Supporting Information

Chloroyttrium 2-(1-(arylimino)alkyl)quinolin-8-olate Complexes: Synthesis, Characterization, and Catalysis of the Ring-Opening Polymerization (ROP) of ε-Caprolactone (ε-CL)

Wenjuan Zhang, Shaofeng Liu, Wenhong Yang, Xiang Hao, Rainer Glaser and Wen-Hua Sun

[a] Key Laboratory of Engineering Plastics and Beijing Natural Laboratory for Molecular Science, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China;

[b] Department of Chemistry, University of Missouri, Columbia, Missouri 65211, USA.

Email: whsun@iccas.ac.cn (WHS) or GlaserR@missouri.edu (RG)

Table of Contents

X-ray Crystallographic Studies.

Table S1 Crystallographic Data, Collection and Refinement Details for complexes **1, 4-6**…….. S2

Computation Study

Details of the Computational Study ……. S3

Table S2. Computed Energies and Thermochemical Parameters …….…….....S3

Cart. Coords. of B3LYP/SDD opt. structs. of model complexes **M1** – **M4**.

(L1)$YCl_2(DMSO)_2$,**M1**…….S4

(L1)$YCl(CH_2SiMe_3)(DMSO)_2$, **M2**…….S5

(L1)$Y(CH_2SiMe_3)_2(DMSO)_2$, **M3**……..…….....S7

(L1)$Y(OCH_2Ph)(CH_2SiMe_3)(DMSO)_2$, **M4a** ……..... S9

(L1)$Y(OCH_2Ph)(CH_2SiMe_3)(DMSO)_2$, **M4b** ……..……..S11

B3LYP/SDD computed vibrational spectra of **M1** – **M4a**

(L1)$YCl_2(DMSO)_2$, **M1** …….....S13

(L1)$YCl(CH_2SiMe_3)(DMSO)_2$, **M2**…….S13

(L1)$Y(CH_2SiMe_3)_2(DMSO)_2$, **M3**…….....S14

(L1)$Y(OCH_2Ph)(CH_2SiMe_3)(DMSO)_2$, **M4a** ……..S14

Overlay **M1** and **M2** ……S15

Overlay **M1** and **M3** ……S15

Overlay **M3** and **M4a** ……..……..……...S15

X-ray Crystallographic Studies.

Crystal Single-crystal X-ray diffraction studies for complexes **1**, **4** - **6** was carried out on a Rigaku Saturn 724+ CCD diffractometer with graphite-monochromated MoKα radiation (λ = 0.71073 Å) and those of **1** and **6** were carried out on Rigaku MM007-HF Saturn 724+ CCD diffractometer with confocal mirror monochromated MoKα radiation (λ = 0.71073 Å). Crystal date and details were collected and shown in the Table S1

Table S1 Crystallographic Data, Collection and Refinement Details for complexes **1, 4-6**

	1	**4**	**5**	**6**
Formula	$C_{22}H_{27}Cl_2N_2O_3S_2Y$	$C_{23}H_{29}Cl_2N_2O_3S_2Y$	$C_{54}H_{74}Cl_4N_4O_6S_4Y_2$	$C_{92}H_{100}Cl_8N_8O_6Y_4$
formula wt.	591.39	605.41	1323.03	2053.04
T (K)	173(2)	173(2)	173(2)	173(2)
wavelength (Å)	0.71073	0.71073	0.71073	0.71073
Cryst. syst.	Monoclinic	Monoclinic	Triclinic	Triclinic
space group	P2(1)/n	C2/c	P-1	P-1
a (Å)	16.683(3)	26.785(5)	12.856(3)	17.277(4)
b (Å)	7.7392(15)	14.369(3)	15.165(3)	20.115(4)
c (Å)	23.361(5)	16.225(3)	18.681(4)	20.357(4)
α (deg)	90.00	90.00	80.81(3)	109.92(3)
β (deg)	106.68(3)	121.89(3)	79.36(3)	107.41(3)
γ (deg)	90.00	90.00	73.60(3)	94.64(3)
V ($Å^3$)	2889.4(10)	5301.8(18)	3411.2(12)	6214(2)
Z	4	8	2	2
D_{calcd} (g cm^{-3})	1.359	1.517	1.288	1.097
μ (mm^{-1})	2.371	2.586	2.016	2.063
F (000)	1208	2480	1368	2096
θ range (deg)	1.34-27.47	2.69-27.48	1.41-27.48	1.10-25.27
Limiting indices	$-19 \le h \le 21$, $-10 \le k \le 0$, $-29 \le l \le 30$	$-34 \le h \le 34$, $-18 \le k \le 16$, $-21 \le l \le 15$	$-16 \le h \le 16$, $-18 \le k \le 19$, $-24 \le l \le 24$	$-20 \le h \le 20$, $-24 \le k \le 24$, $-22 \le l \le 24$
no. of rflns. collected	23011	21363	42311	65763
no. of unique rflns.	6595	6063	15576	22500
completeness to θ (%)	99.8 (θ = 27.47°)	99.8 (θ = 27.48°)	99.5 (θ = 27.48°)	99.7 (θ = 25.27°)
Abs. Corr,	Numerical	Numerical	Numerical	Numerical
no. of params.	289	298	687	1099
goodness of fit on F^2	1.131	1.208	1.085	0.999
final R indices (I > 2σ(I))	R1 = 0.0689, wR2 = 0.1512	R1 = 0.0707, wR2 = 0.1833	R1 = 0.0820, wR2 = 0.1790	R1 = 0.0777, wR2 = 0.1971
R indices (all data)	R1 = 0.0804, wR2 = 0.1577	R1 = 0.0824, wR2 = 0.1902	R1 = 0.1129, wR2 = 0.1947	R1 = 0.1169, wR2= 0.2211
Largest diff. peak, hole (e $Å^{-3}$)	1.513 & -0.555	0.462 & -0.367	0.737 & -0.610	1.416&-0.472

Details of the Computational Study

The basis set notation SDD refers to a set of split-valence basis sets which are employed with Stuttgart/Dresden effective core potentials (ECPs) for Z > 2 to reduce the number of basis functions and to include relativistic effects for heavy atoms. Hydrogen is described with a basis set containing 4 primitive s-functions which are contracted to 2 basis functions (a "31" basis set). The valence shells of C, N, and O are described by [2.2] contractions of (4.4) basis sets and sulfur is described by a [2.3] contraction of a (4.5) basis set. The 28-electron core of yttrium is replaced by effective core potentials and the valence electrons are described by a [6.5.3] contraction of a (8.7.6) basis set.

Table S2. Total Energies and Thermochemistry

Mol.	**Energy**	***VZPE***	***TE***	***S***	ν_1	ν_2	μ
1	-297.730369	284.88	308.65	234.76	16	23	6.967
2	-315.795773	370.55	399.62	271.21	25	26	7.365
3	-333.848069	455.78	490.20	309.81	22	26	8.748
4a	-360.642876	446.62	479.67	308.26	7	16	5.767
4b	-360.638254	446.83	479.25	297.83	-8	18	8.061

Cartesian Coordinates of B3LYP/SDD optimized structures of model complexes **M1** – **M4**.

$(L1)YCl_2(DMSO)_2$, **M1**

```
Stoichiometry    C22H27Cl2N2O3S2Y
Framework group  C1[X(C22H27Cl2N2O3S2Y)]
Deg. of freedom   171
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        4.832638   -0.261432   -0.238518
     2          6           0        3.441250   -0.352738   -0.145978
     3          6           0        2.870063   -1.676684   -0.086940
     4          6           0        3.686737   -2.856968   -0.117536
     5          6           0        5.091479   -2.705997   -0.211741
     6          6           0        5.631769   -1.426045   -0.269315
     7          6           0        3.002698   -4.102746   -0.050834
     8          6           0        1.623043   -4.141412    0.029878
     9          6           0        0.893006   -2.925445    0.051288
    10          6           0       -0.564775   -2.888326    0.102269
    11          1           0        5.293024    0.718948   -0.275988
    12          1           0        5.728949   -3.583102   -0.234554
    13          1           0        6.709287   -1.310798   -0.337674
    14          1           0        3.576608   -5.023739   -0.065742
    15          7           0        1.518031   -1.741204   -0.003447
    16          8           0        2.602405    0.685319   -0.110818
    17          1           0       -1.090598   -3.845655    0.065847
    18          1           0        1.093760   -5.086595    0.079125
    19          7           0       -1.215470   -1.771365    0.164472
    20          6           0       -2.659591   -1.801643    0.081528
    21          6           0       -3.423993   -1.539140    1.239986
    22          6           0       -3.269535   -2.053074   -1.170216
    23          6           0       -4.823177   -1.521825    1.118805
    24          6           0       -4.672861   -2.014305   -1.242144
    25          6           0       -5.448287   -1.750896   -0.110363
    26          1           0       -5.420369   -1.337519    2.006969
    27          1           0       -5.151982   -2.202431   -2.198392
    28          1           0       -6.531248   -1.736610   -0.182945
    29          6           0       -2.458711   -2.329884   -2.420413
    30          1           0       -1.682433   -1.573056   -2.575201
    31          1           0       -1.961650   -3.307290   -2.383293
    32          1           0       -3.113026   -2.334327   -3.297351
    33          6           0       -2.770136   -1.292201    2.577065
    34          1           0       -2.099583   -2.108592    2.866187
    35          1           0       -2.156372   -0.387137    2.561924
    36          1           0       -3.529003   -1.184404    3.358131
    37         39           0        0.349297    0.440208    0.264635
    38         17           0       -0.119870    0.657677   -2.422044
    39         17           0        0.662307    0.009743    2.849991
    40          8           0        0.676514    2.742913    0.365447
    41          8           0       -1.792990    1.282855    0.512619
    42         16           0        2.254999    3.459170    0.276962
    43         16           0       -2.484676    2.618523   -0.329098
    44          6           0        1.711773    5.268936    0.429322
    45          1           0        0.934162    5.450553   -0.311568
    46          1           0        1.315510    5.372468    1.438069
    47          1           0        2.582877    5.909175    0.280429
    48          6           0        2.603837    3.398667   -1.592994
    49          1           0        1.700856    3.728967   -2.104691
    50          1           0        3.466661    4.035581   -1.795839
    51          1           0        2.802286    2.348352   -1.791620
    52          6           0       -3.495648    1.732480   -1.678345
    53          1           0       -4.055900    0.930603   -1.198977
    54          1           0       -4.138177    2.475559   -2.154076
    55          1           0       -2.744375    1.338426   -2.362372
    56          6           0       -3.871388    3.011888    0.905880
    57          1           0       -4.388593    2.076633    1.116312
    58          1           0       -3.368859    3.384162    1.796873
    59          1           0       -4.527493    3.766532    0.469473
---------------------------------------------------------------------
Rotational constants (GHZ):      0.1314553      0.0958464      0.0689584
Standard basis: SDDAll (5D, 10F)
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(L1)YCl(CH_2SiMe_3)$(DMSO)_2$, **M2**

```
 Stoichiometry    C26H38ClN2O3S2SiY
 Framework group  C1[X(C26H38ClN2O3S2SiY)]
 Deg. of freedom   216
 Full point group                 C1      NOp   1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        4.488360    0.649048   -1.241258
      2          6           0        3.153930    0.346684   -0.952516
      3          6           0        2.697899   -0.987951   -1.259822
      4          6           0        3.568456   -1.966940   -1.847667
      5          6           0        4.910265   -1.606279   -2.120392
      6          6           0        5.341076   -0.320153   -1.813717
      7          6           0        2.998136   -3.242479   -2.117067
      8          6           0        1.669391   -3.489288   -1.829545
      9          6           0        0.877708   -2.462605   -1.251493
     10          6           0       -0.544139   -2.643605   -0.987082
     11          1           0        4.863893    1.637756   -1.004255
     12          1           0        5.585503   -2.331605   -2.561057
     13          1           0        6.371461   -0.045591   -2.018467
     14          1           0        3.617560   -4.017732   -2.556495
     15          7           0        1.398590   -1.259048   -0.971734
     16          8           0        2.273509    1.196723   -0.422618
     17          1           0       -0.983938   -3.595914   -1.292687
     18          1           0        1.223762   -4.455372   -2.039312
     19          7           0       -1.272843   -1.715030   -0.453493
     20          6           0       -2.703078   -1.919560   -0.398956
     21          6           0       -3.338384   -2.016437    0.859477
     22          6           0       -3.445070   -1.980252   -1.605625
     23          6           0       -4.732342   -2.178451    0.893378
     24          6           0       -4.840251   -2.129688   -1.518327
     25          6           0       -5.484193   -2.231686   -0.283508
     26          1           0       -5.223125   -2.273099    1.857492
     27          1           0       -5.418208   -2.168920   -2.436782
     28          1           0       -6.561096   -2.359317   -0.238513
     29          6           0       -2.797465   -1.844520   -2.970618
     30          1           0       -2.091315   -1.008449   -3.001699
     31          1           0       -2.256552   -2.751192   -3.268259
     32          1           0       -3.565878   -1.668028   -3.729424
     33          6           0       -2.552212   -1.950363    2.144518
     34          1           0       -1.707574   -2.646221    2.148833
     35          1           0       -2.141036   -0.947007    2.288666
     36          1           0       -3.193842   -2.187634    2.998708
     37         39           0        0.129005    0.587224    0.151701
     38         17           0       -0.844967    1.332378   -2.405151
     39          8           0        0.223309    2.888411    0.583808
     40          8           0       -2.029218    1.130379    0.867093
     41         16           0        1.594271    3.883181    0.204812
     42         16           0       -2.943672    2.480962    0.301338
     43          6           0        0.762994    5.557960    0.519376
     44          1           0       -0.141630    5.602855   -0.086023
     45          1           0        0.518297    5.570490    1.579998
     46          1           0        1.468339    6.351669    0.267471
     47          6           0        1.618421    3.931034   -1.702811
```

48	1	0	0.594088	3.773331	-2.040735
49	1	0	2.033773	4.895042	-2.002249
50	1	0	2.242592	3.093357	-1.998856
51	6	0	-4.116091	1.653502	-0.949664
52	1	0	-4.505527	0.747177	-0.487967
53	1	0	-4.897812	2.373333	-1.199275
54	1	0	-3.477535	1.427624	-1.802833
55	6	0	-4.122233	2.640019	1.780851
56	1	0	-4.550514	1.655578	1.964359
57	1	0	-3.499034	2.951958	2.617099
58	1	0	-4.881027	3.388245	1.546250
59	6	0	0.702363	-0.073878	2.442799
60	1	0	-0.272328	-0.188833	2.950964
61	1	0	1.087455	0.921866	2.747139
62	6	0	1.873236	-1.462617	5.069236
63	1	0	2.581586	-2.212791	5.444347
64	1	0	2.138926	-0.491225	5.504726
65	1	0	0.870716	-1.727778	5.428908
66	6	0	3.723252	-0.977567	2.644539
67	1	0	3.868879	-1.030338	1.559997
68	1	0	4.000110	0.033366	2.969186
69	1	0	4.411030	-1.688959	3.118640
70	6	0	1.509775	-3.163853	2.537972
71	1	0	1.651299	-3.264975	1.455517
72	1	0	2.173424	-3.881342	3.036769
73	1	0	0.474711	-3.440346	2.776070
74	14	0	1.898170	-1.364674	3.133890

Rotational constants (GHZ): 0.0989038 0.0763637 0.0647475
Standard basis: SDDAll (5D, 10F)

(L1)Y(CH_2SiMe_3)$_2$(DMSO)$_2$, **M3**

Stoichiometry C30H49N2O3S2Si2Y
Framework group C1[X(C30H49N2O3S2Si2Y)]
Deg. of freedom 261
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.418885	-0.971993	-0.505383
2	6	0	-3.071985	-0.595059	-0.453262
3	6	0	-2.566474	0.203108	-1.543534
4	6	0	-3.404902	0.598223	-2.638616
5	6	0	-4.760252	0.192553	-2.638786
6	6	0	-5.238913	-0.577758	-1.583419
7	6	0	-2.791329	1.379838	-3.662009
8	6	0	-1.455726	1.714827	-3.577794
9	6	0	-0.692437	1.282339	-2.459317
10	6	0	0.723110	1.567959	-2.332854
11	1	0	-4.828476	-1.567144	0.302891
12	1	0	-5.410414	0.484091	-3.456612
13	1	0	-6.279635	-0.887569	-1.583896
14	1	0	-3.387317	1.704488	-4.508856
15	7	0	-1.253138	0.553976	-1.476137
16	8	0	-2.225356	-0.923339	0.527552
17	1	0	1.200604	2.096680	-3.160951
18	1	0	-0.979143	2.305137	-4.352928
19	7	0	1.412696	1.191334	-1.293809
20	6	0	2.846084	1.369488	-1.324460
21	6	0	3.455029	2.282084	-0.431997
22	6	0	3.626673	0.597885	-2.221277
23	6	0	4.854315	2.392761	-0.437221
24	6	0	5.025576	0.729880	-2.177508
25	6	0	5.641538	1.617827	-1.294128
26	1	0	5.322828	3.107023	0.233747
27	1	0	5.627921	0.132300	-2.855518
28	1	0	6.722370	1.716968	-1.283562
29	6	0	3.008838	-0.363483	-3.216963
30	1	0	2.153302	-0.894430	-2.795265
31	1	0	2.660133	0.153001	-4.120536
32	1	0	3.748560	-1.104178	-3.535309
33	6	0	2.636046	3.132506	0.505921
34	1	0	1.814946	3.639564	-0.009505
35	1	0	2.186877	2.515238	1.288893
36	1	0	3.264850	3.893124	0.979346
37	39	0	-0.042924	-0.144241	0.563463
38	8	0	-0.310831	-1.245038	2.660436
39	8	0	2.080098	0.041788	1.592882
40	16	0	-1.902533	-1.445612	3.318966
41	16	0	2.925212	-1.248982	2.360255
42	6	0	-1.405130	-1.907720	5.090555
43	1	0	-0.650901	-2.691867	5.032234
44	1	0	-0.988499	-1.001837	5.527815
45	1	0	-2.296403	-2.230555	5.631345
46	6	0	-2.374240	-3.168777	2.678000
47	1	0	-1.537140	-3.835491	2.882815
48	1	0	-3.291927	-3.481066	3.179597
49	1	0	-2.516603	-3.016050	1.611274
50	6	0	4.324487	-1.571403	1.107973

51	1	0	4.673081	-0.601672	0.753960
52	1	0	5.103692	-2.147791	1.609648
53	1	0	3.860278	-2.138594	0.303186
54	6	0	3.888404	-0.231744	3.641352
55	1	0	4.381048	0.578607	3.105552
56	1	0	3.136212	0.158536	4.324443
57	1	0	4.595040	-0.886241	4.153834
58	6	0	-0.736570	2.025825	1.693555
59	1	0	0.246660	2.399095	2.028444
60	1	0	-1.187196	1.496189	2.556943
61	6	0	-1.883451	4.866623	2.609852
62	1	0	-2.549567	5.691921	2.325413
63	1	0	-2.229830	4.460642	3.568793
64	1	0	-0.876782	5.276220	2.763548
65	6	0	-3.695385	2.916181	1.061654
66	1	0	-3.818295	2.208478	0.234695
67	1	0	-4.043953	2.422230	1.977725
68	1	0	-4.344636	3.780715	0.874222
69	6	0	-1.348607	4.379111	-0.374490
70	1	0	-1.439472	3.711952	-1.238691
71	1	0	-1.992296	5.251228	-0.544555
72	1	0	-0.310621	4.731534	-0.321541
73	14	0	-1.859000	3.476089	1.256000
74	6	0	0.966051	-2.256215	-0.496445
75	1	0	1.943419	-1.923171	-0.884787
76	1	0	1.140868	-2.764986	0.474547
77	6	0	1.339949	-4.967626	-2.169908
78	1	0	0.843905	-5.660055	-2.862604
79	1	0	2.253116	-4.597051	-2.653461
80	1	0	1.637421	-5.530877	-1.276140
81	6	0	-1.397305	-4.303393	-0.916562
82	1	0	-1.152263	-4.805639	0.028607
83	1	0	-2.163950	-3.545673	-0.721298
84	1	0	-1.816774	-5.052677	-1.599124
85	6	0	-0.361409	-2.697107	-3.361465
86	1	0	-1.125540	-1.927682	-3.205058
87	1	0	0.489072	-2.233635	-3.876637
88	1	0	-0.778490	-3.463865	-4.026184
89	14	0	0.175735	-3.491172	-1.685230

Rotational constants (GHZ): 0.0781019 0.0634393 0.0619560

Standard basis: SDDAll (5D, 10F)

(L1)Y(OCH_2Ph)(CH_2SiMe_3)$(DMSO)_2$, **M4a**

```
Stoichiometry    C33H45N2O4S2SiY
Framework group  C1[X(C33H45N2O4S2SiY)]
Deg. of freedom   258
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.320859   -4.715741   -0.299497
     2          6           0        0.446068   -3.320586   -0.360994
     3          6           0        1.261158   -2.782656   -1.429208
     4          6           0        1.914171   -3.636533   -2.383761
     5          6           0        1.750273   -5.037121   -2.270725
     6          6           0        0.964397   -5.545333   -1.240492
     7          6           0        2.690696   -2.990074   -3.387597
     8          6           0        2.788799   -1.612877   -3.417330
     9          6           0        2.105885   -0.843597   -2.438150
    10          6           0        2.163987    0.613039   -2.421200
    11          1           0       -0.283333   -5.150726    0.488490
    12          1           0        2.235733   -5.697266   -2.981397
    13          1           0        0.839241   -6.620641   -1.153345
    14          1           0        3.205373   -3.593481   -4.128631
    15          7           0        1.374681   -1.431359   -1.479373
    16          8           0       -0.123325   -2.470187    0.487498
    17          1           0        2.807053    1.093899   -3.163548
    18          1           0        3.377614   -1.111977   -4.178279
    19          7           0        1.486688    1.313514   -1.569258
    20          6           0        1.624462    2.747937   -1.556985
    21          6           0        0.535355    3.533844   -1.997047
    22          6           0        2.810398    3.338916   -1.062176
    23          6           0        0.647232    4.930122   -1.910921
    24          6           0        2.872312    4.740940   -0.985752
    25          6           0        1.801278    5.535064   -1.403228
    26          1           0       -0.181159    5.542279   -2.255383
    27          1           0        3.775287    5.204836   -0.599645
    28          1           0        1.869623    6.616799   -1.344205
    29          6           0        3.992662    2.506950   -0.607215
    30          1           0        3.678020    1.649644   -0.006192
    31          1           0        4.569272    2.115112   -1.454902
    32          1           0        4.675293    3.115400   -0.006654
    33          6           0       -0.700568    2.894696   -2.582467
    34          1           0       -0.492073    2.467541   -3.573161
    35          1           0       -1.072590    2.076825   -1.957984
    36          1           0       -1.494578    3.638010   -2.702525
    37         39           0       -0.034993   -0.146062    0.172459
    38          8           0       -1.626292   -0.431674    1.928769
    39          8           0       -0.656390    2.085920    0.737907
    40         16           0       -2.577902   -1.881082    1.877457
    41         16           0       -0.656241    2.698561    2.350430
    42          6           0       -4.056942   -1.291830    2.907850
    43          1           0       -3.665204   -0.788296    3.791342
    44          1           0       -4.602611   -0.600687    2.267346
    45          1           0       -4.670667   -2.157862    3.162201
    46          6           0       -1.688197   -2.933464    3.182492
    47          1           0       -1.558775   -2.314224    4.069653
    48          1           0       -2.287503   -3.824895    3.376458
    49          1           0       -0.735073   -3.169584    2.714869
    50          6           0        0.839283    3.877061    2.316607
```

51	1	0	0.825655	4.395148	1.358184
52	1	0	0.757714	4.554338	3.168639
53	1	0	1.710373	3.230385	2.401803
54	6	0	-2.046269	3.977417	2.161293
55	1	0	-1.825040	4.564610	1.270791
56	1	0	-2.957263	3.398179	2.023333
57	1	0	-2.093744	4.586574	3.065351
58	6	0	1.821243	0.269705	1.906490
59	1	0	2.275863	1.237035	1.624049
60	1	0	1.152736	0.450583	2.773887
61	6	0	4.356647	-0.235930	3.824728
62	1	0	5.121841	-0.971485	4.106198
63	1	0	4.867321	0.671101	3.475671
64	1	0	3.785005	0.025570	4.724414
65	6	0	2.423173	-2.548139	3.181359
66	1	0	1.790807	-2.316218	4.048753
67	1	0	1.807366	-3.057410	2.432339
68	1	0	3.215360	-3.231765	3.510747
69	6	0	4.339572	-1.428630	0.991197
70	1	0	3.779677	-1.941780	0.201448
71	1	0	4.818469	-0.544692	0.550138
72	1	0	5.132912	-2.099869	1.342986
73	14	0	3.173387	-0.927926	2.448317
74	8	0	-1.558956	-0.157717	-1.310539
75	6	0	-2.597586	-0.432318	-2.229859
76	1	0	-2.464206	0.176726	-3.144156
77	1	0	-2.565898	-1.487882	-2.550040
78	6	0	-3.990183	-0.144586	-1.673220
79	6	0	-4.166267	0.746050	-0.602100
80	6	0	-5.125128	-0.744894	-2.244871
81	6	0	-5.451473	1.035278	-0.122199
82	1	0	-3.284137	1.190857	-0.154600
83	6	0	-6.409246	-0.458895	-1.765960
84	1	0	-5.001286	-1.444685	-3.068137
85	6	0	-6.578258	0.435974	-0.701135
86	1	0	-5.576295	1.737303	0.698873
87	1	0	-7.274190	-0.933491	-2.219557
88	1	0	-7.572997	0.663305	-0.330379

Rotational constants (GHZ): 0.0690460 0.0649690 0.0519809

(L1)Y(OCH_2Ph)(CH_2SiMe_3)$(DMSO)_2$, **M4b**

```
Stoichiometry    C33H45N2O4S2SiY
Framework group  C1[X(C33H45N2O4S2SiY)]
Deg. of freedom   258
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
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     2          6           0        3.107736    0.124313   -0.172235
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     4          6           0        3.447398   -0.308655   -2.627283
     5          6           0        4.842005   -0.142594   -2.451629
     6          6           0        5.334981    0.144517   -1.183071
     7          6           0        2.815592   -0.592189   -3.871346
     8          6           0        1.442565   -0.720391   -3.943947
     9          6           0        0.665550   -0.580516   -2.764055
    10          6           0       -0.788605   -0.663550   -2.781008
    11          1           0        4.917382    0.501000    0.915693
    12          1           0        5.508850   -0.242451   -3.301145
    13          1           0        6.405393    0.267325   -1.047422
    14          1           0        3.425590   -0.702244   -4.762196
    15          7           0        1.239352   -0.327654   -1.577802
    16          8           0        2.240355    0.244231    0.833041
    17          1           0       -1.270236   -0.760676   -3.757745
    18          1           0        0.950855   -0.930384   -4.887520
    19          7           0       -1.490758   -0.593456   -1.695039
    20          6           0       -2.927109   -0.509420   -1.811207
    21          6           0       -3.725056   -1.623233   -1.470960
    22          6           0       -3.501844    0.714537   -2.227924
    23          6           0       -5.120172   -1.492664   -1.567110
    24          6           0       -4.902149    0.799818   -2.302359
    25          6           0       -5.709812   -0.293750   -1.979537
    26          1           0       -5.742192   -2.348559   -1.322402
    27          1           0       -5.353678    1.735052   -2.620384
    28          1           0       -6.789819   -0.214487   -2.053126
    29          6           0       -2.645250    1.923000   -2.548175
    30          1           0       -1.875446    2.073681   -1.783466
    31          1           0       -2.131204    1.823804   -3.512598
    32          1           0       -3.266483    2.821951   -2.606657
    33          6           0       -3.103377   -2.920385   -1.016457
    34          1           0       -2.404350   -3.321916   -1.758198
    35          1           0       -2.537842   -2.773364   -0.091657
    36          1           0       -3.876325   -3.673716   -0.836781
    37         39           0       -0.043041   -0.254892    0.589470
    38          8           0        0.279518    0.013787    2.953461
    39          8           0       -2.176093   -0.764666    1.509935
    40         16           0        1.864963   -0.133992    3.634747
    41         16           0       -2.890122    0.451600    2.513452
    42          6           0        1.367884   -0.217584    5.464056
    43          1           0        0.680345    0.604532    5.660498
    44          1           0        0.868169   -1.176608    5.590886
    45          1           0        2.269121   -0.159400    6.076822
    46          6           0        2.475751    1.664511    3.570343
    47          1           0        1.681620    2.293290    3.972238
    48          1           0        3.400631    1.737119    4.145415
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    50          6           0       -4.145567    1.235521    1.322475
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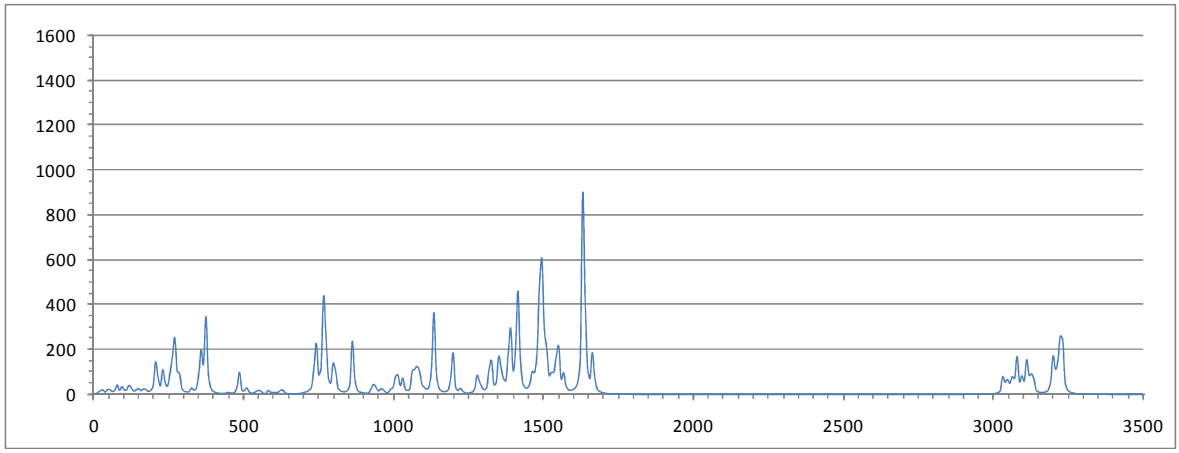
51	1	0	-4.670376	0.429011	0.812031
52	1	0	-4.813034	1.878070	1.899325
53	1	0	-3.539776	1.803595	0.621209
54	6	0	-4.058144	-0.665599	3.505394
55	1	0	-4.621759	-1.266163	2.792417
56	1	0	-3.409329	-1.297576	4.109107
57	1	0	-4.701952	-0.042210	4.127941
58	6	0	0.297749	-2.751097	0.926076
59	1	0	-0.745541	-3.081114	1.080434
60	1	0	0.735087	-2.636296	1.939199
61	6	0	1.027094	-5.872782	0.792665
62	1	0	1.611136	-6.626316	0.247505
63	1	0	1.345886	-5.884032	1.842669
64	1	0	-0.029547	-6.168177	0.760460
65	6	0	3.166565	-3.774128	0.094199
66	1	0	3.434517	-2.849621	-0.429066
67	1	0	3.506602	-3.679801	1.133614
68	1	0	3.715644	-4.603608	-0.369127
69	6	0	0.771432	-4.296580	-1.825012
70	1	0	0.987515	-3.381382	-2.387688
71	1	0	1.329001	-5.122182	-2.284922
72	1	0	-0.299429	-4.515286	-1.924277
73	14	0	1.263629	-4.100272	0.036015
74	8	0	-0.745098	1.793169	0.490623
75	6	0	-0.927128	3.180688	0.723766
76	1	0	-0.860317	3.383118	1.810827
77	1	0	-1.938414	3.503766	0.411085
78	6	0	0.077578	4.084734	0.015287
79	6	0	-0.261716	5.415332	-0.284060
80	6	0	1.361869	3.627108	-0.314801
81	6	0	0.661648	6.273303	-0.892726
82	1	0	-1.258462	5.780078	-0.044846
83	6	0	2.287509	4.482307	-0.926697
84	1	0	1.622702	2.598436	-0.096195
85	6	0	1.942673	5.808414	-1.216352
86	1	0	0.380527	7.297177	-1.120699
87	1	0	3.275701	4.109157	-1.179287
88	1	0	2.659508	6.469235	-1.693550

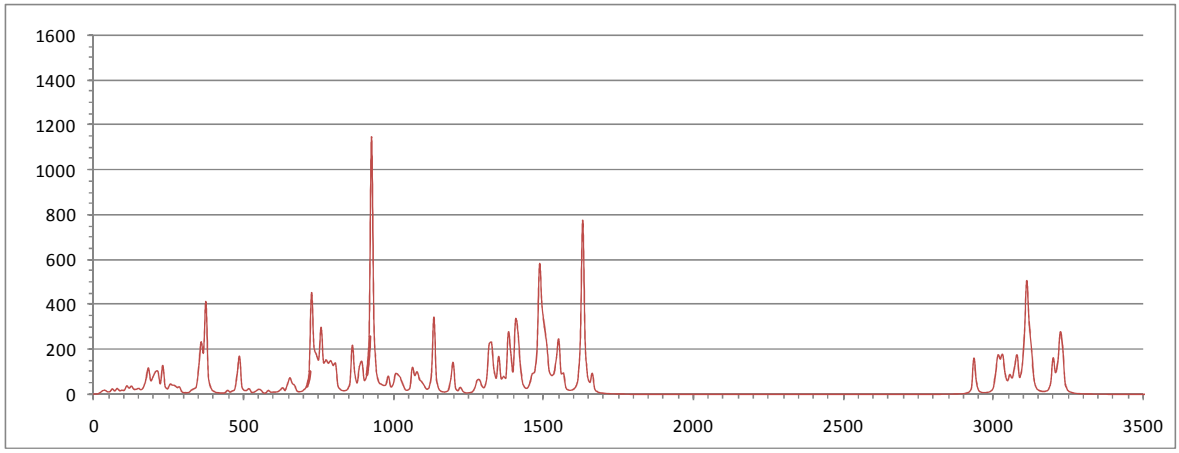
Rotational constants (GHZ): 0.0688364 0.0631497 0.0558143

B3LYP/SDD computed vibrational spectra of **M1** – **M4**

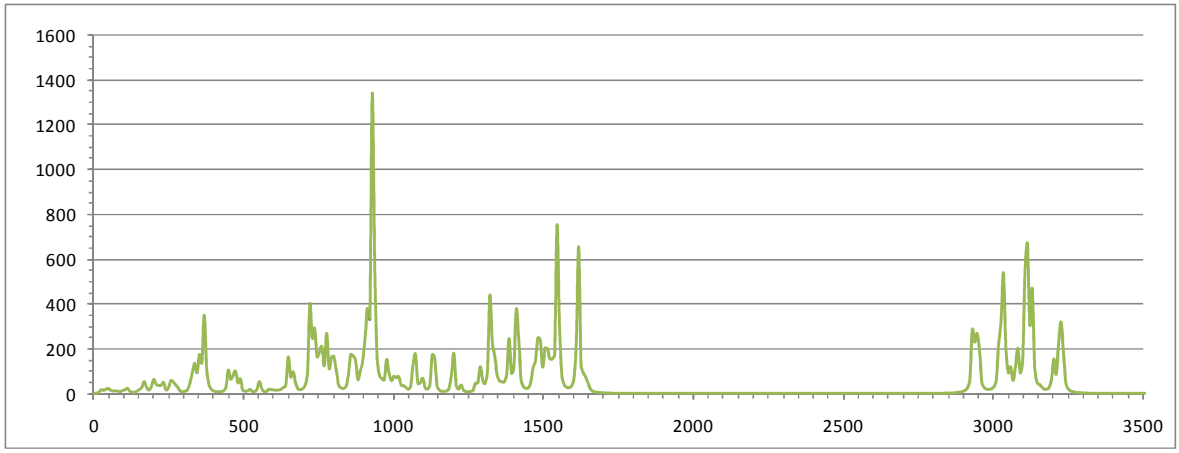
(**L1**)$YCl_2(DMSO)_2$, **M1**



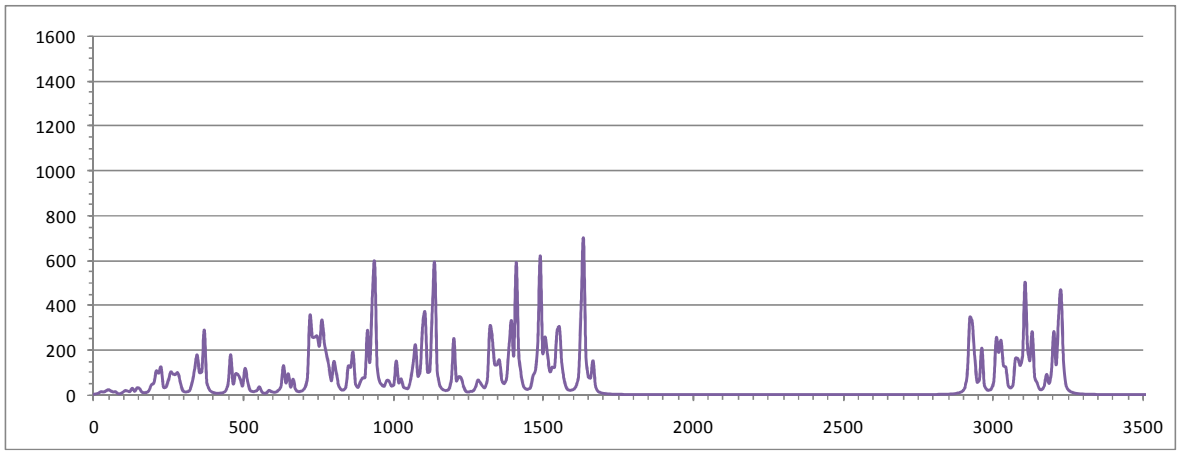
(**L1**)$YCl(CH_2SiMe_3)(DMSO)_2$, **M2**



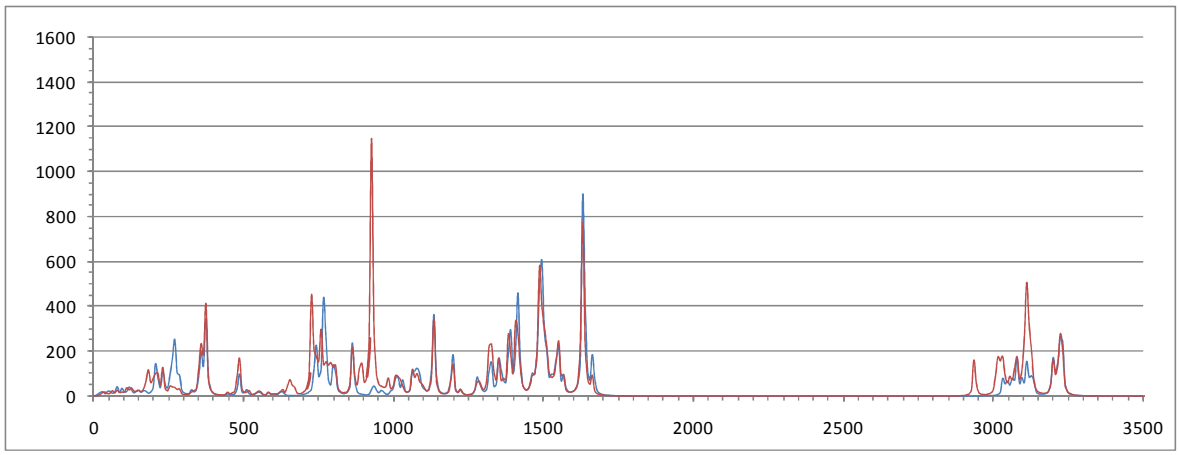
(**L1**)Y(CH_2SiMe_3)$_2$(DMSO)$_2$, **M3**



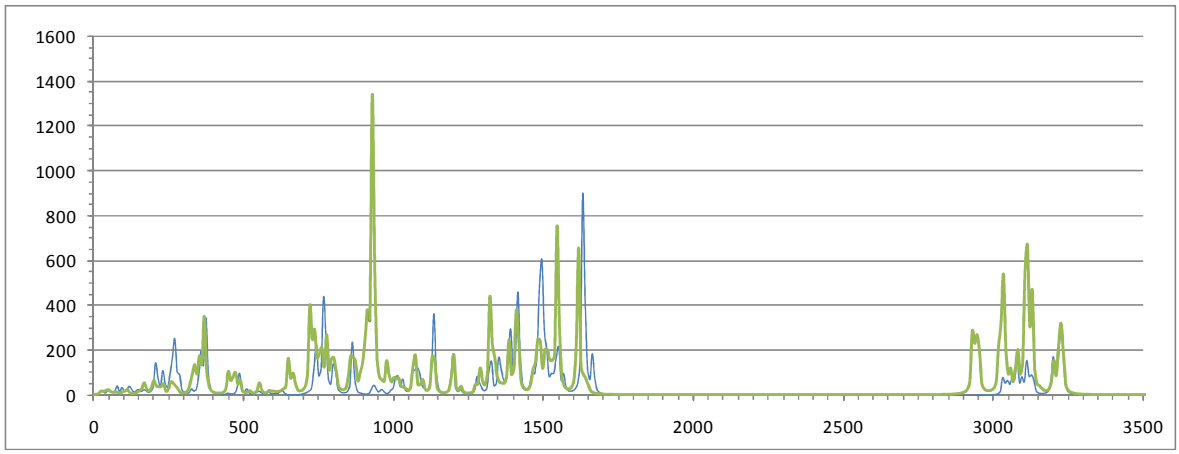
(**L1**)Y(OCH_2Ph)(CH_2SiMe_3)(DMSO)$_2$, **M4a**



Overlay of M1 and M2



Overlay of M1 and M3



Overlay of M3 and M4a