The molecular and crystal structure of Shibasaki's (*R*)-ALB chiral catalyst

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SUPPLEMENTARY INFORMATION

Table of contents

Fig. S1 Ellipsoid plot of **2**·0.67THF
Fig. S2 PXRD pattern of **2**·0.67THF and results of Rietveld refinement
Fig. S3 ^{1}H NMR spectrum of **2**·0.67THF in THF-d_8
Fig. S4 ^{13}C{^{1}H} NMR spectrum of **2**·0.67THF in THF-d_8
Fig. S5 ^{7}Li NMR spectrum of **2**·0.67THF in THF-d_8
Fig. S6 ^{1}H NMR spectrum of **2**·0.67THF in C_6D_6
Fig. S7 ^{13}C{^{1}H} NMR spectrum of **2**·0.67THF in C_6D_6
Fig. S8 ^{7}Li NMR spectrum of **2**·0.67THF in C_6D_6
Table S1 Geometry of non-classical H bonds in **2**·0.67THF

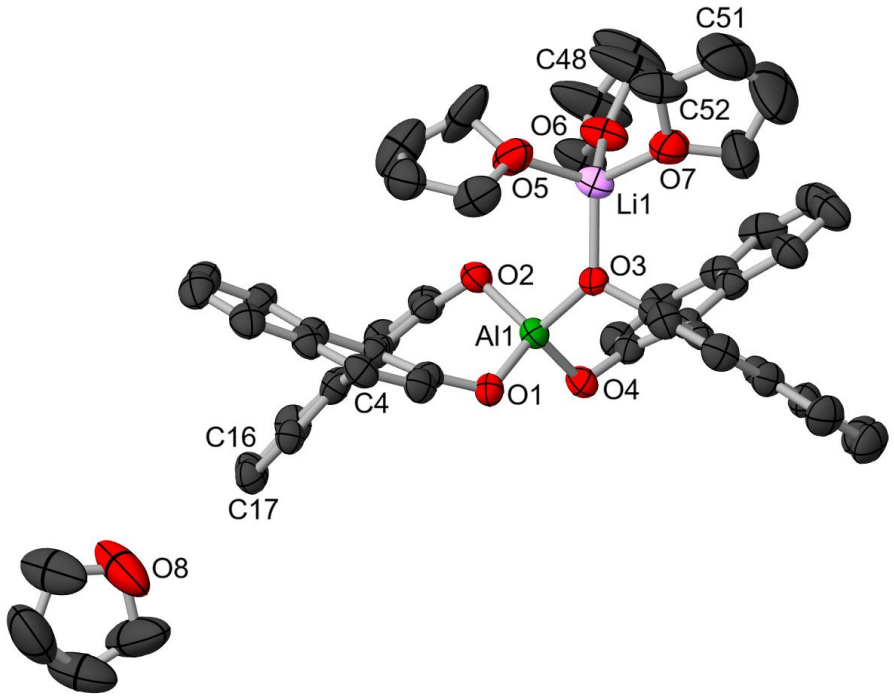


Fig. S1 Ellipsoid plot of **2**·0.67THF, omitting H atoms. Labels are given for heteroatoms and for C atoms involved in the C-H···O contacts listed in **Table S1**. Color code: Al = green, Li = light purple, O = red, C = gray. The planarity of some THF molecules is a consequence of unresolved disorder effects. Ellipsoids are drawn at the 50% probability level

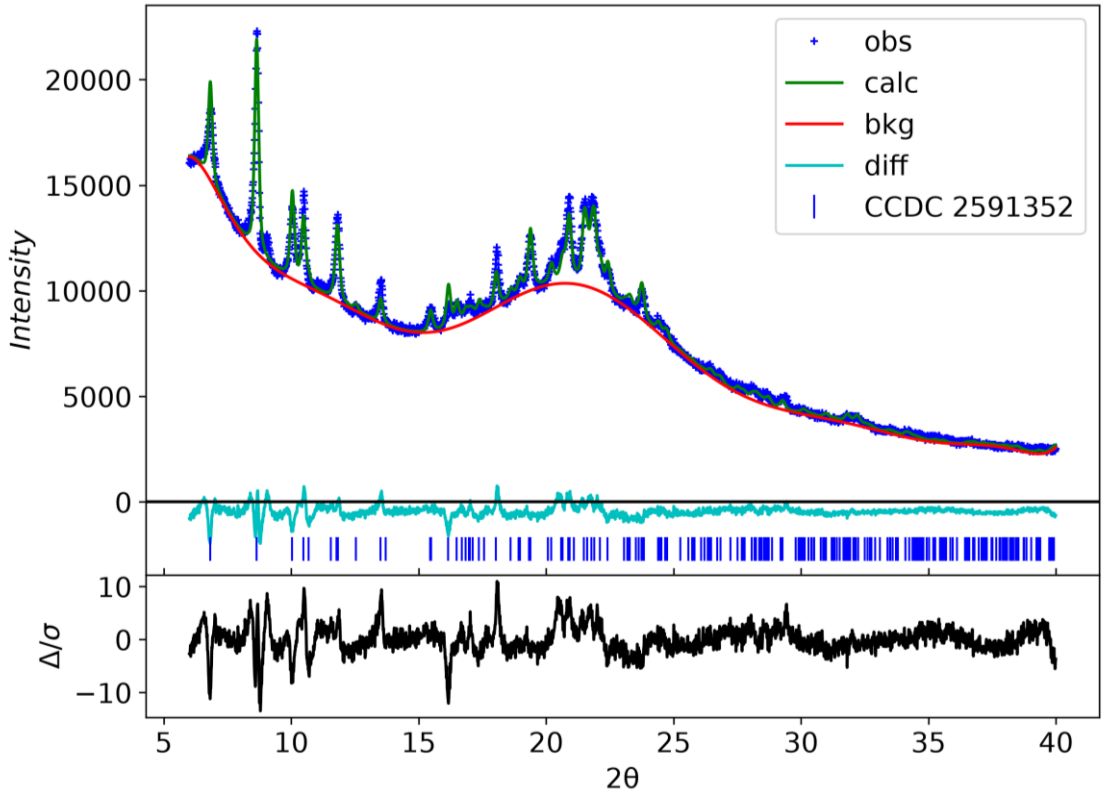


Fig. S2 Observed PXRD pattern of **2**·0.67THF (blue plus symbols), along with calculated (green line), difference (cyan line), and weighted difference curve (black line) from Rietveld refinement. The red curve is the fitted background. The blue ticks indicate the positions of the reflections for the calculated phase

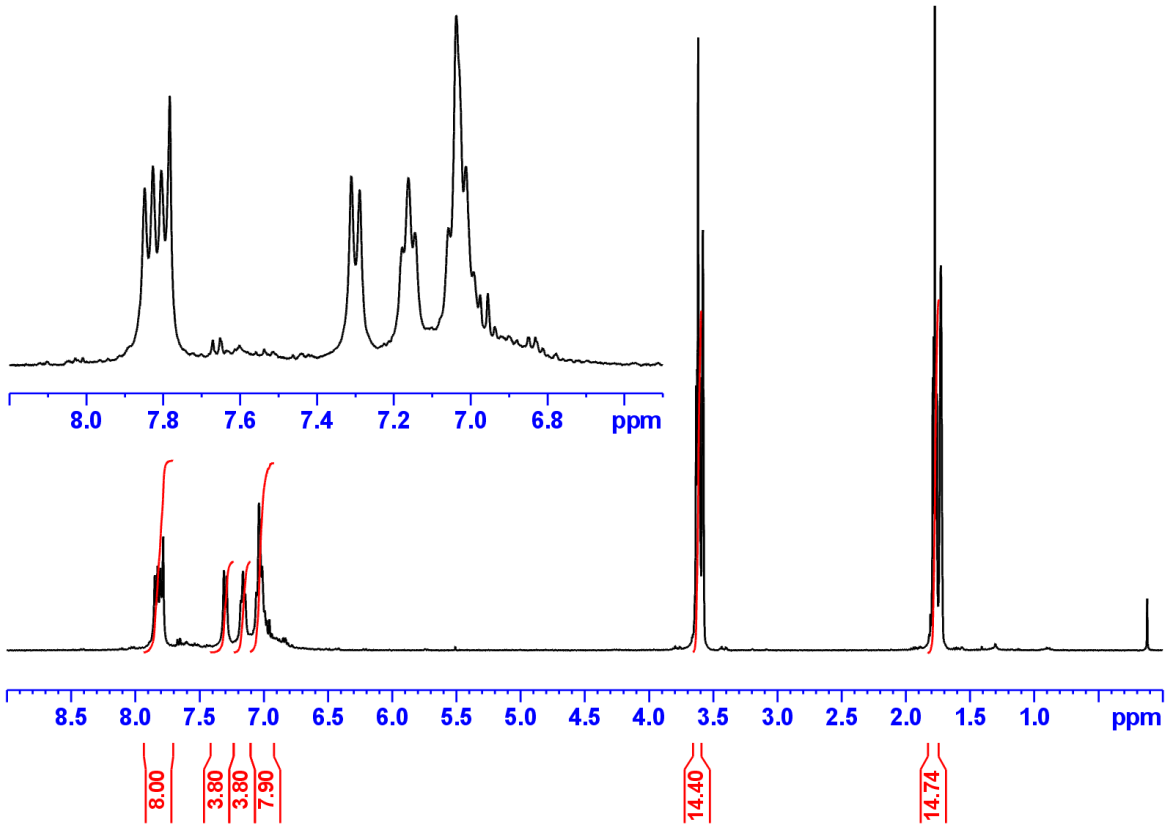


Fig. S3 ^{1}H NMR spectrum (400.13 MHz, 298.0 K, THF-d_8) of **2**·0.67THF. The integral values are indicated in red

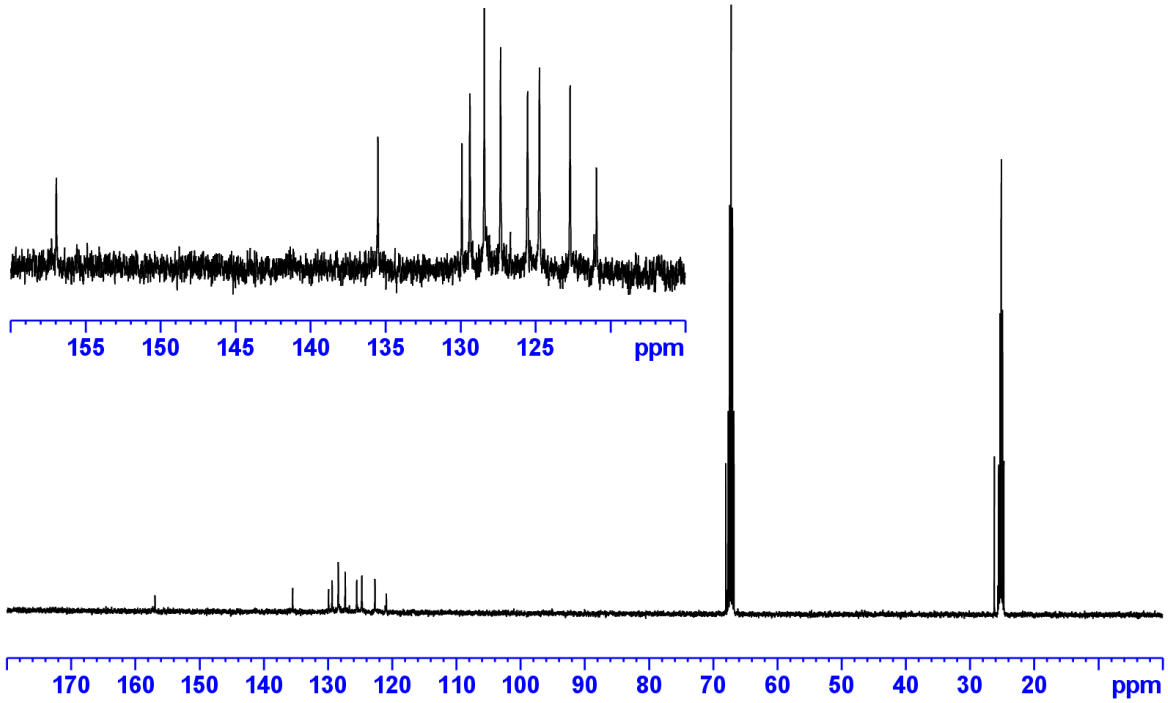


Fig. S4 ^{13}C{^{1}H} NMR spectrum (100.61 MHz, 298.0 K, THF-d_8) of **2**·0.67THF

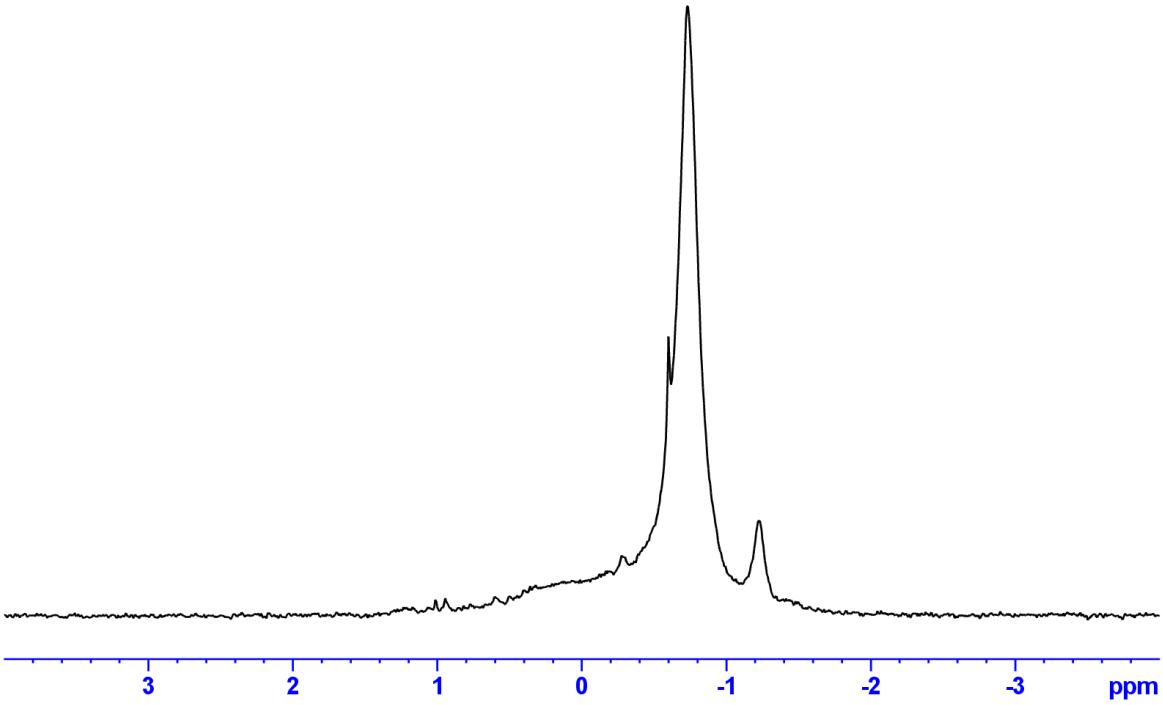


Fig. S5 ^{7}Li NMR spectrum (155.51 MHz, 298.0 K, THF-d_8) of **2**·0.67THF

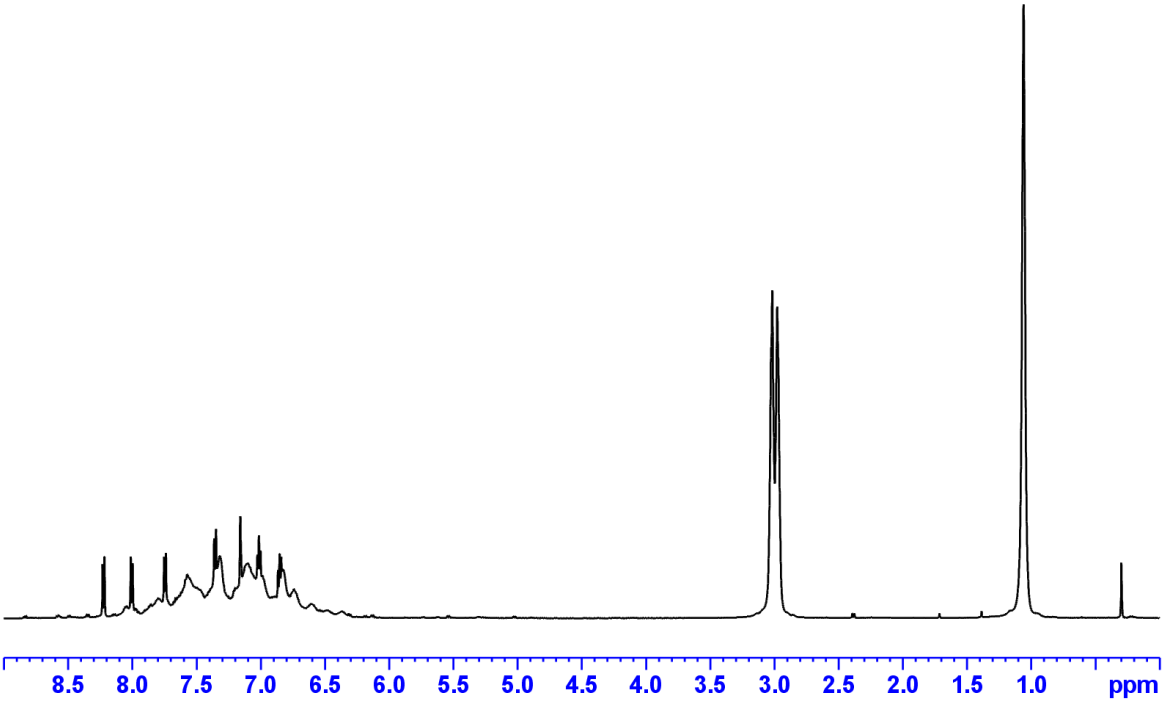


Fig. S6 ^{1}H NMR spectrum (600.13 MHz, 298.0 K, C_6D_6) of **2**·0.67THF

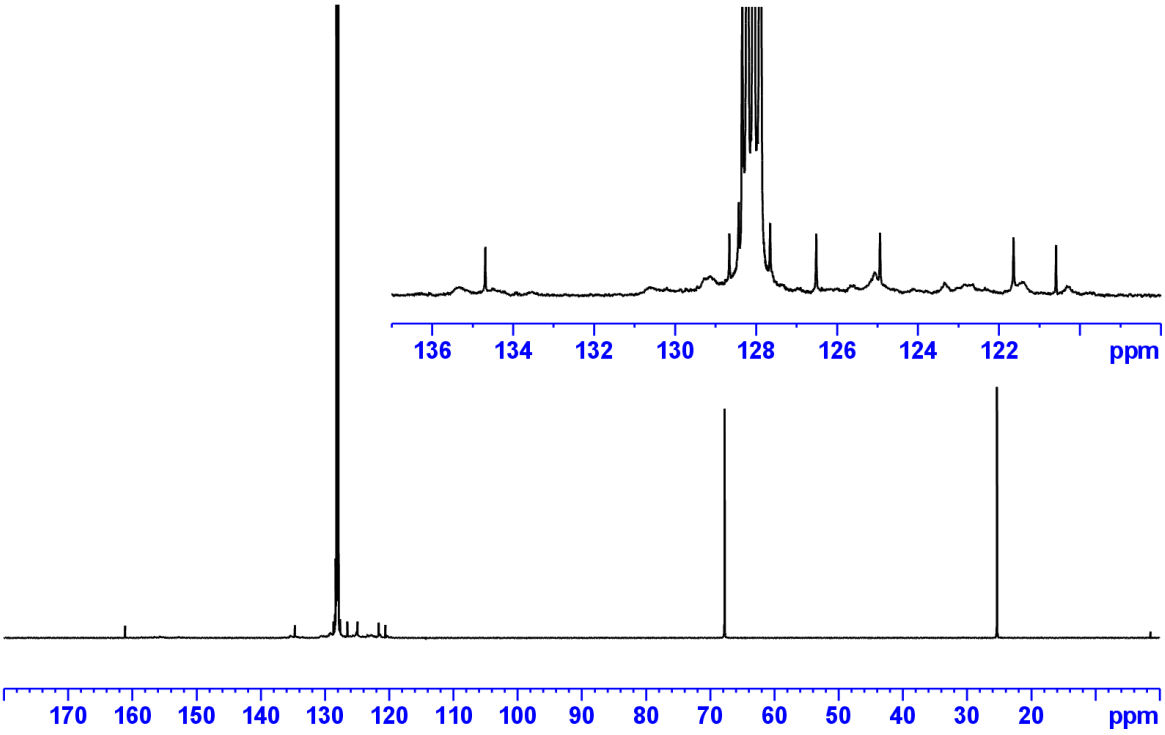


Fig. S7 $^{13}C\{^{1}H\}$ NMR spectrum (150.90 MHz, 298.0 K, C_6D_6) of **2**·0.67THF

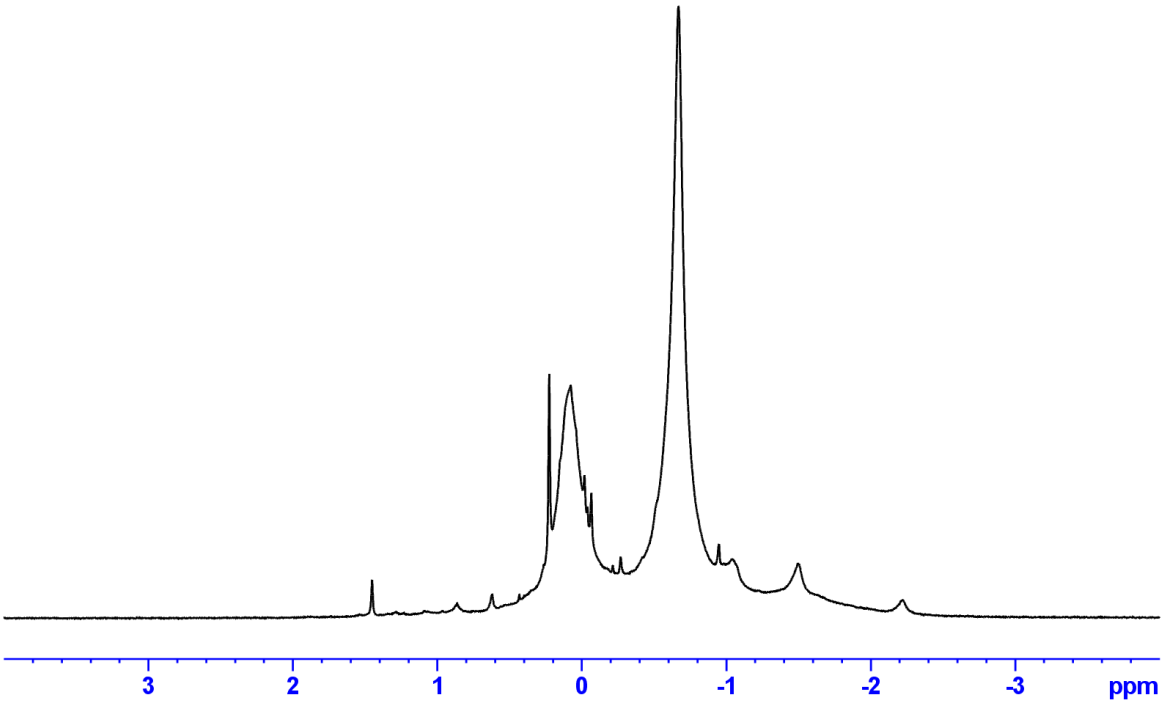


Fig. S8 ^{7}Li NMR spectrum (233.23 MHz, 298.0 K, C_6D_6) of **2**·0.67THF

Table S1 Geometry (Å, °) of non-classical H bonds in **2**·0.67THF

D–H···*A*	*D*–H	H···*A*	*D*···*A*	∠ *D*–H···*A*
C4-H4···O8^{i}	0.95	2.61	3.494(13)	155.9
C16-H16···O8	0.95	2.57	3.225(10)	126.4
C17-H17···O8	0.95	2.77	3.329(10)	118.6
C48-H48B···O1^{ii}	0.99	2.68	3.540(11)	145.2
C51-H51A···O1^{ii}	0.99	3.00	3.712(12)	130.1
C52-H52B···O1^{ii}	0.99	2.71	3.558(8)	144.0

Symmetry codes: (i) *x*, *y*–1, *z*; (ii) *x*–1, *y*, *z*.