ESI*

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S1. Materials and Methods.

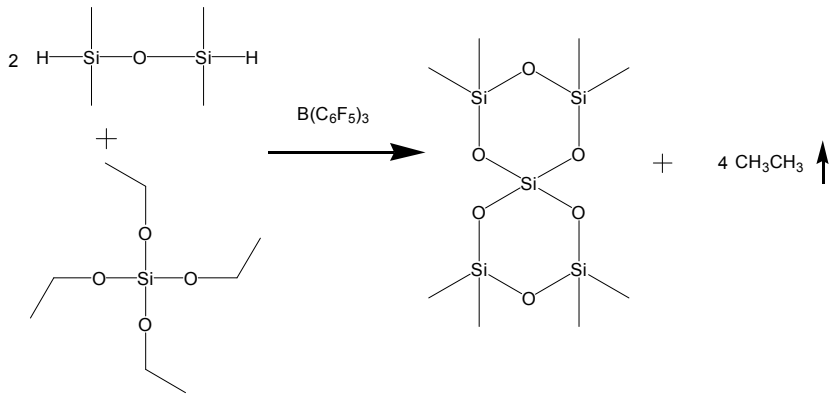
All reactions were carried out under an argon atmosphere in oven-dried glasswares with magnetic stirring bars. Tris(pentafluorophenyl)borane, 1,5,7-triazabicyclo[4.4.0]dec-5-ene, cyclohexane, tetraethylorthosilicate,1,1,3,3-tetramethyldisiloxane, dichloromethane, methanol, sodium were purchased through InnoChem, Inc., China, and then used without any further purification. Tetrahydrofuran was distilled at 94˚C. ^{1}H NMR spectra were recorded in $CDCl_3$ on 300 MHz NMR spectrometer. The ^{1}H NMR spectra were referenced to residual solvent signals at 7.26 ppm ($CHCl_3$). ^{29}Si NMR spectra proton was decoupled and recorded in $CDCl_3$ with a 60s delay at 120 MHz. Gel-permeation chromatography (GPC) analysis was conducted on a Viscotek GPC/SEC 270 max with RI/ UV/ viscosity/ light scattering as the detectors. Raman spectra were recorded on a LabRAM HR Evolution at 532 nm. Atomic force microscope (AFM) images were captured on a Bruker Dimension Icon with ScanAsyst.

Computational Details: All computations were performed using the Gaussian 09[1] software package. Geometry optimizations and vibration analysis were performed using the B3LYP DFT functional with 6-31G+(d) basis set, and the single point energy was then calculated with the 6-311G++(2d,p) level at the optimized geometries. All calculations and vibration analysis include the CPCM solvent model using default parameters. All stationary point structures were confirmed by vibration analysis; no imaginary or negative frequencies were present for intermediates. Electronic energies, enthalpies (298.15K) and free energies (298.15K) were obtained from the single point

energy corrected by zero point vibrational energies (ZPEs).

S2. Reaction Procedure：

(1) Synthesis of compound **1**



Scheme S1. Reaction scheme of compound **1**

Tris(pentafluorophenyl)borane ($B(C_6F_5)_3$) (51.2mg, 0.1mmol) was dissolved in 900 ml cyclohexane in a 2000 ml two-neck glass bottle. A mixture of 1,1,3,3-tetramethyldisiloxane (26.866 g, 0.2mol) and tetraethylorthosilicate (20.833 g, 0.1mol) in 100 ml cyclohexane was slowly added to the catalyst solution via a syringe over 2 h on a syringe pump. After the addition, 2g activated carbon and 3~4 drops triethylamine were added to the reaction mixture to deactivate the catalyst, and then the reaction mixture was filtered and the solvent was removed using a rotovap. The product was then concentrated and dried under an oil pump to give a colorless liquid mixture mixed with solids. The solids was purified through sublimation at reduced pressures to obtain white crystals (yield 17%), compound **1**.

(2) A typical synthesis procedure of cyclic polymer **2**.

Compound **1** (1g, 2.8 mmol) was dissolved in 10 ml tetrahydrofuran (THF) in a 25 ml two-neck glass bottle. At Ar atmosphere 1,5,7-triazabicyclo[4.4.0] dec-5-ene (TBD) (7.8 mg, 0.056mmol) was added to the solution. After 50 min, 0.2mL acetic acid was added to the reaction mixture to deactivate the catalyst, and then the mixture was filtered and the solvent was removed using a rotovap. The product was purified by precipitation in THF:CH_3OH=1:1 (volume ratio) and dried under an oil pump to obtain a colorless liquid. **2** was dialyzed against a membrane with a Mw cut-off around 10 k prior to AFM analysis to remove the small molecular weight molecules.

S3. $^{1}H/^{29}Si$ NMR

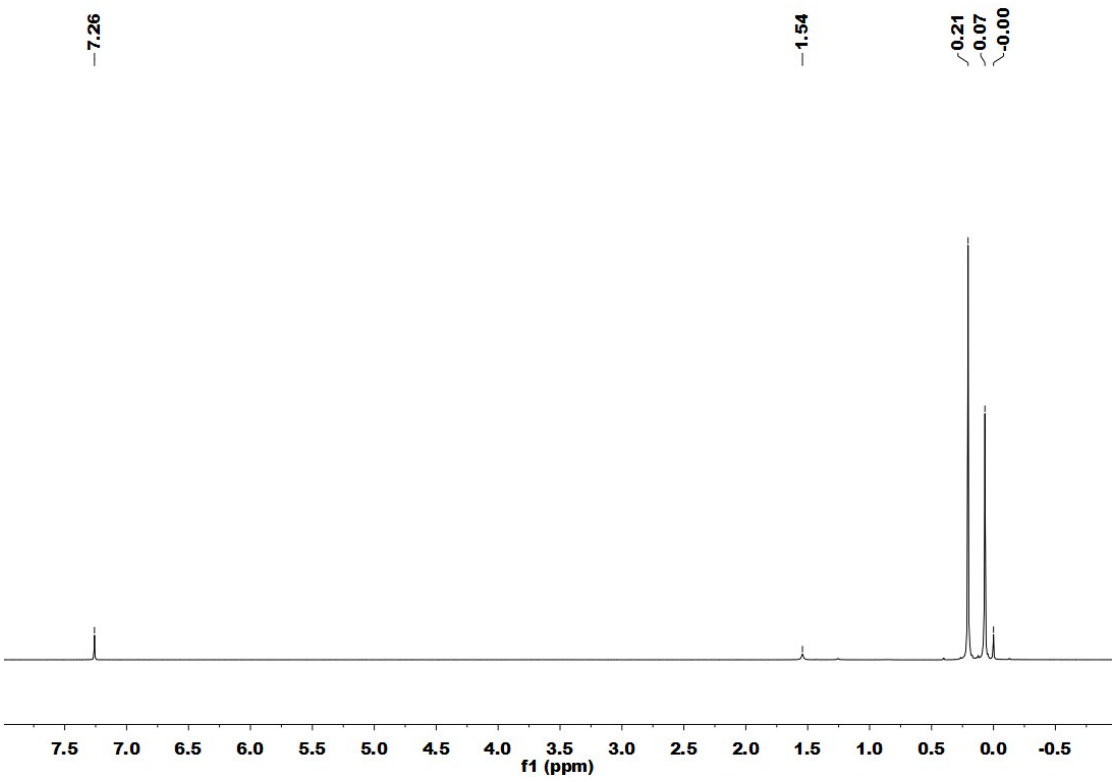


Fig. S1 ^{1}H-NMR of compound **1**. The peaks around 0 ppm refer to $SiCH_3$. The peaks at 7.26 and 1.54 ppm refer to the residual $CHCl_3$ and H_2O molecules in the $CDCl_3$ solvent.

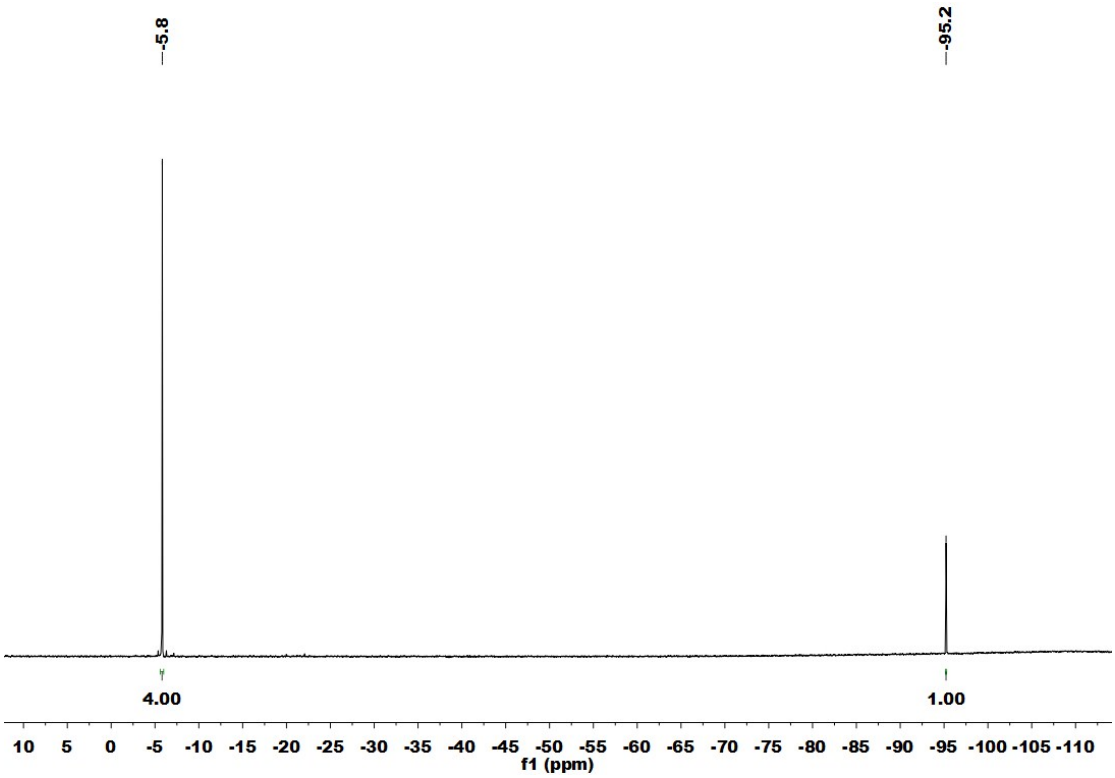


Fig. S2 ^{29}Si-NMR of the compound **1**.

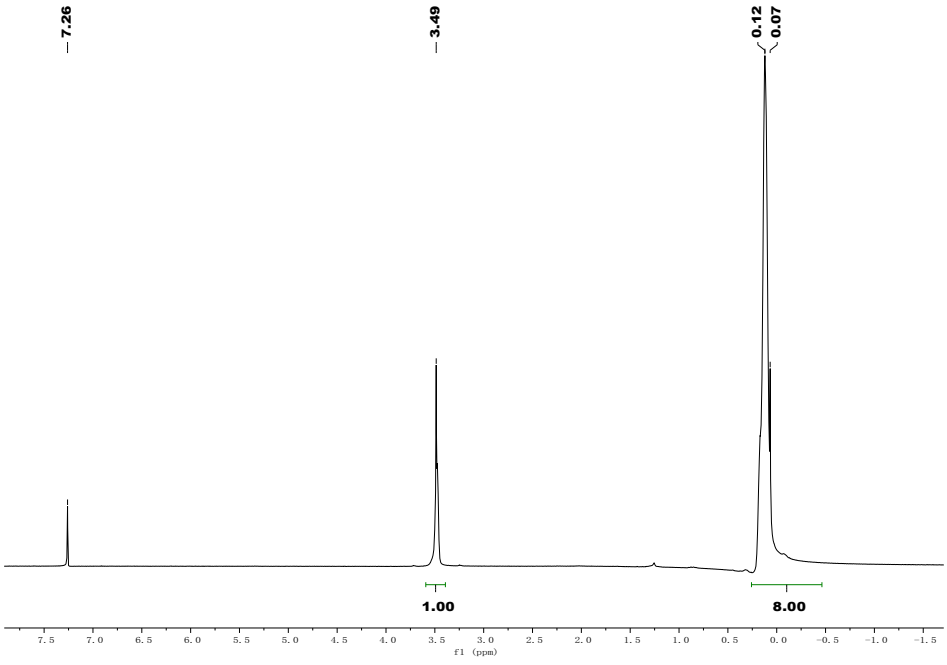


Fig. S3 ^{1}H-NMR of the product from the reaction between compound **1** and methanol.

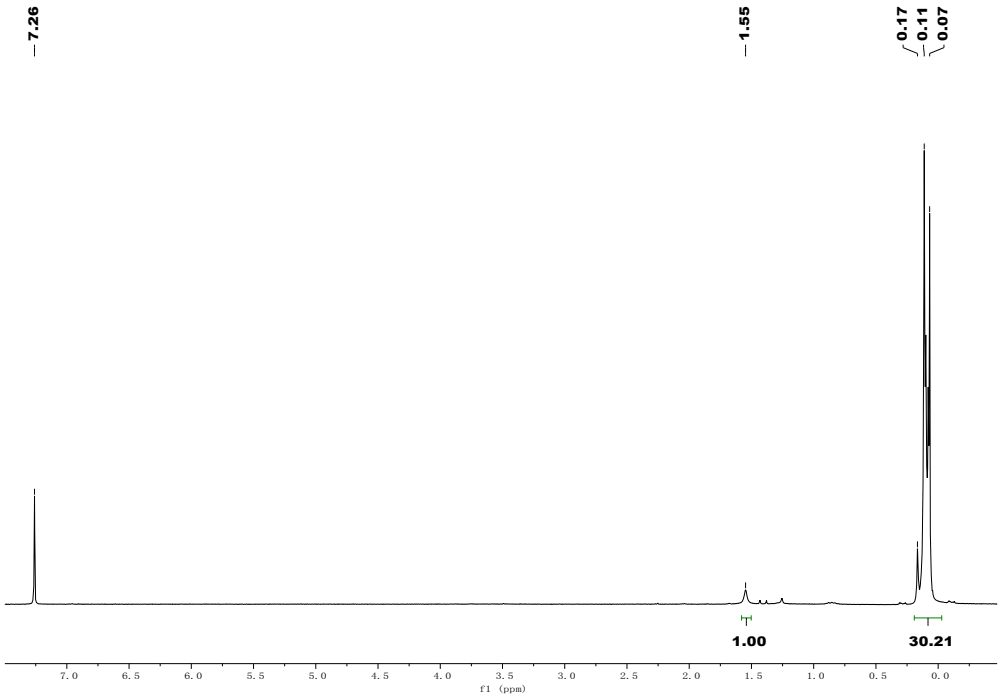


Fig. S4 ^{1}H-NMR of compound **2**. The peaks around 0 ppm refer to $SiCH_3$. The peaks at 7.26 and 1.55 ppm refer to the residual $CHCl_3$ and H_2O molecules in the $CDCl_3$ solvent.

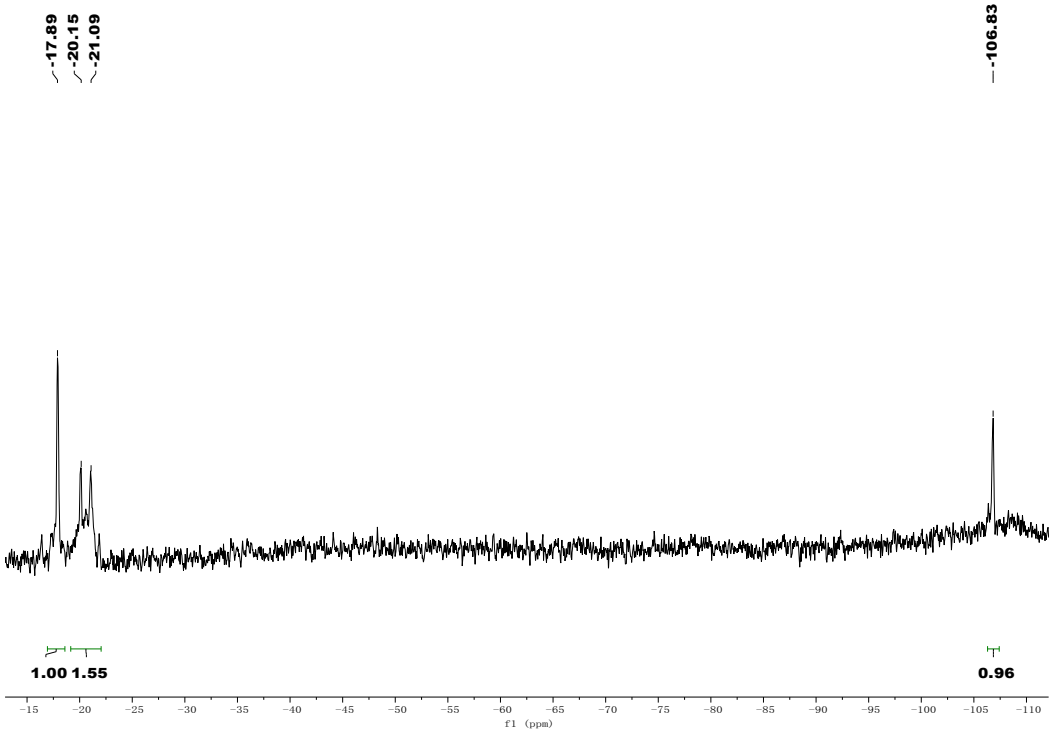


Fig. S5 ^{29}Si-NMR of compound **2**.

S4. X-ray of the spirocyclolsiloxane solids.

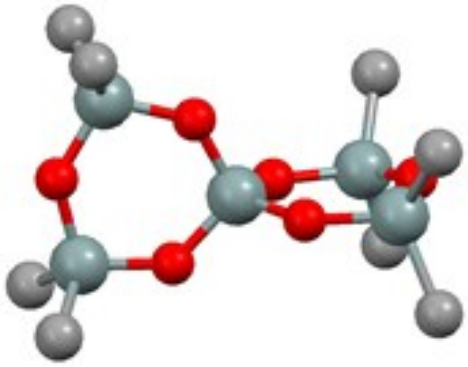
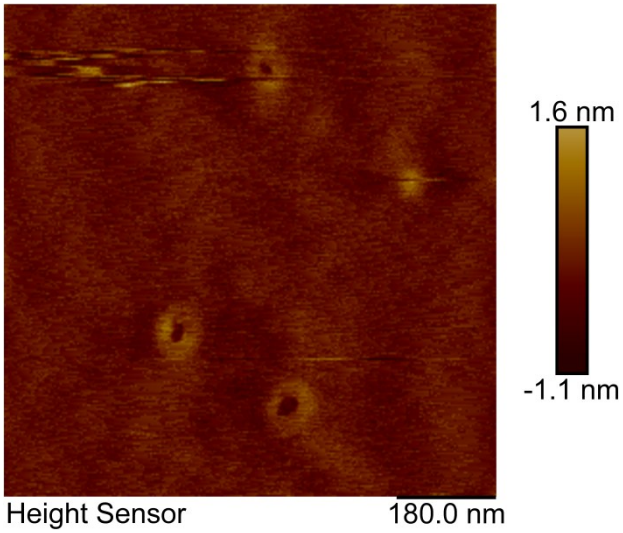


Fig. S6 X-ray of the compound **1**.

S5. AFM of the Compound 2



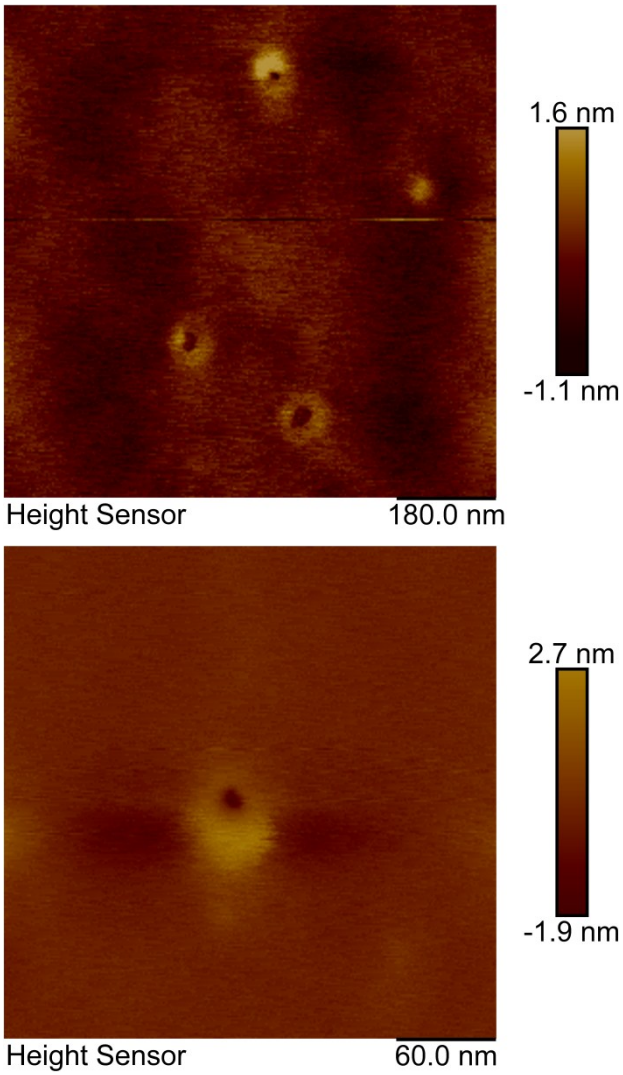


Fig. S7 A collection of several AFM images of compound **2** on the surface of mica deposited from the THF solution at $1*10^{-4}$ mg/ml

S5. IR of the Compounds

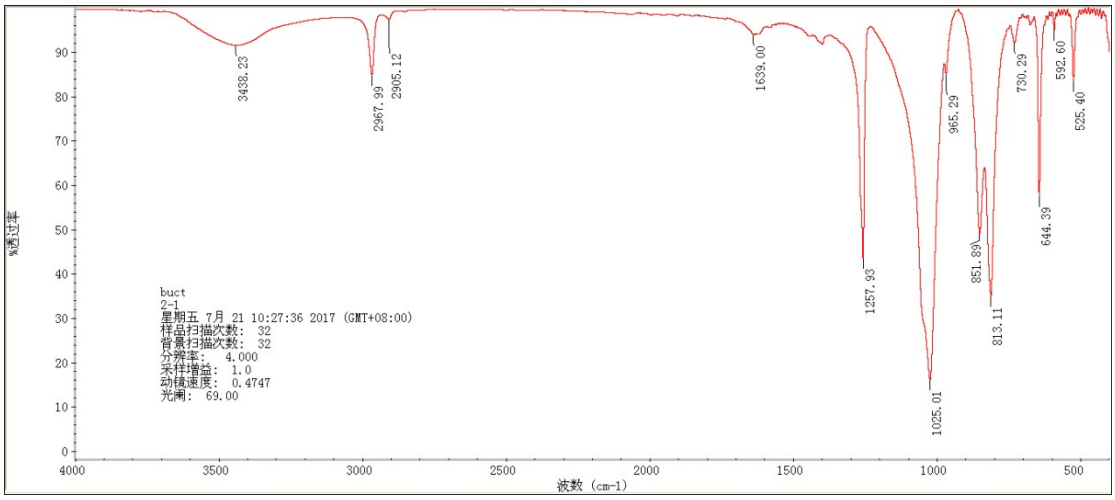


Fig. S8 Infrared spectroscopy of compound **1** on KBr plate

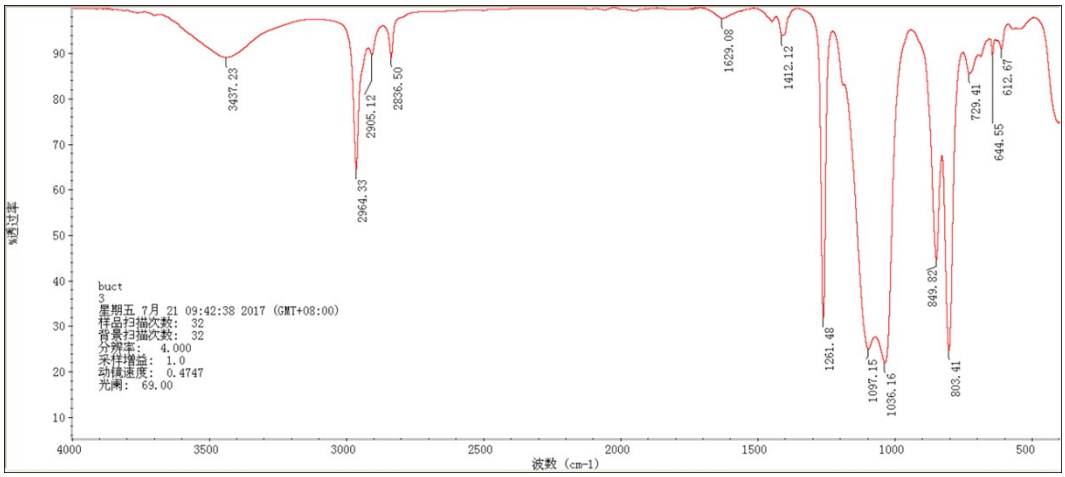


Fig. S9 Infrared spectroscopy of the reaction mixture of compound **1 and methanol** on KBr plate

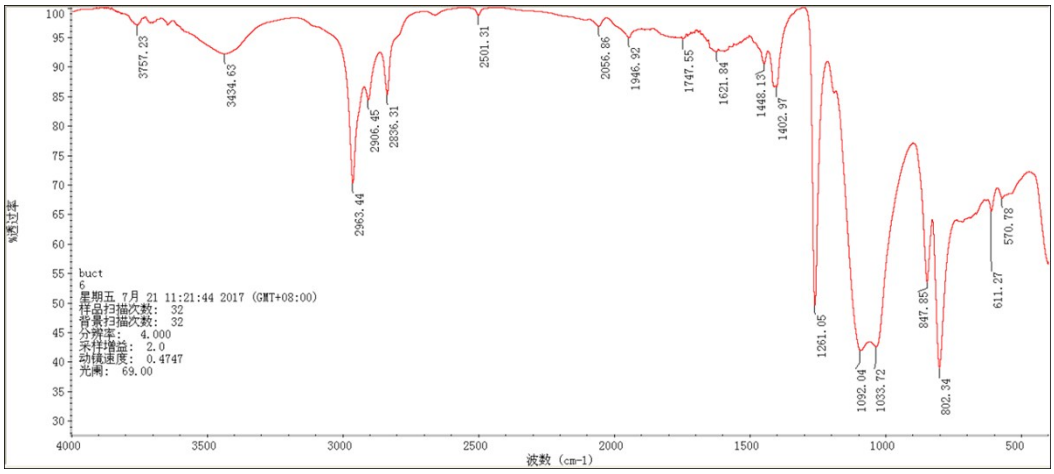


Fig. S10 Infrared spectroscopy of the reaction mixture of compound **2**

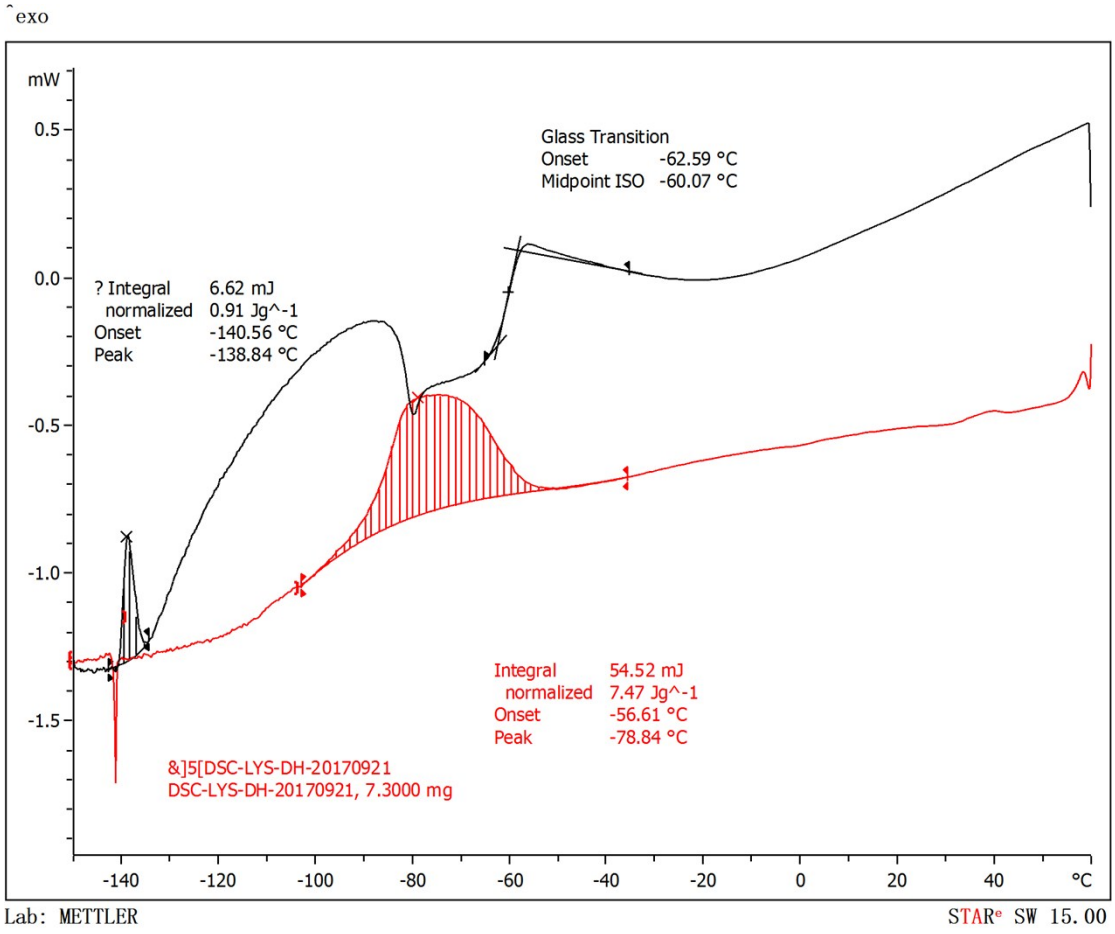


Fig. S11 DSC analysis of **2** under nitrogen at 10°C/min. Temperature is decreased in the red line and increased in the black line.

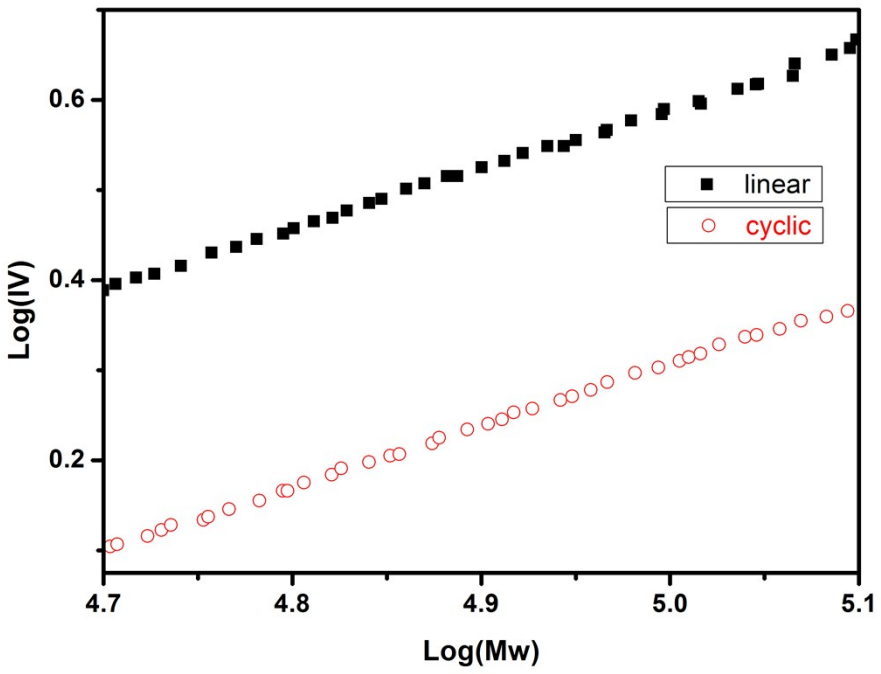


Fig. S12 The Mark-Houwink plot of **2** (red circles) with its linear counterpart (black squares) prepared in the presence of methanol as the alcohol initiator.

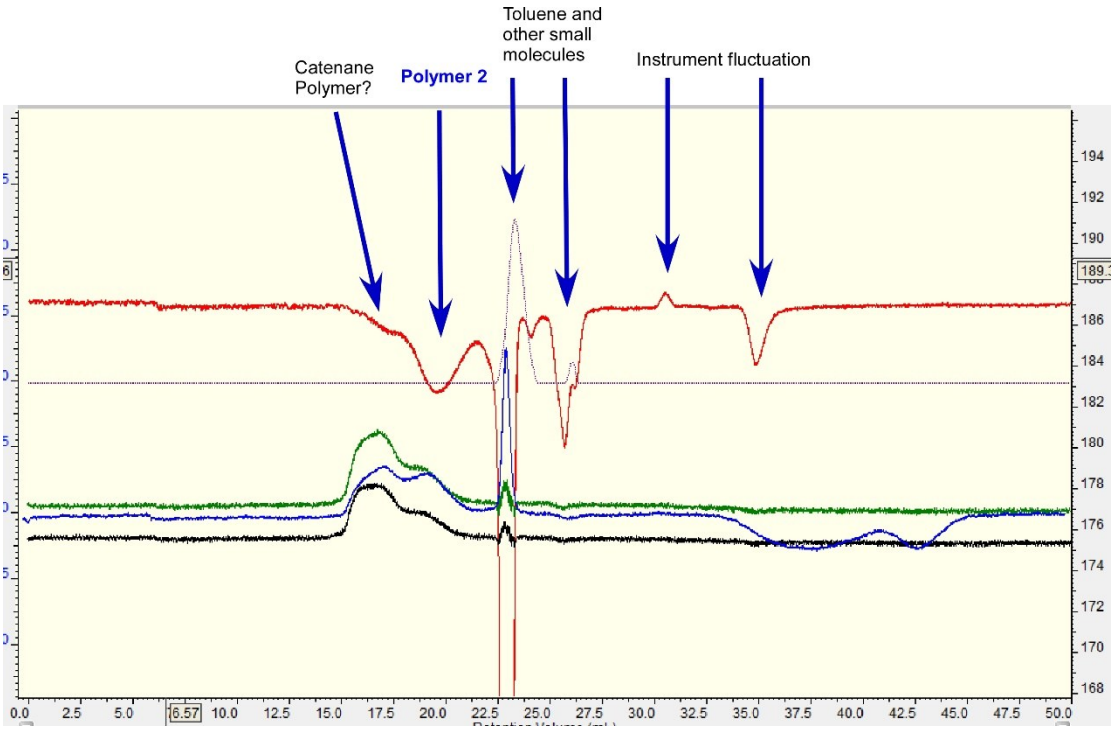


Fig. S13 The GPC trace for polymer **2**, which has small amount of possible catenane polymer.

The peaks eluted out after the cyclic polymer are assigned to solvent peaks and instrument fluctuation, which are confirmed by control GPC measurements done with only the solvents. Red line: differential refractive index, Blue line: viscosity, Green Line: right angle light scattering, Black line: low angle light scattering.

S7. Computation Details

DFT Computed Atomic Coordinates and Energy Profiles of SM0 to R3

Compound SM0

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	8	-0.000000475	-0.000001700	-0.000004188
2	14	-0.000000602	-0.000001091	-0.000001142
3	14	0.000003061	0.000004902	-0.000001530
4	8	-0.000003037	0.000002125	-0.000000425
5	8	-0.000002629	-0.000001628	0.000002353
6	14	0.000002892	0.000001449	0.000002024
7	8	-0.000003543	-0.000004420	-0.000006340
8	8	0.000004578	-0.000004985	0.000003448
9	14	-0.000003323	-0.000000701	0.000011531
10	14	0.000000037	0.000000982	0.000002822
11	8	-0.000000887	0.000001553	0.000000385
12	6	0.000002523	-0.000003729	0.000003198
13	1	0.000001961	-0.000003035	-0.000000277
14	1	0.000002265	-0.000002282	-0.000001155
15	1	0.000000470	-0.000001808	-0.000000101
16	6	0.000005150	0.000002501	-0.000001682
17	1	-0.000000423	-0.000004576	-0.000002288
18	1	0.000007231	-0.000009126	-0.000004059
19	1	0.000004706	-0.000004609	-0.000003973
20	6	0.000000054	0.000000443	-0.000002161
21	1	-0.000000441	0.000003316	-0.000002450
22	1	-0.000001431	0.000003086	-0.000000934
23	1	0.000000287	0.000001106	0.000000596
24	6	-0.000000759	0.000004655	-0.000004538

25	1	0.000000796	0.000002529	-0.000005265
26	1	-0.000001050	0.000000546	-0.000004849
27	1	-0.000000310	0.000003130	-0.000003141
28	6	0.000001758	0.000005505	0.000003109
29	1	-0.000001279	-0.000002819	0.000004135
30	1	-0.000004078	-0.000006968	0.000005229
31	1	-0.000000608	-0.000002624	0.000002981
32	6	-0.000001823	-0.000003781	0.000001995
33	1	-0.000002899	0.000003783	0.000003486
34	1	-0.000003469	0.000003435	0.000003635
35	1	-0.000004720	0.000001287	0.000006774
36	6	0.000002542	-0.000003160	0.000005714
37	1	-0.000000367	-0.000002811	0.000003662
38	1	0.000000118	-0.000002958	0.000004591
39	1	-0.000000925	-0.000003799	0.000003728
40	6	-0.000004337	-0.000001929	0.000004303
41	1	-0.000002571	0.000001240	0.000004946
42	1	-0.000002174	-0.000000058	0.000007013
43	1	-0.000002393	0.000000918	0.000005943
44	6	-0.000000968	0.000000432	0.000005513
45	6	0.000002076	0.000000205	-0.000004580
46	1	0.000005025	-0.000001728	-0.000001326
47	1	0.000000551	-0.000001462	-0.000001668
48	6	0.000003224	-0.000010683	-0.000002863
49	1	0.000005025	-0.000002778	-0.000002634
50	1	0.000000164	-0.000002473	-0.000002600
51	6	0.000004890	0.000003166	-0.000006403
52	1	0.000003407	0.000001650	-0.000001037
53	1	0.000001127	0.000000235	-0.000004571
54	6	0.000000375	0.000004263	-0.000000285
55	1	-0.000001808	0.000001529	-0.000001596
56	1	-0.000000556	-0.000000179	-0.000000152
57	6	-0.000001794	0.000001222	-0.000001077
58	1	-0.000001797	0.000003226	0.000000418
59	1	0.000000098	0.000002697	0.000000623
60	6	-0.000002052	0.000005569	-0.000000410
61	1	-0.000002617	0.000005561	-0.000000244
62	1	-0.000002994	0.000004380	-0.000003241
63	7	-0.000001731	0.000003051	-0.000002178
64	7	-0.000001134	0.000004964	-0.000004834
65	7	0.000000912	-0.000000899	-0.000009062
66	1	0.000000704	0.000004158	-0.000002894

Zero-point correction=	0.537529 (Hartree/Particle)
Thermal correction to Energy=	0.576064
Thermal correction to Enthalpy=	0.577009
Thermal correction to Gibbs Free Energy=	0.465503
Sum of electronic and zero-point Energies=	-2657.332383
Sum of electronic and thermal Energies=	-2657.293848
Sum of electronic and thermal Enthalpies=	-2657.292903
Sum of electronic and thermal Free Energies=	-2657.404409

Compound SM1

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	8	-0.000001069	-0.000006640	-0.000005116
2	14	0.000000488	0.000001761	-0.000002654
3	14	0.000000709	0.000003003	-0.000000642
4	8	-0.000001598	-0.000000969	-0.000007726
5	8	-0.000003482	0.000004469	-0.000001195
6	14	0.000001500	-0.000001972	-0.000000104
7	8	-0.000000479	-0.000000101	0.000006834
8	8	-0.000006388	-0.000001681	0.000003186
9	14	0.000000140	0.000002287	0.000005643
10	14	0.000011002	0.000002517	0.000001578
11	8	0.000002123	-0.000004139	0.000001639
12	6	-0.000002337	0.000000867	-0.000001884
13	1	-0.000004115	0.000002799	-0.000002954
14	1	-0.000003771	0.000000289	-0.000005106
15	1	-0.000003351	0.000000967	-0.000004403
16	6	-0.000000920	0.000000552	-0.000001149
17	1	-0.000003077	0.000001632	-0.000000336
18	1	-0.000003786	0.000003190	0.000000190
19	1	0.000004337	-0.000003696	0.000001867
20	6	0.000003074	-0.000000336	-0.000002302
21	1	-0.000002213	0.000000802	-0.000003601
22	1	-0.000000090	-0.000000412	-0.000000573
23	1	0.000000653	-0.000004070	-0.000007180
24	6	-0.000003841	-0.000004164	-0.000001380
25	1	-0.000001301	-0.000001644	-0.000007070
26	1	0.000000822	-0.000003432	-0.000006310
27	1	0.000005557	-0.000004404	-0.000006315

28	6	0.000006383	-0.000002713	0.000002017
29	1	0.000005903	-0.000002253	-0.000001274
30	1	0.000002217	-0.000002300	-0.000001354
31	1	0.000004690	-0.000002658	0.000003648
32	6	-0.000000429	0.000001892	0.000003923
33	1	-0.000002082	0.000002356	0.000002784
34	1	0.000001391	-0.000001030	0.000003301
35	1	-0.000001689	0.000001086	-0.000002226
36	6	0.000001930	-0.000002308	0.000003493
37	1	0.000002922	-0.000002211	0.000004559
38	1	-0.000000679	0.000002735	0.000003605
39	1	0.000004063	-0.000001234	0.000002324
40	6	-0.000001615	0.000004917	0.000006909
41	1	0.000001084	0.000000696	0.000002970
42	1	0.000000320	0.000002809	0.000005751
43	1	0.000000255	0.000000812	0.000005469
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45	6	-0.000004028	0.000002571	0.000002068
46	1	0.000000734	-0.000001951	-0.000003560
47	1	-0.000000335	0.000001291	0.000006685
48	6	-0.000004093	0.000003995	0.000001258
49	1	0.000000531	0.000001323	0.000005011
50	1	-0.000002578	0.000002701	0.000001883
51	6	-0.000002803	0.000003105	0.000002220
52	1	-0.000001640	0.000001083	-0.000000632
53	1	-0.000001659	0.000002426	0.000000688
54	6	-0.000002993	0.000000215	0.000000815
55	1	-0.000003542	0.000003564	0.000002061
56	1	0.000004617	-0.000003119	0.000003504
57	6	0.000000317	-0.000000684	-0.000001200
58	1	0.000003875	-0.000002233	-0.000000584
59	1	-0.000003636	0.000002185	-0.000001309
60	6	0.000001267	-0.000000790	-0.000002066
61	1	0.000000625	-0.000001092	-0.000001355
62	1	0.000000937	-0.000000073	0.000000642
63	7	0.000003393	-0.000001911	-0.000004049
64	7	0.000000925	-0.000002926	-0.000007796
65	7	0.000000973	0.000000344	0.000000062
66	1	0.000000277	-0.000002739	-0.000001742

Zero-point correction= 0.538509 (Hartree/Particle)

Thermal correction to Energy= 0.576309

Thermal correction to Enthalpy= 0.577253

Thermal correction to Gibbs Free Energy= 0.469065

Sum of electronic and zero-point Energies= -2657.324463

Sum of electronic and thermal Energies= -2657.286663

Sum of electronic and thermal Enthalpies= -2657.285719

Sum of electronic and thermal Free Energies= -2657.393907

Compound R1

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	8	0.000004408	0.000003949	0.000000987
2	14	0.000003789	0.000005032	0.000001756
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4	8	-0.000001350	-0.000000536	0.000002473
5	8	0.000007235	-0.000013281	-0.000000541
6	14	-0.000010631	0.000000286	0.000004576
7	8	0.000008507	0.000005502	0.000001251
8	8	0.000009309	0.000004089	-0.000003441
9	14	-0.000004298	-0.000004468	-0.000009907
10	14	-0.000015341	0.000005046	0.000000119
11	8	0.000000943	-0.000001776	0.000003615
12	6	-0.000003514	-0.000000490	0.000002127
13	1	0.000003453	0.000000106	-0.000001326
14	1	0.000003510	0.000001630	0.000002417
15	1	0.000001419	0.000000446	-0.000000963
16	6	-0.000000968	-0.000000250	-0.000002141
17	1	-0.000001437	0.000000450	-0.000000120
18	1	0.000001780	-0.000002432	-0.000001238
19	1	-0.000000722	0.000001122	-0.000002554
20	6	0.000001024	0.000004890	0.000000167
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22	1	0.000000452	0.000002079	-0.000001710
23	1	-0.000000005	0.000004274	0.000002535
24	6	-0.000002094	0.000003808	0.000000326
25	1	0.000001451	0.000004075	0.000000792
26	1	-0.000000556	0.000002862	0.000001507
27	1	-0.000000524	0.000002856	0.000000499
28	6	-0.000002403	0.000001165	-0.000000964
29	1	-0.000001879	0.000003627	-0.000000105
30	1	0.000002430	0.000001168	0.000000888

31	1	-0.000001755	0.000000145	-0.000000056
32	6	-0.000001004	-0.000000305	-0.000002739
33	1	0.000000304	-0.000002816	-0.000000864
34	1	-0.000002647	-0.000000563	0.000000695
35	1	0.000002664	-0.000001599	0.000002138
36	6	-0.000001044	-0.000001577	0.000000142
37	1	-0.000000077	-0.000001295	0.000001149
38	1	-0.000004790	-0.000002040	-0.000003021
39	1	0.000001837	0.000000440	-0.000001373
40	6	-0.000001912	-0.000001656	-0.000001567
41	1	-0.000002072	-0.000001390	-0.000004903
42	1	-0.000001420	-0.000005033	-0.000001679
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45	6	0.000004282	-0.000002483	0.000003030
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47	1	-0.000001541	-0.000003151	-0.000002850
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51	6	-0.000004777	0.000000758	-0.000003130
52	1	0.000002402	-0.000002462	0.000000915
53	1	0.000000552	-0.000002574	-0.000000129
54	6	0.000002451	0.000001078	0.000001101
55	1	-0.000000188	-0.000003185	-0.000000179
56	1	-0.000003213	0.000002467	-0.000000669
57	6	0.000002237	-0.000000923	0.000002949
58	1	0.000000081	0.000002147	-0.000000802
59	1	0.000000907	-0.000001944	0.000000618
60	6	0.000000435	-0.000000200	0.000001778
61	1	0.000002055	-0.000000408	0.000001819
62	1	0.000001270	-0.000000865	0.000000432
63	7	-0.000001920	-0.000004473	0.000000094
64	7	0.000002692	-0.000004441	0.000001645
65	7	-0.000009718	0.000002372	-0.000005029
66	1	0.000011083	0.000002070	0.000003719

Zero-point correction= 0.537130 (Hartree/Particle)

Thermal correction to Energy= 0.575339

Thermal correction to Enthalpy= 0.576283

Thermal correction to Gibbs Free Energy= 0.467312

Sum of electronic and zero-point Energies= -2657.315644

Sum of electronic and thermal Energies= -2657.277435

Sum of electronic and thermal Enthalpies= -2657.276490

Sum of electronic and thermal Free Energies= -2657.385462

Compound R3

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	8	0.000004964	-0.000004737	0.000001185
2	14	-0.000007840	0.000005445	0.000000088
3	14	-0.000013465	0.000019948	0.000001211
4	8	0.000001422	-0.000001176	0.000000611
5	8	0.000012512	0.000002247	-0.000001636
6	14	-0.000010900	-0.000001910	-0.000003830
7	8	0.000008747	-0.000008912	-0.000017408
8	8	0.000010711	0.000005294	-0.000002234
9	14	-0.000013268	0.000010394	-0.000000615
10	14	-0.000019099	-0.000019682	0.000012101
11	8	0.000005481	0.000001014	-0.000006070
12	6	0.000011526	-0.000003700	-0.000011412
13	1	0.000004720	-0.000001679	-0.000003218
14	1	0.000002059	-0.000001095	0.000000866
15	1	0.000003634	0.000000083	0.000000595
16	6	0.000006482	-0.000001939	0.000000846
17	1	0.000004364	0.000000006	-0.000003678
18	1	-0.000004246	0.000000486	-0.000001336
19	1	-0.000004353	0.000002196	-0.000001364
20	6	0.000005961	0.000003975	0.000009274
21	1	0.000001964	-0.000001823	-0.000003287
22	1	0.000001166	0.000001801	-0.000000247
23	1	-0.000002675	-0.000002376	-0.000001465
24	6	-0.000010043	-0.000004856	0.000006466
25	1	0.000003087	-0.000000537	0.000000196
26	1	-0.000000893	0.000000936	0.000001819
27	1	-0.000000839	0.000002059	-0.000000339
28	6	-0.000004649	-0.000008063	-0.000004359
29	1	-0.000000781	0.000000200	0.000001852
30	1	-0.000001028	0.000002802	0.000006483
31	1	-0.000004227	-0.000003144	-0.000004357
32	6	0.000003606	0.000000925	-0.000016777
33	1	0.000002226	-0.000001149	0.000002859

34	1	-0.000002339	-0.000001101	0.000000291
35	1	0.000001908	0.000001936	0.000004493
36	6	-0.000001231	-0.000008512	-0.000004504
37	1	-0.000001737	-0.000001699	-0.000000500
38	1	0.000002404	-0.000002018	-0.000003852
39	1	-0.000002545	0.000001144	-0.000000152
40	6	0.000002052	-0.000002997	-0.000006447
41	1	-0.000001057	-0.000003387	-0.000000738
42	1	-0.000000091	-0.000004342	-0.000008214
43	1	-0.000003688	0.000002020	-0.000005674
44	6	-0.000005094	-0.000005858	-0.000001653
45	6	0.000004800	0.000011934	0.000007979
46	1	0.000000579	0.000005096	0.000007196
47	1	-0.000002798	-0.000001716	-0.000007831
48	6	0.000001188	-0.000003627	0.000002504
49	1	0.000000799	-0.000002833	-0.000006379
50	1	0.000002876	-0.000000191	0.000002286
51	6	-0.000006958	0.000003461	0.000005451
52	1	0.000003093	0.000000608	0.000006427
53	1	0.000000311	0.000002009	0.000000327
54	6	0.000007097	0.000009842	0.000002062
55	1	0.000005528	-0.000001118	0.000001903
56	1	-0.000007196	0.000000534	-0.000003098
57	6	0.000001920	0.000004257	0.000012768
58	1	-0.000003862	0.000003341	0.000001137
59	1	0.000001898	-0.000001510	-0.000001020
60	6	-0.000002266	-0.000004891	0.000003291
61	1	0.000001187	0.000002651	0.000005753
62	1	0.000001159	0.000001683	0.000007214
63	7	-0.000003575	-0.000010421	0.000006935
64	7	0.000008869	0.000006816	0.000000291
65	7	0.000003853	0.000004762	0.000004157
66	1	-0.000003410	0.000001099	0.000004782

Zero-point correction= 0.539260 (Hartree/Particle)

Thermal correction to Energy= 0.576172

Thermal correction to Enthalpy= 0.577116

Thermal correction to Gibbs Free Energy= 0.472483

Sum of electronic and zero-point Energies= -2657.294512

Sum of electronic and thermal Energies= -2657.257600

Sum of electronic and thermal Enthalpies= -2657.256656

Sum of electronic and thermal Free Energies= -2657.361289

Compound R2

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	8	0.000004304	-0.000002045	-0.000000905
2	14	-0.000004712	0.000005282	-0.000010669
3	14	0.000010005	-0.000002844	-0.000015057
4	8	-0.000012194	-0.000000704	0.000007590
5	8	-0.000002976	0.000007283	0.000001090
6	14	-0.000010819	-0.000009085	0.000011361
7	8	-0.000001133	0.000007654	0.000005182
8	8	0.000001480	0.000009047	-0.000000306
9	14	-0.000013823	-0.000004943	0.000008365
10	14	0.000004652	-0.000006117	-0.000009903
11	8	0.000006801	-0.000000599	0.000005915
12	6	-0.000001759	0.000006288	-0.000005133
13	1	0.000001013	0.000005420	-0.000000735
14	1	0.000012549	0.000009743	-0.000009951
15	1	-0.000001669	0.000000127	0.000003173
16	6	0.000000913	0.000003408	-0.000001966
17	1	-0.000000394	0.000005383	-0.000002763
18	1	-0.000000513	-0.000000147	0.000004714
19	1	-0.000000097	-0.000004743	-0.000002934
20	6	0.000001247	0.000000738	-0.000006098
21	1	0.000000602	0.000002937	-0.000002878
22	1	0.000001191	0.000002228	-0.000000898
23	1	0.000001372	-0.000000404	-0.000004794
24	6	0.000000786	-0.000002252	-0.000003877
25	1	-0.000000827	-0.000001148	-0.000003601
26	1	0.000000556	0.000000653	-0.000006134
27	1	-0.000000385	-0.000002321	-0.000003934
28	6	-0.000000859	-0.000002993	0.000000324
29	1	0.000001031	-0.000001949	-0.000004901
30	1	0.000000353	0.000000561	-0.000000094
31	1	0.000000278	-0.000002608	-0.000000702
32	6	0.000000647	-0.000003940	0.000002043
33	1	-0.000000115	-0.000001103	0.000002249
34	1	-0.000001796	-0.000004300	0.000004678
35	1	-0.000000218	0.000002347	0.000003282
36	6	0.000001838	0.000002051	-0.000000861

37	1	-0.000000322	-0.000003143	0.000000462
38	1	0.000000667	0.000000809	-0.000000532
39	1	0.000001002	-0.000006147	0.000000951
40	6	-0.000000469	0.000002059	0.000002650
41	1	-0.000001919	0.000001869	-0.000001593
42	1	-0.000000665	0.000002316	0.000003287
43	1	-0.000000594	0.000000430	0.000000204
44	6	-0.000003431	-0.000010161	0.000001246
45	6	0.000001062	-0.000001278	0.000000829
46	1	-0.000000360	0.000001484	-0.000000109
47	1	-0.000000159	0.000000708	0.000003657
48	6	-0.000002110	-0.000000448	0.000004206
49	1	-0.000000049	0.000000437	0.000005294
50	1	0.000000218	-0.000000047	0.000005208
51	6	0.000000708	0.000000464	-0.000001726
52	1	-0.000000405	-0.000000416	0.000003971
53	1	0.000003408	-0.000007378	-0.000007921
54	6	-0.000001954	-0.000001622	0.000002728
55	1	-0.000001081	-0.000000889	0.000004942
56	1	0.000001213	-0.000000983	-0.000000021
57	6	0.000001496	0.000000622	0.000001696
58	1	-0.000000550	-0.000001758	-0.000004694
59	1	-0.000000340	0.000001966	0.000003821
60	6	-0.000002988	-0.000001229	-0.000000338
61	1	0.000000205	-0.000000313	0.000001477
62	1	-0.000000313	-0.000001564	0.000001479
63	7	-0.000002363	0.000003926	0.000007375
64	7	0.000002517	0.000004442	-0.000000831
65	7	0.000006465	-0.000003733	-0.000002790
66	1	0.000003781	0.000002669	0.000004198

Zero-point correction= 0.538170 (Hartree/Particle)

Thermal correction to Energy= 0.577102

Thermal correction to Enthalpy= 0.578046

Thermal correction to Gibbs Free Energy= 0.467086

Sum of electronic and zero-point Energies= -2657.322321

Sum of electronic and thermal Energies= -2657.283390

Sum of electronic and thermal Enthalpies= -2657.282445

Sum of electronic and thermal Free Energies= -2657.393405

	SM0	SM1	R1	R3	R2
ZPE @ 6-31+G(d) level (Hatrees)					
	0.537529	0.538509	0.53713	0.53926	0.53817
	0.576064	0.576309	0.575339	0.576172	0.577102
	0.577009	0.577253	0.576283	0.577116	0.578046
	0.465503	0.469065	0.467312	0.472483	0.467086
Single point energy@6-311++G(2d,p) level (Hatrees)					
	−2658.386259	−2658.375464	−2658.36753	−2658.344728	−2658.373978
Eo	−2657.84873	−2657.836955	−2657.8304	−2657.805468	−2657.835808
E	−2657.810195	−2657.799155	−2657.792191	−2657.768556	−2657.796876
H	−2657.80925	−2657.798211	−2657.791247	−2657.767612	−2657.795932
G	−2657.920756	−2657.906399	−2657.900218	−2657.872245	−2657.906892
Energy referenced@SM0 (kcal/mol)					
Eo	0	6.77380255	11.75284618	26.06083599	7.706269207
E	0	7.388761919	11.50246987	27.14705504	8.108502834
H	0	6.927542393	11.29790175	26.12860702	8.35762413
G	0	6.926914883	11.29727424	26.12797951	8.35699662

[1] Frisch, M. J. T., G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision D.1 Wallingford, CT, 2009