

## Supporting information for the manuscript

### Carbon Dioxide Reduction by Dinuclear Yb(II) and Sm(II) Complexes Supported by Siloxide Ligands

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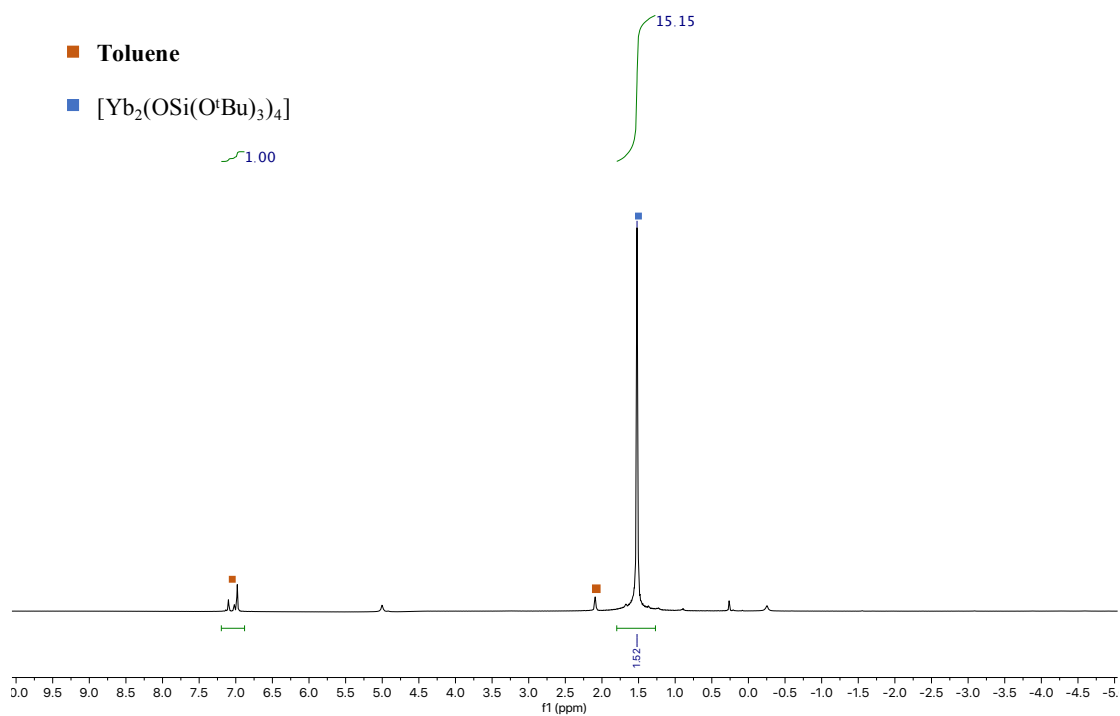
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## Content

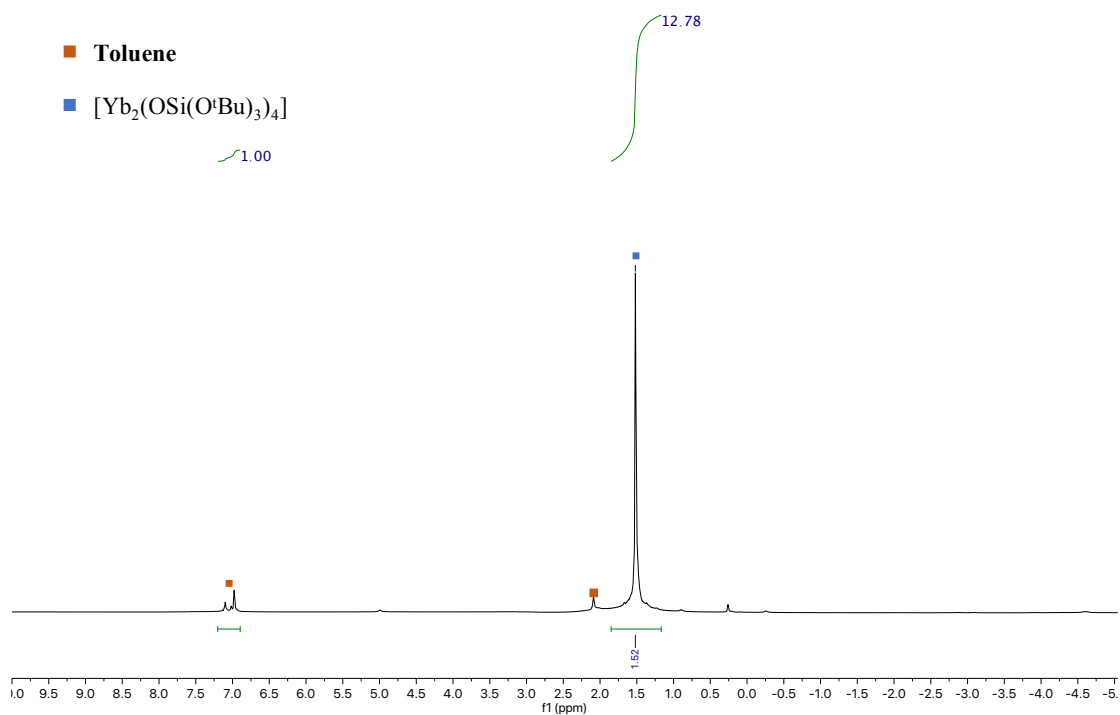
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## A. NMR spectroscopic data

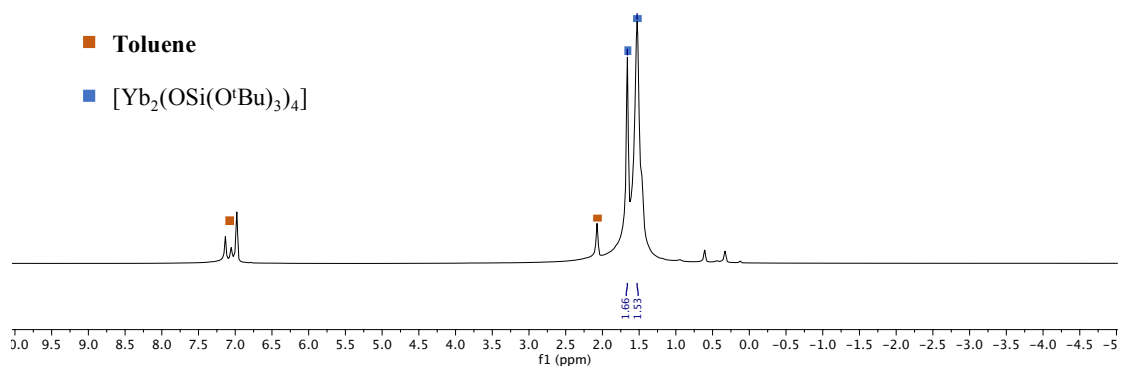
### Syntheses and stability of 1-Yb and 1-Sm.



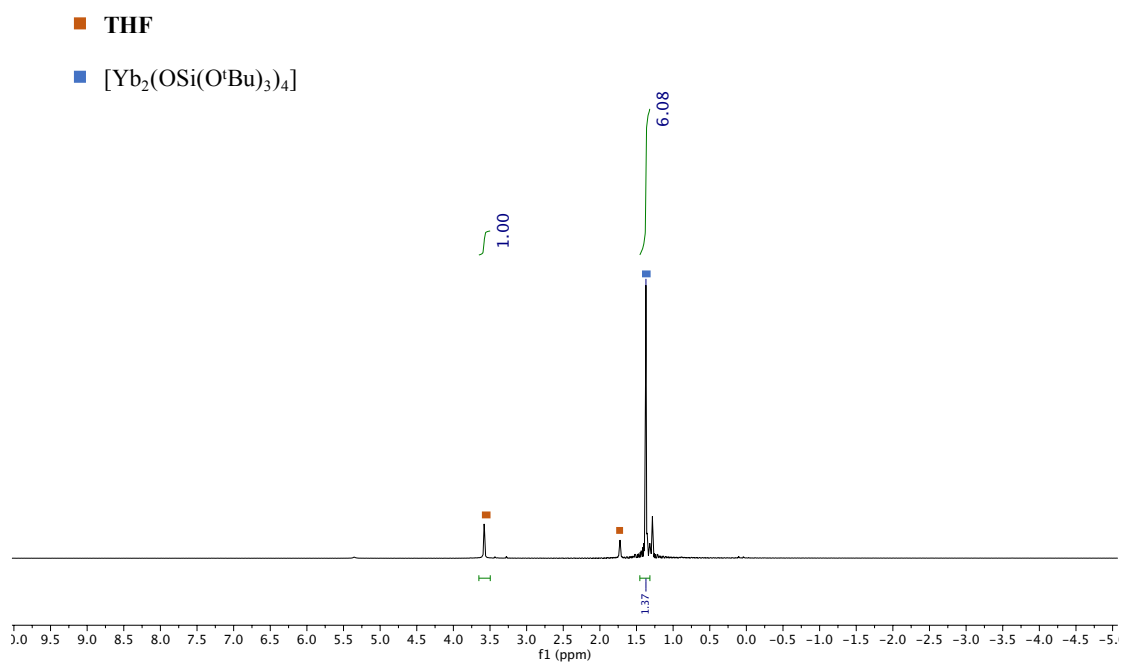
**Figure S 1:**  $^1\text{H}$  NMR spectrum of **1-Yb** ( $\text{Tol-d}_8$ , 400 MHz, 298 K) immediately after the dissolution in  $\text{Tol-d}_8$ .



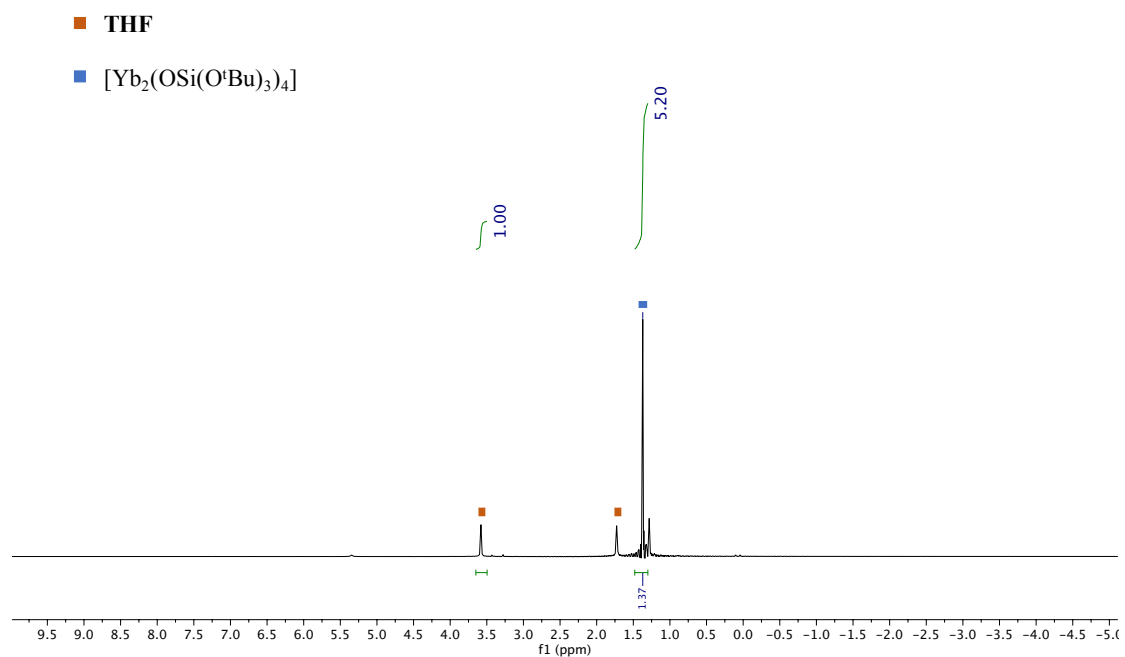
**Figure S 2:**  $^1\text{H}$  NMR spectrum of **1-Yb** ( $\text{Tol-d}_8$ , 400 MHz, 298 K) after 5 days at room temperature in  $\text{Tol-d}_8$ .



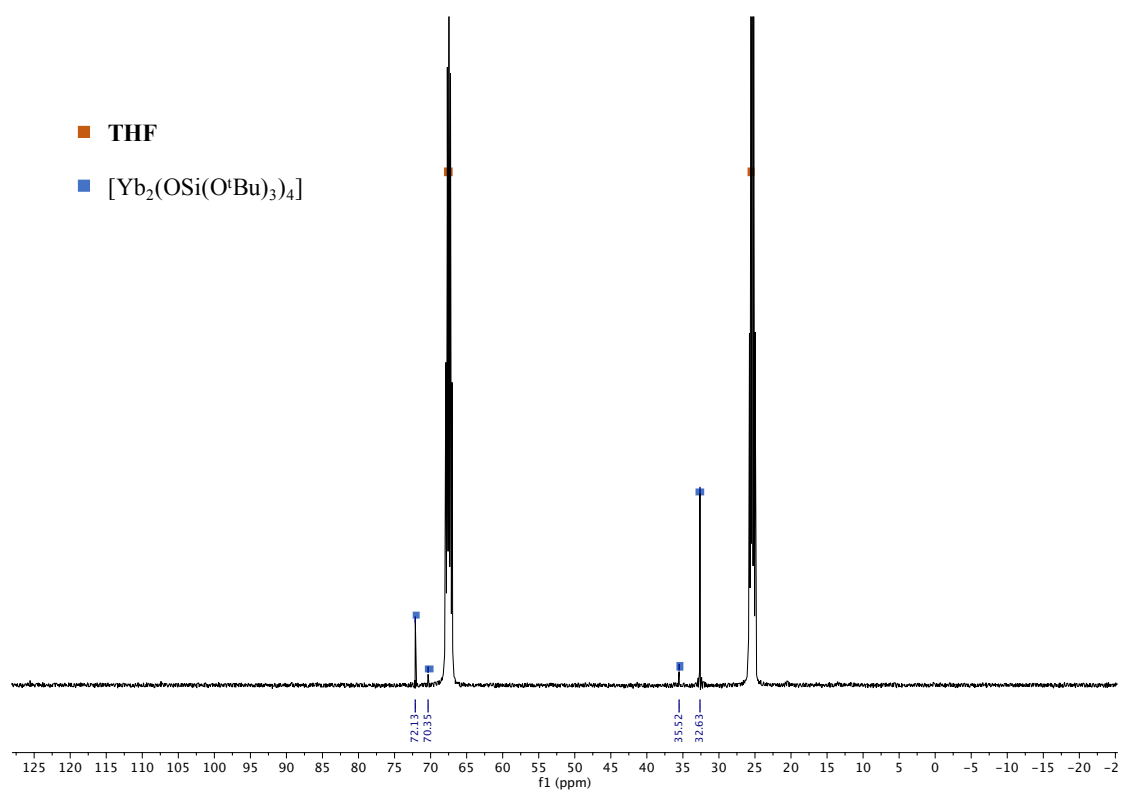
**Figure S 3:**  $^1\text{H}$  NMR spectrum of **1-Yb** (Tol- $d_8$ , 400 MHz, 213 K) recorded at 213 K.



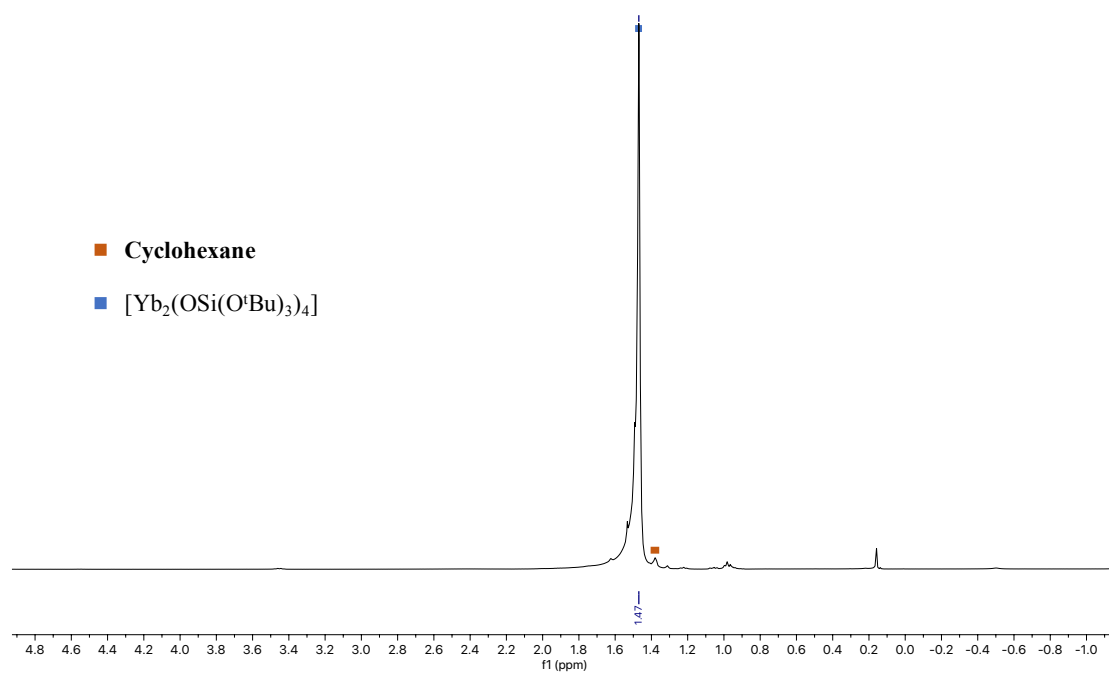
**Figure S 4:**  $^1\text{H}$  NMR spectrum of **1-Yb** (THF- $d_8$ , 400 MHz, 298 K) immediately after the dissolution in THF- $d_8$ .



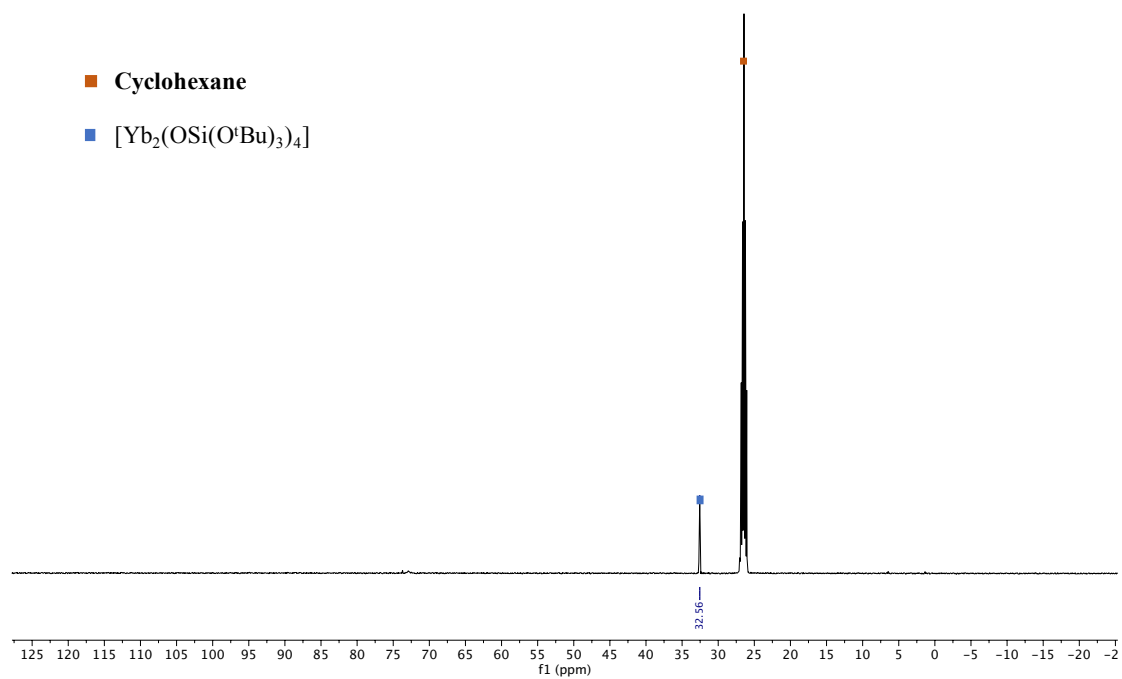
**Figure S 5:**  $^1\text{H}$  NMR spectrum of **1-Yb** (THF- $d_8$ , 400 MHz, 298 K) after 5 days at room temperature in THF- $d_8$ .



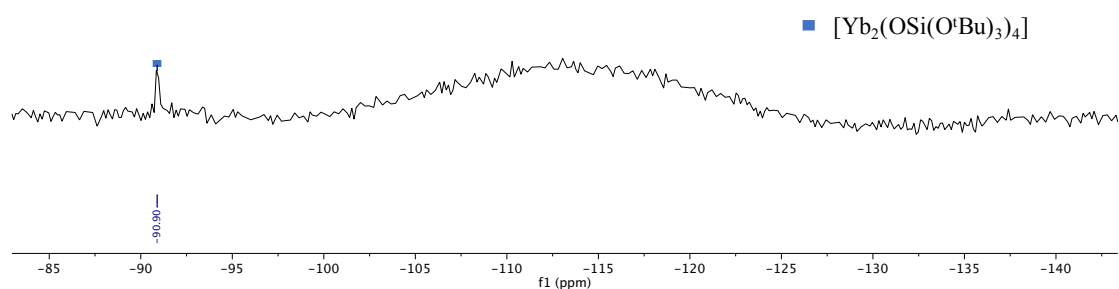
**Figure S 6:**  $^{13}\text{C}$  NMR spectrum of **1-Yb** (THF- $d_8$ , 400 MHz, 298 K).



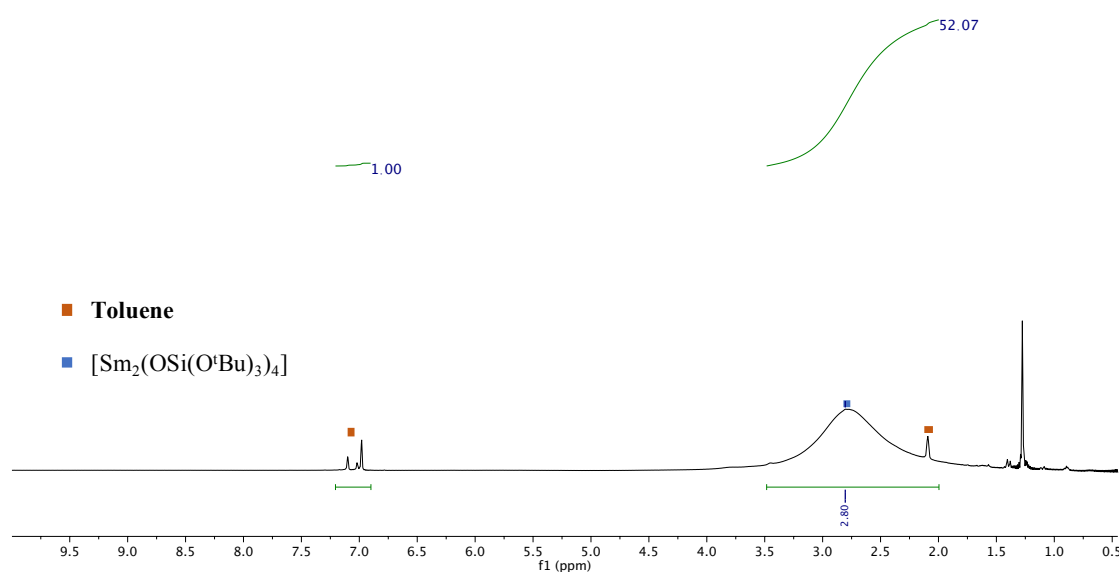
**Figure S 7:**  $^1\text{H}$  NMR spectrum of **1-Yb** ( $\text{C}_6\text{D}_{12}$ , 400 MHz, 298 K).



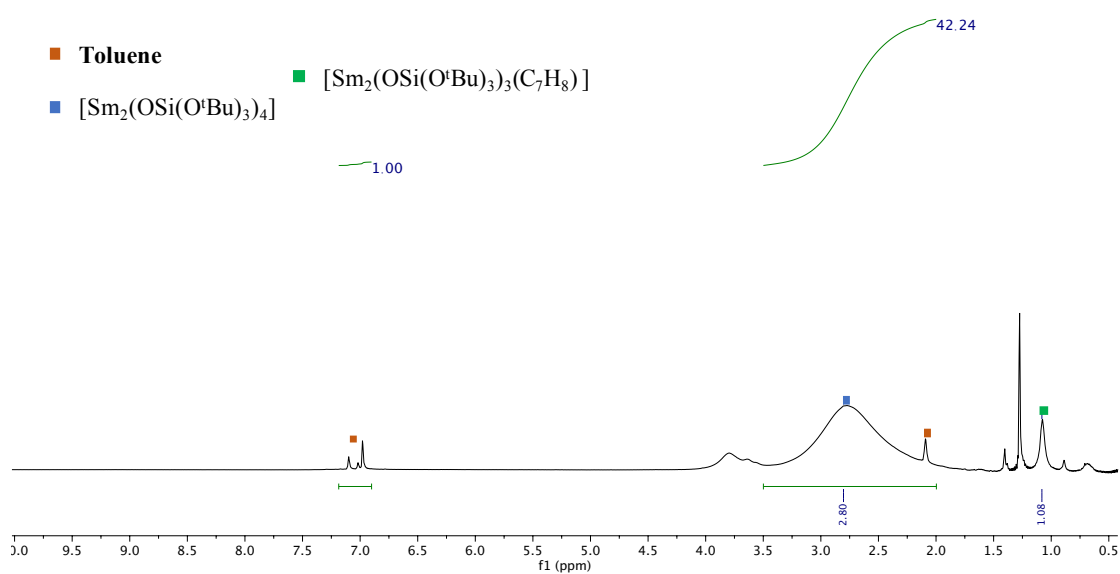
**Figure S 8:**  $^{13}\text{C}$  NMR spectrum of **1-Yb** ( $\text{C}_6\text{D}_{12}$ , 400 MHz, 298 K).



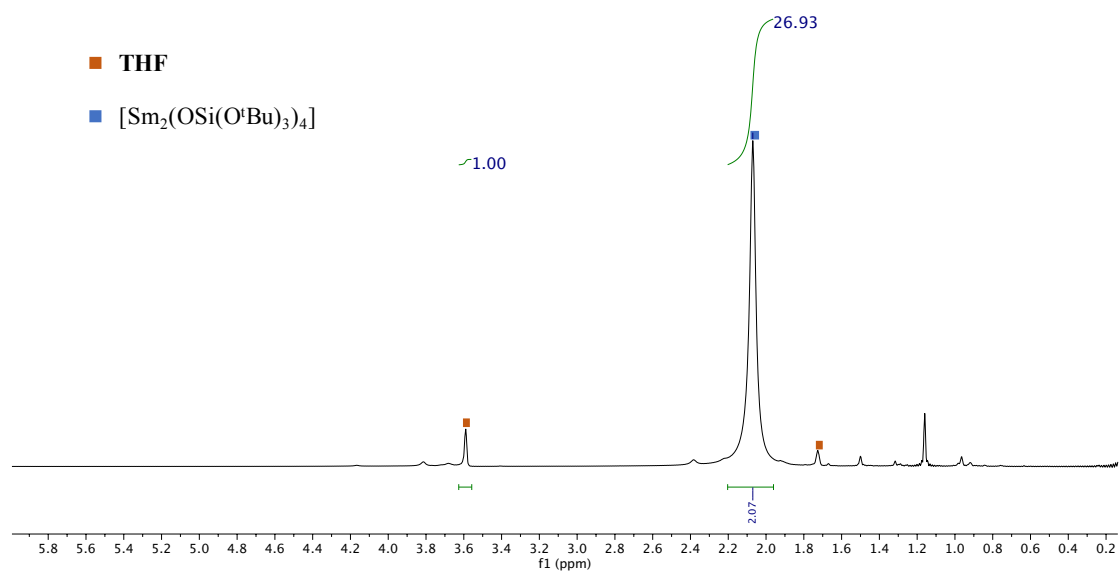
**Figure S 9:**  $^{29}\text{Si}$  NMR spectrum of **1-Yb** (THF- $d_8$ , 400 MHz, 298 K).



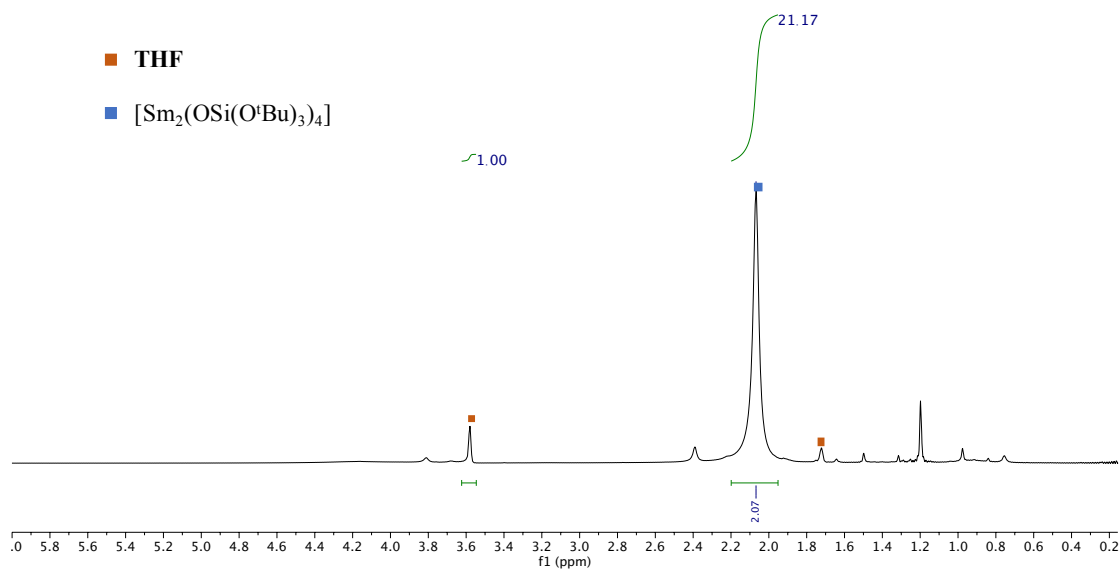
**Figure S 10:**  $^1\text{H}$  NMR spectrum of **1-Sm** (Tol- $d_8$ , 400 MHz, 298 K) immediately after the dissolution in Tol- $d_8$ .



**Figure S 11:**  $^1\text{H}$  NMR spectrum of **1-Sm** (Tol- $d_8$ , 400 MHz, 298 K) after 5 days at room temperature in Tol- $d_8$ .

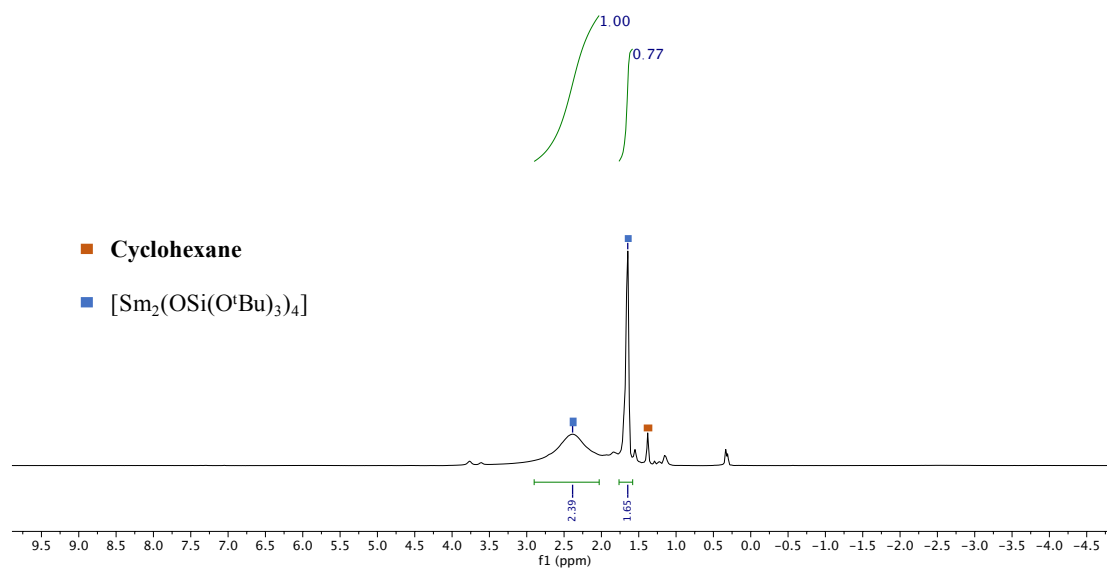


**Figure S 12:**  $^1\text{H}$  NMR spectrum of **1-Sm** (THF- $d_8$ , 400 MHz, 298 K) immediately after the dissolution in THF- $d_8$ .



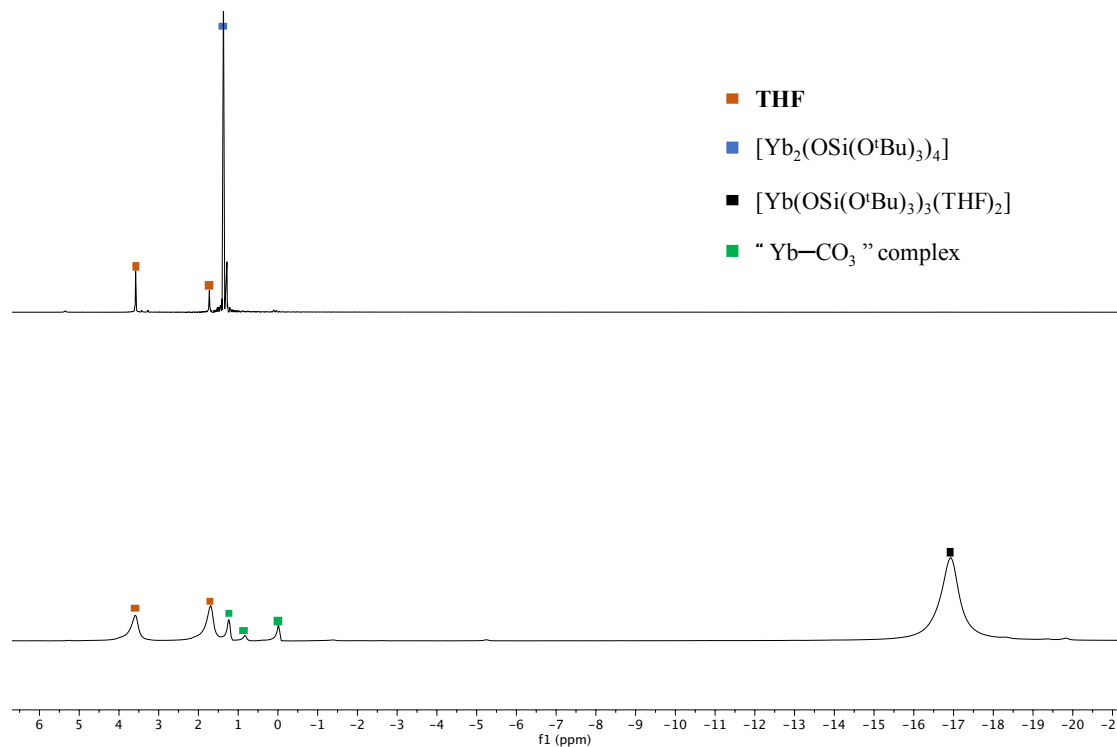
**Figure S 13:**  $^1\text{H}$  NMR spectrum of **1-Sm** (THF- $d_8$ , 400 MHz, 298 K) after 5 days at room temperature in THF- $d_8$ .



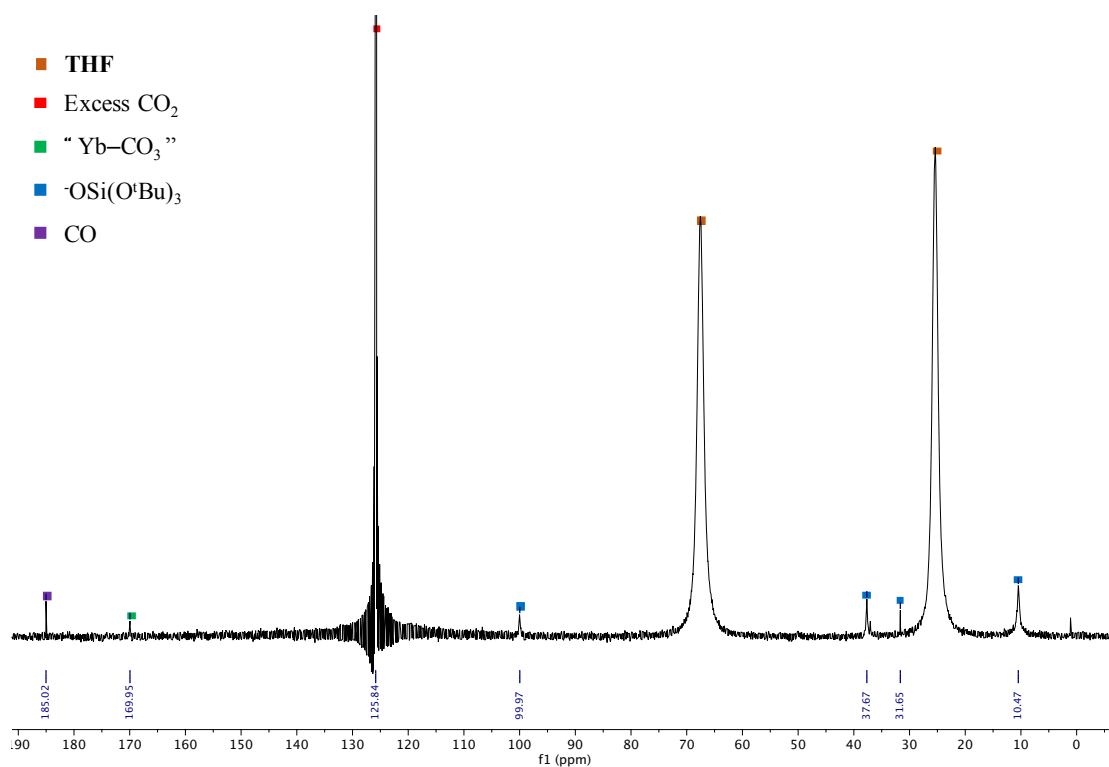


**Figure S 14:** <sup>1</sup>H NMR spectrum of **1-Sm** (C<sub>6</sub>D<sub>12</sub>, 400 MHz, 298 K).

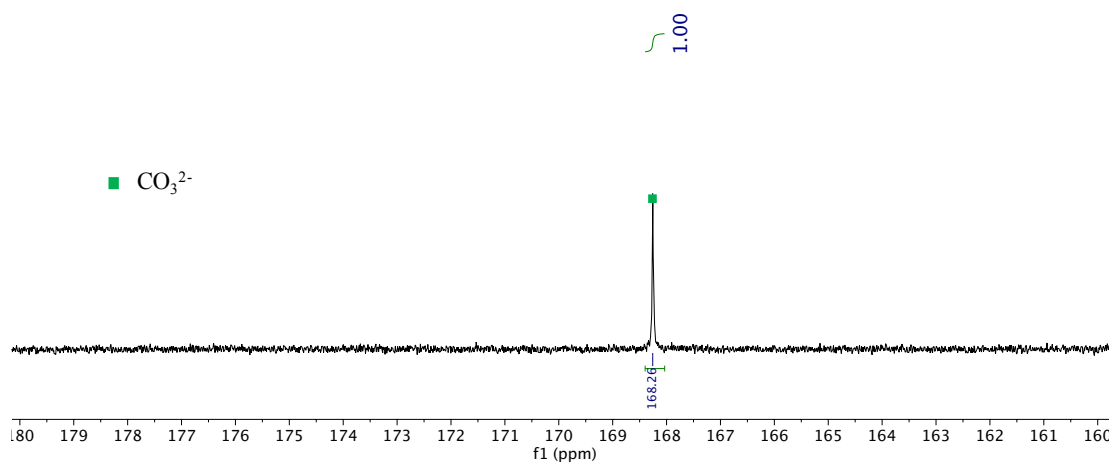
### Reactivity studies



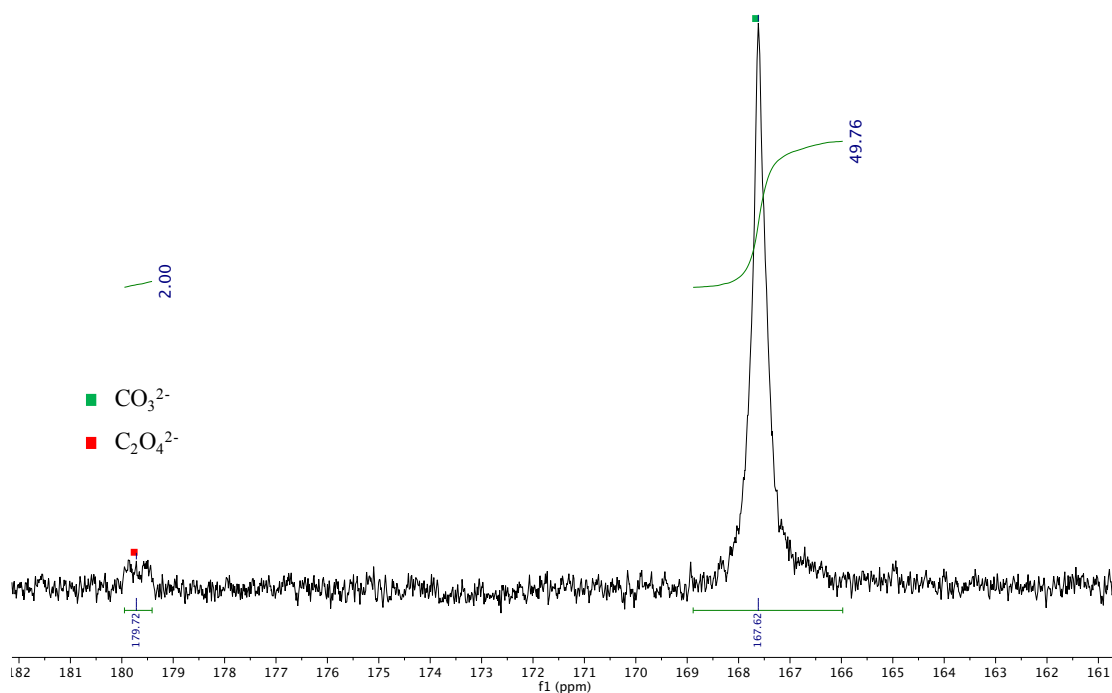
**Figure S 15:** <sup>1</sup>H NMR spectrum of the reaction mixture before the addition of ~5 equivalents <sup>13</sup>CO<sub>2</sub> to a THF-d<sub>8</sub> solution of **1-Yb** at room temperature (above) and 10 days after addition (below) (THF-d<sub>8</sub>, 400 MHz, 298 K).



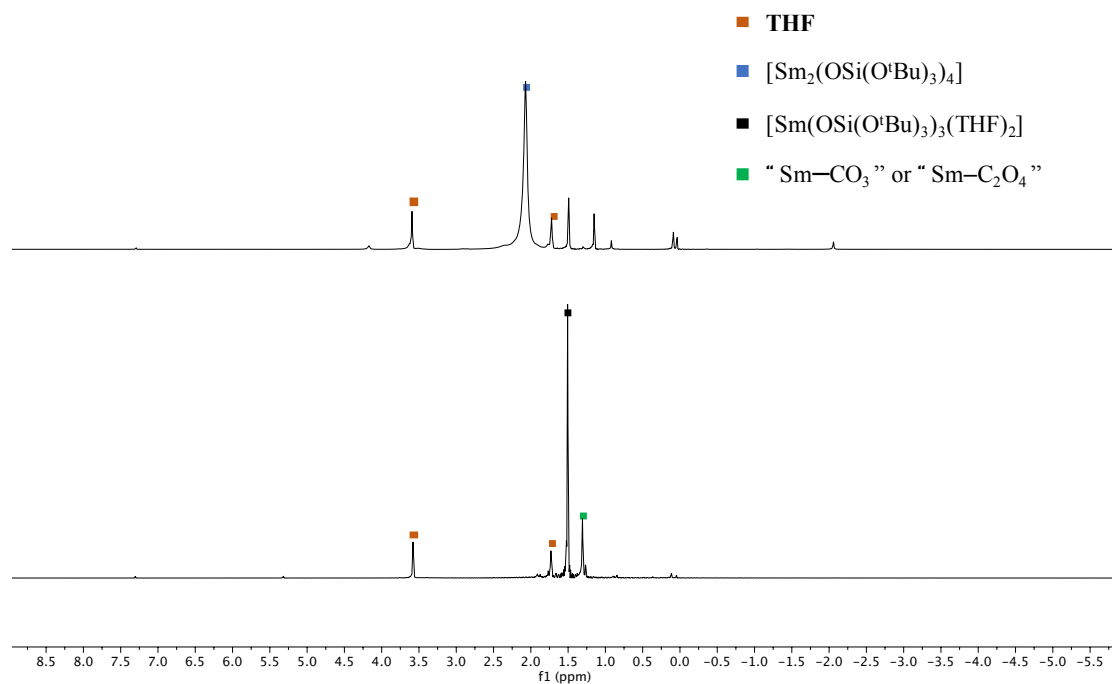
**Figure S 16:**  $^{13}\text{C}$  NMR spectrum of the reaction mixture after addition of  $\sim 5$  equivalents  $^{13}\text{CO}_2$  to a THF- $d_8$  solution of **1-Yb** at room temperature (THF- $d_8$ , 400 MHz, 298 K).



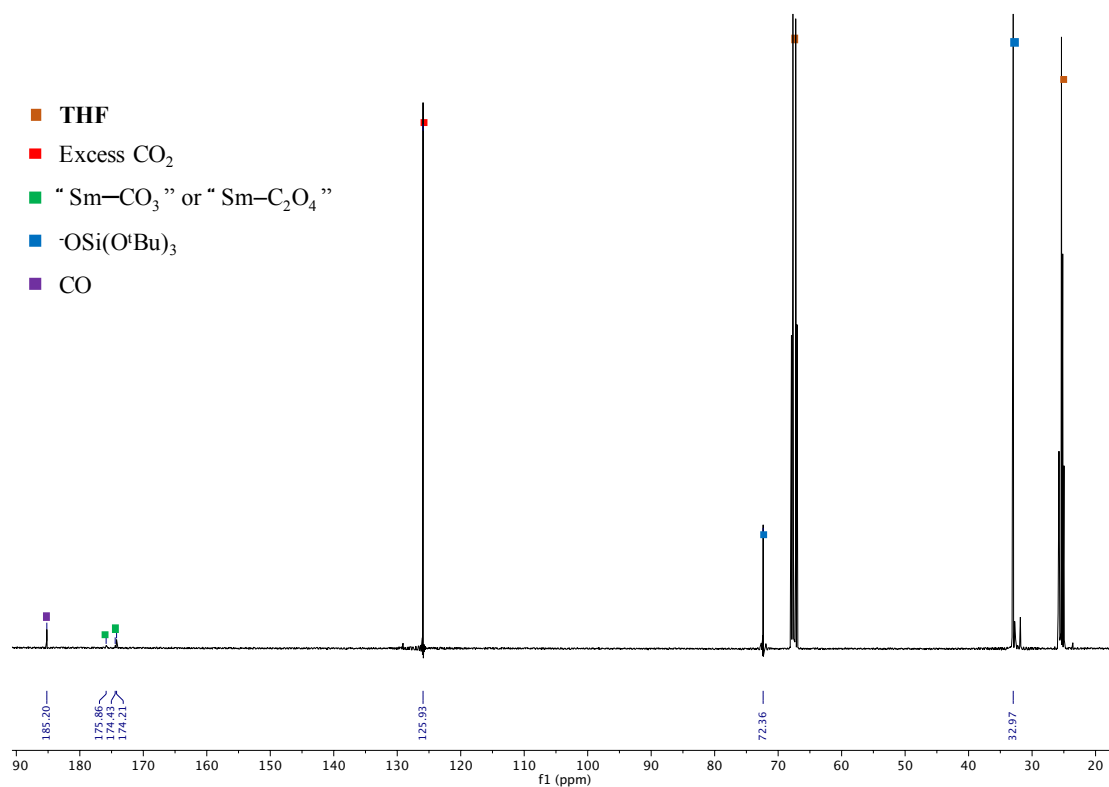
**Figure S 17:** Quantitative  $^{13}\text{C}$  NMR spectrum of the reaction mixture after addition of  $\sim 5$  equivalents  $^{13}\text{CO}_2$  to a THF- $d_8$  solution of **1-Yb** at room temperature after removal of excess  $^{13}\text{CO}_2$  and solvent ( $\text{D}_2\text{O}$ , 600 MHz, 298 K, pD-13).



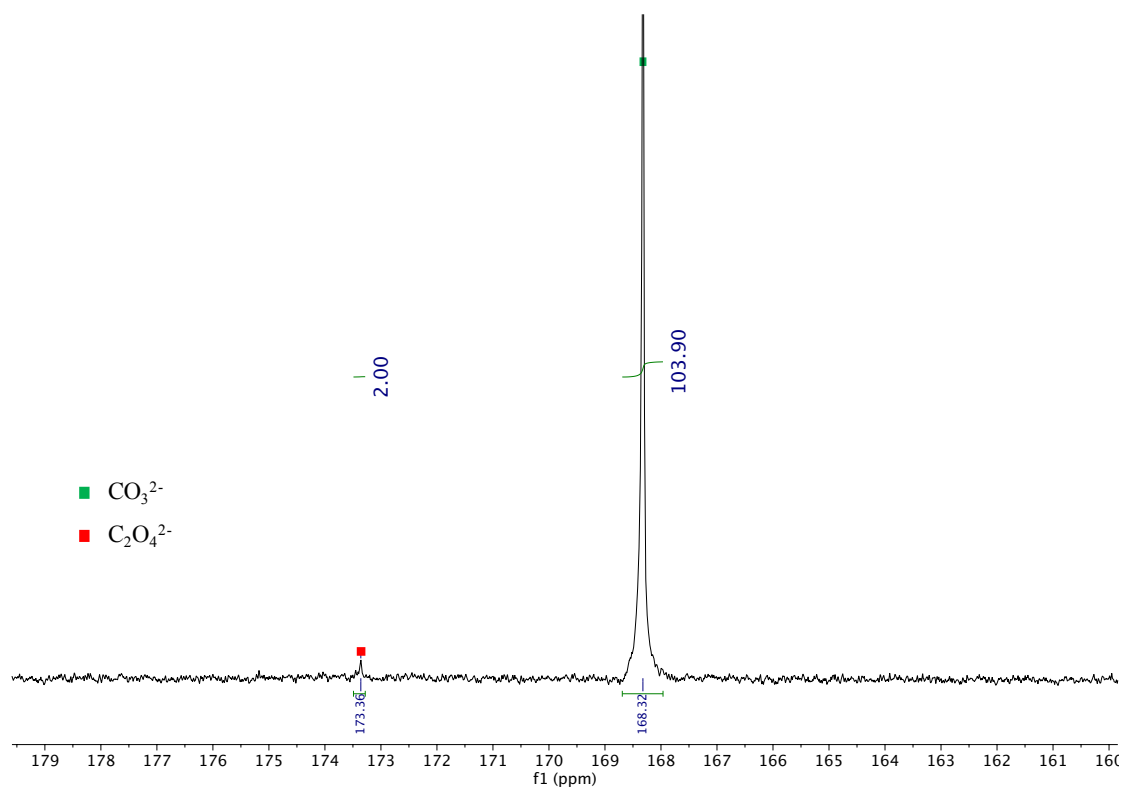
**Figure S 18:** Quantitative  $^{13}\text{C}$  NMR spectrum of the reaction mixture after addition of  $\sim 5$  equivalents  $^{13}\text{CO}_2$  to a  $\text{C}_6\text{D}_{12}$  solution of **1-Yb** at room temperature after removal of excess  $^{13}\text{CO}_2$  and solvent ( $\text{D}_2\text{O}$ , 600 MHz, 298 K, pD-13).



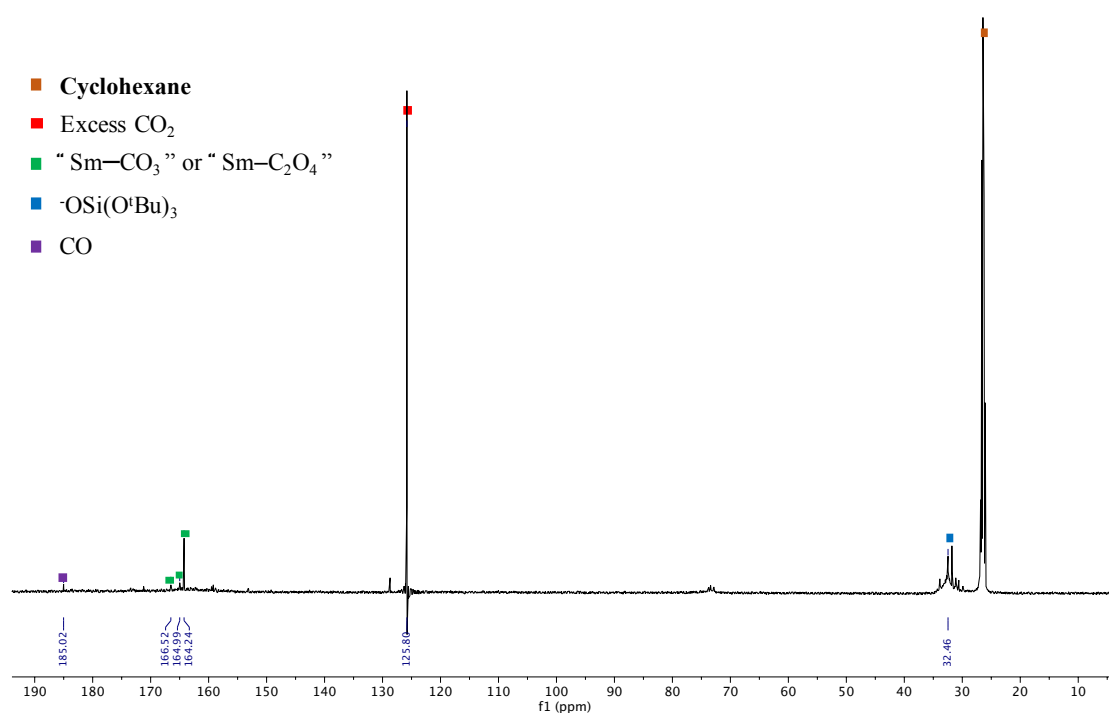
**Figure S 19:**  $^1\text{H}$  NMR spectrum of the reaction mixture before the addition of  $\sim 5$  equivalents  $^{13}\text{CO}_2$  to a  $\text{THF-d}_8$  solution of **1-Sm** at room temperature (above) and 2 days after addition (below) ( $\text{THF-d}_8$ , 400 MHz, 298 K).



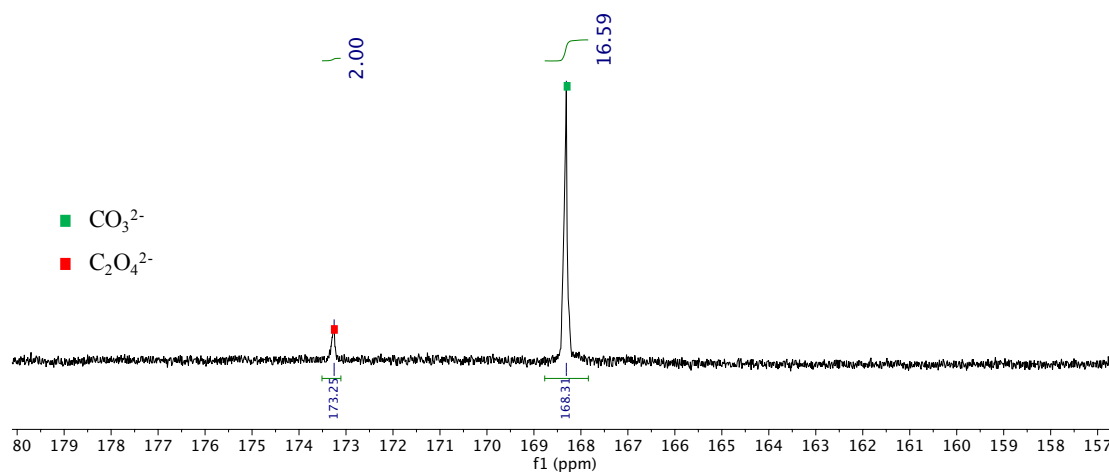
**Figure S 20:** <sup>13</sup>C NMR spectrum of the reaction mixture 2 days after addition of ~5 equivalents <sup>13</sup>CO<sub>2</sub> to a THF-d<sub>8</sub> solution of **1-Sm** at room temperature (THF-d<sub>8</sub>, 400 MHz, 298 K).



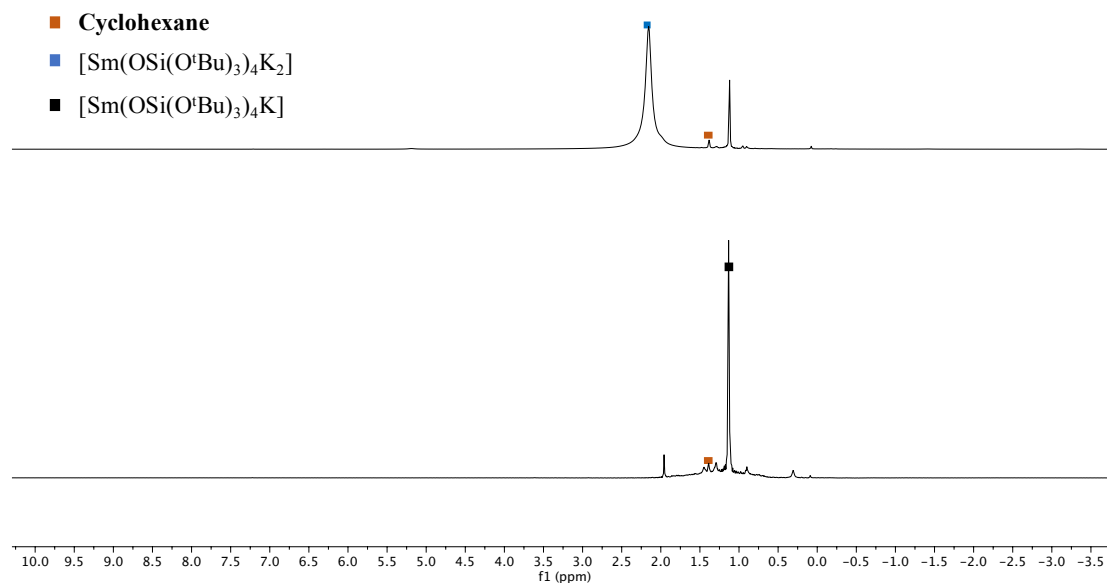
**Figure S 21:** Quantitative <sup>13</sup>C NMR spectrum of the reaction mixture after addition of ~5 equivalents <sup>13</sup>CO<sub>2</sub> to a THF-d<sub>8</sub> solution of **1-Sm** at room temperature, after 10 days, after removal of excess <sup>13</sup>CO<sub>2</sub> and solvent (D<sub>2</sub>O, 600 MHz, 298 K, pD-13).



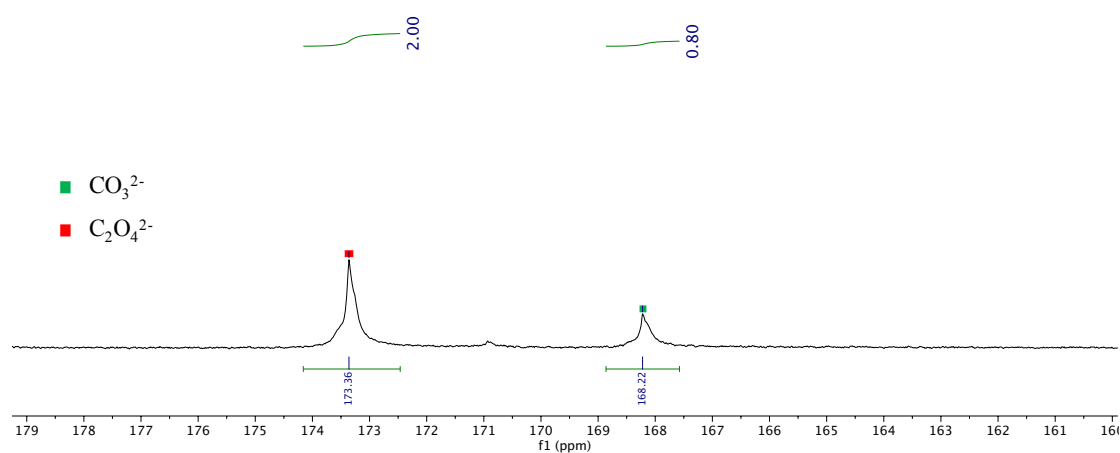
**Figure S 22:** <sup>13</sup>C NMR spectrum of the reaction mixture 2 weeks after addition of ~5 equivalents <sup>13</sup>CO<sub>2</sub> to a C<sub>6</sub>D<sub>12</sub> solution of **1-Sm** at room temperature (C<sub>6</sub>D<sub>12</sub>, 400 MHz, 298 K).



**Figure S 23:** Quantitative <sup>13</sup>C NMR spectrum of the reaction mixture after addition of ~5 equivalents <sup>13</sup>CO<sub>2</sub> to a C<sub>6</sub>D<sub>12</sub> solution of **1-Sm** at room temperature after removal of excess <sup>13</sup>CO<sub>2</sub> and solvent (D<sub>2</sub>O, 600 MHz, 298 K, pD-13).



**Figure S 24:** <sup>1</sup>H NMR spectrum of the reaction mixture before the addition of ~5 equivalents <sup>13</sup>CO<sub>2</sub> to a C<sub>6</sub>D<sub>12</sub> solution of [SmL<sub>4</sub>K<sub>2</sub>] at room temperature (above) and after addition (below) (C<sub>6</sub>D<sub>12</sub>, 400 MHz, 298 K).



**Figure S 25:** Quantitative <sup>13</sup>C NMR spectrum of the reaction mixture after addition of ~5 equivalents <sup>13</sup>CO<sub>2</sub> to a C<sub>6</sub>D<sub>12</sub> solution of [SmL<sub>4</sub>K<sub>2</sub>] at room temperature after removal of excess <sup>13</sup>CO<sub>2</sub> and solvent (D<sub>2</sub>O, 600 MHz, 298 K, pD-12).

### Diffusion coefficient measurement.

DOSY NMR was used to measure the diffusion coefficients ( $D$ ) of **1-Yb** in  $C_6D_{12}$ . The values of the measured coefficient diffusion can be used to estimate the spherical hydrodynamic radius  $r_{sph}$  (Stokes radius) of the complex in solution from the Stokes-Einstein equation.

$$r_{sph} = \frac{k_B T}{6\pi\eta D}$$

$\eta$  = viscosity of the medium (0.86 mPa.s for cyclohexane at 298 K)

$k_B$  = Boltzmann constant ( $1.38 \times 10^{-23} \text{ m}^2 \cdot \text{kg} \cdot \text{s}^{-2} \cdot \text{K}^{-1}$ )

$T$ : absolute temperature (K)

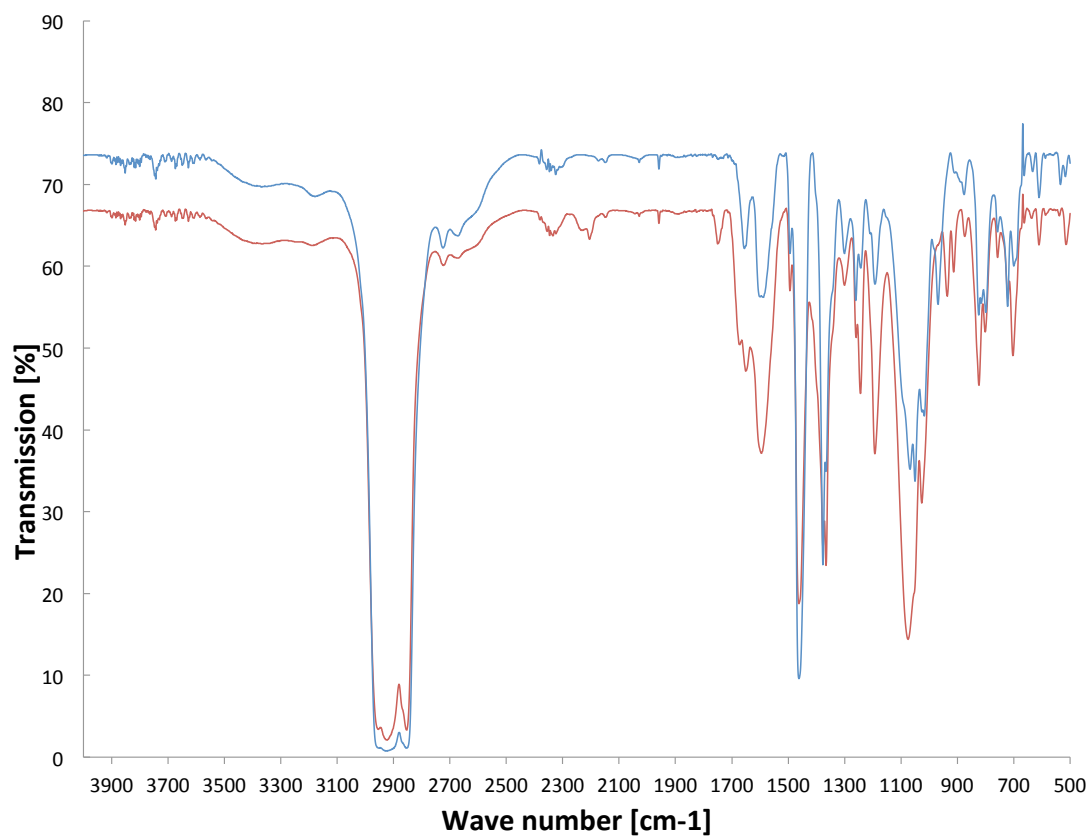
$D$ : diffusion coefficient ( $\text{m}^2 \cdot \text{s}^{-1}$ )

	Diffusion coefficient ( $\text{m}^2 \cdot \text{s}^{-1}$ )	$r_{sph}$ (Å)
<b>1-Yb</b> in $C_6D_{12}$	$3.98 \times 10^{-10}$	<b>6.37</b>

**Table S1:** Diffusion coefficient of **1-Yb** in  $C_6D_{12}$  measured by DOSY NMR and radius of **1-Yb** estimated from the Stokes-Einstein equation.

The value of the radius  $r_{sph}$  obtained by DOSY NMR spectroscopy for **1-Yb** is consistent with the value obtained from the solid-state structure of the dimeric **1-Sm** (~ 6 Å).

## B. IR spectrum



**Figure S 26:** Infrared spectra of complex **1-Yb** (blue) and of the residue of the reaction mixture after addition of  $\sim 5$  equivalents CO<sub>2</sub> to a n-hexane solution of **1-Yb** at room temperature (red).



### C. X-ray Crystal Structure Determination Details

Bragg-intensities of **1-Sm**, **3** and **4** were collected at low temperature (See Table S1) using CuK $\alpha$  radiation. A Rigaku SuperNova dual system diffractometer with an Atlas S2 CCD detector was used for compounds **1-Sm** and **4**, and one equipped with an Atlas CCD detector for compound **3**. The datasets were reduced and corrected for absorption, with the help of a set of faces enclosing the crystals as snugly as possible, with CrysAlis<sup>Pro</sup>.<sup>1</sup>

The X-ray diffraction data of **2** were measured at 120(2) K using MoK $\alpha$  radiation on a Bruker APEX II CCD kappa diffractometer. The datasets were reduced by EvalCCD<sup>2</sup> and corrected for absorption by modelling an empirical transmission surface as sampled by multiple symmetry-equivalent and/or azimuth rotation-equivalent intensity measurements by real spherical harmonic functions of even order.<sup>3</sup>

The solutions and refinements of the structures were performed by the latest available version of ShelXT<sup>4</sup> and ShelXL.<sup>5</sup> All non-hydrogen atoms were refined anisotropically using full-matrix least-squares based on  $|F|^2$ , but the hydrogen atoms were placed at calculated positions by means of the “riding” model where each H-atom was assigned a fixed isotropic displacement parameter with a value equal to 1.2  $U_{eq}$  of its parent C-atom (1.5  $U_{eq}$  for the methyl groups). Crystallographic and refinement data are summarized in Table S1. CCDC numbers 1895385-1895388 for compounds **1-Sm** (1895385), **2**, (1895387), **3** (1895386), and **4** (1895388), contain the supplementary crystallographic data for this paper. These data can be obtained, free of charge, from The Cambridge Crystallographic Data Centre via [www.ccdc.cam.ac.uk/structures](http://www.ccdc.cam.ac.uk/structures).

In the structure of **3**, a solvent mask was calculated with the help of the solvent-masking program in OLEX2<sup>6</sup> and 55.0 electrons were found in a volume of 483.0 Å<sup>3</sup> in three voids. This is consistent with the presence of one hexane solvent molecule per formula unit which accounts for 50.0 electrons.

In the case of **4**, a calculated solvent mask found 356.0 electrons in a volume of 2524.0 Å<sup>3</sup> in two voids. This is consistent with the presence of two hexane solvent molecules per formula unit which account for 400.0 electrons.

**Table S2:** Crystallographic parameters for complexes 1-4.

Compound	[Sm <sub>2</sub> L <sub>4</sub> ] (1-Sm)	[Yb <sub>2</sub> L <sub>4</sub> (μ-OME) <sub>2</sub> (DME) <sub>2</sub> ] (2)	[Yb <sub>4</sub> L <sub>8</sub> (C <sub>2</sub> O <sub>4</sub> )] (3)	[Sm <sub>4</sub> L <sub>8</sub> (CO <sub>3</sub> ) <sub>2</sub> ] (4)
Formula	C <sub>48</sub> H <sub>108</sub> O <sub>16</sub> Si <sub>4</sub> Sm <sub>2</sub>	C <sub>58</sub> H <sub>134</sub> O <sub>22</sub> Si <sub>4</sub> Yb <sub>2</sub>	C <sub>98</sub> H <sub>216</sub> O <sub>36</sub> Si <sub>8</sub> Yb <sub>4</sub>	C <sub>98</sub> H <sub>216</sub> O <sub>38</sub> Si <sub>8</sub> Sm <sub>4</sub>
Crystal size [mm]	0.38 x 0.29 x 0.25	0.25×0.16×0.07	0.38×0.32×0.28	0.19×0.14×0.07
Crystal system	Triclinic	Triclinic	Triclinic	Monoclinic
Space group	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$	<i>C</i> 2/ <i>c</i>
V [Å <sup>3</sup> ]	3355.4(4)	2022.8(6)	3600.41(12)	15088.5(16)
<i>a</i> [Å]	12.9099(7)	9.5823(14)	13.1265(2)	34.217(2)
<i>b</i> [Å]	14.0475(9)	14.4327(18)	15.6137(3)	14.6315(7)
<i>c</i> [Å]	20.4106(8)	16.330(3)	18.8708(4)	30.140(2)
$\alpha$ [°]	88.122(4)	64.364(11)	72.6073(17)	90
$\beta$ [°]	88.122(4)	85.709(14)	80.2421(15)	90.606(6)
$\gamma$ [°]	65.093(6)	83.694(12)	79.3717(13)	90
Z	2	1	1	4
Absorption coefficient [mm <sup>-1</sup> ]	14.134	2.418	5.768	12.626
F(000)	1408	854	1484	5872
T(K)	100.00(10) K	120(2)	140.01(10)	140.00(10)
Total no. reflections	24633	24632	38077	37370
Unique reflexions [ <i>R</i> <sub>int</sub> ]	13518 [0.0548]	7397 [0.0772]	14966 [0.0185]	12866 [0.0919]
Final <i>R</i> <sub>1</sub> [ <i>I</i> >2 $\sigma$ ( <i>I</i> )]	0.0661	0.0564	0.0215	0.0729
Largest diff. peak and hole [eÅ <sup>-3</sup> ]	2.033 and -1.416	0.915 and -0.778	0.596 and -0.796	2.324 and -2.707
GOOF	1.024	1.118	1.049	1.055

## References

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- [3] R. H. Blessing, *Acta Cryst.*, 1995, **A51**, 33-38.
- [4] Sheldrick, G.M., ShelXT-Integrated space-group and crystal-structure determination, *Acta Cryst.*, 2015, **A71**, 3-8.
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- [6] O.V. Dolomanov, L.J. Bourhis, R.J. Gildea, J.A.K. Howard, H. Puschmann, Olex2: A complete structure solution, refinement and analysis program, *J. Appl. Cryst.*, 2009, **42**, 339-341.

## D. Computational Details

Calculations were performed with the GAUSSIAN 09 suite of programs [1]. Density Functional Theory (DFT) was applied by the mean of the B3PW91 hybrid functional [2]. Following our previous work, two kinds of relativistic effective core potential (RECPs) have been used to describe the lanthanide centre: small-core Stuttgart-Dresden RECP [3] (which includes  $1s$ ,  $2s$ ,  $2p$ ,  $3s$ ,  $3p$  and  $3d$  electrons) and large-core Stuttgart-Dresden RECP [4] (which includes, in addition,  $4s$ ,  $4p$ ,  $4d$  and  $4f$  electrons), depending on the size of the system. The large-core RECP was chosen according to the formal oxidation state of the lanthanide. The RECPs were used in combination with their optimized valence basis sets supplemented by an  $f$  polarization function for the large-core RECP. The Stuttgart-Dresden relativistic effective core potential SDD [5] was employed for silicon centers in association with its valence basis set and a  $d$  polarization function, while the 6-31G(d) basis set was used for all other atoms [6]. Geometry optimizations were performed on the whole system and without any symmetry constraints. All stationary points have been identified for the minimum (number of imaginary frequencies,  $\text{Nimag} = 0$ ). The NBO analysis [7] was carried out on the optimized structures using the module included in the Gaussian package and the Chemcraft graphical program was used for the 3D representations of the structures and the orbital plots [8].

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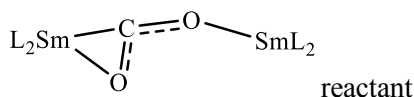
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### Cartesian coordinates of all optimized structures

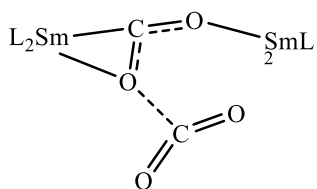


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Sm	21.61352100	2.72065500	14.19212400
Si	25.97768800	5.71542900	20.08169500
Si	18.92178100	3.80176300	15.34679700
O	24.36127800	4.28296100	16.14624500
O	23.03278300	2.50766800	16.10305200
O	24.58702800	5.93243000	19.28583900
O	26.63883000	7.02224800	20.86936100
O	27.00551400	5.55532300	18.68503700
O	26.06872700	4.41750000	21.11154200
O	20.05558600	4.32575400	14.32213400
O	17.33886800	3.91832300	14.83709300
O	19.46950600	2.15981100	15.47970700
O	18.94725400	4.33697100	16.92067400
C	23.42400200	3.59218000	15.55953400
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H	24.36817300	7.97556500	23.22111400
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C	26.62436600	9.06330400	22.08519700
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H	26.36521800	9.56551500	23.02420300
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C	26.93216900	6.85676100	23.27268400
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H	28.01562400	6.96259700	23.14560800
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C	29.02680800	6.81237200	18.27432100
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C	24.77684200	1.79231500	9.90157400
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transition state

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Sm	22.21449700	1.91207000	14.50441800
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Si	19.75507000	1.73636300	16.45722300
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O	24.42184700	1.76687400	15.63749200
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O	28.61740300	5.23518500	20.87373600
O	28.41512600	3.14172300	19.26567200
O	27.15387200	3.20796000	21.81898900
O	20.12563700	2.41502900	15.02832100
O	18.27231900	0.98777000	16.56352500
O	21.09615400	0.65168600	16.54938900
O	19.91022700	2.66107200	17.82692100
C	24.03048100	3.03801000	15.81760900
C	28.40887300	6.30827400	21.83369800
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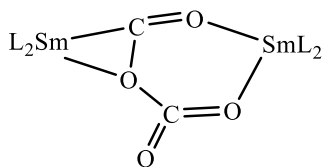
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C	30.05304800	2.26407500	20.90126500
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H	29.28797300	1.63560100	21.36597100
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H	26.81277600	0.73712300	20.83736400
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H	16.31309400	2.17165300	15.19242900
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H	19.14078200	-0.08349200	14.18297900
H	17.71239700	-1.11955900	13.95643700
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C	20.29937900	-0.64819300	18.48532500
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H	20.63733100	-1.26672500	19.32495800
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C	22.35959600	-1.28741300	17.18964900



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C	19.92830900	4.66429400	19.10636400
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C	17.96467200	3.08016700	19.20902800
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Si	28.02086700	6.08381700	15.27054600
O	22.39317700	2.85234900	12.51100900
O	24.11716000	1.48088000	10.73843400
O	22.48089100	0.33999800	12.51899400
O	21.52217700	1.60498700	10.16589900
O	27.29634100	6.12875300	16.71954000
O	27.07152500	6.17520700	13.90935900
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H	23.12908200	1.52406700	8.23033900
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C	24.32371800	-1.24870600	12.55524600
H	24.55073000	-0.98340400	13.59398400
H	24.60890800	-2.29482000	12.39227200
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C	21.97663300	-1.89339200	13.23338400
H	20.91199000	-1.73120300	13.03315300
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C	20.13144700	3.61731300	10.17948100
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C	26.38982300	7.34275700	13.37361200
C	25.94100000	8.28631700	14.49805700
H	26.80951700	8.69456100	15.02632300
H	25.36815400	9.11924900	14.07349700
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H	30.75028500	4.88622400	13.93752400
H	30.37018800	3.85198400	12.53349100
H	29.39241400	5.30401400	12.86423900
C	30.12183800	7.78235200	16.03503800
C	31.24416800	8.46074600	15.23760000
H	30.81213700	9.16985700	14.52307100
H	31.91758800	8.99848500	15.91486900
H	31.81586300	7.70742100	14.68434400
C	29.29205700	8.82504700	16.79621200
H	28.46475500	8.32947100	17.31476200
H	29.92135400	9.34499200	17.52827300
H	28.88696800	9.56220900	16.09342100
C	30.70332300	6.74366800	17.00072100
H	31.24091400	5.97072500	16.44069800
H	31.39843400	7.22781300	17.69656800
H	29.89936300	6.27933700	17.57980000
O	26.68894300	1.72772300	16.62575800
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C 25.87527500 0.93042300 16.17181200

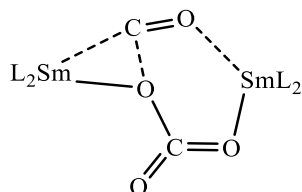


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Si	19.75959900	1.76487600	16.46468300
O	24.69908600	3.95243300	16.45264600
O	24.43879000	1.83788300	15.61399900
O	26.27463100	4.42122200	19.47158000
O	28.55360600	5.22794400	20.92326800
O	28.43777200	3.16554000	19.26923800
O	27.13432600	3.14325200	21.80339100
O	20.10928100	2.40934200	15.01232400
O	18.29557800	0.98722000	16.59808200
O	21.13063700	0.72031100	16.57744800
O	19.90291100	2.73686600	17.80139600
C	23.99756000	3.16728300	15.81613800
C	28.29836600	6.27914000	21.89540100
C	26.82405700	6.70694600	21.87112000
H	26.53666600	7.01025800	20.85920400
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H	26.17886400	5.87899400	22.18614000
C	29.19862500	7.44777400	21.47253600
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H	29.09535100	8.28086300	22.17732300
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H	30.55837900	3.59009800	17.72345700
H	31.78827000	2.99253900	18.86270300
H	30.78740300	4.40967900	19.29114000
C	30.07811700	2.30084300	20.91124900
H	30.12568500	3.25838100	21.43874800
H	31.05217700	1.80322600	20.98562200
H	29.31970200	1.67224700	21.38643100
C	29.66062100	1.17614700	18.69990800
H	28.90491600	0.54143000	19.17397400
H	30.63064600	0.66716000	18.73686800
H	29.37874200	1.32402900	17.65323500
C	26.01505200	2.23360700	21.99203900
C	26.27236900	1.56903300	23.35180000
H	27.22277300	1.02447100	23.32684200
H	25.46297100	0.86971200	23.59042200
H	26.32555100	2.33594200	24.13223200
C	25.98944000	1.17645000	20.88022500
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H	15.75182100	-0.93366400	15.59968400
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C	16.91814200	1.39599200	14.63135800
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H	20.71558500	-1.15727600	19.38795900
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H	21.79186900	1.77054000	18.95492400
C	18.99314600	3.77796300	18.25608600
C	19.86946200	4.77062200	19.03114700
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H	17.27427800	3.90391700	19.57720700
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O	22.49327700	0.39032100	12.53419200
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O	27.31777800	6.11273200	16.68931700
O	27.10269600	6.14272500	13.87815500
O	28.49940000	4.38574400	15.29583700
O	29.31769700	7.10223200	15.00195000

C	24.62853600	2.27196400	9.58476400
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H	26.44638800	2.72648900	10.67015000
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C	24.37605500	-1.15727400	12.55645200
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H	20.98657500	-1.70595300	13.11348600
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H	22.29706800	-1.55291500	14.31799700
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H	21.45435900	-1.23952900	10.66553000
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H	19.64474500	0.46935700	8.74337600
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H	20.18454000	1.98317300	7.97414000
C	20.04953500	3.59682600	10.20295700
H	20.61960600	4.02806300	9.37220300
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C	26.00471200	8.27831300	14.44066000
H	26.87812300	8.67856400	14.96674100
H	25.44602700	9.11539200	14.00542800
H	25.36745200	7.75659600	15.16185700
C	25.21471700	6.77609500	12.58150300
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H	28.30509300	8.32957500	12.89581900
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H	27.32055900	3.94969700	12.90957000

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C	29.32755200	8.79468000	16.75790300
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C	30.73648300	6.71270100	16.96683300
H	31.27201900	5.93704700	16.40863700
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C	25.65608500	1.11776700	16.06805300



transition state

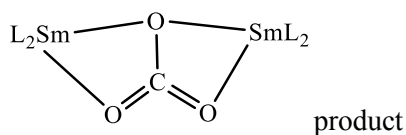
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O	27.25209200	3.15823700	21.81137800
O	20.18384900	2.37257400	14.98350300
O	18.30859700	0.98240400	16.52789400
O	21.12988700	0.62012000	16.53286400
O	19.95220000	2.65532000	17.77948300
C	23.77441700	3.48952600	15.85650900
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C	26.85547100	6.75672100	21.98685000
H	26.55984900	7.08691500	20.98573700
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H	26.21954200	5.91397100	22.28087200
C	29.21967000	7.53463800	21.59916500
H	30.26850500	7.21955200	21.56794500
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H	29.80582200	5.50420100	23.33990400
C	29.79996800	2.63272700	19.36305800
C	30.81463400	3.45745100	18.56605800
H	30.48974600	3.55992800	17.52487000
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C	30.24156100	2.51673800	20.82678700
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C	29.60496200	1.24242100	18.74847700
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H	30.55498400	0.69595500	18.75010900
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C	26.11747000	2.26695700	22.01721700
C	26.43035700	1.53026300	23.32680000
H	27.36047300	0.96072000	23.22188200
H	25.61458200	0.84269100	23.57689600
H	26.55004900	2.25542000	24.13901000
C	26.00008500	1.26806800	20.85950500
H	25.77281500	1.78984300	19.92461100
H	25.19173400	0.55645500	21.06329600
H	26.93677500	0.71297700	20.74105900
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H	23.98279300	2.43467600	22.35974400
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C	16.38406500	-0.36144300	16.19425400
H	15.71824600	-0.83985600	15.46689600
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H	16.80558600	-1.12681200	16.85504800
C	16.94555100	1.49071000	14.57480700
H	16.34272700	2.17932200	15.17770400
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C	18.36059800	-0.60078600	14.65185400
H	18.80149900	-1.35616700	15.31126200
H	19.16178400	-0.06413600	14.13405400
H	17.73281700	-1.10021400	13.90459300
C	21.55721100	-0.12881600	17.72439200
C	20.33078300	-0.64058400	18.49106900
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H	21.79166200	-1.94093200	16.55737500
C	22.40883000	0.79293200	18.60553100
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C	18.43093100	4.45647100	17.05658900
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H	17.40301000	2.36843400	18.56152600
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O	22.43822000	0.27527700	12.52028500
O	21.57606100	1.59630600	10.16170400
O	27.32153300	6.19042800	16.78458300
O	26.97222800	6.25797400	13.98811000
O	28.39970600	4.46016800	15.32102400
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C	24.77422600	1.93852200	9.59674800
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C	26.27430700	1.64027500	9.72280100
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H	26.82133600	2.09567100	8.88932100
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C	24.22186500	1.34580300	8.29273900
H	23.14262400	1.51368900	8.23605700
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H	24.41643300	0.26742600	8.26686400
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C	21.83046100	-1.92097000	13.27034500
H	20.77576800	-1.72358800	13.05187100
H	22.01950900	-2.99636900	13.17668000
H	22.04208700	-1.62629900	14.30409700
C	22.39169400	-1.53379300	10.85182000
H	23.03349800	-0.98787600	10.15457700
H	22.55672000	-2.60932200	10.71801700
H	21.34533600	-1.30184700	10.63000500
C	20.25773500	2.20854200	10.10469600
C	19.36604500	1.67156000	11.23056500
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H	25.39065600	6.22942200	11.92411400
C	27.26231800	8.15987300	12.50840400
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H	26.77100100	9.03778200	12.07236900
H	28.16152700	8.47523400	13.04668100
C	28.80689100	3.63559200	14.17173100
C	27.55107600	3.20968600	13.40329300
H	27.03432200	4.09240500	13.01817800
H	27.82973600	2.55402400	12.57064100
H	26.87081300	2.66195100	14.06343400
C	29.51961600	2.41127500	14.75485700
H	28.83632500	1.85240300	15.40373400
H	29.84041000	1.74918000	13.94249400
H	30.40074500	2.72067600	15.32743800
C	29.75949600	4.43509200	13.27529400
H	30.62633900	4.77553300	13.85070000
H	30.10307000	3.79729700	12.45257000
H	29.24806900	5.30682000	12.85537800
C	30.13048600	7.81540800	15.98552100
C	31.23565600	8.46941500	15.14518400
H	30.79024700	9.17189400	14.43241300
H	31.93351400	9.01048800	15.79433100
H	31.78379100	7.70189100	14.58776900
C	29.33198500	8.87799400	16.75242700
H	28.51473500	8.39934100	17.30199500
H	29.98618900	9.40256700	17.45871000
H	28.91529200	9.60839800	16.04939700
C	30.72935200	6.78641400	16.95057200
H	31.24478600	6.00040600	16.38810800
H	31.44702000	7.27536400	17.61964800
H	29.93724300	6.33772600	17.55772700
O	26.48213700	1.87709700	16.71308700
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C	25.68331500	1.08771000	16.17598600

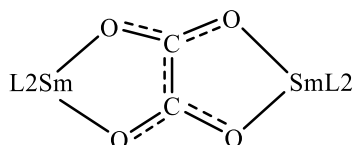


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Si	19.91236000	4.01455300	18.33480400
O	23.89991700	-1.40341000	18.02192300
O	23.47168800	0.60822200	17.16908000
O	21.79001100	-0.83589900	17.40467700
O	25.94505300	1.27228100	19.80306800
O	28.57764500	0.93458600	20.74056400
O	27.05142200	-0.98629200	19.74861400
O	26.54765300	0.16281200	22.30193000
O	20.68063000	2.98111700	17.32245800
O	20.96993700	5.12533000	19.00808200
O	18.70595900	4.73266900	17.43405100
O	19.15444300	3.25821400	19.62064100
C	23.03171100	-0.60882900	17.55647900
C	29.13582900	2.08175700	21.44033500
C	28.12725200	3.23804900	21.50015600
H	27.79622100	3.50463900	20.49112600
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H	27.25185100	2.95274600	22.09445200
C	30.36925900	2.49271400	20.62502400
H	31.06489900	1.64887500	20.55845900
H	30.87603400	3.33756200	21.10527800
H	30.06445800	2.78269900	19.61366500
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H	28.66281200	1.29370000	23.40126200
H	30.00748400	2.47226900	23.39070500
H	30.26565100	0.81495400	22.78473900
C	27.83660900	-2.21086800	19.95908200
C	28.97728100	-2.19782000	18.93676000
H	28.57380800	-2.15154200	17.91917100
H	29.58054200	-3.10807800	19.03229900
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C	28.40063500	-2.26874300	21.38408400
H	29.07092100	-1.42269700	21.56258600
H	28.96328900	-3.20195800	21.50398900
H	27.59290400	-2.24080600	22.12038600
C	26.88113400	-3.38457000	19.71742500
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H	27.41930300	-4.33364900	19.82201200
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C	25.20409000	0.08562200	22.85842500
C	25.40365300	-0.40396300	24.29959300
H	25.88102100	-1.39018500	24.29558900
H	24.43768800	-0.47511900	24.81203700
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C	24.34597500	-0.91334900	22.07176900
H	24.19358200	-0.57010600	21.04368500
H	23.36511700	-1.01737500	22.55016600
H	24.83161300	-1.89501200	22.05018600
C	24.57152100	1.48314900	22.84745800
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C	22.01983200	5.86214100	18.33272500
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H	23.15080200	4.09334600	17.80033600
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H	20.69388100	6.77245600	16.87023500
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C	17.54648300	5.46360900	17.89788500
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H	18.13622900	5.65927900	19.97950600
H	16.97916900	6.89618200	19.42136900
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C	17.14747200	6.37940000	16.73076300
H	16.24167700	6.94392900	16.98052200
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H	17.96129300	7.08117000	16.51619900
C	16.42661500	4.45497300	18.19423400
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H	15.51324200	4.97692100	18.50433900
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H	17.75603700	2.25100400	21.55843100
H	19.06991700	1.34214200	22.35638400
H	18.58184800	0.93396300	20.68754500
C	21.08057200	2.06334400	20.58746900
H	20.94265900	1.22527700	19.89471700
H	21.48485100	1.67226200	21.52786600
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C	19.91829400	3.92970500	21.82861600
H	20.32059600	3.56617500	22.78185600
H	18.94899100	4.40702000	22.01255500
H	20.60282200	4.66620100	21.39796400
Si	19.99134400	0.61064500	13.56829300
Si	27.04131500	0.76201800	15.08449300
O	21.26876400	1.47662700	14.07870700
O	20.26014100	-0.85795900	12.84665500
O	19.41472300	0.18215100	15.15190300
O	18.86208600	1.39796200	12.64237100
O	26.77957700	1.54618000	16.47831000
O	26.01502800	1.03393700	13.80486900
O	26.59285600	-0.82060500	15.63287600
O	28.58732600	0.83945200	14.47393500
C	20.51657600	-1.14203500	11.44317300
C	21.33480700	-0.01764700	10.79413500
H	22.26932000	0.13401400	11.34394000
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C	21.31345300	-2.45362300	11.43737000

H	20.73435800	-3.24074700	11.93258200
H	21.52937000	-2.76102200	10.40772900
H	22.25579700	-2.31521200	11.97824600
C	19.17021700	-1.32226300	10.72962100
H	18.59565100	-0.39260800	10.78591500
H	19.33339400	-1.58626800	9.67799700
H	18.60167100	-2.12565900	11.21191700
C	18.40053600	-0.80060400	15.56341900
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H	19.34777600	-2.43977800	14.51694000
C	18.00855700	-0.40763300	16.99291200
H	17.64068100	0.62397300	17.01875100
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H	17.49268800	-0.96364400	13.60033200
H	16.42273500	-1.41199200	14.95251300
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H	18.99739400	3.26439200	14.72288300
H	17.76952300	4.31411200	14.00874700
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C	17.30615700	2.91553700	11.69879200
H	16.47994500	2.31144800	12.08954800
H	16.98048700	3.95827100	11.61376400
H	17.57760900	2.54288500	10.70489400
C	19.69594900	3.62603800	12.08669700
H	19.93967700	3.28743600	11.07318600
H	19.43273000	4.68961900	12.05031900
H	20.57110400	3.49036100	12.72944300
C	25.97038300	2.20135400	12.93528900
C	26.10942900	3.48938600	13.75857400
H	27.09078100	3.53405500	14.24413500
H	26.00221600	4.36183300	13.10340600
H	25.33580000	3.52500600	14.53258100
C	24.59591600	2.14689100	12.25723900
H	23.79640100	2.16456200	13.00500800
H	24.47536100	3.00060300	11.58045500
H	24.50817900	1.22063100	11.67819400
C	27.08513600	2.09366900	11.88550000
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H	28.06356900	2.08349500	12.37357500
C	26.30564200	-1.99708100	14.79933900
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C	26.46074800	-3.21749900	15.71202800
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H	26.26644300	-4.13322900	15.14211300
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C	27.30360600	-2.06468000	13.63724600
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H	30.73854300	1.59688900	13.23663700
H	31.90372200	1.22563100	14.53711300
H	30.93610500	-0.08176000	13.79829200
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H	28.95786000	2.81584300	16.29724300
H	30.72488500	2.94448500	16.05722900
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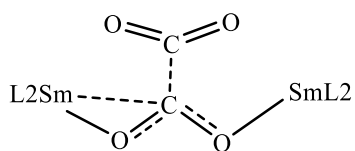


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O	24.99919400	8.80295900	19.25124700
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O	27.14314000	8.82524600	20.77011900
O	24.63081100	9.08915700	21.95728000
O	20.37135800	2.25565700	18.67395800
O	19.04159300	3.12793200	20.89792500
O	18.52379000	0.66250800	19.72604200
O	20.77981100	1.11570700	21.14362200
C	23.72817700	4.94045000	17.18794800
C	24.70033200	12.10146100	20.72025200
C	23.42756200	11.65472800	19.98538800
H	23.65787300	11.43342000	18.93787100
H	22.67833000	12.45413100	20.02445400
H	23.01046100	10.75743100	20.45424900
C	25.27365300	13.36512500	20.06295100
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H	23.65140400	13.14337000	22.31439800
H	25.32704600	12.67804700	22.71056500
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C	28.95162800	10.42238000	20.97730000
H	29.33222000	10.10120600	20.00105200
H	29.79433600	10.74774400	21.59914100
H	28.25855200	11.25622000	20.83175800
C	27.68007500	9.67732900	23.02768700

H	27.01943500	10.54462600	22.93165900
H	28.52072800	9.94111500	23.68035900
H	27.11800500	8.85584100	23.48315200
C	29.13953200	8.04111500	21.78792100
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C	23.99645400	7.82916100	22.28406200
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C	24.89724500	6.63431900	21.93470100
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C	22.65990300	7.73812600	21.53324100
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H	22.13200500	6.81538700	21.80177600
H	22.83996700	7.74939300	20.45367000
C	17.91097100	3.95846800	20.53961800
C	18.10364100	5.26556600	21.32259200
H	17.26743900	5.94898400	21.13625600
H	19.03695700	5.74888600	21.01288200
H	18.15622200	5.04659000	22.39474000
C	17.86581600	4.25113100	19.03181900
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H	17.02281600	4.91722200	18.81417200
H	17.73508300	3.32374900	18.46267900
C	16.61842600	3.25763800	20.98328700
H	16.66557300	3.04644800	22.05736500
H	16.50522900	2.31493400	20.43900800
H	15.75172500	3.89844600	20.78254200
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C	17.94378200	-0.30865600	21.91648500
H	18.87224200	0.04566500	22.37328000
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H	17.16079200	0.44258200	22.06235000
C	16.85359900	-1.01916300	19.75963600
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H	16.08169800	-0.25342000	19.89534700
C	19.26761800	-1.60204300	20.19428500
H	19.41726700	-1.75042500	19.11894100
H	18.98330800	-2.55800000	20.65059500
H	20.20157900	-1.24876300	20.64162300
C	21.75663100	1.77892700	21.98393700
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H	22.42374700	-0.15528400	22.69313900
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H	23.31734000	0.45254700	21.27649000
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H	20.26828200	2.87360300	23.10874700
Si	20.86404500	1.30696200	14.24933300
Si	26.48606600	9.10419700	14.92629800
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O	21.80359700	1.69093400	12.93683900
O	22.04122200	1.01470600	15.49758800
O	19.98602600	-0.03963200	13.84224400
O	25.07221500	9.41038200	15.66308400
O	26.46958400	8.26671600	13.49451800
O	27.03615700	7.91163000	16.06973200
O	27.53659200	10.37253800	14.73756600
C	21.35483200	1.94410500	11.57472400
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H	22.17314000	3.08793700	9.91982500
H	22.45880400	3.80784600	11.52883400
C	21.30575900	0.60705100	10.82388900
H	20.58018200	-0.05952600	11.30016000
H	21.01729200	0.77220500	9.77902700
H	22.29418200	0.13431300	10.84840700
C	23.25372700	0.18313400	15.47125900
C	24.38043100	0.99297000	14.82007100
H	24.56178500	1.90846600	15.39418200
H	25.30192800	0.39921000	14.80386500
H	24.09840200	1.25890500	13.79751200
C	23.57554300	-0.12259500	16.93894400
H	22.72884300	-0.62841600	17.41580200
H	24.45853600	-0.76837100	17.00124000
H	23.79764100	0.80418600	17.48313700
C	22.97354800	-1.10612800	14.69356500
H	22.72412800	-0.87573000	13.65301800
H	23.86669000	-1.74120800	14.71147800
H	22.13882100	-1.65014100	15.14579600
C	18.77975400	-0.56178600	14.47301600
C	19.02033200	-0.81513800	15.96609400
H	19.18541900	0.12266900	16.50625600
H	18.14258400	-1.30313300	16.40496700
H	19.89007300	-1.46751700	16.10090500
C	18.50173400	-1.88587700	13.74785000
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H	18.36933100	-1.69938800	12.67649600
C	17.62100500	0.42135600	14.26204100
H	17.46076200	0.58195100	13.18971900
H	16.70172400	0.01366100	14.69834800
H	17.85352200	1.37959700	14.73674400
C	26.16291300	8.78621800	12.16919900
C	25.11997600	9.90966300	12.24744700

H	25.52554700	10.77190400	12.78840600
H	24.84589200	10.23198900	11.23619600
H	24.22280100	9.55567800	12.76629600
C	25.60154200	7.59068500	11.38783800
H	24.68328100	7.23277400	11.86638800
H	25.37788000	7.88386200	10.35575800
H	26.33590200	6.77781700	11.37776900
C	27.46688300	9.28577800	11.53387900
H	28.19354400	8.46656900	11.49113500
H	27.27691700	9.64545300	10.51577600
H	27.88317100	10.09998600	12.13513300
C	28.20431500	7.01844300	16.02615800
C	27.87863500	5.83438000	15.10916000
H	27.66037500	6.19462000	14.10028900
H	28.73172400	5.14659400	15.07837100
H	27.00638800	5.29553100	15.49565400
C	28.41676200	6.54747200	17.46989400
H	27.55956100	5.95187500	17.80930900
H	29.30777500	5.91204800	17.52595000
H	28.54904700	7.40536900	18.13841100
C	29.42185200	7.79861500	15.52114300
H	29.61558500	8.66009800	16.16750300
H	30.30006500	7.14285600	15.52764600
H	29.25297600	8.15407900	14.49977600
C	27.63683400	11.59351200	15.52882100
C	28.90936800	12.28439900	15.02048900
H	28.81955700	12.47984400	13.94632600
H	29.05902500	13.23430300	15.54593600
H	29.77787900	11.63894100	15.19098800
C	26.40514200	12.46985500	15.26640800
H	25.49960700	11.94480100	15.58676100
H	26.49218000	13.41266000	15.81936900
H	26.33078600	12.69499600	14.19632000
C	27.76720700	11.26519900	17.02027500
H	28.60683000	10.58211700	17.18645400
H	27.94454700	12.18373000	17.59084800
H	26.84973900	10.80595300	17.40198900
O	21.36547900	5.29796800	16.90320000
O	22.69262000	7.10768800	17.05262900
C	22.47712900	5.86966900	17.03352200
O	23.51522900	3.70136300	17.15423900



transition state

Sm	24.87129500	6.61684500	16.97352500
Sm	21.08687500	2.75103100	14.16285500
Si	24.81419300	6.93018400	20.07350800
Si	18.72348900	1.98483200	16.05327300
O	24.62176500	4.16124300	16.51264000
O	23.17719200	2.70700400	15.50401600
O	23.81041900	7.16199800	18.81857100
O	25.69706800	8.22749800	20.62198700
O	26.00026400	6.00794400	19.21791600



O	24.18637600	6.16283200	21.40312800
O	19.18118600	3.24467800	15.15491700
O	17.19314900	1.39030600	15.80455600
O	19.97282400	0.88865600	15.54089400
O	18.93744000	2.07168300	17.70365800
C	23.65348600	3.81794600	15.81147800
C	25.21210000	9.33697100	21.43139500
C	23.75505600	9.67354300	21.09035900
H	23.65649100	9.88304200	20.02529200
H	23.43787300	10.55421200	21.66628200
H	23.09632200	8.83652100	21.34760700
C	26.13087300	10.51650900	21.08689800
H	27.17119000	10.25393400	21.30261200
H	25.85150500	11.39615800	21.68043600
H	26.03491200	10.76159600	20.02228200
C	25.35476700	8.95498700	22.91121800
H	24.73801800	8.07619300	23.12988200
H	25.04499700	9.79148400	23.54892600
H	26.40561900	8.71084800	23.12954300
C	27.23914900	5.40351200	19.72667000
C	28.40438000	6.25621400	19.21614600
H	28.37559900	6.31868800	18.12341800
H	29.35869700	5.81579000	19.52583400
H	28.32240800	7.26622600	19.63025600
C	27.24200400	5.36143500	21.26044100
H	27.18380900	6.37481900	21.66921800
H	28.18187300	4.89648600	21.59486000
H	26.40262600	4.77855400	21.63803700
C	27.29275500	3.98178800	19.15783600
H	26.43819900	3.40436800	19.51312200
H	28.22117100	3.48525500	19.47742200
H	27.27159300	4.00437900	18.06436300
C	23.04776100	5.25592000	21.44224600
C	23.03183000	4.70357200	22.87731900
H	23.96811900	4.16414400	23.07443600
H	22.18846500	4.01858900	23.00960200
H	22.94052100	5.52770800	23.58932700
C	23.23179200	4.11278200	20.43369000
H	23.24495100	4.50885300	19.41318600
H	22.40301400	3.40147700	20.51926400
H	24.17311800	3.58854700	20.62765300
C	21.75737200	6.03719500	21.15739500
H	21.64856500	6.85222300	21.88918700
H	20.89106200	5.37784400	21.24210200
H	21.79634400	6.46495600	20.15038100
C	16.33406500	1.58176500	14.64513200
C	15.11507600	0.68363600	14.91092400
H	14.39228300	0.77744300	14.09596600
H	14.63829400	0.97668600	15.85021500
H	15.43222900	-0.36410300	14.99221500
C	15.91108700	3.05170100	14.56298300
H	15.40154500	3.34407500	15.49533400
H	15.21742900	3.20043200	13.72535700
H	16.79138600	3.68483700	14.42166100
C	17.03907100	1.14528400	13.35647800

H	17.37622200	0.10482900	13.44816700
H	17.90123300	1.78657200	13.15177700
H	16.34626000	1.21630200	12.51354400
C	20.34817000	-0.37881300	16.18210900
C	19.10604800	-1.07099900	16.75664800
H	18.66354700	-0.45618900	17.54966600
H	19.39889000	-2.04067500	17.17599900
H	18.36079700	-1.22511800	15.97142400
C	20.97412500	-1.24316400	15.08465600
H	21.30730000	-2.19736000	15.50871400
H	21.84107000	-0.73811900	14.64643800
H	20.24153500	-1.43488700	14.29505500
C	21.36919600	-0.07099000	17.28657800
H	22.24157500	0.44250500	16.86719700
H	21.69542600	-1.00209300	17.76147900
H	20.90504900	0.57511900	18.04205900
C	18.23971000	2.94552200	18.63199900
C	19.15573400	3.02711200	19.86174000
H	19.31669500	2.01812800	20.26626300
H	18.68940700	3.64864500	20.63771600
H	20.12406500	3.46117200	19.58095400
C	18.04449700	4.34457400	18.01545300
H	18.99786200	4.69262700	17.59195000
H	17.69850700	5.05004800	18.77975000
H	17.30381400	4.31386800	17.20192500
C	16.89203600	2.30684400	19.00150000
H	16.36599500	2.94141800	19.72427600
H	17.05678200	1.32119500	19.45120800
H	16.27099200	2.19345200	18.10308500
Si	21.66943400	2.05983200	11.12123800
Si	26.56784100	8.50078100	15.13391200
O	20.45014400	2.58391600	12.06481500
O	22.60677400	3.20119000	10.36544800
O	22.68488200	1.45719300	12.37293200
O	21.27432200	0.93824300	9.95613600
O	25.49158500	8.63993800	16.33725900
O	25.98453300	8.45444400	13.57743000
O	27.00477500	6.85227000	15.42077700
O	27.85525000	9.55719600	15.13302700
C	22.25664800	4.00644700	9.20495900
C	20.75447400	4.32258700	9.17999900
H	20.45616100	4.81651100	10.11035100
H	20.53229800	4.98460300	8.33463000
H	20.17051800	3.40274000	9.06433300
C	23.07050900	5.29952200	9.34821400
H	24.13867200	5.06011900	9.39744500
H	22.89061100	5.95672900	8.48968100
H	22.78183300	5.82086400	10.26720300
C	22.67636900	3.23938900	7.94400700
H	22.12766200	2.29422400	7.88205600
H	22.46561400	3.83892400	7.05046800
H	23.75073600	3.02610900	7.97782300
C	24.08207100	1.02283000	12.22734300
C	24.98479800	2.25733500	12.31188500
H	24.83746500	2.75433600	13.27527500

H	26.03577800	1.95599400	12.22900400
H	24.73540500	2.95260900	11.50579300
C	24.36036300	0.07358700	13.39715000
H	23.70720800	-0.80329800	13.33828000
H	25.40353100	-0.26128300	13.36204700
H	24.19017500	0.59122100	14.34711400
C	24.28072100	0.28932000	10.89177500
H	24.10105700	0.96848100	10.05280200
H	25.31218300	-0.07802300	10.83427700
H	23.59502400	-0.55995400	10.81777400
C	20.21433800	-0.05351600	9.97489700
C	20.18560300	-0.80123900	11.31374100
H	19.93585800	-0.10987700	12.12462900
H	19.42947800	-1.59475400	11.28339200
H	21.16541200	-1.24811400	11.51809900
C	20.55031900	-1.01840600	8.82930100
H	21.52314600	-1.48827000	9.01630400
H	19.78320200	-1.79716500	8.74981800
H	20.59834400	-0.46484400	7.88523300
C	18.87227900	0.64424100	9.71649400
H	18.90729800	1.16687700	8.75383500
H	18.06218100	-0.09413500	9.68868400
H	18.67464300	1.37040300	10.51120700
C	25.39577200	9.54205000	12.81057400
C	24.58934400	10.48558600	13.71753800
H	25.24875900	10.97690600	14.44151200
H	24.10450500	11.25751600	13.10336100
H	23.82585200	9.92424500	14.25985100
C	24.46422300	8.86143600	11.79916600
H	23.70432300	8.28447700	12.33190600
H	23.97390100	9.61260900	11.16422800
H	25.04055000	8.18202800	11.16128600
C	26.51834600	10.29526400	12.09202600
H	27.07569200	9.60875300	11.44579400
H	26.10129300	11.10128300	11.47662500
H	27.20906800	10.72430200	12.82747800
C	27.72750700	5.97169000	14.49183800
C	26.70894500	5.34203900	13.53177300
H	26.17859800	6.12888900	12.98810400
H	27.22018400	4.68377300	12.81935500
H	25.99212000	4.74207100	14.10116100
C	28.38860800	4.88639900	15.34754900
H	27.62701900	4.32117400	15.89594700
H	28.94132800	4.18991200	14.70222900
H	29.08736900	5.33714200	16.05981900
C	28.79630100	6.76713100	13.73142900
H	29.47443800	7.25879200	14.43598000
H	29.37162700	6.08243000	13.09729000
H	28.32938300	7.52163400	13.09771100
C	28.37114600	10.36143200	16.22770300
C	29.66051800	10.98656300	15.67798500
H	29.43326200	11.57924400	14.78528500
H	30.11733500	11.63606300	16.43336200
H	30.36961800	10.19690200	15.40611400
C	27.34934200	11.45034600	16.58346300

H	26.42322600	10.98037200	16.93859300
H	27.74876300	12.10244600	17.36948200
H	27.13327100	12.05845700	15.69283300
C	28.68098100	9.48795600	17.44750000
H	29.37791300	8.68598400	17.16738300
H	29.14651700	10.09988000	18.22915700
H	27.76574700	9.05186900	17.84642000
O	23.03250700	6.50758400	15.42142300
C	22.62925700	5.39829900	15.01140800
O	21.73037800	5.07185800	14.21656500