Supporting information

Bis(oxazoline)-Derived N-Heterocyclic Carbene Rare-Earth Metal Alkyls: Synthesis, Structure, and Polymerization Performance

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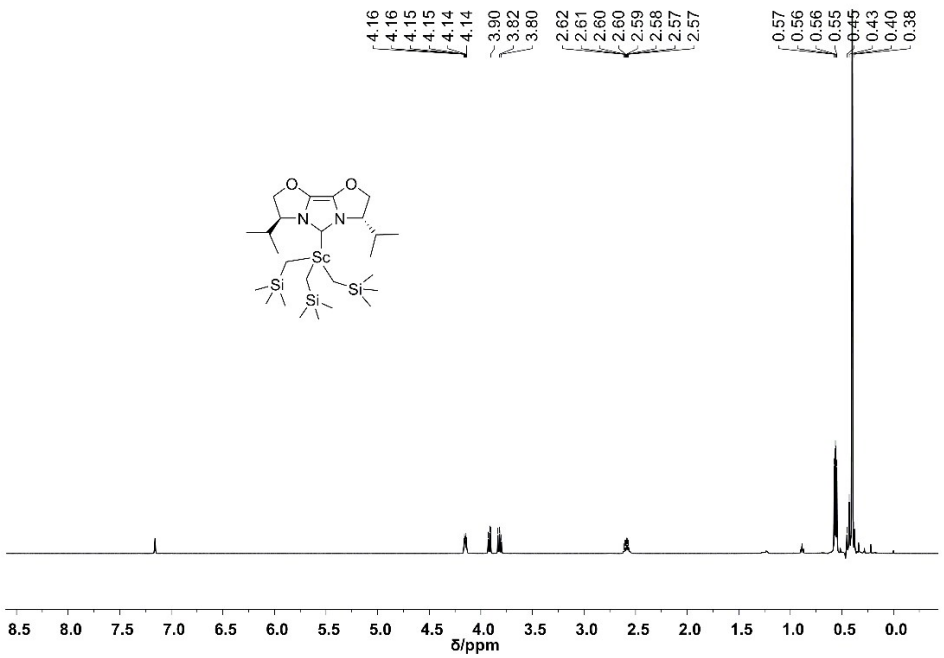

Fig. S1. ^{1}H NMR spectrum (500 MHz, C_6D_6, 25°C) of (IBiox)Sc(CH_2SiMe_3)$_3$ (**1**).

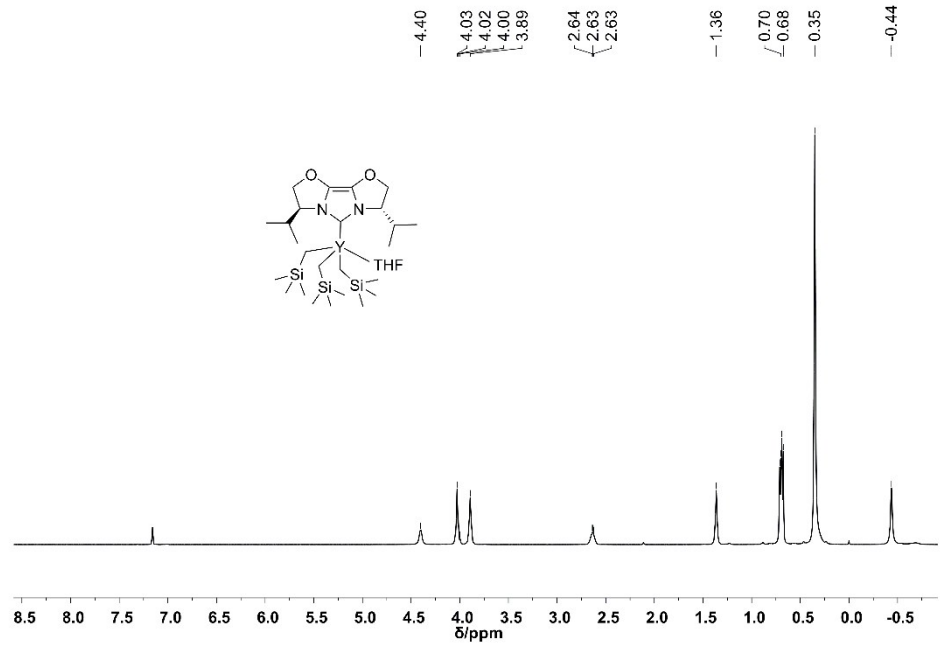

Fig. S2. ^{1}H NMR spectrum (500 MHz, C_6D_6, 25°C) of (IBiox)Y(CH_2SiMe_3)$_3$THF (**2**).

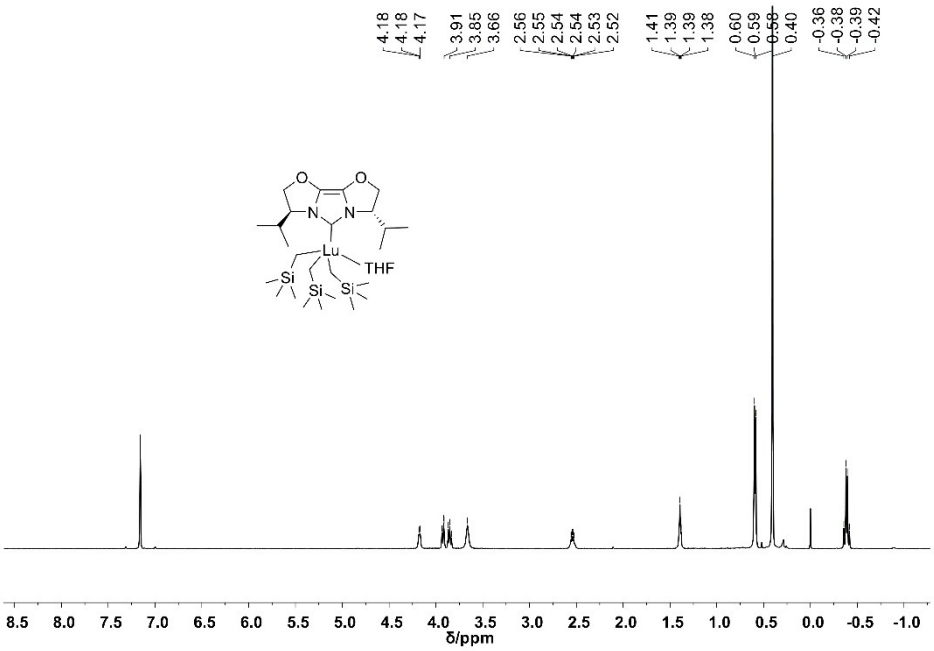

Fig. S3. ^{1}H NMR spectrum (500 MHz, C_6D_6, 25°C) of (IBiox)Lu(CH_2SiMe_3)$_3$THF (**3**).

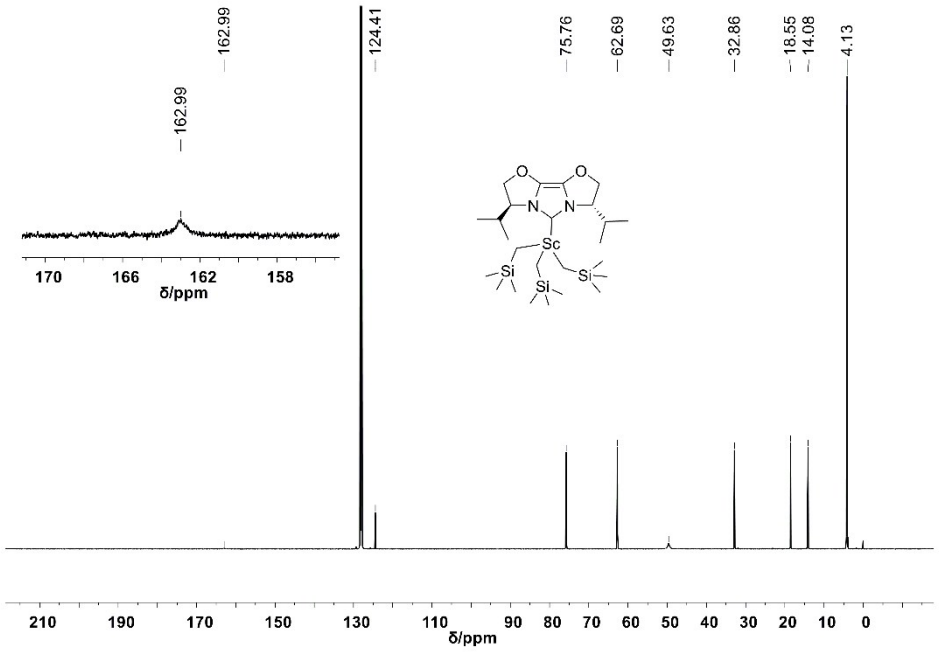

Fig. S4. ^{13}C NMR spectrum (125 MHz, C_6D_6, 25°C) of (IBiox)Sc(CH_2SiMe_3)$_3$ (**1**).

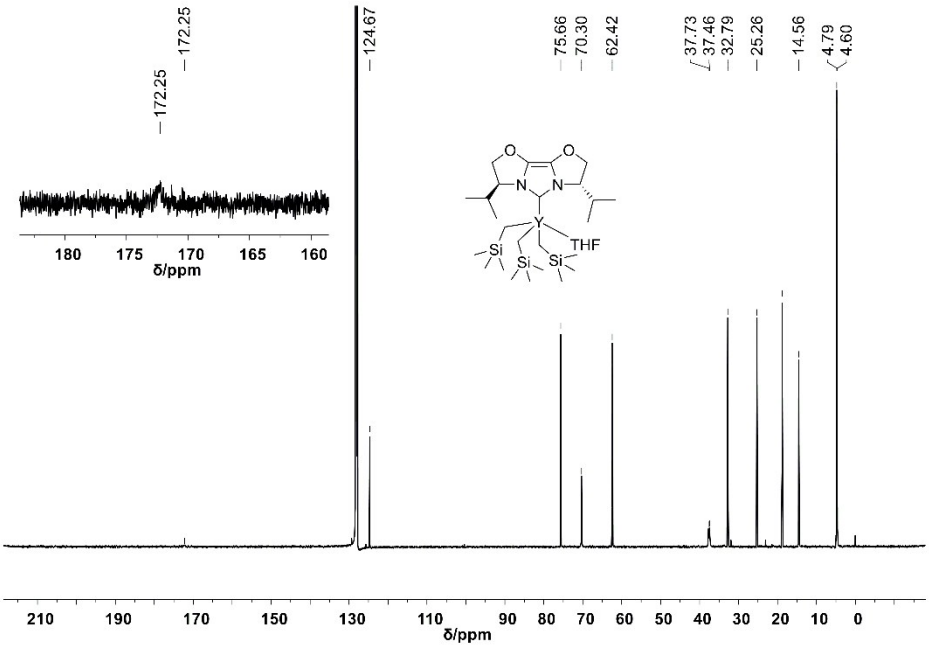

Fig. S5. ^{13}C NMR spectrum (125 MHz, C_6D_6, 25°C) of (IBiox)Y(CH_2SiMe_3)$_3$THF (**2**).

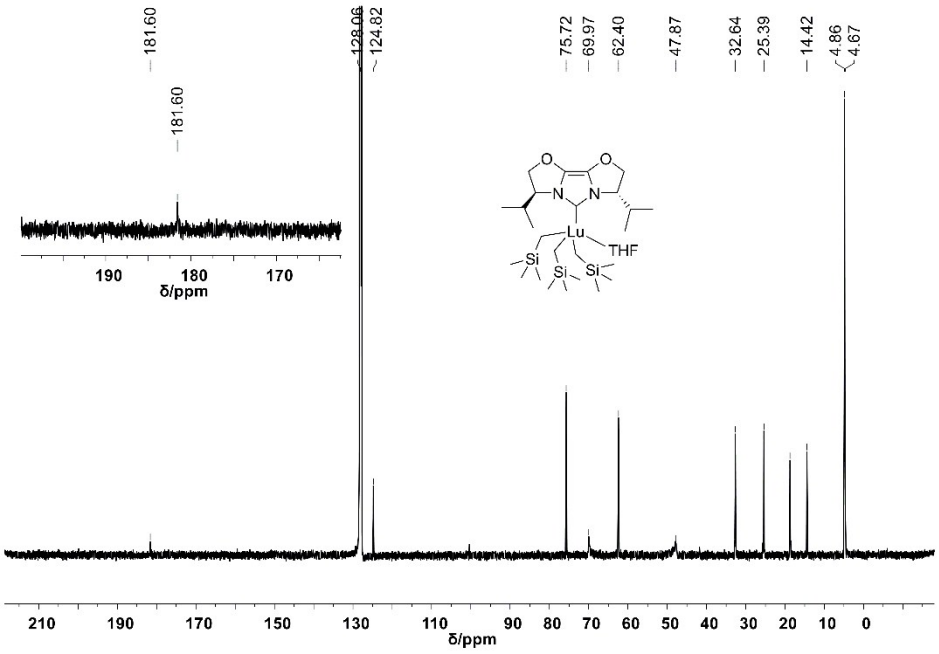

Fig. S6. ^{13}C NMR spectrum (125 MHz, C_6D_6, 25°C) of (IBiox)Lu($CH_2Si\ Me_3$)$_3$ THF (**3**).

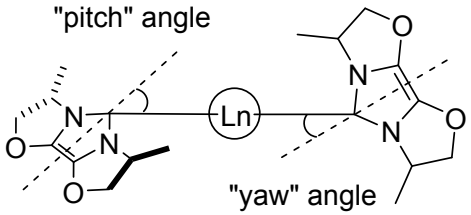

Fig. S7 Distortion angles for the IBiox metal coordination geometry.

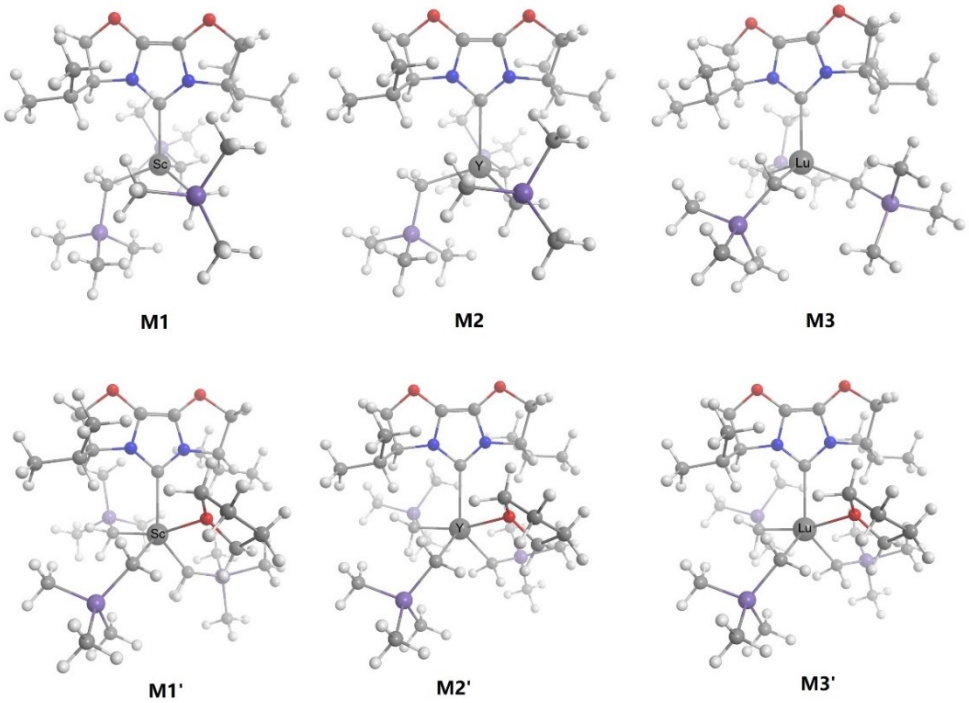

Fig. S8. The model geometry structures of (IBiox)Ln(CH_2SiMe_3)$_3$ (Ln = Sc (**M1**), Y (**M2**), and Lu (**M3**)), and (IBiox)Ln(CH_2SiMe_3)$_3$THF (Ln = Sc (**M1'**), Y (**M2'**), and Lu (**M3'**)).

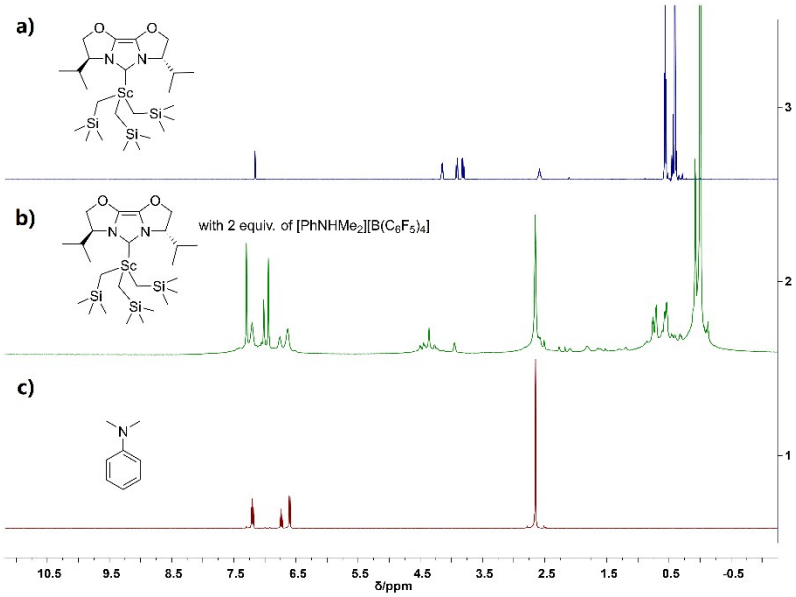

Fig. S9. ^{1}H NMR spectra (500 MHz, 25 °C) of a) **1** in C_6D_6; b) **1**/2[$PhNHMe_2$][$B(C_6F_5)_4$] in C_6D_5Br; c) $PhNMe_2$ in C_6D_5Br.

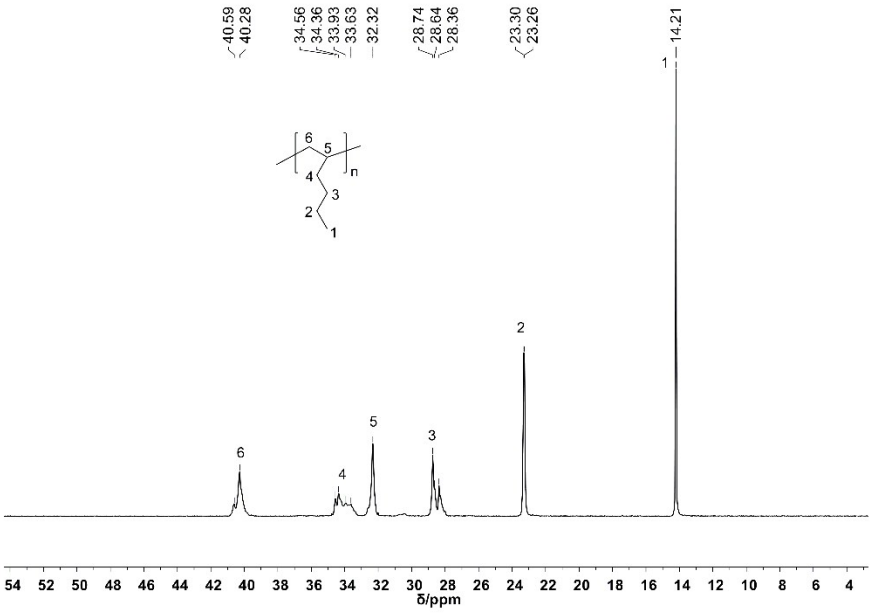

Fig. S10. ^{13}C NMR spectrum (125 MHz, $CDCl_3$, 25°C) of poly(1-hexene) (Table 2, entry 5).

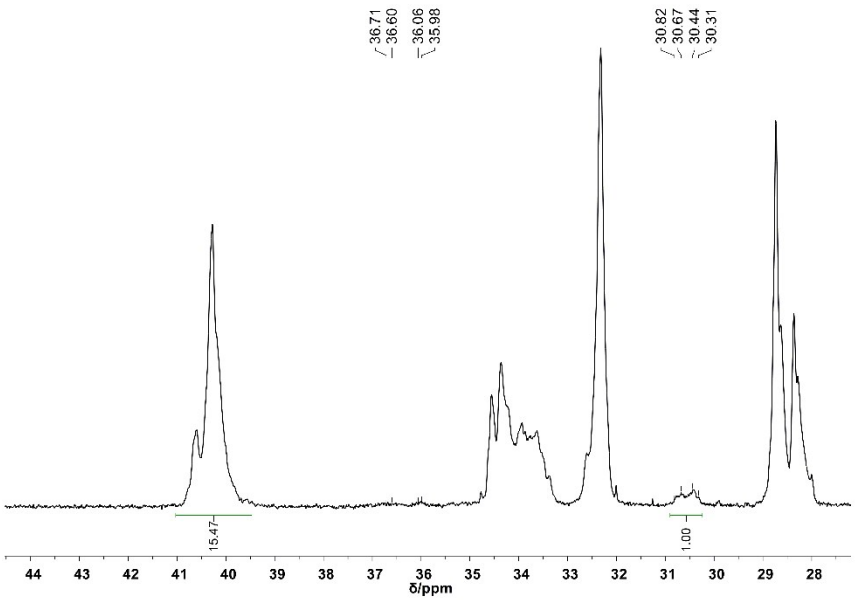

Fig. S11. ^{13}C NMR spectrum (125 MHz, $CDCl_3$, 25°C) of poly(1-hexene) (Table 2, entry 5) at the range of δ = 27 – 44 ppm.

The steric properties of complex **1** and (^{i}Pr-trisox)Sc(CH_2SiMe_3)$_3$ (^{i}Pr-trisox = trisoxazoline), which was with similar chiral oxazoline groups, were evaluated using the percentage of buried volume (%V_{Bur}) as molecular descriptor.[1] The steric maps of two complexes are shown in Fig. S12. %V_{Bur} of **1** was calculated to be 22.3%, while %V_{Bur} of (^{i}Pr-trisox)Sc(CH_2SiMe_3)$_3$ was calculated to be 40.6%, indicating a relative opener space for **1**.

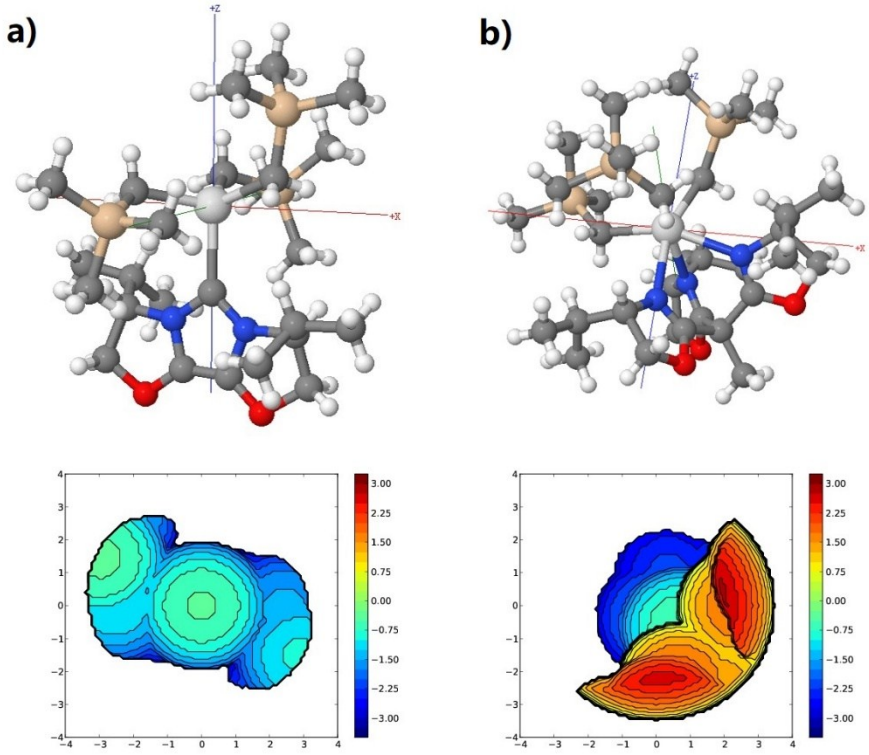

Fig. S12. Steric maps for the two Sc complexes: a) **1**; b) (^{i}Pr-trisox)Sc(CH_2SiMe_3)$_3$. The Sc atom is oriented placing the metal center at the origin of the sphere with the Sc and the center of the carbene ring axis aligned along the z axis at negative z values for **1**, and with the Sc and the vertex carbon axis aligned along the z axis at negative z values for (^{i}Pr-trisox)Sc(CH_2SiMe_3)$_3$.

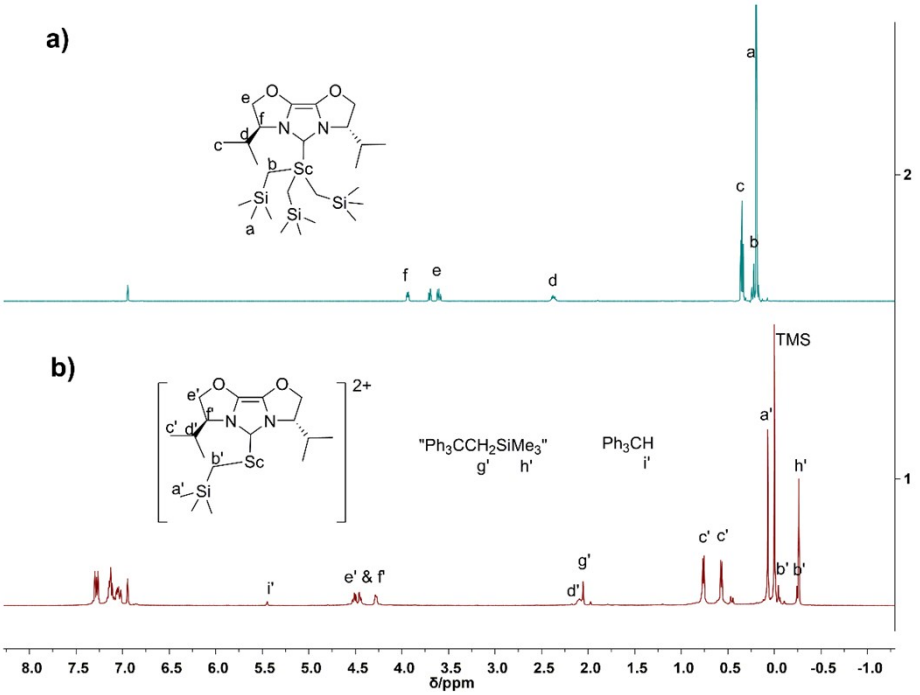

Fig. S13. ^{1}H NMR spectra (500 MHz, 25 °C) of a) **1** in C_6D_6; b) **1**/2[Ph_3C][$B(C_6F_5)_4$] in C_6D_5Br.

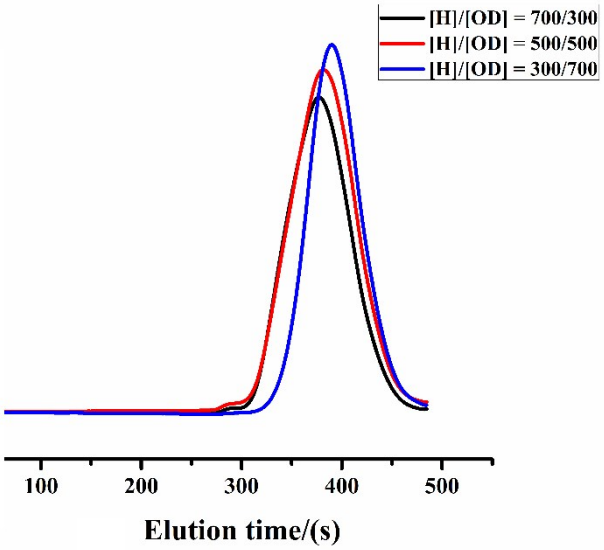

Fig. S14. GPC curves for H/OD copolymers (Table 3, entries 2–4).

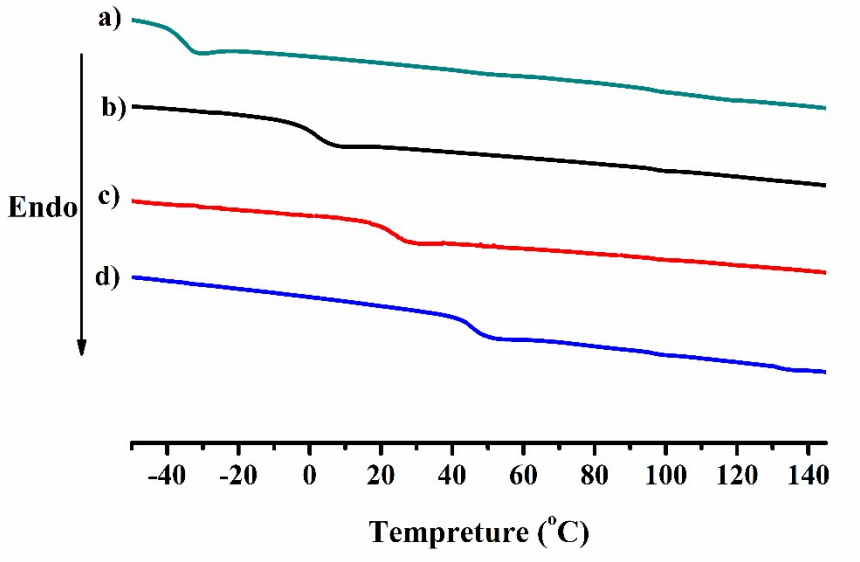

Fig. S15. DSC thermograms for H/OD copolymers: a) [H]/[OD] = 1000/0 (Table 3, entry 1); b) [H]/[OD] = 700/300 (Table 3, entry 2); c) [H]/[OD] = 500/500 (Table 3, entry 3); d) [H]/[OD] = 300/700 (Table 3, entry 4).

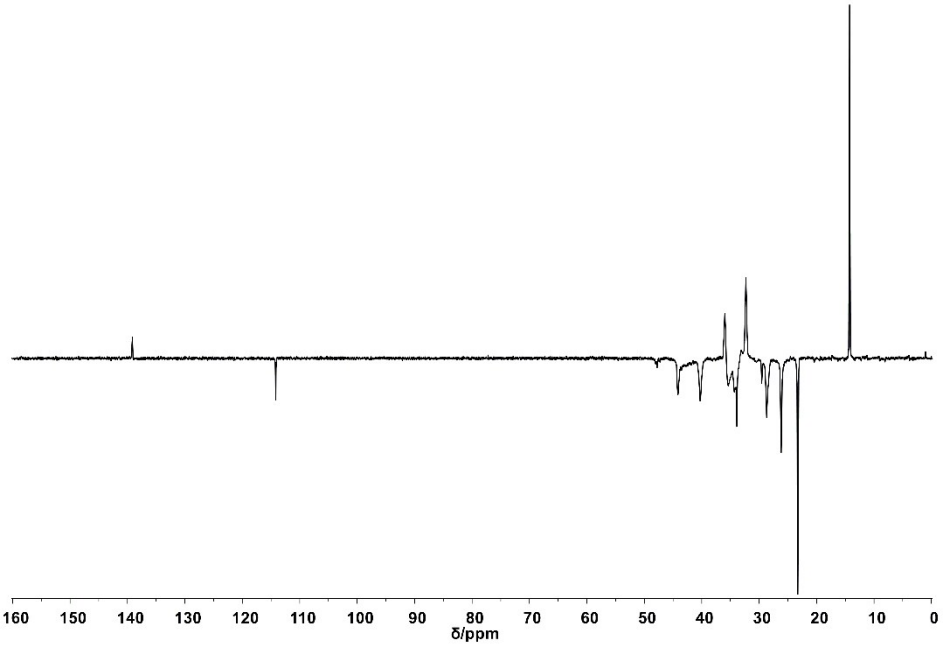

Fig. S16. DEPT 135 spectrum (125 MHz, $CDCl_3$, 25°C) of H/OD copolymer with the feed ratio [H]/[OD] = 700/300 (Table 3, entry 2).

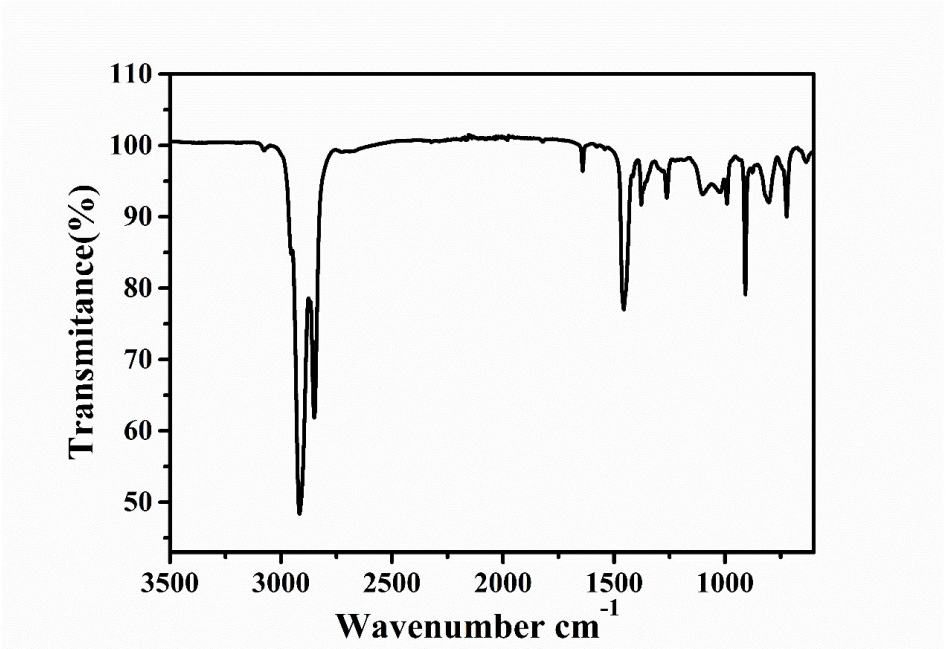

Fig. S17. IR spectrum of H/OD copolymer with the feed ratio [H]/[OD] = 500/500 (Table 3, entry 3).

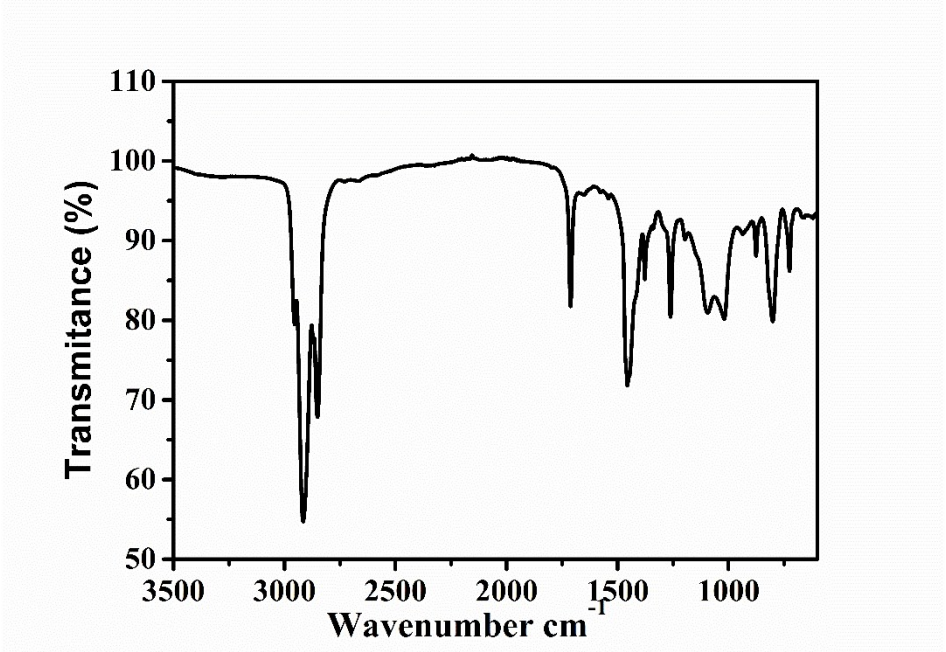

Fig. S18. IR spectrum of functionalized H/OD copolymer modified by light-initiated thiol-ene reaction.

References:

1 (a) L. Falivene, R. Credendino, A. Poater, A. Petta, L. Serra, R. Oliva, V. Scarano and L. Cavallo, *Organometallics*, 2016, **35**, 2286; (*b*) L. Falivene, L. Cavallo and G. Talarico, *ACS Catal.*, 2015, **5**, 6815.

Cartesian coordinates for all of the calculated structures

M1 HF:-2392.8072292

C	0.546794	-4.928453	-0.058157
H	1.217067	-4.705466	-0.896377
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H	-0.104703	-5.760647	-0.353264
C	-0.270353	-3.691283	0.366474
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C	3.372402	1.912644	0.357956
H	2.320374	2.087421	0.625976
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H	4.770690	0.264000	-2.387482
H	5.570042	1.066884	-1.001721
C	3.741220	-1.383329	-0.332527
C	3.109673	-2.508976	0.071600
C	2.095375	-4.317517	1.038486
H	2.260771	-4.287321	2.117709
H	1.954866	-5.343478	0.705699
C	0.954934	-3.346601	0.597164
H	0.339545	-3.078467	1.458448
C	0.035616	-3.864534	-0.537193
H	-0.632205	-3.026411	-0.784272
C	0.803713	-4.259102	-1.811988
H	0.097683	-4.558181	-2.594629
H	1.400844	-3.426479	-2.200155
H	1.478108	-5.105608	-1.635187

C	-0.842521	-5.021655	-0.020862
H	-1.565412	-5.317233	-0.788122
H	-0.242250	-5.907311	0.223538
H	-1.404543	-4.730587	0.873949
C	1.479115	-0.853079	-0.126085
C	-1.646939	2.571681	0.341638
H	-2.173273	2.858929	-0.591342
H	-2.437024	2.242431	1.048835
C	0.293067	5.009965	-0.222404
H	0.722815	5.919810	0.214497
H	1.121382	4.365542	-0.540020
H	-0.280526	5.302843	-1.110942
C	0.263595	3.741717	2.604413
H	0.684374	4.670997	3.009080
H	-0.318854	3.259573	3.397809
H	1.094575	3.074393	2.346045
C	-2.114440	5.454466	1.644254
H	-1.609457	6.338604	2.054363
H	-2.741616	5.776039	0.803344
H	-2.774349	5.046508	2.419802
C	-1.650333	-0.942837	1.766985
H	-2.730471	-0.700696	1.738285
H	-1.573544	-1.998263	1.444610
C	0.822610	-0.374059	3.710901
H	1.125719	-0.344608	4.765124
H	1.427191	-1.136141	3.202720
H	1.058995	0.598320	3.262277
C	-2.016847	0.673018	4.426495
H	-1.607999	0.868855	5.425410
H	-1.955091	1.598115	3.841935
H	-3.077241	0.413424	4.535904
C	-1.353092	-2.344421	4.632730
H	-1.014078	-2.190183	5.665230
H	-2.419657	-2.599631	4.654960
H	-0.809686	-3.206270	4.223090
C	-2.472829	-0.568061	-1.808750
H	-2.462593	0.199903	-2.607791
H	-1.998286	-1.474349	-2.238065
C	-5.137862	0.401701	-0.379500
H	-6.197503	0.163661	-0.223316
H	-4.664607	0.517016	0.602574
H	-5.078292	1.366802	-0.898339
C	-5.363279	-1.218685	-2.994629
H	-6.403336	-1.454133	-2.734343

H	-5.362156	-0.305017	-3.602757
H	-4.970468	-2.036761	-3.611704
C	-4.415713	-2.634067	-0.417152
H	-5.465155	-2.864545	-0.195340
H	-4.000909	-3.468581	-0.997277
H	-3.869086	-2.567573	0.529743
C	-0.180613	2.384713	-2.971010
H	0.155118	3.191642	-2.323123
H	-1.273897	2.384065	-3.024877
C	0.462611	2.350613	-4.356010
H	-0.066238	2.986889	-5.071011
H	1.505363	2.686473	-4.306161
C	0.388755	0.852843	-4.729407
H	1.117267	0.572877	-5.495418
H	-0.610282	0.606934	-5.105189
C	0.652399	0.133308	-3.398931
H	0.052270	-0.768197	-3.268860
H	1.709606	-0.097706	-3.243900
N	2.744367	-0.402983	-0.452170
N	1.756164	-2.165596	0.196954
O	4.993834	-0.912053	-0.654967
O	3.357728	-3.825674	0.380594
O	0.254218	1.104901	-2.328950
Si	-0.838345	4.121921	1.067963
Si	-1.065333	-0.759959	3.557758
Si	-4.280511	-0.986397	-1.407153
Y	-0.886862	0.321895	-0.186270

M2’ HF:-2151.852142

Y	-0.847601	0.319936	-0.624285
Si	-4.391475	0.012340	0.588145
Si	-0.814744	-2.819769	-2.757998
Si	-0.637539	3.999847	-0.016008
O	3.270021	-1.119074	3.369658
O	4.958021	-0.612282	0.348914
N	2.703331	-0.315478	-0.067486
N	1.679152	-0.618769	1.769708
C	-2.561141	0.183738	1.078501
H	-2.315433	-0.645883	1.768893
H	-2.427474	1.125904	1.646192
C	1.424015	-0.304296	0.451100
C	3.691009	-0.612039	0.880619
C	3.037786	-0.809106	2.050793
C	-1.389671	-1.024040	-2.560494

H	-2.497268	-1.002083	-2.573751
H	-1.055811	-0.437433	-3.439130
C	-0.675080	2.626001	-1.328795
H	0.227155	2.701512	-1.965535
H	-1.540168	2.798804	-1.997437
C	3.323254	-0.012088	-1.382247
H	2.818013	-0.594801	-2.157045
C	0.101011	-2.248895	2.882341
H	-0.530625	-2.174372	1.985946
C	0.859734	-0.899655	2.974920
H	0.139834	-0.089219	3.118079
C	1.030292	-3.464426	2.709185
H	1.664962	-3.369132	1.821520
H	1.681780	-3.607588	3.579256
H	0.431023	-4.373768	2.591994
C	1.967815	-0.833124	4.071065
H	2.047632	0.163579	4.510761
H	1.865195	-1.585983	4.848920
C	3.261779	1.491657	-1.750050
H	2.195893	1.758760	-1.743678
C	1.107237	-2.903209	-2.934025
H	1.433192	-3.929941	-3.140377
H	1.452081	-2.265783	-3.758393
H	1.593700	-2.573927	-2.007179
C	-4.853910	1.163922	-0.889001
H	-5.929448	1.099566	-1.096567
H	-4.612787	2.210356	-0.666558
H	-4.317234	0.877003	-1.802082
C	-0.832645	-2.412707	4.098024
H	-1.519295	-1.563519	4.193792
H	-1.434498	-3.320782	3.989821
H	-0.267108	-2.503897	5.034000
C	4.755221	-0.585929	-1.143023
H	4.846564	-1.614019	-1.500364
H	5.551900	0.031303	-1.551342
C	-5.610685	0.445889	2.022302
H	-6.653643	0.332143	1.700099
H	-5.444046	-0.212484	2.883821
H	-5.467177	1.481663	2.354280
C	-1.276874	-3.884825	-1.216192
H	-0.972032	-4.928062	-1.365957
H	-0.777383	-3.513593	-0.311888
H	-2.358396	-3.868065	-1.036371
C	0.334645	3.460260	1.568310

H	0.406515	4.295914	2.275909
H	-0.173310	2.630726	2.077282
H	1.353618	3.138787	1.318371
C	-2.422547	4.455111	0.543899
H	-2.400171	5.216417	1.333313
H	-2.999405	4.854691	-0.299145
H	-2.950849	3.575995	0.930653
C	-4.772623	-1.800080	0.055991
H	-5.829143	-1.907345	-0.218857
H	-4.164338	-2.092612	-0.807641
H	-4.561900	-2.498892	0.875339
C	3.788486	1.705755	-3.183089
H	3.249425	1.083808	-3.907925
H	3.660552	2.752165	-3.478416
H	4.857611	1.471107	-3.261779
C	3.982439	2.399622	-0.736843
H	3.839048	3.449869	-1.012773
H	3.592224	2.266904	0.277896
H	5.061863	2.208741	-0.713311
C	-1.547917	-3.726746	-4.295880
H	-1.182805	-4.759857	-4.357634
H	-2.643184	-3.752781	-4.242093
H	-1.268162	-3.207121	-5.220530
C	0.205796	5.626537	-0.625003
H	0.204134	6.390160	0.163180
H	1.246945	5.442701	-0.918978
H	-0.324988	6.029613	-1.495986

M3 HF:-3582.357566

C	4.317752	2.844776	-0.194187
H	3.828442	3.299428	-1.063944
H	4.316174	3.586632	0.610497
H	5.365195	2.647527	-0.455452
C	3.595345	1.562587	0.267792
H	2.581443	1.846444	0.582115
C	4.306706	0.919747	1.472282
H	3.757465	0.052787	1.851644
H	5.324095	0.597254	1.220081
H	4.380742	1.645533	2.289303
C	3.410411	0.594638	-0.929010
H	2.855127	1.108345	-1.717785
C	4.732109	-0.018357	-1.488714
H	4.690299	-0.156621	-2.572971
H	5.626239	0.536328	-1.213922

C	3.587351	-1.725472	-0.498377
C	2.862914	-2.788641	-0.082837
C	1.726208	-4.486146	0.935346
H	1.942476	-4.455192	2.006106
H	1.475327	-5.498825	0.627751
C	0.662184	-3.419051	0.528646
H	0.101431	-3.094426	1.407012
C	-0.333208	-3.859899	-0.574171
H	-0.925637	-2.966782	-0.817289
C	0.358712	-4.342485	-1.862148
H	-0.393566	-4.584268	-2.621041
H	1.020919	-3.576086	-2.279557
H	0.957134	-5.245395	-1.690599
C	-1.304941	-4.919077	-0.016569
H	-2.071471	-5.156308	-0.761421
H	-0.788133	-5.855125	0.232060
H	-1.815990	-4.558570	0.883226
C	1.398133	-0.975548	-0.196205
C	-1.241058	2.604157	0.464294
H	-1.810156	2.986313	-0.407544
H	-2.009583	2.344617	1.222494
C	0.897484	4.862954	-0.150465
H	1.459168	5.695958	0.289692
H	1.621817	4.141572	-0.546912
H	0.311537	5.263186	-0.987458
C	0.871616	3.549300	2.658480
H	1.417028	4.422071	3.038845
H	0.274653	3.141362	3.481949
H	1.606178	2.787080	2.373333
C	-1.374204	5.487893	1.828616
H	-0.772994	6.312459	2.232490
H	-2.003680	5.884465	1.022735
H	-2.036571	5.126715	2.624469
C	-1.551432	-0.811104	1.770013
H	-2.585359	-0.417626	1.825792
H	-1.666725	-1.857695	1.431748
C	1.060725	-0.615325	3.613337
H	1.406459	-0.627052	4.654392
H	1.559226	-1.437280	3.083465
H	1.385793	0.327754	3.158406
C	-1.610925	0.687454	4.521133
H	-1.156431	0.770659	5.515626
H	-1.451833	1.633213	3.991083
H	-2.691519	0.552411	4.650109

C	-1.270066	-2.397544	4.529504
H	-0.868993	-2.345201	5.549612
H	-2.354858	-2.543440	4.593901
H	-0.841557	-3.285717	4.045543
C	-2.442615	-0.341522	-1.673029
H	-2.392372	0.387324	-2.506719
H	-2.112774	-1.310775	-2.101978
C	-4.939342	0.957144	-0.199492
H	-6.012036	0.843797	-0.000138
H	-4.421671	1.045596	0.762329
H	-4.794449	1.897730	-0.744922
C	-5.409451	-0.669495	-2.782113
H	-6.463788	-0.783230	-2.499647
H	-5.320155	0.229630	-3.404662
H	-5.125096	-1.534065	-3.394709
C	-4.581488	-2.146056	-0.197867
H	-5.646431	-2.254465	0.041317
H	-4.273852	-3.031707	-0.768585
H	-4.018860	-2.129545	0.741373
C	-0.059835	2.410880	-2.864887
H	0.410315	3.188667	-2.267414
H	-1.147702	2.495401	-2.789587
C	0.409832	2.328334	-4.316595
H	-0.157126	2.997036	-4.970587
H	1.470868	2.593858	-4.397332
C	0.192014	0.837535	-4.660080
H	0.793309	0.506044	-5.511601
H	-0.862017	0.654723	-4.895502
C	0.578431	0.111467	-3.364748
H	-0.037774	-0.764207	-3.158806
H	1.637037	-0.162551	-3.333333
N	2.689158	-0.648927	-0.567233
N	1.555141	-2.314937	0.099078
O	4.867209	-1.376439	-0.867273
O	2.993367	-4.124807	0.212541
O	0.344741	1.100435	-2.265181
Si	-0.253088	4.057329	1.177450
Si	-0.862946	-0.786384	3.536729
Si	-4.281018	-0.539785	-1.217061
Lu	-0.780772	0.370995	-0.136762

M3’ HF:-3349.834676

Lu	-0.820290	0.094855	0.207502
Si	-2.154345	3.552565	-0.291925

Si	-0.208657	-1.170133	3.656841
Si	-3.579933	-1.680092	-1.572520
C	2.684269	4.522332	0.029986
H	1.825384	4.847033	-0.568654
H	2.635487	5.043490	0.991502
H	3.599709	4.855681	-0.475304
C	2.679233	2.997070	0.256520
H	1.753643	2.744503	0.791864
C	3.870380	2.549262	1.123739
H	3.838335	1.475710	1.337050
H	4.831549	2.770872	0.644912
H	3.848404	3.077296	2.083046
C	2.593942	2.254465	-1.103233
H	1.720857	2.612000	-1.656307
C	3.871915	2.347670	-1.993750
H	3.625327	2.368964	-3.058287
H	4.528274	3.176397	-1.739007
C	3.733163	0.185537	-1.272492
C	3.588641	-1.134944	-1.006238
C	3.453472	-3.282676	-0.240274
H	3.880465	-3.320572	0.764870
H	3.545451	-4.248953	-0.730477
C	1.998731	-2.714767	-0.232005
H	1.570457	-2.790860	0.771216
C	1.026422	-3.361574	-1.250747
H	0.094069	-2.781865	-1.193805
C	1.534659	-3.298285	-2.702636
H	0.785987	-3.727497	-3.376885
H	1.716977	-2.267357	-3.023941
H	2.464399	-3.864663	-2.835225
C	0.699742	-4.805538	-0.819823
H	-0.076664	-5.223948	-1.467564
H	1.577739	-5.460254	-0.892365
H	0.326930	-4.844007	0.210532
C	1.570052	-0.109702	-0.470341
C	-1.349250	2.280952	0.869616
H	-2.029013	2.133839	1.732338
H	-0.429138	2.727433	1.297321
C	-1.179250	3.701614	-1.954274
H	-1.683813	4.397773	-2.635119
H	-0.165050	4.086099	-1.782276
H	-1.104599	2.731320	-2.460875
C	-2.220727	5.332985	0.450680
H	-2.676352	6.039404	-0.254597

H	-2.813081	5.341413	1.373313
H	-1.214360	5.695611	0.694620
C	-3.960740	3.046887	-0.717525
H	-4.422424	3.783392	-1.385985
H	-3.993301	2.070011	-1.212079
H	-4.570112	2.986612	0.192228
C	-1.069055	-1.422829	1.980711
H	-2.160234	-1.458687	2.169846
H	-0.806889	-2.427910	1.592371
C	1.709590	-1.048193	3.446558
H	2.188854	-0.890451	4.420345
H	2.124431	-1.971292	3.020284
H	1.990832	-0.213640	2.792449
C	-0.799878	0.456327	4.498769
H	-0.297426	0.595851	5.463553
H	-0.591957	1.331754	3.873012
H	-1.880698	0.426831	4.682510
C	-0.519818	-2.605045	4.909285
H	-0.000045	-2.421564	5.858087
H	-1.591022	-2.705916	5.120615
H	-0.166459	-3.561973	4.505851
C	-2.039783	-0.566210	-1.673061
H	-2.343518	0.400232	-2.123101
H	-1.334971	-1.025339	-2.394661
C	-4.787335	-1.091991	-0.191977
H	-5.685644	-1.720956	-0.172208
H	-4.314465	-1.148707	0.796049
H	-5.104816	-0.055653	-0.357430
C	-4.582505	-1.732549	-3.220584
H	-5.459397	-2.385806	-3.129704
H	-4.931388	-0.729797	-3.494999
H	-3.959063	-2.108272	-4.041018
C	-3.069087	-3.495281	-1.171440
H	-3.952890	-4.142340	-1.118804
H	-2.406169	-3.894806	-1.949595
H	-2.548091	-3.553473	-0.208666
N	2.506729	0.781225	-0.947267
N	2.283865	-1.287806	-0.521862
O	4.656217	1.090730	-1.740241
O	4.284574	-2.319167	-1.041747

THF HF:-232.5174389

C	1.195071	-0.424229	0.129743
H	1.963728	-0.816646	-0.541903

H	1.562370	-0.485874	1.162639
C	0.739532	1.001123	-0.224340
H	1.336398	1.770393	0.275054
H	0.807102	1.167853	-1.306157
C	-0.739437	1.001219	0.224268
H	-1.336217	1.770443	-0.275293
H	-0.807013	1.168191	1.306047
C	-1.195138	-0.424165	-0.129567
H	-1.963585	-0.816498	0.542372
H	-1.562776	-0.485902	-1.162327
O	-0.000022	-1.274456	-0.000132