

## Supporting Information

### **Sodium Complexes as Precise Tools for Cutting Polymer Chains. Exploration of PLA Degradation by Unique Cooperation of Sodium Centers**

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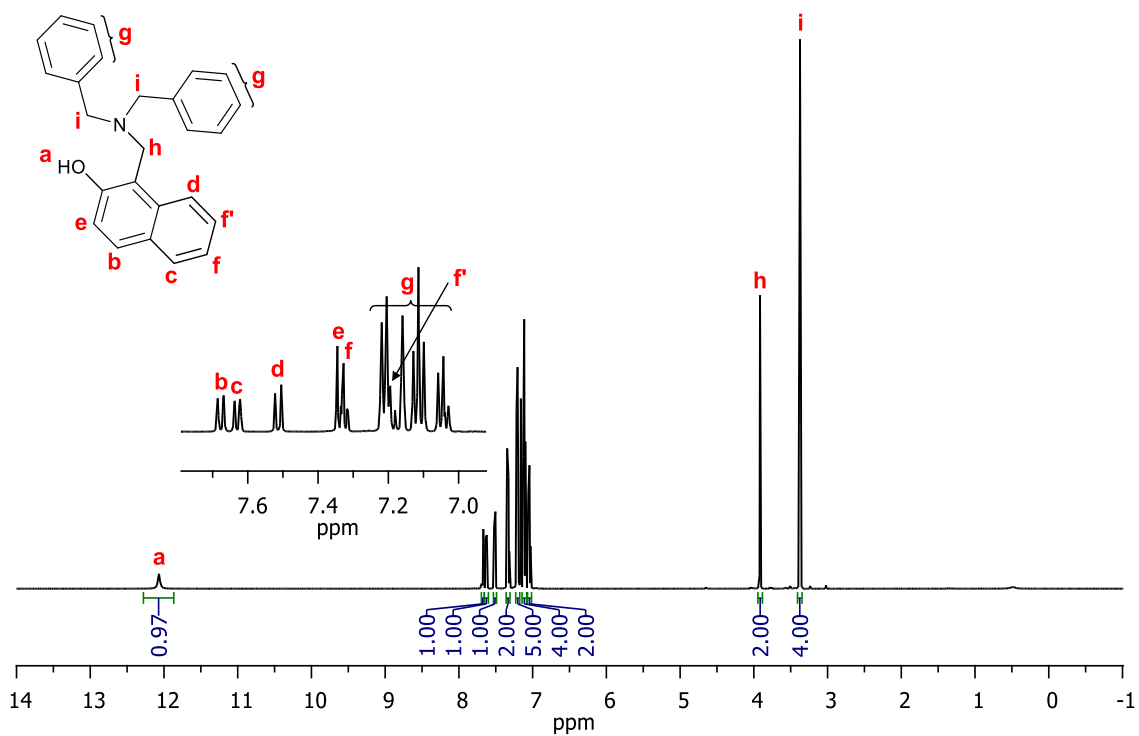


Figure S1.  $^1\text{H}$  NMR of  ${}_{2np}\text{L}^{\text{Bn}}\text{-H}$  ( $\text{C}_6\text{D}_6$ ).

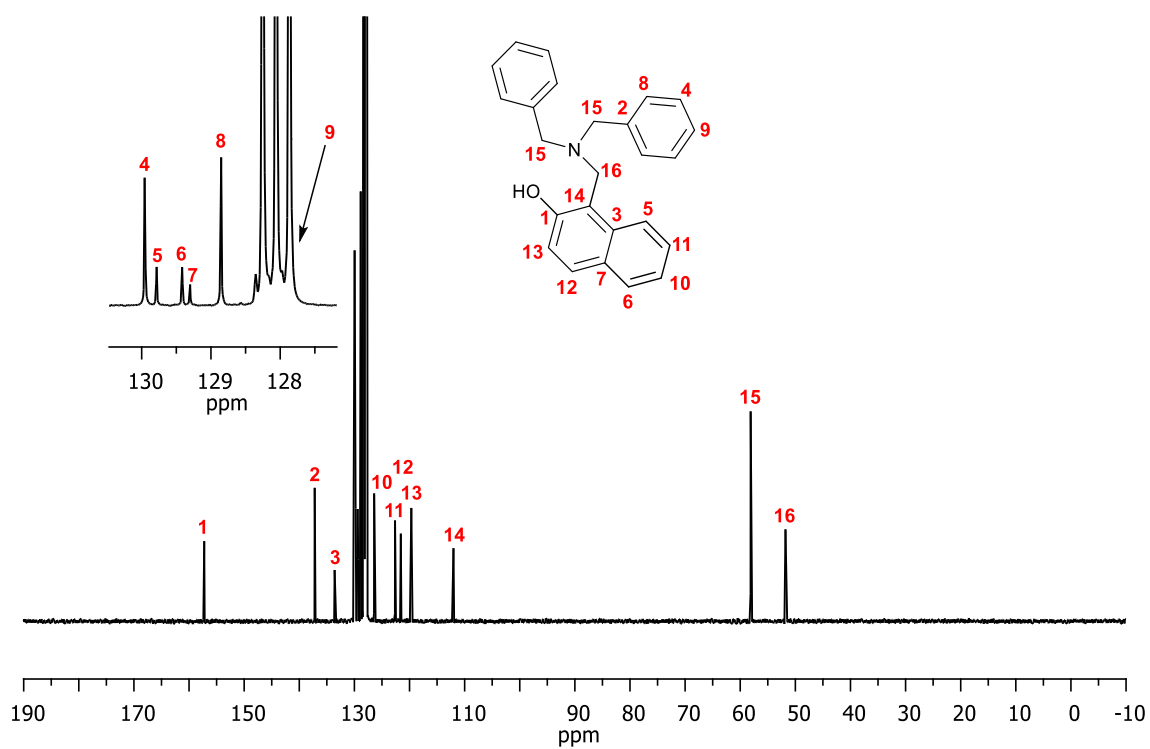


Figure S2.  $^{13}\text{C}$  NMR of  ${}_{2np}\text{L}^{\text{Bn}}\text{-H}$  ( $\text{C}_6\text{D}_6$ ).

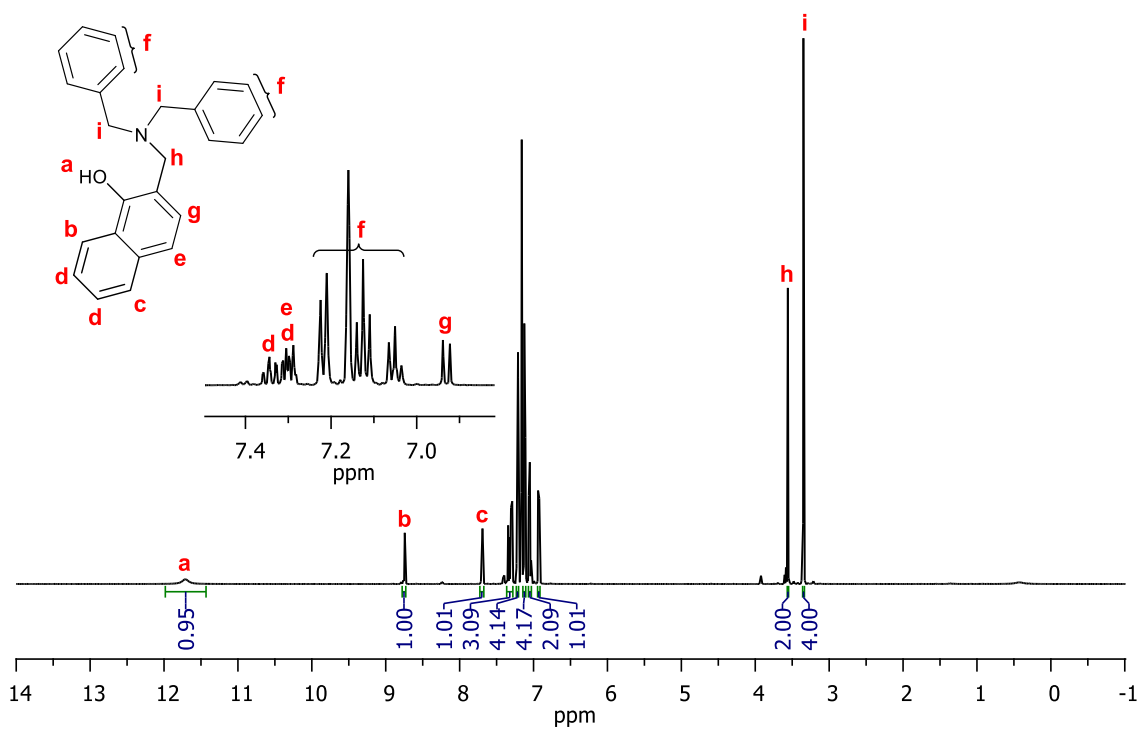


Figure S3.  $^1\text{H}$  NMR of  ${}_{1np}\text{L}^{\text{Bn}}\text{-H}$  ( $\text{C}_6\text{D}_6$ ).

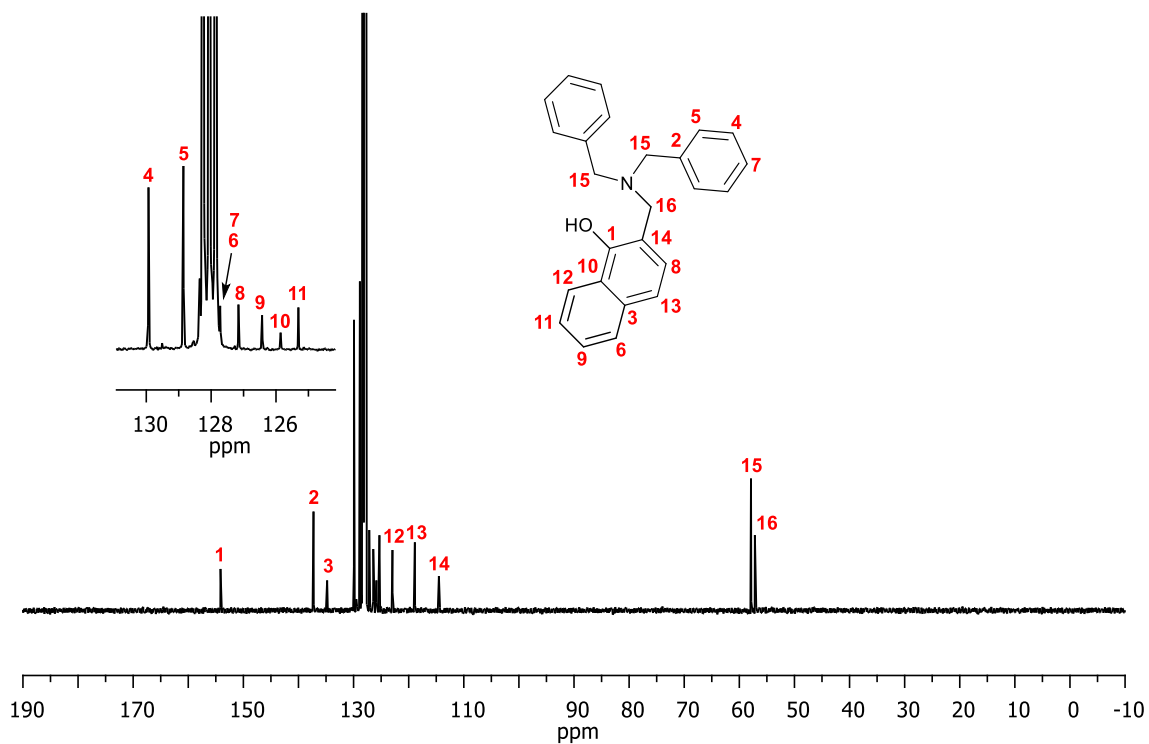
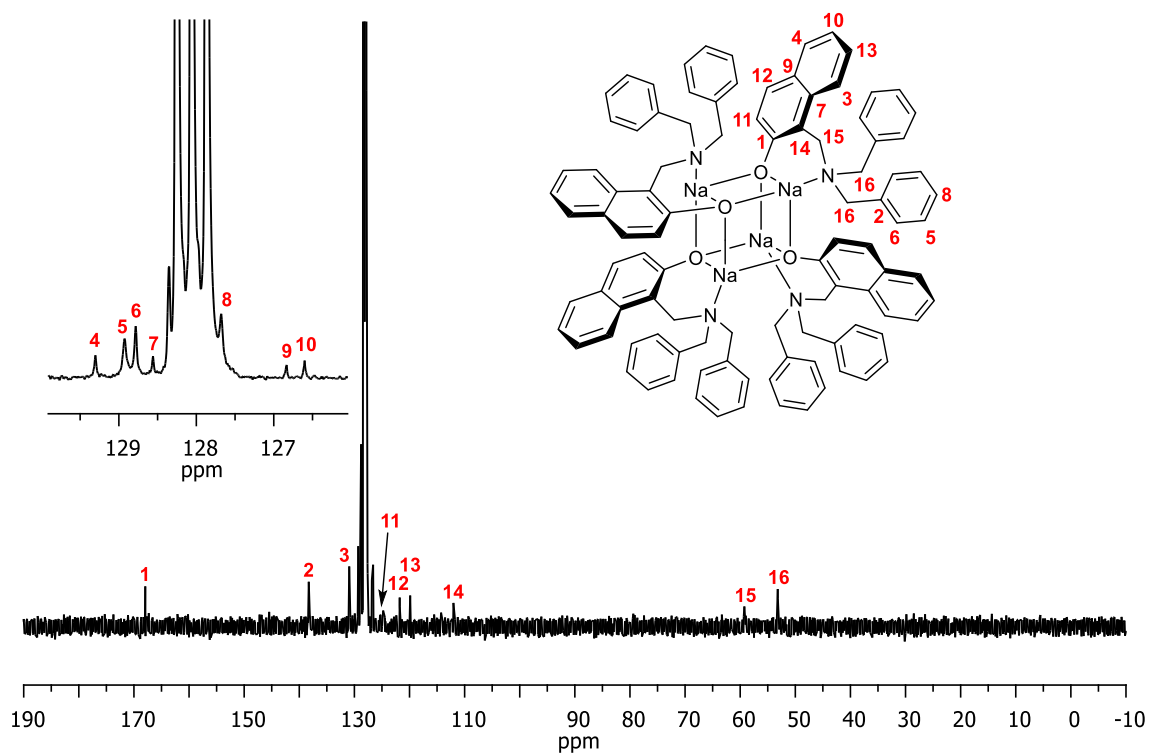
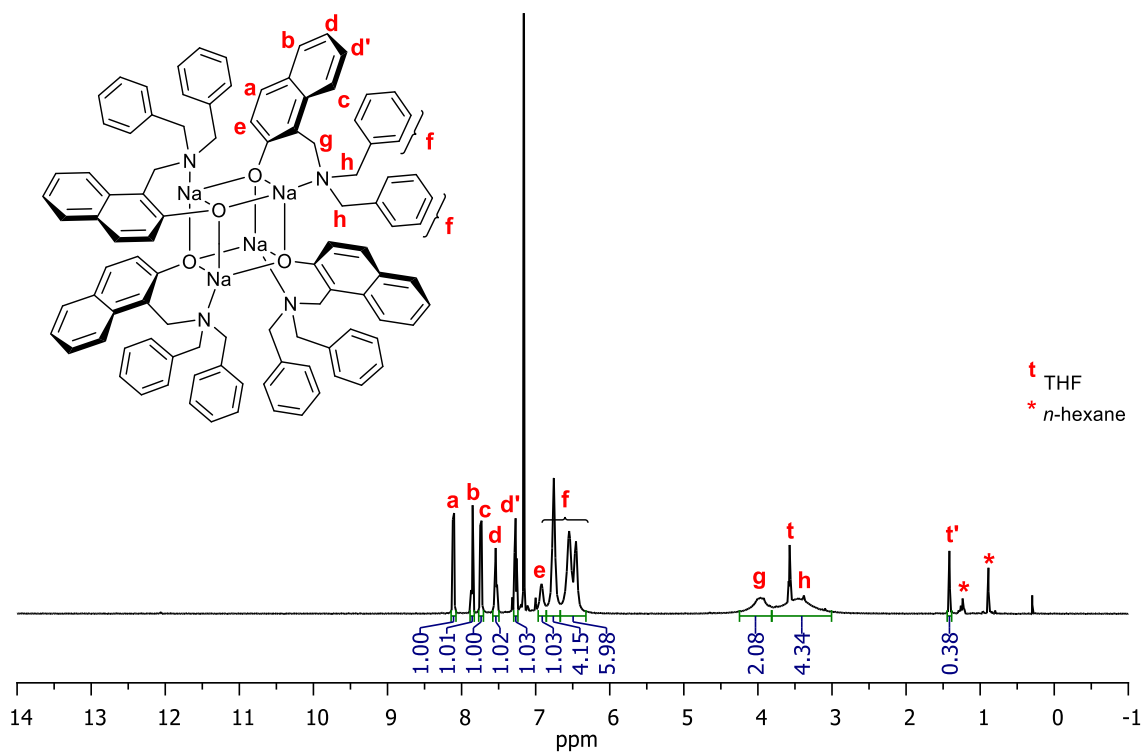


Figure S4.  $^{13}\text{C}$  NMR of  ${}_{1np}\text{L}^{\text{Bn}}\text{-H}$  ( $\text{C}_6\text{D}_6$ ).



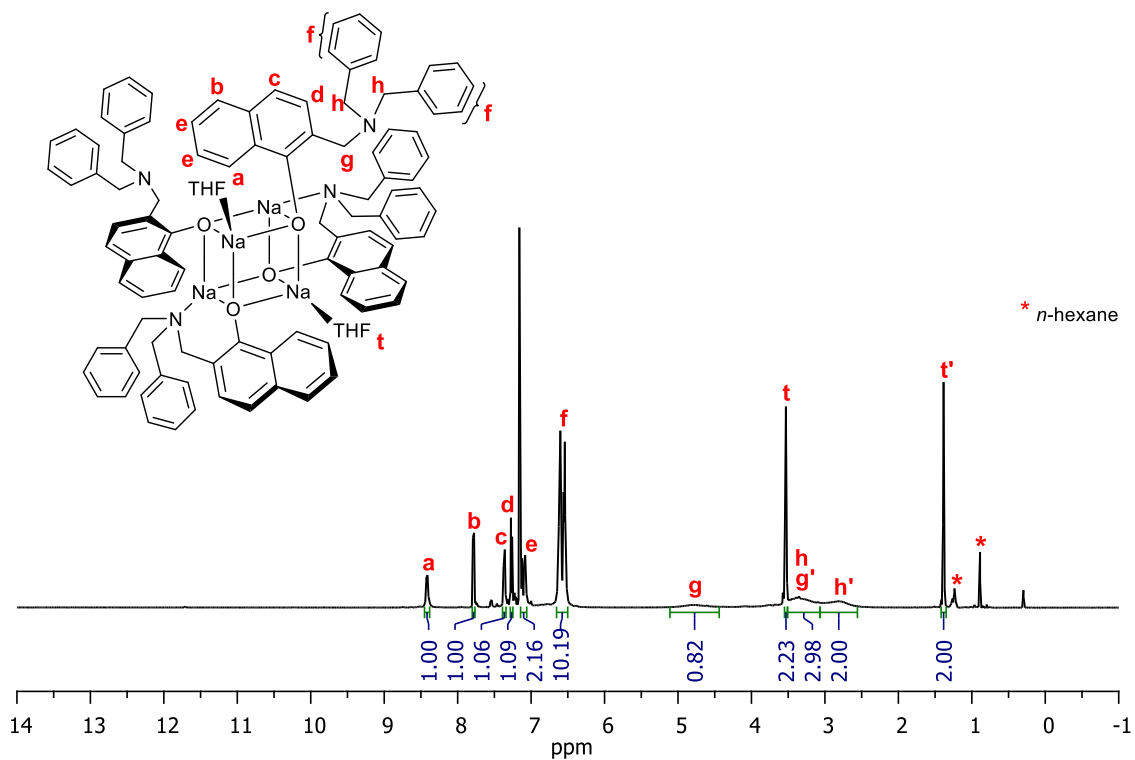


Figure S7.  $^1\text{H}$  NMR of  $[(1\text{-npL}^{\text{Bn}})\text{-Na(THF)}_{0.5}]_4$  ( $\text{C}_6\text{D}_6$ ).

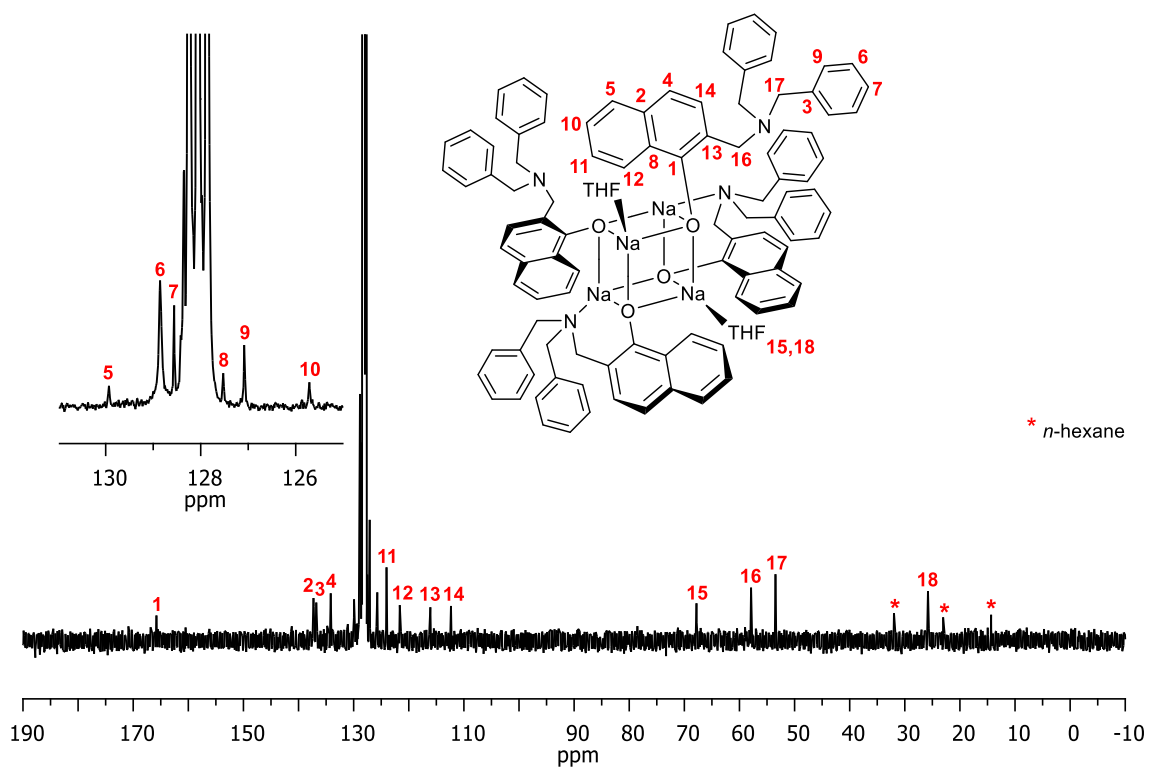
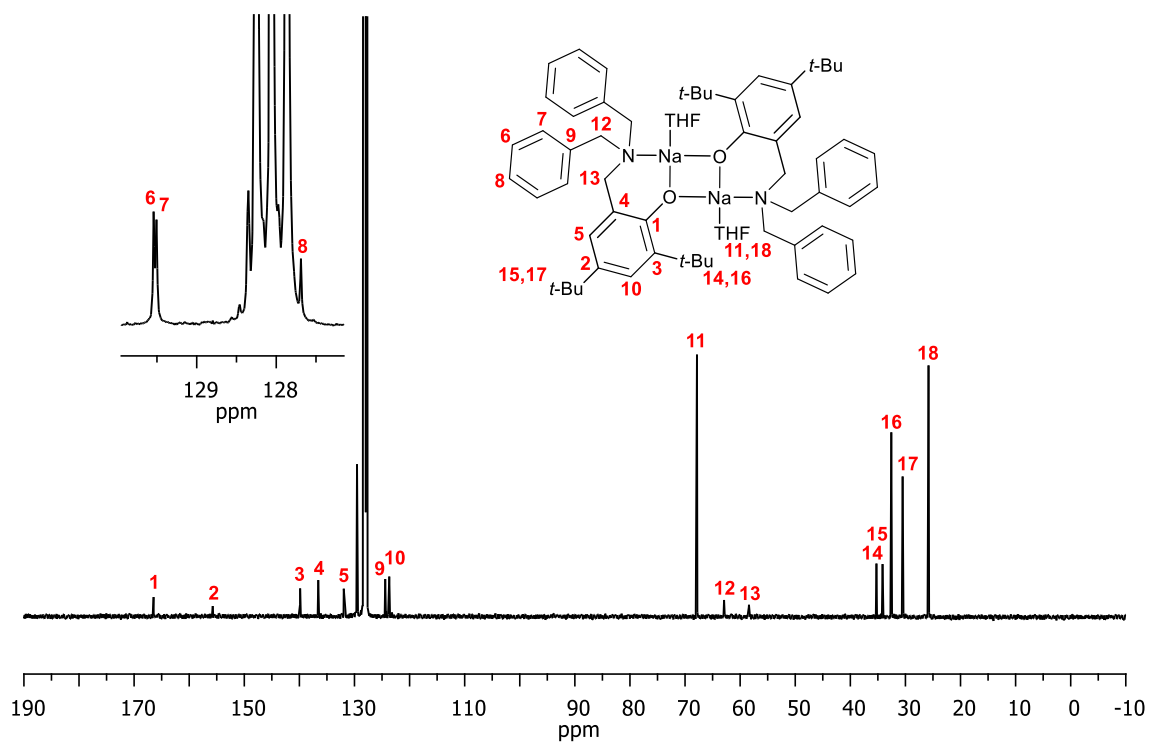
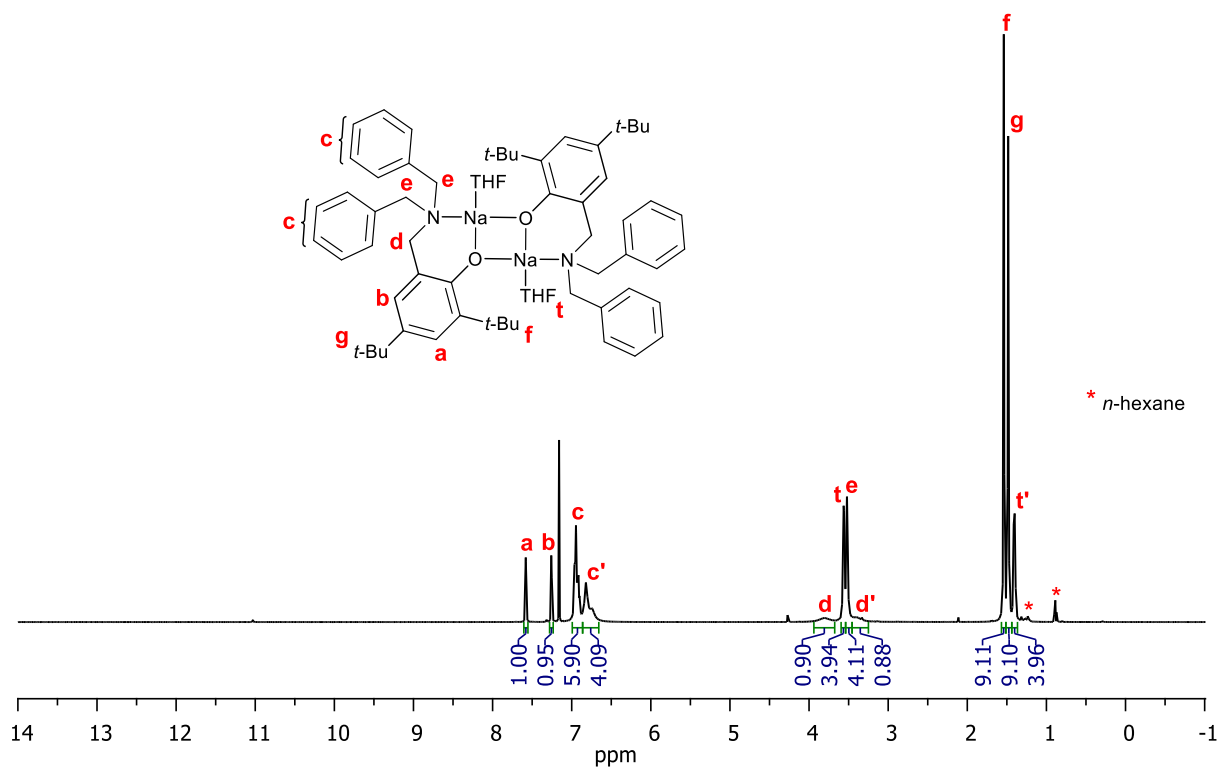


Figure S8.  $^{13}\text{C}$  NMR of  $[(1\text{-npL}^{\text{Bn}})\text{-Na(THF)}_{0.5}]_4$  ( $\text{C}_6\text{D}_6$ ).



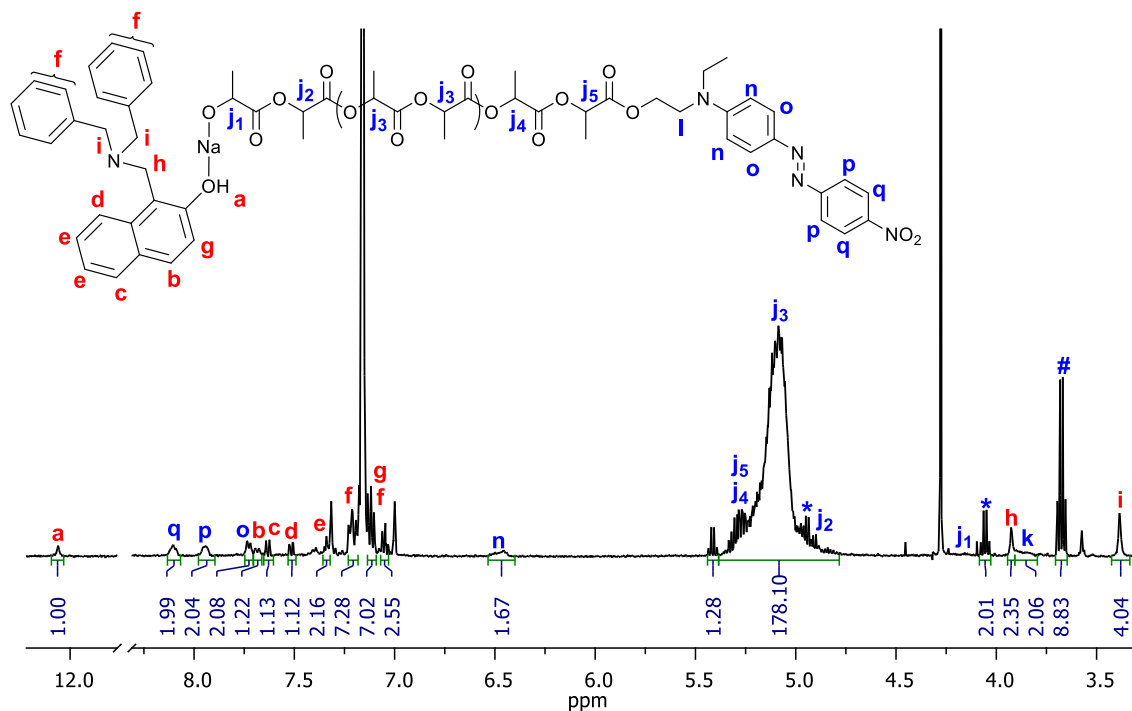


Figure S11. Fragment of  $^1\text{H}$  NMR spectrum for mixture of 0.25 eq.  $[(2\text{-npL}^{\text{Bn}})\text{-Na}]_4$  with 1.0 eq. PLA-100-D ( $\text{C}_6\text{D}_6$ ).

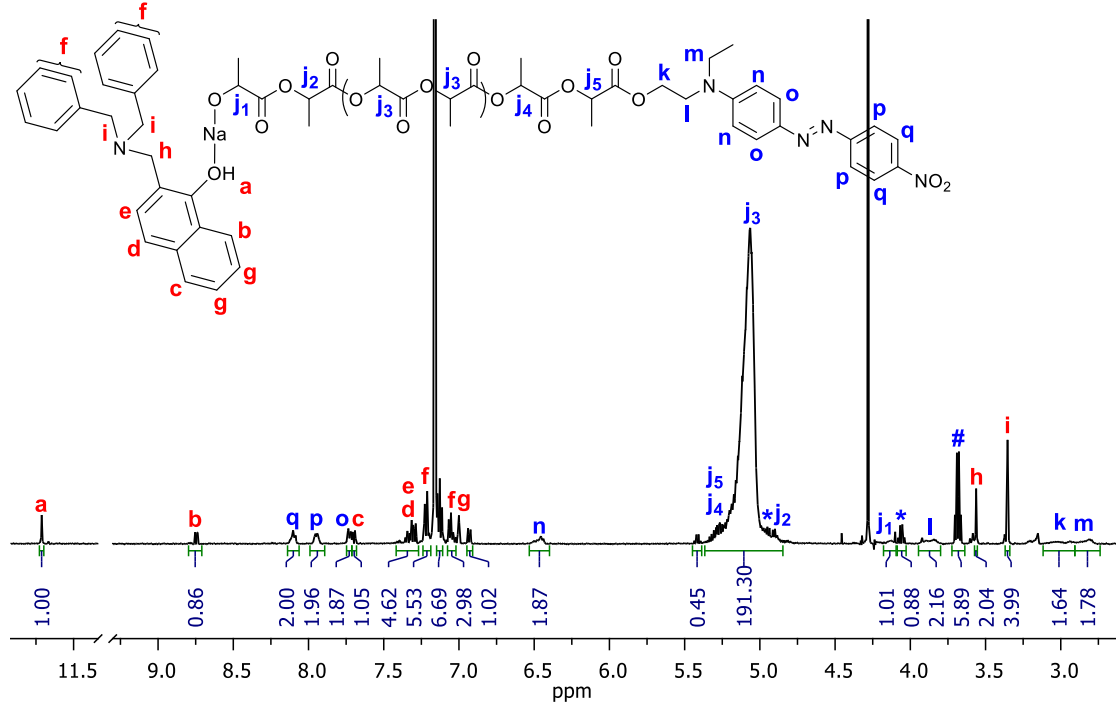
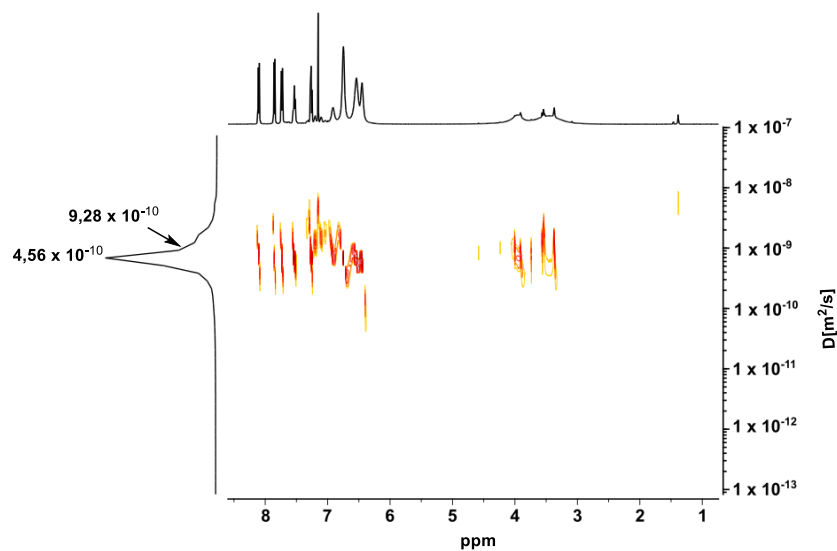
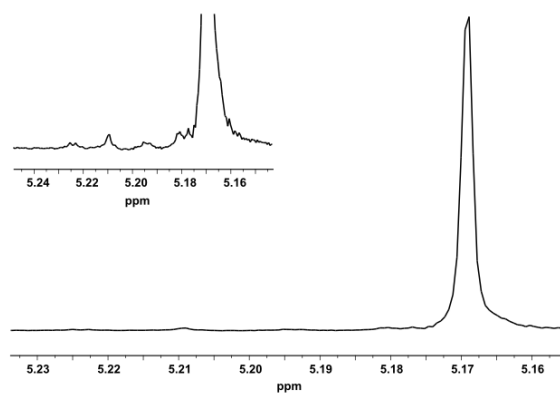


Figure S12. Fragment of  $^1\text{H}$  NMR spectrum for mixture of 0.25 eq.  $[(1\text{-npL}^{\text{Bn}})\text{-Na}(\text{THF})_{0.5}]_4$  with 1.0 eq. PLA-100-D ( $\text{C}_6\text{D}_6$ ).

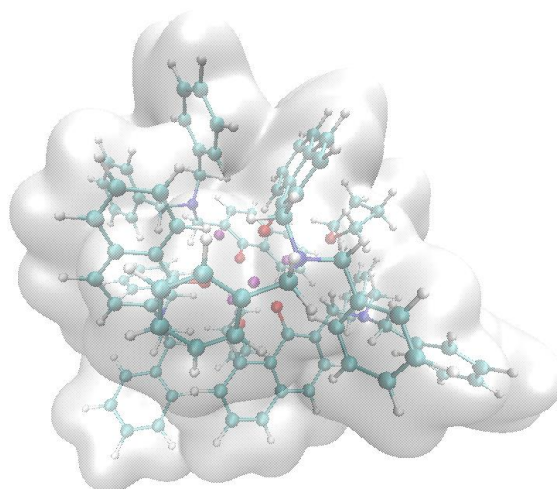




**Figure S13.** DOSY NMR spectrum of  $[(2\text{-npL}^{\text{Bn}})\text{Na}(\text{THF})_4]$  ( $\text{C}_6\text{D}_6$ ).



**Figure S14.** Deconvoluted homonuclear decoupled  $^1\text{H}$  NMR of the methine region of isotactic depolymerized PLA produced by  $[(2\text{-npL}^{\text{Bn}})\text{Na}]_4$  ( $\text{CDCl}_3$ ).



**Figure S15.** Van der Waals surface generated around DFT optimized  $[(1\text{-npL}^{\text{Bn}})\text{Na}(\text{THF})_{0.5}]_4$  structure.

	$[(2\text{-npL}^{\text{Bn}})\text{-Na(THF)}]_4$	$[(1\text{-npL}^{\text{Bn}})\text{-Na(THF)}_{0.5}]_4$
Empirical formula	$\text{C}_{116}\text{H}_{120}\text{N}_4\text{O}_8\text{Na}_4, \text{C}_4\text{H}_8\text{O}$	$2(\text{C}_{108}\text{H}_{104}\text{N}_4\text{O}_6\text{Na}_4), 3(\text{C}_4\text{H}_8\text{O})$
Formula weight	1862.22	3508.12
Crystal system	Triclinic	Monoclinic
Space group	<i>P</i> -1	<i>Cc</i>
<i>a</i> (Å)	14.765(5)	12.952(2)
<i>b</i> (Å)	15.491(5)	23.117(5)
<i>c</i> (Å)	25.112(8)	64.350(13)
$\alpha$ (°)	100.61(4)	90
$\beta$ (°)	98.40(4)	94.38(2)
$\gamma$ (°)	111.87(5)	90
<i>V</i> (Å <sup>3</sup> )	5092(3)	19211(6)
<i>Z</i>	2	4
Crystal description	Block, colourless	Twinned block, colourless
Crystal size (mm)	0.52 × 0.24 × 0.14	0.42 × 0.31 × 0.16
<i>d</i> <sub>calc</sub> (g/cm <sup>3</sup> )	1.215	1.213
$\mu$ (mm <sup>-1</sup> )	0.09	0.744
<i>F</i> (000)	1984	7456
Diffractometer	Kuma KM-4 CCD	Xcalibur, CCD Ruby
$\lambda$ (Å)	0.71073 (Mo)	1.54184 (Cu)
<i>T</i> (K)	100	100
$\theta$ min/max (°)	2.8/25.0	3.4/68.2
<i>h, k, l</i> min/max	-17/17, -18/14, -29/29	-14/15, -27/27, -73/77
Reflections collected	48393	46411
Independent reflections	17919	22743
Reflections [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )]	7257	21781
<i>R</i> (int.)	0.194	0.064
data/restraints/params	17919/676/1374	22743/1375/2610
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )]	0.096	0.129
<i>wR</i> ( <i>F</i> <sup>2</sup> )	0.290	0.364
Goof	1.04	1.681
$\Delta\rho_{\text{max}}/\Delta\rho_{\text{min}}$ (e·Å <sup>-3</sup> )	0.41/-0.38	0.74/-0.52

**Table S1.** X-ray experimental data and refinement for  $[(2\text{-npL}^{\text{Bn}})\text{-Na(THF)}]_4$  and  $[(1\text{-npL}^{\text{Bn}})\text{-Na(THF)}_{0.5}]_4$ .

Atoms / Distances (Å)							
Na1A-O1A	2.252(5)	Na1B-O1B	2.243(5)	Na1C-O1C	2.283(5)	Na1D-O1D	2.305(5)
Na1A-O1B	2.304(4)	Na1B-O1A	2.309(4)	Na1C-O1A	2.388(6)	Na1D-O1B	2.297(6)
Na1A-O1C	2.300(6)	Na1B-O1D	2.401(6)	Na1C-O1D	2.286(4)	Na1D-O1C	2.311(4)

Na1A-O2A	2.315(5)	Na1B-O2B	2.308(6)	Na1C-O2C	2.276(6)	Na1D-O2D	2.303(6)
Na1A-Na1B <sup>a</sup>	3.195(4)	Na1B-Na1D <sup>a</sup>	3.329(4)	O1A-O1B <sup>a</sup>	3.245(6)	O1B-O1C <sup>a</sup>	3.411(7)
Na1A-Na1C <sup>a</sup>	3.284(4)	Na1B-Na1C <sup>a</sup>	3.237(4)	O1A-O1C <sup>a</sup>	3.218(7)	O1B-O1D <sup>a</sup>	3.190(7)
Na1A-Na1D <sup>a</sup>	3.091(4)	Na1C-Na1D <sup>a</sup>	3.130(4)	O1A-O1D <sup>a</sup>	3.395(6)	O1C-O1D <sup>a</sup>	3.361(6)

**Atoms / Angles (°)**

O1A-Na1A-O1B	90.8(2)	O1B-Na1B-O1A	90.9(2)	O1C-Na1C-O1A	87.1(2)	O1D-Na1D-O1B	87.8(2)
O1A-Na1A-O1C	90.0(2)	O1B-Na1B-O1D	86.7(2)	O1C-Na1C-O1D	94.7(2)	O1D-Na1D-O1C	93.4(2)
O1A-Na1A-O2A	146.5(2)	O1B-Na1B-O2B	121.6(2)	O1C-Na1C-O2C	122.5(2)	O1D-Na1D-O2D	156.1(2)
O1B-Na1A-O1C	95.6(2)	O1A-Na1B-O1D	92.2(2)	O1A-Na1C-O1D	93.1(2)	O1B-Na1D-O1C	95.5(2)
O1B-Na1A-O2A	115.1(2)	O1A-Na1B-O2B	101.2(2)	O1A-Na1C-O2C	143.8(2)	O1B-Na1D-O2D	104.9(2)
O1C-Na1A-O2A	107.0(2)	O1D-Na1B-O2B	148.0(2)	O1D-Na1C-O2C	103.5(2)	O1C-Na1D-O2D	105.2(2)
Na1A-O1A-Na1B	88.9(2)	Na1A-O1C-Na1C	91.5(2)	Na1B-O1A-Na1C	87.1(2)	Na1B-O1D-Na1D	90.0(2)
Na1A-O1B-Na1B	89.3(2)	Na1A-O1B-Na1D	84.4(2)	Na1B-O1D-Na1C	87.3(2)	Na1C-O1C-Na1D	85.9(2)
Na1A-O1A-Na1C	90.1(2)	Na1A-O1C-Na1D	84.2(2)	Na1B-O1B-Na1D	94.3(2)	Na1C-O1D-Na1D	86.0(2)

<sup>a</sup> Non-bonding interactions

**Table S2.** Selected bond distances (Å) and angles (°) for [(<sub>2-np</sub>L<sup>Bn</sup>)-Na(THF)]<sub>4</sub>.

Atoms / Distances (Å)							
Na1A-O1A	2.277(8)	Na1B-O1B	2.259(8)	Na1C-O1C	2.340(7)	Na1D-O1D	2.269(8)
Na1A-O1B	2.258(8)	Na1B-O1C	2.331(8)	Na1C-O1A	2.220(8)	Na1D-O1A	2.503(8)
Na1A-O1C	2.295(8)	Na1B-O1D	2.409(7)	Na1C-O1D	2.331(8)	Na1D-O1B	2.383(7)
Na1A-N1A	2.40(1)	Na1B-N1B	2.51(1)	Na1C-O2C	2.256(9)	Na1D-O2D	2.377(9)
Na1A-Na1B <sup>a</sup>	3.189(5)	Na1B-Na1C <sup>a</sup>	3.251(6)	O1A-O1B <sup>a</sup>	3.33(1)	O1B-O1C <sup>a</sup>	3.27(1)
Na1A-Na1C <sup>a</sup>	3.097(6)	Na1B-Na1D <sup>a</sup>	3.274(5)	O1A-O1C <sup>a</sup>	3.35(1)	O1B-O1D <sup>a</sup>	3.315(9)
Na1A-Na1D <sup>a</sup>	3.329(5)	Na1C-Na1D <sup>a</sup>	3.291(6)	O1A-O1D <sup>a</sup>	3.30(1)	O1C-O1D <sup>a</sup>	3.399(9)
Na1E-O1E	2.271(8)	Na1F-O1F	2.284(8)	Na1G-O1G	2.342(8)	Na1H-O1H	2.266(8)
Na1E-O1F	2.266(7)	Na1F-O1G	2.334(8)	Na1G-O1E	2.197(8)	Na1H-O1E	2.493(8)
Na1E-O1G	2.289(8)	Na1F-O1H	2.399(8)	Na1G-O1H	2.335(8)	Na1H-O1F	2.365(8)
Na1E-N1E	2.37(1)	Na1F-N1F	2.487(9)	Na1G-O2G	2.238(8)	Na1H-O2H	2.323(9)
Na1E-Na1F <sup>a</sup>	3.172(5)	Na1F-Na1G <sup>a</sup>	3.247(5)	O1E-O1F <sup>a</sup>	3.343(9)	O1F-O1G <sup>a</sup>	3.31(1)
Na1E-Na1G <sup>a</sup>	3.131(5)	Na1F-Na1H <sup>a</sup>	3.240(6)	O1E-O1G <sup>a</sup>	3.30(1)	O1F-O1H <sup>a</sup>	3.35(1)
Na1E-Na1H <sup>a</sup>	3.295(5)	Na1G-Na1H <sup>a</sup>	3.271(5)	O1E-O1H <sup>a</sup>	3.300(9)	O1G-O1H <sup>a</sup>	3.40(1)
Atoms / Angles (°)							
O1A-Na1A-O1B	94.4(3)	O1B-Na1B-O1C	91.0(3)	O1C-Na1C-O1A	94.7(3)	O1D-Na1D-O1A	87.4(3)
O1A-Na1A-O1C	94.4(3)	O1B-Na1B-O1D	90.4(3)	O1C-Na1C-O1D	93.4(3)	O1D-Na1D-O1B	90.9(3)
O1A-Na1A-N1A	93.4(3)	O1B-Na1B-N1B	86.2(3)	O1C-Na1C-O2C	139.5(3)	O1D-Na1D-O2D	121.5(3)
O1B-Na1A-O1C	91.9(3)	O1C-Na1B-O1D	91.6(3)	O1A-Na1C-O1D	93.0(3)	O1A-Na1D-O1B	85.8(3)
O1B-Na1A-N1A	135.0(3)	O1C-Na1B-N1B	146.5(3)	O1A-Na1C-O2C	102.5(3)	O1A-Na1D-O2D	146.4(3)
O1C-Na1A-N1A	131.5(3)	O1D-Na1B-N1B	121.8(3)	O1D-Na1C-O2C	121.5(3)	O1B-Na1D-O2D	108.6(3)
Na1A-O1A-Na1C	87.0(3)	Na1A-O1B-Na1D	91.6(3)	Na1B-O1B-Na1D	89.7(3)	Na1B-O1D-Na1D	88.8(3)

Na1A-O1A-Na1D	88.1(3)	Na1A-O1C-Na1B	87.1(3)	Na1B-O1C-Na1C	88.2(3)	Na1C-O1A-Na1D	88.2(3)
Na1A-O1B-Na1B	89.8(3)	Na1A-O1C-Na1C	83.8(3)	Na1B-O1D-Na1C	86.6(3)	Na1C-O1D-Na1D	91.4(3)
O1E-Na1E-O1F	94.9(3)	O1F-Na1F-O1G	91.6(3)	O1G-Na1G-O1E	93.1(3)	O1H-Na1H-O1E	87.6(3)
O1E-Na1E-O1G	92.6(3)	O1F-Na1F-O1H	91.2(3)	O1G-Na1G-O1H	93.4(3)	O1H-Na1H-O1F	92.5(3)
O1E-Na1E-N1E	94.1(3)	O1F-Na1F-N1F	85.6(3)	O1G-Na1G-O2G	142.8(3)	O1H-Na1H-O2H	123.9(3)
O1F-Na1E-O1G	93.2(3)	O1G-Na1F-O1F	91.6(3)	O1E-Na1G-O1H	93.4(3)	O1E-Na1H-O1F	86.9(3)
O1F-Na1E-N1E	134.5(3)	O1G-Na1F-N1H	91.9(3)	O1E-Na1G-O2G	104.3(3)	O1E-Na1H-O1H	87.6(3)
O1G-Na1E-N1E	130.8(3)	O1H-Na1F-N1F	121.1(3)	O1H-Na1G-O2G	117.6(3)	O1F-Na1H-O2H	143.6(3)
Na1E-O1E-Na1G	89.0(3)	Na1E-O1F-Na1H	90.7(3)	Na1F-O1F-Na1H	88.3(3)	Na1F-O1H-Na1H	87.9(3)
Na1E-O1E-Na1H	87.4(3)	Na1E-O1G-Na1F	86.6(3)	Na1F-O1G-Na1G	88.0(3)	Na1G-O1E-Na1H	88.2(3)
Na1E-O1F-Na1F	88.4(3)	Na1E-O1G-Na1G	85.1(3)	Na1F-O1H-Na1G	86.6(3)	Na1G-O1H-Na1H	90.6(3)

<sup>a</sup> Non-bonding interactions

**Table S3.** Selected bond distances (Å) and angles (°) for  $[(1\text{-npL}^{\text{Bn}})\text{-Na}(\text{THF})_{0.5}]_4$ .

	$E_{\text{tot}}$	$E_{\text{tot}}$ with ZPE correction	H	G	$S^{\text{a}}$
$[(d\text{-tbL}^{\text{Bn}})\text{Na}(\text{THF})]_2$	-2072953	-2072065	-2072016	-2072139	0.414
INT1	-2072938	-2072052	-2072002	-2072131	0.433
INT2	-2364721	-2363681	-2363625	-2363763	0.466
$[(d\text{-tbL}^{\text{Bn}})\text{Na}(\text{THF})_2]_2$	-2364724	-2363687	-2363630	-2363773	0.483
THF	-145869	-145795	-145791	-145813	0.072

<sup>a</sup> data are given in kcal/mol\*K

**Table S4.** Energies of calculated models for transformation pathways from “closed”  $[(d\text{-tbL}^{\text{Bn}})\text{Na}(\text{THF})]_2$  to “opened”  $[(d\text{-tbL}^{\text{Bn}})\text{Na}(\text{THF})_2]_2$  structures. Data are given in kcal/mol.

		$E_{\text{tot}}$	$E_{\text{tot}}$ with ZPE correction	H	G	$S^{\text{a}}$
$[(d\text{-tbL}^{\text{Bn}})\text{Na}(\text{THF})]_2$	Gas phase	-2072953	-2072065	-2072016	-2072139	0.414
	PCM	-2072962	-2072074	-2072025	-2072147	0.409
CH <sub>3</sub> OH	Gas phase	-72613	-72580	-72578	-72595	0.057
	PCM	-72615	-72583	-72580	-72597	0.057
INT1	Gas phase	-2218218	-2217262	-2217208	-2217342	0.449
	PCM	-2218227	-2217272	-2217218	-2217353	0.454
2	Gas phase	-2218211	-2217256	-2217201	-2217339	0.463
	PCM	-2218223	-2217268	-2217214	-2217349	0.455
INT2	Gas phase	-2218150	-2217196	-2217141	-2217277	0.455
	PCM <sup>b</sup>	-2218167	-2217207	-2217152	-2217287	0.452
3	Gas phase	-2218182	-2217227	-2217173	-2217308	0.453
	PCM	-2218192	-2217237	-2217183	-2217316	0.446

<sup>a</sup> data are given in kcal/mol\*K

<sup>b</sup> The total energy was calculated without optimization for the geometry taken from the gas phase calculations. Corrections to the energies have been estimated.

**Table S5.** Energies of calculated models for proposed mechanism of the reaction between  $[(d\text{-tbL}^{\text{Bn}})\text{Na}(\text{THF})]_2$  and methanol in gas phase and in Polarizable Continuum Model with dichloromethane as a solvent. Data are given in kcal/mol.

	$E_{\text{tot}}$	$E_{\text{tot}}$ with ZPE correction	H	G	$S^a$
$[(d\text{-tbL}^{\text{Bn}})\text{Na}(\text{THF})]_2$	-2072953	-2072065	-2072016	-2072139	0.414
LA	-240288	-240210	-240204	-240231	0.089
A	-2553561	-2552515	-2552454	-2552602	0.495
B	-2553560	-2552512	-2552452	-2552598	0.491
C	-1276749	-1276227	-1276196	-1276280	0.280
D	-2553585	-2552539	-2552478	-2552628	0.504

<sup>a</sup> data are given in kcal/mol\*K

**Table S6.** Energies of calculated models for proposed compounds obtained between  $[(d\text{-tbL}^{\text{Bn}})\text{Na}(\text{THF})]_2$  and methyl lactate.

Data are given in kcal/mol.

	$E_{\text{tot}}$	$E_{\text{tot}}$ with ZPE correction	H	G	$S^a$
$[(d\text{-tbL}^{\text{Bn}})\text{Na}(\text{THF})]_2$	-2072953	-2072065	-2072016	-2072139	0.414
LLA	-407954	-407832	-407822	-407858	0.119
$\text{CH}_3\text{OH}$	-72613	-72580	-72578	-72595	0.057
1	-2888937	-2887801	-2887733	-2887898	0.553
2	-3034191	-3032987	-3032914	-3033090	0.591
3	-3034183	-3032978	-3032905	-3033081	0.592
4	-3179440	-3178168	-3178089	-3178280	0.639
5	-2553585	-2552539	-2552478	-2552628	0.504
La-Me	-312907	-312795	-312787	-312820	0.110

<sup>a</sup> data are given in kcal/mol\*K

**Table S7.** Energies of calculated models for proposed polylactide degradation process by using sodium compounds. Data are given in kcal/mol.

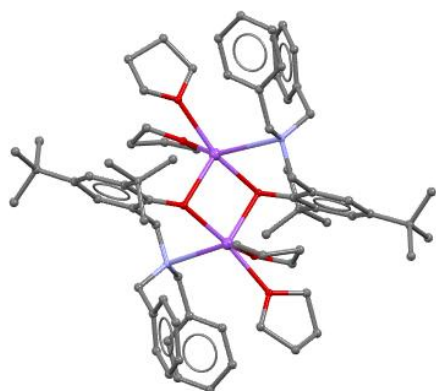
$[(d\text{-tbL}^{\text{Bn}})\text{Na}(\text{THF})]_2$				INT1			
Na	0.25021400	0.54848300	-1.45718900	Na	9.71050000	10.54635100	10.14632900
O	1.87645800	1.97225700	-2.23565700	O	10.85229900	9.26329800	8.70643700
C	3.29189500	1.67662100	-2.31973200	O	11.31493000	11.72184400	11.27183300
H	3.47785200	0.74187200	-1.78905600	N	13.15455000	12.05437800	6.87970500
H	3.56419700	1.55398800	-3.37798800	C	12.15043200	9.18457100	8.93154300
C	3.98600900	2.88152300	-1.69323400	C	12.76128900	8.00904400	9.47769300
H	5.01979700	2.99521800	-2.03275600	C	14.13660900	8.02403900	9.74682400
H	3.99147200	2.77104200	-0.60389600	H	14.58286000	7.13604800	10.17268900
C	3.06643400	4.03286400	-2.12894300	C	14.96798500	9.12306500	9.48984300

H	3.28255200	4.32273400	-3.16426000	C	14.35843500	10.24838000	8.92529900
H	3.15614900	4.92440500	-1.50111900	H	14.96658600	11.11586300	8.68182100
C	1.67706000	3.39224600	-2.03343800	C	12.99438300	10.30235700	8.65248900
H	0.97035100	3.75101100	-2.78685300	C	11.91471700	6.74676900	9.74075100
H	1.23430900	3.53789100	-1.03816400	C	12.73710600	5.59765100	10.35727500
Na	-0.18150900	-0.38231700	1.48053600	H	13.55942900	5.28462900	9.70404000
O	-1.41926800	0.84968800	-0.03083600	H	12.08997100	4.72621100	10.51249300
O	-1.78677300	-1.95418000	1.95344200	H	13.15978400	5.87425500	11.33050300
N	-1.26420000	-1.02990900	-2.74083200	C	11.32812700	6.23332800	8.40350900
C	-2.67939300	0.60064500	-0.31726400	H	10.73515100	7.01327500	7.92185500
C	-3.74857700	1.51071500	-0.00712600	H	10.68869700	5.35603400	8.57245100
C	-5.07032700	1.09891200	-0.22213900	H	12.13358400	5.93992300	7.71946600
H	-5.86264000	1.78318400	0.04691900	C	10.75779100	7.05797100	10.72014700
C	-5.43026000	-0.13997700	-0.76825300	H	11.14624500	7.48717200	11.65256000
C	-4.37552900	-0.96669300	-1.16575500	H	10.20703400	6.14162200	10.97252100
H	-4.58992600	-1.91788800	-1.65126200	H	10.06043200	7.76816200	10.27500600
C	-3.03738200	-0.61898700	-0.97950500	C	16.47458600	9.13687200	9.79434600
C	-3.45184100	2.91821200	0.55172200	C	16.78543100	10.26200500	10.80964200
C	-4.72055600	3.77599400	0.72545100	H	16.49505400	11.24439600	10.42192200
H	-5.25553500	3.91443600	-0.22139400	H	17.85835200	10.29697400	11.03918200
H	-4.43888800	4.76860100	1.09639800	H	16.23995600	10.09769700	11.74678200
H	-5.41575800	3.34082200	1.45275800	C	17.26984000	9.39860500	8.49327100
C	-2.50853000	3.68245900	-0.40778700	H	17.06241400	8.61822000	7.75175800
H	-1.58208900	3.12565300	-0.56196000	H	18.34946400	9.40403400	8.69208900
H	-2.26091100	4.66853600	0.00738700	H	17.01105800	10.36326400	8.04444700
H	-2.99352300	3.83929900	-1.37843300	C	16.96578100	7.80621900	10.39355600
C	-2.77610000	2.79368900	1.92919300	H	16.46127900	7.57713800	11.33937900
H	-3.43152500	2.28420400	2.64440800	H	18.04189800	7.86203000	10.59560700
H	-2.52825500	3.78083200	2.34215900	H	16.79889300	6.96842700	9.70691000
H	-1.85901600	2.21750300	1.82563600	C	12.40426200	11.56474000	8.05204200
C	-6.88628700	-0.58933600	-0.96587800	H	11.36765700	11.37163600	7.76787900
C	-7.13091300	-1.90201300	-0.18512500	H	12.34987700	12.35791000	8.81258600
H	-6.46734200	-2.70401800	-0.52646900	C	13.94820200	13.25312300	7.11487400
H	-8.16503100	-2.24659600	-0.31462000	H	14.30084900	13.21541300	8.15272400
H	-6.95078600	-1.75381300	0.88619300	H	13.34605600	14.18110700	7.03359800
C	-7.15805100	-0.83460400	-2.46862400	C	15.15782100	13.34933300	6.20127100
H	-6.99480600	0.08335400	-3.04475200	C	15.89299100	12.19929100	5.88192900
H	-8.19352200	-1.16171600	-2.62930000	H	15.54473300	11.23919800	6.24918700
H	-6.49754300	-1.60665400	-2.87789200	C	17.04056300	12.28802500	5.09475900
C	-7.89747400	0.45765600	-0.46324600	H	17.60123000	11.38741600	4.85743500
H	-7.76889000	0.66322900	0.60573000	C	17.46812900	13.52761500	4.61088300
H	-8.91960000	0.09015900	-0.61169600	H	18.36106400	13.59626000	3.99502800
H	-7.80334600	1.40478400	-1.00643300	C	16.73656100	14.67614500	4.91672600
C	-1.97207100	-1.53790500	-1.52033500	H	17.05534800	15.64345300	4.53664800
H	-1.19103700	-1.71747500	-0.77296400	C	15.58686500	14.58419200	5.70487500
C	-2.18947300	-0.54234300	-3.80433000	H	15.01602800	15.48150200	5.93596200
H	-3.18692900	-0.44757500	-3.37078200	C	12.36605900	12.14108100	5.65881700
H	-2.25981800	-1.27868700	-4.61632700	H	13.02277200	12.53910600	4.87325900
C	-1.77671000	0.80819000	-4.35513300	H	11.52746300	12.85856400	5.75579300
C	-1.91382800	1.94686500	-3.54769500	C	11.82137800	10.80113200	5.19937200
H	-2.35544200	1.84566300	-2.56105000	C	12.51652900	9.60953900	5.45084200
C	-1.50511500	3.19930500	-4.00608400	H	13.43405100	9.64904400	6.02653900
H	-1.62391200	4.07022000	-3.36643000	C	12.01073000	8.38554600	5.00958400
C	-0.96099400	3.33311800	-5.28723500	H	12.55223100	7.47069600	5.23382200
H	-0.64512700	4.30856200	-5.64884700	C	10.81017400	8.33241700	4.29482500
C	-0.84029300	2.20779100	-6.10480200	H	10.42031700	7.37868100	3.94839500
H	-0.42225000	2.30119400	-7.10386900	C	10.11151000	9.51503700	4.03375700
C	-1.24710300	0.95482300	-5.64075700	H	9.17021100	9.48520700	3.49255900

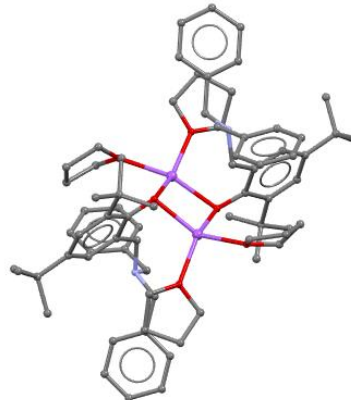
H	-1.12368100	0.07889000	-6.27212700	C	10.61015700	10.73891300	4.49284300
C	-3.15388800	-1.66312700	2.33202700	H	10.05126100	11.65356100	4.30700000
H	-3.47392500	-0.76309300	1.80208900	C	12.46468700	11.12469200	11.90970700
H	-3.18063600	-1.48342000	3.41513600	H	12.71996100	10.21935300	11.35641200
C	-3.95326100	-2.90812600	1.95512900	H	12.20957300	10.86408200	12.94848800
H	-4.86289600	-3.01965600	2.55271500	C	13.53184500	12.21036900	11.85184100
H	-4.23777300	-2.85470200	0.89955100	H	14.33475600	12.05816100	12.57876400
C	-2.92245700	-4.02315000	2.18687400	H	13.97289600	12.22435600	10.85024600
H	-2.83854600	-4.25232600	3.25624800	C	12.70107800	13.47782400	12.11391200
H	-3.15406100	-4.95023100	1.65382000	H	12.55488400	13.61927500	13.19109100
C	-1.63571200	-3.36676000	1.68449000	H	13.16194500	14.38685200	11.71661300
H	-0.73357000	-3.71372300	2.19279300	C	11.36138600	13.15736400	11.42613500
H	-1.51326000	-3.50641300	0.60234300	H	10.49229700	13.48204200	12.01023500
H	-2.42989200	-2.51939800	-1.74209600	H	11.28773300	13.60092600	10.42706900
C	-0.38900800	-2.10890000	-3.24512700	Na	9.39623300	9.60060400	7.12542000
H	0.28680000	-2.38859000	-2.42794500	O	8.34264100	10.99295300	8.50923000
H	-0.99082700	-3.00987100	-3.47043000	O	7.57695400	8.88214500	5.88954200
C	0.41478500	-1.75345000	-4.48061100	N	5.68302400	8.42710500	10.22964200
C	1.26859900	-0.64281700	-4.52322900	C	7.06759200	11.30759400	8.38261200
H	1.34676000	0.02638400	-3.67528600	C	6.63778700	12.60788200	7.96307200
C	2.00421100	-0.34692600	-5.66805500	C	5.26512600	12.84733200	7.80784700
H	2.65089600	0.52655800	-5.67660700	H	4.95232300	13.82854200	7.47860100
C	1.89772400	-1.15456000	-6.80273100	C	4.27498100	11.88775700	8.05748500
H	2.46855300	-0.92120100	-7.69756800	C	4.71485800	10.63147200	8.48927700
C	1.04737300	-2.26014100	-6.77876700	H	3.98176500	9.86322600	8.71932000
H	0.94984500	-2.89472500	-7.65574100	C	6.06357000	10.32781300	8.64824300
C	0.31448500	-2.55265400	-5.62556100	C	7.67427500	13.71449000	7.67824300
H	-0.35022600	-3.41359200	-5.61652300	C	7.02188300	15.04046400	7.23934200
O	1.51259400	-0.57252000	0.03202500	H	6.34969700	15.43995500	8.00737300
N	1.32615300	1.09157500	2.87436600	H	7.80132200	15.79034500	7.05909500
C	2.76996900	-0.44745000	0.39609300	H	6.45100600	14.92791000	6.31027800
C	3.78982300	-1.39733800	0.04234800	C	8.50171800	14.00659700	8.95313500
C	5.11807500	-1.12978800	0.39830400	H	9.02623000	13.10798000	9.27990100
H	5.87282200	-1.84622500	0.10588700	H	9.24361800	14.79362300	8.75998300
C	5.53064800	0.00798600	1.10311500	H	7.84956700	14.34568700	9.76718900
C	4.51876700	0.88561900	1.50104000	C	8.63020100	13.27372700	6.54398800
H	4.77119100	1.76883800	2.08622700	H	8.06688500	13.04167400	5.63108700
C	3.17502300	0.67329100	1.19033600	H	9.34460100	14.07341400	6.30667200
C	3.44586200	-2.65860300	-0.77509400	H	9.19188100	12.38808900	6.84209800
C	4.62853700	-3.64040200	-0.89591900	C	2.77183000	12.15166500	7.87425100
H	4.98505000	-3.97107200	0.08689300	C	2.20813900	11.18932400	6.80194300
H	4.30664000	-4.52886300	-1.45197200	H	2.35177100	10.14163500	7.08778300
H	5.47536100	-3.20737800	-1.44016300	H	1.13226300	11.35186400	6.65633200
C	2.27559200	-3.43837300	-0.13026700	H	2.71158500	11.34577700	5.84031600
H	1.39544500	-2.80324300	-0.02793400	C	2.02952200	11.90880000	9.20978300
H	2.01945000	-4.31244800	-0.74365400	H	2.41631100	12.57273600	9.99174900
H	2.56124500	-3.80050100	0.86447500	H	0.95469600	12.10163500	9.09732100
C	3.05364600	-2.21477900	-2.19768600	H	2.14551500	10.87744200	9.55886300
H	3.90195900	-1.74392300	-2.70835100	C	2.47862300	13.59390900	7.42169300
H	2.71891800	-3.06180300	-2.81026800	H	2.94904700	13.81976100	6.45772900
H	2.24482400	-1.48852800	-2.14844500	H	1.39785600	13.73663100	7.30545300
C	6.99766200	0.30902700	1.44575400	H	2.83472900	14.32693700	8.15461200
C	7.40759100	1.65381000	0.80025500	C	6.48078200	8.94179000	9.10262200
H	6.78374400	2.47949500	1.15941800	H	7.53303300	8.97483400	9.39419600
H	8.45230400	1.89696400	1.03353900	H	6.43812900	8.23410800	8.25946700
H	7.30195100	1.60626200	-0.29010500	C	4.69857000	7.41605800	9.86652000
C	7.16786100	0.40845900	2.97976200	H	4.33265000	7.66060100	8.86195900
H	6.88713700	-0.53540200	3.46112200	H	5.14534100	6.40388500	9.78703900

H	8.21012900	0.63116100	3.24239900	C	3.51170100	7.37599500	10.81338500
H	6.54118200	1.19933200	3.40588500	C	2.99456300	8.56327200	11.34977700
C	7.95699200	-0.77944200	0.92991900	H	3.49627700	9.49902200	11.12528700
H	7.90558400	-0.88074000	-0.16026700	C	1.86618600	8.53810500	12.16897300
H	8.98960000	-0.52068800	1.19176100	H	1.47619900	9.46753700	12.57612800
H	7.73641400	-1.75672700	1.37422000	C	1.23990400	7.32500400	12.46746400
C	2.14976600	1.63091700	1.73915100	H	0.36198300	7.30532700	13.10787500
H	1.43382500	1.92927900	0.96273700	C	1.75397400	6.13737300	11.94455900
C	2.13616200	0.40355100	3.92617200	H	1.27995300	5.18765200	12.17919600
H	3.16456000	0.31690100	3.57189700	C	2.88505000	6.16531100	11.12555200
H	2.16226100	1.01106500	4.83892500	H	3.28600100	5.23615000	10.72513700
C	1.61665400	-0.98636700	4.24565300	C	6.47747800	8.03955100	11.38588500
C	1.95073800	-2.06350900	3.40986400	H	5.78678400	7.63321400	12.13711100
H	2.60350000	-1.89632000	2.55728400	H	7.18974700	7.22325100	11.14677800
C	1.46231200	-3.34474300	3.67149700	C	7.24169500	9.19515600	12.00634400
H	1.73924700	-4.16890600	3.01920000	C	6.76159500	10.51068300	11.93560600
C	0.62987900	-3.57004200	4.77106700	H	5.85174300	10.70912300	11.38030400
H	0.25123300	-4.56848300	4.97569000	C	7.46879100	11.55754700	12.53356300
C	0.30199700	-2.50650300	5.61394700	H	7.08954700	12.57295900	12.45439200
H	-0.33545500	-2.67071800	6.47914100	C	8.66003300	11.30497200	13.22018900
C	0.79627800	-1.22669200	5.35488800	H	9.21172300	12.11948200	13.68141000
H	0.53613900	-0.40755400	6.01808200	C	9.14669300	9.99618600	13.29626500
H	2.66678800	2.54988500	2.06903500	H	10.07916400	9.78895400	13.81452900
C	0.54839700	2.21588600	3.44193500	C	8.44509600	8.95250500	12.68627600
H	-0.02889100	2.65647400	2.62211300	H	8.83906100	7.94044200	12.73188300
H	1.23254800	3.00631500	3.80356000	C	6.60070200	9.77345600	5.30939000
C	-0.37748800	1.82604700	4.57499400	H	6.53943300	10.65813500	5.94406400
C	-1.46433500	0.96423400	4.37680300	H	6.92595500	10.06556700	4.29833900
H	-1.67564500	0.57609200	3.38744500	C	5.32134400	8.94748800	5.26936500
C	-2.28833700	0.59442300	5.43723100	H	4.58142800	9.34115300	4.56645900
H	-3.12715800	-0.07302000	5.26011800	H	4.87480800	8.93531400	6.26843900
C	-2.03842200	1.07682100	6.72439000	C	5.85734200	7.55998000	4.87541000
H	-2.67920900	0.78512700	7.55210500	H	5.95641700	7.48588200	3.78645900
C	-0.96291600	1.93954400	6.93728600	H	5.21484400	6.73975600	5.20836500
H	-0.75869700	2.32407400	7.93302600	C	7.24581100	7.52038100	5.54593500
C	-0.14376800	2.30986400	5.86775500	H	8.02339200	7.11701800	4.88558900
H	0.69715100	2.97745400	6.04110000	H	7.24440100	6.93802000	6.47472000

INT2



Na	0.73488500	0.34448400	-1.37866800
O	1.74884100	2.70861200	-1.48082600
C	3.15399100	2.94274000	-1.67864400
H	3.69374100	2.06899400	-1.31524400
H	3.35599100	3.07695000	-2.75106900

[(d-tb<sup>Bn</sup>)Na(THF)<sub>2</sub>]<sub>2</sub>

Na	10.17653400	11.35369100	9.84534000
O	10.41225400	9.21076500	9.08354600
O	9.17308500	12.66016300	11.48122000
O	12.23201300	12.10194300	10.66992400
N	12.65328700	11.53908100	6.41799900



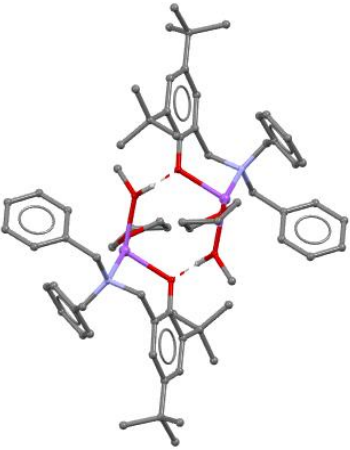
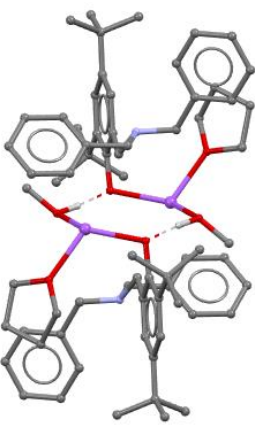
C	3.46048300	4.22670700	-0.91651500	C	11.70378500	8.96865000	9.00581200
H	4.37030000	4.71982800	-1.27235600	C	12.38769300	8.13328500	9.94903900
H	3.58193700	4.00857300	0.14821100	C	13.76132300	7.90876400	9.77686300
C	2.18396200	5.04450900	-1.16705800	H	14.26760600	7.26933500	10.48676600
H	2.25063200	5.56297300	-2.13081200	C	14.52076900	8.48053800	8.74594100
H	1.99150800	5.79634200	-0.39596500	C	13.84227600	9.32046200	7.85412000
C	1.08890800	3.96350700	-1.21228000	H	14.37729800	9.81259500	7.04773700
H	0.34841700	4.15225600	-1.99574500	C	12.48092700	9.57416000	7.96585800
H	0.55763700	3.86467100	-0.26017000	C	11.62612000	7.52870700	11.14874100
Na	-0.30989900	-0.33055200	1.71619400	C	12.53888600	6.68716100	12.06220500
O	-1.15490100	0.75878600	-0.27213300	H	12.98348200	5.84011800	11.52717500
O	-1.11325400	-2.85433600	1.80167900	H	11.95101500	6.28005900	12.89338300
N	-1.34329100	-1.63167700	-2.54251500	H	13.35140300	7.28434700	12.49274900
C	-2.44815900	0.56436000	-0.37479400	C	10.47807500	6.61445000	10.66346500
C	-3.42653900	1.58372500	-0.09384800	H	9.77815300	7.18902700	10.05484300
C	-4.78290600	1.23939000	-0.08818000	H	9.93349800	6.19103400	11.51810900
H	-5.50038700	2.01008000	0.15684700	H	10.87079500	5.78098700	10.06820700
C	-5.26848100	-0.04498800	-0.36759500	C	11.01950400	8.65777100	12.01871200
C	-4.31445400	-0.99454800	-0.74401800	H	11.79405700	9.35818700	12.35141100
H	-4.63422500	-1.99718000	-1.02518900	H	10.53930600	8.23592000	12.91175800
C	-2.94657700	-0.71667000	-0.77643600	H	10.26335100	9.20798600	11.45599700
C	-2.99567700	3.04276800	0.15655300	C	16.03315700	8.26384200	8.58484900
C	-4.17565200	3.97289200	0.49881600	C	16.76530500	9.61411900	8.77437400
H	-4.91273200	4.02173800	-0.31067000	H	16.42294600	10.36490900	8.05438900
H	-3.80020400	4.98988200	0.66332600	H	17.84933300	9.49415700	8.64765300
H	-4.69141000	3.65937200	1.41453900	H	16.58128700	10.01387100	9.77886400
C	-2.33467900	3.57565200	-1.13377100	C	16.33421500	7.71637400	7.17001400
H	-1.48024000	2.95134800	-1.39611400	H	15.82447400	6.75901000	7.01043900
H	-1.98362800	4.60750000	-0.99733800	H	17.41206900	7.55923300	7.03400500
H	-3.04670100	3.56298500	-1.96714500	H	15.99701500	8.40635000	6.38919000
C	-1.98164700	3.13773500	1.31628000	C	16.59833000	7.26466600	9.61086700
H	-2.42310000	2.80165900	2.26176500	H	16.46233900	7.61894400	10.63916000
H	-1.65736200	4.17803600	1.45669300	H	17.67385700	7.12856300	9.44742000
H	-1.11351500	2.51683600	1.09725400	H	16.11940000	6.28260800	9.52281400
C	-6.75304300	-0.42938600	-0.27875800	C	11.79060900	10.47843700	6.96013300
C	-6.92618100	-1.54794900	0.77654100	H	11.44384200	9.87846900	6.11245100
H	-6.33784000	-2.43596200	0.52059700	H	10.89038800	10.93151100	7.40609500
H	-7.97768500	-1.85310800	0.85690700	C	12.86616200	12.56993200	7.43171300
H	-6.59461900	-1.20114300	1.76313200	H	12.98873700	12.05224300	8.38585600
C	-7.24913100	-0.94408200	-1.64992300	H	11.96757600	13.20985800	7.54510800
H	-7.14005000	-0.16723900	-2.41526200	C	14.08377300	13.43776000	7.20118400
H	-8.30762500	-1.23058700	-1.59930900	C	15.26637000	12.89307100	6.68355400
H	-6.68257500	-1.82050100	-1.98227900	H	15.26799300	11.85419000	6.37070500
C	-7.64351800	0.75626600	0.13609900	C	16.41635200	13.67388800	6.56418000
H	-7.36014900	1.15030500	1.11901600	H	17.32577100	13.23511100	6.16150100
H	-8.69000300	0.43482600	0.19518500	C	16.40248700	15.01323100	6.96146300
H	-7.58783500	1.57652400	-0.58853400	H	17.29886500	15.62079400	6.86987000
C	-2.00301300	-1.80808300	-1.21523500	C	15.22614100	15.56829100	7.46885600
H	-1.19601100	-1.94158900	-0.48775100	H	15.20027300	16.61318000	7.76771200
C	-2.26404400	-1.16412700	-3.60850200	C	14.07536200	14.78530200	7.58135000
H	-3.18153700	-0.81064100	-3.13197600	H	13.15701500	15.22523100	7.96550900
H	-2.55250000	-1.98999400	-4.27306700	C	12.09494000	12.12847000	5.19765600
C	-1.69217700	-0.01805200	-4.41939100	H	12.75247500	12.96144100	4.91614600
C	-1.58944000	1.24650800	-3.82153400	H	11.09613400	12.56547900	5.38234200
H	-1.90257400	1.36379900	-2.79025900	C	12.01191600	11.14884100	4.04662800
C	-1.11794900	2.34315300	-4.54143000	C	13.08683600	10.29863400	3.75411100
H	-1.06209400	3.31696400	-4.06051700	H	13.96630900	10.32953200	4.39058500
C	-0.73664700	2.19049900	-5.87808200	C	13.01940400	9.41215700	2.67961000

H	-0.37479900	3.04396100	-6.44617300	H	13.85886600	8.75422700	2.46985800
C	-0.82638300	0.93318100	-6.47953000	C	11.87661200	9.36609400	1.87556800
H	-0.52636600	0.80253600	-7.51635100	H	11.82504300	8.67579800	1.03775500
C	-1.30155200	-0.16397600	-5.75428200	C	10.80061800	10.20928400	2.15905600
H	-1.35826100	-1.14112700	-6.22615500	H	9.90497200	10.17760100	1.54386600
C	-2.50262200	-3.24583500	1.78309300	C	10.86690000	11.08913200	3.24296700
H	-3.06537800	-2.49543000	1.22604500	H	10.02144300	11.73425900	3.46992700
H	-2.87668200	-3.27099400	2.81489500	C	9.15423000	12.23937300	12.86600900
C	-2.54587900	-4.63995500	1.15337600	H	10.12767500	12.46633500	13.31780800
H	-3.39913900	-5.22967500	1.50210300	H	9.00645900	11.15378000	12.88770700
H	-2.60459400	-4.56552600	0.06189700	C	7.98891100	12.98675500	13.53685100
C	-1.18618600	-5.21569000	1.57290900	H	7.46026500	12.35535400	14.25427100
H	-1.22640200	-5.57271800	2.60941500	H	8.35610500	13.87598100	14.06309200
H	-0.84454400	-6.04061600	0.94056000	C	7.11382700	13.40070000	12.34133400
C	-0.28521200	-3.98422100	1.46837900	H	6.46178300	12.57948200	12.02689200
H	0.56021300	-4.00572700	2.15752800	H	6.48820900	14.27429700	12.54824000
H	0.10789300	-3.85293600	0.45199600	C	8.16281200	13.67062700	11.26834900
H	-2.57525700	-2.75436500	-1.22527000	H	7.79368700	13.56392800	10.24761800
C	-0.72364100	-2.92894600	-2.88376300	H	8.61529400	14.66704200	11.39042100
H	0.01157300	-3.15071000	-2.10268000	C	13.45030200	11.42785000	11.05134800
H	-1.48391800	-3.73423900	-2.83740600	H	13.51950200	10.51539700	10.46017500
C	-0.05786800	-2.98861600	-4.23958500	H	13.40104100	11.16220000	12.11828800
C	1.11652700	-2.27242900	-4.49312000	C	14.55473100	12.44550800	10.78438200
H	1.53736100	-1.65585300	-3.70917700	H	15.46269700	12.23920300	11.35910700
C	1.72335800	-2.32300300	-5.74685400	H	14.81967600	12.45064900	9.72283200
H	2.63807200	-1.76455000	-5.92555700	C	13.87822000	13.76953600	11.18542400
C	1.16189000	-3.08771700	-6.77279800	H	14.00474000	13.95494800	12.25805700
H	1.63473700	-3.12395900	-7.75075100	H	14.28405700	14.62661500	10.64094600
C	-0.00768200	-3.80898700	-6.53050100	C	12.39234700	13.52622800	10.85227800
H	-0.45249900	-4.41067100	-7.31889200	H	11.71152000	13.86235900	11.64252700
C	-0.60827500	-3.75984000	-5.26977900	H	12.09547200	14.01012700	9.91471200
H	-1.52022700	-4.32328600	-5.08525800	Na	9.00798900	9.48315400	7.31252000
O	1.59556500	-0.69760900	0.62182200	O	8.65212500	11.55019200	8.21851400
N	1.54011600	1.58846700	2.98928100	O	9.96816000	7.67938600	6.11837800
C	2.86345200	-0.36731500	0.68869800	O	7.03028300	9.01284000	6.15247600
C	3.92756500	-1.24597100	0.27586100	N	6.44034700	8.92203200	10.48902300
C	5.23640300	-0.75060900	0.23834100	C	7.38247100	11.85600400	8.38746500
H	6.01855400	-1.41124800	-0.10945400	C	6.74168500	12.89659900	7.63557400
C	5.59585700	0.54922800	0.62165300	C	5.36882600	13.11599000	7.81774300
C	4.56812000	1.34815500	1.12969400	H	4.89441000	13.89233400	7.23294300
H	4.79554200	2.35067000	1.48833100	C	4.57573300	12.38066000	8.70976900
C	3.23842900	0.92618800	1.17575200	C	5.22850900	11.40666300	9.47347100
C	3.65023700	-2.73180400	-0.03535600	H	4.67464700	10.81712400	10.19874900
C	4.89630500	-3.48574800	-0.53979800	C	6.58820200	11.14342800	9.34322000
H	5.70431500	-3.49566000	0.20027600	C	7.56093000	13.74213400	6.63815600
H	4.63000500	-4.52874100	-0.74811000	C	6.72020700	14.84514900	5.96587300
H	5.28681900	-3.05243200	-1.46876800	H	6.29851800	15.54165600	6.69993600
C	3.18836300	-3.40244600	1.27732100	H	7.35406700	15.42485900	5.28434000
H	2.29203900	-2.90336100	1.64426400	H	5.89506500	14.43023500	5.37510900
H	2.95473900	-4.46397200	1.11645600	C	8.73478500	14.43671700	7.37123500
H	3.96624000	-3.33329600	2.04625200	H	9.38584300	13.69298100	7.83373100
C	2.54696900	-2.90897800	-1.10039400	H	9.32727400	15.03556900	6.66647900
H	2.85591900	-2.48666000	-2.06005600	H	8.35722500	15.10948100	8.15149400
H	2.33968700	-3.97564700	-1.26189300	C	8.12866300	12.84298500	5.51377700
H	1.63364100	-2.41141500	-0.77600800	H	7.31903800	12.36282200	4.95141300
C	7.02012700	1.10921000	0.48913600	H	8.72048600	13.44193100	4.80808900
C	6.99942300	2.31449700	-0.48209600	H	8.77018300	12.06806400	5.93548500
H	6.33767500	3.10928400	-0.12090700	C	3.06537200	12.60181000	8.88489200

H	8.00391700	2.74116600	-0.60169900	C	2.31119300	11.29272900	8.55175700
H	6.63940400	2.00512100	-1.47136200	H	2.62052700	10.47234300	9.20825400
C	7.53878800	1.57724600	1.86823300	H	1.22747900	11.42407000	8.66860100
H	7.56850600	0.73891100	2.57348100	H	2.51064900	10.98351400	7.51907400
H	8.55189800	1.99128200	1.78349800	C	2.76455400	13.00047700	10.34905200
H	6.89766600	2.35294900	2.30023200	H	3.28008800	13.93261600	10.60816900
C	8.01166700	0.06987600	-0.06550800	H	1.68748500	13.15009600	10.50045900
H	7.71874100	-0.27679600	-1.06338800	H	3.09813300	12.23006600	11.05272100
H	9.01087800	0.51343400	-0.14775600	C	2.52119200	13.71096200	7.96618400
H	8.08851700	-0.80511500	0.58991800	H	2.68015600	13.47263600	6.90811900
C	2.19632100	1.89358100	1.67803500	H	1.44264700	13.83106800	8.12245400
H	1.38744800	1.99378500	0.94690400	H	2.99681400	14.67654900	8.17278700
C	2.45685200	1.02291500	4.00935000	C	7.23823500	10.14303000	10.28086600
H	3.34714000	0.65883100	3.49078700	H	7.36662700	10.61001700	11.26262900
H	2.79499700	1.79807500	4.71265000	H	8.24457400	9.87480300	9.93025900
C	1.84874400	-0.14117000	4.76792900	C	6.52986600	8.05638000	9.31639500
C	1.71340400	-1.37629200	4.11671200	H	6.46044300	8.70842900	8.44028300
H	2.02715000	-1.45817500	3.08096300	H	7.51518700	7.55162900	9.25696500
C	1.19760600	-2.48544000	4.78621300	C	5.42508000	7.02907900	9.22830100
H	1.11513500	-3.43783500	4.26914000	C	4.09195800	7.41603200	9.42234600
C	0.80045600	-2.37576200	6.12167200	H	3.88570800	8.44397500	9.70490700
H	0.40170900	-3.23962500	6.64780000	C	3.05517500	6.49989300	9.25320900
C	0.92348100	-1.14848200	6.77591100	H	2.02559000	6.81625200	9.40004100
H	0.61335900	-1.04954300	7.81325000	C	3.33672200	5.17869700	8.89155400
C	1.44807600	-0.04095000	6.10420100	H	2.52845500	4.46448500	8.75840100
H	1.53367500	0.91069500	6.61995300	C	4.66222200	4.78027500	8.71059800
H	2.67662700	2.88559000	1.74863300	H	4.89122700	3.75227700	8.44155800
C	0.92828600	2.85493500	3.44701500	C	5.69868600	5.70153700	8.88306100
H	0.22326700	3.16784000	2.67220900	H	6.73220900	5.38870900	8.74650600
H	1.70427500	3.64375500	3.50087600	C	6.83837100	8.21182600	11.70543900
C	0.22368000	2.80211100	4.78269700	H	6.29767900	7.25626500	11.71270300
C	-0.97548000	2.09830500	4.94200600	H	7.91588600	7.96198500	11.69887300
H	-1.39956700	1.57103000	4.09440600	C	6.50174600	8.97964000	12.96721700
C	-1.60272000	2.04206700	6.18624100	C	5.27458400	9.64578300	13.09025700
H	-2.52419100	1.47791000	6.30102300	H	4.58339200	9.62358700	12.25369000
C	-1.04894900	2.69713500	7.28922600	C	4.95168500	10.33206500	14.26035800
H	-1.54044600	2.64973100	8.25747700	H	3.99760000	10.84733300	14.33773800
C	0.13620700	3.41714600	7.13688000	C	5.84818700	10.35474300	15.33328300
H	0.57407800	3.93694500	7.98516200	H	5.59473800	10.88567200	16.24720800
C	0.76410700	3.46678500	5.88998500	C	7.07298300	9.69385600	15.22045400
H	1.69214300	4.02260400	5.77635100	H	7.78007200	9.70984300	16.04607100
O	2.48420400	0.27331000	-3.08478400	C	7.39775400	9.01789000	14.04137000
C	3.83742800	-0.19987200	-3.21016500	H	8.35704200	8.51297900	13.95313400
H	4.26671400	-0.24153000	-2.20782100	C	10.68532100	7.55343800	4.88117600
H	3.83543700	-1.21567700	-3.63408100	H	10.19120200	6.79813300	4.24869400
C	4.52094800	0.77927800	-4.16183300	H	10.65010200	8.51645700	4.37053300
H	5.38869400	0.33684800	-4.66072400	C	12.09432900	7.10583700	5.29249800
H	4.86044100	1.66462200	-3.61576100	H	12.72096100	7.97739000	5.49270500
C	3.38155200	1.13246100	-5.13653200	H	12.57869900	6.51669300	4.50806400
H	3.34784600	0.41062700	-5.95972400	C	11.85857900	6.30725700	6.60169400
H	3.49080000	2.12794500	-5.57729400	H	12.49894100	6.68087200	7.40386800
C	2.11311200	1.01922900	-4.27139900	H	12.05697400	5.23811100	6.47568300
H	1.30173900	0.49578200	-4.78166500	C	10.36929600	6.55614800	6.92316300
H	1.73769100	1.98811600	-3.93451800	H	10.18583100	6.82458700	7.96187100
O	-2.17332400	-0.37456000	3.18966600	H	9.74868700	5.68675200	6.65428100
C	-2.03889600	-1.12771400	4.42125800	C	5.91217500	9.85125900	5.80315900
H	-1.55998600	-2.08166300	4.19201500	H	5.98255000	10.75964100	6.40056700
H	-1.37532500	-0.56842600	5.08574400	H	5.96870700	10.11238800	4.73453400

C	-3.45762200	-1.27470100	4.99404200	C	4.68926700	8.99195500	6.10700700
H	-3.46706600	-1.21442200	6.08668200	H	3.79695600	9.32289300	5.56679100
H	-3.89329000	-2.23941500	4.70863800	H	4.46970300	9.02955100	7.17738600
C	-4.22941700	-0.13017200	4.31465700	C	5.15637100	7.58076300	5.69138800
H	-4.08039900	0.81356100	4.85128600	H	4.86329500	7.36325000	4.65870600
H	-5.30591300	-0.31594200	4.24680900	H	4.73392600	6.80416600	6.33406200
C	-3.56093800	-0.06624700	2.94479500	C	6.69782000	7.64961100	5.81051800
H	-3.60646700	0.91013400	2.46533400	H	7.20286000	7.37939500	4.87499600
H	-3.98788500	-0.79699900	2.24793000	H	7.09027800	7.01143400	6.60711600

**Table S8.** DFT optimized structures and atom coordinates of complexes for transformation pathways from “closed”  $[(d\text{-}t\text{b}^{\text{Bn}})\text{Na}(\text{THF})_2]$  to “opened”  $[(d\text{-}t\text{b}^{\text{Bn}})\text{Na}(\text{THF})_2]_2$  structures.

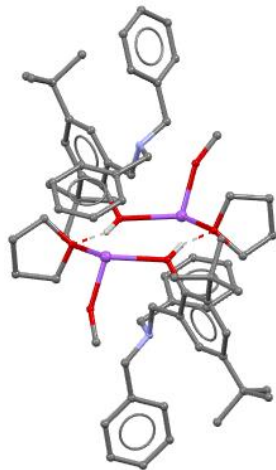
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Na	9.82233700	6.61627000	-8.03924000	Na	10.17680000	10.74210000	-10.34170000
O	8.96971800	8.76644100	-7.61394700	O	10.42300000	8.72930000	-9.38320000
C	10.00810100	9.53419900	-6.95504400	O	12.15520000	11.56360000	-11.12550000
H	10.60274300	8.84687700	-6.34578700	N	12.27990000	11.39040000	-6.69400000
H	10.64955100	9.96957500	-7.72694600	C	11.73140000	8.56710000	-9.15920000
C	9.28845500	10.61276400	-6.14089700	C	12.52280000	7.60340000	-9.85650000
H	9.88328800	11.52664000	-6.04934500	C	13.89990000	7.54580000	-9.59130000
H	9.06410900	10.24672800	-5.13440400	H	14.49110000	6.81780000	-10.12900000
C	7.98937800	10.80726800	-6.93909500	C	14.54850000	8.37600000	-8.66930000
H	8.16749500	11.44804800	-7.81123500	C	13.74770000	9.28380000	-7.96820000
H	7.17784100	11.24566100	-6.35041000	H	14.18320000	9.94150000	-7.22440000
C	7.68642700	9.37622300	-7.38365300	C	12.37880000	9.38640000	-8.18950000
H	7.10979100	9.30853800	-8.31088900	C	11.87380000	6.64710000	-10.87580000
H	7.15579700	8.81517600	-6.60435000	C	12.87810000	5.64930000	-11.48480000
O	10.53914800	6.13170300	-6.01013300	H	13.34040000	5.01550000	-10.71930000
N	9.96368500	4.04910700	-8.48350400	H	12.35520000	4.99080000	-12.18840000
C	10.02800500	5.09154100	-5.36957800	H	13.67720000	6.15520000	-12.03930000
C	9.40090900	5.21022200	-4.09053100	C	10.75660000	5.82500000	-10.18980000
C	8.86056200	4.06207100	-3.49899100	H	9.99990000	6.48410000	-9.76150000
H	8.37333700	4.16679700	-2.53957500	H	10.27220000	5.15680000	-10.91390000
C	8.92302600	2.78284100	-4.07005400	H	11.17730000	5.20510000	-9.38840000
C	9.57535600	2.68291500	-5.30336300	C	11.26820000	7.46670000	-12.03650000
H	9.66957800	1.71164400	-5.78648000	H	12.04210000	8.05520000	-12.54530000
C	10.10509900	3.79445600	-5.95776000	H	10.79650000	6.80820000	-12.77780000
C	9.30038800	6.58330300	-3.39862000	H	10.51170000	8.14480000	-11.64270000

C	8.67290700	6.49699200	-1.99326900	C	16.05760000	8.31290000	-8.38280000
H	7.64190700	6.12519800	-2.02283600	C	16.70320000	9.68630000	-8.68130000
H	8.64780800	7.49667700	-1.54353400	H	16.25260000	10.48750000	-8.08590000
H	9.25243400	5.84780000	-1.32639500	H	17.77780000	9.66670000	-8.45770000
C	8.40986000	7.51571700	-4.25066900	H	16.58040000	9.94910000	-9.73810000
H	8.81730800	7.62676400	-5.25542900	C	16.28510000	7.96220000	-6.89340000
H	8.33498400	8.50658300	-3.78192600	H	15.83650000	6.99180000	-6.65150000
H	7.39618500	7.10711800	-4.33652800	H	17.35750000	7.91170000	-6.66490000
C	10.70627200	7.21037300	-3.23771500	H	15.83760000	8.71110000	-6.23090000
H	11.34358200	6.57566400	-2.60965500	C	16.77510000	7.25290000	-9.23840000
H	10.63588200	8.19392600	-2.75457300	H	16.66790000	7.45890000	-10.30970000
H	11.18773400	7.32910500	-4.20795900	H	17.84640000	7.24760000	-9.00610000
C	8.31844700	1.53228700	-3.41162700	H	16.38780000	6.24610000	-9.04450000
C	9.43039100	0.48913700	-3.15339300	C	11.53110000	10.30480000	-7.33030000
H	9.92868000	0.19174300	-4.08232100	H	11.09950000	9.68880000	-6.53580000
H	9.01508600	-0.41621500	-2.69209100	H	10.67300000	10.69830000	-7.89660000
H	10.19404100	0.89705400	-2.48118400	C	12.52490000	12.46610000	-7.65390000
C	7.25479600	0.91909300	-4.35285200	H	12.74710000	11.98080000	-8.60940000
H	6.45040400	1.63817500	-4.54768600	H	11.61330000	13.06400000	-7.83120000
H	6.81024400	0.02012700	-3.90655500	C	13.68340000	13.37180000	-7.29600000
H	7.68662300	0.63360600	-5.31817000	C	14.81590000	12.88100000	-6.63360000
C	7.63757100	1.84609600	-2.06654100	H	14.82110000	11.84800000	-6.30200000
H	8.34708600	2.25776100	-1.33972600	C	15.91170000	13.70940000	-6.38780000
H	7.21775400	0.92828400	-1.63848900	H	16.78210000	13.31180000	-5.87190000
H	6.81697000	2.56285200	-2.18594600	C	15.89290000	15.04330000	-6.80150000
C	10.77238000	3.62231900	-7.29965500	H	16.74680000	15.68790000	-6.61120000
H	11.69181500	4.21293500	-7.33351800	C	14.76430000	15.54560000	-7.45260000
C	8.58440100	3.48107300	-8.46621700	H	14.73320000	16.58600000	-7.76630000
H	8.51652100	2.65973300	-7.74552800	C	13.66700000	14.71570000	-7.69040000
H	8.36350300	3.05898700	-9.44929700	H	12.78350000	15.11330000	-8.18640000
C	7.53926900	4.53541800	-8.15458900	C	11.63550000	11.88770000	-5.47520000
C	6.99766800	4.67733000	-6.87029800	H	12.26780000	12.69500000	-5.08280000
H	7.31949600	4.01409100	-6.07353800	H	10.64840000	12.33680000	-5.69290000
C	6.05760100	5.67637400	-6.60625300	C	11.48020000	10.80350000	-4.42290000
H	5.64688000	5.77201400	-5.60488600	C	12.44590000	9.79710000	-4.27210000
C	5.65052800	6.54845300	-7.61720500	H	13.31650000	9.80510000	-4.91990000
H	4.91794100	7.32375800	-7.40819900	C	12.26970000	8.77480000	-3.34040000
C	6.18790300	6.41808800	-8.90103100	H	13.02510000	7.99890000	-3.24610000
H	5.87044700	7.08659800	-9.69761500	C	11.12670000	8.73920000	-2.53560000
C	7.12373000	5.41653900	-9.16795100	H	10.99010000	7.93930000	-1.81280000
H	7.53519900	5.31011300	-10.16943800	C	10.16730000	9.74450000	-2.66330000
H	11.05313000	2.55954100	-7.41990600	H	9.27950000	9.73850000	-2.03570000
C	10.70973800	3.66705500	-9.70769400	C	10.34580000	10.76880000	-3.59960000
H	11.72008100	4.07782600	-9.59856400	H	9.60010000	11.55460000	-3.68240000
H	10.81582600	2.56792900	-9.77265800	C	13.39780000	10.89450000	-11.41920000
C	10.09334000	4.19638200	-10.98358500	H	13.35990000	9.91120000	-10.94900000
C	10.24120700	5.54777500	-11.32246200	H	13.50290000	10.77640000	-12.50920000
H	10.83801900	6.19017000	-10.68383300	C	14.46810000	11.82140000	-10.84990000
C	9.62964500	6.06674000	-12.46327500	H	15.44670000	11.66630000	-11.31360000
H	9.75840200	7.11718900	-12.71090700	H	14.57510000	11.64530000	-9.77640000
C	8.86519700	5.23783000	-13.28975500	C	13.89030000	13.22560000	-11.12800000
H	8.38878500	5.64105900	-14.17942900	H	14.27550000	13.62430000	-12.07230000
C	8.73000500	3.88509600	-12.97374200	H	14.14510000	13.93370000	-10.33520000
H	8.14813400	3.22969800	-13.61642300	C	12.36420000	12.99090000	-11.22490000
C	9.34475600	3.36967100	-11.82966200	H	11.95680000	13.34780000	-12.18030000
H	9.23870100	2.31363000	-11.59044700	H	11.79620000	13.44660000	-10.40970000
Na	14.67955200	6.92363400	-7.08367900	Na	8.61860000	9.96010000	-6.15700000
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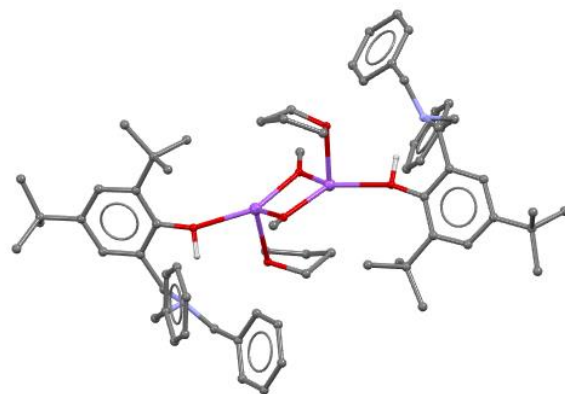
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H	13.85196700	3.57008300	-7.39479600	C	7.06570000	12.13450000	-7.34070000
C	15.21302700	2.92572800	-8.98041400	C	6.27400000	13.09740000	-6.64260000
H	14.61806200	2.01189100	-9.07150400	C	4.89690000	13.15480000	-6.90780000
H	15.43751900	3.29118100	-9.98708200	H	4.30540000	13.88210000	-6.36950000
C	16.51194900	2.73142200	-8.18192100	C	4.24850000	12.32510000	-7.83050000
H	16.33356500	2.09109800	-7.30950300	C	5.04970000	11.41830000	-8.53240000
H	17.32350800	2.29259000	-8.77025000	H	4.61430000	10.76090000	-9.27660000
C	16.81512600	4.16263400	-7.73798500	C	6.41860000	11.31590000	-8.31120000
H	17.39139200	4.23054700	-6.81052600	C	6.92260000	14.05300000	-5.62240000
H	17.34625800	4.72312500	-8.51733100	C	5.91800000	15.05000000	-5.01270000
O	13.96263200	7.40759200	-9.11255800	H	5.45560000	15.68430000	-5.77780000
N	14.53857300	9.49117900	-6.64048900	H	6.44060000	15.70820000	-4.30860000
C	14.47366400	8.44736000	-9.75385100	H	5.11900000	14.54340000	-4.45860000
C	15.10041100	8.32792900	-11.03299100	C	8.03970000	14.87600000	-6.30760000
C	15.64083500	9.47569700	-11.62521300	H	8.79660000	14.21740000	-6.73640000
H	16.12783500	9.37041900	-12.58468100	H	8.52390000	15.54360000	-5.58280000
C	15.57870900	10.75522300	-11.05476600	H	7.61890000	15.49640000	-7.10840000
C	14.92661700	10.85588300	-9.82139000	C	7.52830000	13.23260000	-4.46240000
H	14.83264500	11.82741200	-9.33874700	H	6.75460000	12.64300000	-3.95450000
C	14.39682500	9.74474900	-9.16633100	H	7.99920000	13.89060000	-3.72020000
C	15.20062600	6.95445600	-11.72418600	H	8.28540000	12.55540000	-4.85660000
C	15.82766300	7.03991400	-13.12978200	C	2.73930000	12.38740000	-8.11630000
H	16.85874000	7.41153300	-13.10076200	C	2.09470000	11.01360000	-7.81780000
H	15.85244200	6.03998500	-13.57899300	H	2.54560000	10.21280000	-8.41360000
H	15.24802500	7.68885800	-13.79680100	H	1.02000000	11.03240000	-8.04080000
C	16.09134300	6.02248000	-10.87187900	H	2.21830000	10.75070000	-6.76110000
H	15.68428800	5.91211400	-9.86688000	C	2.51090000	12.73840000	-9.60560000
H	16.16592100	5.03130200	-11.34001800	H	2.95880000	13.70910000	-9.84740000
H	17.10510800	6.43099200	-10.78667900	H	1.43830000	12.78820000	-9.83350000
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H	13.31351000	6.20921700	-10.91381300	H	0.95010000	13.45170000	-7.49230000
C	16.18330700	12.00535700	-11.71396900	H	2.40830000	14.45380000	-7.45380000
C	15.07132700	13.04830800	-11.97290700	C	7.26630000	10.39820000	-9.17110000
H	14.57302900	13.34627000	-11.04416600	H	7.69580000	11.01430000	-9.96680000
H	15.48659700	13.95337300	-12.43480500	H	8.12560000	10.00630000	-8.60560000
H	14.30770100	12.63991000	-12.64484900	C	6.27430000	8.23660000	-8.84430000
C	17.24691300	12.61919500	-10.77312200	H	6.05310000	8.72290000	-7.88910000
H	18.05134400	11.90027900	-10.57783100	H	7.18620000	7.63910000	-8.66730000
H	17.69141600	13.51790200	-11.21998800	C	5.11570000	7.33010000	-9.19960000
H	16.81508700	12.90528400	-9.80798300	C	3.98240000	7.81940000	-9.86170000
C	16.86424700	11.69069100	-13.05882100	H	3.97680000	8.85190000	-10.19520000
H	16.15477300	11.27857400	-13.78542000	C	2.88650000	6.99050000	-10.10490000
H	17.28408900	12.60822900	-13.48743700	H	2.01550000	7.38700000	-10.62070000
H	17.68483200	10.97400000	-12.93891200	C	2.90590000	5.65740000	-9.68860000
C	13.72983400	9.91769300	-7.82439800	H	2.05180000	5.01230000	-9.87690000
H	12.81021600	9.32738600	-7.79010800	C	4.03520000	5.15640000	-9.03770000
C	15.91796400	10.05891800	-6.65814700	H	4.06670000	4.11670000	-8.72200000
H	15.98589800	10.88020600	-7.37890900	C	5.13260000	5.98690000	-8.80260000
H	16.13912000	10.48104400	-5.67514900	H	6.01670000	5.59040000	-8.30670000
C	16.96286300	9.00433000	-6.96976200	C	7.16200000	8.81280000	-11.02420000
C	17.50425900	8.86202000	-8.25408900	H	6.53000000	8.00450000	-11.41520000
H	17.18251800	9.52516000	-9.05096000	H	8.14950000	8.36460000	-10.80630000
C	18.44412500	7.86274400	-8.51800100	C	7.31610000	9.89580000	-12.07790000
H	18.85467700	7.76678000	-9.51940500	C	6.34870000	10.90020000	-12.23070000

C	18.85117500	6.99085000	-7.50689300	H	5.47760000	10.89140000	-11.58340000
H	19.58362100	6.21537700	-7.71577400	C	6.52350000	11.92150000	-13.16360000
C	18.31398000	7.12159900	-6.22302400	H	5.76670000	12.69590000	-13.25960000
H	18.63146400	6.45323100	-5.42633100	C	7.66690000	11.95800000	-13.96780000
C	17.37836800	8.12337500	-5.95623300	H	7.80260000	12.75720000	-14.69160000
H	16.96699000	8.23013000	-4.95473700	C	8.62820000	10.95480000	-13.83810000
H	13.44945200	10.98061400	-7.70456800	H	9.51640000	10.96160000	-14.46510000
C	13.79274600	9.87385800	-5.41635500	C	8.45100000	9.93140000	-12.90040000
H	12.78220800	9.46353600	-5.52536400	H	9.19810000	9.14710000	-12.81610000
H	13.68717300	10.97304700	-5.35162400	C	5.39660000	9.80530000	-5.08280000
C	14.40891100	9.34447600	-4.14036100	H	5.43350000	10.78730000	-5.55580000
C	14.26012300	7.99327200	-3.80109400	H	5.29050000	9.92640000	-3.99330000
H	13.66284100	7.35106100	-4.43948200	C	4.32780000	8.87530000	-5.65010000
C	14.87142600	7.47421200	-2.66018200	H	3.34860000	9.03100000	-5.18790000
H	14.74197700	6.42392500	-2.41223200	H	4.22180000	9.04730000	-6.72430000
C	15.63652400	8.30282700	-1.83399800	C	4.90700000	7.47310000	-5.36620000
H	16.11272000	7.89951700	-0.94424500	H	4.52440000	7.07950000	-4.41870000
C	15.77263200	9.65537300	-2.15040600	H	4.65070000	6.76040000	-6.15440000
H	16.35500400	10.31055500	-1.50795800	C	6.43310000	7.70930000	-5.27440000
C	15.15813700	10.17090100	-3.29458100	H	6.84440000	7.35220000	-4.32070000
H	15.26490700	11.22680200	-3.53410000	H	6.99850000	7.25450000	-6.09190000
C	13.35457700	4.76640600	-4.95017100	H	9.66780000	8.27020000	-8.05060000
H	14.41968900	4.51544900	-4.99377500	O	9.27180000	8.02380000	-7.14800000
H	12.76698800	3.86199500	-5.15052800	C	10.08030000	6.99670000	-6.57970000
H	13.10593500	5.10866200	-3.93546300	H	9.63800000	6.71240000	-5.61880000
O	13.10952000	5.77582100	-5.92146100	H	10.11220000	6.11250000	-7.22850000
H	12.11237300	5.95517500	-5.96590000	H	11.11030000	7.33730000	-6.40650000
C	11.14713500	8.77436900	-10.17227300	H	9.12920000	12.43240000	-8.44880000
H	10.08193300	9.02496400	-10.12897200	H	7.68680000	13.36530000	-10.09380000
H	11.73435900	9.67892000	-9.97147500	O	9.52510000	12.67920000	-9.35120000
H	11.39627400	8.43245000	-11.18697000	H	9.15960000	13.99250000	-10.87900000
O	11.39213900	7.76479200	-9.20113800	H	8.68300000	14.58960000	-9.26900000
H	12.38916300	7.58500300	-9.15692300	C	8.71640000	13.70640000	-9.91900000

**INT2**



**3**



Na	10.36264900	11.24024000	11.43206100
O	11.03763800	9.17935800	10.53569000
O	9.66834800	12.91400200	9.62343700
N	13.70733300	11.63025400	8.35367800
C	12.41856200	8.93116500	10.64416000
C	12.91347000	7.94709700	11.51655900
C	14.30612900	7.74986700	11.52074000
H	14.71347000	7.00017600	12.18231900

Na	0.20227400	1.16731500	-0.11920700
O	-1.03547200	0.46153800	1.76064100
C	-0.54740200	1.17468700	2.92317400
H	0.17816000	1.92210700	2.58448200
H	-1.39128200	1.69146800	3.39680800
C	0.10384600	0.12580200	3.83472700
H	-0.62024200	-0.25324600	4.56645400
H	0.96175200	0.53134500	4.37812200

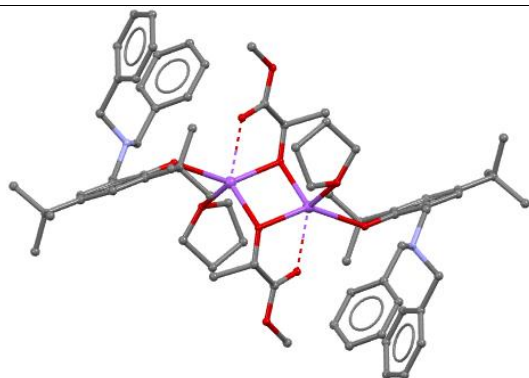
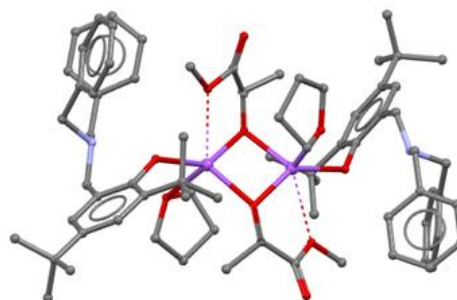
C	15.18580400	8.47686800	10.71448800	C	0.48631800	-0.97784200	2.83674100
C	14.63682600	9.44722900	9.87055500	H	0.62357600	-1.95659000	3.30656300
H	15.27564300	10.05120300	9.24169500	H	1.40093400	-0.70204800	2.30329500
C	13.26891900	9.69394000	9.83352200	C	-0.69230100	-0.94534500	1.86958100
C	12.00178100	7.15205100	12.47225000	H	-1.56207300	-1.49456100	2.25747400
C	12.76408700	6.04163300	13.22446400	H	-0.45023500	-1.29194700	0.86049100
H	13.20649800	5.31275500	12.53557400	O	-1.15508600	3.02814400	0.01601400
H	12.06724600	5.50354500	13.87694700	N	-3.69391900	2.33946300	0.43487000
H	13.56029300	6.44331000	13.85993800	C	-1.54258400	4.34805000	0.07708900
C	10.84218600	6.46525800	11.71233800	C	-0.74989500	5.37379500	-0.47161100
H	10.18018700	7.19287000	11.24458600	C	-1.25055000	6.68179100	-0.36003200
H	10.24807200	5.85529400	12.40409900	H	-0.65697700	7.48253700	-0.77431400
H	11.22987600	5.80028700	10.93062700	C	-2.47181400	7.00820000	0.23867400
C	11.44365000	8.13414600	13.52722700	C	-3.22318500	5.95144600	0.76407200
H	12.25728600	8.55918500	14.12492800	H	-4.18142800	6.14309100	1.24086600
H	10.74828000	7.62140500	14.20540400	C	-2.77155700	4.63699100	0.70284800
H	10.91538700	8.96126000	13.05307500	C	0.60179100	5.09434000	-1.15560800
C	16.71109600	8.29136900	10.75282000	C	1.25850800	6.38198600	-1.69623200
C	17.35089400	9.57779100	11.32744000	H	0.63746500	6.87700300	-2.45189700
H	17.11160900	10.45538400	10.72101600	H	2.21381300	6.12595200	-2.16752400
H	18.44331100	9.47896300	11.36125800	H	1.47103100	7.10097800	-0.89706200
H	16.99180300	9.76623100	12.34564200	C	0.40778700	4.14878600	-2.36345900
C	17.24684200	8.05570900	9.32124200	H	0.02515700	3.17154300	-2.06727800
H	16.78543700	7.16895700	8.87009400	H	1.36630600	3.99413500	-2.87159200
H	18.33259400	7.90200400	9.34330600	H	-0.29517700	4.57901600	-3.08673800
H	17.05112900	8.91259800	8.66885500	C	1.58980700	4.46992300	-0.14506700
C	17.13611000	7.09743600	11.62678100	H	1.76168200	5.15562800	0.69322300
H	16.84392000	7.23563400	12.67391300	H	2.55273100	4.27882800	-0.63071000
H	18.22644300	6.99063000	11.60285700	H	1.24400000	3.51894200	0.26043500
H	16.69978000	6.15675300	11.26979300	C	-3.00254600	8.44879200	0.32847900
C	12.68758400	10.74171600	8.90295600	C	-3.20156100	8.83208600	1.81339200
H	12.19494500	10.22953200	8.06887000	H	-3.91414500	8.16685700	2.31250900
H	11.90535600	11.30595700	9.42690700	H	-3.58592100	9.85621200	1.89765600
C	14.18434200	12.60804500	9.34372300	H	-2.25297500	8.77619300	2.35942000
H	13.76695600	12.33716100	10.32099500	C	-4.35787200	8.54317500	-0.41041600
H	13.76386900	13.60492300	9.12610200	H	-4.24306400	8.27862700	-1.46775900
C	15.69518200	12.71922200	9.43619200	H	-4.75632600	9.56379200	-0.35362500
C	16.55136900	12.24356500	8.43650600	H	-5.10459400	7.86962300	0.02343300
H	16.12962700	11.75420100	7.56362600	C	-2.04081300	9.47151800	-0.30441600
C	17.93766800	12.36049400	8.56814500	H	-1.06513500	9.47441200	0.19475900
H	18.58705500	11.97798900	7.78444000	H	-2.46176600	10.47933400	-0.21478600
C	18.48754300	12.95740000	9.70306900	H	-1.88063300	9.27304800	-1.37028700
H	19.56570600	13.04201200	9.81028900	C	-3.56150200	3.51304600	1.33351300
C	17.64007400	13.43506200	10.70663300	H	-3.03698200	3.15643600	2.22987200
H	18.05812400	13.88886900	11.60164100	H	-4.54930400	3.87589100	1.66367500
C	16.25701300	13.31602500	10.57315800	C	-4.55418700	2.65550500	-0.73374000
H	15.59873100	13.66739500	11.36498500	H	-4.39634300	3.71675400	-0.95484200
C	13.34979500	12.22384000	7.07510800	H	-5.61599900	2.53840700	-0.46454600
H	14.16008700	12.91065300	6.79749700	C	-4.23203700	1.84496700	-1.97388800
H	12.43410100	12.84494100	7.13776400	C	-2.93988200	1.86750500	-2.51625600
C	13.16771000	11.19606000	5.97183600	H	-2.17073300	2.47019400	-2.04858300
C	13.87999500	9.98740800	5.97162600	C	-2.62726800	1.10834400	-3.64250900
H	14.57272700	9.78874500	6.78390300	H	-1.61419900	1.12231600	-4.03436700
C	13.66701200	9.03659100	4.97049000	C	-3.60973900	0.32670400	-4.25561400
H	14.21765400	8.09975900	4.99369400	H	-3.36466700	-0.27410500	-5.12742600
C	12.74310700	9.27845400	3.94895300	C	-4.90531900	0.31924200	-3.73806100
H	12.56747500	8.53277000	3.17894900	H	-5.67597000	-0.28997900	-4.20278600
C	12.04361200	10.48933800	3.92808500	C	-5.21247800	1.07608900	-2.60642100



H	11.31923300	10.69043500	3.14351900	H	-6.21331300	1.03429900	-2.18584200
C	12.25841800	11.43867700	4.93317400	C	-4.16264900	1.17944600	1.23498400
H	11.70122100	12.37035600	4.92179900	H	-5.05107300	1.48036400	1.81731400
C	10.73618000	13.92069000	9.72974200	H	-3.35581200	0.95131400	1.93756200
H	11.03147200	14.20813300	8.71463100	C	-4.50061500	-0.05951900	0.44035800
H	11.54380800	13.42578600	10.27853900	C	-3.51289300	-0.77155700	-0.25455600
C	10.13484300	15.10113800	10.52153800	H	-2.48592800	-0.42367800	-0.24597000
H	10.74054600	15.33014000	11.40155100	C	-3.85071500	-1.90632200	-0.98875300
H	10.07972500	16.00134100	9.90012900	H	-3.07712800	-2.43593400	-1.53359200
C	8.71930800	14.61905300	10.90425200	C	-5.17472300	-2.35209100	-1.03208600
H	8.73316600	14.10968900	11.87428300	H	-5.43269600	-3.23667500	-1.60868600
H	7.98525500	15.42960700	10.95127200	C	-6.16177800	-1.65812000	-0.33361600
C	8.41129900	13.61260900	9.80569900	H	-7.19394100	-1.99845500	-0.35798900
H	7.65725800	12.86656800	10.05338500	C	-5.82167000	-0.51789100	0.39747200
H	8.12448600	14.10239800	8.86638000	H	-6.59383000	0.02699100	0.93677600
Na	10.22791600	9.60669900	6.37109200	O	0.30227200	-0.66213300	-1.28038400
O	9.35929400	11.60293800	7.20799600	C	-0.42107100	-1.57979200	-2.01425400
O	10.85540000	7.89800200	8.08859300	H	-0.78158800	-2.44129600	-1.40618100
N	6.59838200	9.20343400	9.37735800	H	-1.32430100	-1.14758400	-2.49169300
C	7.98607800	11.89393600	7.10578900	H	0.15868700	-2.04208200	-2.84820700
C	7.52231600	12.92758900	6.27449700	H	-2.00489600	2.49001300	0.13332500
C	6.14380500	13.20650400	6.31960500	Na	2.41899100	-0.60529800	-0.69429600
H	5.76278300	14.00163800	5.69642100	O	3.23868000	0.07792700	-2.82309300
C	5.24792700	12.50615200	7.13164000	C	2.78614100	-0.82872100	-3.85576800
C	5.75867700	11.45643000	7.90150400	H	2.29947900	-1.67855800	-3.36561400
H	5.10240100	10.86066100	8.52290900	H	3.65856800	-1.19583700	-4.41136700
C	7.10982200	11.12817200	7.88743800	C	1.80643000	-0.04020800	-4.74048500
C	8.45077700	13.68233200	5.30227700	H	2.31435300	0.33682300	-5.63629700
C	7.72052900	14.81260500	4.54845900	H	0.96139600	-0.65607800	-5.06100400
H	7.32512200	15.57124900	5.23382200	C	1.38466300	1.12101900	-3.82571000
H	8.42529100	15.31031300	3.87286000	H	1.02714000	1.99574500	-4.37639900
H	6.89405900	14.43458000	3.93745900	H	0.61807700	0.77693600	-3.12467000
C	9.64422000	14.33132400	6.04112200	C	2.67184500	1.38948100	-3.05079500
H	10.27240000	13.58359600	6.52318600	H	3.38512400	1.99755500	-3.62729100
H	10.26397700	14.89582800	5.33328900	H	2.53298900	1.85162900	-2.06974900
H	9.29286300	15.03254500	6.80793700	O	4.39791800	-1.71623000	-0.37218900
C	8.95831700	12.67048400	4.24807200	N	6.50142800	-0.58658300	-1.54560800
H	8.12033800	12.26887300	3.66817800	C	5.09403200	-2.90207400	-0.39122900
H	9.65684600	13.15485300	3.55263200	C	4.77736600	-3.94328400	0.50039500
H	9.46673300	11.82813800	4.71829600	C	5.55723600	-5.10817200	0.40671900
C	3.74482800	12.81943800	7.19865600	H	5.33072300	-5.92082000	1.08061300
C	2.94116200	11.56889500	6.76902500	C	6.61832100	-5.26967100	-0.49115000
H	3.13110800	10.71459600	7.42687600	C	6.89964500	-4.19759700	-1.34705400
H	1.86482000	11.77931200	6.79862000	H	7.71687500	-4.26566000	-2.06106400
H	3.20441400	11.27094600	5.74790300	C	6.14832700	-3.02735200	-1.31742600
C	3.36901700	13.19016400	8.65276600	C	3.63309200	-3.81783300	1.52634500
H	3.92806300	14.07205700	8.98770600	C	3.55141300	-5.04590300	2.45669100
H	2.29804400	13.41573400	8.72671300	H	4.47216800	-5.18078200	3.03575500
H	3.58471200	12.37010700	9.34603700	H	2.72986800	-4.90503100	3.16788900
C	3.34584600	13.99099200	6.28344700	H	3.35063000	-5.97121400	1.90511200
H	3.55927300	13.77275400	5.23084500	C	3.84583200	-2.57824400	2.43085400
H	2.27002100	14.18011900	6.37056700	H	3.81861600	-1.64319100	1.87098600
H	3.86840400	14.91566500	6.55527300	H	3.06354100	-2.53723500	3.19706700
C	7.64581500	9.93716300	8.65769100	H	4.81382500	-2.64364500	2.94245500
H	8.39793100	10.27275400	9.38072900	C	2.27944700	-3.72003400	0.78343000
H	8.14795500	9.28586300	7.92236800	H	2.08270700	-4.63882300	0.21879600
C	5.92561200	8.23320700	8.51309800	H	1.45882400	-3.57433800	1.49555400
H	5.85653100	8.67869700	7.51583800	H	2.25226700	-2.89150200	0.07435600

H	6.52997100	7.31734700	8.38053800	C	7.46981700	-6.54871400	-0.55858200
C	4.52571100	7.86544300	8.96945000	C	7.36695400	-7.16074000	-1.97507400
C	3.78234000	8.68305400	9.82980000	H	7.72072300	-6.46619800	-2.74437700
H	4.24500300	9.57532800	10.23914800	H	7.97330600	-8.07239000	-2.04449900
C	2.46983900	8.35033900	10.17368300	H	6.32888600	-7.42103600	-2.21131800
H	1.90998800	8.99646800	10.84529100	C	8.94601900	-6.19889200	-0.25790800
C	1.87995700	7.19474400	9.66094900	H	9.04605000	-5.76427400	0.74319500
H	0.85872600	6.93557400	9.92737300	H	9.57135600	-7.09906800	-0.30495100
C	2.61551800	6.36948300	8.80611300	H	9.34713900	-5.47705100	-0.97725800
H	2.16776600	5.46397200	8.40455300	C	7.01509800	-7.61388100	0.45633100
C	3.92718500	6.70138000	8.46925300	H	5.97945700	-7.92649900	0.28054600
H	4.49551400	6.05569000	7.80270900	H	7.64910000	-8.50327100	0.36754800
C	7.04831500	8.62906600	10.63471000	H	7.09457600	-7.25242600	1.48790800
H	6.25124100	7.96797000	10.99803100	C	6.42193200	-1.88120700	-2.26610700
H	7.94363100	7.98836200	10.51031700	H	5.58997000	-1.78939400	-2.97513000
C	7.32980500	9.67504200	11.69841700	H	7.33314100	-2.07430800	-2.85602600
C	6.71763500	10.93560400	11.66773000	C	7.72314700	-0.51108300	-0.70110600
H	6.05000600	11.17091400	10.84513400	H	7.98967300	-1.54089800	-0.44149000
C	6.98427700	11.88215000	12.66090100	H	8.55812800	-0.10004700	-1.29019100
H	6.50564600	12.85679100	12.61590300	C	7.53563200	0.27767900	0.57818400
C	7.86812400	11.58550100	13.70259400	C	6.65976800	-0.19826100	1.56177800
H	8.08322800	12.32439300	14.46927600	H	6.13394500	-1.13341800	1.40608400
C	8.47540000	10.32538400	13.74870700	C	6.44595400	0.52484600	2.73357500
H	9.16721300	10.08063500	14.55007700	H	5.74836200	0.14873200	3.47708500
C	8.20487600	9.38089000	12.75325000	C	7.11873600	1.73112200	2.94408900
H	8.68694800	8.40864800	12.78814400	H	6.94537600	2.30171600	3.85263000
C	9.79399900	6.86991000	8.00354400	C	8.01151800	2.20036500	1.97962300
H	9.39499400	6.71896300	9.01230600	H	8.53584500	3.14006400	2.13119600
H	9.04045100	7.28525100	7.32017500	C	8.22044800	1.47402800	0.80659600
C	10.46980000	5.60611100	7.44363500	H	8.89020800	1.86125500	0.04409600
H	9.85888600	5.14092900	6.66519300	C	6.37481000	0.54008800	-2.49551200
H	10.64079200	4.86482200	8.23306200	H	7.21991000	0.52471800	-3.20672600
C	11.81654000	6.12311700	6.90687900	H	5.45400000	0.36187500	-3.05751400
H	11.69797600	6.54452400	5.90162500	C	6.29413800	1.89853500	-1.83673300
H	12.59376300	5.35320800	6.87391700	C	5.29544400	2.18658900	-0.89580900
C	12.13213200	7.23346800	7.89654900	H	4.55543100	1.44209500	-0.61979800
H	12.84303000	7.98040500	7.54157900	C	5.25127900	3.43522400	-0.27856300
H	12.48866700	6.83864300	8.85583800	H	4.49397400	3.62652300	0.47356600
H	10.77294200	8.80468200	9.65943700	C	6.18442300	4.42175700	-0.60993000
O	8.53714600	8.51614700	5.88890300	H	6.14632100	5.39318300	-0.12367300
C	7.33838200	8.54479400	5.21707700	C	7.16508500	4.15260200	-1.56427500
H	6.68426300	7.66706200	5.43617100	H	7.89426200	4.91329400	-1.83174400
H	7.44023600	8.54940900	4.10738300	C	7.21887000	2.89435000	-2.16841300
H	6.71422200	9.43990000	5.45435000	H	7.99683700	2.67915100	-2.89832600
H	9.64815600	11.99887800	8.06766600	O	2.27000100	1.11742600	0.60199100
H	12.27832700	13.51917700	13.55111200	C	2.92813600	1.62660300	1.70286300
O	12.08503600	12.30305200	11.85739800	H	4.03109100	1.54536100	1.63795500
H	13.79185400	12.84185300	12.93285500	H	2.65940800	1.11718700	2.65840000
H	12.99969800	14.16834000	12.06849100	H	2.71952400	2.70664600	1.88373900
C	12.78996400	13.20795500	12.60981000	H	5.04610800	-1.01895800	-0.71535400

**Table S9.** DFT optimized structures and atom coordinates of complexes for proposed mechanism of the reaction between  $[(\text{d-}t\text{bL}^{\text{Bn}})\text{Na}(\text{THF})_2]$  and methanol.

**A****B**

Na	0.20416100	1.30712700	-0.28320100
O	-0.59951500	0.70808400	1.94573900
C	-0.51199100	1.41397600	3.18785200
H	-0.49546000	2.48346000	2.96502500
H	-1.40614300	1.19494500	3.79435200
C	0.76406400	0.89420600	3.87434700
H	0.63184600	0.82670500	4.95887300
H	1.60532800	1.56683200	3.68456800
C	1.00013900	-0.48780500	3.20592600
H	1.04173400	-1.30476600	3.93299100
H	1.94057800	-0.48256200	2.65235100
C	-0.18560600	-0.64701400	2.24063500
H	-1.02776800	-1.17616800	2.71384900
H	0.08145500	-1.10666100	1.28545600
O	-1.56950700	2.82751000	-0.78524100
N	-3.81314400	1.99450400	0.46340000
C	-2.02078300	4.10988800	-0.57196100
C	-1.60679800	5.17417400	-1.39527000
C	-2.12849800	6.44249400	-1.08552700
H	-1.81817100	7.27563700	-1.69779600
C	-3.03743600	6.68765700	-0.05088500
C	-3.44346200	5.58841600	0.71532000
H	-4.16089500	5.71600400	1.52249500
C	-2.94252800	4.31332800	0.47490400
C	-0.63107900	4.97826200	-2.57445000
C	-0.48118100	6.26347700	-3.41599400
H	-1.43979400	6.59668800	-3.83114800
H	0.19370100	6.06445300	-4.25595900
H	-0.04712100	7.08916800	-2.84077200
C	-1.13474000	3.86917900	-3.53099200
H	-1.21547900	2.90003400	-3.03989900
H	-0.43804700	3.76816700	-4.37240500
H	-2.11572000	4.13894900	-3.94266000
C	0.76884300	4.61657300	-2.03185100
H	1.15615000	5.42920300	-1.40534600
H	1.46980800	4.47602200	-2.86389100
H	0.78300200	3.70520800	-1.43310000
C	-3.60172200	8.08554600	0.25361600
C	-3.23714300	8.48091900	1.70354500
H	-3.64636000	7.77320500	2.43229400
H	-3.63581300	9.47468800	1.94286800
H	-2.14966900	8.50657600	1.83700000
C	-5.14052300	8.06349500	0.10033200
H	-5.42497000	7.78736600	-0.92146100

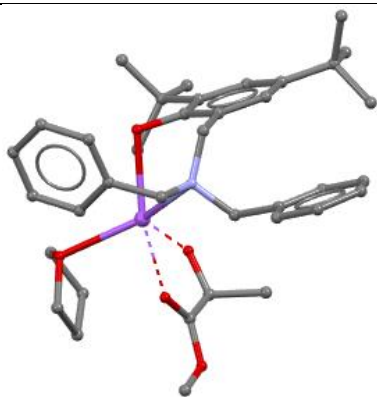
Na	0.22000500	1.28311500	-0.12322500
O	-0.74053300	0.82564000	2.11594600
C	-0.73524400	1.77571600	3.20517500
H	-0.61286900	2.77012900	2.76717900
H	-1.70208100	1.73657200	3.72573300
C	0.43060700	1.38088000	4.13998300
H	0.04382600	0.94886200	5.06985800
H	1.05490100	2.23818200	4.40717800
C	1.18807800	0.31672600	3.32572500
H	1.72353100	-0.40105200	3.95219500
H	1.90123000	0.79114400	2.64282900
C	0.06018400	-0.31436300	2.51617800
H	-0.55011600	-0.99368400	3.13281900
H	0.38321000	-0.81157200	1.59768600
O	-1.59830100	2.70396700	-0.90565200
N	-3.80097600	1.51104500	0.12630900
C	-2.15771000	3.92058900	-0.56329300
C	-1.74181200	5.12309700	-1.17098400
C	-2.39835100	6.29551600	-0.75679900
H	-2.09014200	7.22668000	-1.20653900
C	-3.43253600	6.33103400	0.18293400
C	-3.81756000	5.10961000	0.74507300
H	-4.61802600	5.07184400	1.47989300
C	-3.18934700	3.91765000	0.39781100
C	-0.63608100	5.18383400	-2.24546900
C	-0.44626400	6.60856800	-2.80807000
H	-1.35957700	6.99277000	-3.27723100
H	0.33533000	6.58693800	-3.57565200
H	-0.12579200	7.31913300	-2.03795800
C	-1.00625900	4.27411900	-3.43683500
H	-1.10942200	3.23490000	-3.13246200
H	-0.23149400	4.33347500	-4.21048000
H	-1.95279200	4.59679200	-3.88393200
C	0.71515200	4.75171000	-1.63854300
H	1.00516900	5.43093600	-0.82988600
H	1.50072600	4.79205900	-2.40295100
H	0.70252600	3.74027300	-1.23102000
C	-4.14432900	7.62889900	0.59854900
C	-3.97054500	7.84498800	2.11993300
H	-4.39218800	7.01628900	2.69862800
H	-4.47678700	8.76506700	2.43723500
H	-2.90970000	7.92992500	2.38139300
C	-5.65046700	7.51632400	0.26574700
H	-5.80068800	7.36449500	-0.80929600

H	-5.56285700	9.05234200	0.31836900	H	-6.17823500	8.43212800	0.55935200
H	-5.60649600	7.34478700	0.78283800	H	-6.12102700	6.67824900	0.79086100
C	-3.04307000	9.16573000	-0.69108900	C	-3.58470800	8.86612000	-0.12765100
H	-1.95322300	9.24961800	-0.61210700	H	-2.52136800	9.01799400	0.08968300
H	-3.47051700	10.14086300	-0.43140400	H	-4.12157300	9.76256900	0.20240900
H	-3.29667900	8.96101400	-1.73744900	H	-3.70570500	8.78902900	-1.21422900
C	-3.36386200	3.12673000	1.31077100	C	-3.57459400	2.62531100	1.07817500
H	-2.50521100	2.76007100	1.88221600	H	-2.75580800	2.30527500	1.72651200
H	-4.13908400	3.42077900	2.03799700	H	-4.45599300	2.78459700	1.72202400
C	-5.09947500	2.29480900	-0.21894000	C	-5.01768600	1.73700200	-0.71290800
H	-5.20335100	3.38443100	-0.24014300	H	-5.37870200	2.75070400	-0.51178700
H	-5.93885600	1.90246100	0.37524300	H	-5.80950200	1.04694300	-0.39685000
C	-5.17337800	1.78173200	-1.64324400	C	-4.77481900	1.59897500	-2.20443100
C	-4.36830100	2.36710500	-2.62872300	C	-4.32577400	2.70178500	-2.94388600
H	-3.70577500	3.18453000	-2.36510200	H	-4.14567100	3.64807900	-2.44052800
C	-4.41523400	1.91499900	-3.94615700	C	-4.10250200	2.59552700	-4.31753900
H	-3.77850000	2.37875800	-4.69502800	H	-3.75654200	3.46035700	-4.87614000
C	-5.27498400	0.87044700	-4.29856200	C	-4.32413500	1.38283000	-4.97304700
H	-5.31118600	0.51470700	-5.32522900	H	-4.14865600	1.29918700	-6.04231700
C	-6.08759900	0.28797600	-3.32452800	C	-4.77843200	0.28090100	-4.24588400
H	-6.75528800	-0.52860200	-3.58591800	H	-4.95623100	-0.66830600	-4.74440700
C	-6.03907700	0.74648500	-2.00729400	C	-5.00559500	0.39032500	-2.87367300
H	-6.65439100	0.27193100	-1.24874400	H	-5.35916400	-0.47288200	-2.32054600
C	-3.85387300	0.74619000	1.25413700	C	-3.84614900	0.23650000	0.88851500
H	-4.59685700	0.83684900	2.06714100	H	-4.68332100	0.26427500	1.60860200
H	-2.86542200	0.63737300	1.71097800	H	-2.91467200	0.18830000	1.46139900
C	-4.15144800	-0.48421900	0.42918100	C	-3.96796800	-0.98754000	0.01503000
C	-3.30598700	-0.83957300	-0.62918000	C	-2.90380900	-1.34899900	-0.81805200
H	-2.45407900	-0.21214900	-0.86414100	H	-1.99753900	-0.75672700	-0.80908100
C	-3.57306200	-1.96555800	-1.40496000	C	-3.00761000	-2.44243200	-1.67558000
H	-2.90976000	-2.22315600	-2.22509000	H	-2.17650700	-2.69870000	-2.32725400
C	-4.68993500	-2.75894400	-1.12490900	C	-4.18106600	-3.20278100	-1.69635800
H	-4.89983500	-3.63688400	-1.73019300	H	-4.26592800	-4.05605800	-2.36390200
C	-5.53001800	-2.42233300	-0.06360300	C	-5.23924600	-2.86791300	-0.84956500
H	-6.39778900	-3.03653200	0.16308700	H	-6.15026500	-3.46062700	-0.85345100
C	-5.25934900	-1.28918700	0.70852700	C	-5.13160900	-1.76336200	0.00092600
H	-5.92126800	-1.02316200	1.53012600	H	-5.96260500	-1.49702500	0.65066100
H	-2.33301400	2.23355900	-0.51864400	H	-2.31007400	2.02002600	-0.70581000
Na	2.91517000	0.03309100	-0.42364400	Na	3.10152000	0.31732200	-0.20436500
O	3.71847300	0.63235400	-2.65340900	O	3.61308200	0.81394200	-2.56932900
C	3.63159700	-0.07247600	-3.89617200	C	3.30256700	0.07936900	-3.77648700
H	3.61290200	-1.14204500	-3.67398700	H	2.82856000	-0.85712700	-3.48029800
H	4.52693300	0.14550200	-4.50131600	H	4.23516800	-0.15090800	-4.30995100
C	2.35723100	0.44958600	-4.58397400	C	2.36644200	0.96684300	-4.62259300
H	2.49094600	0.51770600	-5.66827700	H	2.88229800	1.32908900	-5.51847700
H	1.51489600	-0.22214200	-4.39575400	H	1.48173300	0.40990600	-4.94137600
C	2.12211500	1.83138900	-3.91485400	C	2.03339700	2.13706200	-3.67928700
H	2.08278600	2.64895000	-4.64136000	H	1.84617100	3.07470000	-4.20912300
H	1.18092300	1.82699600	-3.36260000	H	1.15548900	1.90753700	-3.07000500
C	3.30659300	1.98821100	-2.94761500	C	3.26174300	2.19982800	-2.77887400
H	4.15012000	2.51689900	-3.41891300	H	4.10102400	2.72409600	-3.26171000
H	3.03856600	2.44716500	-1.99238300	H	3.05379300	2.62536200	-1.79548900
O	4.69205700	-1.48418500	0.07306000	O	4.91668900	-1.07482800	0.32867000
N	6.93413700	-0.65138800	-1.17812700	N	6.83891100	-0.72352700	-1.51725200
C	5.14352200	-2.76664900	-0.13947900	C	5.07343300	-2.43381300	0.15845800
C	4.73059100	-3.83045300	0.68502500	C	4.67726500	-3.35852000	1.13979500
C	5.25266700	-5.09879400	0.37598600	C	4.90620900	-4.71525700	0.84016500
H	4.94312200	-5.93155100	0.98917300	H	4.59915200	-5.44510100	1.57356700

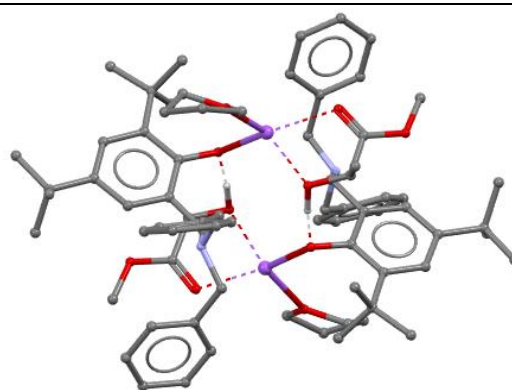
C	6.16099800	-5.34445600	-0.65906200	C	5.51235000	-5.17848600	-0.32969500
C	6.56597000	-4.24569000	-1.42649200	C	5.89628300	-4.21340500	-1.26911700
H	7.28289600	-4.37363200	-2.23406200	H	6.37149700	-4.51011300	-2.20086300
C	6.06463800	-2.97062500	-1.18680600	C	5.67080200	-2.86173000	-1.04489200
C	3.75555600	-3.63417300	1.86472000	C	3.96027000	-2.99377800	2.46047700
C	3.60700900	-4.91873300	2.70750700	C	4.23438700	-4.05628500	3.55227800
H	4.56610800	-5.25100600	3.12228400	H	5.31022200	-4.19459900	3.71286600
H	2.93260000	-4.71933200	3.54776400	H	3.78950800	-3.72702000	4.49764900
H	3.17301600	-5.74519800	2.13335000	H	3.79351600	-5.03097500	3.32079800
C	4.25919700	-2.52398700	2.81997900	C	4.40642400	-1.63726700	3.04960000
H	4.33921900	-1.55521000	2.32807100	H	4.04244600	-0.79430300	2.46632000
H	3.56293900	-2.42258000	3.66170900	H	4.00388000	-1.53644800	4.06497100
H	5.24054700	-2.79293200	3.23130100	H	5.49703400	-1.56765800	3.10821300
C	2.35504200	-3.27386500	1.32277500	C	2.43914200	-2.95179900	2.18694400
H	1.96745600	-4.08764700	0.69793300	H	2.08288400	-3.92534800	1.82856500
H	1.65472300	-3.13204900	2.15513500	H	1.89459400	-2.71364000	3.10979400
H	2.34005400	-2.36359700	0.72242200	H	2.18241500	-2.20174000	1.43238300
C	6.72570300	-6.74235000	-0.96275200	C	5.76708400	-6.66815100	-0.60971200
C	6.36023700	-7.13916100	-2.41206300	C	5.02661900	-7.08088900	-1.90308600
H	6.76860000	-6.43190400	-3.14173300	H	5.36726300	-6.50262000	-2.76838200
H	6.75917800	-8.13296000	-2.65080600	H	5.19837400	-8.14212500	-2.12203900
H	5.27267600	-7.16542500	-2.54469600	H	3.94740700	-6.92160300	-1.79965200
C	8.26460600	-6.71944100	-0.81062900	C	7.28518200	-6.90185700	-0.79043500
H	8.54968200	-6.44231200	0.21071800	H	7.83213900	-6.61970400	0.11679500
H	8.68724900	-7.70827200	-1.02814400	H	7.48992200	-7.95938800	-0.99844300
H	8.72972900	-6.00108700	-1.49408800	H	7.69018100	-6.31471500	-1.62155300
C	6.16825300	-7.82196300	-0.01668600	C	5.27614500	-7.57526900	0.53357900
H	5.07837400	-7.90634200	-0.09470200	H	4.19636100	-7.47756500	0.69342700
H	6.59587100	-8.79714500	-0.27590700	H	5.48119000	-8.62336400	0.28792400
H	6.42264100	-7.61627600	1.02929400	H	5.78502100	-7.35036500	1.47791100
C	6.48486100	-1.78463000	-2.02408400	C	6.03380600	-1.82929400	-2.08531400
H	5.62565300	-1.41900800	-2.59534100	H	5.11543100	-1.37790400	-2.47342600
H	7.25974500	-2.07901200	-2.75153700	H	6.55024200	-2.30743800	-2.93457800
C	8.22118400	-0.95018700	-0.49651600	C	8.17155700	-1.19103900	-1.03100400
H	8.32618900	-2.03970200	-0.47499100	H	8.35100400	-2.20774100	-1.40133200
H	9.05978300	-0.55721700	-1.09137700	H	8.94336600	-0.55223400	-1.46991000
C	8.29553600	-0.43649100	0.92755100	C	8.30798900	-1.16560400	0.47886600
C	7.49188800	-1.02241600	1.91387100	C	8.11410300	-2.32574500	1.23851400
H	6.83009100	-1.84069600	1.65109100	H	7.86239700	-3.25818400	0.74072300
C	7.53937200	-0.56981200	3.23110200	C	8.21701500	-2.28923400	2.63010900
H	6.90371200	-1.03399300	3.98061700	H	8.05230600	-3.19656500	3.20540000
C	8.39823200	0.47581500	3.58248700	C	8.52311000	-1.09134900	3.27917000
H	8.43481800	0.83194000	4.60900900	H	8.60132800	-1.06144700	4.36273500
C	9.20941500	1.05886600	2.60761000	C	8.73204700	0.06781100	2.52769500
H	9.87641900	1.87626500	2.86818700	H	8.97561000	1.00363900	3.02404800
C	9.16037300	0.59983500	1.29057000	C	8.62407200	0.03063800	1.13707600
H	9.77457300	1.07481100	0.53138500	H	8.77724400	0.93742000	0.55836600
C	6.97330900	0.59626800	-1.97002700	C	6.92721000	0.40501000	-2.47264500
H	7.71529200	0.50525200	-2.78389600	H	7.54532000	0.12570200	-3.34370300
H	5.98418900	0.70415700	-2.42554500	H	5.90976100	0.59093200	-2.82383400
C	7.27126400	1.82747900	-1.14646900	C	7.45954900	1.66786000	-1.83696700
C	6.42631600	2.18372900	-0.08798200	C	6.64496200	2.40178500	-0.96416700
H	5.57447200	1.55653700	0.14790100	H	5.63267400	2.06314800	-0.76637700
C	6.69385700	3.31033900	0.68671600	C	7.12382100	3.55241900	-0.33745100
H	6.03106300	3.56859900	1.50704200	H	6.48139000	4.10150700	0.34478300
C	7.81058700	4.10348600	0.40540800	C	8.43329800	3.98140000	-0.57714500
H	8.02081400	4.98191400	1.00986900	H	8.81025000	4.87438800	-0.08591700
C	8.65008600	3.76601600	-0.65608200	C	9.25081200	3.26467400	-1.45199300

H	9.51771400	4.38004500	-0.88377900	H	10.26703000	3.59704100	-1.64720000
C	8.37900400	2.63221100	-1.42709900	C	8.76217300	2.11613100	-2.08071000
H	9.04045600	2.36550000	-2.24885300	H	9.40013600	1.56145400	-2.76569900
H	5.45500800	-0.89020200	-0.19509400	H	5.65188000	-0.64876000	-0.21093300
C	0.27371000	-1.61136800	-1.55142700	C	0.79305600	-1.73080500	-1.22512400
H	-0.56185500	-2.20454300	-1.10156400	H	-0.07794400	-2.31024600	-0.82548500
C	1.17678700	-2.63318400	-2.27936600	C	1.87504200	-2.77615300	-1.55681300
H	1.66009700	-3.26228300	-1.52759900	H	2.16726300	-3.29650400	-0.64224600
H	0.62018000	-3.26617000	-2.97854700	H	1.52787100	-3.50708800	-2.29420600
H	1.96407900	-2.10873400	-2.83102100	H	2.77265600	-2.28717200	-1.95151300
O	-0.65655500	0.47622700	-2.43153000	O	0.25625300	-1.67649100	-3.63990700
O	-0.96943300	-1.39412000	-3.63494800	O	-0.47254600	0.00282700	-2.32623200
C	-1.77171900	-0.61372900	-4.54403100	C	-1.30126600	0.44790500	-3.41918300
H	-1.19015900	0.21955600	-4.94819800	H	-1.87844300	-0.38521000	-3.82182300
H	-2.06250200	-1.30169800	-5.33914600	H	-1.96543200	1.19827300	-2.99943800
H	-2.65297800	-0.21970300	-4.03284300	H	-0.68894700	0.88285200	-4.21277000
O	0.92705800	-0.84823400	-0.63712700	O	1.19723500	-0.75449300	-0.35627900
C	-0.46998100	-0.72473500	-2.57358100	C	0.21089900	-1.16424300	-2.53805600
C	2.84731000	2.95307200	0.84189600	C	2.70065100	3.37330100	0.79375600
H	3.68133600	3.54595000	0.38870400	H	2.99623400	4.12642500	0.02339700
C	1.94615200	3.97548000	1.57138300	C	1.78252900	4.12386000	1.78793900
H	1.16251900	3.45142100	2.12858300	H	1.56383200	3.47731200	2.64348600
H	2.50520200	4.61121900	2.26610600	H	2.24225300	5.04720400	2.15519700
H	1.45816700	4.60170600	0.82025100	H	0.83845700	4.35920500	1.28633200
O	3.78168900	0.86705300	1.72124700	O	4.69298500	3.98125700	2.08742600
O	4.09469200	2.73844100	2.92304500	O	4.42670300	1.81793800	1.50627100
C	4.89884600	1.95937200	3.83160500	C	5.63820200	1.52110700	2.23168700
H	5.78022800	1.56651500	3.31974800	H	5.45661300	1.60511900	3.30718700
H	5.18930500	2.64789800	4.62636000	H	5.89724900	0.50174400	1.96536900
H	4.31883500	1.12530600	4.23638300	H	6.43628800	2.20573000	1.94567500
O	2.19138200	2.18869300	-0.06947700	O	2.12705000	2.26424000	0.25218900
C	3.59416700	2.06790500	1.86293500	C	4.03231400	3.12290000	1.53432800

C



D



Na	3.73109900	-1.42035100	-2.16433600	Na	10.20102600	11.27878500	10.54781000
O	1.47129500	-0.77341000	-3.15197800	O	10.62521300	9.22079500	9.79984600
C	0.41159500	-1.36584700	-2.37743600	O	12.31852500	12.12977400	11.14040000
H	0.68250300	-2.40417700	-2.18063900	N	12.28200900	11.46000300	6.75106500
H	-0.52360100	-1.34482000	-2.96124000	C	11.86903400	8.91401000	9.42316300
C	0.33300300	-0.48477400	-1.13036400	C	12.69772800	8.03314100	10.19246500
H	-0.62952700	-0.56375700	-0.61542600	C	13.99275300	7.75744900	9.73109000
H	1.14563300	-0.77224000	-0.45410200	H	14.61218700	7.09512400	10.31936800
C	0.59581200	0.92899200	-1.70905100	C	14.52542500	8.28298200	8.54614300
H	-0.33001000	1.50334600	-1.82029200	C	13.69301000	9.12117800	7.80192300
H	1.26546200	1.50424500	-1.06435800	H	14.03687100	9.55464900	6.86693300

C	1.22975200	0.64689700	-3.09466000	C	12.39988800	9.44028100	8.21005100
H	0.54477800	0.92291600	-3.91009200	C	12.16889600	7.38383500	11.49088100
H	2.18705800	1.14746500	-3.24581800	C	13.18983300	6.42486400	12.13667100
O	4.43168700	-3.63971000	-2.92423800	H	13.45337200	5.59707100	11.46832100
N	6.52596900	-1.41069300	-3.07269200	H	12.75613900	5.99131900	13.04557900
C	5.33622700	-4.05837100	-1.95187500	H	14.11348300	6.93942200	12.42610400
C	4.86473300	-4.85491400	-0.89332800	C	10.89975200	6.55077000	11.18760500
C	5.81361000	-5.23991900	0.06728000	H	10.13474300	7.15981700	10.70648700
H	5.47367400	-5.84477700	0.89377600	H	10.48308500	6.13331400	12.11315800
C	7.16789500	-4.89382400	0.01317300	H	11.14611300	5.71133200	10.52522200
C	7.57795100	-4.09827500	-1.06054200	C	11.84785900	8.47068000	12.54438500
H	8.61475000	-3.78898300	-1.15166600	H	12.76636400	8.96277000	12.88294400
C	6.68112200	-3.65879100	-2.03174000	H	11.36152500	8.02583200	13.42215700
C	3.39906000	-5.32870800	-0.80188200	H	11.18330900	9.23095400	12.13388100
C	3.12491500	-6.09929300	0.50560000	C	15.93821100	7.96036300	8.03542200
H	3.29873600	-5.47353800	1.38830400	C	16.74344700	9.27048300	7.87020000
H	2.07578000	-6.41399800	0.52288800	H	16.27472100	9.94086800	7.14217500
H	3.73694700	-7.00432200	0.59219100	H	17.76265100	9.06043300	7.52091200
C	2.41966000	-4.13058500	-0.84103300	H	16.81055000	9.80776500	8.82344000
H	2.37163600	-3.70926200	-1.84725700	C	15.83600600	7.25363900	6.66256000
H	1.40817500	-4.47153600	-0.58578000	H	15.26650500	6.32102200	6.75321900
H	2.70614600	-3.33330400	-0.14613200	H	16.83303300	7.01207900	6.27167200
C	3.10457700	-6.28082900	-1.98598400	H	15.32909300	7.88443600	5.92412600
H	3.75059900	-7.16590100	-1.94425600	C	16.71577600	7.03920800	8.99302100
H	2.06144200	-6.61911400	-1.94658700	H	16.83798500	7.49645800	9.98171800
H	3.26508300	-5.78113000	-2.94474300	H	17.71635500	6.84085100	8.59132600
C	8.19343500	-5.36361200	1.05872000	H	16.21306800	6.07415300	9.12371500
C	9.22778500	-6.28521600	0.37125500	C	11.55571200	10.30198600	7.29121400
H	9.75081400	-5.76689000	-0.43975900	H	11.26530400	9.70168400	6.42303400
H	9.98033400	-6.62610100	1.09336200	H	10.62674300	10.60679500	7.79329900
H	8.73859400	-7.16803000	-0.05600600	C	12.41954600	12.51971200	7.74904300
C	8.92533300	-4.14217300	1.66210900	H	12.60877500	12.02124000	8.70509200
H	8.21270500	-3.44849100	2.12296600	H	11.48525600	13.08619100	7.88122900
H	9.63590100	-4.46519600	2.43284400	C	13.56706700	13.45983100	7.45962500
H	9.49146200	-3.59225300	0.90344000	C	14.83661900	12.94919900	7.15451400
C	7.53984300	-6.14558700	2.21304000	H	14.95680300	11.87275100	7.07975300
H	7.04596700	-7.05750300	1.85885600	C	15.92009800	13.80422300	6.96102600
H	8.30611400	-6.44634600	2.93641000	H	16.90003000	13.39215700	6.73309100
H	6.79891000	-5.53777500	2.74465300	C	15.74907600	15.18858500	7.06366600
C	7.14436200	-2.74907900	-3.14579800	H	16.59317400	15.85631900	6.91233700
H	6.87940800	-3.17946000	-4.12066000	C	14.48667100	15.70813700	7.35460800
H	8.24361900	-2.68325200	-3.13866900	H	14.34246100	16.78336300	7.42506200
C	6.59863300	-0.70158500	-4.36638700	C	13.40314700	14.84624500	7.54764900
H	6.41303300	0.35855700	-4.16760700	H	12.41779900	15.25154500	7.76973500
H	7.59576200	-0.78141400	-4.83050500	C	11.67703400	11.94634700	5.50762100
C	5.53288200	-1.23112600	-5.30517600	H	12.12941600	12.92126500	5.28706600
C	4.19578100	-0.85004400	-5.11067400	H	10.59127100	12.11582600	5.61813200
H	3.96438900	-0.09785300	-4.35917200	C	11.95205800	11.00018300	4.35640200
C	3.16968900	-1.42222300	-5.86173700	C	13.27000300	10.59859700	4.09030700
H	2.14223800	-1.14102300	-5.65555800	H	14.06738900	10.97672500	4.72368300
C	3.47246800	-2.37169300	-6.84301200	C	13.55059800	9.73141100	3.03549700
H	2.67630200	-2.82310000	-7.42852800	H	14.57785400	9.43487600	2.83731900
C	4.80074000	-2.73543600	-7.06980300	C	12.51288000	9.24185000	2.23359100
H	5.04291300	-3.46570200	-7.83729900	H	12.73020700	8.56268700	1.41311300
C	5.82433200	-2.16906700	-6.30298900	C	11.19933100	9.63136500	2.49412000
H	6.85778400	-2.46025400	-6.47819400	H	10.38489100	9.25187500	1.88242100
C	6.97505700	-0.62769000	-1.89908700	C	10.92391200	10.50681500	3.54852000
H	6.47569200	0.34199600	-1.96401500	H	9.89842100	10.81191500	3.74163800

H	6.56629000	-1.12571800	-1.01435000	C	13.52935100	11.40403100	11.43979700
C	8.47354800	-0.45180100	-1.71728300	H	13.41987400	10.39949400	11.03137100
C	9.11101600	-1.03364200	-0.61411600	H	13.65908800	11.34162100	12.53106200
H	8.51710000	-1.59333900	0.10250000	C	14.64051200	12.21906600	10.78770200
C	10.48768700	-0.90253900	-0.42411900	H	15.62070100	12.02159400	11.23234500
H	10.95888200	-1.36100100	0.44170800	H	14.69870400	11.98578700	9.72123000
C	11.25318300	-0.18348700	-1.34346400	C	14.16379300	13.66759800	11.00752600
H	12.32580200	-0.08079700	-1.20221400	H	14.54566300	14.05709100	11.95757000
C	10.62904000	0.41480900	-2.44089000	H	14.48992700	14.33725000	10.20769000
H	11.21535900	0.99026000	-3.15279600	C	12.62539600	13.54084100	11.05660900
C	9.25115900	0.28625500	-2.62170000	H	12.19306300	14.05431200	11.92519400
H	8.77625600	0.77687700	-3.46659400	H	12.14484100	13.92144900	10.15148100
H	4.91162200	-3.27231900	-3.68540300	Na	8.59005900	9.46156600	6.35582600
O	3.41132700	-1.05391100	-0.08721800	O	8.28229900	11.53822400	7.13119400
C	3.64139600	0.17995100	0.40171000	O	6.62220600	8.88343500	5.22585000
H	2.77170500	0.62618400	0.94575800	N	6.13433300	9.08273300	9.62836000
C	4.83770400	0.24531700	1.39425400	C	7.01109000	11.87533300	7.36192700
H	4.63322100	-0.46155700	2.20401800	C	6.33777600	12.86642500	6.57848500
H	5.75732100	-0.07796200	0.89188000	C	5.01415900	13.19117900	6.90791300
H	4.99096000	1.24677500	1.81537400	H	4.51194600	13.94259800	6.31502300
C	3.92819200	1.21906600	-0.71539300	C	4.30928300	12.60602400	7.96917100
O	4.16866300	0.94938600	-1.89093800	C	4.98843200	11.64502200	8.72215300
O	3.87829600	2.49887800	-0.29188900	H	4.50136900	11.15146000	9.55920000
C	4.14698800	3.50896400	-1.27697100	C	6.30104300	11.27285000	8.44145900
H	3.41111100	3.46488500	-2.08583500	C	7.06714200	13.58972900	5.42421600
H	4.07563000	4.46145300	-0.75033600	C	6.16004600	14.59691600	4.68916000
H	5.14755500	3.38132800	-1.70114100	H	5.80959100	15.39573800	5.35287100
				H	6.72420500	15.06856600	3.87605200
				H	5.28333700	14.11080700	4.24512300
				C	8.27822600	14.38039800	5.97633300
				H	8.97135400	13.72399700	6.50262100
				H	8.82018300	14.87036200	5.15692300
				H	7.94223000	15.16346700	6.66770200
				C	7.56130500	12.57124400	4.37132400
				H	6.71650800	12.05459600	3.90303700
				H	8.12654600	13.08019100	3.57983500
				H	8.21086000	11.83099300	4.83805900
				C	2.86476500	12.98365700	8.33229700
				C	1.95692700	11.73855700	8.20239900
				H	2.28706000	10.92936300	8.86166900
				H	0.91889800	11.98245600	8.46335000
				H	1.97146900	11.35473100	7.17559700
				C	2.82031600	13.49647000	9.79153400
				H	3.47244500	14.36966900	9.91144900
				H	1.79940300	13.78538700	10.07279600
				H	3.15668600	12.72902800	10.49687300
				C	2.29565100	14.08749200	7.42217200
				H	2.27033300	13.77326400	6.37244600
				H	1.26842600	14.32576100	7.72196800
				H	2.88453600	15.00954800	7.48810200
				C	6.97952200	10.25423300	9.33559500
				H	7.20457600	10.71486900	10.30155000
				H	7.94546400	9.96082000	8.90319800
				C	5.86817500	8.29791300	8.42102700
				H	5.69700100	9.01197500	7.61145900
				H	6.74782100	7.70005600	8.13393700
				C	4.65329400	7.40540100	8.54233700
				C	3.44550400	7.92022200	9.03317500

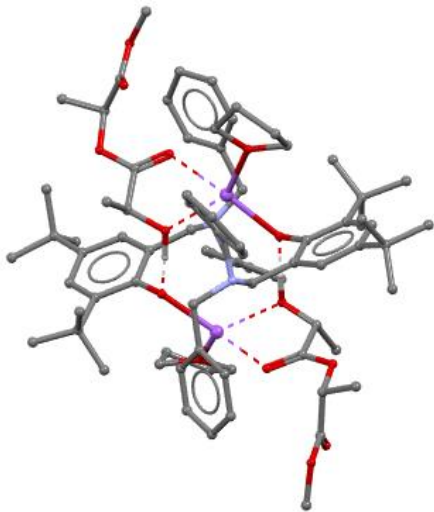
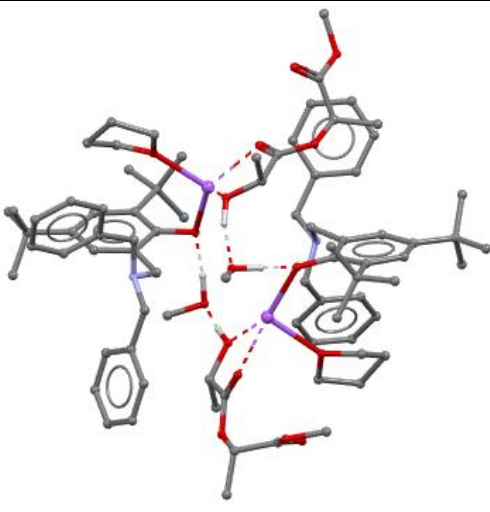


H	3.42484100	8.94766300	9.38220500
C	2.29966500	7.12757300	9.07760300
H	1.36922900	7.54374200	9.45590700
C	2.34386000	5.80198700	8.63479400
H	1.45044000	5.18400400	8.66858200
C	3.54453400	5.27482500	8.15726500
H	3.59288000	4.24063800	7.82545000
C	4.69118300	6.07273300	8.11716800
H	5.62981900	5.65459700	7.75908700
C	6.74139700	8.22466100	10.65660800
H	6.06849100	7.36898500	10.79570100
H	7.70966500	7.82215800	10.31163300
C	6.92998600	8.94246500	11.97196400
C	5.82899000	9.45841100	12.66710500
H	4.83419500	9.32969800	12.24772600
C	6.00943000	10.13426200	13.87477500
H	5.14703000	10.52370100	14.41109000
C	7.29463000	10.30984700	14.39826500
H	7.43333400	10.83792800	15.33816600
C	8.39613200	9.80086500	13.70880700
H	9.40091800	9.93340300	14.10298300
C	8.21114000	9.12102300	12.50327000
H	9.06490100	8.73640600	11.95437000
C	5.44602800	9.66436400	4.91474300
H	5.43326500	10.52533100	5.58552700
H	5.51460600	10.02121900	3.87705500
C	4.27364300	8.70375500	5.09165300
H	3.39064800	9.01706900	4.52650400
H	3.99312300	8.62540300	6.14603400
C	4.86824300	7.37692500	4.58822300
H	4.77176100	7.30304300	3.49905800
H	4.38530500	6.50402000	5.03620500
C	6.34931000	7.48263600	4.99264000
H	7.03353500	7.10985400	4.22199400
H	6.55221400	6.94819000	5.92623800
H	9.71033800	8.47915600	8.78576000
O	9.19359400	7.94664100	8.07878000
C	9.98014800	6.83714900	7.68938200
H	10.81548100	6.69219000	8.37961400
H	9.04248500	12.32683900	8.24862600
O	9.46192500	12.87040900	9.00665600
C	8.52518400	13.82321700	9.47093100
H	7.72362200	13.97072400	8.74255000
C	9.23096100	15.15601100	9.73464900
H	9.66968700	15.51399200	8.79850300
H	8.52752400	15.90608900	10.11082000
H	10.03303800	15.02017800	10.46759500
C	9.11730400	5.57277600	7.65106000
H	8.28106600	5.71094200	6.95715200
H	9.70257100	4.70296100	7.33397200
H	8.71304500	5.38929200	8.65066100
C	10.57329900	7.10567600	6.30634200
C	7.88256300	13.31304900	10.75993100
O	10.04717100	7.82467800	5.46597400
O	11.72389700	6.46791500	6.11166600
C	12.41050900	6.76434900	4.87379700
H	12.61259700	7.83459100	4.80918200
H	13.34036600	6.19890500	4.91992300

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H	11.80440800	6.45929700	4.01738200
O	8.40981100	12.50804500	11.51557000
O	6.68638600	13.85605200	10.97789900
C	5.96983900	13.37178700	12.13497000
H	5.00043000	13.86760900	12.09838700
H	5.85649200	12.28735200	12.07769300
H	6.50897500	13.62663400	13.05120000

**Table S10.** DFT optimized structures and atom coordinates of proposed complexes obtained between  $[(d\text{-tbL}^{\text{Bn}})\text{Na}(\text{THF})_2]$  and methyl lactate.

1				2			
							
Na	10.15782700	11.61957900	10.54622400	Na	10.45371200	11.37122400	10.48509900
O	10.72454900	9.54154400	9.99965100	O	10.75866700	9.15003300	10.26254100
O	12.17566100	12.62301500	11.19440300	O	12.36357200	12.54531000	11.09335900
N	12.39661600	11.67492800	6.87374000	N	13.19590400	10.69475600	7.21313900
C	11.99932500	9.28524700	9.69581300	C	12.08105200	9.04400300	10.40769100
C	12.83719000	8.49795300	10.55070800	C	12.69038500	8.57306800	11.61235700
C	14.16518700	8.26861800	10.16303900	C	14.08871100	8.46905600	11.65940300
H	14.79119000	7.67661500	10.81595800	H	14.54290000	8.10243800	12.56936400
C	14.72130500	8.75321400	8.97164300	C	14.92809200	8.83307800	10.59898900
C	13.87985100	9.49986600	8.14421300	C	14.30905800	9.30597600	9.43678100
H	14.24170500	9.89364500	7.19936900	H	14.90778500	9.62985300	8.59324200
C	12.55516500	9.77142100	8.47770100	C	12.92596800	9.40329800	9.31836200
C	12.27857900	7.88809600	11.85467200	C	11.82623500	8.20889200	12.83686100
C	13.31989800	7.03517900	12.60761200	C	12.66917000	7.75103700	14.04355700
H	13.66946300	6.18875100	12.00526600	H	13.25766400	6.85481600	13.81573000
H	12.86522800	6.62754000	13.51820100	H	12.00411700	7.50418700	14.87935000
H	14.19316800	7.62441000	12.91091800	H	13.35583300	8.53411600	14.38657200
C	11.08538600	6.95735600	11.52699000	C	10.84616500	7.06292600	12.49111600
H	10.30813700	7.49080600	10.98037000	H	10.23387900	7.31544100	11.62481000
H	10.64806600	6.55190700	12.44832500	H	10.18084100	6.86056000	13.34071300
H	11.42180600	6.11053600	10.91552600	H	11.39749900	6.13947000	12.27533800
C	11.82926700	9.00613900	12.82548700	C	11.02153400	9.45069900	13.28656200
H	12.69374900	9.57963800	13.17881700	H	11.68934200	10.29159000	13.51134600
H	11.32882600	8.57641800	13.70280500	H	10.43430300	9.22920900	14.18692100
H	11.13749400	9.69401600	12.33950400	H	10.32851800	9.74729700	12.49818600
C	16.16693600	8.47297500	8.53323700	C	16.46194600	8.75547300	10.66274500

C	16.90556700	9.80873800	8.28374200	C	17.05767300	10.17396000	10.49996900
H	16.42905400	10.39037000	7.48767100	H	16.75449200	10.63790600	9.55541300
H	17.94651000	9.62851300	7.98585900	H	18.15478600	10.13991100	10.52107300
H	16.90912000	10.42495000	9.19037700	H	16.72183900	10.82854600	11.31240900
C	16.14980900	7.65123900	7.22145000	C	16.98367100	7.85362000	9.51930900
H	15.64526000	6.69038900	7.37996600	H	16.57503800	6.84031600	9.60877000
H	17.17061100	7.44910700	6.87160900	H	18.07884700	7.78574400	9.54697100
H	15.61774300	8.18123700	6.42342000	H	16.69901800	8.24297300	8.53585000
C	16.96004100	7.67894300	9.58712200	C	16.96647400	8.17462000	11.99628300
H	17.01738700	8.21946800	10.53899100	H	16.66207600	8.79388400	12.84792700
H	17.98491300	7.51063400	9.23609000	H	18.06184000	8.12951800	11.99382300
H	16.51010600	6.69820700	9.77894400	H	16.59080800	7.15838200	12.16243600
C	11.70636000	10.52350100	7.47010800	C	12.29569400	9.85228200	8.00925700
H	11.47700600	9.84413100	6.64406700	H	12.02481000	8.97559100	7.41030600
H	10.74631300	10.82045800	7.91851100	H	11.33537500	10.36225800	8.19432100
C	12.41909100	12.81163800	7.79355200	C	13.23855500	12.05094100	7.75150200
H	12.59081800	12.39718700	8.79210200	H	13.17778600	11.96308900	8.84109000
H	11.44514000	13.32419200	7.83946600	H	12.35308300	12.63651100	7.44881000
C	13.51931000	13.80195000	7.48907800	C	14.49413800	12.82623300	7.41033200
C	14.83071000	13.35440600	7.27607000	C	15.70415100	12.18240700	7.12519700
H	15.02019600	12.28522500	7.27947600	H	15.71787200	11.09905300	7.06802200
C	15.86808200	14.26283100	7.07303700	C	16.86735800	12.92178200	6.90117900
H	16.88116800	13.90049700	6.91678000	H	17.79821400	12.40536700	6.68078800
C	15.60826500	15.63706400	7.07422600	C	16.83834400	14.31642200	6.95886900
H	16.41652900	16.34624900	6.91586500	H	17.74454800	14.89112000	6.78694300
C	14.30395900	16.09264900	7.27335300	C	15.63283300	14.96860000	7.22948200
H	14.09144900	17.15876300	7.26528800	H	15.59572400	16.05460100	7.26389200
C	13.26673800	15.17779600	7.47592500	C	14.47092800	14.22690200	7.44587400
H	12.24904600	15.53230500	7.62739200	H	13.53129100	14.73784700	7.64892000
C	11.83574600	12.03514600	5.56890300	C	12.90806400	10.67485500	5.78385200
H	12.28968300	12.99040000	5.27605700	H	13.44557100	11.51930900	5.33312500
H	10.74532900	12.20753000	5.62373900	H	11.83633800	10.84630900	5.58207700
C	12.15544200	10.98776000	4.52043700	C	13.34853400	9.40763500	5.07359300
C	13.47397800	10.53206600	4.37483800	C	14.08666600	8.40082400	5.70672100
H	14.24304400	10.94846600	5.01853800	H	14.37136000	8.52449000	6.74542600
C	13.79170000	9.56021300	3.42701700	C	14.44056500	7.23664800	5.01747700
H	14.81939000	9.21937000	3.32559600	H	15.00198800	6.46052800	5.53147600
C	12.79159000	9.02351200	2.60816300	C	14.07804600	7.06896400	3.68061200
H	13.03074200	8.24950400	1.88492600	H	14.35175700	6.16343600	3.14592700
C	11.47729300	9.46955500	2.74755900	C	13.36428900	8.08159900	3.03296600
H	10.68987700	9.04776300	2.12820600	H	13.08639300	7.96813000	1.98800000
C	11.16431700	10.44717000	3.69552200	C	13.00061300	9.23515800	3.72594300
H	10.13723600	10.78689600	3.79819100	H	12.42558800	10.01065700	3.22431300
C	13.40793700	11.99881300	11.60800100	C	13.55938300	12.12978600	11.78017100
H	13.37809800	10.96097200	11.27602100	H	13.69566000	11.06701400	11.58769000
H	13.48493900	12.02800400	12.70586500	H	13.43822600	12.28920200	12.86347500
C	14.50077800	12.83089100	10.94579000	C	14.65309900	13.02409500	11.20603500
H	15.46827400	12.72749600	11.44656300	H	15.53374100	13.08518100	11.85249600
H	14.62352100	12.52357200	9.90368100	H	14.97341800	12.64393300	10.23117200
C	13.93052300	14.26027600	11.03226300	C	13.92186700	14.37117000	11.05658100
H	14.25361900	14.74739900	11.95867600	H	14.00018900	14.95436300	11.98080400
H	14.24667800	14.88274400	10.19147000	H	14.32851800	14.97354600	10.23980300
C	12.40041800	14.04435300	11.04284400	C	12.45616500	13.95969600	10.79925600
H	11.91209000	14.57476900	11.87047900	H	11.74892100	14.50462100	11.43711500
H	11.92362500	14.34577700	10.10652000	H	12.14633300	14.08530600	9.75929500
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O	8.31880700	11.64775600	7.21164000	O	7.67875200	11.68056300	6.77127500
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N	6.18628200	9.01181100	9.59237300	N	6.64192900	9.21168900	9.77087300
C	6.99225000	11.80430100	7.25107100	C	6.39913300	11.74864300	7.10564300
C	6.29947100	12.62807000	6.30771600	C	5.41938800	12.42003400	6.30623500
C	4.89942300	12.67183500	6.35963700	C	4.06823800	12.30397400	6.66407000
H	4.38148200	13.27444200	5.62719200	H	3.33123600	12.78633500	6.03705600
C	4.13155500	11.96066500	7.29204100	C	3.61906500	11.58761500	7.78162700
C	4.83223300	11.21067000	8.24131800	C	4.60310500	11.02370600	8.59941200
H	4.29919500	10.63196300	8.99005500	H	4.32786600	10.48658000	9.50216200
C	6.22320300	11.11782800	8.23705700	C	5.95936000	11.10989500	8.30051000
C	7.07163500	13.40865400	5.22116200	C	5.84557700	13.26167400	5.08484800
C	6.14302900	14.25268900	4.32496400	C	4.64951600	13.93366700	4.38047000
H	5.58163600	14.99616300	4.90273500	H	4.10242800	14.60384200	5.05298100
H	6.74479400	14.79336900	3.58510400	H	5.01145100	14.53385700	3.53707500
H	5.42566900	13.63276300	3.77468700	H	3.94236500	13.19683700	3.98194000
C	8.09132200	14.37822100	5.86422500	C	6.79221900	14.39397100	5.54969300
H	8.80783400	13.84357000	6.48739700	H	7.67622100	13.99012200	6.04328100
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H	7.57560700	15.12539200	6.48047800	H	6.27997200	15.05366500	6.25967500
C	7.82318600	12.41971300	4.30074500	C	6.55763000	12.38498000	4.02737500
H	7.12078200	11.75323100	3.78759800	H	5.87637300	11.60962300	3.65872500
H	8.39915600	12.96057100	3.53838700	H	6.87270900	12.99481000	3.16985200
H	8.51298500	11.81505500	4.88911800	H	7.43634100	11.89455100	4.44690100
C	2.59542700	11.90466300	7.24627500	C	2.13467600	11.39574200	8.13055400
C	2.16618800	10.46494200	6.87152400	C	1.80744900	9.88333500	8.13710400
H	2.53567900	9.73166600	7.59609600	H	2.41288800	9.34523000	8.87474200
H	1.07223800	10.38015700	6.83051400	H	0.75080800	9.71265200	8.38133100
H	2.56679600	10.18800400	5.88894200	H	2.00993600	9.43946400	7.15558100
C	1.99633700	12.26650200	8.62361700	C	1.84106400	11.98106100	9.53176500
H	2.27621300	13.28599000	8.91307700	H	2.04468400	13.05806000	9.55138900
H	0.90078400	12.20907400	8.59559600	H	0.78900100	11.82740000	9.80496900
H	2.34087700	11.58531800	9.40871400	H	2.45924300	11.51102900	10.30429700
C	2.00077500	12.87055800	6.20455900	C	1.19845700	12.08268500	7.11981300
H	2.32685900	12.62295500	5.18809900	H	1.33693000	11.68539000	6.10764100
H	0.90624000	12.81127400	6.22269600	H	0.15289400	11.91471700	7.40366500
H	2.28415900	13.90943100	6.40998300	H	1.36419300	13.16573400	7.08657800
C	6.91709500	10.25071500	9.27058000	C	6.95349800	10.56868500	9.30828200
H	7.01295300	10.80114400	10.21069100	H	6.92322900	11.20465500	10.19602500
H	7.94539600	10.03933900	8.94489800	H	7.97908600	10.63801000	8.90775200
C	6.05279000	8.13184800	8.42893000	C	7.03302400	8.22425400	8.76952700
H	5.85336700	8.76992600	7.56462300	H	6.70627000	8.61576100	7.79973800
H	6.99680500	7.60524700	8.21656300	H	8.12933600	8.10633400	8.71982400
C	4.92082700	7.13340800	8.55240300	C	6.38486600	6.87476200	8.97439300
C	3.70425100	7.49334400	9.14772200	C	4.99993800	6.78707400	9.17225100
H	3.61578800	8.47937800	9.59235300	H	4.42322400	7.70585500	9.23601800
C	2.63556800	6.59749000	9.18289900	C	4.37763000	5.54446300	9.28327300
H	1.69840800	6.89410800	9.64749200	H	3.30179800	5.48870000	9.43043600
C	2.76566900	5.32344900	8.62385100	C	5.13511700	4.37147100	9.20084500
H	1.93256000	4.62599400	8.65032900	H	4.65053900	3.40202600	9.28475300
C	3.97717700	4.94980700	8.03979400	C	6.51736500	4.45268100	9.02165900
H	4.09491700	3.95601700	7.61494800	H	7.11378500	3.54478800	8.97365300
C	5.04617900	5.84798800	8.01139200	C	7.14117200	5.69892600	8.91511500
H	5.99277800	5.54617000	7.56814800	H	8.21998300	5.77250700	8.79782300
C	6.83503900	8.27765500	10.69049300	C	7.22109600	8.92855200	11.08909000
H	6.24411600	7.36823900	10.85763600	H	7.06076300	7.86146100	11.28762000
H	7.84909600	7.95562800	10.39780800	H	8.31471100	9.08497100	11.10490800
C	6.90994900	9.07540000	11.97090300	C	6.54664800	9.74662800	12.17319100
C	5.74309300	9.50876900	12.61452000	C	5.14696600	9.82477100	12.22271500
H	4.77801800	9.26376000	12.17780300	H	4.56902100	9.28024200	11.48248800

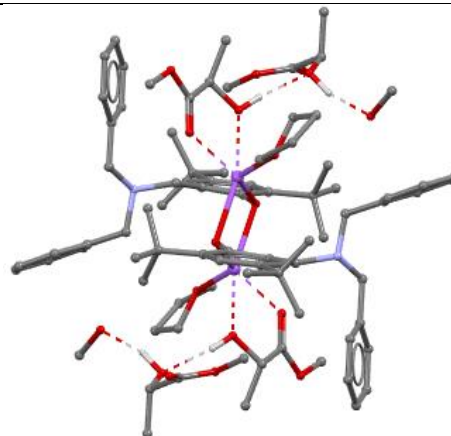
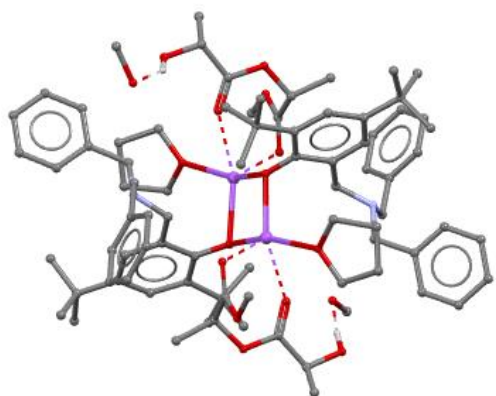
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H	4.91148800	10.60095700	14.27672800	H	3.42224200	10.65258800	13.20956200
C	7.06662700	10.58427700	14.33417700	C	5.26051600	11.29943200	14.13901600
H	7.12359100	11.17374000	15.24537800	H	4.76637600	11.91627000	14.88420300
C	8.23225700	10.15565400	13.69911600	C	6.65306100	11.21594000	14.10820300
H	9.20711800	10.41087300	14.10748100	H	7.24863800	11.76831300	14.83033600
C	8.15096700	9.40681900	12.52327500	C	7.28923100	10.44933500	13.12817700
H	9.05503200	9.09130800	12.01176500	H	8.37274400	10.41197300	13.09580400
C	5.85177100	9.27841600	4.85927100	C	5.41351200	8.99355200	5.04037900
H	5.60443500	10.06503100	5.57414000	H	5.28539000	10.01679600	5.39194400
H	5.93103200	9.72584100	3.85874800	H	5.31595500	8.96024800	3.94363300
C	4.88625700	8.09541800	4.86008500	C	4.49072700	7.98485600	5.71747800
H	4.01774000	8.26665300	4.21684700	H	3.49033700	7.95789700	5.27384800
H	4.52442200	7.89021100	5.87245300	H	4.38961500	8.24404200	6.77556400
C	5.78916300	6.95150700	4.37066000	C	5.26606500	6.66197900	5.54887200
H	5.87434000	6.97182400	3.27747700	H	4.94426100	6.13750400	4.64281300
H	5.42605800	5.96315100	4.66722700	H	5.12444200	5.99179200	6.40035900
C	7.13545000	7.28958200	5.02128100	C	6.73828600	7.11605400	5.41111300
H	8.00528200	7.01286500	4.41988000	H	7.18398700	6.77311100	4.47165800
H	7.23442500	6.81001500	6.00187600	H	7.36349500	6.80170200	6.24787900
H	9.90021800	8.69992200	9.00181000	H	10.07274100	7.49534700	7.32798700
O	9.43992600	8.11853100	8.29447000	O	9.81871200	7.89588900	6.44168600
C	10.27924400	7.02717300	7.98345000	C	10.48229700	7.22927500	5.38465300
H	11.17036000	7.02742600	8.62146000	H	11.57337600	7.35556100	5.47128800
H	8.99611700	12.55151900	8.24678800	H	10.18518600	12.74809800	7.86092600
O	9.38508400	13.17798300	8.96284200	O	10.05803300	12.94061600	8.82467200
C	8.34144400	14.01726600	9.41388500	C	8.87724800	13.72608200	8.92861000
H	7.57439700	14.13324100	8.64144800	H	8.15965000	13.40858200	8.16666800
C	8.90475800	15.38816600	9.79552800	C	9.17830100	15.22129900	8.78237600
H	9.35226300	15.84658600	8.90856500	H	9.61994000	15.40216600	7.79687600
H	8.11814700	16.04012100	10.18740500	H	8.26290800	15.81221600	8.87555200
H	9.67782100	15.27350500	10.56186100	H	9.88887900	15.54245700	9.55044200
C	9.52965200	5.70134500	8.16150700	C	10.16581500	5.73331700	5.32864900
H	8.64154100	5.68262600	7.52207000	H	9.10266600	5.56252200	5.14699900
H	10.16620600	4.85046700	7.90263400	H	10.74420400	5.24927000	4.53742400
H	9.21091000	5.61645600	9.20395400	H	10.43234600	5.27716800	6.28662900
C	10.76524300	7.16486400	6.54463100	C	10.10265100	7.98507900	4.11759900
C	7.67233500	13.39139400	10.63273700	C	8.22739600	13.43008600	10.26837400
O	10.33404500	7.97292000	5.73776400	O	9.73798900	9.14954000	4.09752300
O	11.73014000	6.28461200	6.24637900	O	10.23554800	7.25246400	3.00408200
C	12.21323000	6.32461600	4.89071900	C	9.93994600	7.94044000	1.77291100
H	12.44669800	7.35776300	4.61967300	H	10.57730200	8.82503700	1.69924300
O	8.22237800	12.60914700	11.39280900	O	8.73375800	12.78289200	11.17122100
O	6.40662200	13.79491100	10.77204800	O	6.99210400	13.93542600	10.31136200
C	5.67939900	13.27067900	11.89823700	C	6.22177000	13.71361700	11.50911300
H	5.91375500	12.20953400	12.01847600	H	6.38810000	12.69474400	11.86743200
C	13.46107800	5.45320900	4.83237900	C	10.21402800	6.95216300	0.64780600
H	13.86604800	5.46067400	3.81712500	H	10.02753700	7.42818600	-0.31960500
H	14.21339200	5.84946000	5.51990700	H	11.25633600	6.62285700	0.68751700
H	13.22788800	4.42283900	5.11822000	H	9.56259700	6.07930700	0.74923300
C	11.10883000	5.83396800	3.95398800	C	8.47364300	8.38148000	1.76830700
O	11.48177800	6.01702900	2.67344200	O	8.33058700	9.50945800	1.05667900
O	10.05623200	5.34361600	4.29514800	O	7.56764200	7.76326300	2.27919100
C	10.50772200	5.62736200	1.68743300	C	6.97983100	10.00733600	0.96172400
H	9.59602300	6.22018800	1.80423500	H	6.60249400	10.24902800	1.95766000
H	10.97390700	5.82535000	0.72220600	H	7.04302500	10.90488400	0.34684200
H	10.26036900	4.56744900	1.78940600	H	6.33007500	9.26098000	0.49666400
C	4.19962500	13.46403800	11.59836400	C	4.75871200	13.91542100	11.13849100

H	3.95619400	12.94592400	10.66801000
H	3.60017100	13.04996300	12.41276700
H	3.96100100	14.52596700	11.48236600
C	6.14658400	13.99036600	13.16062500
O	6.98993200	14.85538900	13.20822000
O	5.47866400	13.51645300	14.23148700
C	5.87512700	14.07476700	15.49695100
H	5.23769100	13.59560500	16.24042100
H	6.92865300	13.85561900	15.69227600
H	5.72940800	15.15825100	15.50180800

H	4.49822800	13.22731900	10.33022200
H	4.13163100	13.70267500	12.00705000
H	4.57890000	14.94172200	10.80283000
C	6.72406900	14.67410000	12.58427100
O	7.62546700	15.46962600	12.44964800
O	6.01851200	14.50758700	13.71915700
C	6.42960600	15.33234200	14.82413100
H	5.76611400	15.06829100	15.64797100
H	7.47134300	15.12578000	15.08505700
H	6.32958700	16.39131500	14.57080800
C	10.35629500	13.28930200	5.12678500
H	11.44765100	13.30839700	5.05550200
H	9.99665100	14.31229300	5.30510100
H	9.94664300	12.93664300	4.17098800
C	11.60696800	6.24044600	8.91773400
H	11.42850200	5.25730400	8.46898500
H	11.89915700	6.10400800	9.96316500
H	12.43761800	6.73086500	8.39180900
O	10.00907900	12.41107200	6.18928900
H	9.00956300	12.31903100	6.27520100
O	10.39662700	6.98953900	8.81964000
H	10.47299700	7.83201200	9.38237500

3

4



O	-0.14188000	-1.32309700	-1.02685300
N	2.36800200	-3.56435800	1.44720500
C	0.44068800	-2.38339800	-1.55168600
C	0.42528100	-2.67416900	-2.95835200
C	1.04621100	-3.84705200	-3.41258200
H	1.01952200	-4.05761400	-4.47264900
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C	1.73498200	-4.44702900	-1.21392800
H	2.23442700	-5.10201900	-0.50695300
C	1.13573200	-3.30148900	-0.70133600
C	-0.24485800	-1.70770400	-3.95433600
C	-0.11820600	-2.17754300	-5.41754300
H	-0.59908300	-3.14920200	-5.58145500
H	-0.61114500	-1.45169000	-6.07531400
H	0.92820700	-2.25609300	-5.73572300
C	-1.74965000	-1.57706000	-3.63875600
H	-1.89242100	-1.19893700	-2.62763300
H	-2.24446500	-0.89678500	-4.34088000
H	-2.23632800	-2.55925800	-3.71901600
C	0.40688600	-0.30906300	-3.86515300

O	0.10782000	-0.89005600	-1.25024200
N	3.53021700	-1.66860700	1.03870100
C	1.09897600	-1.48887000	-1.86876100
C	1.07455500	-1.79137800	-3.27097900
C	2.23081600	-2.31538600	-3.86963400
H	2.20132800	-2.52785600	-4.92961000
C	3.41577300	-2.59183900	-3.17036100
C	3.39862400	-2.35663700	-1.78638000
H	4.27552500	-2.56734500	-1.18003800
C	2.27828800	-1.85365300	-1.13748600
C	-0.20760400	-1.53764400	-4.09052900
C	-0.08970600	-2.04156500	-5.54200600
H	0.12730300	-3.11550500	-5.58042400
H	-1.03941600	-1.87427600	-6.06483200
H	0.68985000	-1.50960700	-6.10074400
C	-1.40070800	-2.28221900	-3.44535500
H	-1.50189800	-2.00319800	-2.39527500
H	-2.33594100	-2.04572500	-3.97145900
H	-1.24871500	-3.36239400	-3.51674400
C	-0.52049100	-0.02640300	-4.12792800

H	1.48153900	-0.36015500	-4.07409300	H	0.31625800	0.53931900	-4.55240500
H	-0.04477200	0.36077400	-4.60662800	H	-1.41240800	0.16677900	-4.74197600
H	0.26677400	0.13174400	-2.87853300	H	-0.70081300	0.35043000	-3.12220800
C	2.38691800	-6.03842100	-3.08227700	C	4.66611500	-3.19702200	-3.82990400
C	3.90107600	-5.97659700	-2.77191600	C	5.88342000	-2.26971400	-3.61116100
H	4.08890000	-5.86868700	-1.69873300	H	6.06959400	-2.09570100	-2.54546400
H	4.40924500	-6.88826600	-3.11305300	H	6.79346700	-2.70821600	-4.04133200
H	4.36254200	-5.11824100	-3.27376100	H	5.71651100	-1.29761200	-4.08842500
C	1.77283300	-7.26614000	-2.36861100	C	4.96949200	-4.57658800	-3.19642800
H	0.70058400	-7.34159700	-2.58651400	H	4.13390900	-5.26686700	-3.35923500
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C	1.15357700	-3.06870000	0.79580200	C	2.21845000	-1.76268400	0.37499200
H	0.30211600	-3.57600900	1.25427000	H	1.71161300	-2.66138900	0.74343500
H	0.99369600	-2.00083200	1.02984000	H	1.59368600	-0.91351300	0.68664700
C	3.47205400	-2.62555500	1.24025600	C	3.92501200	-0.25717500	1.09220800
H	3.39379900	-2.29260000	0.20121100	H	3.69356800	0.17366700	0.11449100
H	3.36015200	-1.72379500	1.86182100	H	3.31013200	0.29028800	1.83553900
C	4.84324600	-3.22766200	1.45101500	C	5.39376200	-0.04942700	1.37592500
C	5.12917200	-4.52627200	1.00805400	C	6.33318800	-0.27209800	0.35781700
H	4.32859500	-5.11431400	0.57092300	H	5.98092300	-0.61773800	-0.61065900
C	6.41519800	-5.05298400	1.12639600	C	7.69095800	-0.05558700	0.58221200
H	6.62055000	-6.06078800	0.77360000	H	8.40578700	-0.22644400	-0.21851800
C	7.43790500	-4.28668200	1.69179500	C	8.13464000	0.38308900	1.83525600
H	8.44110200	-4.69523400	1.78335500	H	9.19363000	0.55353600	2.00943100
C	7.16049500	-2.99441900	2.14238400	C	7.21316100	0.59368200	2.86065100
H	7.94756100	-2.39254400	2.59022100	H	7.55016700	0.92058800	3.84092100
C	5.87059700	-2.46951800	2.02781300	C	5.84992100	0.37442200	2.63060600
H	5.66512100	-1.45974000	2.37500000	H	5.13315300	0.52581300	3.43621000
C	2.13367600	-3.87529800	2.85700000	C	3.52316600	-2.26944700	2.37076600
H	3.10733600	-4.09917000	3.31000200	H	4.49373300	-2.05076200	2.83538600
H	1.71830100	-3.00978400	3.40475600	H	2.75498400	-1.80890000	3.02163700
C	1.20822400	-5.06631900	3.00169300	C	3.32281300	-3.77282700	2.36068900
C	1.54567900	-6.28847000	2.40293600	C	3.69397000	-4.56153600	1.26370300
H	2.48195500	-6.36249700	1.85704600	H	4.11425700	-4.07851000	0.38903000
C	0.68993700	-7.38579400	2.49163100	C	3.49638900	-5.94342400	1.28181900
H	0.96544400	-8.32630600	2.02131000	H	3.77791500	-6.53606500	0.41506600
C	-0.52419800	-7.27538800	3.17778700	C	2.93402100	-6.56269600	2.40123800
H	-1.19491900	-8.12824100	3.24177500	H	2.77389800	-7.63746800	2.41123900
C	-0.87160900	-6.06161900	3.77196500	C	2.57591300	-5.78688700	3.50546900
H	-1.81711000	-5.96382700	4.30050000	H	2.12678200	-6.25290100	4.37810100
C	-0.00925600	-4.96513200	3.68196600	C	2.76812300	-4.40457900	3.47982000
H	-0.29550000	-4.01284300	4.12106500	H	2.47384600	-3.80213900	4.33622700
Na	-1.71835900	-0.86819800	0.56812700	Na	-0.72919000	-1.35609500	0.79945400
O	-4.03366400	-0.33098800	1.52995600	O	-2.95457400	-1.59221300	1.58224100
C	-4.23441200	0.49618900	2.68712600	C	-3.31828900	-1.16469300	2.90699100
H	-3.28029600	0.95830800	2.93590300	H	-3.05949100	-0.11201900	2.99884700
H	-4.57757800	-0.12372300	3.53372500	H	-2.73109200	-1.74387000	3.63386800
C	-5.30396300	1.49533800	2.25427800	C	-4.82510300	-1.46493100	3.02120900
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C	-6.22539000	0.63960600	1.35755500	C	-5.07986300	-2.53624100	1.92469400
H	-7.10050300	0.28536500	1.91280100	H	-5.54357900	-3.44775700	2.31482300
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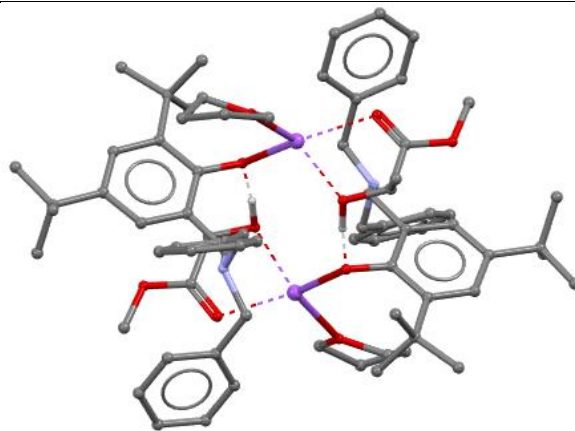
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H	-6.42218400	-3.42999600	-0.88938600	H	-2.00497700	-7.63425100	-1.34221300
H	-5.70934100	-4.90967200	-1.57901600	H	-2.25372700	-7.87320300	-3.09046400
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C	-3.73943900	-3.01022200	-1.34117900	O	-0.16423000	-5.91486300	-3.92158200
O	-3.34197200	-1.99919400	-0.79585500	C	-0.28546600	-4.65780300	1.48053300
O	-3.24045400	-4.23086500	-1.08965300	H	0.78500000	-4.89566700	1.37072700
C	-2.14567800	-4.26625500	-0.13533900	C	-1.07124400	-5.96825600	1.47006700
H	-1.35232300	-3.61738800	-0.50398700	H	-0.73574300	-6.61679500	2.28266800
C	-1.65756200	-5.70234200	-0.04029800	H	-0.90086500	-6.47202600	0.51625800
H	-0.82211700	-5.76284100	0.66218300	H	-2.14445000	-5.78278000	1.57214500
H	-1.30180900	-6.02524400	-1.02226800	C	-0.38862300	-3.88298900	2.78970600
H	-2.45846400	-6.36422900	0.30105500	O	-0.47839100	-4.67309400	3.87074100
C	-2.59021300	-3.71293300	1.21780500	O	-0.36515700	-2.66842300	2.86188600
O	-3.79181800	-4.15800100	1.59537300	C	-0.51623300	-3.98446700	5.13508100
O	-1.91025800	-2.95813700	1.89115400	H	0.35423600	-3.33306300	5.24348300
C	-4.27603100	-3.61306300	2.84379500	H	-0.51517800	-4.76789100	5.89309100
H	-3.65954300	-3.97427100	3.67144700	H	-1.42223300	-3.37656900	5.20956900
H	-5.29975500	-3.97424400	2.93926000	C	-5.58218300	-3.84543100	-1.74859700
H	-4.23795500	-2.52236900	2.80492300	H	-5.50209800	-4.91141100	-1.97356000
C	-5.50648700	-0.25828600	-5.42607400	H	-5.78104800	-3.72435300	-0.67641300
H	-5.11858100	-1.13404500	-5.95230200	H	-6.41261600	-3.41137700	-2.31663600
H	-6.45487000	-0.52737900	-4.94328300	O	-4.33654200	-3.25538100	-2.12935900
H	-5.68259600	0.54215700	-6.15659800	H	-4.39529800	-2.29563400	-1.99761000
O	-4.51507100	0.11582900	-4.46737800	O	-0.04536600	0.87271900	1.32334400
H	-4.84682600	0.89781900	-3.99282200	N	-3.46761100	1.65151500	-0.96590500
O	-0.32808800	0.86199600	1.33414900	C	-1.03653900	1.47166900	1.94171800
N	-2.72441700	2.48327000	-1.73740400	C	-1.01222400	1.77439700	3.34387900
C	-1.07155400	1.91680900	1.61919500	C	-2.16848500	2.29862800	3.94233800
C	-1.21364100	2.45179700	2.94431400	H	-2.13908300	2.51124900	5.00228700
C	-2.01556700	3.58797200	3.14032000	C	-3.35334700	2.57508100	3.24290900
H	-2.10319000	3.98166500	4.14363400	C	-3.33610400	2.33962500	1.85897000
C	-2.70173500	4.24230700	2.11201100	H	-4.21295000	2.55023200	1.25251900
C	-2.56305900	3.70242600	0.82775300	C	-2.21576500	1.83639100	1.21028800
H	-3.08051500	4.15177000	-0.01361400	C	0.26985500	1.52073200	4.16357200
C	-1.78830600	2.57784200	0.57074500	C	0.15174300	2.02460200	5.61504400
C	-0.42397300	1.84948300	4.12329400	H	-0.06532100	3.09853200	5.65348100
C	-0.81040200	2.45700700	5.48580700	H	1.10138800	1.85734000	6.13799800
H	-0.58904500	3.52856600	5.54017600	H	-0.62787300	1.49259800	6.17365700
H	-0.23692100	1.96537700	6.28119300	C	1.46291000	2.26547000	3.51851200
H	-1.87523500	2.31625600	5.70578300	H	1.56432200	1.98639500	2.46847000
C	1.07119000	2.14737500	3.87792400	H	2.39812300	2.02923500	4.04478300
H	1.37784100	1.69053200	2.93721600	H	1.31062800	3.34561000	3.58973700
H	1.70168900	1.75998700	4.68890800	C	0.58291300	0.00952100	4.20097700
H	1.24044200	3.22810800	3.80845800	H	-0.25391800	-0.55634500	4.62509500
C	-0.63556000	0.31953400	4.23052200	H	1.47463000	-0.18358400	4.81534500
H	-1.68783700	0.08194900	4.42638700	H	0.76368800	-0.36718600	3.19528800
H	-0.05202500	-0.09025900	5.06684600	C	-4.60374800	3.18036500	3.90223700
H	-0.35200800	-0.17511700	3.29918100	C	-5.82101900	2.25301000	3.68347100
C	-3.53926100	5.51477400	2.31681900	H	-6.00717700	2.07899100	2.61777600
C	-4.99154000	5.28492900	1.83640000	H	-6.73109100	2.69147200	4.11363000



H	-5.03109500	4.96727100	0.78888000	H	-5.65406600	1.28091800	4.16074900
H	-5.58017300	6.20699300	1.92869100	C	-4.90706000	4.55984100	3.26853800
H	-5.48023700	4.50975700	2.43686100	H	-4.07150000	5.25015100	3.43134100
C	-2.91513000	6.66732300	1.49379700	H	-5.80758200	5.00558900	3.71125100
H	-1.88187700	6.85220700	1.81062900	H	-5.07055000	4.47855600	2.18827600
H	-3.48616600	7.59601600	1.62370500	C	-4.43006600	3.38408600	5.41857900
H	-2.89808800	6.43102100	0.42415400	H	-4.22684600	2.43668600	5.93121500
C	-3.59098000	5.95352400	3.79159300	H	-5.34656300	3.80665300	5.84751400
H	-4.03338500	5.17722700	4.42674800	H	-3.60890600	4.07440600	5.64140800
H	-4.20392500	6.85693800	3.89284500	C	-2.15584000	1.74494500	-0.30215600
H	-2.59262100	6.18396100	4.18105300	H	-1.64838700	2.64323000	-0.67079000
C	-1.62919400	2.07630100	-0.85108300	H	-1.53157400	0.89532100	-0.61357900
H	-0.69793200	2.46868300	-1.26279000	C	-3.86319900	0.24031800	-1.01943200
H	-1.49621100	0.98282600	-0.88485900	H	-3.63141400	-0.19084300	-0.04193700
C	-3.90671900	1.66496200	-1.48899000	H	-3.24900100	-0.30728100	-1.76326100
H	-3.98576200	1.55316600	-0.40211500	C	-5.33225000	0.03348000	-1.30228300
H	-3.78767600	0.63743400	-1.87963600	C	-6.27076300	0.25591300	-0.28328100
C	-5.20097200	2.27055600	-1.99853600	H	-5.91753800	0.60037000	0.68527200
C	-5.33630300	3.65403400	-2.17934600	C	-7.62885900	0.04060400	-0.50688200
H	-4.47565800	4.28851400	-1.99483000	H	-8.34297900	0.21127800	0.29451900
C	-6.54810500	4.20234700	-2.60049500	C	-8.07375800	-0.39658900	-1.76000500
H	-6.63292700	5.27748200	-2.73676800	H	-9.13300100	-0.56605200	-1.93359600
C	-7.64792600	3.37749100	-2.84948800	C	-7.15315600	-0.60703900	-2.78622200
H	-8.59053400	3.80607600	-3.17930900	H	-7.49111200	-0.93288700	-3.76651700
C	-7.52489500	1.99841200	-2.67336800	C	-5.78959200	-0.38906800	-2.55695300
H	-8.37295700	1.34513400	-2.86264900	H	-5.07348600	-0.54057000	-3.36312100
C	-6.31108800	1.44715300	-2.25223500	C	-3.46039200	2.25249800	-2.29788900
H	-6.22799000	0.37193800	-2.11377900	H	-4.43101100	2.03410800	-2.76254100
C	-2.31378100	2.49914000	-3.14098600	H	-2.69231400	1.79184100	-2.94879800
H	-3.20557400	2.70798500	-3.74694000	C	-3.25966700	3.75583100	-2.28765000
H	-1.93960200	1.51463600	-3.47166300	C	-3.63043000	4.54449500	-1.19051200
C	-1.26588900	3.56322000	-3.42397200	H	-4.05068800	4.06147900	-0.31582200
C	-1.21400400	4.75011700	-2.67976600	C	-3.43252300	5.92634600	-1.20850100
H	-1.92557600	4.89510100	-1.87360600	H	-3.71375000	6.51894100	-0.34162000
C	-0.23799300	5.71355900	-2.93823700	C	-2.87019600	6.54561400	-2.32793200
H	-0.21117000	6.62425600	-2.34457000	H	-2.70977500	7.62034200	-2.33782700
C	0.70111500	5.51146100	-3.95299600	C	-2.51249700	5.76984500	-3.43233500
H	1.46250600	6.26090200	-4.15349800	H	-2.06342200	6.23586400	-4.30499200
C	0.64721700	4.33958700	-4.71049200	C	-2.70505400	4.38759000	-3.40682200
H	1.36654500	4.17156000	-5.50867500	H	-2.41113000	3.78518400	-4.26337300
C	-0.32639900	3.37500800	-4.44332100	Na	0.79155700	1.33884800	-0.72637300
H	-0.34801100	2.45894100	-5.02613900	O	3.01656200	1.57539800	-1.50947800
Na	1.28785100	0.21098400	-0.21738700	C	3.38067200	1.14805400	-2.83411600
O	3.60910200	-0.40899100	-1.36718100	H	3.11993800	0.09593700	-2.92698600
C	3.76175600	-1.28411000	-2.50120600	H	2.79538400	1.72890500	-3.56124000
H	2.82883200	-1.83304000	-2.62300700	C	4.88806500	1.44551800	-2.94634000
H	3.94867900	-0.68533700	-3.40836000	H	5.15518300	1.79447900	-3.94869200
C	4.96316700	-2.16130100	-2.16220700	H	5.47093600	0.54382700	-2.74423400
H	5.42549900	-2.60344500	-3.05035300	C	5.14272200	2.51841200	-1.85129900
H	4.65677900	-2.97705500	-1.50168500	H	5.60579900	3.42962300	-2.24289800
C	5.88992900	-1.17470600	-1.42721300	H	5.79746600	2.11497500	-1.07259900
H	6.54944400	-0.66682500	-2.14050200	C	3.73985400	2.78811400	-1.28378400
H	6.51419400	-1.66717900	-0.67710900	H	3.24429500	3.61516600	-1.81324300
C	4.91118600	-0.16943200	-0.78321900	H	3.71225100	3.00037400	-0.21467800
H	5.20379900	0.87219800	-0.97611600	H	3.03604600	4.22565900	1.70561900
H	4.81590500	-0.29466000	0.29587300	O	2.48809300	4.98662300	1.41086100
H	4.12940800	0.33407900	3.22984900	C	2.16787600	5.77366900	2.55174200
O	4.94382000	0.80256700	2.93790900	H	2.68476100	5.39186700	3.43937400

C	4.61595300	2.12264200	2.59542900	C	2.57735500	7.22861100	2.30572700
H	4.27679900	2.70285000	3.47116100	H	2.06978300	7.61704500	1.41685900
C	5.85953700	2.78948300	2.00317100	H	2.31787800	7.85479500	3.16537700
H	6.17629300	2.24935500	1.10489600	H	3.65711800	7.28133300	2.13435300
H	5.65925300	3.83230200	1.74456300	O	0.22631100	5.89920200	3.99418200
H	6.66967500	2.74369700	2.73612300	C	0.34859000	4.64057500	-1.40684200
C	3.46593500	2.16030000	1.59200500	H	-0.72172100	4.87901900	-1.29683200
O	2.95779800	1.16680700	1.10556100	C	1.13509900	5.95059300	-1.39623000
O	3.06155500	3.40924200	1.31440000	H	0.79975800	6.59948800	-2.20862300
C	1.91882500	3.51406400	0.42164800	H	0.96522900	6.45423200	-0.44227000
H	1.11085000	2.89462500	0.81470100	H	2.20817800	5.76457200	-1.49858700
C	1.50245600	4.97468300	0.37663100	C	0.45118300	3.86595100	-2.71619700
H	0.63530000	5.07976400	-0.28166700	O	0.54164100	4.65621100	-3.79706600
H	1.21914700	5.30179200	1.38082500	O	0.42699900	2.65141700	-2.78864200
H	2.31755700	5.60035000	0.00194900	C	0.57907800	3.96782800	-5.06154300
C	2.26094400	2.96731900	-0.96397600	H	-0.29174000	3.31691800	-5.17007900
O	3.44259500	3.38288100	-1.42090900	H	0.57844700	4.75140700	-5.81939500
O	1.51576700	2.23404100	-1.58759500	H	1.48474400	3.35944700	-5.13617000
C	3.80327700	2.84832100	-2.71978000	C	5.64573700	3.83176000	1.82043900
H	3.10821100	3.22341600	-3.47523000	H	5.56493200	4.89726400	2.04739500
H	4.81631700	3.20472100	-2.90481700	H	5.84350000	3.71276000	0.74780500
H	3.76046300	1.75741600	-2.68594600	H	6.47718600	3.39746900	2.38681300
C	2.71879400	-0.98539700	5.23153000	O	4.40109200	3.23976400	2.20150100
H	3.74767500	-1.23632900	5.49897300	H	4.46158800	2.28009800	2.06975000
H	2.08558900	-1.86566100	5.39899200	O	0.75489700	3.73254100	-0.39588900
H	2.37293500	-0.16411600	5.87275400	H	1.06376500	4.24187300	0.38396300
O	2.74162600	-0.61373500	3.85504700	C	0.67480800	5.71206200	2.88357600
H	1.85148000	-0.35886400	3.56434500	O	-0.06779600	5.47129200	1.79081700
				C	-1.48557200	5.30489000	2.01124600
				H	-1.89334700	4.98886600	1.05355800
				H	-1.65655700	4.53771300	2.76511400
				H	-1.92590700	6.25325000	2.33346100
				O	-0.69211800	-3.75029800	0.46925000
				H	-1.00167200	-4.26013600	-0.31000200
				C	-0.61230500	-5.72894100	-2.81059900
				O	0.13069300	-5.48890400	-1.71795100
				C	1.54837500	-5.32231200	-1.93887300
				H	1.71903600	-4.55392400	-2.69157000
				H	1.95670800	-5.00793400	-0.98086900
				H	1.98840400	-6.27019200	-2.26290400

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Na	10.20102600	11.27878500	10.54781000	H	16.83798500	7.49645800	9.98171800
O	10.62521300	9.22079500	9.79984600	H	17.71635500	6.84085100	8.59132600

O	12.31852500	12.12977400	11.14040000	H	16.21306800	6.07415300	9.12371500
N	12.28200900	11.46000300	6.75106500	C	11.55571200	10.30198600	7.29121400
C	11.86903400	8.91401000	9.42316300	H	11.26530400	9.70168400	6.42303400
C	12.69772800	8.03314100	10.19246500	H	10.62674300	10.60679500	7.79329900
C	13.99275300	7.75744900	9.73109000	C	12.41954600	12.51971200	7.74904300
H	14.61218700	7.09512400	10.31936800	H	12.60877500	12.02124000	8.70509200
C	14.52542500	8.28298200	8.54614300	H	11.48525600	13.08619100	7.88122900
C	13.69301000	9.12117800	7.80192300	C	13.56706700	13.45983100	7.45962500
H	14.03687100	9.55464900	6.86693300	C	14.83661900	12.94919900	7.15451400
C	12.39988800	9.44028100	8.21005100	H	14.95680300	11.87275100	7.07975300
C	12.16889600	7.38383500	11.49088100	C	15.92009800	13.80422300	6.96102600
C	13.18983300	6.42486400	12.13667100	H	16.90003000	13.39215700	6.73309100
H	13.45337200	5.59707100	11.46832100	C	15.74907600	15.18858500	7.06366600
H	12.75613900	5.99131900	13.04557900	H	16.59317400	15.85631900	6.91233700
H	14.11348300	6.93942200	12.42610400	C	14.48667100	15.70813700	7.35460800
C	10.89975200	6.55077000	11.18760500	H	14.34246100	16.78336300	7.42506200
H	10.13474300	7.15981700	10.70648700	C	13.40314700	14.84624500	7.54764900
H	10.48308500	6.13331400	12.11315800	H	12.41779900	15.25154500	7.76973500
H	11.14611300	5.71133200	10.52522200	C	11.67703400	11.94634700	5.50762100
C	11.84785900	8.47068000	12.54438500	H	12.12941600	12.92126500	5.28706600
H	12.76636400	8.96277000	12.88294400	H	10.59127100	12.11582600	5.61813200
H	11.36152500	8.02583200	13.42215700	C	11.95205800	11.00018300	4.35640200
H	11.18330900	9.23095400	12.13388100	C	13.27000300	10.59859700	4.09030700
C	15.93821100	7.96036300	8.03542200	H	14.06738900	10.97672500	4.72368300
C	16.74344700	9.27048300	7.87020000	C	13.55059800	9.73141100	3.03549700
H	16.27472100	9.94086800	7.14217500	H	14.57785400	9.43487600	2.83731900
H	17.76265100	9.06043300	7.52091200	C	12.51288000	9.24185000	2.23359100
H	16.81055000	9.80776500	8.82344000	H	12.73020700	8.56268700	1.41311300
C	15.83600600	7.25363900	6.66256000	C	11.19933100	9.63136500	2.49412000
H	15.26650500	6.32102200	6.75321900	H	10.38489100	9.25187500	1.88242100
H	16.83303300	7.01207900	6.27167200	C	10.92391200	10.50681500	3.54852000
H	15.32909300	7.88443600	5.92412600	H	9.89842100	10.81191500	3.74163800
C	16.71577600	7.03920800	8.99302100	C	13.52935100	11.40403100	11.43979700
H	13.41987400	10.39949400	11.03137100	C	2.29966500	7.12757300	9.07760300
H	13.65908800	11.34162100	12.53106200	H	1.36922900	7.54374200	9.45590700
C	14.64051200	12.21906600	10.78770200	C	2.34386000	5.80198700	8.63479400
H	15.62070100	12.02159400	11.23234500	H	1.45044000	5.18400400	8.66858200
H	14.69870400	11.98578700	9.72123000	C	3.54453400	5.27482500	8.15726500
C	14.16379300	13.66759800	11.00752600	H	3.59288000	4.24063800	7.82545000
H	14.54566300	14.05709100	11.95757000	C	4.69118300	6.07273300	8.11716800
H	14.48992700	14.33725000	10.20769000	H	5.62981900	5.65459700	7.75908700
C	12.62539600	13.54084100	11.05660900	C	6.74139700	8.22466100	10.65660800
H	12.19306300	14.05431200	11.92519400	H	6.06849100	7.36898500	10.79570100
H	12.14484100	13.92144900	10.15148100	H	7.70966500	7.82215800	10.31163300
Na	8.59005900	9.46156600	6.35582600	C	6.92998600	8.94246500	11.97196400
O	8.28229900	11.53822400	7.13119400	C	5.82899000	9.45841100	12.66710500
O	6.62220600	8.88343500	5.22585000	H	4.83419500	9.32969800	12.24772600
N	6.13433300	9.08273300	9.62836000	C	6.00943000	10.13426200	13.87477500
C	7.01109000	11.87533300	7.36192700	H	5.14703000	10.52370100	14.41109000
C	6.33777600	12.86642500	6.57848500	C	7.29463000	10.30984700	14.39826500
C	5.01415900	13.19117900	6.90791300	H	7.43333400	10.83792800	15.33816600
H	4.51194600	13.94259800	6.31502300	C	8.39613200	9.80086500	13.70880700
C	4.30928300	12.60602400	7.96917100	H	9.40091800	9.93340300	14.10298300
C	4.98843200	11.64502200	8.72215300	C	8.21114000	9.12102300	12.50327000
H	4.50136900	11.15146000	9.55920000	H	9.06490100	8.73640600	11.95437000
C	6.30104300	11.27285000	8.44145900	C	5.44602800	9.66436400	4.91474300
C	7.06714200	13.58972900	5.42421600	H	5.43326500	10.52533100	5.58552700
C	6.16004600	14.59691600	4.68916000	H	5.51460600	10.02121900	3.87705500

H	5.80959100	15.39573800	5.35287100	C	4.27364300	8.70375500	5.09165300
H	6.72420500	15.06856600	3.87605200	H	3.39064800	9.01706900	4.52650400
H	5.28333700	14.11080700	4.24512300	H	3.99312300	8.62540300	6.14603400
C	8.27822600	14.38039800	5.97633300	C	4.86824300	7.37692500	4.58822300
H	8.97135400	13.72399700	6.50262100	H	4.77176100	7.30304300	3.49905800
H	8.82018300	14.87036200	5.15692300	H	4.38530500	6.50402000	5.03620500
H	7.94223000	15.16346700	6.66770200	C	6.34931000	7.48263600	4.99264000
C	7.56130500	12.57124400	4.37132400	H	7.03353500	7.10985400	4.22199400
H	6.71650800	12.05459600	3.90303700	H	6.55221400	6.94819000	5.92623800
H	8.12654600	13.08019100	3.57983500	H	9.71033800	8.47915600	8.78576000
H	8.21086000	11.83099300	4.83805900	O	9.19359400	7.94664100	8.07878000
C	2.86476500	12.98365700	8.33229700	C	9.98014800	6.83714900	7.68938200
C	1.95692700	11.73855700	8.20239900	H	10.81548100	6.69219000	8.37961400
H	2.28706000	10.92936300	8.86166900	H	9.04248500	12.32683900	8.24862600
H	0.91889800	11.98245600	8.46335000	O	9.46192500	12.87040900	9.00665600
H	1.97146900	11.35473100	7.17559700	C	8.52518400	13.82321700	9.47093100
C	2.82031600	13.49647000	9.79153400	H	7.72362200	13.97072400	8.74255000
H	3.47244500	14.36966900	9.91144900	C	9.23096100	15.15601100	9.73464900
H	1.79940300	13.78538700	10.07279600	H	9.66968700	15.51399200	8.79850300
H	3.15668600	12.72902800	10.49687300	H	8.52752400	15.90608900	10.11082000
C	2.29565100	14.08749200	7.42217200	H	10.03303800	15.02017800	10.46759500
H	2.27033300	13.77326400	6.37244600	C	9.11730400	5.57277600	7.65106000
H	1.26842600	14.32576100	7.72196800	H	8.28106600	5.71094200	6.95715200
H	2.88453600	15.00954800	7.48810200	H	9.70257100	4.70296100	7.33397200
C	6.97952200	10.25423300	9.33559500	H	8.71304500	5.38929200	8.65066100
H	7.20457600	10.71486900	10.30155000	C	10.57329900	7.10567600	6.30634200
H	7.94546400	9.96082000	8.90319800	C	7.88256300	13.31304900	10.75993100
C	5.86817500	8.29791300	8.42102700	O	10.04717100	7.82467800	5.46597400
H	5.69700100	9.01197500	7.61145900	O	11.72389700	6.46791500	6.11166600
H	6.74782100	7.70005600	8.13393700	C	12.41050900	6.76434900	4.87379700
C	4.65329400	7.40540100	8.54233700	H	12.61259700	7.83459100	4.80918200
C	3.44550400	7.92022200	9.03317500	H	13.34036600	6.19890500	4.91992300
H	3.42484100	8.94766300	9.38220500	H	11.80440800	6.45929700	4.01738200
O	8.40981100	12.50804500	11.51557000	H	5.00043000	13.86760900	12.09838700
O	6.68638600	13.85605200	10.97789900	H	5.85649200	12.28735200	12.07769300
C	5.96983900	13.37178700	12.13497000	H	6.50897500	13.62663400	13.05120000

**Table S11.** DFT optimized structures and atom coordinates of complexes for proposed polylactide degradation process by using sodium compounds.

**CheckCif Alert B explanation:**

B Alert explanation for  $[(2\text{-npL}^{\text{Bn}})\text{-Na(THF)}]_4$ :

**RINTA01\_ALERT\_3\_B** The value of Rint is greater than 0.18      Rint given   0.194

**PLAT020\_ALERT\_3\_B** The Value of Rint is Greater Than 0.12 .....      0.194 Report

**PLAT340\_ALERT\_3\_B** Low Bond Precision on C-C Bonds .....      0.01082 Ang.

**PLAT910\_ALERT\_3\_B** Missing # of FCF Reflection(s) Below Theta(Min).      26 Note

**RESPONSE:** Crystals diffracted weakly. Data was collected with radiation sources of Mo and Cu. All results were consistent with the model in this report (from the Mo data collection), however all yielded serious problems due to weak diffraction.

B Alert explanation for [(1-n0L<sup>Bn</sup>)-Na(THF)<sub>0.5</sub>]<sub>4</sub>:

**PLAT084\_ALERT\_3\_B** High wR2 Value (i.e. > 0.25) ..... 0.36 Report

**PLAT340\_ALERT\_3\_B** Low Bond Precision on C-C Bonds ..... 0.01652 Ang.

**RESPONSE:** Crystals diffracted weakly. Data was collected with radiation sources of Mo and Cu. All results were consistent with the model in this report (from the Cu data collection), however all yielded serious problems due to weak diffraction.