6.01763	0.06778	2.60866
H	4.78219	1.09349	1.86959
C	6.70289	1.05319	0.82422
H	7.47156	0.30925	0.5995
H	7.17226	1.86323	1.39019
C	5.19526	3.1812	-0.39733
H	5.48168	3.50834	0.60836
H	5.53057	3.96189	-1.08824
C	3.67625	3.00444	-0.51564
H	3.32424	2.2727	0.22154
H	3.44613	2.57796	-1.50005
C	2.93066	4.33775	-0.35342
H	3.16839	4.77891	0.62486
H	3.31146	5.04638	-1.10332
C	1.40612	4.22718	-0.50124
H	0.99654	3.62184	0.31698
H	1.16745	3.68962	-1.42982
C	0.7256	5.60335	-0.53327
H	0.96845	6.16235	0.37941
H	1.14651	6.18144	-1.36731
C	-0.79666	5.58102	-0.71826

H	-1.0651	4.95317	-1.5752
H	-1.15754	6.59603	-0.91616
C	-3.39809	5.39282	0.37339
H	-3.92925	5.41602	1.32774
H	-3.42125	6.40033	-0.05287
C	-4.09114	4.39261	-0.55873
H	-5.07211	4.79628	-0.84572
H	-3.52631	4.22382	-1.47804
C	-4.34119	3.07135	0.14771
C	-4.18403	0.69329	-0.05467
H	-5.09127	0.68316	0.55458
C	-4.25425	-0.28808	-1.21069
H	-3.39421	-0.09848	-1.8629
H	-5.1571	-0.10891	-1.80471
C	-4.23039	-1.7754	-0.77754
C	-2.88061	-1.02298	1.33527
C	-2.95158	0.42037	0.79301
H	-2.92178	1.11575	1.63585
H	-2.06911	0.61289	0.17197
C	-3.99234	-2.59946	-2.05714
H	-3.00114	-2.40835	-2.47225
H	-4.74175	-2.31805	-2.804
H	-4.08778	-3.67083	-1.872
C	-5.59603	-2.20802	-0.19364
H	-6.3579	-2.19848	-0.98049
H	-5.94734	-1.55829	0.6093
H	-5.53061	-3.22806	0.19637
C	-1.47321	-1.20385	1.93533
H	-0.71532	-1.29496	1.15502
H	-1.41552	-2.09122	2.56771
H	-1.2402	-0.33264	2.55607
C	-3.89706	-1.22883	2.48463
H	-3.59828	-0.63183	3.35261
H	-3.91391	-2.2797	2.78876

H	-4.91383	-0.93173	2.22413



L(C_6)-S

atom	X	Y	Z
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C	-0.25899	-7.70376	-1.055
C	-0.91929	-7.64499	0.31861
C	-1.91774	-6.47642	0.49309
N	-1.27118	-5.18702	0.03951
C	-0.41809	-5.13567	-1.20787
S	-1.90945	-3.73546	0.60297
S	-3.76049	-3.11064	-0.60502
N	-4.35734	-1.90115	0.43683
C	-2.23427	-6.38729	1.99794
C	0.53426	-3.92622	-1.13487
C	-1.27247	-5.00032	-2.48884
O	0.71614	-8.74155	-1.13956
C	-4.09004	-0.48008	-0.00343
C	-4.46072	0.49465	1.13921
C	-5.83619	0.23808	1.72114
C	-5.87725	-1.17362	2.2812
C	-5.59641	-2.26364	1.22072
C	-2.58215	-0.30185	-0.25899
C	-5.34476	-3.57063	1.99449

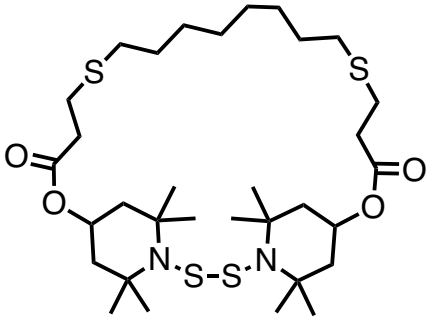
C	-6.83052	-2.46321	0.31187
O	-6.03302	1.20709	2.79175
C	-3.23237	-6.77216	-0.26504
C	-4.85354	-0.11053	-1.29558
C	-7.31352	1.43992	3.17404
O	-8.27722	0.91885	2.6568
C	-7.37831	2.37412	4.36856
C	-6.48959	3.62207	4.30493
C	-2.75448	2.73827	-4.4702
C	-1.88802	1.53106	-4.10488
C	-0.46893	1.93928	-3.74471
O	-0.01049	1.24219	-2.68435
O	0.17779	2.76345	-4.35648
C	1.3568	1.51287	-2.25893
C	1.38055	2.70277	-1.31596
C	2.78202	2.99281	-0.72317
N	3.36272	1.71118	-0.17453
C	3.27135	0.42771	-0.95584
C	1.83753	0.27878	-1.52267
S	4.496	1.84699	1.08617
C	3.48457	-0.76878	-0.00934
C	4.30571	0.34749	-2.10118
C	2.56249	4.00819	0.41585
C	3.69243	3.65483	-1.78347
S	6.50794	2.70776	0.53103
N	7.86024	1.73592	0.86727
C	8.23038	1.54199	2.31767
C	9.74754	1.24717	2.42049
C	10.24388	0.15746	1.47592
C	9.90263	0.56752	0.05399
C	8.39543	0.8109	-0.19407
C	8.28856	1.49199	-1.57172
C	7.63999	-0.53615	-0.24698
C	7.98915	2.84413	3.10738

C	7.41062	0.41759	2.99309
O	11.6615	0.0035	1.52998
C	12.13361	-0.71743	2.64995
C	0.18284	-10.03801	-1.31918
C	-3.93014	5.18353	-3.74775
C	-4.07202	6.38899	-2.80652
C	-5.18129	6.32272	-1.74204
C	-4.90298	5.41657	-0.53416
C	-5.70894	4.61781	1.74402
C	-5.98766	5.5294	0.54746
H	0.97562	-6.41264	-2.25427
H	1.26113	-6.32414	-0.51802
H	-1.01458	-7.86315	-1.841
H	-0.11791	-7.55132	1.06127
H	-1.45674	-8.57371	0.53881
H	-1.35177	-6.06914	2.56002
H	-3.04508	-5.68907	2.20732
H	-2.534	-7.37731	2.35683
H	1.07603	-3.91832	-0.18495
H	1.2629	-4.00345	-1.94882
H	0.00525	-2.97798	-1.23614
H	-0.61833	-4.88048	-3.35931
H	-1.90631	-5.8706	-2.66988
H	-1.91426	-4.11665	-2.43204
H	-3.72549	0.3992	1.94684
H	-4.3887	1.51658	0.75293
H	-6.63274	0.39534	0.99059
H	-5.12394	-1.24166	3.07523
H	-6.85531	-1.37364	2.72728
H	-2.00247	-0.61965	0.61223
H	-2.24717	-0.87856	-1.12252
H	-2.36708	0.75357	-0.45316
H	-4.42197	-3.50243	2.57604
H	-6.17937	-3.74919	2.68018

H	-5.26994	-4.42788	1.3234
H	-7.154	-1.53978	-0.17271
H	-6.60809	-3.19871	-0.46663
H	-7.67443	-2.8377	0.90036
H	-3.7294	-7.63997	0.18224
H	-3.91308	-5.92036	-0.20032
H	-3.0709	-6.99509	-1.32187
H	-4.5603	0.88845	-1.63636
H	-4.61419	-0.82609	-2.08774
H	-5.93736	-0.10805	-1.15997
H	-8.42754	2.64619	4.49926
H	-7.08059	1.78171	5.24611
H	-6.53083	4.13618	5.26889
H	-5.44811	3.34873	4.12197
H	-3.68009	2.40654	-4.9493
H	-2.20181	3.37841	-5.16385
H	-2.32752	0.94135	-3.29732
H	-1.81452	0.87529	-4.98206
H	1.94173	1.71372	-3.15909
H	0.68196	2.49663	-0.49648
H	1.03052	3.59926	-1.8352
H	1.14401	0.07972	-0.6976
H	1.81519	-0.5934	-2.18488
H	2.82667	-0.69457	0.86075
H	3.24597	-1.69283	-0.54563
H	4.51198	-0.83916	0.34833
H	5.30027	0.60022	-1.7327
H	4.34057	-0.67025	-2.50473
H	4.07549	1.02094	-2.92873
H	2.02854	3.5491	1.25199
H	3.49937	4.41937	0.79354
H	1.9586	4.8362	0.0306
H	3.77866	3.06904	-2.70034
H	3.28493	4.6333	-2.05873

H	4.69861	3.80602	-1.38434
H	10.30674	2.16061	2.18536
H	9.96602	0.99326	3.4634
H	9.77524	-0.80876	1.72264
H	10.45849	1.48636	-0.16676
H	10.25335	-0.19784	-0.64642
H	8.73637	2.48914	-1.54473
H	8.83034	0.88934	-2.30764
H	7.25687	1.5937	-1.9095
H	7.92162	-1.08844	-1.14999
H	7.85657	-1.17718	0.60965
H	6.56299	-0.36774	-0.27451
H	8.44624	3.69848	2.60139
H	6.92878	3.05768	3.24732
H	8.44781	2.74095	4.09634
H	7.63032	-0.57246	2.58929
H	7.63138	0.39325	4.06593
H	6.33938	0.59823	2.87328
H	11.94942	-0.19788	3.60152
H	11.67883	-1.71882	2.71133
H	13.21314	-0.83037	2.52345
H	-0.40775	-10.38042	-0.45705
H	-0.45301	-10.09623	-2.21665
H	1.03057	-10.71572	-1.446
H	-3.28398	5.46134	-4.58688
H	-4.90803	4.90284	-4.15549
H	-3.10531	6.59254	-2.32878
H	-4.27884	7.25246	-3.45205
H	-5.34936	7.34377	-1.37391
H	-6.12304	6.01804	-2.21989
H	-4.82013	4.37268	-0.85833
H	-3.92923	5.68334	-0.10028
H	-4.73249	4.85184	2.18199
H	-5.70196	3.56878	1.43716

H	-6.05721	6.57012	0.88998
H	-6.96585	5.27676	0.1191



MM(C_8)-S

atom	X	Y	Z
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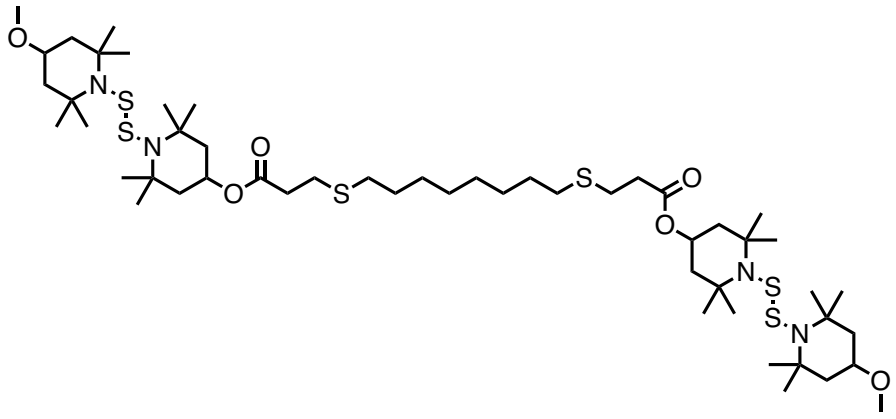
S	4.23875	4.32638	-0.94078
S	1.42539	-4.14911	-0.44261
O	-4.1813	-0.04034	-0.82606
O	-6.31453	-0.78896	-0.61437
O	5.90706	1.08952	-1.30128
O	4.87511	0.54779	0.64325
N	-1.44124	-3.00278	0.36595
N	2.42863	-2.79749	-0.12451
C	-2.53804	-3.48878	-0.54946
C	-3.25657	-2.26059	-1.16004
H	-2.58575	-1.78104	-1.88251
H	-4.139	-2.60888	-1.70668
C	-3.66049	-1.21286	-0.13584
H	-4.45186	-1.58208	0.51924
C	-2.44269	-0.75011	0.64177
H	-2.73643	0.00158	1.38194
H	-1.75041	-0.26743	-0.05818
C	-1.70764	-1.90142	1.36426
C	-1.92233	-4.2642	-1.72961
H	-1.13529	-3.68275	-2.21426
H	-2.70574	-4.47048	-2.46604
H	-1.5009	-5.21986	-1.41232
C	-3.54639	-4.4262	0.15513

H	-4.16756	-3.91475	0.89208
H	-3.01518	-5.23928	0.65867
H	-4.21948	-4.8726	-0.58429
C	-0.3779	-1.32741	1.89135
H	0.33382	-1.15487	1.08216
H	0.09118	-1.99618	2.61461
H	-0.5776	-0.37529	2.3939
C	-2.52026	-2.37881	2.59276
H	-2.55221	-1.58571	3.34761
H	-2.04161	-3.25205	3.04568
H	-3.5515	-2.64209	2.35339
C	-5.51994	0.04891	-0.98371
C	-5.9074	1.33279	-1.69504
H	-6.30794	1.04836	-2.67733
H	-5.0235	1.94951	-1.86854
C	-6.99533	2.09908	-0.93453
H	-7.84376	1.4342	-0.75258
H	-7.34983	2.94298	-1.53388
C	-5.23181	3.96046	0.35922
H	-5.38878	4.31471	-0.66593
H	-5.44074	4.80862	1.01946
C	-3.79452	3.47131	0.56785
H	-3.59789	2.60904	-0.07955
H	-3.69458	3.10323	1.59692
C	-2.74959	4.56743	0.31441
H	-2.86814	4.96216	-0.70486
H	-2.9372	5.41365	0.99069
C	-1.3086	4.07487	0.50188
H	-1.20462	3.63588	1.50434
H	-1.11113	3.25874	-0.20717
C	-0.25121	5.17121	0.32231
H	-0.4307	5.96961	1.05674
H	-0.37077	5.63663	-0.66627
C	1.18595	4.65537	0.46859

H	1.38152	3.89642	-0.29869
H	1.29249	4.14454	1.4364
C	2.2389	5.7674	0.37525
H	2.1344	6.30397	-0.57683
H	2.04848	6.50777	1.16407
C	3.68796	5.28979	0.53145
H	3.78286	4.66821	1.42896
H	4.35788	6.14901	0.64194
C	5.92926	3.84687	-0.40595
H	6.46291	3.59344	-1.3247
H	6.4176	4.71758	0.04174
C	5.97173	2.64867	0.54635
H	6.99945	2.51738	0.914
H	5.33466	2.79243	1.42192
C	5.58784	1.3611	-0.16241
C	4.43945	-0.72328	0.07836
H	5.25522	-1.1012	-0.54245
C	4.1401	-1.63563	1.25246
H	3.41178	-1.12883	1.89602
H	5.04471	-1.7958	1.849
C	3.56854	-3.01369	0.83928
C	2.5726	-1.8315	-1.27808
C	3.17957	-0.51363	-0.74653
H	3.396	0.1412	-1.59499
H	2.44134	-0.0078	-0.11309
C	3.03948	-3.66963	2.12891
H	2.1904	-3.11389	2.53203
H	3.83774	-3.67665	2.87826
H	2.72845	-4.70233	1.96104
C	4.68103	-3.92528	0.26993
H	5.40039	-4.17326	1.05776
H	5.237	-3.46455	-0.54832
H	4.24954	-4.86175	-0.09527
C	1.18688	-1.48678	-1.85713

H	0.4677	-1.26231	-1.06757
H	0.78472	-2.30518	-2.45622
H	1.28279	-0.60979	-2.50539
C	3.42802	-2.39528	-2.4388
H	3.37694	-1.71937	-3.29877
H	3.04198	-3.36931	-2.75385
H	4.48185	-2.51279	-2.18242



L(C_8)-S

atom	X	Y	Z
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C	3.76013	-4.28674	-0.5721
C	4.21065	-3.98476	0.85229
C	3.3456	-2.86335	1.39816
C	1.83303	-3.18432	1.41602
N	1.41145	-3.71829	0.06442
C	2.27422	-4.7	-0.69504
S	-0.21777	-3.6351	-0.34199
S	-1.42102	-5.35815	0.59308
N	-2.96685	-4.84101	0.09509
C	1.10624	-1.85467	1.69275
C	1.92454	-4.64258	-2.19451
C	2.07133	-6.1525	-0.20605
O	5.57033	-3.53754	0.8926
C	-3.56198	-5.59271	-1.07201
C	-4.80933	-4.83606	-1.58486
C	-5.78461	-4.46829	-0.48419
C	-5.08136	-3.58872	0.53523
C	-3.84182	-4.25305	1.17851
C	-2.55484	-5.61407	-2.23686
C	-3.07318	-3.13312	1.90401
C	-4.27126	-5.30585	2.22518
O	-6.85978	-3.71036	-1.10803

C	1.49813	-4.16749	2.56066
C	-3.91947	-7.05314	-0.71318
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O	0.04019	6.13497	0.44979
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C	1.99149	5.35847	1.57044
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C	3.26201	3.89328	-1.76281
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H	-2.2094	-4.60387	-2.47058
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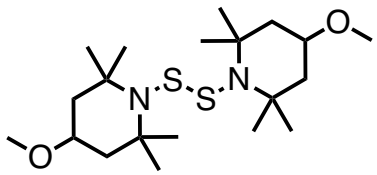

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C	-5.0835	0.14744	-0.09534
C	-4.44103	-1.07155	0.55859
C	-2.91997	-1.20035	0.30749
C	-2.3075	2.57034	1.05718
C	-2.40097	-2.27302	1.284
C	-2.64751	-1.68488	-1.13513
O	-6.46535	0.27031	0.23791
C	-7.32372	-0.59041	-0.48266
C	-2.57623	1.76787	-1.29658
C	2.1447	2.36624	0.18477
O	6.13664	-0.31136	1.17744
C	1.91355	-2.46614	0.29461
C	3.20915	-1.88701	-1.76516
C	3.37686	1.57369	-1.84257
C	2.85528	-1.4222	-0.33382
C	4.12035	-1.37778	0.5514
C	5.03646	-0.19838	0.27555
C	4.23855	1.08238	0.49857
C	2.98151	1.20945	-0.39287
N	2.18147	-0.06984	-0.32326
S	0.63333	-0.01004	-1.03175
C	7.25955	0.47586	0.83784
H	-4.5788	1.42932	1.51961
H	-4.84477	2.28374	0.0019

H	-4.98742	0.0938	-1.19169
H	-4.62448	-0.99598	1.63709
H	-4.91243	-1.99881	0.21534
H	-2.3889	2.31883	2.11832
H	-1.26148	2.78363	0.8345
H	-2.89047	3.47833	0.87153
H	-2.47181	-1.92138	2.31708
H	-3.01641	-3.17293	1.18219
H	-1.36371	-2.54411	1.08446
H	-3.06401	-2.68876	-1.27312
H	-3.09422	-1.03623	-1.8915
H	-1.57265	-1.73857	-1.32586
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H	-7.22378	-0.44849	-1.57038
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H	-2.95394	2.76941	-1.52935
H	-1.49985	1.76332	-1.48743
H	-3.04785	1.06923	-1.99081
H	1.77519	2.11626	1.18246
H	2.77132	3.26107	0.25979
H	1.28987	2.60292	-0.45116
H	1.56832	-2.13373	1.27675
H	1.04116	-2.65326	-0.33398
H	2.45447	-3.41027	0.41632
H	3.58921	-2.914	-1.74426
H	2.31664	-1.87115	-2.39736
H	3.97138	-1.26249	-2.23635
H	3.85662	2.55814	-1.86683
H	4.07131	0.85607	-2.28473
H	2.48536	1.61879	-2.47468
H	3.82305	-1.32349	1.6053
H	4.67203	-2.31454	0.42107
H	5.42031	-0.24013	-0.75657
H	3.93694	1.09755	1.5526

H	4.85766	1.96968	0.32698
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H	7.62589	0.24783	-0.17572
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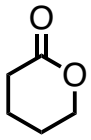

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C	1.73427	-0.06411	0.32077
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O	-0.46178	-1.19416	0.04283
C	-1.13817	-0.0147	0.0109
O	-2.34507	-0.03628	-0.01511
H	-0.89966	2.03636	-0.46078
H	-0.42787	1.58851	1.16618
H	1.66102	2.09791	0.03443
H	1.21688	1.15458	-1.38308
H	2.78849	-0.17955	0.04493
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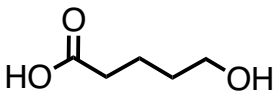
H	1.12819	-1.4184	-1.25155
H	1.2734	-2.19456	0.33397



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C	1.55421	-0.44299	0.00017
C	2.75833	0.48963	-0.00025
O	-3.35137	-0.77626	-0.00023
C	-2.3086	0.09248	-0.00002
O	-2.46507	1.29372	0.00029
O	3.93337	-0.3136	0.00017
H	-0.96743	-1.30031	-0.87208
H	-0.96734	-1.29956	0.87297
H	0.15664	0.96888	0.87385
H	0.15673	0.96801	-0.87503
H	1.62422	-1.09648	-0.87871
H	1.62415	-1.0956	0.87972
H	2.7208	1.14421	0.88629
H	2.72085	1.14335	-0.88744
H	-4.15523	-0.22948	-0.00014
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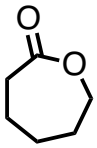

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C	0.53555	1.631	-0.29477
C	1.38914	0.74935	0.65012
C	1.76153	-0.63888	0.08312
C	0.57927	-1.58883	-0.11512
O	-0.46336	-0.90907	-0.84777
C	-1.25642	-0.12121	-0.04074
O	-2.009	-0.58239	0.78018
H	-1.44308	1.66003	-1.21443
H	-1.4897	1.89887	0.53459
H	0.68341	2.68434	-0.0325
H	0.90913	1.50962	-1.31698
H	2.32453	1.27977	0.86143
H	0.88231	0.63759	1.61904
H	2.48674	-1.12587	0.74817
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H	0.1722	-1.94393	0.83862
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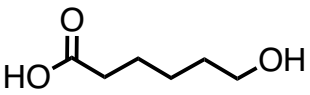

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C	2.17411	0.34124	-0.00014
O	-3.99289	-0.6894	-0.00027
C	-2.91663	0.13833	0.00003
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C	3.47355	-0.45322	0.00015
O	4.5546	0.47253	-0.00016
H	-1.63302	-1.30619	-0.87232
H	-1.63294	-1.3057	0.87299
H	-0.41203	0.91465	0.87368
H	-0.41198	0.91408	-0.87439
H	0.94786	-1.21098	-0.87767
H	0.94783	-1.21039	0.87841
H	2.16944	0.99784	0.87867
H	2.16947	0.99724	-0.87939
H	-4.77438	-0.11111	-0.00025
H	3.50844	-1.10832	-0.88653
H	3.50842	-1.10771	0.88729
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atom	X	Y	Z
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H	-0.75938	-0.47669	0

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C	-1.66909	0.7558	0.14694
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S	1.13142	1.00015	0.31445
S	1.13142	-1.00015	-0.31445
H	-0.55277	-2.59303	0.18768
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H	-1.71058	0.91875	1.23097
H	-0.40515	1.41998	-1.51001
H	-0.55278	2.59303	-0.18768

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C	0.00002	0.67558	-0.00006
C	1.25519	-0.19426	0.13293
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S	-4.29482	-0.45564	-0.57328
C	-4.82662	-0.81891	1.14634
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H	1.38813	-0.82011	-0.75417
H	1.1953	-0.8427	1.01101
H	-5.68646	-1.48925	1.05742
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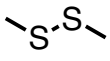

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S	0.98404	-0.34023	-0.4949
C	0.98404	-1.64447	0.79733
H	-1.99083	2.07219	0.79068
H	-0.78045	1.22635	1.78476
H	-0.25794	2.42286	0.559
H	1.99083	-2.07219	0.79068
H	0.78045	-1.22635	1.78476
H	0.25794	-2.42286	0.559

[1] D. Sathe, J. Zhou, H. Chen, H. W. Su, W. Xie, T. G. Hsu, B. R. Schrage, T. Smith, C. J. Ziegler, J. Wang, *Nat. Chem.* **2021**, *13*, 743–750.

[2] CrystalStructure 4.3: Crystal Structure Analysis Package, Rigaku Corporation, Tokyo 196-8666, Japan, **2000**–**2018**.

[3] G. M. Sheldrick, *Acta Crystallogr., Sect. A* **2015**, *71*, 3–8.

[4] G. M. Sheldrick, *Acta Crystallogr., Sect. C* **2015**, *71*, 3–8.