Supplementary Information for:

Labilized Ligands Under Ultra-Confinement: A Solid-State ^{2}H NMR Investigation of $Ln(BH_4)_2(THF)_2/HY_{30}$

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1. Experimental Details

1.1. Synthesis

1.1.1. $Sc(BH_4)_3(THF)_2$

$Sc(BH_4)_3(THF)_2$ was synthesized using literature methods.[1,2] Briefly, $ScCl_3$ (1.516 g, 10.01 mmol) and excess sodium borohydride (1.515 g, 40.05 mmol) were heated at reflux in dry THF (100 mL) for 5 days. The solution was filtered through a cannula wrapped with filter paper to remove the residual $NaBH_4$ and NaCl. The filtrate was concentrated to saturated solution by evaporating under reduced pressure and then cooled at –30 °C for 2 days, providing 1.905 g (81% yield) $Sc(BH_4)_3(THF)_3$. The colorless powders were stored at –30 °C freezer in a N_2 glovebox. $Y(BH_4)_3(THF)_3$ and $La(BH_4)_3(THF)_3$ complexes were prepared via the same protocol. To deuterate the compound, 0.100 g of $Sc(BH_4)_3(THF)_2$ was stirred with 0.2 mL THF-d_8 at room temperature for 30 h and then was evacuated under vacuum (10^{-3} mbar) for 12 h.

1.1.2. $Ln(BH_4)_2(THF)_2/Y_{30}$

0.020 g of $Sc(BH_4)_3(THF)_3$ (0.075 mmol) was dissolved in toluene (10 mL) and added to 0.300 g of zeolite HY_{30} that had been capped by Ph_3SiCl (namely $Ph_3Si\text{-}HY_{30}$).[2,3] The mixtures were stirred at room temperature for 20 h. The supernatant was decanted and the solids were washed with toluene (3×10 mL). The obtained solids were then dried under vacuum (10^{-3} mbar) at room temperature for 24 h, giving $Sc(BH_4)_2(THF)_2/Y_{30}$. The material was subsequently deuterated by taking 0.100 g $Sc(BH_4)_2(THF)_2/Y_{30}$ and stirring it with 0.2 mL THF-d_8 at room temperature for 30 h. The material was then evacuated under vacuum (10^{-3} mbar) for 12 h. The procedure was repeated to prepare the Y and La analogues. Metal loadings were measured using inductively-coupled plasma optical emission spectroscopy (ICP-OES) and equaled 0.16, 0.069, and 0.076 mmol/g for Sc, Y, and La, respectively.

1.2. Solid-State ^2H NMR Spectroscopy

All solid-state NMR experiments were performed using an Agilent DD2 400 MHz NMR spectrometer equipped with a Chemagnetics 5 mm magic-angle spinning (MAS) probe operated as a static probe. Samples were flame-sealed into 5 mm NMR tubes to prevent their degradation and inserted directly into the coil of the probe. Samples were cooled using a nitrogen heat exchanger in a temperature range of 20 to -120 °C. The ^2H NMR spectra were acquired using a quadrupolar echo sequence with 2 µs excitation and refocusing pulses and a 30 µs delay. The number of scans was varied for each sample and temperature to obtain a reasonable signal-to-noise ratio and varied between 1024 and 10240 scans. The recycle delay was set to 2 s.

1.3. Density Functional Theory

1.3.1. Cluster Model Calculations

Density functional theory (DFT) calculations were performed on a large cluster model of the micropore in zeolite Y consisting of 37 interconnected silicon tetrahedral sites that were hydride-terminated. The desired $Ln(BH_4)_2(THF)_2$ was coordinated to an oxide site bonded to an aluminum tetrahedral site, to mirror the experimental chemical environment as closely as possible. Geometry optimizations froze the positions of the silicon atoms to those from the crystal structure to prevent the pore from relaxing in response to the grafted complex, which could influence the computed steric effects. The geometry-optimized structure for the La analogue is depicted in **Figure S1** and the coordinates are also given for the three supported complexes below. Calculations were all performed at the PBE-D3/TZP[4,5] level of theory using the Amsterdam Density Functional (ADF) program.[6]

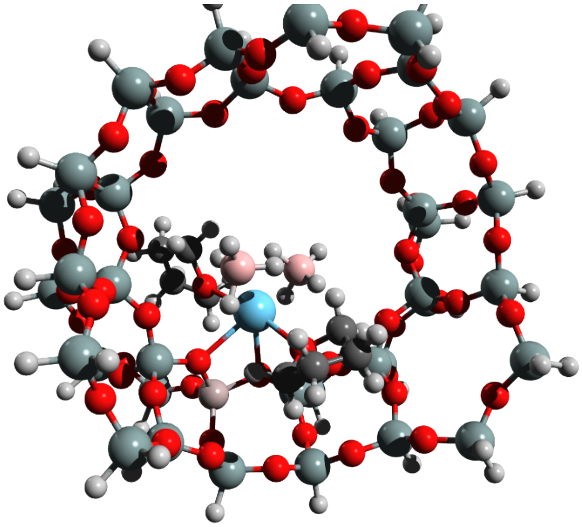


Figure S1. Geometry-optimized structure of $La(BH_4)_2(THF)_2/Y_{30}$.

1.3.2. Plane Wave Calculations

The activation energy barrier for intramolecular THF exchange was investigated using the nudged elastic band (NEB) method[7,8] as implemented in the neb.x module of the Quantum ESPRESSO (v7.1).[9,10] Calculations used the PBE exchange-correlation functional.[4]

Pseudopotentials were taken from the SSSP library.[11] Kinetic energy cutoffs for wavefunctions and charge density were set to 544 eV and 2177 eV, respectively. Brillouin zone integration was performed using Gamma-point sampling due to the large size of the simulation cell. To determine the energy barrier, the climbing-image NEB (CI-NEB) scheme[9,10] was used with 11 images to identify the saddle point. Calculations were considered converged when the forces on the climbing image fell below 0.05 eV/Å.

2. Density Functional Theory

2.1. THF Rotation

We performed potential energy surface scans as a function of the O-Ln-O-C dihedral angle in a Ln-bonded THF to rotate the ligand around its metal-oxygen bond. The scan was performed in 10° increments and yielded rotation barriers of 17.4, 17.5, and 20.6 kJ/mol for the La, Y, and Sc complexes, respectively. The full list of relative energies are listed below in **Table S1**.

Table S1. Relative bonding energy as a function of THF rotation.

$\varphi_{\text{O-Ln-O-C}}$ / °	**Sc Δ*E* / kJ mol^{-1}**	**Y Δ*E* / kJ mol^{-1}**	**La Δ*E* / kJ mol^{-1}**
0	7.358016	2.163648	2.926199
10	9.178669	3.518879	3.493018
20	10.52416	4.742126	4.001288
30	11.39735	5.882406	4.783766
40	13.03558	8.063173	6.374793
50	15.42216	10.33693	8.277545
60	18.23869	13.78096	11.58764
70	22.12795	17.59972	15.39079
80	20.88793	15.62939	17.32951
90	18.93954	14.35673	12.66518
100	18.28894	13.49179	11.65638
110	17.18983	12.51395	11.40864
120	16.20217	11.87319	10.90417
130	15.51203	11.45443	10.62133
140	15.12086	10.23895	9.342868
150	12.83021	8.735616	8.079215
160	9.545189	6.978500	6.706525
170	8.736955	4.874241	4.931135
180	7.095729	2.109432	2.833807
190	5.688671	0.260712	1.583728
200	5.167010	0.000000	1.861086
210	5.832286	1.667508	3.660131
220	8.155538	2.806371	4.914831
230	12.83835	6.617284	8.614055
240	10.92686	12.39139	13.28603
250	17.89549	17.47121	17.38837
260	18.97982	16.55504	14.36889
270	14.86133	14.80315	13.28692
280	12.00751	12.78800	12.31753
290	10.70296	11.56031	11.27587
300	10.46902	10.47325	10.51426
310	8.401626	7.415305	5.155721
320	5.804088	3.769142	1.267408
330	2.408686	0.830708	0.000000
340	0.159630	0.135423	0.414750
350	0.000000	0.482409	1.346540

2.2. THF Dissociation

To estimate the free energy change associated with THF dissociation, geometry optimizations were performed on both $Ln(BH_4)_2(THF)_2/Y_{30}$ and $Ln(BH_4)_2(THF)/Y_{30}$ (Ln = Sc, Y, or La). Given that all silicon atoms' positions needed to be frozen, we could not estimate the free energy of the solid species because vibrational framework contributions to entropy have been neglected, however, we did estimate the entropy contributions from the THF translational and rotational degrees of freedom for the released THF as these are likely important. The translational entropy contribution was calculated as 0.1621 kJ/mol K, and the rotational entropy contribution as 0.1043 kJ/mol K, using the ideal gas rigid-rotor approximation. The bonding energies are listed in **Table S2** for the six complexes. Dissociation enthalpies equal 118, 111, and 87 kJ/mol for the La, Y, and Sc analogues, respectively, which are reduced to 40.3, 32.6, and 8.7 kJ/mol at 20 °C when considering the new degrees of freedom of the free THF.

Table S2. Bonding energies of $Ln(BH_4)_2(THF)_2/Y_{30}$ and $Ln(BH_4)_2(THF)/Y_{30}$

Model	E / kJ mol^{-1}
$La(BH_4)_2(THF)_2/Y_{30}$	-99845.35406
$Y(BH_4)_2(THF)_2/Y_{30}$	-99785.62787
$Sc(BH_4)_2(THF)_2/Y_{30}$	-99713.09967
$La(BH_4)_2(THF)/Y_{30}$	-92802.43295
$Y(BH_4)_2(THF)/Y_{30}$	-92750.38491
$Sc(BH_4)_2(THF)/Y_{30}$	-92701.73143
THF	-6924.567608

2.3. Intramolecular THF Exchange

The energy barrier for the intramolecular THF exchange in $La(BH_4)_2(THF)_2/Y_{30}$ was estimated using a minimum energy path (MEP) search via the climbing-image nudged elastic band (CI-NEB) method. The energy profile reaches its maximum when the two THF ligands pass each other in a sterically constrained configuration (**Figure S2**), resulting in a calculated energy barrier of approximately 150 kJ/mol. The conformational rearrangement requires the two BH_4 ligands to move in synchronization with the THF ligands; however, this collective motion is severely hindered by steric repulsion with the zeolite walls, which significantly increases the overall energy of the transition state.

In configurations where steric hindrance becomes excessive, the system alleviates the energy strain through the dissociation of one THF ligand from the La center, which occurs well before the system reaches the highest energy intermediate. Along this part of the MEP, a pronounced elongation of one La–O is observed, reaching 3.0 Å, indicating that one of the THF ligand is already in a nearly dissociated state. While the current DFT-based MEP calculation focuses on electronic energy at 0 K, in a real-world scenario, the dissociation of a ligand provides a significant entropic gain. This additional entropic contribution lowers the free energy barrier for dissociation, making it even more favorable than the positional exchange. Consequently, it is expected that the ligands will dissociate at an earlier stage than predicted by the static energy profile, effectively pre-empting the intramolecular THF exchange.

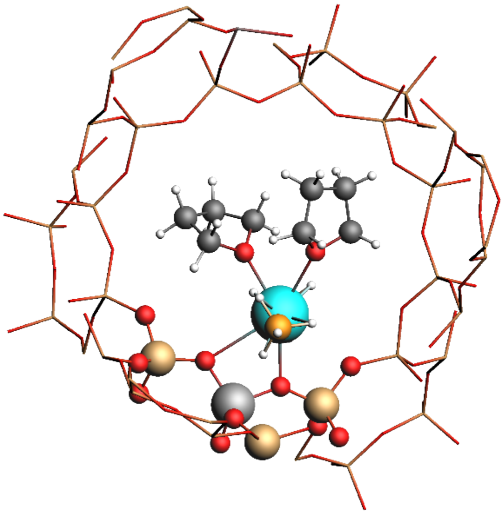


Figure. S2 Highest energy geometry of $La(BH_4)_2(THF)_2/Y_{30}$ as it performs intramolecular THF exchange.

3. Lineshape Simulations

All lineshape simulations were performed using an open-source program developed in our lab that is available in the following repository.[12] They assumed a quadrupolar coupling constant of 163 kHz and no axial asymmetry, consistent with the expected C_Q for C-D bonds in a cyclic ether environment. Polar angles were calculation from a given structure using the approach described by Bryce.[13] Briefly, the polar angles for a given internuclear vector were calculated as:

$$\beta = cos^{-1}\left(\frac{z}{\sqrt{x^2+y^2+z^2}}\right)$$

$$\gamma = \begin{cases} cos^{-1}\left(\frac{x}{\sqrt{x^2+y^2}}\right) & if\ y > 0 \\ 60° - cos^{-1}\left(\frac{x}{\sqrt{x^2+y^2}}\right) & if\ y \leq 0 \end{cases}$$

Calculations were performed using a 3-angle powder average comprising a 678-angle REPULSION grid[14] interleaved with a 15-step γ angle average. 256 time increments were considered with a spectral width of 400 kHz and 5 kHz of Lorentzian broadening. The full set of polar angles describing a single molecule are listed in **Table S3**. Additional tetrahedral averaging was performed to emulate the isotropic motion seen in the grafted species.

Table S3. Polar angles describing the rotation-related C-H bonds in $Ln(BH_4)_2(THF)_2/Y_{30}$

Site[a]	***β* / °**	***γ* / °**

α1	94	101
α1	141	287
α2	26	289
α2	150	264
β1	61	135
β1	84	252
β2	43	99
β2	134	336

[a]α and β refer to the respective positions of the two chemically distinct deuterons on THF. The numbers refer to ligands 1 and 2 on either side of the molecule.

Exchange rates were calculated on-the-fly for a given temperature and energy barrier using the Eyring relationship below. T refers to the temperature, k_B to the Boltzmann constant, h to the Planck constant, and $\Delta G^{\ddagger}$ to the free energy barrier.

$$k_{ex} = \frac{k_B T}{h} exp \left(\frac{-\Delta G^{\ddagger}}{RT} \right)$$

Component-based fits were also performed for the $Sc(BH_4)_3(THF)_3$ complex using the fast-motion limit lineshapes associated to libration, intramolecular exchange, and a combination of intramolecular exchange and THF rotation. THF libration was approximated with a lineshape having an averaged C_Q of 145 kHz and a 0.14 asymmetry parameter, which corresponds to a discrete case with a 30° libration angle. As the temperature was increased, the librating component was observed to narrow, suggesting an increase in librational amplitude. This was accounted for using a temperature-dependent order parameter ($\langle S \rangle$). The temperature dependent weights are listed in **Table S4** and are plotted in **Figure S3**.

Table S4. Weights used in the fit shown in Figure 3 for $Sc(BH_4)_3(THF)_2$

***T* / K**	**static**	**librating**	**exchange**	**exchange and rotation**	$\langle S \rangle_{libration}$
-120	56	39	6	0	1.00
-100	33	53	13	0	1.00
-90	15	62	23	0	1.00
-80	0	67	27	7	1.00
-70	0	61	30	7	0.95
-60	0	56	11	29	0.90
-50	0	52	0	45	0.90
-40	0	48	0	48	0.88
-30	0	44	0	52	0.85
-20	0	43	0	53	0.83
-10	0	36	0	60	0.75
0	0	31	0	65	0.72
10	0	18	0	82	0.72

20	0	0	0	100	0.72

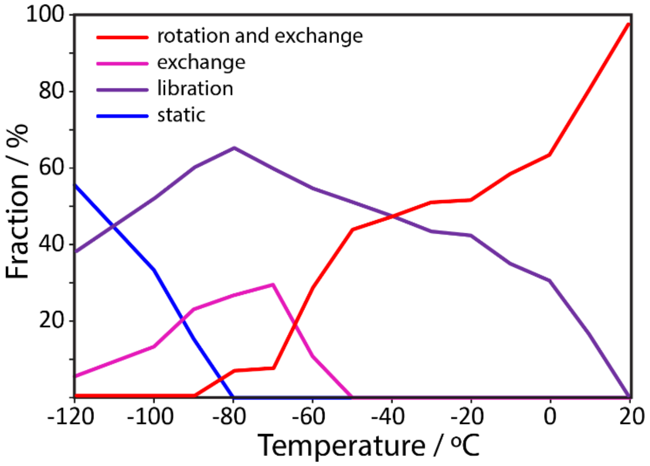


Figure S3. Temperature dependence of the weights used in the fit shown in Figure 3 for $Sc(BH_4)_3(THF)_2$.

Simulations of the variable temperature NMR data for the HY_{30}-supported complexes undertook a time-domain approach as only this method can simulate the narrowing of the isotropic resonance from intermolecular exchange. Nevertheless, these simulations incorporate a component from a purely rotating THF group that is visible as a baseline feature in the spectra and thought to originate from silanol-grafted sites that are visible by ^{11}B NMR.

4. Supplementary Figures

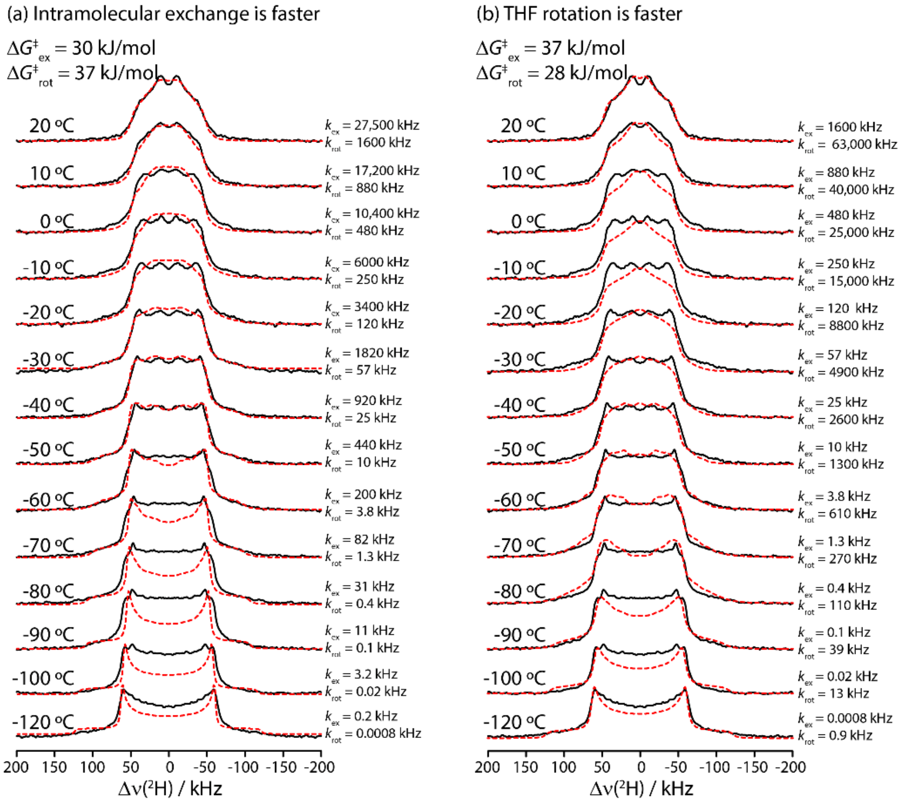
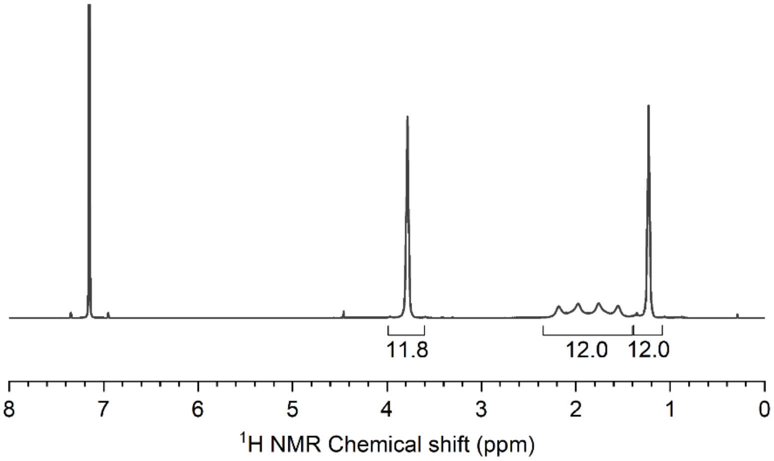


Figure S4. Variable temperature ^2H NMR spectra of $Sc(BH_4)_3(THF)_2$ with time-domain simulations assuming constant $\Delta G^{\ddagger}$ and that either (a) intramolecular exchange or (b) THF rotation is faster. The intermediate lineshapes have a cusp in the center and do not match the experimental result in (b) suggesting that THF rotation has the higher barrier.


(a) $La(BH_4)_3(THF)_3$

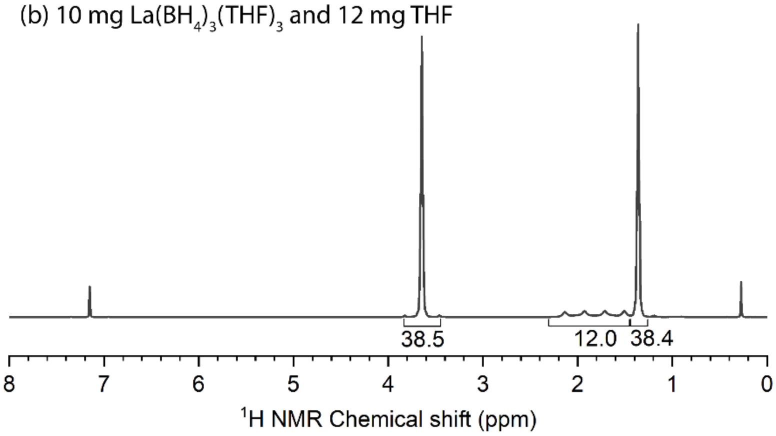

(b) 10 mg $La(BH_4)_3(THF)_3$ and 12 mg THF

Figure S5. Liquid-state ^1H NMR spectra acquired for C_6D_6 solutions of $La(BH_4)_3(THF)_3$ acquired without (a) and with (b) the addition of excess THF. As is evident from the spectrum and integrals, the excess THF is in rapid chemical exchange with the La-bound THF.

5. Geometry-Optimized Coordinates

5.1. $Sc(BH_4)_2(THF)_2/Y_{30}$

Sc	18.82325582801248	7.882464776531349	6.368538960153203
O	19.75020945829827	6.400044498581743	8.270558188712583
O	17.32500447640999	6.18331184580245	6.646229724860877
B	17.79948924507838	8.373394752749633	4.376676039017444
B	18.14587056465124	9.471422717708549	7.876485094275379
O	20.75205317999711	9.014652040565661	6.114441744959668
H	19.22816674017682	8.988733031264287	8.213834997127426
H	17.37764440658761	8.504086148507819	7.747424933790826
H	17.03463332175281	8.377037189322321	5.356016793320886
H	18.69844346972966	9.165701918422	4.679270979972886
H	18.28301164352391	9.900744249240342	6.722716443666361
C	15.49686960079504	4.796967902687604	5.956028079254798
Si	18.17039236111365	3.670904667623998	10.56821250977811

Si	16.08298507918421	5.274972788485146	12.19765473006501
Si	21.30777063098081	8.177328528424047	2.224290360708302
Si	19.83034330648602	10.47435528811806	0.8539809458493575
Si	18.494187349613	9.881468233758914	13.80418263901107
Si	13.41633800444066	11.68575293321304	9.949332174471733
Si	14.91892180604226	9.393209929388473	11.33423157194002
Si	22.74906296161497	6.601091327088554	10.62701218066163
Si	21.0410121424635	5.941662577004375	4.271742937360798
Si	17.5811833336759	7.926885367331652	11.53693984404205
Si	19.68358898635822	6.35703219482746	9.906124239924727
Si	24.08493298078833	6.188396541070476	5.008869029902728
Si	18.87698065889061	2.488932934351078	7.897700099083481
Si	23.52133086268682	5.462304697900136	7.926597821978866
Al	20.44347263326601	5.148373005955044	7.202613617537454
O	24.11914630745845	6.318403612109321	6.633877235839795
O	17.84829506467298	2.995490174503729	9.115259617872933
O	24.32847709066255	7.710074611067413	4.423878994377674
O	22.18480083254721	8.932279747240715	13.62195833798876
O	21.10987621900277	6.797960448511829	10.5789996237484
O	22.82489551393375	8.752666144541113	2.420755052235075
O	22.0955221355332	4.77611037574352	7.60963219613446
O	22.64343802066474	5.605798312058214	4.437107541047047
O	23.36631822273399	7.927094344134625	11.37967812091568
O	16.73453192216632	4.303713013478919	11.0569795990562
O	20.28517816830456	6.141766668606945	5.717432493161168
O	20.80755453926336	7.374299108435398	3.531268719170574
O	18.37980333177888	11.05875965529338	1.313446704816383
O	20.35252327677203	4.698950941771802	3.46605605642948
O	20.28132470344152	9.426254990726086	2.020344750268743
O	16.3467792302363	8.756830971512768	10.85496424977953
O	23.41303132593761	6.598272332723641	9.128709302578276
O	13.86615796856777	12.45808297925897	8.575077919959321
O	17.45326078068486	11.13099330780119	13.59340509529066
O	14.58086463049772	5.63438256836113	11.62444388053558
O	18.47034786048811	8.852107499572343	12.53067848295619
O	13.7586778552472	8.241063748897087	11.40575760835124
O	19.48050224678441	3.722606509400368	7.042248638495002
H	23.07305519491893	5.361462577519608	11.36860991435836
O	16.97243587802759	6.656548774097875	12.40999317864353
O	19.33536900193661	4.83850849721988	10.4539627532421
O	15.06536747596652	10.08171846122941	12.82919510309424
O	18.51040110420783	7.405379980486505	10.32237629660046
O	19.99329551239175	10.5426297938802	13.86971333952279
O	14.51589216742796	10.49601776684166	10.20212837989296
C	22.49889246752786	10.21836375358339	7.221103277394091
H	16.81019830784976	6.261943082918061	8.658949094748833
H	20.08346263466663	10.99717989668904	6.010893861032371
H	15.29930328483697	3.770177651570263	5.621138710232731
H	16.95147253947322	5.786264797132978	4.626436103465918

C	15.48121120586913	4.939082174881494	7.484887479229342
H	20.60895332943867	10.26699386831652	4.45929536857203
H	17.63620112072156	4.426252319213209	5.582291419095811
H	18.3343605653719	7.262898223297828	4.354109166766355
H	14.74787686206178	5.459946476590673	5.497942778614509
H	15.68401109368768	7.114662408347154	7.560972324924549
C	16.29098538446072	6.205563997063731	7.69601789552163
C	21.84030800953769	8.852109463090736	7.101453266471456
H	17.72068068102637	10.29490684597912	8.636639742760938
H	17.25563735779403	8.660438859145545	3.346301235720345
H	23.56264892396616	10.12527431654942	7.473984719245848
H	14.46878491954571	5.037431968791372	7.898864058263842
C	20.84229078573585	10.36475080377024	5.525502121353027
H	15.97330845476467	4.085268860018074	7.969035519043825
H	22.33319859867686	11.92238012243224	5.82349836497396
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H	22.00346875223456	10.81888643502012	7.99799405383331
C	22.25601863695498	10.82725321799374	5.832444158487859
H	22.52946578614912	8.101133035170909	6.701469924799821
H	21.40109304459322	8.487954726565267	8.03776128906868
C	16.9051008982379	5.24604469021247	5.578596063728931
Si	20.14813849983376	3.95907653282789	2.00159450400948
Si	23.61803910669732	8.499798403550928	12.9059533807259
H	18.66071082571554	2.676795332262826	11.54419803330269
H	16.00600578825363	4.602022143088683	13.50919840799943
H	19.96202528514853	1.684056099157537	8.537771271724608
H	24.51731890527972	4.436668947214915	8.306794716560713
H	25.13302028532887	5.271013293316582	4.519769553775865
H	18.02281494344453	1.650738821807056	7.010795253176046
Si	13.41161157448859	6.735130455453435	12.01198116602707
H	12.05994605765219	11.12174859315991	9.806486412240682
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Si	20.35336841367202	6.224753548041149	-0.01019091238314268
Si	17.17047174853669	11.96569406600497	0.690450180692907
Si	15.12530476500975	13.54757639052923	2.307652399720728
Si	14.33431729544196	14.67762936089485	4.995983672759918
Si	13.65812962954835	13.9570828432801	7.934000485629821
Si	24.35086004922854	8.421095862204451	2.94355766547118
O	19.62183668801614	5.051695989834167	0.8750613002895602
O	19.13792539293354	7.090907987995722	-0.6829722988163359
O	16.31187882900322	12.47080845758523	1.976491564458011
O	17.77508336021484	13.23260590899137	-0.1759757584107
O	15.13083786630288	13.70154073312342	3.941891832777959
O	17.28137478986026	8.791002418082316	-1.313104133395089
O	20.95178076976182	11.65092510302189	0.7562926137946716
O	16.20943072009608	11.09040210109364	-0.2985162656955105
O	21.33231572506961	7.18114467946401	0.9120821220405936
O	19.73273138326871	9.750230140694381	-0.6205517667369043

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H 13.81880076984796 13.07586778650288 1.810249073131662
O 14.3163528949505 13.89785383185922 6.43410963264518
Si 21.47336788011123 10.15060875075224 14.49075184538873
Si 15.82767610573598 11.32846620811171 13.61467750741988
Si 14.31946855112148 13.62784957924152 12.23691062543555
O 15.02693668682799 14.8719204593281 11.44255360400724
H 22.31072865970459 11.37722455894331 14.41325579351224
O 14.45384190287395 15.08864165847621 8.802734274600146
H 18.17570107795384 9.1425874857346 15.0475543492068
O 13.36728328415668 12.737755554762 11.22391759933169
O 15.55578008577374 12.75363255427636 12.85854711359336
Si 25.81289455869415 11.00987967644201 2.222681391322872
O 24.681264876498 11.83150691157178 1.334961283278103
O 25.10035156071605 9.86317695605219 3.17243561986419
H 25.05575966614836 7.584066378264489 1.947228097568173
H 24.49154953505514 9.697670737980129 12.78347819014082
H 24.23070822229105 7.425423316205149 13.73483291262415
H 21.29316800285494 9.666123509542404 15.88744672985955
O 15.10074966927529 16.11745591834317 5.163726141828489
H 21.44660607362712 3.375638317579622 1.562046290984502
H 19.08010747336447 2.945880760392744 2.168231319982299
H 13.28727673441662 6.834402758643248 13.49338654380222
H 19.37561648446512 8.541868398479135 -2.789986361722159
H 21.21414652622266 5.631181155048632 -1.053411224090878
O 15.41883663754884 15.00798766713672 1.581166858714784
H 12.94983312497287 14.91935375953842 4.524313794085709
H 12.21820664150706 14.29673473323709 7.862354060380294
Si 18.67168144054911 14.60623764783076 0.03180100296158797
Si 16.23379940197917 10.03870576251072 -1.579814239941245
Si 21.32583788300103 13.14874387616199 0.1976237123766612
H 15.30878591044903 11.34286621922329 14.99613774181082
H 13.44011129847711 14.12768226268753 13.31282856850667
Si 14.58948637419795 15.88104241024539 10.22806493002782
H 26.51077798038988 11.9516089047 3.138099079535125
H 26.74131420510746 10.33708102121441 1.272614612895059
Si 24.30197840506262 13.37697511266461 0.8688264254103431
Si 15.78106563249047 17.34598434276356 4.314903783013697
Si 16.57255165627347 16.19634464681085 1.603344259413794
O 20.17079366512093 14.24316499107884 0.5842594204726773
H 18.73323410750152 15.2734407263657 -1.283639496656469
O 18.03610593330898 15.60208300759997 1.166372576252714
H 16.65213229921861 10.78359111774888 -2.8008927757882
H 14.87291211705372 9.463660526851024 -1.688773430264813
O 22.67769277258538 13.63973759248276 0.9853351102305595
H 21.53803255859364 13.0920039713374 -1.266741925199107
H 13.31608781534752 16.56774342191118 10.54908446003496
O 15.82537184905693 16.94714814574585 10.07556868313514
H 24.96552820167034 14.34902794171596 1.777968677202915
H 24.71869806979692 13.54195249291514 -0.551312468550209
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O	16.75737836603589	16.7936440283267	3.114835072003264
O	16.78198769085177	18.16549727452767	5.317480091523035
H	14.71724932796508	18.22025355896489	3.768485158462326
H	16.13010703379439	17.24567314308411	0.6634277844353932
Si	16.07265967883708	18.47998078543554	9.524252542603971
Si	16.67469752390994	19.24701771075589	6.55361585756662
H	17.44827495688155	18.87046009662543	9.931591288514625
O	15.94048390062914	18.56029882818721	7.872891156554532
H	15.02909602068341	19.37103206882683	10.10388835282613
H	18.06271642224856	19.64954501834693	6.902980705745343
H	15.84043501480082	20.40054710341955	6.114802594363984

5.2. $Y(BH_4)_2(THF)_2/Y_{30}$

Y	18.83923283084387	7.976858857180677	6.469369656744343
O	19.75967773942869	6.415885187437509	8.266906734076708
O	17.1391787947831	6.296928634879324	6.791807752957689
B	17.70242104669606	8.512592725878871	4.352517015689383
B	18.18827113139691	9.750626094766394	8.042229345965181
O	20.91540678720848	9.142994020200518	6.147713044186768
H	19.26062129642802	9.225234323079455	8.376041198006604
H	17.36142186998581	8.823534759533747	7.962712283964728
H	16.95014118954954	8.576164541626689	5.340896424269426
H	18.64634708228833	9.278653253966537	4.599948178380974
H	18.32712814132988	10.16521197400399	6.880612552771235
C	15.29760022083849	4.893489511190124	6.182505871893131
Si	18.17039236111365	3.670904667623998	10.56821250977811
Si	16.08298507918421	5.274972788485146	12.19765473006501
Si	21.30777063098081	8.177328528424047	2.224290360708302
Si	19.83034330648602	10.47435528811806	0.8539809458493575
Si	18.494187349613	9.881468233758914	13.80418263901107
Si	13.41633800444066	11.68575293321304	9.949332174471733
Si	14.91892180604226	9.393209929388473	11.33423157194002
Si	22.74906296161497	6.601091327088554	10.62701218066163
Si	21.04101121424635	5.941662577004375	4.271742937360798
Si	17.5811833336759	7.926885367331652	11.53693984404205
Si	19.68358898635822	6.35703219482746	9.906124239924727
Si	24.08493298078833	6.188396541070476	5.008869029902728
Si	18.87698065889061	2.488932934351078	7.897700099083481
Si	23.52133086268682	5.462304697900136	7.926597821978866
Al	20.45763099817885	5.136961328554025	7.211988276870096
O	24.06610134463929	6.345567634797317	6.631960393111449
O	17.84675749404052	2.978307212000902	9.122954803702678
O	24.35762374208173	7.701338708745439	4.418504293695334
O	22.1860650074633	8.930044576413479	13.62557136456509
O	21.10932302906223	6.797883815091907	10.57506261543071
O	22.82148323496461	8.752144108301625	2.436365520584731
O	22.09667004340634	4.751540449355946	7.649409590920392
O	22.65137304444543	5.612677239232215	4.40672056598678
O	23.36166965386298	7.92969405769215	11.37870748672181

O	16.73640572699355	4.306875614878519	11.05482595741542
O	20.31907246290785	6.127077798707258	5.729627859893296
O	20.79392961847691	7.379201655941252	3.537548074330036
O	18.38275138456037	11.06337764071142	1.312871988247962
O	20.34525720671695	4.703006547095742	3.465982338454141
O	20.28505303250705	9.425981739292448	2.016169581065468
O	16.34353356149003	8.7492243215525	10.8543368919946
O	23.42248410815636	6.591343599452412	9.134814071031757
O	13.86419239115135	12.45765968395669	8.575105140010262
O	17.45344384532039	11.1306913315663	13.59660003622688
O	14.583183705295	5.637009658742014	11.62133550197685
O	18.47096765677869	8.852895946806436	12.52795718976218
O	13.75720125381166	8.241496529495629	11.40750980578296
O	19.45012349336243	3.744561341129685	7.04993204108088
H	23.06693268544091	5.363672404271765	11.37491562112388
O	16.97783440331714	6.653426371350517	12.41042885515424
O	19.33801550933318	4.834617576626775	10.43422993158273
O	15.06907958058313	10.07925263286904	12.82937732714218
O	18.50589358035068	7.401015198724153	10.31754121227838
O	19.99365162906204	10.5410364116856	13.86873003103043
O	14.51518996426129	10.49467469067998	10.20248004328269
C	22.40138139348504	10.9555170710326	5.815177713394331
H	16.66059347288432	6.45514402438824	8.806848033203631
H	22.66004705103054	8.253286038550629	6.861152108958366
H	15.09730240468289	3.855798731391488	5.884966218729236
H	16.71531233987087	5.861002968152876	4.791998811761376
C	15.31992193300938	5.082892221332894	7.706842655912689
H	21.49815573126232	8.753511986420957	8.132077981722858
H	17.42607342830049	4.518627876898433	5.756023578086212
H	18.18142985861489	7.36999564783138	4.334258858427809
H	14.53289418625173	5.537822218712946	5.724116281831345
H	15.51451596516827	7.264909998583185	7.696720408047147
C	16.12532690092574	6.361756375216568	7.855756719763217
C	20.98809106180645	10.48051790478843	5.528422197544725
H	17.8348967621287	10.60724614180484	8.80543935209919
H	17.1466299106693	8.790674656849003	3.324207280791751
H	22.48065675122509	12.04931637609004	5.759327368763688
H	14.31795986558975	5.181763365634651	8.145006836249255
C	21.96978956826901	9.041088154000416	7.182467158393153
H	15.83568931431608	4.248273247876952	8.201249606296217
H	23.70534445285884	10.31985909436376	7.48538330717662
H	22.15465816139446	11.05182099432592	7.979007141283994
H	23.11193405671578	10.51744748466139	5.098999125560048
C	22.64123397761256	10.40872084453005	7.230990938398266
H	20.22826387065769	11.12274187551437	6.002228286825192
H	20.74934910354016	10.35330746718233	4.465408776482756
C	16.69428302192879	5.338630231974641	5.756373669285756
Si	20.14813849983376	3.95907653282789	2.00159450400948
Si	23.61803910669732	8.499798403550928	12.9059533807259

H	18.66572166403169	2.689299345098874	11.5541536245271
H	16.00405014137731	4.599400748656825	13.50756657525143
H	19.98213930491771	1.704244619941643	8.527599057225865
H	24.5417141096194	4.448749515958386	8.273054047415329
H	25.13721142364065	5.253794569011887	4.563634551263549
H	18.03453703131802	1.639960549206495	7.011120670163232
Si	13.41161157448859	6.735130455453435	12.01198116602707
H	12.06017655658223	11.1205772290958	9.808094818647454
H	12.16075788185531	6.29333496158816	11.35060599542048
Si	18.9027779477544	8.547381883468464	-1.391490884147836
Si	20.35336841367202	6.224753548041149	-0.01019091238314268
Si	17.17047174853669	11.96569406600497	0.690450180692907
Si	15.12530476500975	13.54757639052923	2.307652399720728
Si	14.33431729544196	14.67762936089485	4.995983672759918
Si	13.65812962954835	13.9570828432801	7.934000485629821
Si	24.35086004922854	8.421095862204451	2.94355766547118
O	19.62466091347015	5.045458322209508	0.8684231423257187
O	19.13705883494394	7.09435913458234	-0.6749974191012018
O	16.31105453153887	12.47119156096558	1.975392600937345
O	17.77286102176479	13.23426176903445	-0.1765711362619531
O	15.13142712392497	13.70296521731215	3.94175198014728
O	17.28139735065642	8.789804330534764	-1.319351388473828
O	20.95457618511529	11.64935379201031	0.7535828386124996
O	16.2109346403589	11.08869892564533	-0.2979848195259899
O	21.33617674499919	7.173695875647979	0.9185737779961596
O	19.73077462248606	9.752179454676183	-0.6220575875345105
H	13.81800102607625	13.07712262579973	1.811077995815132
O	14.31580866474104	13.89833884520484	6.434398377612641
Si	21.47336788011123	10.15060875075224	14.49075184538873
Si	15.82767610573598	11.32846620811171	13.61467750741988
Si	14.31946855112148	13.62784957924152	12.23691062543555
O	15.02606435555367	14.8727472287544	11.44391581194346
H	22.31095736029125	11.37679845195065	14.41064957452766
O	14.45438828085322	15.08744163806358	8.803805593573776
H	18.17657107902608	9.138510347221796	15.04530125886926
O	13.36763397252955	12.73664762379069	11.22480246434864
O	15.55594295021239	12.7527177116557	12.8580062937111
Si	25.81289455869415	11.00987967644201	2.222681391322872
O	24.68202328533863	11.83125686153092	1.334083482017169
O	25.09858490813363	9.864688610381833	3.173044920017849
H	25.04755030855591	7.593542229058946	1.933378866198696
H	24.4911692382721	9.697766219600556	12.78295637323163
H	24.23265080725757	7.423340851898127	13.73057009539595
H	21.292820170622	9.66855712753121	15.88820907135698
O	15.09911558571741	16.11861400643686	5.164001700856787
H	21.45044016617261	3.377643576185175	1.570460085595349
H	19.08260246737008	2.943116368413995	2.166486100586142
H	13.28779242090095	6.830202777232369	13.49360847836329
H	19.38012665942238	8.535613539228114	-2.788490315134611

H	21.21376725279734	5.638669982441038	-1.058010828905361
O	15.41903168508615	15.00819523042199	1.580761361901379
H	12.94954314726967	14.91868792393163	4.524594471005209
H	12.21833145721307	14.29772518017612	7.863309408926719
Si	18.67168144054911	14.60623764783076	0.03180100296158797
Si	16.23379940197917	10.03870576251072	-1.579814239941245
Si	21.32583788300103	13.14874387616199	0.1976237123766612
H	15.30700172270715	11.34217737914757	14.9954849977062
H	13.44041155997624	14.12597002498762	13.3138964302063
Si	14.58948637419795	15.88104241024539	10.22806493002782
H	26.51082412256319	11.95174041127228	3.13806951473552
H	26.74172915695288	10.33576498787966	1.273955644508154
Si	24.30197840506262	13.37697511266461	0.8688264254103431
Si	15.78106563249047	17.34598434276356	4.314903783013697
Si	16.57255165627347	16.19634464681085	1.603344259413794
O	20.1700124666484	14.24155613286419	0.5861370888537355
H	18.73633070547432	15.2729432360909	-1.283818600477806
O	18.03656673862798	15.60415471536465	1.164966129373656
H	16.64990780037848	10.7854201399263	-2.800669489958096
H	14.87289485457716	9.463495240895	-1.688136230438319
O	22.67800580184515	13.63987847140036	0.9857557028468568
H	21.53871523057505	13.09530737245543	-1.266841643762174
H	13.31587425719141	16.56768107784331	10.54854953317961
O	15.82513800518364	16.94734664422675	10.07603236990518
H	24.96607135334203	14.34809647420254	1.778676468219069
H	24.71925181520201	13.54263610025547	-0.5510953716842451
O	16.75755801319457	16.7931045737156	3.115289175291114
O	16.78207140208309	18.16554382706851	5.317708626400747
H	14.71826076747731	18.22124966773302	3.767980451550079
H	16.12947896821899	17.24651848380914	0.664549322168832
Si	16.07265967883708	18.47998078543554	9.524252542603971
Si	16.67469752390994	19.24701771075589	6.55361585756662
H	17.44843611192728	18.8701152231422	9.931431121151624
O	15.94005321224202	18.56082223710788	7.873072451986793
H	15.02948210374646	19.37124500526972	10.1043480373263
H	18.06265533760351	19.64946492864961	6.903431064396025
H	15.84075461987532	20.40082745679901	6.11483552427825

5.3. $La(BH_4)_2(THF)_2/Y_{30}$

La	18.93514934854764	8.190783666774111	6.558395701026415
O	19.81170713998769	6.410454990873427	8.274343630037755
O	16.90812850789806	6.725170514919354	7.146328150254925
B	17.5892591926862	8.752998598325775	4.386839035971406
B	18.49961261197378	10.20638870886163	8.179732052691103
O	21.18078005786165	9.329701658492139	6.11339458989008
H	19.49396397510832	9.541965311440649	8.521283307239894
H	17.55089382653902	9.406469056708151	8.134735066360939
H	16.95301863919926	8.981760409509191	5.432493816493556
H	18.63709904535661	9.416052257704983	4.482977109620762

H	18.68605915627153	10.56049155624798	7.002206205577704
C	15.4509907523822	4.870952237499367	7.125791673140343
Si	18.17039236111365	3.670904667623998	10.56821250977811
Si	16.08298507918421	5.274972788485146	12.19765473006501
Si	21.30777063098081	8.177328528424047	2.224290360708302
Si	19.83034330648602	10.47435528811806	0.8539809458493575
Si	18.494187349613	9.881468233758914	13.80418263901107
Si	13.41633800444066	11.68575293321304	9.949332174471733
Si	14.91892180604226	9.393209929388473	11.33423157194002
Si	22.74906296161497	6.601091327088554	10.62701218066163
Si	21.04101121424635	5.941662577004375	4.271742937360798
Si	17.5811833336759	7.926885367331652	11.53693984404205
Si	19.68358898635822	6.35703219482746	9.906124239924727
Si	24.08493298078833	6.188396541070476	5.008869029902728
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