

Electronic Supplementary Information

**Redox Activity of a Dissymmetric Ligand Bridging Divalent
Ytterbium and Reactive Nickel Fragments**

Ding Wang,[†] Maxime Tricoire,[†] Valeriu Cemortan,[†] Jules Moutet[†] and Grégory Nocton^{*,†}

[†]LCM, CNRS, Ecole Polytechnique, Institut Polytechnique Paris, Route de Saclay, 91128 Palaiseau, France.

*** Corresponding Author**

Email: gregory.nocton@polytechnique.edu

Table of Contents

1.	<i>NMR spectra</i>	S3
2.	<i>Magnetism</i>	S17
3.	<i>DFT calculation data</i>	S20
4.	<i>Crystallographic data</i>	S29

1. NMR spectra

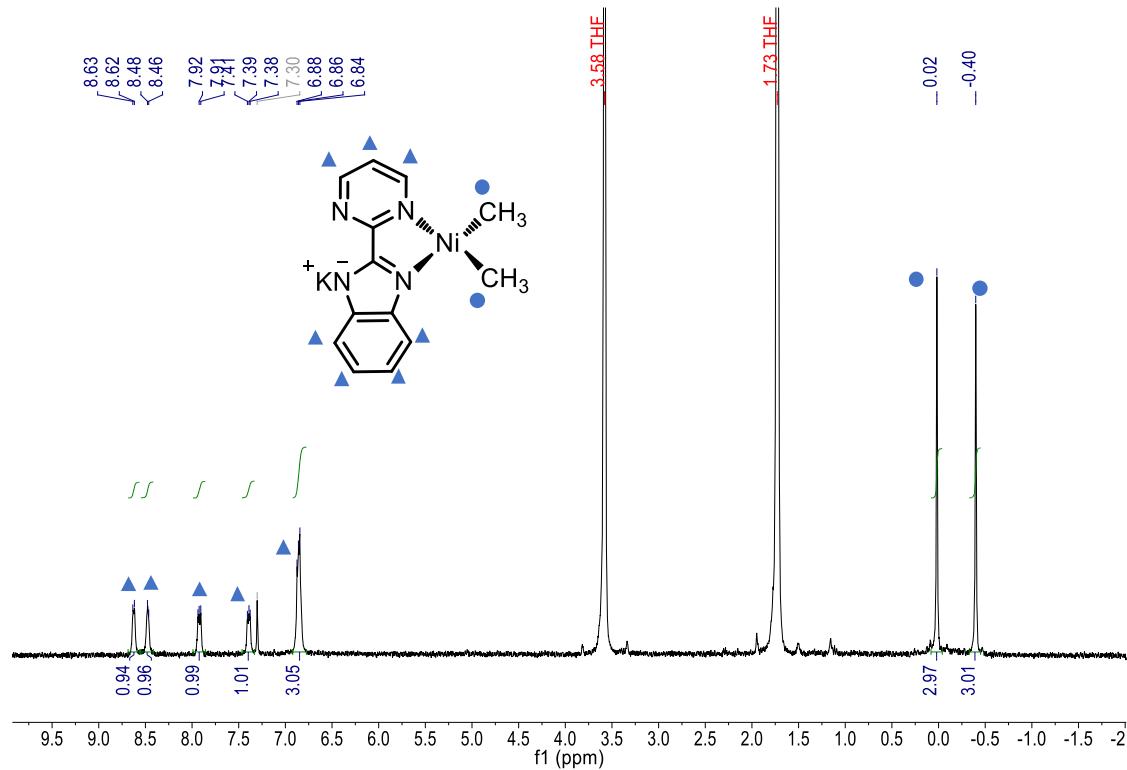


Figure S1. ^1H NMR (300 MHz, $\text{THF}-\text{d}^8$, 20°C) spectrum of $\text{K}(\text{bimpm})\text{Ni}(\text{CH}_3)_2$ (**1**). Benzene impurity is indicated in grey.

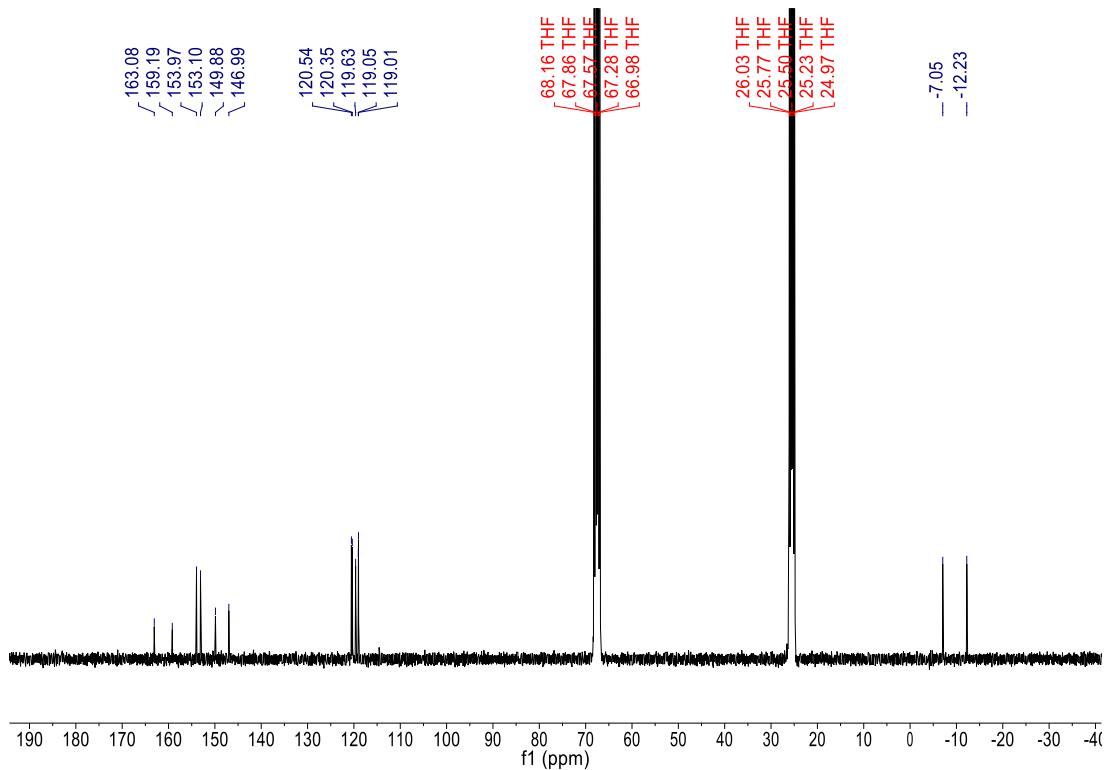


Figure S2. ^{13}C NMR (75 MHz, THF- d^8 , 20°C) spectrum of $\text{K}(\text{bimpm})\text{Ni}(\text{CH}_3)_2$ (**1**).

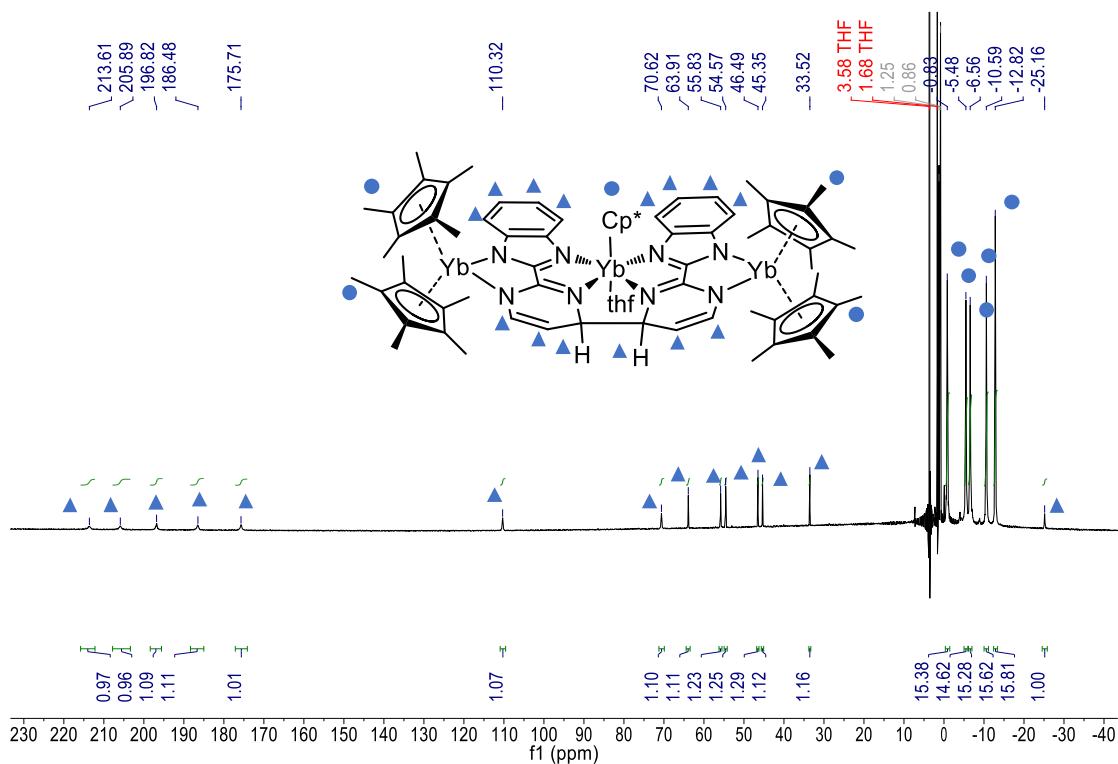


Figure S3. ^1H NMR (300 MHz, THF- d^8 , 20°C) spectrum of $\text{Cp}^*\text{Yb}(\text{thf})[\text{Cp}^*{}_{\text{2}}\text{Yb}(\text{bimpm})]_2$ (**2**). *n*-Pentane impurities are indicated in grey.

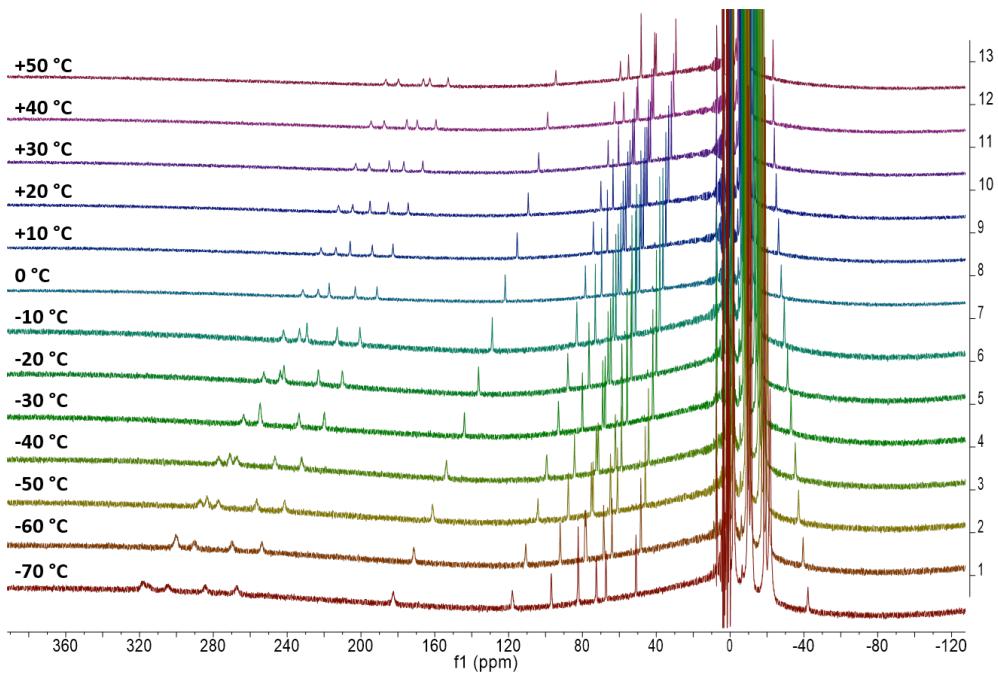


Figure S4. Variable temperature ^1H NMR (300 MHz, THF-d⁸) spectra of Cp*Yb(thf)[Cp*₂Yb(bimpm)]₂ (**2**) from -70°C to 50°C: δ vs T.

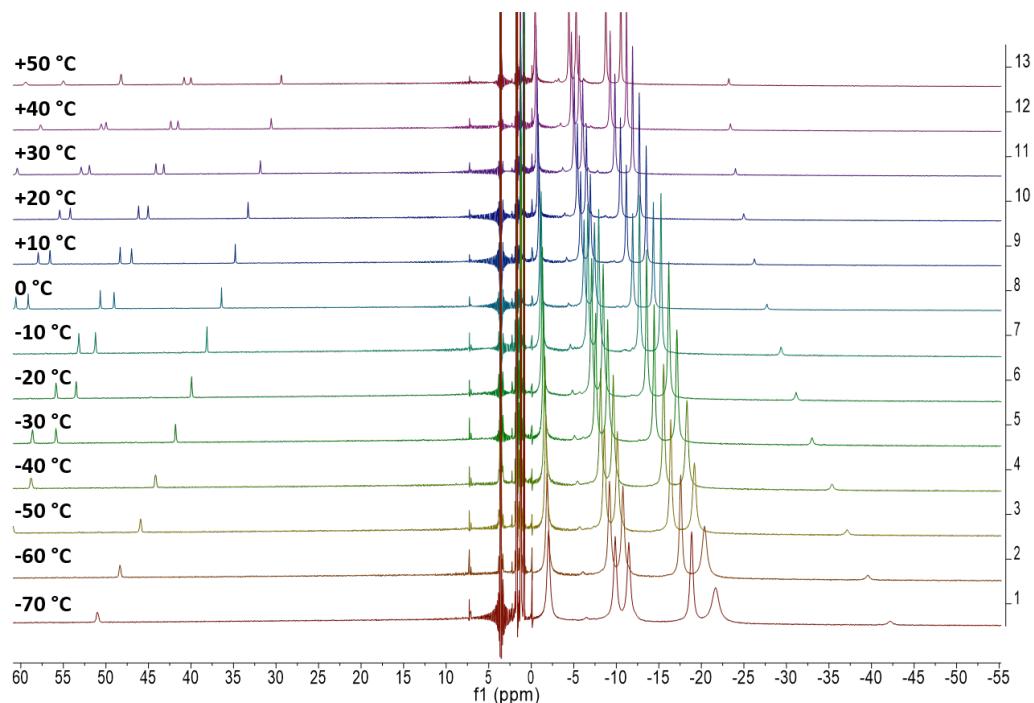


Figure S5. Variable temperature ^1H NMR (300 MHz, THF-d⁸) spectra of Cp*Yb(thf)[Cp*₂Yb(bimpm)]₂ (**2**) from -70°C to 50°C: δ vs T zoom.

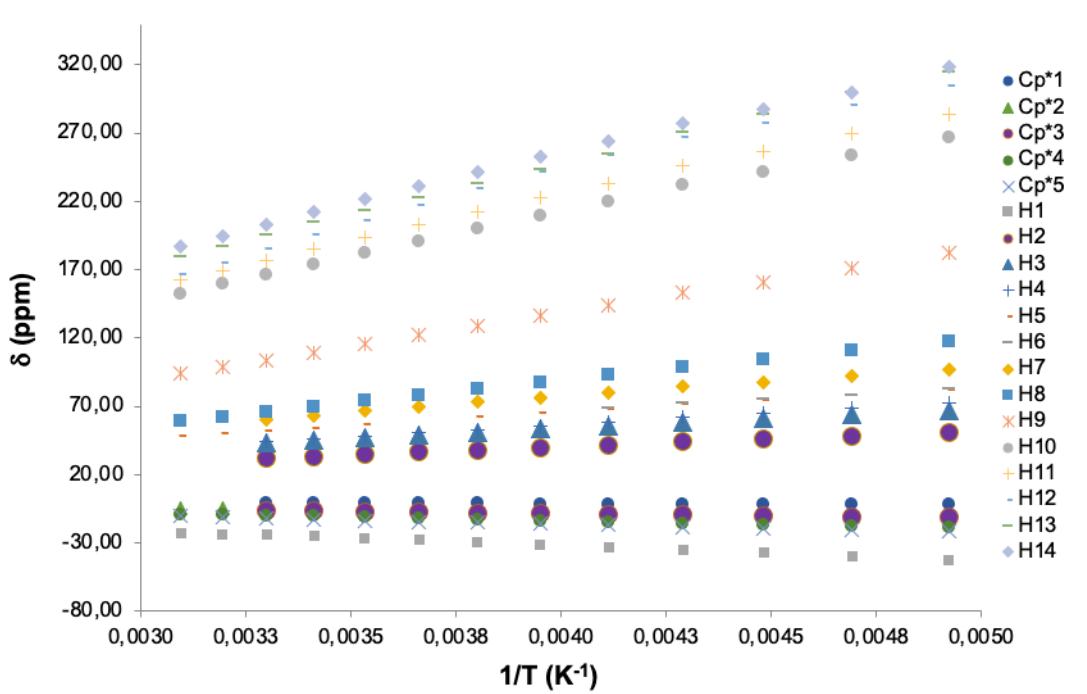


Figure S6. Variable temperature ^1H NMR of $\text{Cp}^*\text{Yb}(\text{thf})[\text{Cp}^*_2\text{Yb}(\text{bimpm})]_2$ (**2**) in THF-d^8 from -70°C to 50°C : δ vs $1/\text{T}$.

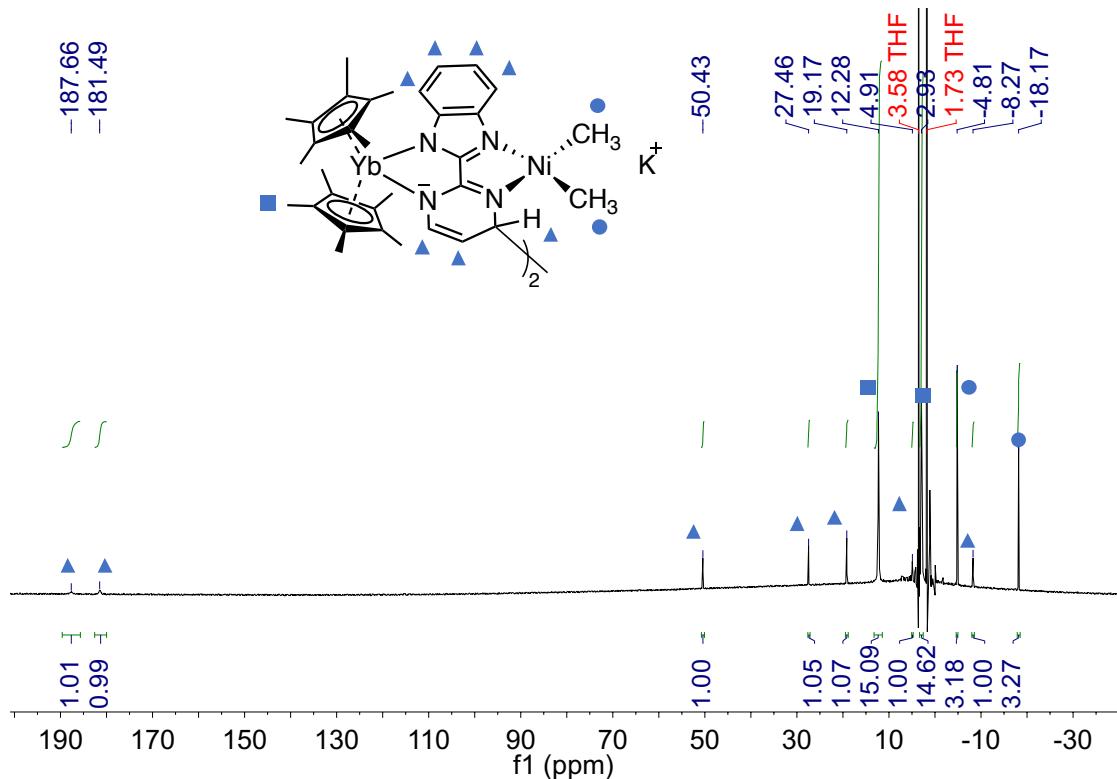


Figure S7. ^1H NMR (300 MHz, THF-d^8 , 20°C) spectrum of $[\text{KCp}^*_2\text{Yb}(\text{bimpm})\text{NiMe}_2]_2$ (**3**).

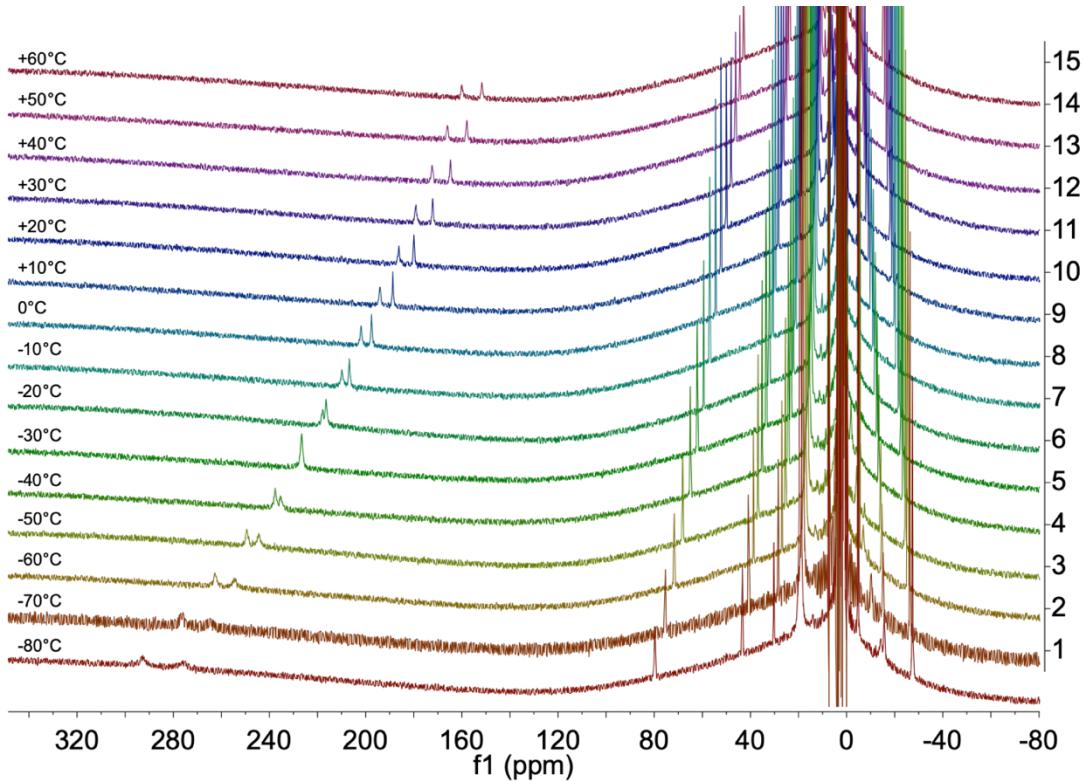


Figure S8. Variable temperature ^1H NMR (300 MHz, THF- d^8) spectrum of $[\text{KCp}^*_2\text{Yb}(\text{bimpm})\text{NiMe}_2]_2$ (**3**) from -80°C to 60°C : δ vs T .

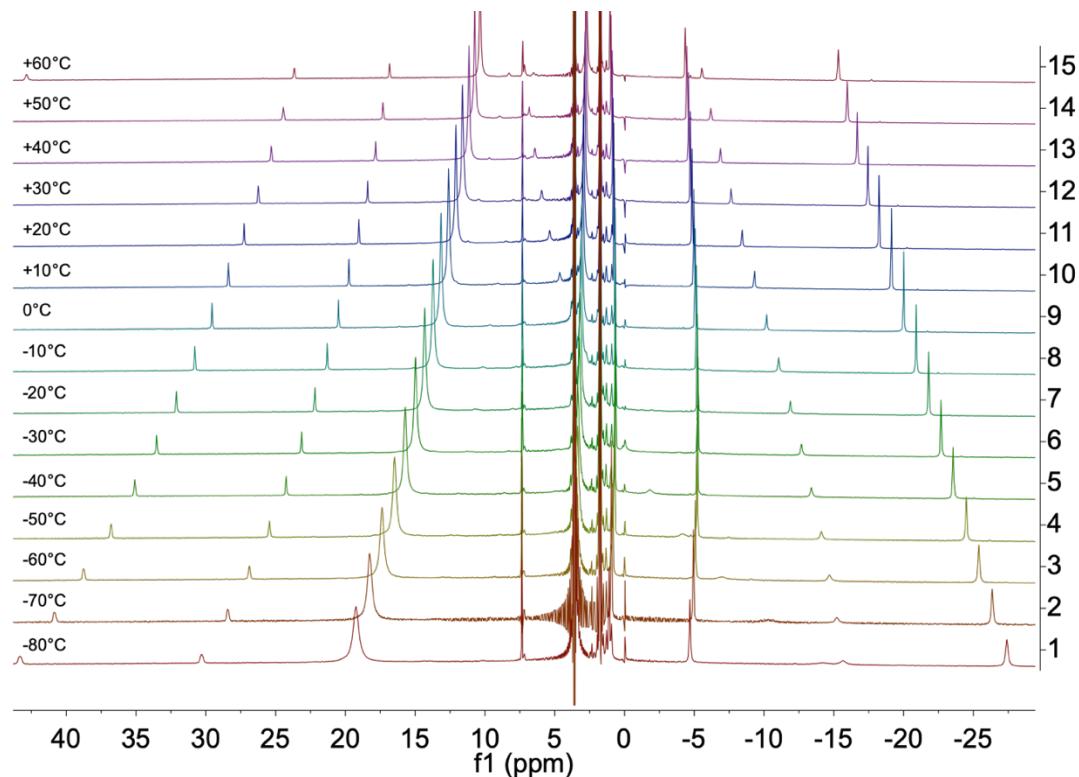


Figure S9. Variable temperature ^1H NMR (300 MHz, THF- d^8) spectrum of $[\text{KCp}^*_2\text{Yb}(\text{bimpm})\text{NiMe}_2]_2$ (**3**) from -80°C to 60°C : δ vs T zoom.

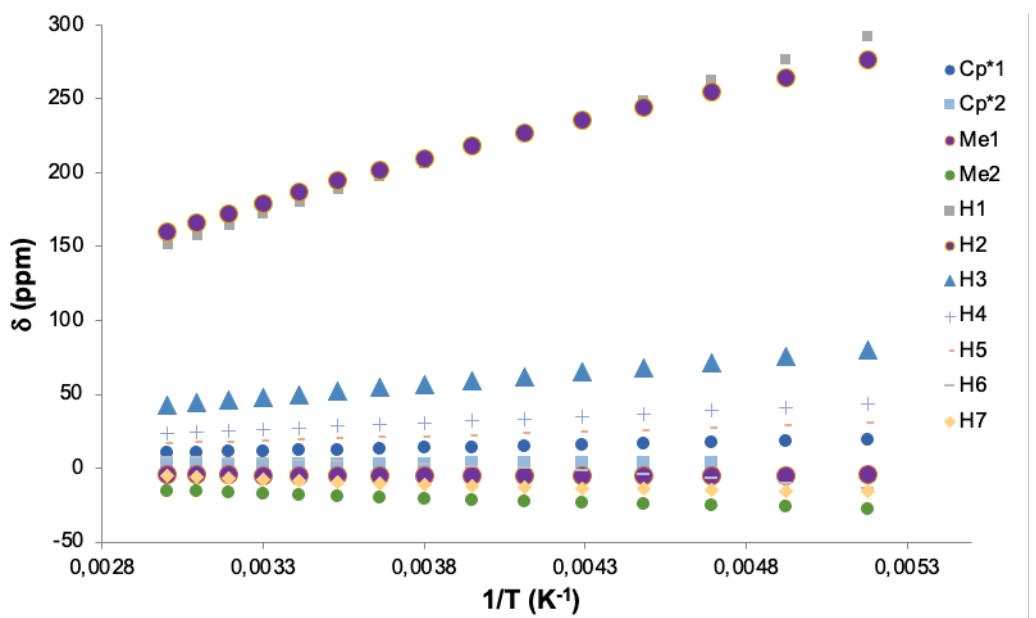


Figure S10. Variable temperature ^1H NMR of $[\text{KCp}^*_2\text{Yb(bimpm)}\text{NiMe}_2]_2$ (**3**) in THF-d^8 from -80°C to 60°C : δ vs $1/T$.

Note: Some protons signals are overlapped in the temperature range with the THF-d^8 signals.

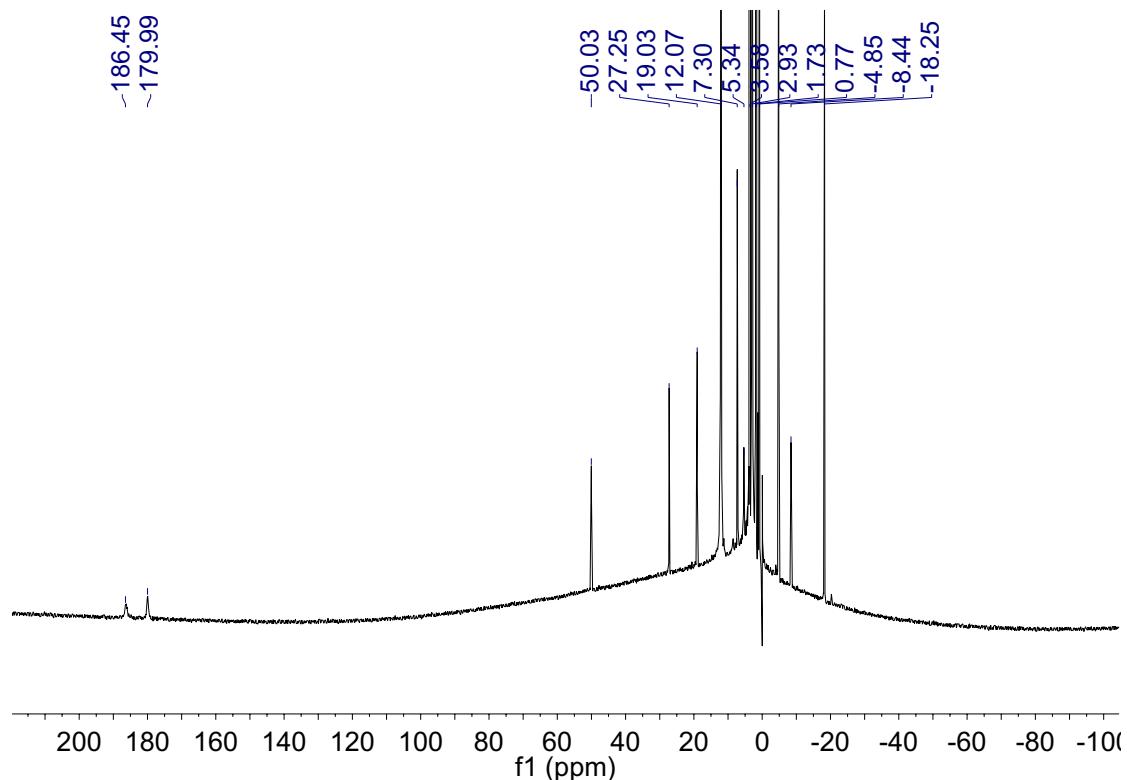


Figure S11. ^1H NMR (300 MHz, THF-d^8 , 20°C) spectrum of **3** for hours: slow ethane formation.

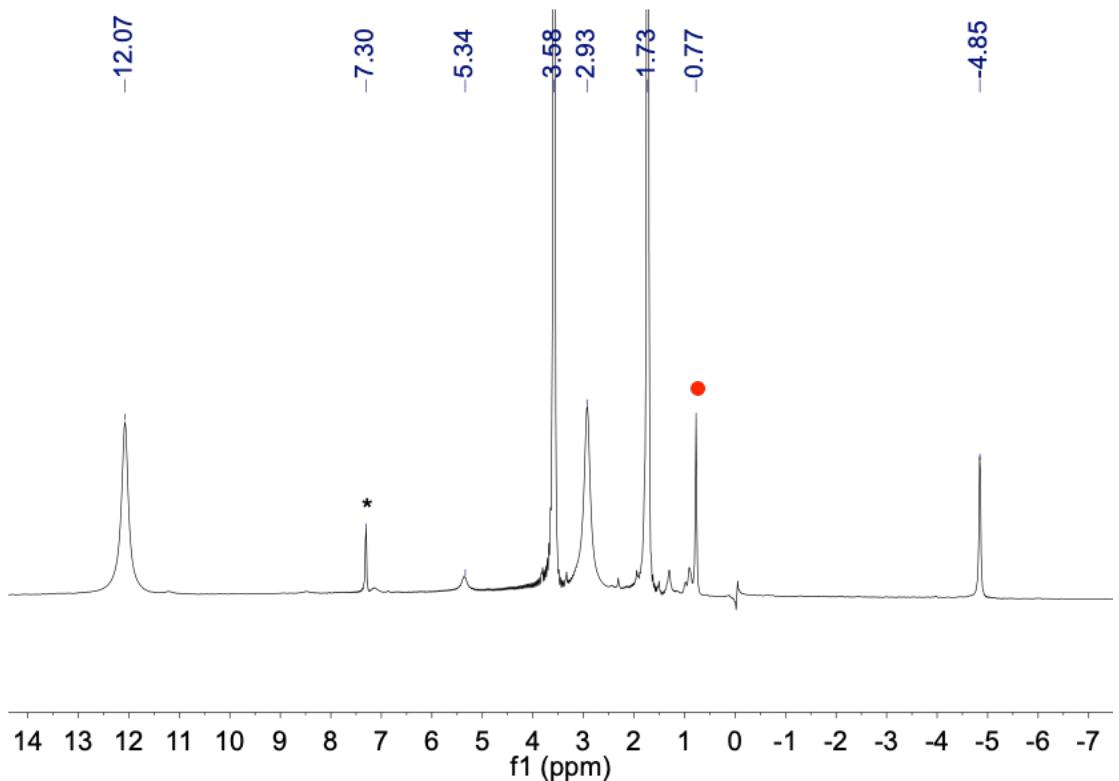


Figure S12. ^1H NMR (300 MHz, THF- d^8 , 20°C) spectrum of **3** for hours: slow ethane formation. The signal of ethane is indicated by a red dot. Benzene impurity from THF- d^8 is indicated by an asterisk.

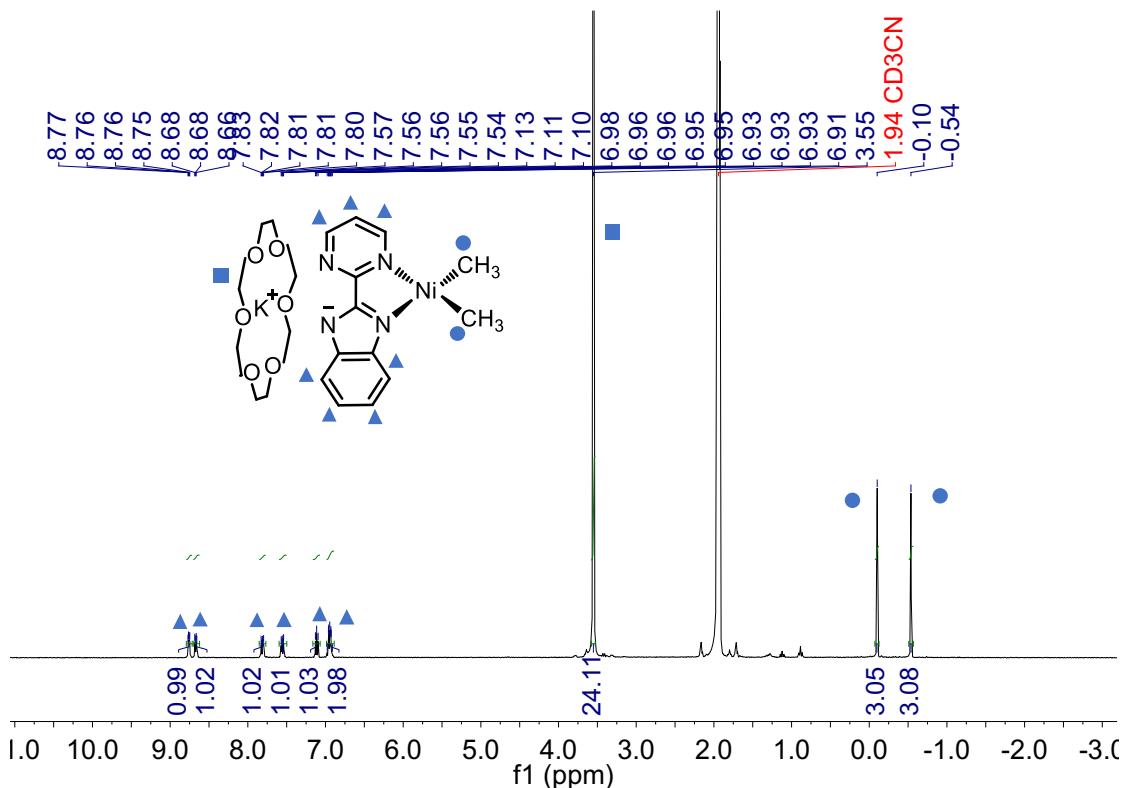


Figure S13. ^1H NMR (300 MHz, CD_3CN , 20°C) spectrum of $\text{K}(18\text{-c-}6)(\text{bimpm})\text{Ni}(\text{CH}_3)_2$ (**4**).

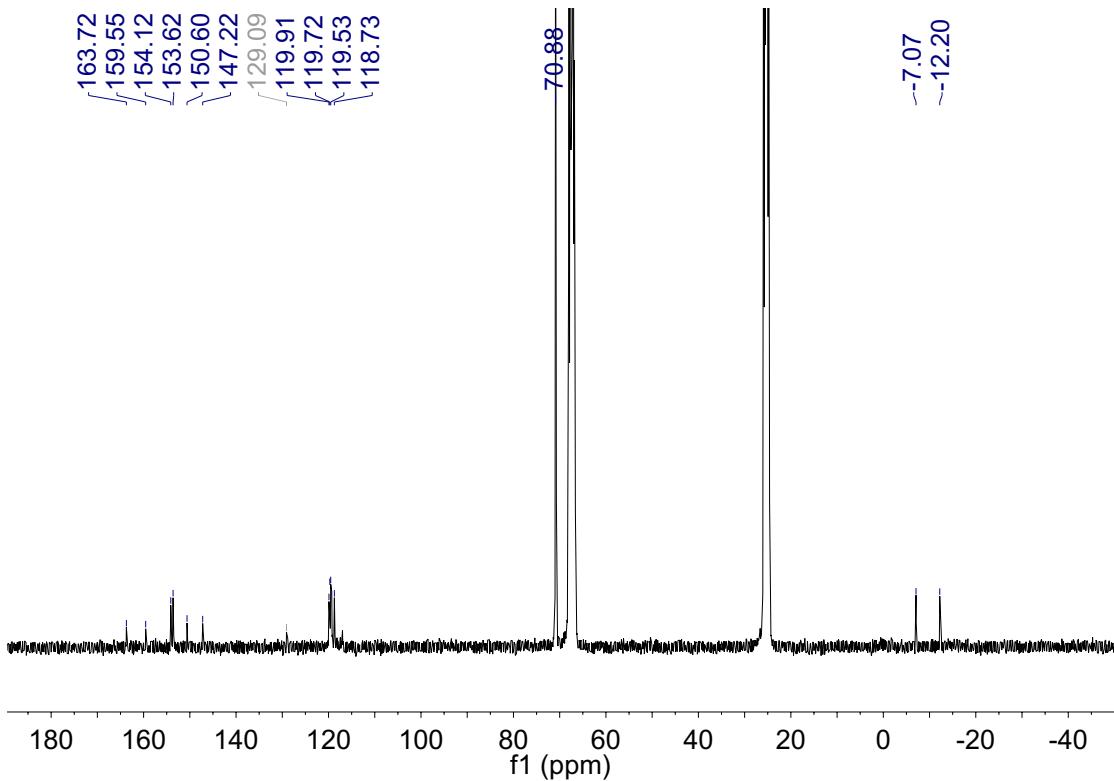


Figure S14. ^{13}C NMR (75 MHz, THF-d⁸, 20°C) spectrum of K(18-c-6)(bimpm)Ni(CH₃)₂ (**4**). Benzene impurity is indicated in grey.

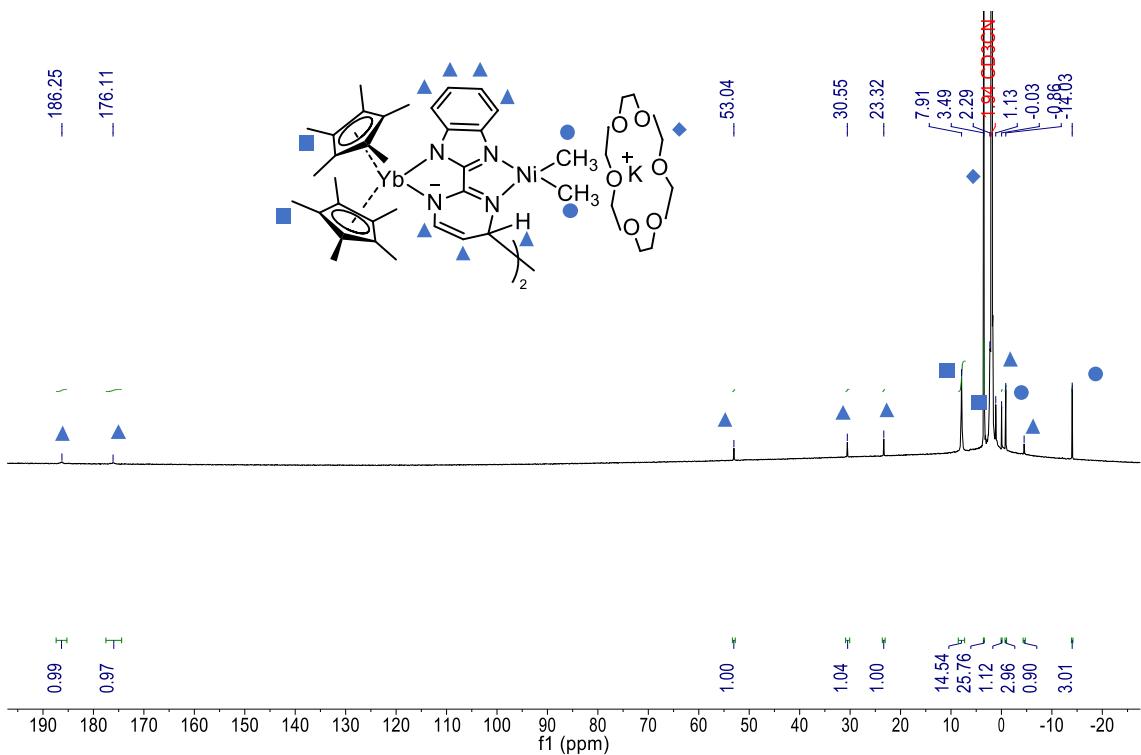


Figure S15. ^1H NMR (300 MHz, CD₃CN, 20°C) spectrum of [K(18-c-6)Cp*₂Yb(bimpm)NiMe₂]₂ (**5**).

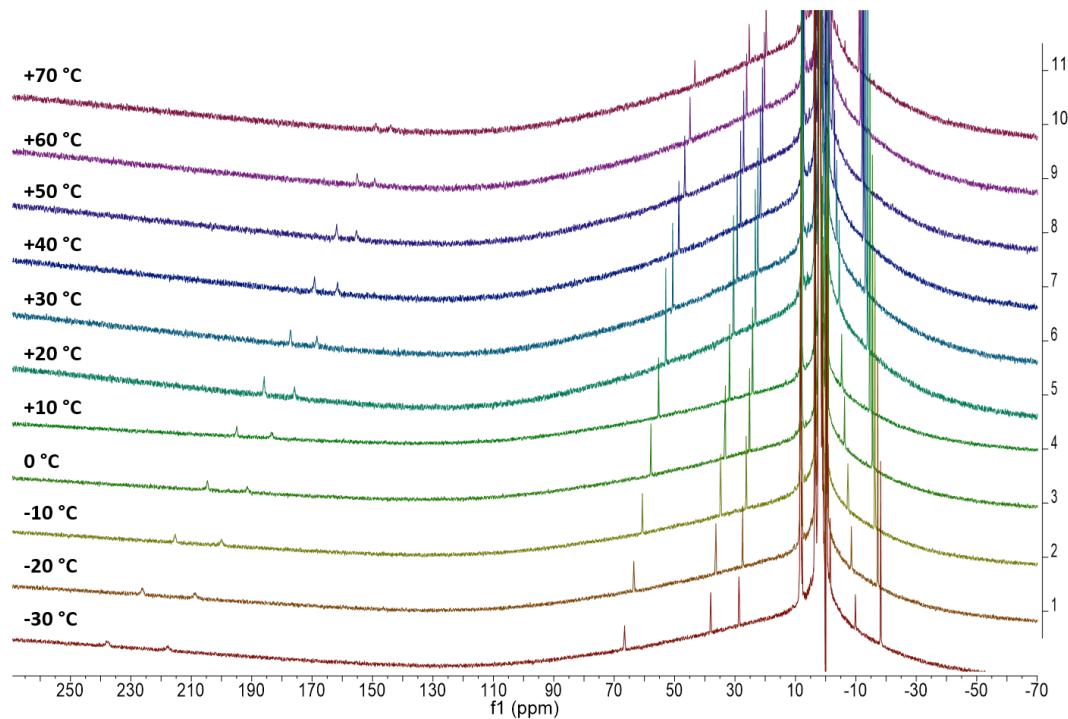


Figure S16. Variable temperature ^1H NMR (300 MHz, CD_3CN) spectra of $[\text{K}(18\text{-c-}6)\text{Cp}^*_2\text{Yb(bimpm)}\text{NiMe}_2]_2$ (**5**) in the range of -30°C and 70°C: δ vs T.

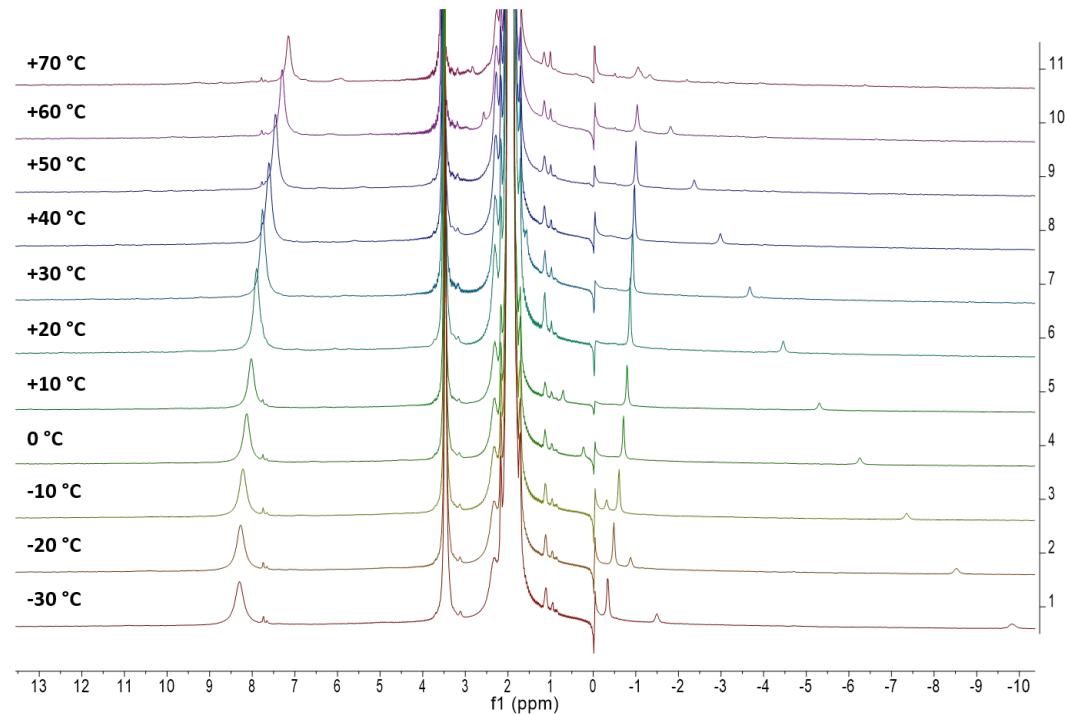


Figure S17. Variable temperature ^1H NMR (300 MHz, CD_3CN) spectrum of $[\text{K}(18\text{-c-}6)\text{Cp}^*_2\text{Yb(bimpm)}\text{NiMe}_2]_2$ (**5**) in the range of -30°C to 70°C: δ vs T zoom.

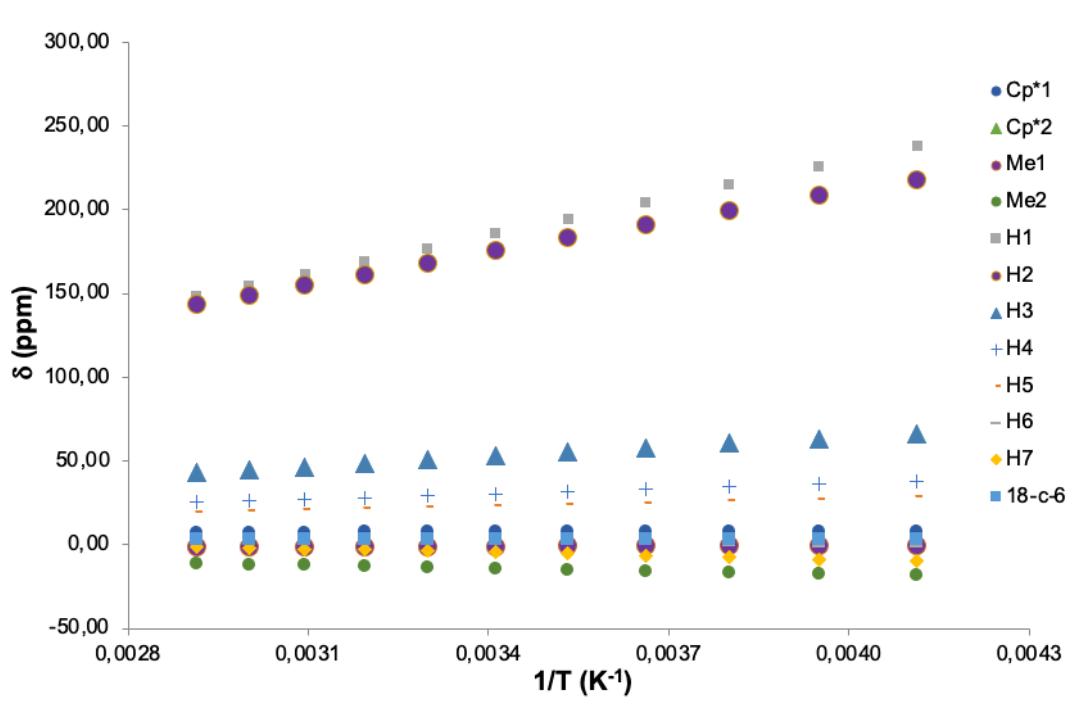


Figure S18. Variable temperature ^1H NMR of $[\text{K}(18\text{-}c\text{-}6)\text{Cp}^*\text{Yb(bimpm)}\text{NiMe}_2]_2$ (**5**) in CD_3CN from -30°C to 70°C : δ vs $1/T$.

Note: Most of resonances of one Cp^ protons as well as one proton on the bimpm ligand are overlapped in the temperature range with the CD_3CN signal.*

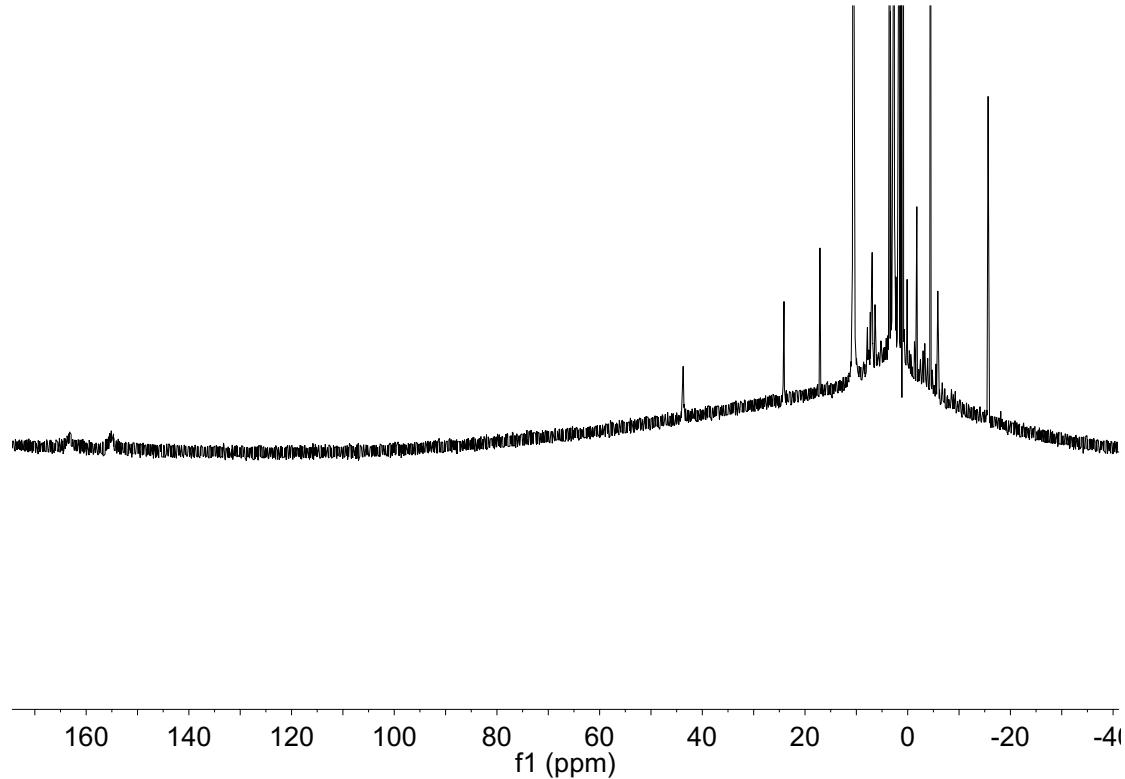


Figure S19. ^1H NMR (300 MHz, THF-d^8 , 60°C) spectrum of **3**.

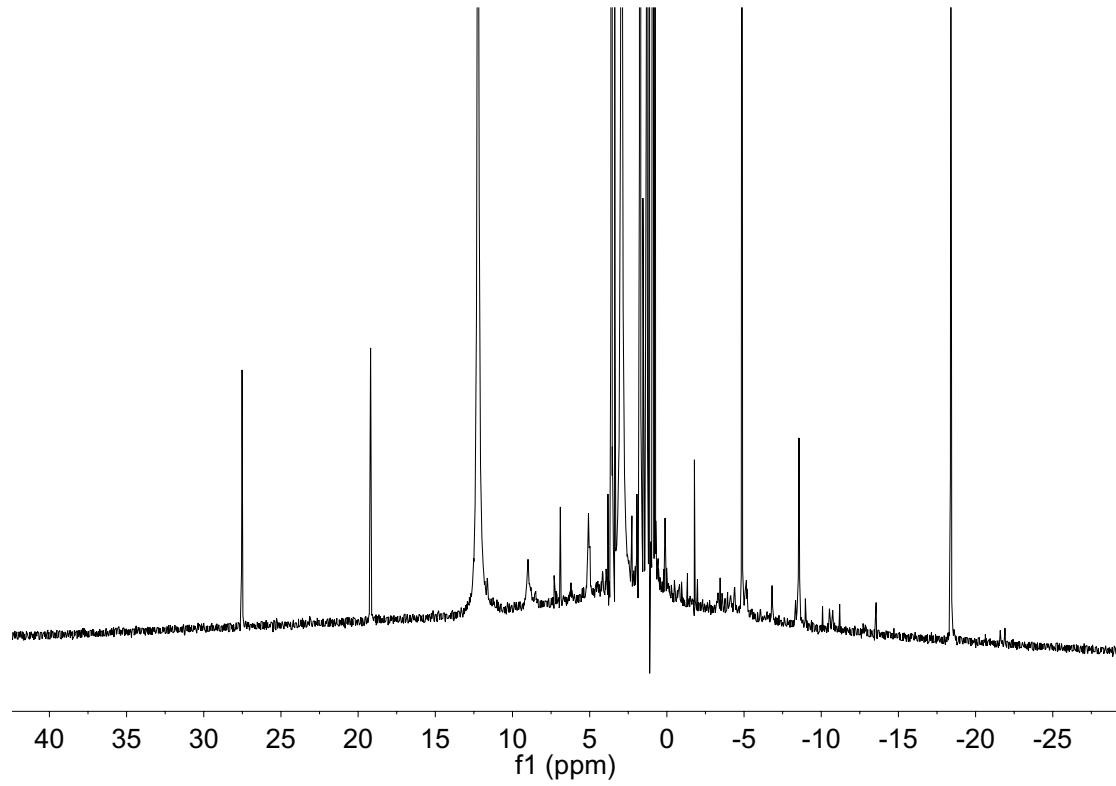


Figure S20. Zoomed ^1H NMR (300 MHz, THF- d^8 , 60°C) spectrum of **3**.

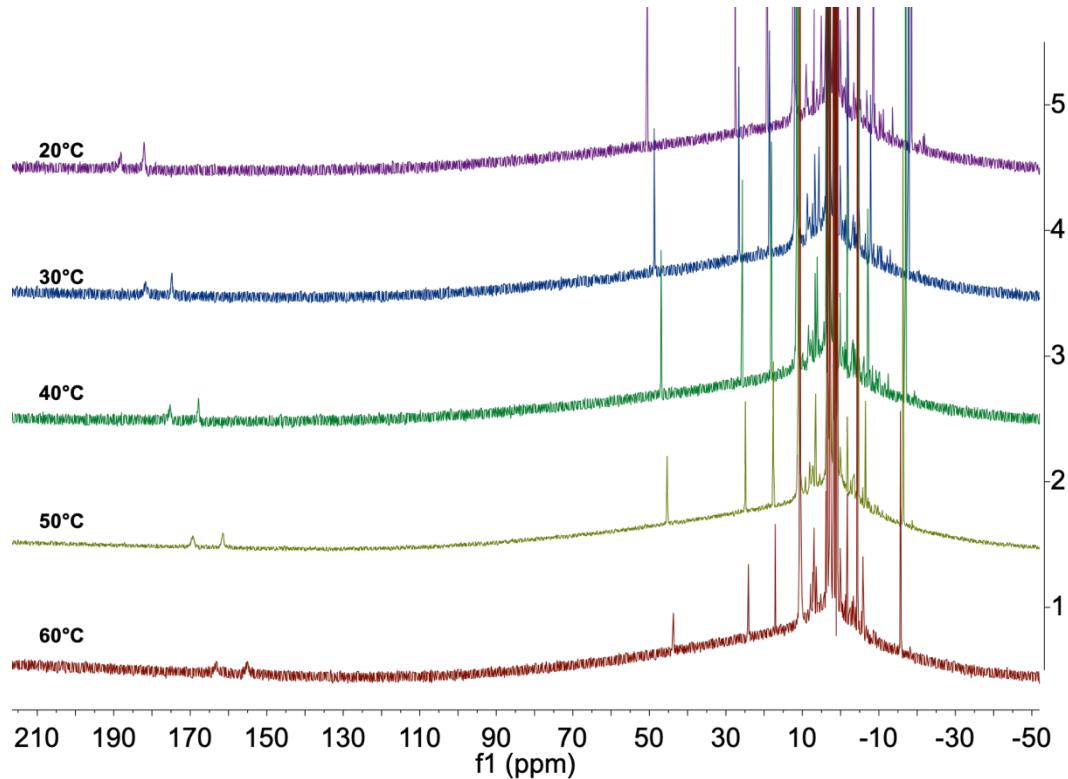


Figure S21. Variable temperature ^1H NMR (300 MHz, THF- d^8) spectra of **3** from 60°C to 20°C: δ vs T.

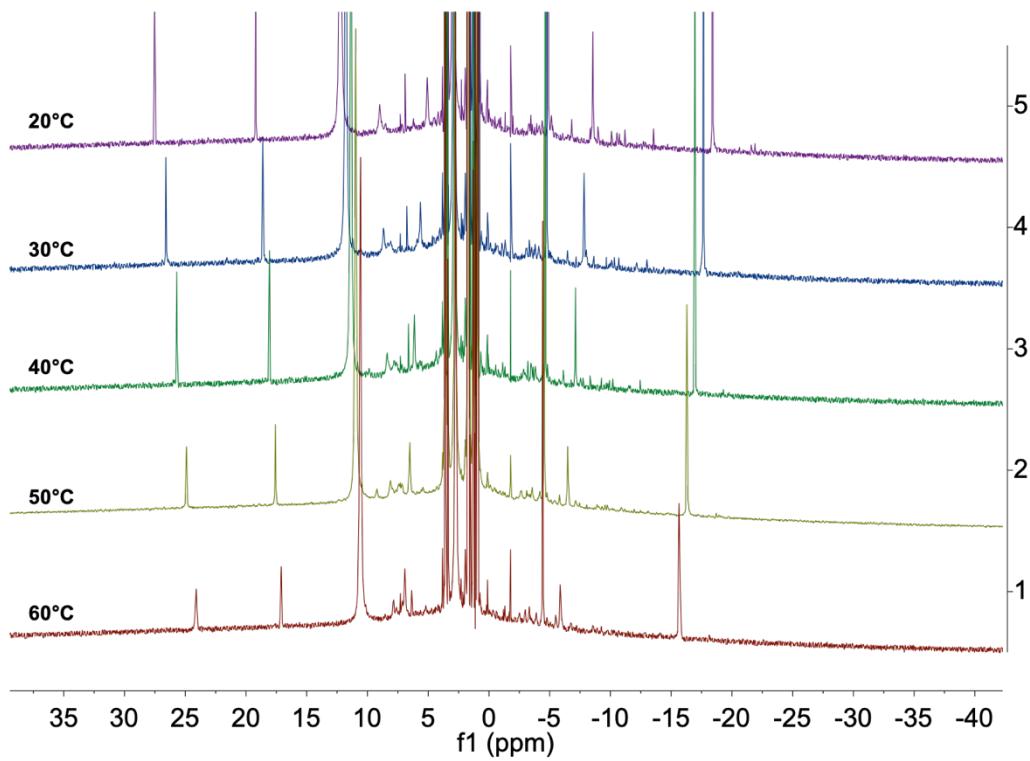


Figure S22. Variable temperature ^1H NMR (300 MHz, THF-d⁸) spectra of **3** from 60°C to 20°C: δ vs T. Zoom.

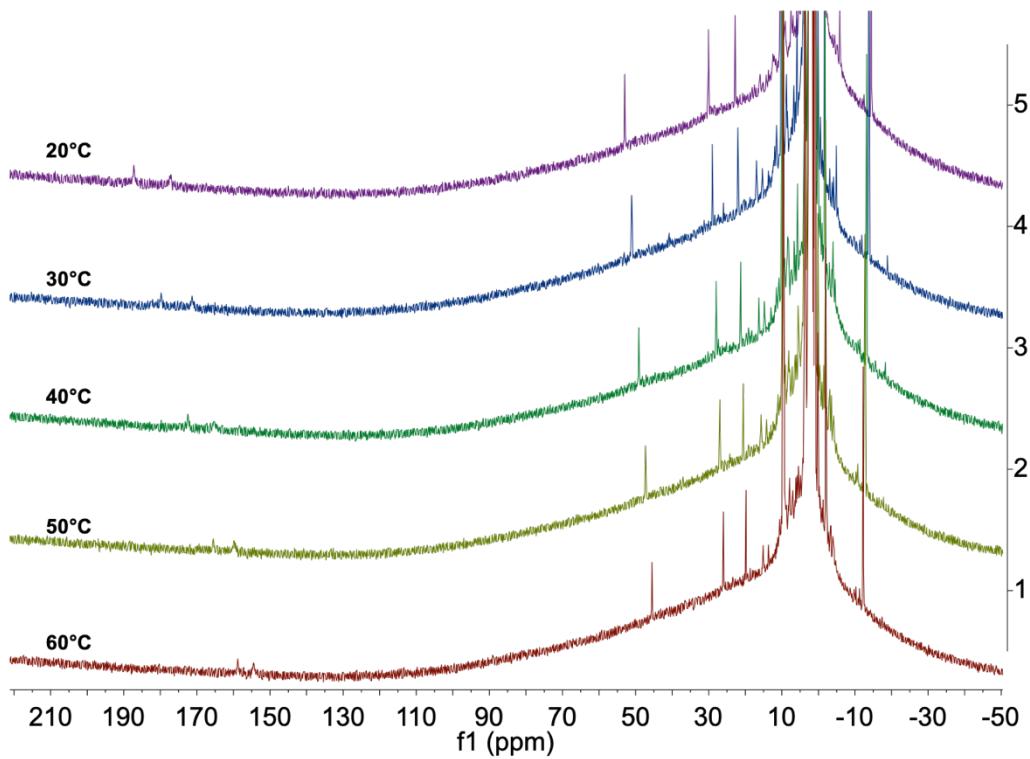


Figure S23. Variable temperature ^1H NMR (300 MHz, THF-d⁸) spectra of **5** from 60°C to 20°C: δ vs T.

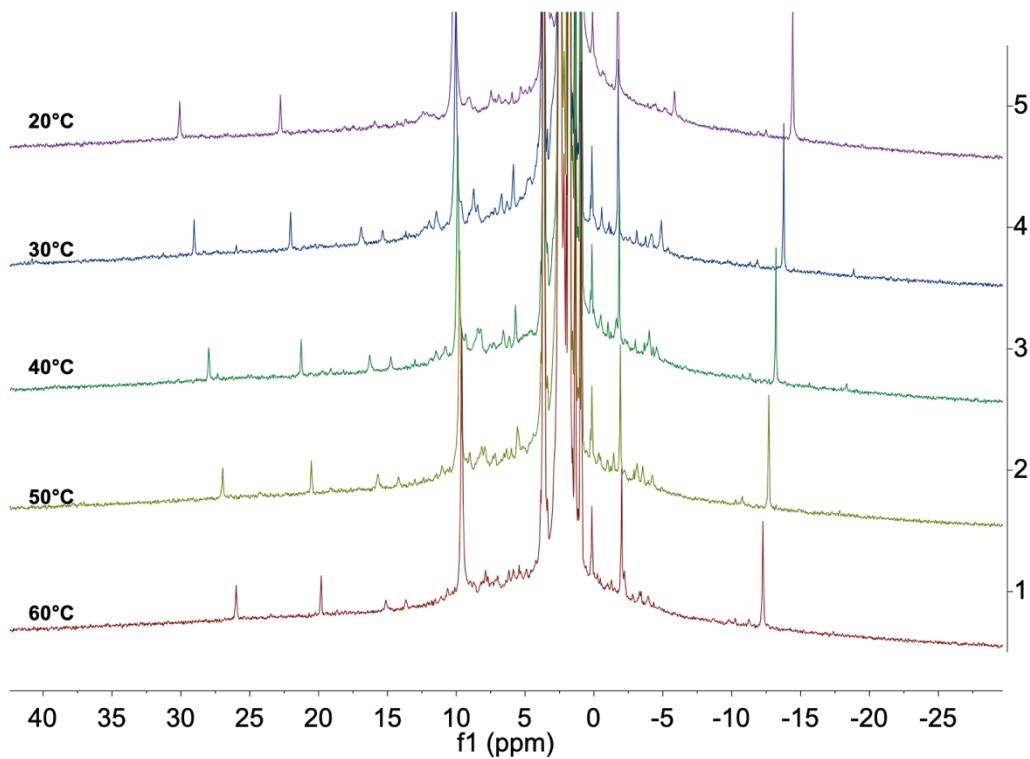


Figure S24. Variable temperature ^1H NMR (300 MHz, THF- d^8) spectrum of **5** from 60°C to 20°C: δ vs T. Zoom.

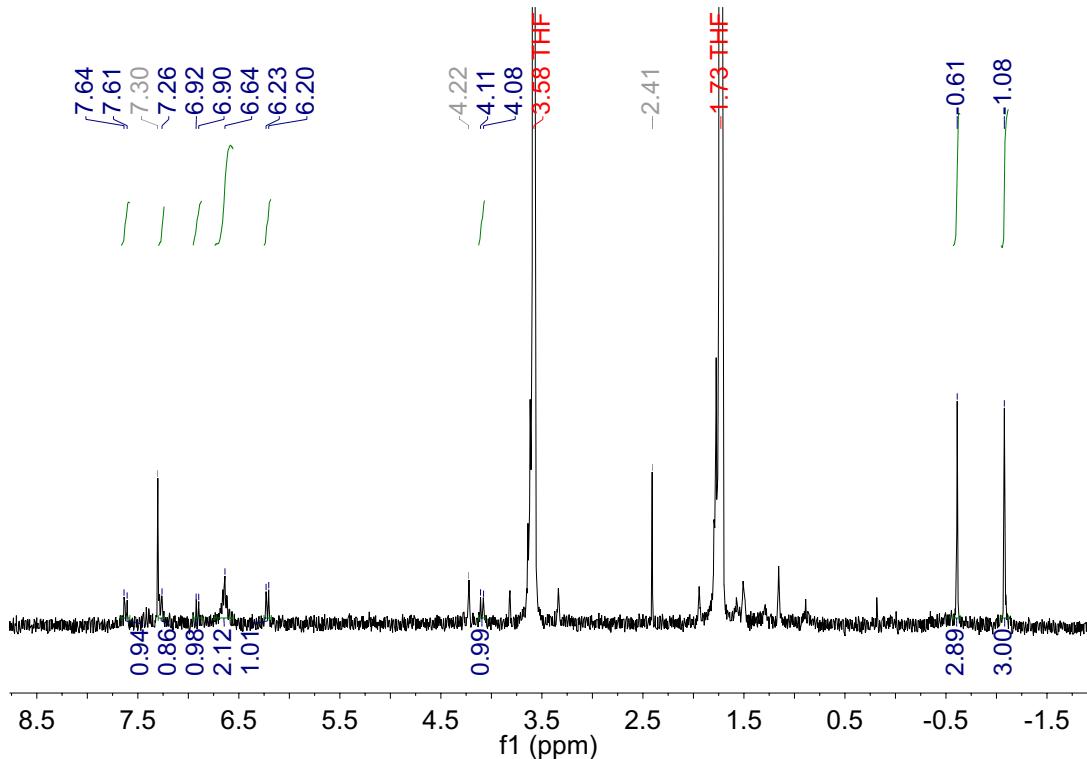


Figure S25. ^1H NMR (300 MHz, THF- d^8 , 20°C) spectrum of $[\text{K}_2(\text{bimpm})\text{NiMe}_2]_2$ (**6**). Residue impurity, which is hardly removed from crystallization, as well as benzene solvate from deuterated solvent are indicated in grey.

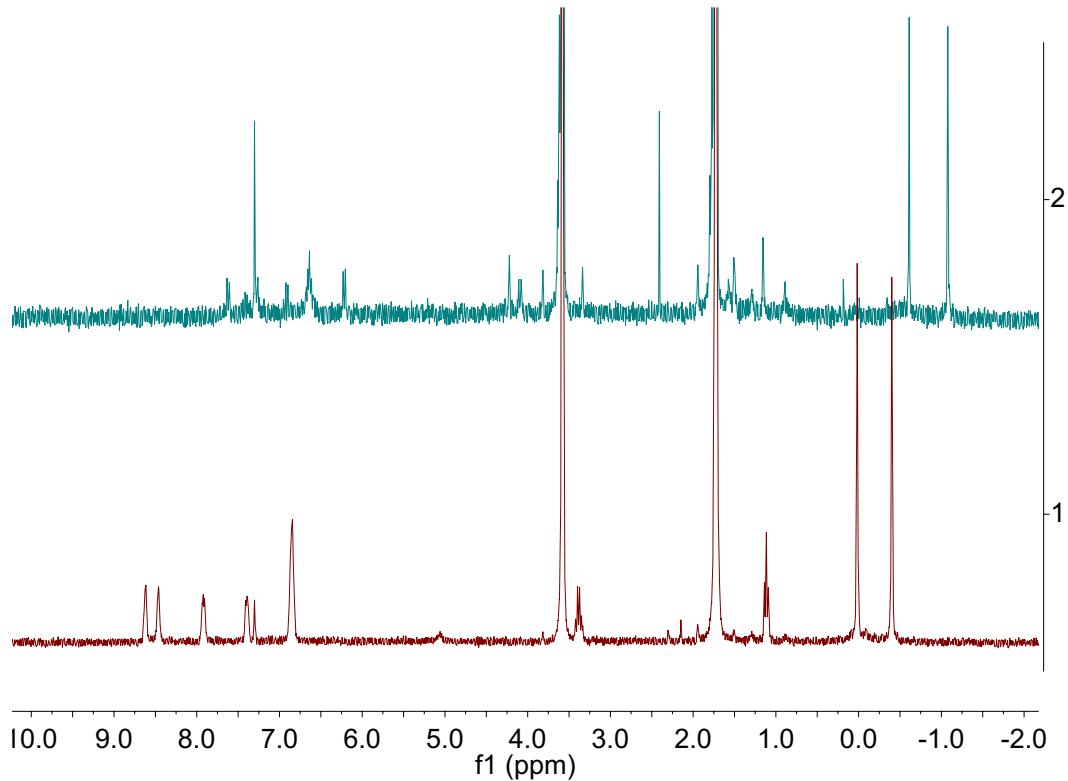


Figure S26. ^1H NMR (300 MHz, THF-d⁸, 20°C) comparison between **6** (top, in green) and **1** (bottom, in red).

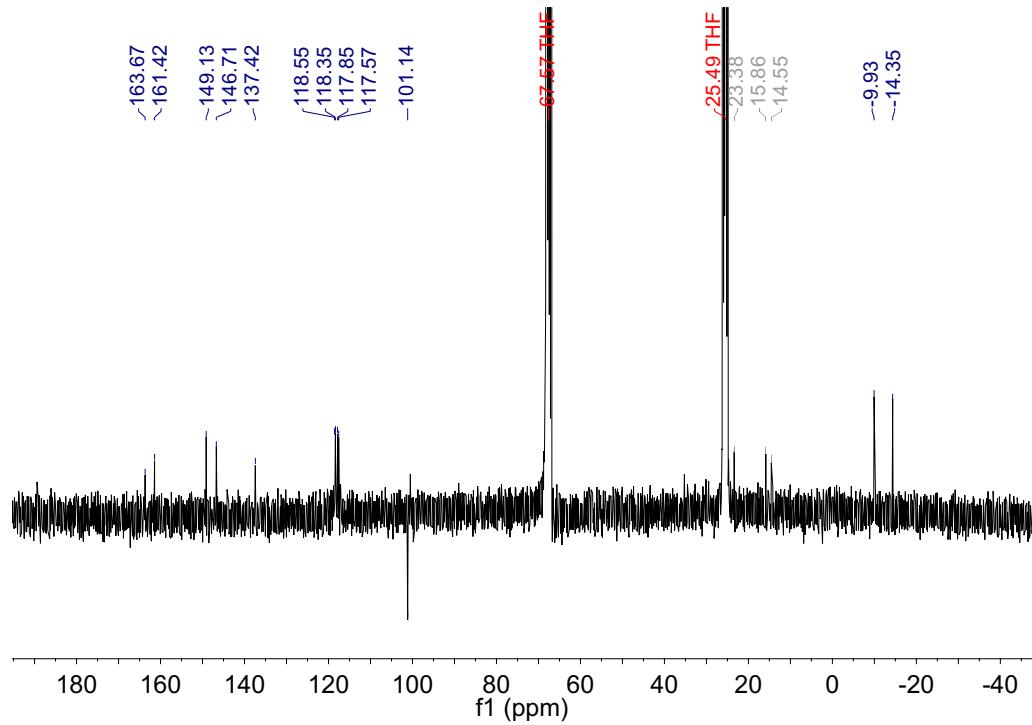


Figure S27. ^{13}C NMR (75 MHz, THF-d⁸, 20°C) spectrum of $[\text{K}_2(\text{bimpm})\text{NiMe}_2]_2$ (**6**). Resonances of *n*-pentane and diethyl ether impurities are indicated in grey.

2. Magnetism

Magnetic properties of **2**, **3** and **5** were measured on crushed crystals in sealed quartz tubes.

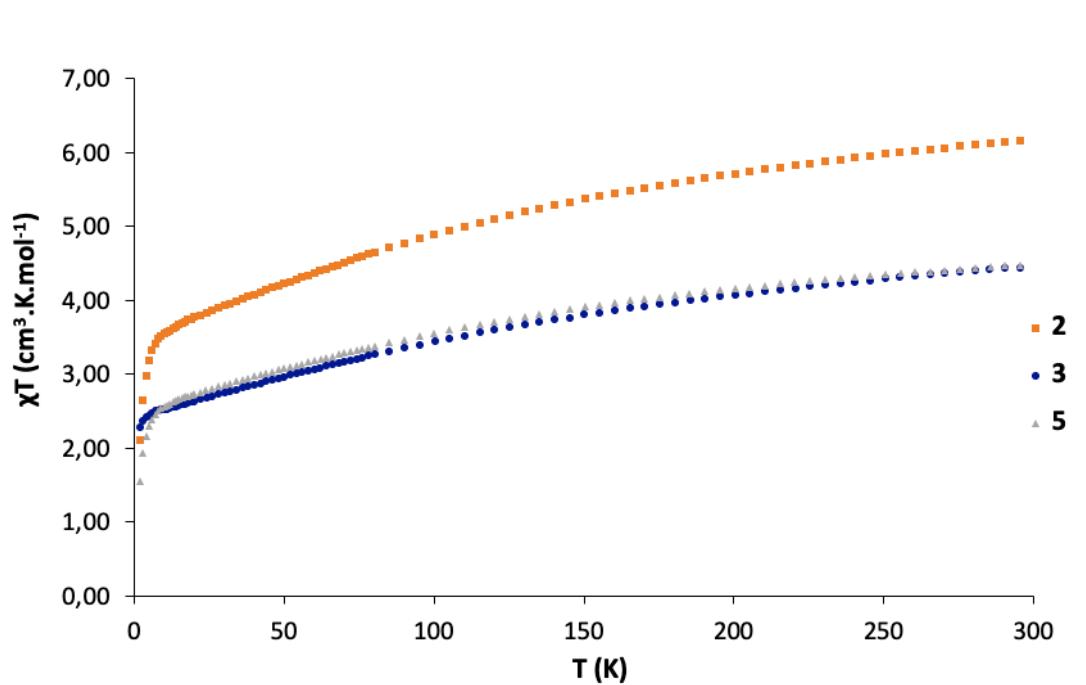


Figure S28. Solid-state temperature-dependent magnetic data for **2** (squares), **3** (circles) and **5** (triangles) at 2 T: plot of χT versus T.

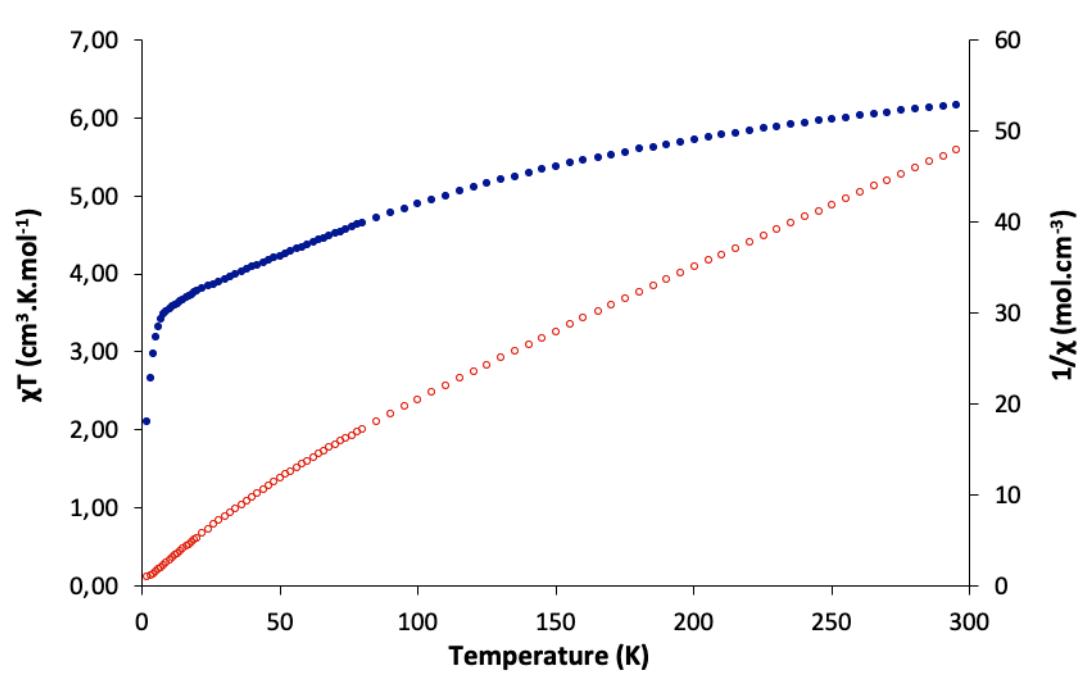


Figure S29. Temperature-dependent magnetic data for **2** at 2 T. $1/\chi$ vs T is given as unfilled red dots, and χT vs. T as filled blue dots.

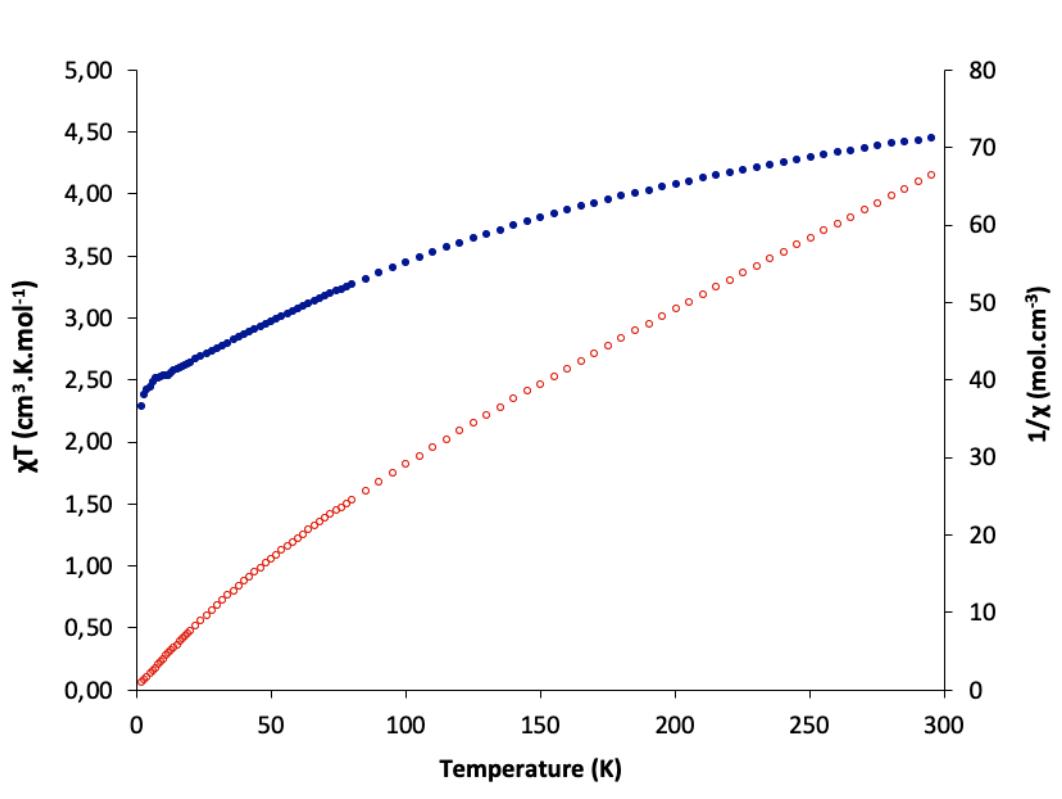


Figure S30. Temperature-dependent magnetic data for **3** at 2 T. $1/\chi$ vs T is given as unfilled red dots, and χT vs. T as filled blue dots.

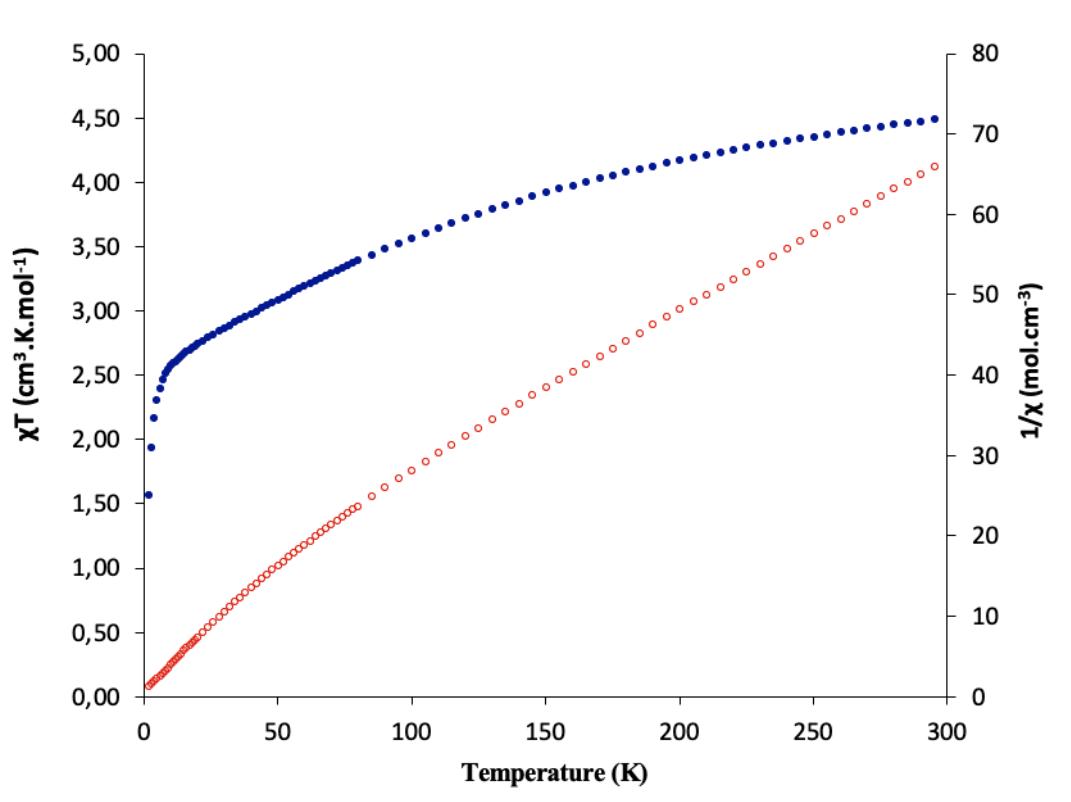


Figure S31. Temperature-dependent magnetic data for **5** at 2 T. $1/\chi$ vs T is given as unfilled red dots, and χT vs. T as filled blue dots.

3. DFT calculation data

Table S1. Main average distances (\AA) and angles ($^\circ$) in the compounds $[\text{bimpm}]^-$, $[(\text{bimpm})\text{NiMe}_2]^-$ and $[\text{Cp}^*_2\text{Yb}(\text{bimpm})\text{NiMe}_2]^-$. Geometries were optimized with the PBE functional.

	$[\text{bimpm}]^-$	$[(\text{bimpm})\text{NiMe}_2]^-$	$[\text{Cp}^*_2\text{Yb}(\text{bimpm})\text{NiMe}_2]^-$
Ni-CH ₃	-	1.921	1.922
Ni-N	-	1.959	1,9725
Yb-N	-	-	2,39855
Yb-Cp* _{centr}	-	-	2.379
Bridging C-C _{bimpm}	1.46119	1.443	1.45(6)
Coupled C-C _{bimpm}	-	-	1.40139
bimpm [^] NiMe ₂	-	1.56	13.55

Table S2. Cartesian coordinates for the PBE optimized geometry for compound [bimpm]⁻.

N	10.96939429243430	5.56793491400100	8.32405298785742
N	9.10821178716916	7.59068238655870	8.92344824145940
N	9.12262317600363	8.30171024547728	6.69773453292266
N	10.96971838079360	6.29286313861084	6.02821040104677
C	11.85977850903180	5.34415616264287	5.75402181630087
H	12.19141900602610	5.28182791582472	4.70859015662691
C	12.36574418052770	4.46224082440688	6.71257247458056
H	13.10037667788650	3.69235299054774	6.46929205933975
C	11.86050112917730	4.63417621927497	8.00396943081854
H	12.19210804314950	3.98286470361457	8.82402266831438
C	10.54666927944640	6.38668323416213	7.32020110590324
C	9.58286705308764	7.43424232633364	7.65001927210445
C	8.26677362468822	8.65060610200981	8.79018263661858
C	7.46294972346363	9.31122181108609	9.74172660447988
H	7.45366013842814	8.97987397178864	10.78387879934960
C	6.69156747282486	10.38860770021320	9.32009696906957
H	6.06186904308575	10.91854340975720	10.04039035515020
C	6.70266557521504	10.82243616797390	7.96836269775326
H	6.08364731254276	11.67754091920770	7.68208304215277
C	7.48357548695074	10.18665211303540	7.00952980891279
H	7.49169368984768	10.52354490587110	5.96920900635484
C	8.27608641821909	9.09170783760120	7.41083493288330

Table S3. Cartesian coordinates for the PBE optimized geometry for compound [(bimpm)NiMe₂]⁻.

Ni	-10.85795270488540	-2.45740262521130	-6.57935426882062
----	--------------------	-------------------	-------------------

N	-12.16690938027450	-2.47617400645348	-8.02848767309177
N	-9.63104288187552	-0.98924629496297	-10.19297569602920
N	-9.72190513164585	-1.67784842361876	-7.97877934398171
N	-12.46603543931090	-1.87008588432823	-10.35303098582760
C	-10.35483787957940	-1.52205420376669	-9.19096651394813
C	-11.72804155261930	-1.96256742857989	-9.23842460493234
C	-8.41833447966368	-0.77438005535526	-9.59887705420482
C	-13.43898642383910	-2.91715654354570	-8.00446671102704
H	-13.78280493081610	-3.32493148992910	-7.05348346371986
C	-8.45849025645250	-1.19818253643805	-8.21929767910621
C	-7.23911396604844	-0.23336095848478	-10.14545110920170
H	-7.21816133290692	0.08499896421989	-11.19005705938840
C	-14.26708679409540	-2.85864896297681	-9.12068589740189
H	-15.29345282976310	-3.22425455654789	-9.07469775017968
C	-6.16597411403526	-0.53635024547288	-7.97167460508340
H	-5.26872830288447	-0.43039336329760	-7.35641269722556
C	-6.12418176307088	-0.11943702116715	-9.32462379430804
H	-5.19653391075010	0.29838548510648	-9.72395705729421
C	-13.72617664086060	-2.31585067378255	-10.28796512632440
H	-14.31955675621730	-2.23306177029168	-11.20537559305620
C	-7.31676040488315	-1.07487759059319	-7.40524923123936
H	-7.33371636792981	-1.39219404724718	-6.36440803125959
C	-9.51730015881202	-2.37213474562474	-5.20749482385873
H	-8.66106683383841	-2.97420385339203	-5.55934331431786
H	-9.80407210279150	-2.72512383352885	-4.20659008874281
H	-9.19618709629966	-1.31902674576451	-5.13163817508685
C	-12.08303369501440	-3.23157898342586	-5.31638360137583

H	-12.96604234310390	-2.56531401659679	-5.24312130412955
H	-11.71021274944740	-3.40299288536415	-4.29655101771715
H	-12.41863377628410	-4.20885870357825	-5.71782272811903

Table S4. Cartesian coordinates for the PBE optimized geometry for compound $[\text{Cp}^*_2\text{Yb(bimpm)}\text{NiMe}_2]^-$.

Yb	2.39641272031517	6.15729270118101	2.17623539274325
Ni	5.86072236274985	8.61550105486300	6.03309031529828
N	4.11237202236377	9.08842011923908	5.19547893787800
N	5.71563672389365	7.01104788159994	4.93506825566606
N	2.48387516240986	8.12681684414460	3.62414364774130
N	4.36326531994733	5.88241491594803	3.43456679111152
C	4.54136719860743	6.98787997471363	4.21991992281914
C	1.71137087533012	9.19017889340959	3.81688174439116
H	0.78103974564572	9.22692173513074	3.24522255993999
C	3.66724710196465	8.07740751881191	4.33272936282232
C	2.05945456175369	10.22916801393730	4.70438084352796
H	1.40953707271138	11.08784260415250	4.85852450720239
C	3.36825109753380	8.03193116469782	0.52328658233750
C	3.29814949401944	10.12239074919770	5.36169038605642
H	3.64889984481953	10.90603609057970	6.03835193750379
C	5.51688322209105	5.14948120084789	3.63260872420609
C	1.07047736769470	5.14865045031667	4.25255626421903
C	7.17602242788496	3.42387181138627	3.42307661635628
H	7.51346149845632	2.48014550129935	2.99013124452023
C	3.54417898589444	5.84844897342900	-0.20267074690117
C	0.92346318428311	3.93028499704512	2.29679588397145
C	2.10415288491797	7.64273885842900	-0.01257621564896
C	2.21787107957549	6.29693508829315	-0.48013760040722
C	5.92335426665246	3.93893290491699	3.06233011328329
H	5.27790037074100	3.41440877006212	2.35424516845242
C	7.41643002350605	8.04898118182051	7.00686229010992

H	7.28328807187182	6.98093079639079	7.24095609771287
H	7.58798213636076	8.60574856580025	7.93916726488627
H	8.30007310946648	8.16863193748175	6.35578534230198
C	4.25757497661698	6.92445313919276	0.40594274555639
C	7.61332011183881	5.32159005453330	4.90662056304681
H	8.26972086883253	5.85120365875788	5.59478429262628
C	8.00360243484257	4.10566803658788	4.32701510300378
H	8.97770514897346	3.68399279593937	4.58333028729923
C	4.12447257781091	4.52639338340720	-0.61116575210817
H	4.95669276573238	4.22742325090820	0.04358016605098
H	4.52400283505917	4.55358276840978	-1.64162604834321
H	3.37372799109757	3.72157661955813	-0.58389318034125
C	2.58697781879088	3.04210121135381	4.09789344096194
H	3.13613014393777	2.52044122501607	3.30107477998948
H	2.09086919354623	2.26433332563434	4.70718061168830
H	3.33941440580214	3.52608849928554	4.73644761728281
C	5.71586213732072	6.94091667203119	0.74893462921725
H	5.91770431324628	7.49339863748183	1.67738645280602
H	6.30750032747332	7.42087000283874	-0.05135857144106
H	6.11550431842012	5.92840455077550	0.89085461674529
C	1.06992272524842	2.79926397732262	1.32196440054742
H	0.66735909715695	3.05438728868776	0.33111655930116
H	0.53273525843273	1.89582744016537	1.66266760130067
H	2.12151618113693	2.50564877875339	1.17992431556064
C	1.22639133945835	5.58154915635379	-1.34507019616007
H	0.20310059124306	5.94891344896402	-1.19087393465549
H	1.22004038132427	4.49619973526261	-1.16507892164361

H	1.46130402328226	5.72432312468086	-2.41706886853748
C	-0.83875281480479	6.87622075489877	3.81972147254907
H	-0.41749630536220	7.46958344226592	4.64309788328965
H	-1.82351933227440	6.50544361812122	4.15784196568667
H	-1.03553301921867	7.56425915450630	2.98154128887365
C	0.90523077201579	8.53267165200117	-0.16283986106713
H	0.93684459510962	9.11908389862296	-1.09977800668563
H	0.83024952241699	9.26192591395969	0.65946486086599
H	-0.03331291575853	7.95741456860572	-0.17921589023261
C	-1.10489655830724	5.17498883972956	1.19876904781476
H	-1.22666416968764	6.22408779624994	0.88617484112156
H	-2.08544242553667	4.84893292182627	1.59219013276248
H	-0.91038557245085	4.58503096703050	0.29347683911357
C	0.06810483038516	5.74776829058412	3.43341787314285
C	1.59531006602882	4.02345129097902	3.55125045074993
C	6.36206717604535	5.84707048353001	4.56227693222938
C	3.74830341105638	9.40049687177665	1.00114069746180
H	2.88319322612116	9.95957800171721	1.38431761057975
H	4.18937486397982	10.00160062434140	0.18541421681186
H	4.49102973912560	9.35914945206526	1.81186529118388
C	-0.02663332654978	4.99856984182425	2.22572926351211
C	1.47259294741769	5.58064266879634	5.63026205712258
H	2.55133314652206	5.44478219138609	5.79600208739841
H	0.94616258526837	5.00357695038904	6.41038748739249
H	1.25186419149996	6.64369529459219	5.80231364785171
C	6.09119399067120	10.36117578750750	6.81064540498873
H	7.10480848110940	10.59205380065770	7.16393738485188

H	5.79237331651299	11.11452246967220	6.06198970042898
H	5.39945612157676	10.41610773233380	7.67220496734523

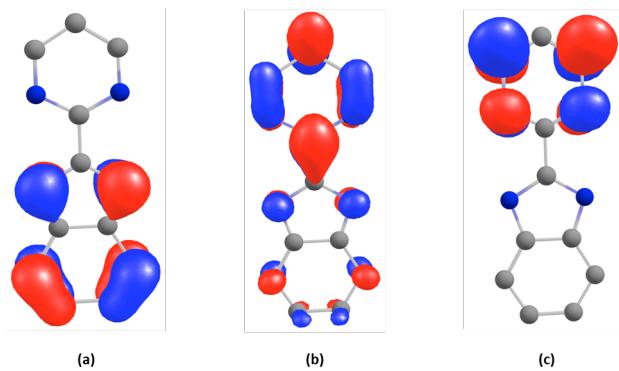


Figure S32. Main Kohn-Sham orbitals of the $[\text{bimpmp}]^-$ compound obtained with PBE0 functional starting from a geometry optimized in PBE: (a) HOMO, (b) LUMO, and (c) LUMO +1.

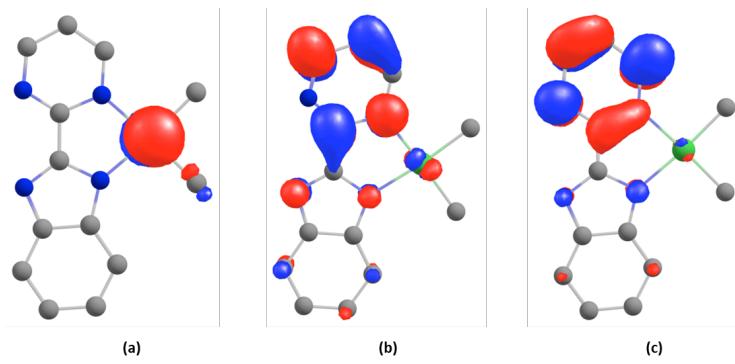


Figure S33. Main Kohn-Sham orbitals of the $[(\text{bimpmp})\text{NiMe}_2]^-$ compound obtained with PBE0 functional starting from a geometry optimized in PBE: (a) HOMO, (b) LUMO, and (c) LUMO +1.

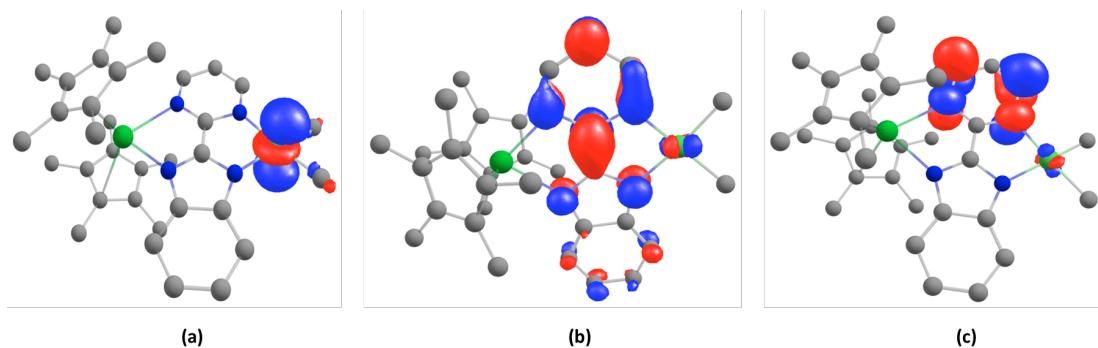


Figure S34. Main Kohn-Sham alpha orbitals of the $[\text{Cp}^*_2\text{Yb}(\text{bimpmp})\text{NiMe}_2]^-$ compound obtained with PBE0 functional starting from a geometry optimized in PBE: (a) SOMO-1, (b) SOMO, and (c) LUMO.

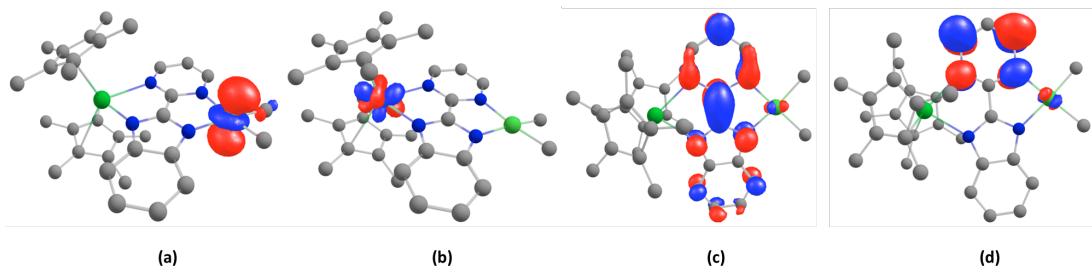


Figure S35. Main Kohn-Sham beta orbitals of the $[\text{Cp}^*_2\text{Yb}(\text{bimpm})\text{NiMe}_2]^-$ compound obtained with PBE0 functional starting from a geometry optimized in PBE: (a) SOMO, (b) LUMO, (c) LUMO +1, and (d) LUMO +2.

4. Crystallographic data

Table S5. Crystallographic data for compounds **1 - 6**.

	1	2	3	4	5	6
Empirical formula	C ₁₇ H ₂₁ KN ₄ NiO	C ₈₄ H ₁₁₇ N ₈ O ₃ Y	C ₁₀₀ H ₁₆₁ K ₃ N ₈ N	C ₅₀ H ₇₃ K ₂ N ₈ N	C ₉₄ H ₁₄₄ K ₂ N ₈ Ni	C ₆₂ H ₉₈ K ₄ N ₈ Ni ₂ O
Formula weight	395.19	1805.97	2152.16	1173.78	2135.86	1373.3
Temperature/K	150.15	150.0	150.01	150.0	150.0	150.0
Crystal system	monoclinic	tetragonal	triclinic	triclinic	triclinic	monoclinic
Space group	P2 ₁ /n	I4/m	P-1	P-1	P-1	P21/n
a/Å	13.7210(7)	26.3931(15)	15.4720(13)	13.9055(13)	17.575(6)	14.7527(11)
b/Å	7.1655(4)	26.3931(15)	18.3028(16)	14.5462(13)	17.768(6)	17.6187(14)
c/Å	18.9082(8)	22.8754(13)	20.4081(17)	16.4926(15)	18.319(6)	26.226(2)
α/°	90	90	98.073(2)	93.346(3)	111.847(7)	90
β/°	106.036(5)	90	102.959(2)	104.115(3)	101.994(9)	96.607(2)
γ/°	90	90	99.279(3)	118.509(3)	95.118(10)	90
Volume/Å ³	1786.68(16)	15935(2)	5463.8(8)	2782.5(4)	5106(3)	6771.5(9)
Z	4	8	2	2	2	4
ρ _{calc} g/cm ³	1.469	1.506	1.308	1.401	1.389	1.347
μ/mm ⁻¹	1.330	3.544	2.200	0.892	2.319	0.86
F(000)	824.0	7288.0	2236.0	1238.0	2204.0	2920
Crystal size/mm ³	0.32 × 0.2 × 0.1	0.34 × 0.25 × 0.12	0.22 × 0.1 × 0.04	0.32 × 0.32 × 0.15	0.12 × 0.12 × 0.04	0.26 × 0.18 × 0.12
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71069)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.482 to 60.054	4.712 to 60.154	2.294 to 54.97	2.602 to 61.998	2.41 to 52.044	3.888 to 52.044
Index ranges	-19 ≤ h ≤ 19, -10 ≤ k ≤ 10, -26 ≤ l ≤ 26	-37 ≤ h ≤ 37, -37 ≤ k ≤ 37, -32 ≤ l ≤ 32	-20 ≤ h ≤ 20, -23 ≤ k ≤ 23, -26 ≤ l ≤ 26	-20 ≤ h ≤ 20, -21 ≤ k ≤ 21, -23 ≤ l ≤ 23	-21 ≤ h ≤ 20, -21 ≤ k ≤ 21, -22 ≤ l ≤ 22	-18 ≤ h ≤ 17, -21 ≤ k ≤ 21, -32 ≤ l ≤ 30
Reflections collected	85107	326142	188869	117733	55476	75848
Independent reflections	5228 [R _{int} = 0.0586, R _{sigma} = 0.0263]	11978 [R _{int} = 0.1064, R _{sigma} = 0.0343]	25047 [R _{int} = 0.0902, R _{sigma} = 0.0600]	17709 [R _{int} = 0.0609, R _{sigma} = 0.0431]	20057 [R _{int} = 0.1761, R _{sigma} = 0.2547]	13329 [R _{int} = 0.0899, R _{sigma} = 0.0738]
Data/restraints/p	5228/36/238	11978/54/487	25047/307/12	17709/0/671	20057/598/10	13329/892/10

arameters	26	71	00
Goodness-of-fit on F^2	1.081	1.167	1.055
Final R indexes $[I \geq 2\sigma (I)]$	$R_1 = 0.0535$, $wR_2 = 0.1330$	$R_1 = 0.0376$, $wR_2 = 0.0788$	$R_1 = 0.0411$, $wR_2 = 0.0836$
Final R indexes [all data]	$R_1 = 0.0667$, $wR_2 = 0.1429$	$R_1 = 0.0738$, $wR_2 = 0.0992$	$R_1 = 0.0777$, $wR_2 = 0.1013$
Largest diff. peak/hole / e Å ⁻³	1.84/-0.58	2.59/-2.00	2.45/-1.37
	2.55/-0.68	4.70/-2.54	0.72/-0.45

Comments on the way the structures were solved.

A solvent mask was used for the structures of **2**, **3** and **5**.

In **2**, 422 electrons were found in a volume of 1064 Å³ in 3 voids per unit cell. This is consistent with the presence of 1.5 [C₄H₁₀O] per asymmetric unit, which account for 504 electrons per unit cell.

In **3**, 28 electrons were found in a volume of 477 Å³ in 2 voids per unit cell. This is consistent with the presence of 0.333 [C₄H₁₀O] per asymmetric unit, which account for 28 electrons per unit cell.

In **5**, 152 electrons were found in a volume of 476 Å³ in 2 voids per unit cell. This is consistent with the presence of 2 [C₄H₁₀O] per asymmetric unit, which account for 168 electrons per unit cell.

Moreover, after several crystallization and acquisition tries, no better data set was recorded for compound **5**. We choose however to present it as a qualitative characterization while taking care not to expect too much precision on the distances observed. Two A alerts and three B alerts are signaled by checkcif and are all resulting from the lack of data at high angle.

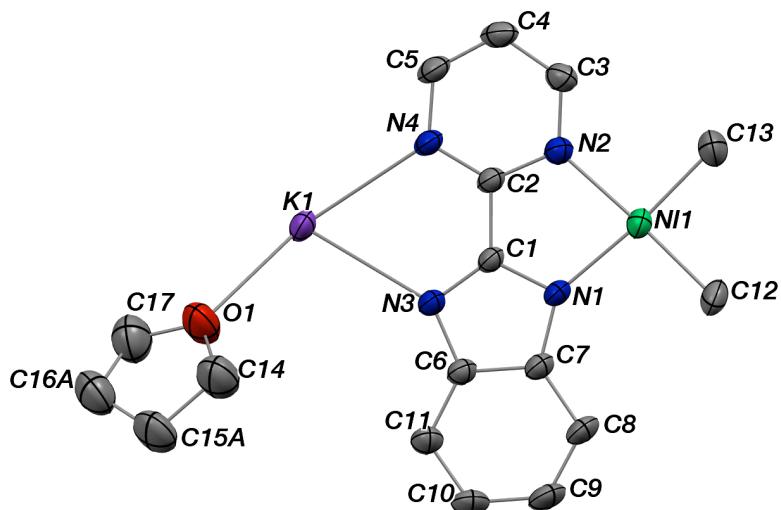


Figure S36. ORTEPs of K(bimpm)Ni(CH₃)₂ (**1**) when each one position disorder of C(15) and C(16) is allowed.

Thermal ellipsoids are at 50 % level. Carbon atoms are in grey, nitrogen atoms in blue, oxygen atoms in red, nickel atom in green and potassium atom in purple. Hydrogen atoms have been removed for clarity.

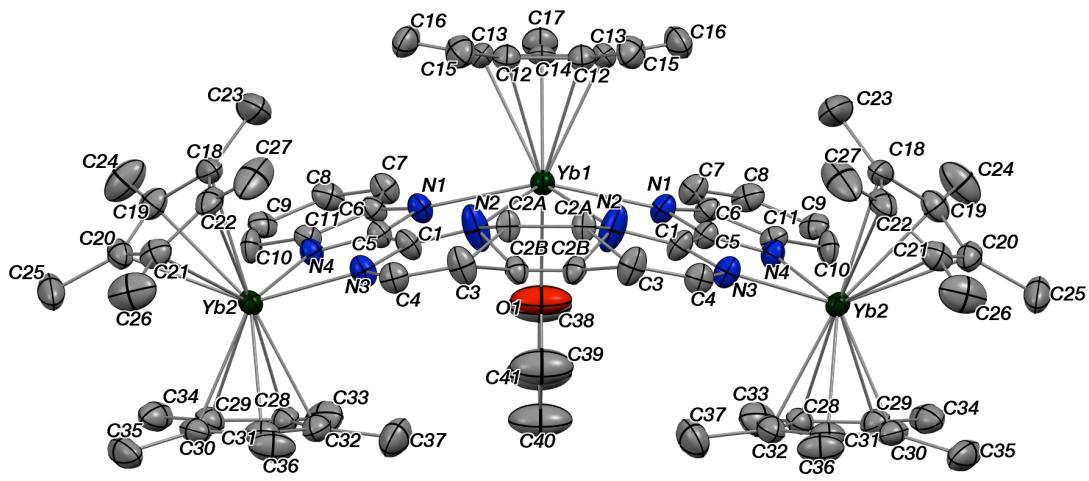


Figure S37. ORTEPs of $\text{Cp}^*\text{Yb}(\text{thf})[\text{Cp}^*{}_{\text{2}}\text{Yb}(\text{bimpm})]_2$ (**2**). Thermal ellipsoids are at 50 % level. Carbon atoms are in grey, nitrogen in blue, and ytterbium in deep green. H-atoms and two co-crystallized diethyl ether solvate molecules are removed for clarity.

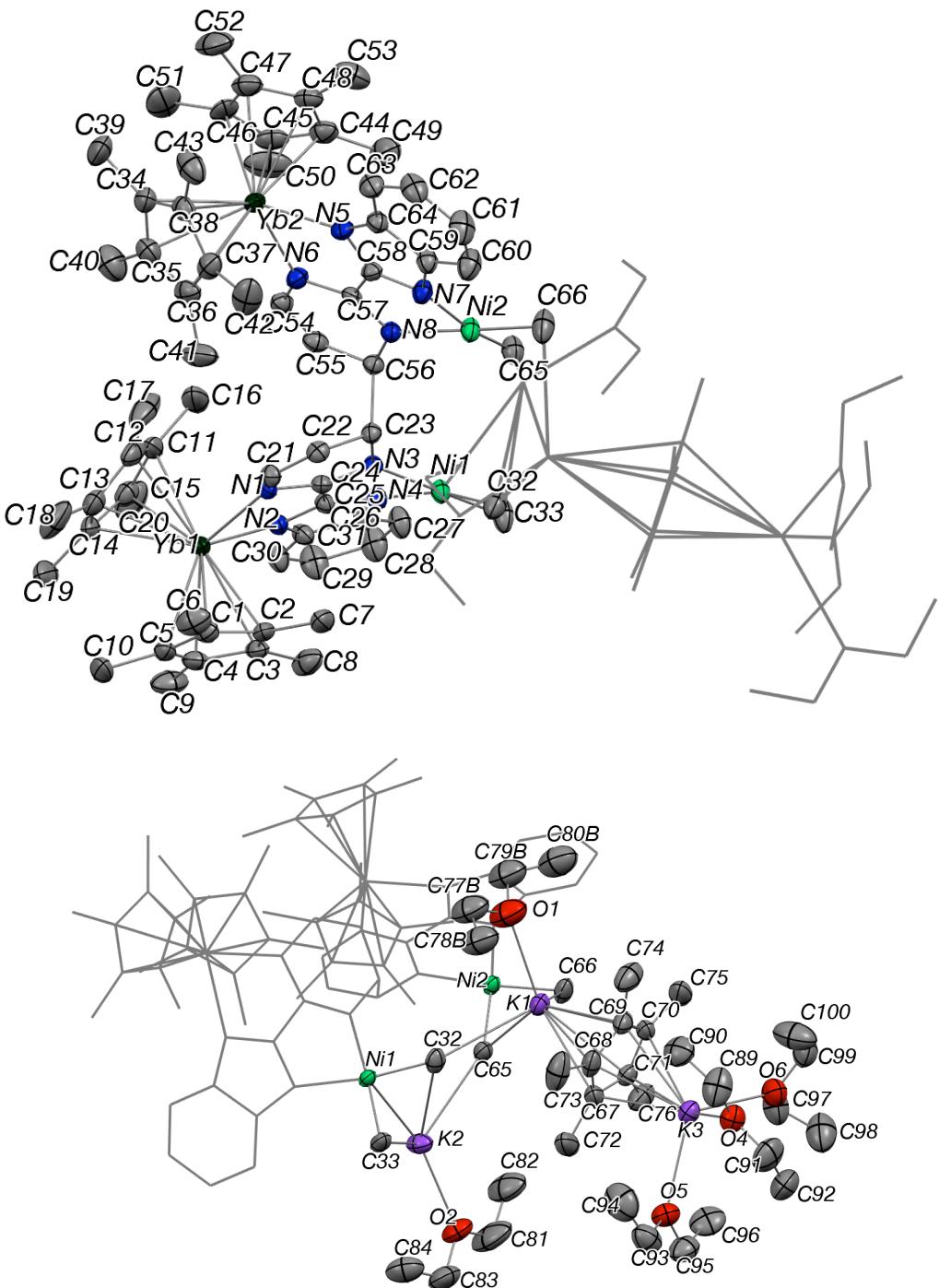


Figure S38. ORTEPs of $[KCP^*_2Yb(\text{bimpm})\text{NiMe}_2]_2 \bullet KCP^*$ (**3**) when each one position disorder of C(77–80) and O(1) is allowed. Thermal ellipsoids are at 50 % level. Carbon atoms are in grey, potassium in purple, nitrogen in blue, nickel in bright green and ytterbium atoms in deep green. One co-crystallized diethyl ether solvate molecule with disorder and hydrogen atoms are removed and pentamethylcyclopentadienyl ligands on ytterbium are presented in wireframe style for clarity.

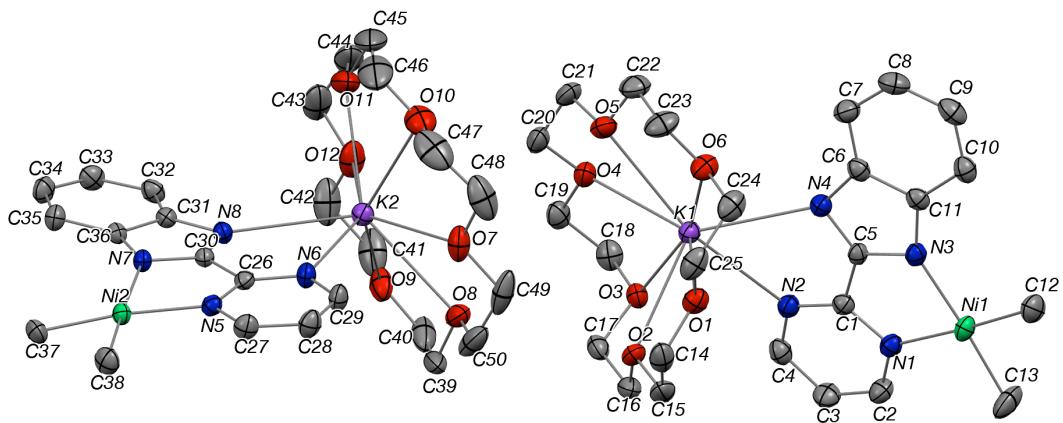


Figure S39. ORTEPs of $\text{K}(18\text{-c-}6)(\text{bimpmp})\text{Ni}(\text{CH}_3)_2$ (**4**). Thermal ellipsoids are at 50 % level. Carbon atoms are in grey, nitrogen atoms in blue, oxygen atoms in red, nickel atom in green and potassium atom in purple. Hydrogen atoms have been removed for clarity.

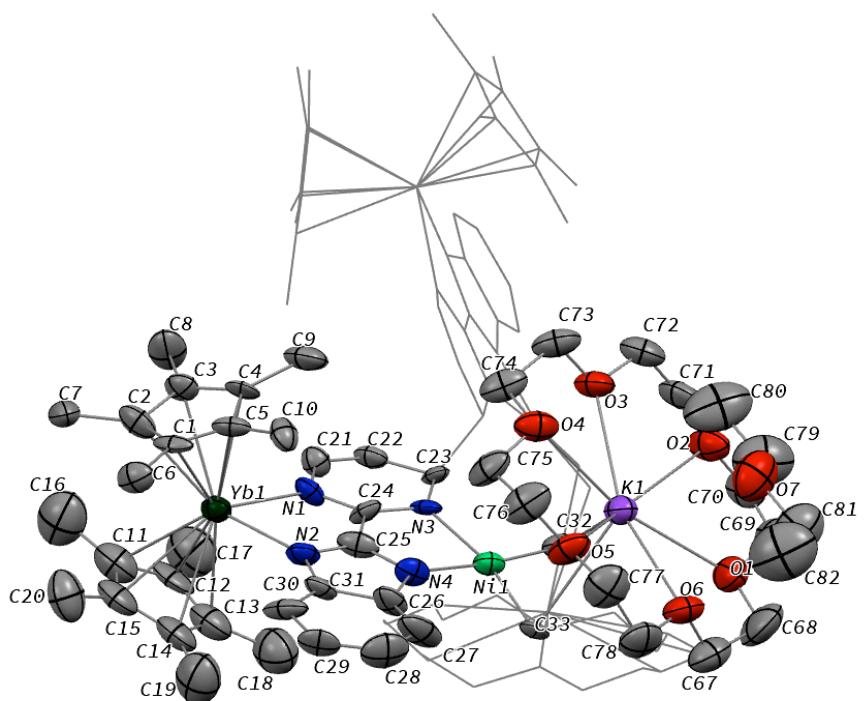
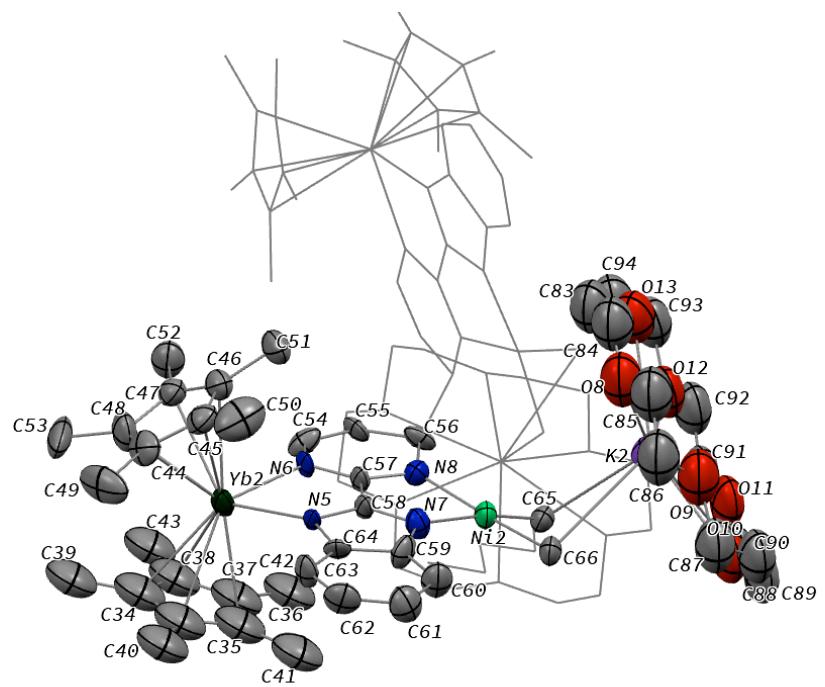


Figure S40. ORTEPs of $[\text{K}(18\text{-c-6})\text{Cp}^*{}_{\text{2}}\text{Yb}(\text{bimpm})\text{NiMe}_2]_2$ (**5**). Thermal ellipsoids are at 50 % level. Carbon atoms are in grey, potassium in purple, nitrogen in blue, nickel in bright green and ytterbium atoms in deep green. H-atoms are omitted and pentamethylcyclopentadienyl ligands on ytterbium and 18-c-6 chelating compounds are presented in wireframe style for clarity.

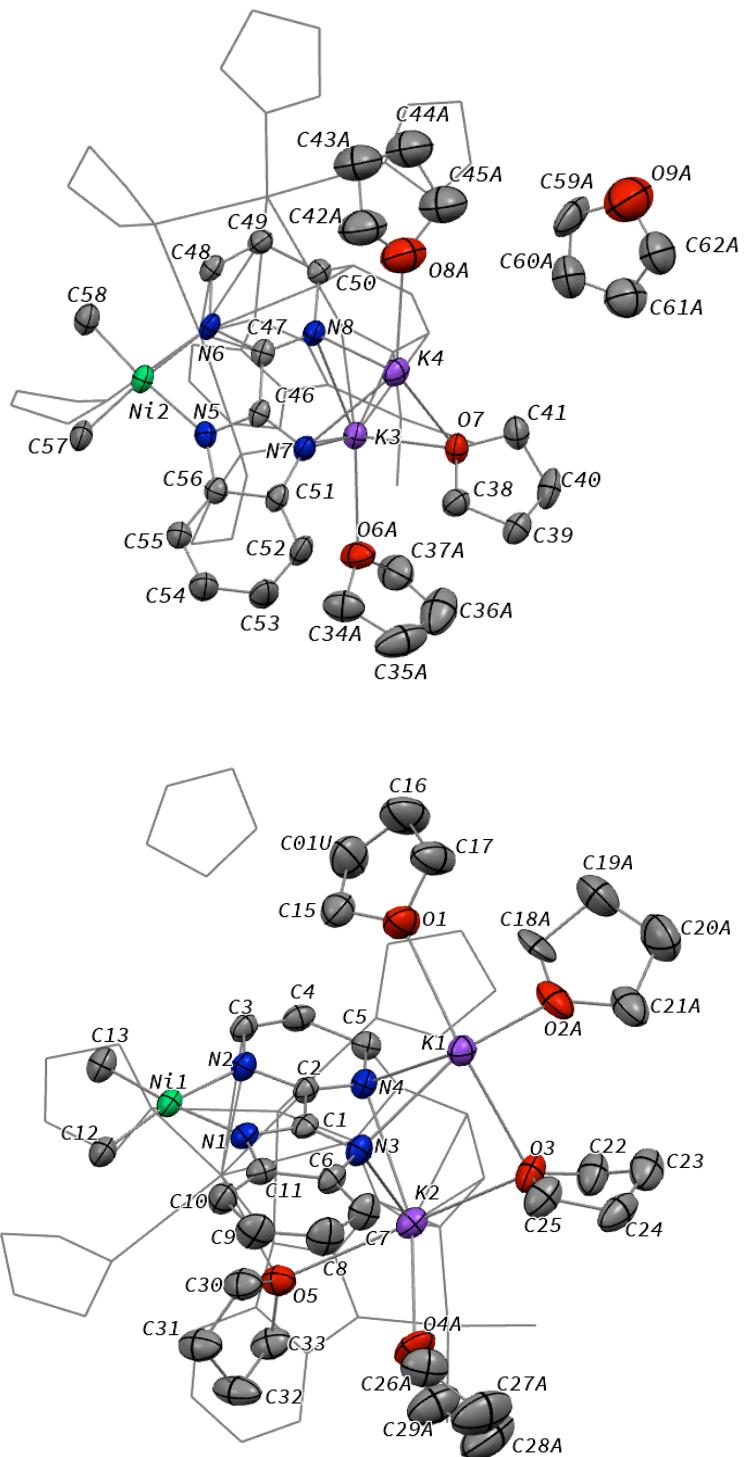


Figure S41. ORTEPs of $[K_2(\text{bimpm})\text{NiMe}_2]_2$ (**6**) when each one position disorder of C(18-21, 26-29, 34-37, 42-45, 59-62) and O(2, 4, 6, 8, 9) is allowed. One co-crystallized THF solvate and four THF solvate molecules on potassium atoms are with disorder. Thermal ellipsoids are at 50 % level. Carbon atoms are in grey, potassium in purple, nitrogen in blue and nickel in bright green. Hydrogen atoms are removed for clarity.

Table S6. Distances (Å) and angles (deg) for K(bimpmp)Ni(CH₃)₂ (**1**).

Ni(1)-K(1) ¹	3.1643(9)	N(4)-C(5)	1.339(3)
Ni(1)-N(2)	1.981(2)	C(1)-C(2)	1.451(3)
Ni(1)-N(1)	1.969(2)	C(6)-C(7)	1.419(4)
Ni(1)-C(12)	1.925(3)	C(6)-C(11)	1.400(4)
Ni(1)-C(13)	1.920(3)	C(3)-C(4)	1.380(4)
K(1)-O(1)	2.691(3)	C(7)-C(8)	1.406(3)
K(1)-N(3)	2.770(2)	C(11)-C(10)	1.382(4)
K(1)-N(4)	2.775(2)	C(4)-C(5)	1.367(4)
O(1)-C(14)	1.428(5)	C(9)-C(10)	1.405(5)
O(1)-C(17)	1.407(5)	C(9)-C(8)	1.376(5)
N(2)-C(2)	1.355(3)	C(14)-C(15A)	1.522(13)
N(2)-C(3)	1.337(3)	C(14)-C(15B)	1.337(14)
N(3)-C(1)	1.336(3)	C(17)-C(16A)	1.475(11)
N(3)-C(6)	1.376(3)	C(17)-C(16B)	1.510(13)
N(1)-C(1)	1.356(3)	C(15A)-C(16A)	1.419(17)
N(1)-C(7)	1.378(3)	C(16B)-C(15B)	1.48(2)
N(4)-C(2)	1.331(3)		

¹-2-X,-Y,-Z

N(2)-Ni(1)-K(1) ¹	99.33(7)	N(3)-C(1)-K(1)	46.22(12)
N(1)-Ni(1)-K(1) ¹	79.33(7)	N(3)-C(1)-N(1)	117.6(2)
N(1)-Ni(1)-N(2)	82.13(9)	N(3)-C(1)-C(2)	125.9(2)
C(12)-Ni(1)-K(1) ¹	80.69(11)	N(1)-C(1)-K(1)	163.09(18)
C(12)-Ni(1)-N(2)	177.38(11)	N(1)-C(1)-C(2)	116.5(2)
C(12)-Ni(1)-N(1)	95.31(11)	C(2)-C(1)-K(1)	79.95(13)
C(13)-Ni(1)-K(1) ¹	100.13(14)	N(2)-C(2)-C(1)	113.4(2)
C(13)-Ni(1)-N(2)	92.58(12)	N(4)-C(2)-N(2)	125.9(2)
C(13)-Ni(1)-N(1)	174.50(12)	N(4)-C(2)-C(1)	120.7(2)
C(13)-Ni(1)-C(12)	89.99(14)	N(3)-C(6)-C(7)	109.7(2)
O(1)-K(1)-Ni(1) ¹	100.61(9)	N(3)-C(6)-C(11)	129.3(2)
O(1)-K(1)-N(3)	101.87(8)	C(11)-C(6)-C(7)	121.0(2)
O(1)-K(1)-N(4)	152.83(9)	N(2)-C(3)-C(4)	122.0(3)
N(3)-K(1)-Ni(1) ¹	88.34(5)	N(1)-C(7)-C(6)	107.7(2)
N(3)-K(1)-N(4)	63.45(6)	N(1)-C(7)-C(8)	132.1(3)
N(4)-K(1)-Ni(1) ¹	101.58(5)	C(8)-C(7)-C(6)	120.2(3)
C(14)-O(1)-K(1)	121.1(2)	C(10)-C(11)-C(6)	118.1(3)
C(17)-O(1)-K(1)	129.4(3)	C(5)-C(4)-C(3)	117.7(3)
C(17)-O(1)-C(14)	108.8(3)	C(8)-C(9)-C(10)	122.3(3)
C(2)-N(2)-Ni(1)	114.65(16)	C(11)-C(10)-C(9)	120.7(3)
C(3)-N(2)-Ni(1)	129.5(2)	N(4)-C(5)-C(4)	122.1(2)
C(3)-N(2)-C(2)	115.8(2)	C(9)-C(8)-C(7)	117.7(3)
C(1)-N(3)-K(1)	113.39(15)	Ni(1)-C(12)-K(1) ²	164.54(17)

C(1)-N(3)-C(6)	102.2(2)	Ni(1)-C(12)-K(1) ¹	65.65(9)
C(6)-N(3)-K(1)	143.96(18)	K(1) ² -C(12)-K(1) ¹	127.77(10)
Ni(1)-N(1)-K(1) ¹	66.02(6)	Ni(1)-C(13)-K(1) ³	96.32(15)
C(1)-N(1)-Ni(1)	113.25(16)	O(1)-C(14)-C(15A)	103.9(6)
C(1)-N(1)-K(1) ¹	109.30(16)	C(15B)-C(14)-O(1)	107.7(9)
C(1)-N(1)-C(7)	102.8(2)	O(1)-C(17)-C(16A)	108.3(6)
C(7)-N(1)-Ni(1)	143.82(17)	O(1)-C(17)-C(16B)	99.9(6)
C(7)-N(1)-K(1) ¹	105.37(17)	C(16A)-C(15A)-C(14)	106.3(8)
C(2)-N(4)-K(1)	116.10(16)	C(15A)-C(16A)-C(17)	102.6(8)
C(2)-N(4)-C(5)	116.5(2)	C(15B)-C(16B)-C(17)	106.8(9)
C(5)-N(4)-K(1)	127.37(18)	C(14)-C(15B)-C(16B)	106.8(11)

¹2-X,-Y,-1-Z; ²1/2+X,-1/2-Y,1/2+Z; ³2-X,-1-Y,-1-Z

Table S7. Distances (Å) and angles (deg) for Cp*Yb(thf)[Cp*₂Yb(bimpm)]₂ (**2**).

Yb1-O1	2.397(6)	C7-C8	1.383(7)
Yb1-N1 ¹	2.441(4)	C8-C9	1.399(7)
Yb1-N1	2.441(4)	C9-C10	1.380(7)
Yb1-N2	2.343(4)	C10-C11	1.407(6)
Yb1-N2 ¹	2.343(4)	C12-C12 ¹	1.413(10)
Yb1-C12 ¹	2.638(5)	C12-C13	1.421(7)
Yb1-C12	2.638(5)	C12-C15	1.502(7)
Yb1-C13 ¹	2.669(5)	C13-C14	1.422(6)
Yb1-C13	2.669(5)	C13-C16	1.494(7)
Yb1-C14	2.668(6)	C14-C17	1.512(10)
Yb2-N3	2.326(4)	C18-C19	1.425(8)
Yb2-N4	2.347(4)	C18-C22	1.408(8)
Yb2-C18	2.613(5)	C18-C23	1.498(8)
Yb2-C19	2.627(5)	C19-C20	1.396(7)
Yb2-C20	2.651(5)	C19-C24	1.517(8)
Yb2-C21	2.627(5)	C20-C21	1.410(7)
Yb2-C22	2.624(5)	C20-C25	1.513(8)
Yb2-C28	2.636(5)	C21-C22	1.405(8)
Yb2-C29	2.601(5)	C21-C26	1.507(8)
Yb2-C30	2.622(5)	C22-C27	1.504(8)
Yb2-C31	2.621(5)	C28-C29	1.420(7)
Yb2-C32	2.654(5)	C28-C32	1.412(7)
O1-C38	1.456(13)	C28-C33	1.504(7)
O1-C41	1.373(13)	C29-C30	1.430(8)
N1-C5	1.344(6)	C29-C34	1.510(8)
N1-C6	1.391(6)	C30-C31	1.424(8)
N2-C1	1.308(6)	C30-C35	1.509(8)
N2-C2A	1.507(9)	C31-C32	1.412(8)
N2-C2B	1.563(11)	C31-C36	1.506(8)

N3-C1	1.340(6)	C32-C37	1.510(8)
N3-C4	1.407(6)	C38-C39	1.296(14)
N4-C5	1.353(6)	C39-C40	1.556(16)
N4-C11	1.390(6)	C40-C41	1.450(15)
C1-C5	1.476(6)	O2-C43	1.355(16)
C2A-C2B ¹	1.521(12)	O2-C44	1.369(16)
C2A-C3	1.488(10)	C42-C43	1.471(18)
C2B-C3	1.600(10)	C44-C45	1.42(2)
C3-C4	1.320(7)	O3-C46 ¹	1.412(6)
C6-C7	1.398(6)	O3-C46	1.412(6)
C6-C11	1.412(6)	C46-C47	1.497(9)

¹+X,+Y,-Z

O1-Yb1-N1 ¹	72.36(10)	C1-N3-C4	113.2(4)
O1-Yb1-N1	72.36(10)	C4-N3-Yb2	130.3(3)
O1-Yb1-C12	164.41(11)	C5-N4-Yb2	112.6(3)
O1-Yb1-C12 ¹	164.40(11)	C5-N4-C11	102.7(4)
O1-Yb1-C13 ¹	139.28(17)	C11-N4-Yb2	144.5(3)
O1-Yb1-C13	139.28(17)	N2-C1-Yb2	169.7(4)
O1-Yb1-C14	129.0(2)	N2-C1-N3	129.3(5)
N1 ¹ -Yb1-N1	137.99(19)	N2-C1-C5	114.3(4)
N1 ¹ -Yb1-C12 ¹	92.14(15)	N3-C1-Yb2	41.2(2)
N1-Yb1-C12	92.15(15)	N3-C1-C5	116.4(4)
N1-Yb1-C12 ¹	122.51(15)	C5-C1-Yb2	75.2(3)
N1 ¹ -Yb1-C12	122.51(15)	N2-C2A-C2B ¹	98.1(6)
N1 ¹ -Yb1-C13	122.53(14)	C3-C2A-N2	110.2(6)
N1-Yb1-C13	74.58(14)	C3-C2A-C2B ¹	109.2(7)
N1-Yb1-C13 ¹	122.53(14)	N2-C2B-C3	101.8(6)
N1 ¹ -Yb1-C13 ¹	74.58(14)	C2A ¹ -C2B-N2	104.1(7)
N1-Yb1-C14	92.42(11)	C2A ¹ -C2B-C3	112.5(7)
N1 ¹ -Yb1-C14	92.42(11)	C2A-C3-C2B	32.8(5)
N2-Yb1-O1	88.9(2)	C4-C3-C2A	121.0(5)
N2 ¹ -Yb1-O1	88.9(2)	C4-C3-C2B	116.8(5)
N2-Yb1-N1 ¹	131.74(16)	C3-C4-N3	124.5(5)
N2 ¹ -Yb1-N1	131.74(16)	N1-C5-Yb2	160.8(3)
N2 ¹ -Yb1-N1 ¹	69.06(14)	N1-C5-N4	117.2(4)
N2-Yb1-N1	69.06(14)	N1-C5-C1	121.4(4)
N2 ¹ -Yb1-N2	66.5(2)	N4-C5-Yb2	43.8(2)
N2 ¹ -Yb1-C12 ¹	83.76(18)	N4-C5-C1	121.5(4)
N2-Yb1-C12	83.76(18)	C1-C5-Yb2	77.6(3)
N2-Yb1-C12 ¹	100.65(18)	N1-C6-C7	130.8(4)
N2 ¹ -Yb1-C12	100.64(18)	N1-C6-C11	108.7(4)
N2 ¹ -Yb1-C13	131.32(18)	C7-C6-C11	120.6(4)
N2-Yb1-C13 ¹	131.32(18)	C8-C7-C6	117.6(5)

N2 ¹ -Yb1-C13 ¹	100.87(18)	C7-C8-C9	121.9(5)
N2-Yb1-C13	100.87(18)	C10-C9-C8	121.4(4)
N2 ¹ -Yb1-C14	131.43(18)	C9-C10-C11	117.3(5)
N2-Yb1-C14	131.43(18)	N4-C11-C6	108.6(4)
C12-Yb1-C12 ¹	31.1(2)	N4-C11-C10	130.2(4)
C12-Yb1-C13	31.04(15)	C10-C11-C6	121.2(4)
C12-Yb1-C13 ¹	51.23(15)	C12 ¹ -C12-Yb1	74.47(11)
C12 ¹ -Yb1-C13	51.22(15)	C12 ¹ -C12-C13	108.1(3)
C12 ¹ -Yb1-C13 ¹	31.04(15)	C12 ¹ -C12-C15	126.7(3)
C12 ¹ -Yb1-C14	51.33(18)	C13-C12-Yb1	75.7(3)
C12-Yb1-C14	51.33(18)	C13-C12-C15	124.8(5)
C13 ¹ -Yb1-C13	51.0(2)	C15-C12-Yb1	121.6(3)
C14-Yb1-C13 ¹	30.89(13)	C12-C13-Yb1	73.3(3)
C14-Yb1-C13	30.89(13)	C12-C13-C14	108.0(4)
N3-Yb2-N4	72.95(13)	C12-C13-C16	125.3(5)
N3-Yb2-C18	89.02(16)	C14-C13-Yb1	74.5(3)
N3-Yb2-C19	119.95(16)	C14-C13-C16	125.8(5)
N3-Yb2-C20	134.03(15)	C16-C13-Yb1	126.6(3)
N3-Yb2-C21	108.31(16)	C13 ¹ -C14-Yb1	74.6(3)
N3-Yb2-C22	82.83(16)	C13-C14-Yb1	74.6(3)
N3-Yb2-C28	98.78(15)	C13 ¹ -C14-C13	107.8(6)
N3-Yb2-C29	128.94(16)	C13-C14-C17	125.7(3)
N3-Yb2-C30	124.17(16)	C13 ¹ -C14-C17	125.7(3)
N3-Yb2-C31	92.73(16)	C17-C14-Yb1	125.2(5)
N3-Yb2-C32	78.79(16)	C19-C18-Yb2	74.7(3)
N4-Yb2-C18	82.84(16)	C19-C18-C23	125.7(6)
N4-Yb2-C19	87.13(15)	C22-C18-Yb2	74.8(3)
N4-Yb2-C20	116.63(15)	C22-C18-C19	107.3(5)
N4-Yb2-C21	133.87(15)	C22-C18-C23	126.7(6)
N4-Yb2-C22	109.95(16)	C23-C18-Yb2	121.2(4)
N4-Yb2-C28	79.94(15)	C18-C19-Yb2	73.7(3)
N4-Yb2-C29	98.03(15)	C18-C19-C24	126.2(6)
N4-Yb2-C30	129.02(15)	C20-C19-Yb2	75.6(3)
N4-Yb2-C31	127.23(16)	C20-C19-C18	108.3(5)
N4-Yb2-C32	96.39(16)	C20-C19-C24	124.7(6)
C18-Yb2-C19	31.55(17)	C24-C19-Yb2	124.5(4)
C18-Yb2-C20	51.49(16)	C19-C20-Yb2	73.7(3)
C18-Yb2-C21	51.56(17)	C19-C20-C21	107.9(5)
C18-Yb2-C22	31.19(18)	C19-C20-C25	124.0(5)
C18-Yb2-C28	158.04(18)	C21-C20-Yb2	73.6(3)
C18-Yb2-C30	137.27(16)	C21-C20-C25	127.3(5)
C18-Yb2-C31	148.93(17)	C25-C20-Yb2	126.1(4)
C18-Yb2-C32	167.41(17)	C20-C21-Yb2	75.4(3)
C19-Yb2-C20	30.67(16)	C20-C21-C26	126.3(6)

C19-Yb2-C28	133.30(16)	C22-C21-Yb2	74.4(3)
C19-Yb2-C32	161.00(17)	C22-C21-C20	108.2(5)
C20-Yb2-C32	137.61(17)	C22-C21-C26	124.6(5)
C21-Yb2-C19	51.19(16)	C26-C21-Yb2	124.9(4)
C21-Yb2-C20	31.00(16)	C18-C22-Yb2	74.0(3)
C21-Yb2-C28	141.28(16)	C18-C22-C27	126.9(6)
C21-Yb2-C32	129.57(17)	C21-C22-Yb2	74.6(3)
C22-Yb2-C19	51.50(17)	C21-C22-C18	108.2(5)
C22-Yb2-C20	51.26(16)	C21-C22-C27	124.5(6)
C22-Yb2-C21	31.05(17)	C27-C22-Yb2	122.9(4)
C22-Yb2-C28	169.93(17)	C29-C28-Yb2	72.9(3)
C22-Yb2-C32	141.66(17)	C29-C28-C33	125.8(5)
C28-Yb2-C20	126.76(16)	C32-C28-Yb2	75.2(3)
C28-Yb2-C32	30.96(16)	C32-C28-C29	108.2(5)
C29-Yb2-C18	140.81(18)	C32-C28-C33	125.6(5)
C29-Yb2-C19	109.27(17)	C33-C28-Yb2	123.0(4)
C29-Yb2-C20	95.55(16)	C28-C29-Yb2	75.6(3)
C29-Yb2-C21	112.60(17)	C28-C29-C30	107.5(5)
C29-Yb2-C22	143.47(17)	C28-C29-C34	125.7(5)
C29-Yb2-C28	31.47(16)	C30-C29-Yb2	74.9(3)
C29-Yb2-C30	31.79(16)	C30-C29-C34	126.6(5)
C29-Yb2-C31	52.40(17)	C34-C29-Yb2	119.0(3)
C29-Yb2-C32	51.78(17)	C29-C30-Yb2	73.3(3)
C30-Yb2-C19	112.52(18)	C29-C30-C35	126.5(5)
C30-Yb2-C20	86.28(17)	C31-C30-Yb2	74.2(3)
C30-Yb2-C21	89.67(17)	C31-C30-C29	107.8(5)
C30-Yb2-C22	119.16(17)	C31-C30-C35	124.3(5)
C30-Yb2-C28	51.86(16)	C35-C30-Yb2	129.2(4)
C30-Yb2-C32	51.51(17)	C30-C31-Yb2	74.3(3)
C31-Yb2-C19	139.79(17)	C30-C31-C36	125.6(5)
C31-Yb2-C20	109.64(17)	C32-C31-Yb2	75.8(3)
C31-Yb2-C21	98.90(17)	C32-C31-C30	107.9(5)
C31-Yb2-C22	118.40(18)	C32-C31-C36	126.2(5)
C31-Yb2-C28	51.72(16)	C36-C31-Yb2	120.5(4)
C31-Yb2-C30	31.51(17)	C28-C32-Yb2	73.8(3)
C31-Yb2-C32	31.05(17)	C28-C32-C31	108.5(5)
C38-O1-Yb1	118.8(6)	C28-C32-C37	125.8(5)
C41-O1-Yb1	131.9(6)	C31-C32-Yb2	73.2(3)
C41-O1-C38	109.3(8)	C31-C32-C37	125.4(5)
C5-N1-Yb1	113.4(3)	C37-C32-Yb2	123.9(4)
C5-N1-C6	102.8(4)	C39-C38-O1	109.1(10)
C6-N1-Yb1	143.7(3)	C38-C39-C40	110.0(10)
C1-N2-Yb1	121.9(3)	C41-C40-C39	101.9(9)
C1-N2-C2A	118.6(5)	O1-C41-C40	109.6(10)

C1-N2-C2B	114.8(5)	C43-O2-C44	118.0(12)
C2A-N2-Yb1	118.6(4)	O2-C43-C42	116.3(12)
C2A-N2-C2B	33.3(5)	O2-C44-C45	113.9(14)
C2B-N2-Yb1	117.8(4)	C46-O3-C46 ¹	112.5(6)
C1-N3-Yb2	116.5(3)	O3-C46-C47	109.4(5)

¹+X,+Y,-Z

Table S8. Distances (Å) and angles (deg) for [KCp*₂Yb(bimpm)NiMe₂]₂ • KCp* (**3**).

Yb1-N1	2.320(4)	C25-C24	1.469(6)
Yb1-N2	2.332(4)	C55-C56	1.502(6)
Yb1-C2	2.635(5)	C31-C30	1.386(7)
Yb1-C5	2.604(4)	C22-C23	1.503(6)
Yb1-C4	2.595(5)	C5-C4	1.410(7)
Yb1-C1	2.600(5)	C5-C1	1.419(7)
Yb1-C3	2.636(5)	C5-C10	1.517(7)
Yb1-C14	2.644(5)	C36-C35	1.411(8)
Yb1-C13	2.630(5)	C36-C37	1.411(8)
Yb1-C15	2.631(5)	C36-C41	1.511(7)
Yb1-C11	2.603(5)	C56-C23	1.566(6)
Yb1-C12	2.605(5)	C27-C28	1.374(7)
Yb2-N6	2.317(4)	C70-C71	1.406(7)
Yb2-N5	2.353(4)	C70-C69	1.417(8)
Yb2-C36	2.615(5)	C70-C75	1.518(7)
Yb2-C45	2.623(5)	C64-C59	1.415(7)
Yb2-C48	2.630(5)	C64-C63	1.389(7)
Yb2-C44	2.621(5)	C71-C67	1.396(8)
Yb2-C38	2.621(5)	C71-C76	1.514(8)
Yb2-C47	2.641(5)	C4-C3	1.425(7)
Yb2-C35	2.620(5)	C4-C9	1.511(7)
Yb2-C34	2.639(5)	C1-C6	1.497(7)
Yb2-C37	2.614(5)	C3-C8	1.509(7)
Yb2-C46	2.641(5)	C30-C29	1.379(7)
Ni1-K2	3.0966(13)	C45-C44	1.404(8)
Ni1-N4	1.976(4)	C45-C46	1.420(8)
Ni1-N3	1.991(4)	C45-C50	1.512(8)
Ni1-C33	1.938(5)	C14-C13	1.404(8)
Ni1-C32	1.918(5)	C14-C15	1.407(7)
Ni2-K1	3.3335(14)	C14-C19	1.522(7)
Ni2-N8	2.006(4)	C48-C44	1.421(7)
Ni2-N7	1.977(4)	C48-C47	1.407(8)

Ni2-C65	1.919(5)	C48-C53	1.499(8)
Ni2-C66	1.938(5)	C59-C60	1.401(7)
K1-C70	2.997(5)	C44-C49	1.504(8)
K1-C71	3.030(5)	C62-C63	1.380(7)
K1-C68	3.000(6)	C62-C61	1.389(8)
K1-C67	3.027(5)	C38-C34	1.413(7)
K1-C69	2.972(6)	C38-C37	1.415(7)
K1-O1	2.745(12)	C38-C43	1.496(7)
K1-O1A	2.716(9)	C47-C46	1.416(8)
K3-O4 ¹	2.881(4)	C47-C52	1.511(8)
K3-O5 ¹	2.853(4)	C35-C34	1.399(7)
K3-O6 ²	2.789(5)	C35-C40	1.526(8)
K3-C70 ³	3.105(5)	C68-C67	1.413(8)
K3-C71 ³	3.065(5)	C68-C69	1.404(8)
K3-C68 ³	2.952(5)	C68-C73	1.509(8)
K3-C67 ³	2.973(6)	C67-C72	1.511(8)
K3-C69 ³	3.043(6)	C28-C29	1.403(7)
K3-C96 ¹	3.416(7)	C69-C74	1.522(8)
K3-C100 ²	3.514(10)	C13-C12	1.405(8)
K2-O2	2.675(4)	C13-C18	1.520(8)
K2-O3A	2.696(13)	C34-C39	1.510(7)
K2-O3B	2.781(12)	C15-C11	1.423(7)
N4-C26	1.378(6)	C15-C20	1.496(8)
N4-C25	1.339(5)	C37-C42	1.500(8)
O4-C91	1.413(8)	C60-C61	1.376(7)
O4-C89	1.428(8)	C11-C12	1.388(8)
N1-C21	1.403(6)	C11-C16	1.514(7)
N1-C24	1.357(5)	C12-C17	1.500(8)
N2-C25	1.345(5)	O1-C77B	1.383(17)
N2-C31	1.388(6)	O1-C79B	1.461(16)
N8-C57	1.316(6)	C46-C51	1.513(8)
N8-C56	1.474(6)	C99-C100	1.483(10)
N7-C58	1.332(6)	C92-C91	1.469(10)
N7-C59	1.380(6)	C95-C96	1.492(10)
N3-C24	1.312(5)	C90-C89	1.484(10)
N3-C23	1.474(5)	C93-C94	1.482(10)
O5-C95	1.429(7)	C97-C98	1.466(10)
O5-C93	1.419(8)	C83-C84	1.416(9)
N6-C54	1.402(6)	C77B-C78B	1.454(18)
N6-C57	1.354(6)	C79B-C80B	1.423(18)

O6-C99	1.406(8)	C82-C81	1.492(10)
O6-C97	1.445(8)	C86A-C85A	1.474(14)
N5-C58	1.355(5)	C85A-O3A	1.451(14)
N5-C64	1.370(6)	O3A-C87A	1.575(15)
C21-C22	1.330(6)	C87A-C88A	1.296(14)
C58-C57	1.451(6)	C86B-C85B	1.508(14)
C54-C55	1.324(7)	C85B-O3B	1.392(13)
C2-C1	1.412(7)	O3B-C87B	1.803(14)
C2-C3	1.403(7)	C87B-C88B	1.362(15)
C2-C7	1.508(7)	C78A-C77A	1.452(15)
O2-C83	1.472(8)	C77A-O1A	1.354(13)
O2-C81	1.399(8)	O1A-C79A	1.462(13)
C26-C31	1.425(6)	C79A-C80A	1.396(15)
C26-C27	1.396(6)		

¹1-X,2-Y,1-Z; ²+X,+Y,1+Z; ³-1+X,+Y,+Z

N1-Yb1-N2	75.36(13)	C64-N5-Yb2	147.6(3)
N1-Yb1-C2	79.74(14)	C22-C21-N1	123.7(4)
N1-Yb1-C5	122.17(15)	N7-C58-Yb2	162.5(3)
N1-Yb1-C4	131.13(15)	N7-C58-N5	116.2(4)
N1-Yb1-C1	90.55(14)	N7-C58-C57	118.8(4)
N1-Yb1-C3	102.16(14)	N5-C58-Yb2	46.3(2)
N1-Yb1-C14	133.16(14)	N5-C58-C57	125.0(4)
N1-Yb1-C13	106.93(15)	C57-C58-Yb2	78.6(3)
N1-Yb1-C15	120.25(15)	C55-C54-N6	124.2(4)
N1-Yb1-C11	89.19(15)	C1-C2-Yb1	73.0(3)
N1-Yb1-C12	81.88(14)	C1-C2-C7	125.7(5)
N2-Yb1-C2	91.61(14)	C3-C2-Yb1	74.6(3)
N2-Yb1-C5	127.49(14)	C3-C2-C1	108.6(4)
N2-Yb1-C4	97.66(15)	C3-C2-C7	125.4(5)
N2-Yb1-C1	122.84(14)	C7-C2-Yb1	123.4(3)
N2-Yb1-C3	77.13(14)	C83-O2-K2	121.6(4)
N2-Yb1-C14	118.06(15)	C81-O2-K2	124.9(4)
N2-Yb1-C13	135.84(15)	C81-O2-C83	113.4(5)
N2-Yb1-C15	88.53(15)	N4-C26-C31	108.2(4)
N2-Yb1-C11	85.18(16)	N4-C26-C27	131.8(4)
N2-Yb1-C12	112.00(17)	C27-C26-C31	120.0(4)
C2-Yb1-C3	30.88(15)	N8-C57-Yb2	170.6(3)
C2-Yb1-C14	138.38(15)	N8-C57-N6	130.5(4)
C5-Yb1-C2	51.73(15)	N8-C57-C58	113.2(4)

C5-Yb1-C3	51.85(15)	N6-C57-Yb2	42.4(2)
C5-Yb1-C14	86.66(15)	N6-C57-C58	116.3(4)
C5-Yb1-C13	89.62(16)	C58-C57-Yb2	74.3(2)
C5-Yb1-C15	113.29(16)	N4-C25-Yb1	161.5(3)
C5-Yb1-C12	119.00(17)	N4-C25-N2	117.0(4)
C4-Yb1-C2	51.79(15)	N4-C25-C24	117.9(4)
C4-Yb1-C5	31.47(16)	N2-C25-Yb1	47.0(2)
C4-Yb1-C1	52.29(16)	N2-C25-C24	125.0(4)
C4-Yb1-C3	31.59(15)	C24-C25-Yb1	78.9(2)
C4-Yb1-C14	93.34(16)	C54-C55-C56	121.9(4)
C4-Yb1-C13	110.39(17)	N2-C31-C26	108.2(4)
C4-Yb1-C15	107.59(16)	C30-C31-N2	130.8(4)
C4-Yb1-C11	139.14(17)	C30-C31-C26	121.0(4)
C4-Yb1-C12	141.30(17)	C21-C22-C23	120.8(4)
C1-Yb1-C2	31.28(14)	C4-C5-Yb1	73.9(3)
C1-Yb1-C5	31.65(15)	C4-C5-C1	108.0(4)
C1-Yb1-C3	51.78(15)	C4-C5-C10	127.2(5)
C1-Yb1-C14	111.77(16)	C1-C5-Yb1	74.0(3)
C1-Yb1-C13	101.32(16)	C1-C5-C10	123.6(5)
C1-Yb1-C15	142.01(16)	C10-C5-Yb1	127.4(3)
C1-Yb1-C11	150.85(17)	C35-C36-Yb2	74.6(3)
C1-Yb1-C12	120.45(18)	C35-C36-C37	108.2(5)
C3-Yb1-C14	124.21(15)	C35-C36-C41	126.2(6)
C13-Yb1-C2	132.52(16)	C37-C36-Yb2	74.3(3)
C13-Yb1-C3	140.46(16)	C37-C36-C41	125.5(5)
C13-Yb1-C14	30.86(17)	C41-C36-Yb2	121.4(3)
C13-Yb1-C15	51.30(17)	N8-C56-C55	111.6(4)
C15-Yb1-C2	159.20(16)	N8-C56-C23	109.3(4)
C15-Yb1-C3	130.00(16)	C55-C56-C23	112.1(4)
C15-Yb1-C14	30.93(16)	C28-C27-C26	118.3(5)
C11-Yb1-C2	168.92(15)	K1-C70-K3 ⁵	130.17(17)
C11-Yb1-C5	137.40(15)	C71-C70-K1	77.8(3)
C11-Yb1-C3	155.64(18)	C71-C70-K3 ⁵	75.2(3)
C11-Yb1-C14	51.40(15)	C71-C70-C69	107.8(5)
C11-Yb1-C13	51.28(17)	C71-C70-C75	127.4(6)
C11-Yb1-C15	31.55(16)	C69-C70-K1	75.3(3)
C11-Yb1-C12	30.90(18)	C69-C70-K3 ⁵	74.3(3)
C12-Yb1-C2	145.11(17)	C69-C70-C75	124.7(5)
C12-Yb1-C3	170.79(17)	C75-C70-K1	110.1(3)
C12-Yb1-C14	51.29(15)	C75-C70-K3 ⁵	119.6(4)

C12-Yb1-C13	31.13(17)	N5-C64-C59	108.7(4)
C12-Yb1-C15	51.59(17)	N5-C64-C63	131.7(5)
N6-Yb2-N5	74.66(13)	C63-C64-C59	119.6(4)
N6-Yb2-C36	80.79(15)	K1-C71-K3 ⁵	130.46(19)
N6-Yb2-C45	83.12(15)	C70-C71-K1	75.2(3)
N6-Yb2-C48	113.71(15)	C70-C71-K3 ⁵	78.4(3)
N6-Yb2-C44	84.27(15)	C70-C71-C76	125.8(5)
N6-Yb2-C38	130.27(15)	C67-C71-K1	76.6(3)
N6-Yb2-C47	133.31(15)	C67-C71-K3 ⁵	73.0(3)
N6-Yb2-C35	96.23(15)	C67-C71-C70	108.2(5)
N6-Yb2-C34	126.93(15)	C67-C71-C76	126.0(5)
N6-Yb2-C37	99.90(15)	C76-C71-K1	114.1(4)
N6-Yb2-C46	111.50(17)	C76-C71-K3 ⁵	115.4(3)
N5-Yb2-C36	98.16(16)	C5-C4-Yb1	74.6(3)
N5-Yb2-C45	114.88(17)	C5-C4-C3	107.8(4)
N5-Yb2-C48	83.67(15)	C5-C4-C9	127.1(5)
N5-Yb2-C44	85.57(16)	C3-C4-Yb1	75.8(3)
N5-Yb2-C38	96.16(15)	C3-C4-C9	124.9(5)
N5-Yb2-C47	111.28(16)	C9-C4-Yb1	118.8(3)
N5-Yb2-C35	128.67(15)	C2-C1-Yb1	75.8(3)
N5-Yb2-C34	126.96(15)	C2-C1-C5	107.7(4)
N5-Yb2-C37	79.60(15)	C2-C1-C6	126.6(5)
N5-Yb2-C46	133.89(16)	C5-C1-Yb1	74.3(3)
C36-Yb2-C45	137.61(18)	C5-C1-C6	125.3(5)
C36-Yb2-C48	165.21(16)	C6-C1-Yb1	121.9(3)
C36-Yb2-C44	163.01(17)	C2-C3-Yb1	74.5(3)
C36-Yb2-C38	51.68(16)	C2-C3-C4	107.8(4)
C36-Yb2-C47	138.99(17)	C2-C3-C8	125.2(5)
C36-Yb2-C35	31.27(17)	C4-C3-Yb1	72.6(3)
C36-Yb2-C34	51.29(16)	C4-C3-C8	126.5(5)
C36-Yb2-C46	127.86(18)	C8-C3-Yb1	124.8(3)
C45-Yb2-C48	51.46(17)	N1-C24-Yb1	43.7(2)
C45-Yb2-C47	51.61(17)	N1-C24-C25	116.2(4)
C45-Yb2-C34	115.44(18)	N3-C24-Yb1	168.3(3)
C45-Yb2-C46	31.30(18)	N3-C24-N1	130.2(4)
C48-Yb2-C47	30.96(17)	N3-C24-C25	113.5(4)
C48-Yb2-C34	116.26(16)	C25-C24-Yb1	73.4(2)
C48-Yb2-C46	51.28(17)	C29-C30-C31	117.9(5)
C44-Yb2-C45	31.06(17)	C44-C45-Yb2	74.4(3)
C44-Yb2-C48	31.39(16)	C44-C45-C46	108.3(5)

C44-Yb2-C38	144.72(16)	C44-C45-C50	126.1(6)
C44-Yb2-C47	51.68(17)	C46-C45-Yb2	75.1(3)
C44-Yb2-C34	137.27(16)	C46-C45-C50	124.9(6)
C44-Yb2-C46	51.57(17)	C50-C45-Yb2	124.1(4)
C38-Yb2-C45	140.68(18)	C13-C14-Yb1	74.0(3)
C38-Yb2-C48	113.57(16)	C13-C14-C15	108.3(4)
C38-Yb2-C47	95.94(16)	C13-C14-C19	127.3(5)
C38-Yb2-C34	31.17(16)	C15-C14-Yb1	74.0(3)
C38-Yb2-C46	109.42(18)	C15-C14-C19	123.3(5)
C35-Yb2-C45	113.84(18)	C19-C14-Yb1	127.6(3)
C35-Yb2-C48	141.84(17)	C44-C48-Yb2	73.9(3)
C35-Yb2-C44	144.78(18)	C44-C48-C53	125.5(5)
C35-Yb2-C38	51.60(16)	C47-C48-Yb2	74.9(3)
C35-Yb2-C47	110.89(18)	C47-C48-C44	108.4(5)
C35-Yb2-C34	30.86(16)	C47-C48-C53	125.8(5)
C35-Yb2-C46	96.85(17)	C53-C48-Yb2	122.3(4)
C34-Yb2-C47	87.81(17)	N7-C59-C64	108.0(4)
C34-Yb2-C46	87.21(17)	N7-C59-C60	131.1(5)
C37-Yb2-C36	31.31(17)	C60-C59-C64	120.8(4)
C37-Yb2-C45	165.40(18)	N3-C23-C22	110.5(3)
C37-Yb2-C48	136.68(17)	N3-C23-C56	108.4(3)
C37-Yb2-C44	162.85(18)	C22-C23-C56	113.3(4)
C37-Yb2-C38	31.35(16)	C45-C44-Yb2	74.6(3)
C37-Yb2-C47	126.78(17)	C45-C44-C48	107.7(5)
C37-Yb2-C35	51.77(17)	C45-C44-C49	126.1(5)
C37-Yb2-C34	51.52(16)	C48-C44-Yb2	74.7(3)
C37-Yb2-C46	138.34(17)	C48-C44-C49	126.1(6)
C46-Yb2-C47	31.09(18)	C49-C44-Yb2	119.6(4)
N4-Ni1-K2	113.95(11)	C63-C62-C61	120.6(5)
N4-Ni1-N3	82.68(15)	C34-C38-Yb2	75.1(3)
N3-Ni1-K2	107.21(11)	C34-C38-C37	107.7(5)
C33-Ni1-K2	72.94(18)	C34-C38-C43	126.2(5)
C33-Ni1-N4	94.03(19)	C37-C38-Yb2	74.1(3)
C33-Ni1-N3	176.5(2)	C37-C38-C43	125.9(5)
C32-Ni1-K2	80.46(18)	C43-C38-Yb2	121.1(3)
C32-Ni1-N4	165.4(2)	C48-C47-Yb2	74.1(3)
C32-Ni1-N3	95.47(19)	C48-C47-C46	107.8(5)
C32-Ni1-C33	88.0(2)	C48-C47-C52	125.5(6)
N8-Ni2-K1	117.33(11)	C46-C47-Yb2	74.4(3)
N7-Ni2-K1	128.75(12)	C46-C47-C52	126.0(6)

N7-Ni2-N8	82.11(15)	C52-C47-Yb2	124.9(4)
C65-Ni2-K1	64.42(17)	C36-C35-Yb2	74.2(3)
C65-Ni2-N8	92.74(19)	C36-C35-C40	124.9(5)
C65-Ni2-N7	166.8(2)	C34-C35-Yb2	75.3(3)
C65-Ni2-C66	92.1(2)	C34-C35-C36	108.0(5)
C66-Ni2-K1	64.78(18)	C34-C35-C40	126.9(5)
C66-Ni2-N8	175.2(2)	C40-C35-Yb2	121.0(4)
C66-Ni2-N7	93.2(2)	K3 ⁵ -C68-K1	136.8(2)
C70-K1-Ni2	126.33(12)	C67-C68-K1	77.5(3)
C70-K1-C71	26.98(14)	C67-C68-K3 ⁵	77.0(3)
C70-K1-C68	44.67(15)	C67-C68-C73	124.8(6)
C70-K1-C67	44.27(14)	C69-C68-K1	75.3(3)
C71-K1-Ni2	115.24(11)	C69-C68-K3 ⁵	80.1(3)
C68-K1-Ni2	155.16(13)	C69-C68-C67	107.8(5)
C68-K1-C71	44.36(15)	C69-C68-C73	127.3(6)
C68-K1-C67	27.12(16)	C73-C68-K1	111.2(4)
C67-K1-Ni2	128.08(12)	C73-C68-K3 ⁵	111.9(4)
C67-K1-C71	26.64(14)	K3 ⁵ -C67-K1	134.5(2)
C69-K1-Ni2	153.50(12)	C71-C67-K1	76.8(3)
C69-K1-C70	27.46(15)	C71-C67-K3 ⁵	80.3(3)
C69-K1-C71	44.67(15)	C71-C67-C68	108.3(5)
C69-K1-C68	27.18(16)	C71-C67-C72	124.4(6)
C69-K1-C67	44.59(15)	C68-C67-K1	75.4(3)
O1-K1-Ni2	92.6(6)	C68-C67-K3 ⁵	75.4(3)
O1-K1-C70	115.3(6)	C68-C67-C72	127.3(6)
O1-K1-C71	141.9(6)	C72-C67-K1	115.0(4)
O1-K1-C68	112.2(6)	C72-C67-K3 ⁵	110.3(4)
O1-K1-C67	139.3(6)	C27-C28-C29	121.4(5)
O1-K1-C69	99.7(6)	K1-C69-K3 ⁵	133.9(2)
O1A-K1-Ni2	84.1(4)	C70-C69-K1	77.3(3)
O1A-K1-C70	120.4(4)	C70-C69-K3 ⁵	79.1(3)
O1A-K1-C71	147.4(4)	C70-C69-C74	126.2(6)
O1A-K1-C68	120.7(4)	C68-C69-K1	77.5(3)
O1A-K1-C67	147.8(4)	C68-C69-K3 ⁵	72.9(3)
O1A-K1-C69	107.2(4)	C68-C69-C70	107.8(5)
O4 ¹ -K3-C70 ²	137.59(14)	C68-C69-C74	125.9(6)
O4 ¹ -K3-C71 ²	161.22(14)	C74-C69-K1	108.4(4)
O4 ¹ -K3-C68 ²	119.59(15)	C74-C69-K3 ⁵	117.6(4)
O4 ¹ -K3-C67 ²	143.68(15)	C14-C13-Yb1	75.1(3)
O4 ¹ -K3-C69 ²	117.38(14)	C14-C13-C12	108.0(5)

O4 ¹ -K3-C96 ¹	110.03(16)	C14-C13-C18	126.0(5)
O4 ¹ -K3-C100 ³	69.87(18)	C12-C13-Yb1	73.4(3)
O5 ¹ -K3-O4 ¹	84.37(13)	C12-C13-C18	125.4(6)
O5 ¹ -K3-C70 ²	133.43(14)	C18-C13-Yb1	124.6(4)
O5 ¹ -K3-C71 ²	107.80(14)	C38-C34-Yb2	73.7(3)
O5 ¹ -K3-C68 ²	104.46(15)	C38-C34-C39	125.1(5)
O5 ¹ -K3-C67 ²	91.54(14)	C35-C34-Yb2	73.8(3)
O5 ¹ -K3-C69 ²	131.37(15)	C35-C34-C38	108.4(5)
O5 ¹ -K3-C96 ¹	43.63(16)	C35-C34-C39	125.4(5)
O5 ¹ -K3-C100 ³	137.17(19)	C39-C34-Yb2	128.1(4)
O6 ³ -K3-O4 ¹	99.75(14)	C62-C63-C64	119.3(5)
O6 ³ -K3-O5 ¹	115.99(13)	C14-C15-Yb1	75.0(3)
O6 ³ -K3-C70 ²	81.57(14)	C14-C15-C11	107.1(5)
O6 ³ -K3-C71 ²	87.89(15)	C14-C15-C20	126.5(5)
O6 ³ -K3-C68 ²	125.68(15)	C11-C15-Yb1	73.1(3)
O6 ³ -K3-C67 ²	114.25(16)	C11-C15-C20	126.0(5)
O6 ³ -K3-C69 ²	103.10(15)	C20-C15-Yb1	123.2(4)
O6 ³ -K3-C96 ¹	76.96(17)	C36-C37-Yb2	74.4(3)
O6 ³ -K3-C100 ³	41.82(17)	C36-C37-C38	107.7(5)
C70 ² -K3-C96 ¹	111.48(18)	C36-C37-C42	126.1(5)
C70 ² -K3-C100 ³	85.55(19)	C38-C37-Yb2	74.6(3)
C71 ² -K3-C70 ²	26.34(14)	C38-C37-C42	125.7(5)
C71 ² -K3-C96 ¹	88.34(17)	C42-C37-Yb2	123.0(4)
C71 ² -K3-C100 ³	106.86(19)	C61-C60-C59	117.7(5)
C68 ² -K3-C70 ²	44.11(14)	C30-C29-C28	121.4(5)
C68 ² -K3-C71 ²	44.42(16)	C60-C61-C62	122.0(5)
C68 ² -K3-C67 ²	27.59(16)	C15-C11-Yb1	75.3(3)
C68 ² -K3-C69 ²	27.02(15)	C15-C11-C16	126.5(6)
C68 ² -K3-C96 ¹	116.8(2)	C12-C11-Yb1	74.6(3)
C68 ² -K3-C100 ³	117.9(2)	C12-C11-C15	108.3(5)
C67 ² -K3-C70 ²	43.79(14)	C12-C11-C16	125.2(6)
C67 ² -K3-C71 ²	26.67(15)	C16-C11-Yb1	116.9(3)
C67 ² -K3-C69 ²	44.45(15)	C13-C12-Yb1	75.4(3)
C67 ² -K3-C96 ¹	90.53(18)	C13-C12-C17	125.4(6)
C67 ² -K3-C100 ³	129.3(2)	C11-C12-Yb1	74.5(3)
C69 ² -K3-C70 ²	26.62(15)	C11-C12-C13	108.4(5)
C69 ² -K3-C71 ²	43.86(15)	C11-C12-C17	125.9(6)
C69 ² -K3-C96 ¹	131.63(18)	C17-C12-Yb1	121.8(4)
C69 ² -K3-C100 ³	91.29(19)	C77B-O1-K1	121.5(16)
C96 ¹ -K3-C100 ³	114.2(2)	C77B-O1-C79B	113.4(14)

O2-K2-Ni1	151.30(11)	C79B-O1-K1	114.6(11)
O3A-K2-Ni1	99.7(3)	C45-C46-Yb2	73.6(3)
O3B-K2-Ni1	90.5(2)	C45-C46-C51	123.0(6)
C26-N4-Ni1	143.8(3)	C47-C46-Yb2	74.5(3)
C25-N4-Ni1	108.2(3)	C47-C46-C45	107.8(5)
C25-N4-C26	103.6(4)	C47-C46-C51	128.5(6)
C91-O4-K3 ¹	124.3(4)	C51-C46-Yb2	124.9(4)
C91-O4-C89	113.1(5)	O6-C99-C100	108.8(6)
C89-O4-K3 ¹	122.4(4)	O5-C95-C96	109.6(6)
C21-N1-Yb1	131.8(3)	O4-C91-C92	111.6(6)
C24-N1-Yb1	112.5(3)	O4-C89-C90	109.9(6)
C24-N1-C21	112.2(4)	O5-C93-C94	110.4(6)
C25-N2-Yb1	108.0(3)	C95-C96-K3 ¹	89.7(4)
C25-N2-C31	103.0(4)	O6-C97-C98	114.7(7)
C31-N2-Yb1	147.1(3)	C84-C83-O2	109.6(6)
C57-N8-Ni2	112.4(3)	C99-C100-K3 ⁴	85.8(5)
C57-N8-C56	118.3(4)	O1-C77B-C78B	110.8(18)
C56-N8-Ni2	129.1(3)	C80B-C79B-O1	107.2(17)
C58-N7-Ni2	108.8(3)	O2-C81-C82	111.6(6)
C58-N7-C59	103.8(4)	O3A-C85A-C86A	112.3(13)
C59-N7-Ni2	142.7(3)	C85A-O3A-K2	119.5(10)
C24-N3-Ni1	111.3(3)	C85A-O3A-C87A	104.3(11)
C24-N3-C23	116.8(4)	C87A-O3A-K2	128.7(8)
C23-N3-Ni1	131.8(3)	C88A-C87A-O3A	92.5(13)
C95-O5-K3 ¹	116.7(4)	O3B-C85B-C86B	111.6(12)
C93-O5-K3 ¹	129.1(4)	C85B-O3B-K2	132.1(9)
C93-O5-C95	112.9(5)	C85B-O3B-C87B	100.2(9)
C54-N6-Yb2	132.1(3)	C87B-O3B-K2	124.1(7)
C57-N6-Yb2	114.5(3)	C88B-C87B-O3B	70.3(10)
C57-N6-C54	112.6(4)	O1A-C77A-C78A	115.8(11)
C99-O6-K3 ⁴	121.0(4)	C77AO1A-K1	130.6(9)
C99-O6-C97	113.2(5)	C77A-O1A-C79A	113.4(10)
C97-O6-K3 ⁴	119.7(4)	C79A-O1A-K1	115.0(8)
C58-N5-Yb2	109.1(3)	C80A-C79A-O1A	113.6(14)
C58-N5-C64	103.3(4)		

¹1-X,2-Y,1-Z; ²-1+X,+Y,+Z; ³+X,+Y,1+Z; ⁴+X,+Y,-1+Z; ⁵1+X,+Y,+Z

Table S9. Distances (Å) and angles (deg) for K(18-c-6)(bimpmp)Ni(CH₃)₂ (**4**).

Ni(2)-N(5)	1.9712(17)	Ni(1)-N(1)	1.9853(19)
Ni(2)-N(7)	1.9635(17)	Ni(1)-N(3)	1.9633(19)

Ni(2)-C(37)	1.931(2)	Ni(1)C(12)	1.921(2)
Ni(2)-C(38)	1.924(2)	Ni(1)-C(13)	1.920(3)
K(2)-O(12)	2.8195(19)	K(1)-O(6)	2.8091(18)
K(2)-O(7)	2.9331(18)	K(1)-O(3)	2.8395(17)
K(2)-O(8)	3.0075(18)	K(1)-O(2)	2.9067(17)
K(2)-O(9)	2.9007(19)	K(1)-O(5)	3.0549(18)
K(2)-O(11)	2.8719(19)	K(1)-O(1)	2.8982(17)
K(2)-O(10)	3.007(2)	K(1)-O(4)	3.0419(18)
K(2)-N(6)	2.9780(19)	K(1)-N(2)	2.990(2)
K(2)-N(8)	3.0411(18)	K(1)-N(4)	2.9139(19)
O(12)-C(42)	1.414(4)	O(6)-C(23)	1.406(3)
O(12)-C(43)	1.429(4)	O(6)-C(24)	1.424(3)
O(7)-C(48)	1.414(4)	O(3)-C(17)	1.426(3)
O(7)-C(49)	1.434(4)	O(3)-C(18)	1.424(3)
O(8)-C(39)	1.436(4)	O(2)-C(15)	1.425(3)
O(8)-C(50)	1.411(4)	O(2)-C(16)	1.423(3)
O(9)-C(40)	1.412(4)	O(5)-C(21)	1.423(3)
O(9)-C(41)	1.427(4)	O(5)-C(22)	1.413(3)
O(11)-C(44)	1.415(4)	O(1)-C(14)	1.420(3)
O(11)-C(45)	1.437(4)	O(1)-C(25)	1.426(3)
O(10)-C(46)	1.419(4)	O(4)-C(19)	1.430(3)
O(10)-C(47)	1.413(4)	O(4)-C(20)	1.421(3)
N(5)-C(26)	1.358(3)	N(1)-C(1)	1.358(3)
N(5)-C(27)	1.340(3)	N(1)-C(2)	1.338(3)
N(6)-C(26)	1.335(3)	N(2)-C(1)	1.331(3)
N(6)-C(29)	1.342(3)	N(2)-C(4)	1.343(3)
N(7)-C(30)	1.357(2)	N(3)-C(5)	1.356(3)
N(7)-C(36)	1.373(3)	N(3)-C(11)	1.384(3)
N(8)-C(30)	1.339(3)	N(4)-C(5)	1.336(3)
N(8)-C(31)	1.383(3)	N(4)-C(6)	1.377(3)
C(26)-C(30)	1.457(3)	C(1)-C(5)	1.455(3)
C(27)-C(28)	1.374(3)	C(2)-C(3)	1.377(3)
C(28)-C(29)	1.376(3)	C(3)-C(4)	1.384(4)
C(31)-C(32)	1.403(3)	C(6)-C(7)	1.403(3)
C(31)-C(36)	1.425(3)	C(6)-C(11)	1.426(3)
C(32)-C(33)	1.378(3)	C(7)-C(8)	1.369(4)
C(33)-C(34)	1.401(3)	C(8)-C(9)	1.398(4)
C(34)-C(35)	1.378(3)	C(9)-C(10)	1.378(4)
C(35)-C(36)	1.404(3)	C(10)-C(11)	1.400(3)
C(39)-C(40)	1.479(5)	C(14)-C(15)	1.487(4)
C(41)-C(42)	1.481(5)	C(16)-C(17)	1.495(4)
C(43)-C(44)	1.480(5)	C(18)-C(19)	1.506(4)
C(45)-C(46)	1.471(6)	C(20)-C(21)	1.494(4)
C(47)-C(48)	1.483(6)	C(22)-C(23)	1.494(4)

C(49)-C(50)	1.478(5)	C(24)-C(25)	1.495(4)
N(7)-Ni(2)-N(5)	81.30(7)	N(3)-Ni(1)-N(1)	81.92(8)
C(37)-Ni(2)-N(5)	171.45(9)	C(12)-Ni(1)-N(1)	176.27(10)
C(37)-Ni(2)-N(7)	97.15(9)	C(12)-Ni(1)-N(3)	94.58(10)
C(38)-Ni(2)-N(5)	94.13(9)	C(13)-Ni(1)-N(1)	93.21(10)
C(38)-Ni(2)-N(7)	173.93(9)	C(13)-Ni(1)-N(3)	175.03(10)
C(38)-Ni(2)-C(37)	87.96(11)	C(13)-Ni(1)-C(12)	90.31(12)
O(12)-K(2)-O(7)	139.46(5)	O(6)-K(1)-O(3)	163.20(5)
O(12)-K(2)-O(8)	104.74(6)	O(6)-K(1)-O(2)	113.38(5)
O(12)-K(2)-O(9)	57.93(7)	O(6)-K(1)-O(5)	56.07(5)
O(12)-K(2)-O(11)	59.45(7)	O(6)-K(1)-O(1)	60.42(5)
O(12)-K(2)-O(10)	108.31(7)	O(6)-K(1)-O(4)	110.13(5)
O(12)-K(2)-N(6)	151.01(5)	O(6)-K(1)-N(2)	125.31(5)
O(12)-K(2)-N(8)	92.25(5)	O(6)-K(1)-N(4)	70.30(5)
O(7)-K(2)-O(8)	56.37(6)	O(3)-K(1)-O(2)	59.62(5)
O(7)-K(2)-O(10)	55.47(6)	O(3)-K(1)-O(5)	110.62(5)
O(7)-K(2)-N(6)	69.53(5)	O(3)-K(1)-O(1)	116.69(5)
O(7)-K(2)-N(8)	128.22(5)	O(3)-K(1)-O(4)	58.85(5)
O(8)-K(2)-O(10)	106.08(6)	O(3)-K(1)-N(2)	70.55(5)
O(8)-K(2)-N(8)	125.95(5)	O(3)-K(1)-N(4)	126.49(5)
O(9)-K(2)-O(7)	111.28(6)	O(2)-K(1)-O(5)	112.55(5)
O(9)-K(2)-O(8)	55.32(6)	O(2)-K(1)-O(4)	97.33(5)
O(9)-K(2)-O(10)	144.56(6)	O(2)-K(1)-N(2)	82.39(5)
O(9)-K(2)-N(6)	120.14(6)	O(2)-K(1)-N(4)	124.09(5)
O(9)-K(2)-N(8)	97.45(5)	O(1)-K(1)-O(2)	57.38(5)
O(11)-K(2)-O(7)	111.41(6)	O(1)-K(1)-O(5)	98.11(5)
O(11)-K(2)-O(8)	142.46(5)	O(1)-K(1)-O(4)	134.72(5)
O(11)-K(2)-O(9)	117.08(7)	O(1)-K(1)-N(2)	95.47(5)
O(11)-K(2)-O(10)	56.72(7)	O(1)-K(1)-N(4)	85.87(5)
O(11)-K(2)-N(6)	116.94(6)	O(4)-K(1)-O(5)	54.31(5)
O(11)-K(2)-N(8)	90.30(5)	N(2)-K(1)-O(5)	163.73(5)
O(10)-K(2)-N(8)	116.55(6)	N(2)-K(1)-O(4)	119.60(5)
N(6)-K(2)-O(8)	93.05(5)	N(4)-K(1)-O(5)	113.18(5)
N(6)-K(2)-O(10)	87.87(6)	N(4)-K(1)-O(4)	135.55(5)
N(6)-K(2)-N(8)	58.79(5)	N(4)-K(1)-N(2)	58.88(5)
C(42)-O(12)-K(2)	110.57(18)	C(23)-O(6)-K(1)	124.79(15)
C(42)-O(12)-C(43)	112.2(2)	C(23)-O(6)-C(24)	113.1(2)
C(43)-O(12)-K(2)	111.82(18)	C(24)-O(6)-K(1)	111.21(14)
C(48)-O(7)-K(2)	121.58(19)	C(17)-O(3)-K(1)	115.83(13)
C(48)-O(7)-C(49)	112.4(2)	C(18)-O(3)-K(1)	113.46(14)
C(49)-O(7)-K(2)	120.15(17)	C(18)-O(3)-C(17)	112.29(18)
C(39)-O(8)-K(2)	110.38(15)	C(15)-O(2)-K(1)	113.83(13)
C(50)-O(8)-K(2)	109.55(15)	C(16)-O(2)-K(1)	112.17(13)

C(50)-O(8)-C(39)	111.9(2)	C(16)-O(2)-C(15)	111.42(19)
C(40)-O(9)-K(2)	124.53(18)	C(21)-O(5)-K(1)	118.83(15)
C(40)-O(9)-C(41)	111.1(2)	C(22)-O(5)-K(1)	111.03(15)
C(41)-O(9)-K(2)	117.53(18)	C(22)-O(5)-C(21)	111.85(19)
C(44)-O(11)-K(2)	115.58(19)	C(14)-O(1)-K(1)	119.79(14)
C(44)-O(11)-C(45)	112.8(3)	C(14)-O(1)-C(25)	112.6(2)
C(45)-O(11)-K(2)	120.6(2)	C(25)-O(1)-K(1)	115.24(14)
C(46)-O(10)-K(2)	105.43(18)	C(19)-O(4)-K(1)	114.44(13)
C(47)-O(10)-K(2)	109.08(17)	C(20)-O(4)-K(1)	118.76(14)
C(47)-O(10)-C(46)	112.1(3)	C(20)-O(4)-C(19)	111.09(19)
C(26)-N(5)-Ni(2)	114.83(14)	C(1)-N(1)-Ni(1)	114.48(15)
C(27)-N(5)-Ni(2)	129.13(15)	C(2)-N(1)-Ni(1)	129.90(16)
C(27)-N(5)-C(26)	115.62(18)	C(2)-N(1)-C(1)	115.62(19)
C(26)-N(6)-K(2)	119.06(13)	C(1)-N(2)-K(1)	113.73(14)
C(26)-N(6)-C(29)	116.06(19)	C(1)-N(2)-C(4)	116.4(2)
C(29)-N(6)-K(2)	124.87(14)	C(4)-N(2)-K(1)	127.32(15)
C(30)-N(7)-Ni(2)	113.49(13)	C(5)-N(3)-Ni(1)	113.87(15)
C(30)-N(7)-C(36)	102.83(16)	C(5)-N(3)-C(11)	102.66(18)
C(36)-N(7)-Ni(2)	142.17(14)	C(11)-N(3)-Ni(1)	143.47(15)
C(30)-N(8)-K(2)	113.78(12)	C(5)-N(4)-K(1)	113.17(13)
C(30)-N(8)-C(31)	101.81(16)	C(5)-N(4)-C(6)	101.68(18)
C(31)-N(8)-K(2)	143.60(13)	C(6)-N(4)-K(1)	140.27(15)
N(5)-C(26)-C(30)	112.92(17)	N(1)-C(1)-C(5)	113.44(19)
N(6)-C(26)-N(5)	125.98(19)	N(2)-C(1)-N(1)	126.4(2)
N(6)-C(26)-C(30)	121.10(18)	N(2)-C(1)-C(5)	120.13(19)
N(5)-C(27)-C(28)	122.7(2)	N(1)-C(2)-C(3)	122.2(2)
C(27)-C(28)-C(29)	117.0(2)	C(2)-C(3)-C(4)	117.8(2)
N(6)-C(29)-C(28)	122.6(2)	N(2)-C(4)-C(3)	121.6(2)
N(7)-C(30)-C(26)	115.08(18)	N(3)-C(5)-C(1)	115.93(19)
N(8)-C(30)-N(7)	117.88(18)	N(4)-C(5)-N(3)	118.27(19)
N(8)-C(30)-C(26)	127.03(18)	N(4)-C(5)-C(1)	125.63(19)
N(8)-C(31)-C(32)	130.44(19)	N(4)-C(6)-C(7)	129.1(2)
N(8)-C(31)-C(36)	109.53(18)	N(4)-C(6)-C(11)	110.2(2)
C(32)-C(31)-C(36)	120.03(19)	C(7)-C(6)-C(11)	120.7(2)
C(33)-C(32)-C(31)	118.2(2)	C(8)-C(7)-C(6)	117.8(2)
C(32)-C(33)-C(34)	121.5(2)	C(7)-C(8)-C(9)	121.7(2)
C(35)-C(34)-C(33)	121.6(2)	C(10)-C(9)-C(8)	122.0(2)
C(34)-C(35)-C(36)	117.9(2)	C(9)-C(10)-C(11)	117.6(2)
N(7)-C(36)-C(31)	107.87(17)	N(3)-C(11)-C(6)	107.22(18)
N(7)-C(36)-C(35)	131.51(19)	N(3)-C(11)-C(10)	132.4(2)
C(35)-C(36)-C(31)	120.57(19)	C(10)-C(11)-C(6)	120.3(2)
O(8)-C(39)-C(40)	109.7(2)	O(1)-C(14)-C(15)	109.1(2)
O(9)-C(40)-C(39)	109.0(3)	O(2)-C(15)-C(14)	109.7(2)
O(9)-C(41)-C(42)	108.7(2)	O(2)-C(16)-C(17)	109.34(19)

O(12)-C(42)-C(41)	108.5(2)	O(3)-C(17)-C(16)	109.58(18)
O(12)-C(43)-C(44)	108.7(3)	O(3)-C(18)-C(19)	113.6(2)
O(11)-C(44)-C(43)	109.1(2)	O(4)-C(19)-C(18)	108.4(2)
O(11)-C(45)-C(46)	108.8(3)	O(4)-C(20)-C(21)	108.8(2)
O(10)-C(46)-C(45)	107.9(3)	O(5)-C(21)-C(20)	108.7(2)
O(10)-C(47)-C(48)	108.1(3)	O(5)-C(22)-C(23)	108.8(2)
O(7)-C(48)-C(47)	109.0(2)	O(6)-C(23)-C(22)	109.2(2)
O(7)-C(49)-C(50)	109.3(2)	O(6)-C(24)-C(25)	112.5(2)
O(8)-C(50)-C(49)	109.3(2)	O(1)-C(25)-C(24)	108.1(2)

Table S10. Distances (\AA) and angles (deg) for $[\text{K}(18\text{-c-}6)\text{Cp}^*\text{Yb(bimpmp)}\text{NiMe}_2]_2$ (**5**).

Yb(1)-N(1)	2.341(14)	C(36)-C(35)	1.416(8)
Yb(1)-N(2)	2.297(15)	C(36)-C(41)	1.506(8)
Yb(1)-C(1)	2.610(16)	C(37)-C(38)	1.417(8)
Yb(1)-C(2)	2.58(2)	C(37)-C(42)	1.506(8)
Yb(1)-C(3)	2.596(19)	C(38)-C(34)	1.416(8)
Yb(1)-C(4)	2.627(18)	C(38)-C(43)	1.506(8)
Yb(1)-C(5)	2.640(19)	C(34)-C(35)	1.417(8)
Yb(1)-C(11)	2.711(12)	C(34)-C(39)	1.506(8)
Yb(1)-C(12)	2.674(12)	C(35)-C(40)	1.506(8)
Yb(1)-C(13)	2.658(12)	C(44)-C(45)	1.40(3)
Yb(1)-C(14)	2.685(12)	C(44)-C(48)	1.44(3)
Yb(1)-C(15)	2.717(11)	C(44)-C(49)	1.51(3)
Yb(2)-N(5)	2.331(14)	C(45)-C(46)	1.40(3)
Yb(2)-N(6)	2.336(12)	C(45)-C(50)	1.50(3)
Yb(2)-C(36)	2.669(13)	C(46)-C(47)	1.41(3)
Yb(2)-C(37)	2.659(13)	C(46)-C(51)	1.47(3)
Yb(2)-C(38)	2.688(13)	C(47)-C(48)	1.43(3)
Yb(2)-C(34)	2.714(12)	C(47)-C(52)	1.48(3)
Yb(2)-C(35)	2.702(12)	C(48)-C(53)	1.54(3)
Yb(2)-C(44)	2.648(19)	C(54)-C(55)	1.34(2)
Yb(2)-C(45)	2.68(2)	C(55)-C(56)	1.49(3)
Yb(2)-C(46)	2.65(2)	C(57)-C(58)	1.45(2)
Yb(2)-C(47)	2.605(19)	C(59)-C(60)	1.39(3)
Yb(2)-C(48)	2.63(2)	C(59)-C(64)	1.43(3)
Ni(1)-N(3)	2.083(14)	C(60)-C(61)	1.38(3)
Ni(1)-N(4)	1.967(16)	C(61)-C(62)	1.37(3)
Ni(1)-C(32)	1.89(2)	C(62)-C(63)	1.34(3)
Ni(1)-C(33)	1.903(18)	C(63)-C(64)	1.39(2)
Ni(1)-K(1)	3.389(6)	C(65)-K(2)	3.13(2)
Ni(2)-N(7)	1.992(15)	C(66)-K(2)	3.24(2)
Ni(2)-N(8)	2.013(15)	K(2)-O(8)	2.84(3)
Ni(2)-C(65)	1.924(18)	K(2)-O(9)	2.88(3)

Ni(2)-C(66)	1.937(18)	K(2)-O(10)	2.88(2)
Ni(2)-K(2)	3.809(6)	K(2)-O(11)	2.96(2)
N(1)-C(21)	1.42(2)	K(2)-O(12)	2.68(2)
N(1)-C(24)	1.30(2)	K(2)-O(13)	2.91(3)
Yb(1)-N(1)	2.341(14)	C(36)-C(35)	1.416(8)
Yb(1)-N(2)	2.297(15)	C(36)-C(41)	1.506(8)
Yb(1)-C(1)	2.610(16)	C(37)-C(38)	1.417(8)
Yb(1)-C(2)	2.58(2)	C(37)-C(42)	1.506(8)
Yb(1)-C(3)	2.596(19)	C(38)-C(34)	1.416(8)
Yb(1)-C(4)	2.627(18)	C(38)-C(43)	1.506(8)
Yb(1)-C(5)	2.640(19)	C(34)-C(35)	1.417(8)
Yb(1)-C(11)	2.711(12)	C(34)-C(39)	1.506(8)
Yb(1)-C(12)	2.674(12)	C(35)-C(40)	1.506(8)
Yb(1)-C(13)	2.658(12)	C(44)-C(45)	1.40(3)
Yb(1)-C(14)	2.685(12)	C(44)-C(48)	1.44(3)
Yb(1)-C(15)	2.717(11)	C(44)-C(49)	1.51(3)
Yb(2)-N(5)	2.331(14)	C(45)-C(46)	1.40(3)
Yb(2)-N(6)	2.336(12)	C(45)-C(50)	1.50(3)
Yb(2)-C(36)	2.669(13)	C(46)-C(47)	1.41(3)
Yb(2)-C(37)	2.659(13)	C(46)-C(51)	1.47(3)
Yb(2)-C(38)	2.688(13)	C(47)-C(48)	1.43(3)
Yb(2)-C(34)	2.714(12)	C(47)-C(52)	1.48(3)
Yb(2)-C(35)	2.702(12)	C(48)-C(53)	1.54(3)
Yb(2)-C(44)	2.648(19)	C(54)-C(55)	1.34(2)
Yb(2)-C(45)	2.68(2)	C(55)-C(56)	1.49(3)
Yb(2)-C(46)	2.65(2)	C(57)-C(58)	1.45(2)
Yb(2)-C(47)	2.605(19)	C(59)	C(60)
Yb(2)-C(48)	2.63(2)	C(59)-C(64)	1.43(3)
Ni(1)-N(3)	2.083(14)	C(60)	C(61)
Ni(1)-N(4)	1.967(16)	C(61)	C(62)
Ni(1)-C(32)	1.89(2)	C(62)-C(63)	1.34(3)
Ni(1)-C(33)	1.903(18)	C(63)-C(64)	1.39(2)
Ni(1)-K(1)	3.389(6)	C(65)-K(2)	3.13(2)
Ni(2)-N(7)	1.992(15)	C(66)-K(2)	3.24(2)
Ni(2)-N(8)	2.013(15)	K(2)-O(8)	2.84(3)
Ni(2)-C(65)	1.924(18)	K(2)-O(9)	2.88(3)
Ni(2)-C(66)	1.937(18)	K(2)-O(10)	2.88(2)
Ni(2)-K(2)	3.809(6)	K(2)-O(11)	2.96(2)
N(1)-C(21)	1.42(2)	K(2)-O(12)	2.68(2)
N(1)-C(24)	1.30(2)	K(2)-O(13)	2.91(3)
N(2)-C(25)	1.29(3)	O(8)-C(84)	1.27(4)
N(2)-C(31)	1.40(2)	O(8)-C(85)	1.24(4)
N(3)-C(23)	1.48(2)	O(9)-C(86)	1.38(4)
N(3)-C(24)	1.33(2)	O(9)-C(87)	1.51(4)

N(4)-C(25)	1.35(3)	O(10)-C(88)	1.37(4)
N(4)-C(26)	1.35(2)	O(10)-C(89)	1.43(4)
N(5)-C(58)	1.39(2)	O(11)-C(90)	1.11(3)
N(5)-C(64)	1.40(2)	O(11)-C(91)	1.45(4)
N(6)-C(54)	1.39(2)	O(12)-C(92)	1.25(3)
N(6)-C(57)	1.31(2)	O(12)-C(93)	1.53(3)
N(7)-C(58)	1.31(2)	O(13)-C(83)	1.46(4)
N(7)-C(59)	1.34(2)	O(13)-C(94)	1.24(4)
N(8)-C(56)	1.55(2)	C(83)-C(84)	1.39(2)
N(8)-C(57)	1.33(2)	C(85)-C(86)	1.39(2)
C(1)-C(2)	1.42(3)	C(87)-C(88)	1.38(2)
C(1)-C(5)	1.24(3)	C(89)-C(90)	1.38(2)
C(1)-C(6)	1.54(2)	C(91)-C(92)	1.38(2)
C(2)-C(3)	1.39(3)	C(93)-C(94)	1.36(2)
C(2)-C(7)	1.53(3)	K(1)-O(1)	2.755(16)
C(3)-C(4)	1.41(3)	K(1)-O(2)	2.825(14)
C(3)-C(8)	1.53(3)	K(1)-O(3)	2.792(14)
C(4)-C(5)	1.43(2)	K(1)-O(4)	2.841(16)
C(4)-C(9)	1.51(3)	K(1)-O(5)	2.823(14)
C(5)-C(10)	1.52(3)	K(1)-O(6)	2.920(14)
C(11)-C(12)	1.415(6)	O(1)-C(68)	1.45(3)
C(11)-C(15)	1.416(6)	O(1)-C(69)	1.36(3)
C(11)-C(16)	1.505(7)	O(2)-C(70)	1.39(3)
C(12)-C(13)	1.415(6)	O(2)-C(71)	1.41(3)
C(12)-C(17)	1.505(7)	O(3)-C(72)	1.38(3)
C(13)-C(14)	1.416(6)	O(3)-C(73)	1.41(3)
C(13)-C(18)	1.504(7)	O(4)-C(74)	1.42(2)
C(14)-C(15)	1.416(6)	O(4)-C(75)	1.46(3)
C(14)-C(19)	1.505(7)	O(5)-C(76)	1.45(2)
C(15)-C(20)	1.504(7)	O(5)-C(77)	1.41(3)
C(21)-C(22)	1.29(2)	O(6)-C(67)	1.38(3)
C(22)-C(23)	1.50(3)	O(6)-C(78)	1.40(3)
C(23)-C(56)	1.56(3)	C(67)-C(68)	1.52(4)
C(24)-C(25)	1.50(2)	C(69)-C(70)	1.46(4)
C(26)-C(27)	1.40(3)	C(71)-C(72)	1.44(3)
C(26)-C(31)	1.45(3)	C(73)-C(74)	1.53(3)
C(27)-C(28)	1.30(3)	C(75)-C(76)	1.47(3)
C(28)-C(29)	1.36(3)	C(77)-C(78)	1.55(4)
C(29)-C(30)	1.41(3)	O(7)-C(79)	1.38(3)
C(30)-C(31)	1.36(2)	O(7)-C(81)	1.47(3)
C(32)-K(1)	3.14(2)	C(79)-C(80)	1.48(4)
C(33)-K(1)	3.13(2)	C(81)-C(82)	1.47(4)
C(36)-C(37)	1.417(8)		

N(1)-Yb(1)-C(1)	129.4(6)	C(19)-C(14)-Yb(1)	116.4(4)
N(1)-Yb(1)-C(2)	127.4(6)	C(11)-C(15)-Yb(1)	74.6(4)
N(1)-Yb(1)-C(3)	96.3(5)	C(11)-C(15)-C(20)	126
N(1)-Yb(1)-C(4)	82.1(6)	C(14)-C(15)-Yb(1)	73.6(4)
N(1)-Yb(1)-C(5)	103.1(6)	C(14)-C(15)-C(11)	108
N(1)-Yb(1)-C(11)	113.9(5)	C(14)-C(15)-C(20)	126
N(1)-Yb(1)-C(12)	85.3(5)	C(20)-C(15)-Yb(1)	117.8(4)
N(1)-Yb(1)-C(13)	84.0(4)	C(22)-C(21)-N(1)	122.5(18)
N(1)-Yb(1)-C(14)	111.9(4)	C(21)-C(22)-C(23)	124.5(17)
N(1)-Yb(1)-C(15)	133.0(5)	N(3)-C(23)-C(22)	110.4(13)
N(2)-Yb(1)-N(1)	72.3(5)	N(3)-C(23)-C(56)	114.0(15)
N(2)-Yb(1)-C(1)	94.5(6)	C(22)-C(23)-C(56)	111.8(14)
N(2)-Yb(1)-C(2)	125.7(7)	N(1)-C(24)-Yb(1)	40.8(8)
N(2)-Yb(1)-C(3)	124.5(6)	N(1)-C(24)-N(3)	132.4(15)
N(2)-Yb(1)-C(4)	93.5(6)	N(1)-C(24)-C(25)	112.1(16)
N(2)-Yb(1)-C(5)	78.1(6)	N(3)-C(24)-Yb(1)	172.9(11)
N(2)-Yb(1)-C(11)	132.3(5)	N(3)-C(24)-C(25)	115.4(16)
N(2)-Yb(1)-C(12)	115.2(5)	C(25)-C(24)-Yb(1)	71.4(11)
N(2)-Yb(1)-C(13)	85.8(5)	N(2)-C(25)-Yb(1)	44.1(10)
N(2)-Yb(1)-C(14)	82.8(5)	N(2)-C(25)-N(4)	117.9(16)
N(2)-Yb(1)-C(15)	109.6(4)	N(2)-C(25)-C(24)	124.8(19)
C(1)-Yb(1)-C(4)	49.4(6)	N(4)-C(25)-Yb(1)	161.9(13)
C(1)-Yb(1)-C(5)	27.4(6)	N(4)-C(25)-C(24)	116.9(18)
C(1)-Yb(1)-C(11)	110.7(6)	C(24)-C(25)-Yb(1)	80.7(11)
C(1)-Yb(1)-C(12)	141.1(6)	N(4)-C(26)-C(27)	135(2)
C(1)-Yb(1)-C(13)	145.0(5)	N(4)-C(26)-C(31)	107.7(15)
C(1)-Yb(1)-C(14)	114.5(5)	C(27)-C(26)-C(31)	117(2)
C(1)-Yb(1)-C(15)	97.6(5)	C(28)-C(27)-C(26)	120(3)
C(2)-Yb(1)-C(1)	31.7(6)	C(27)-C(28)-C(29)	125(2)
C(2)-Yb(1)-C(3)	31.1(6)	C(28)-C(29)-C(30)	118.8(18)
C(2)-Yb(1)-C(4)	51.2(6)	C(31)-C(30)-C(29)	118(2)
C(2)-Yb(1)-C(5)	49.8(7)	N(2)-C(31)-C(26)	106.7(15)
C(2)-Yb(1)-C(11)	89.5(6)	C(30)-C(31)-N(2)	132(2)
C(2)-Yb(1)-C(12)	116.3(6)	C(30)-C(31)-C(26)	121.1(18)
C(2)-Yb(1)-C(13)	138.9(6)	Ni(1)-C(32)-K(1)	80.6(7)
C(2)-Yb(1)-C(14)	118.8(5)	Ni(1)-C(33)-K(1)	80.8(6)
C(2)-Yb(1)-C(15)	90.9(5)	C(37)-C(36)-Yb(2)	74.2(4)
C(3)-Yb(1)-C(1)	51.0(5)	C(37)-C(36)-C(41)	126
C(3)-Yb(1)-C(4)	31.3(6)	C(35)-C(36)-Yb(2)	76.0(4)
C(3)-Yb(1)-C(5)	51.1(6)	C(35)-C(36)-C(37)	108
C(3)-Yb(1)-C(11)	102.4(5)	C(35)-C(36)-C(41)	126
C(3)-Yb(1)-C(12)	117.7(5)	C(41)-C(36)-Yb(2)	115.9(4)
C(3)-Yb(1)-C(13)	148.5(5)	C(36)-C(37)-Yb(2)	74.9(4)
C(3)-Yb(1)-C(14)	146.4(5)	C(36)-C(37)-C(42)	126

C(3)-Yb(1)-C(15)	116.1(5)	C(38)-C(37)-Yb(2)	75.7(4)
C(4)-Yb(1)-C(5)	31.4(5)	C(38)-C(37)-C(36)	108
C(4)-Yb(1)-C(11)	133.7(5)	C(38)-C(37)-C(42)	126
C(4)-Yb(1)-C(12)	143.2(5)	C(42)-C(37)-Yb(2)	115.5(4)
C(4)-Yb(1)-C(13)	165.5(4)	C(37)-C(38)-Yb(2)	73.5(4)
C(4)-Yb(1)-C(14)	163.4(4)	C(37)-C(38)-C(43)	126
C(4)-Yb(1)-C(15)	141.9(5)	C(34)-C(38)-Yb(2)	75.8(4)
C(5)-Yb(1)-C(11)	137.3(5)	C(34)-C(38)-C(37)	108
C(5)-Yb(1)-C(12)	166.2(5)	C(34)-C(38)-C(43)	126
C(5)-Yb(1)-C(13)	159.3(4)	C(43)-C(38)-Yb(2)	116.7(4)
C(5)-Yb(1)-C(14)	132.5(4)	C(38)-C(34)-Yb(2)	73.8(4)
C(5)-Yb(1)-C(15)	123.6(5)	C(38)-C(34)-C(35)	108
C(11)-Yb(1)-C(15)	30.24(16)	C(38)-C(34)-C(39)	126
C(12)-Yb(1)-C(11)	30.46(17)	C(35)-C(34)-Yb(2)	74.4(4)
C(12)-Yb(1)-C(14)	50.6(3)	C(35)-C(34)-C(39)	126
C(12)-Yb(1)-C(15)	50.3(3)	C(39)-C(34)-Yb(2)	117.8(4)
C(13)-Yb(1)-C(11)	50.5(3)	C(36)-C(35)-Yb(2)	73.4(4)
C(13)-Yb(1)-C(12)	30.78(17)	C(36)-C(35)-C(34)	108
C(13)-Yb(1)-C(14)	30.72(17)	C(36)-C(35)-C(40)	126
C(13)-Yb(1)-C(15)	50.4(3)	C(34)-C(35)-Yb(2)	75.3(4)
C(14)-Yb(1)-C(11)	50.2(3)	C(34)-C(35)-C(40)	126
C(14)-Yb(1)-C(15)	30.38(16)	C(40)-C(35)-Yb(2)	117.3(4)
N(5)-Yb(2)-N(6)	74.4(5)	C(45)-C(44)-Yb(2)	75.9(12)
N(5)-Yb(2)-C(36)	79.2(5)	C(45)-C(44)-C(48)	108.6(18)
N(5)-Yb(2)-C(37)	97.7(5)	C(45)-C(44)-C(49)	129(2)
N(5)-Yb(2)-C(38)	127.4(5)	C(48)-C(44)-Yb(2)	73.6(12)
N(5)-Yb(2)-C(34)	125.3(5)	C(48)-C(44)-C(49)	122(2)
N(5)-Yb(2)-C(35)	95.3(5)	C(49)-C(44)-Yb(2)	122.8(16)
N(5)-Yb(2)-C(44)	104.0(7)	C(44)-C(45)-Yb(2)	73.6(13)
N(5)-Yb(2)-C(45)	81.0(6)	C(44)-C(45)-C(50)	129(2)
N(5)-Yb(2)-C(46)	90.5(6)	C(46)-C(45)-Yb(2)	73.8(13)
N(5)-Yb(2)-C(47)	121.3(6)	C(46)-C(45)-C(44)	108(2)
N(5)-Yb(2)-C(48)	132.4(7)	C(46)-C(45)-C(50)	123(2)
N(6)-Yb(2)-C(36)	99.1(5)	C(50)-C(45)-Yb(2)	121.9(16)
N(6)-Yb(2)-C(37)	80.6(5)	C(45)-C(46)-Yb(2)	75.7(12)
N(6)-Yb(2)-C(38)	96.6(5)	C(45)-C(46)-C(47)	108.8(19)
N(6)-Yb(2)-C(34)	126.7(5)	C(45)-C(46)-C(51)	123(2)
N(6)-Yb(2)-C(35)	128.8(5)	C(47)-C(46)-Yb(2)	72.6(13)
N(6)-Yb(2)-C(44)	132.5(6)	C(47)-C(46)-C(51)	128(2)
N(6)-Yb(2)-C(45)	106.8(6)	C(51)-C(46)-Yb(2)	118.5(14)
N(6)-Yb(2)-C(46)	81.8(6)	C(46)-C(47)-Yb(2)	76.4(12)
N(6)-Yb(2)-C(47)	87.7(5)	C(46)-C(47)-C(48)	108.5(18)
N(6)-Yb(2)-C(48)	118.6(6)	C(46)-C(47)-C(52)	126.7(19)
C(36)-Yb(2)-C(38)	50.7(3)	C(48)-C(47)-Yb(2)	75.3(12)

C(36)-Yb(2)-C(34)	50.4(3)	C(48)-C(47)-C(52)	124(2)
C(36)-Yb(2)-C(35)	30.58(19)	C(52)-C(47)-Yb(2)	120.9(15)
C(36)-Yb(2)-C(45)	141.5(5)	C(44)-C(48)-Yb(2)	74.8(12)
C(37)-Yb(2)-C(36)	30.85(19)	C(44)-C(48)-C(53)	130(2)
C(37)-Yb(2)-C(38)	30.73(19)	C(47)-C(48)-Yb(2)	73.1(11)
C(37)-Yb(2)-C(34)	50.5(3)	C(47)-C(48)-C(44)	106(2)
C(37)-Yb(2)-C(35)	50.6(3)	C(47)-C(48)-C(53)	123(2)
C(37)-Yb(2)-C(45)	171.6(5)	C(53)-C(48)-Yb(2)	127.8(19)
C(38)-Yb(2)-C(34)	30.40(18)	C(55)-C(54)-N(6)	123.3(19)
C(38)-Yb(2)-C(35)	50.3(3)	C(54)-C(55)-C(56)	122.5(18)
C(35)-Yb(2)-C(34)	30.32(18)	N(8)-C(56)-C(23)	108.4(15)
C(44)-Yb(2)-C(36)	127.7(6)	C(55)-C(56)-N(8)	110.9(14)
C(44)-Yb(2)-C(37)	144.2(6)	C(55)-C(56)-C(23)	111.0(15)
C(44)-Yb(2)-C(38)	117.9(7)	N(6)-C(57)-Yb(2)	43.5(8)
C(44)-Yb(2)-C(34)	93.8(6)	N(6)-C(57)-N(8)	131.2(16)
C(44)-Yb(2)-C(35)	98.7(6)	N(6)-C(57)-C(58)	118.7(14)
C(44)-Yb(2)-C(45)	30.6(7)	N(8)-C(57)-Yb(2)	171.3(15)
C(44)-Yb(2)-C(46)	50.8(6)	N(8)-C(57)-C(58)	110.2(15)
C(45)-Yb(2)-C(38)	147.8(6)	C(58)-C(57)-Yb(2)	75.7(9)
C(45)-Yb(2)-C(34)	123.9(6)	N(5)-C(58)-Yb(2)	45.5(8)
C(45)-Yb(2)-C(35)	121.1(5)	N(5)-C(58)-C(57)	122.3(15)
C(46)-Yb(2)-C(36)	168.9(6)	N(7)-C(58)-Yb(2)	159.3(12)
C(46)-Yb(2)-C(37)	157.8(5)	N(7)-C(58)-N(5)	115.4(15)
C(46)-Yb(2)-C(38)	140.4(6)	N(7)-C(58)-C(57)	122.2(15)
C(46)-Yb(2)-C(34)	137.0(5)	C(57)-C(58)-Yb(2)	77.2(10)
C(46)-Yb(2)-C(35)	149.3(5)	N(7)-C(59)-C(60)	135.5(18)
C(46)-Yb(2)-C(45)	30.5(6)	N(7)-C(59)-C(64)	109.9(15)
C(47)-Yb(2)-C(36)	159.5(6)	C(60)-C(59)-C(64)	114.6(18)
C(47)-Yb(2)-C(37)	134.5(6)	C(61)-C(60)-C(59)	120(2)
C(47)-Yb(2)-C(38)	109.6(6)	C(62)-C(61)-C(60)	123(2)
C(47)-Yb(2)-C(34)	110.4(6)	C(63)-C(62)-C(61)	121.4(19)
C(47)-Yb(2)-C(35)	135.7(6)	C(62)-C(63)-C(64)	116.2(18)
C(47)-Yb(2)-C(44)	51.7(6)	N(5)-C(64)-C(59)	106.3(15)
C(47)-Yb(2)-C(45)	51.2(7)	C(63)-C(64)-N(5)	128.4(17)
C(47)-Yb(2)-C(46)	31.0(7)	C(63)-C(64)-C(59)	125.3(17)
C(47)-Yb(2)-C(48)	31.6(6)	Ni(2)-C(65)-K(2)	94.8(8)
C(48)-Yb(2)-C(36)	134.6(6)	Ni(2)-C(66)-K(2)	91.3(7)
C(48)-Yb(2)-C(37)	128.6(7)	O(8)-K(2)-O(9)	56.0(8)
C(48)-Yb(2)-C(38)	97.9(7)	O(8)-K(2)-O(10)	115.5(8)
C(48)-Yb(2)-C(34)	85.5(6)	O(8)-K(2)-O(11)	158.3(7)
C(48)-Yb(2)-C(35)	105.3(6)	O(8)-K(2)-O(13)	64.2(8)
C(48)-Yb(2)-C(44)	31.6(7)	O(9)-K(2)-O(10)	59.6(8)
C(48)-Yb(2)-C(45)	51.6(8)	O(9)-K(2)-O(11)	114.2(7)
C(48)-Yb(2)-C(46)	51.5(7)	O(9)-K(2)-O(13)	111.8(8)

N(3)-Ni(1)-K(1)	126.8(4)	O(10)-K(2)-O(11)	59.5(6)
N(4)-Ni(1)-N(3)	83.1(6)	O(10)-K(2)-O(13)	151.0(7)
N(4)-Ni(1)-K(1)	111.5(5)	O(12)-K(2)-O(8)	119.3(8)
C(32)-Ni(1)-N(3)	94.4(7)	O(12)-K(2)-O(9)	148.2(7)
C(32)-Ni(1)-N(4)	174.2(8)	O(12)-K(2)-O(10)	115.7(7)
C(32)-Ni(1)-C(33)	91.4(8)	O(12)-K(2)-O(11)	57.0(7)
C(32)-Ni(1)-K(1)	65.9(7)	O(12)-K(2)-O(13)	55.2(8)
C(33)-Ni(1)-N(3)	167.7(7)	O(13)-K(2)-O(11)	109.1(7)
C(33)-Ni(1)-N(4)	92.1(7)	C(84)-O(8)-K(2)	108(2)
C(33)-Ni(1)-K(1)	65.6(6)	C(85)-O(8)-K(2)	114(3)
N(7)-Ni(2)-N(8)	81.4(6)	C(85)-O(8)-C(84)	124(4)
N(7)-Ni(2)-K(2)	135.3(5)	C(86)-O(9)-K(2)	112(2)
N(8)-Ni(2)-K(2)	121.5(4)	C(86)-O(9)-C(87)	115(2)
C(65)-Ni(2)-N(7)	169.1(8)	C(87)-O(9)-K(2)	109(2)
C(65)-Ni(2)-N(8)	95.4(7)	C(88)-O(10)-K(2)	112(2)
C(65)-Ni(2)-C(66)	87.9(8)	C(88)-O(10)-C(89)	124(2)
C(65)-Ni(2)-K(2)	55.0(6)	C(89)-O(10)-K(2)	113.2(17)
C(66)-Ni(2)-N(7)	95.9(7)	C(90)-O(11)-K(2)	101(2)
C(66)-Ni(2)-N(8)	175.4(8)	C(90)-O(11)-C(91)	137(4)
C(66)-Ni(2)-K(2)	58.1(6)	C(91)-O(11)-K(2)	103.3(17)
C(21)-N(1)-Yb(1)	129.4(12)	C(92)-O(12)-K(2)	131(2)
C(24)-N(1)-Yb(1)	117.9(11)	C(92)-O(12)-C(93)	108(2)
C(24)-N(1)-C(21)	112.7(15)	C(93)-O(12)-K(2)	120.1(18)
C(25)-N(2)-Yb(1)	112.8(12)	C(83)-O(13)-K(2)	97.1(19)
C(25)-N(2)-C(31)	103.6(16)	C(94)-O(13)-K(2)	118(3)
C(31)-N(2)-Yb(1)	143.6(13)	C(94)-O(13)-C(83)	113(3)
C(23)-N(3)-Ni(1)	131.3(11)	O(13)-C(83)-K(2)	57.8(18)
C(24)-N(3)-Ni(1)	110.6(10)	C(84)-C(83)-K(2)	79(3)
C(24)-N(3)-C(23)	117.1(14)	C(84)-C(83)-O(13)	116(3)
C(25)-N(4)-Ni(1)	112.9(11)	O(8)-C(84)-K(2)	52(2)
C(26)-N(4)-Ni(1)	142.9(14)	O(8)-C(84)-C(83)	124(4)
C(26)-N(4)-C(25)	103.8(16)	C(83)-C(84)-K(2)	77(3)
C(58)-N(5)-Yb(2)	109.4(11)	O(8)-C(85)-K(2)	47(2)
C(58)-N(5)-C(64)	102.9(14)	O(8)-C(85)-C(86)	118(4)
C(64)-N(5)-Yb(2)	145.9(11)	C(86)-C(85)-K(2)	82(3)
C(54)-N(6)-Yb(2)	129.1(12)	O(9)-C(86)-C(85)	103(3)
C(57)-N(6)-Yb(2)	113.8(10)	C(88)-C(87)-O(9)	106(3)
C(57)-N(6)-C(54)	115.1(14)	O(10)-C(88)-C(87)	113(3)
C(58)-N(7)-Ni(2)	109.9(12)	C(90)-C(89)-O(10)	110(3)
C(58)-N(7)-C(59)	105.4(15)	O(11)-C(90)-K(2)	60(2)
C(59)-N(7)-Ni(2)	142.6(12)	O(11)-C(90)-C(89)	136(4)
C(56)-N(8)-Ni(2)	129.1(11)	C(89)-C(90)-K(2)	92(2)
C(57)-N(8)-Ni(2)	114.9(12)	C(92)-C(91)-O(11)	119(3)
C(57)-N(8)-C(56)	115.8(15)	O(12)-C(92)-C(91)	109(3)

C(2)-C(1)-Yb(1)	73.1(11)	C(94)-C(93)-O(12)	114(3)
C(2)-C(1)-C(6)	118.4(19)	O(13)-C(94)-C(93)	106(3)
C(5)-C(1)-Yb(1)	77.7(12)	O(1)-K(1)-O(2)	60.2(5)
C(5)-C(1)-C(2)	111.4(17)	O(1)-K(1)-O(3)	119.1(5)
C(5)-C(1)-C(6)	130(2)	O(1)-K(1)-O(4)	162.3(5)
C(6)-C(1)-Yb(1)	122.2(12)	O(1)-K(1)-O(5)	117.3(5)
C(1)-C(2)-Yb(1)	75.2(12)	O(1)-K(1)-O(6)	59.5(5)
C(1)-C(2)-C(7)	129.0(18)	O(2)-K(1)-O(4)	114.7(5)
C(3)-C(2)-Yb(1)	74.9(12)	O(2)-K(1)-O(6)	113.0(5)
C(3)-C(2)-C(1)	105.7(19)	O(3)-K(1)-O(2)	58.9(5)
C(3)-C(2)-C(7)	122.1(19)	O(3)-K(1)-O(4)	60.0(4)
C(7)-C(2)-Yb(1)	130.8(15)	O(3)-K(1)-O(5)	119.1(4)
C(2)-C(3)-Yb(1)	73.9(12)	O(3)-K(1)-O(6)	156.7(5)
C(2)-C(3)-C(4)	107.1(17)	O(4)-K(1)-O(6)	113.5(4)
C(2)-C(3)-C(8)	127(2)	O(5)-K(1)-O(2)	155.4(6)
C(4)-C(3)-Yb(1)	75.5(11)	O(5)-K(1)-O(4)	59.2(4)
C(4)-C(3)-C(8)	125.8(17)	O(5)-K(1)-O(6)	57.9(4)
C(8)-C(3)-Yb(1)	119.0(16)	C(68)-O(1)-K(1)	121.5(14)
C(3)-C(4)-Yb(1)	73.2(11)	C(69)-O(1)-K(1)	116.9(14)
C(3)-C(4)-C(5)	105.6(16)	C(69)-O(1)-C(68)	112(2)
C(3)-C(4)-C(9)	128.0(17)	C(70)-O(2)-K(1)	111.8(13)
C(5)-C(4)-Yb(1)	74.8(10)	C(70)-O(2)-C(71)	113.9(19)
C(5)-C(4)-C(9)	126.3(19)	C(71)-O(2)-K(1)	113.8(13)
C(9)-C(4)-Yb(1)	119.3(13)	C(72)-O(3)-K(1)	118.6(13)
C(1)-C(5)-Yb(1)	75.0(12)	C(72)-O(3)-C(73)	113.5(17)
C(1)-C(5)-C(4)	110.1(18)	C(73)-O(3)-K(1)	117.8(11)
C(1)-C(5)-C(10)	128.0(17)	C(74)-O(4)-K(1)	107.5(11)
C(4)-C(5)-Yb(1)	73.8(11)	C(74)-O(4)-C(75)	110.1(18)
C(4)-C(5)-C(10)	121.5(18)	C(75)-O(4)-K(1)	106.8(11)
C(10)-C(5)-Yb(1)	123.0(12)	C(76)-O(5)-K(1)	117.4(11)
C(12)-C(11)-Yb(1)	73.4(4)	C(77)-O(5)-K(1)	120.9(14)
C(12)-C(11)-C(15)	108	C(77)-O(5)-C(76)	111.9(17)
C(12)-C(11)-C(16)	126	C(67)-O(6)-K(1)	106.1(13)
C(15)-C(11)-Yb(1)	75.1(4)	C(67)-O(6)-C(78)	110.8(19)
C(15)-C(11)-C(16)	126	C(78)-O(6)-K(1)	113.2(13)
C(16)-C(11)-Yb(1)	117.5(4)	O(6)-C(67)-C(68)	112(2)
C(11)-C(12)-Yb(1)	76.2(4)	O(1)-C(68)-C(67)	107(2)
C(11)-C(12)-C(13)	108	O(1)-C(69)-C(70)	114(2)
C(11)-C(12)-C(17)	126	O(2)-C(70)-C(69)	110(2)
C(13)-C(12)-Yb(1)	74.0(4)	O(2)-C(71)-C(72)	110(2)
C(13)-C(12)-C(17)	126	O(3)-C(72)-C(71)	112.2(18)
C(17)-C(12)-Yb(1)	116.0(4)	O(3)-C(73)-C(74)	107.5(18)
C(12)-C(13)-Yb(1)	75.2(4)	O(4)-C(74)-K(1)	50.0(9)
C(12)-C(13)-C(14)	108	O(4)-C(74)-C(73)	106(2)

C(12)-C(13)-C(18)	126	C(73)-C(74)-K(1)	82.3(12)
C(14)-C(13)-Yb(1)	75.7(4)	O(4)-C(75)-C(76)	106(2)
C(14)-C(13)-C(18)	126	O(5)-C(76)-C(75)	107.2(17)
C(18)-C(13)-Yb(1)	115.3(4)	O(5)-C(77)-C(78)	106(2)
C(13)-C(14)-Yb(1)	73.6(4)	O(6)-C(78)-C(77)	109(2)
C(13)-C(14)-C(19)	126	C(79)-O(7)-C(81)	113(2)
C(15)-C(14)-Yb(1)	76.1(4)	O(7)-C(79)-C(80)	109(3)
C(15)-C(14)-C(13)	108	C(79)-C(80)-K(1)	93(2)
C(15)-C(14)-C(19)	126	O(7)-C(81)-C(82)	112(3)

Table S11. Distances (\AA) and angles (deg) for $\text{K}_2(\text{bimpmp})\text{Ni}(\text{CH}_3)_2$ (**6**)

Ni(1)-K(3)	3.6114(13)	C(10)-C(11)	1.391(7)
Ni(1)-K(4) ¹	3.3702(13)	C(16)-C(17)	1.510(9)
Ni(1)-N(1)	1.969(4)	C(22)-C(23)	1.504(8)
Ni(1)-N(2)	1.975(4)	C(23)-C(24)	1.505(10)
Ni(1)-C(12)	1.936(5)	C(24)-C(25)	1.517(8)
Ni(1)-C(13)	1.938(5)	C(30)-C(31)	1.482(8)
Ni(2)-K(1) ²	3.4379(13)	C(31)-C(32)	1.498(8)
Ni(2)-K(2)	3.7744(13)	C(32)-C(33)	1.491(8)
Ni(2)-N(5)	1.967(4)	C(38)-C(39)	1.519(8)
Ni(2)-N(6)	1.984(4)	C(39)-C(40)	1.501(9)
Ni(2)-C(57)	1.924(6)	C(40)-C(41)	1.486(8)
Ni(2)-C(58)	1.922(5)	C(46)-C(47)	1.481(7)
K(1)-O(1)	2.830(4)	C(48)-C(49)	1.327(7)
K(1)-O(3)	2.818(4)	C(49)-C(50)	1.510(7)
K(1)-N(3)	2.897(4)	C(51)-C(52)	1.399(7)
K(1)-N(4)	2.848(4)	C(51)-C(56)	1.409(7)
K(1)-O(2A)	2.88(4)	C(52)-C(53)	1.364(8)
K(1)-O(2B)	3.07(5)	C(53)-C(54)	1.390(8)
K(2)-O(3)	2.855(4)	C(54)-C(55)	1.375(8)
K(2)-O(5)	2.919(4)	C(55)-C(56)	1.380(7)
K(2)-N(3)	2.860(4)	O(2A)-C(18A)	1.48(3)
K(2)-N(4)	2.939(4)	O(2A)-C(21A)	1.49(3)
K(2)-O(4A)	2.747(10)	O(4A)-C(26A)	1.414(14)
K(2)-O(4B)	2.821(13)	O(4A)-C(29A)	1.425(14)
K(3)-O(5)	2.873(4)	O(6A)-C(34A)	1.392(10)
K(3)-O(7)	2.870(4)	O(6A)-C(37A)	1.398(9)
K(3)-N(7)	2.898(4)	O(8A)-C(42A)	1.49(3)
K(3)-N(8)	2.927(4)	O(8A)-C(45A)	1.50(3)
K(3)-O(6A)	2.786(7)	C(18A)-C(19A)	1.57(2)
K(3)-O(6B)	2.59(11)	C(19A)-C(20A)	1.60(2)
K(4)-O(7)	2.804(4)	C(20A)-C(21A)	1.58(2)

K(4)-N(7)	2.816(4)	C(26A)-C(27A)	1.452(16)
K(4)-N(8)	2.803(4)	C(27A)-C(28A)	1.428(17)
K(4)-O(8A)	2.70(3)	C(28A)-C(29A)	1.443(18)
K(4)-O(8B)	2.777(10)	C(34A)-C(35A)	1.527(11)
O(1)-C(15)	1.405(7)	C(35A)-C(36A)	1.516(11)
O(1)-C(17)	1.426(7)	C(36A)-C(37A)	1.508(11)
O(3)-C(22)	1.442(7)	C(42A)-C(43A)	1.503(16)
O(3)-C(25)	1.445(7)	C(43A)-C(44A)	1.511(16)
O(5)-C(30)	1.434(7)	C(44A)-C(45A)	1.481(16)
O(5)-C(33)	1.444(6)	O(2B)-C(18B)	1.33(4)
O(7)-C(38)	1.446(6)	O(2B)-C(21B)	1.34(4)
O(7)-C(41)	1.429(6)	O(4B)-C(26B)	1.416(17)
N(1)-C(1)	1.351(6)	O(4B)-C(29B)	1.40(2)
N(1)-C(11)	1.384(6)	O(6B)-C(34B)	1.53(11)
N(2)-C(2)	1.360(6)	O(6B)-C(37B)	1.54(11)
N(2)-C(3)	1.405(6)	O(8B)-C(42B)	1.397(12)
N(3)-C(1)	1.346(6)	O(8B)-C(45B)	1.418(13)
N(3)-C(6)	1.375(6)	C(18B)-C(19B)	1.29(3)
N(4)-C(2)	1.315(6)	C(19B)-C(20B)	1.29(3)
N(4)-C(5)	1.466(6)	C(20B)-C(21B)	1.28(3)
N(5)-C(46)	1.350(6)	C(26B)-C(27B)	1.50(2)
N(5)-C(56)	1.384(6)	C(27B)-C(28B)	1.52(2)
N(6)-C(47)	1.358(6)	C(28B)-C(29B)	1.54(2)
N(6)-C(48)	1.396(6)	C(34B)-C(35B)	1.51(8)
N(7)-C(46)	1.334(6)	C(35B)-C(36B)	1.51(8)
N(7)-C(51)	1.388(6)	C(36B)-C(37B)	1.52(8)
N(8)-C(47)	1.307(6)	C(42B)-C(43B)	1.483(12)
N(8)-C(50)	1.474(6)	C(43B)-C(44B)	1.465(13)
C(1)-C(2)	1.454(7)	C(44B)-C(45B)	1.491(12)
C(01U)-C(15)	1.475(9)	O(9A)-C(59A)	1.407(16)
C(01U)-C(16)	1.504(10)	O(9A)-C(62A)	1.40(2)
C(3)-C(4)	1.329(7)	C(59A)-C(60A)	1.380(16)
C(4)-C(5)	1.498(7)	C(60A)-C(61A)	1.39(2)
C(5)-C(50)	1.537(7)	C(61A)-C(62A)	1.38(2)
C(6)-C(7)	1.400(7)	O(9B)-C(59B)	1.25(2)
C(6)-C(11)	1.406(7)	O(9B)-C(62B)	1.26(2)
C(7)-C(8)	1.352(8)	C(59B)-C(60B)	1.72(5)
C(8)-C(9)	1.392(8)	C(60B)-C(61B)	1.71(5)
C(9)-C(10)	1.372(8)	C(61B)-C(62B)	1.72(5)

¹1/2-X,-1/2+Y,1/2-Z; ²3/2-X,1/2+Y,1/2-Z

K(4) ¹ -Ni(1)-K(3)	142.75(3)	N(2)-C(2)-C(1)	111.8(4)
N(1)-Ni(1)-K(3)	98.37(12)	N(4)-C(2)-K(1)	51.7(2)

N(1)-Ni(1)-K(4) ¹	118.87(12)	N(4)-C(2)-K(2)	58.9(3)
N(1)-Ni(1)-N(2)	82.39(16)	N(4)-C(2)-K(3)	98.4(3)
N(2)-Ni(1)-K(3)	56.66(12)	N(4)-C(2)-N(2)	130.1(4)
N(2)-Ni(1)-K(4) ¹	125.45(12)	N(4)-C(2)-C(1)	118.1(4)
C(12)-Ni(1)-K(3)	117.41(17)	C(1)-C(2)-K(1)	77.6(3)
C(12)-Ni(1)-K(4) ¹	63.05(16)	C(1)-C(2)-K(2)	73.3(3)
C(12)-Ni(1)-N(1)	93.0(2)	C(1)-C(2)-K(3)	111.3(3)
C(12)-Ni(1)-N(2)	171.5(2)	N(2)-C(3)-K(3)	73.7(3)
C(12)-Ni(1)-C(13)	92.4(2)	C(4)-C(3)-K(3)	95.7(3)
C(13)-Ni(1)-K(3)	80.07(17)	C(4)-C(3)-N(2)	123.2(5)
C(13)-Ni(1)-K(4) ¹	62.95(17)	C(3)-C(4)-K(3)	62.0(3)
C(13)-Ni(1)-N(1)	174.5(2)	C(3)-C(4)-C(5)	122.6(5)
C(13)-Ni(1)-N(2)	92.4(2)	C(5)-C(4)-K(3)	94.5(3)
K(1) ² -Ni(2)-K(2)	146.02(3)	N(4)-C(5)-C(4)	112.1(4)
N(5)-Ni(2)-K(1) ²	116.36(12)	N(4)-C(5)-C(50)	111.5(4)
N(5)-Ni(2)-K(2)	96.51(12)	C(4)-C(5)-C(50)	112.7(4)
N(5)-Ni(2)-N(6)	81.93(16)	N(3)-C(6)-C(7)	129.2(5)
N(6)-Ni(2)-K(1) ²	120.28(12)	N(3)-C(6)-C(11)	109.6(4)
N(6)-Ni(2)-K(2)	53.13(12)	C(7)-C(6)-C(11)	121.3(5)
C(57)-Ni(2)-K(1) ²	65.25(18)	C(8)-C(7)-C(6)	117.5(5)
C(57)-Ni(2)-K(2)	123.48(19)	C(7)-C(8)-C(9)	122.2(5)
C(57)-Ni(2)-N(5)	94.3(2)	C(10)-C(9)-C(8)	121.0(6)
C(57)-Ni(2)-N(6)	174.3(2)	C(9)-C(10)-C(11)	118.6(5)
C(58)-Ni(2)-K(1) ²	66.27(17)	N(1)-C(11)-C(6)	108.0(4)
C(58)-Ni(2)-K(2)	80.26(17)	N(1)-C(11)-C(10)	132.5(5)
C(58)-Ni(2)-N(5)	174.5(2)	C(10)-C(11)-C(6)	119.5(5)
C(58)-Ni(2)-N(6)	92.6(2)	Ni(1)-C(12)-K(4) ¹	82.25(18)
C(58)-Ni(2)-C(57)	91.2(2)	Ni(1)-C(13)-K(4) ¹	82.31(18)
O(1)-K(1)-N(3)	109.67(13)	O(1)-C(15)-C(01U)	105.6(5)
O(1)-K(1)-N(4)	81.36(12)	C(01U)-C(16)-C(17)	104.8(6)
O(1)-K(1)-O(2A)	83.8(5)	O(1)-C(17)-C(16)	105.8(6)
O(1)-K(1)-O(2B)	81.5(7)	O(3)-C(22)-C(23)	104.4(5)
O(3)-K(1)-O(1)	165.31(14)	C(22)-C(23)-C(24)	101.9(6)
O(3)-K(1)-N(3)	77.18(12)	C(23)-C(24)-C(25)	103.2(5)
O(3)-K(1)-N(4)	91.69(12)	O(3)-C(25)-K(1)	52.4(3)
O(3)-K(1)-O(2A)	83.6(6)	O(3)-C(25)-C(24)	106.0(5)
O(3)-K(1)-O(2B)	86.5(8)	C(24)-C(25)-K(1)	129.5(5)
N(3)-K(1)-O(2B)	149.7(9)	O(5)-C(30)-C(31)	107.0(5)
N(4)-K(1)-N(3)	59.56(12)	C(30)-C(31)-C(32)	103.6(5)
N(4)-K(1)-O(2A)	92.7(7)	C(33)-C(32)-C(31)	103.9(5)

N(4)-K(1)-O(2B)	96.2(8)	O(5)-C(33)-C(32)	106.5(4)
O(2A)-K(1)-N(3)	145.2(7)	O(7)-C(38)-K(4)	53.3(2)
O(3)-K(2)-O(5)	162.60(12)	O(7)-C(38)-C(39)	107.0(5)
O(3)-K(2)-N(3)	77.18(11)	C(39)-C(38)-K(4)	136.0(4)
O(3)-K(2)-N(4)	89.09(12)	C(40)-C(39)-C(38)	104.7(5)
O(5)-K(2)-N(4)	93.44(11)	C(41)-C(40)-C(39)	103.0(5)
N(3)-K(2)-O(5)	89.39(11)	O(7)-C(41)-C(40)	106.0(5)
N(3)-K(2)-N(4)	58.94(12)	K(3)-C(46)-K(4)	68.64(10)
O(4A)-K(2)-O(3)	96.2(3)	N(5)-C(46)-K(3)	134.0(3)
O(4A)-K(2)-O(5)	74.4(3)	N(5)-C(46)-K(4)	152.1(3)
O(4A)-K(2)-N(3)	97.6(2)	N(5)-C(46)-C(47)	116.8(4)
O(4A)-K(2)-N(4)	154.2(2)	N(7)-C(46)-K(3)	62.0(3)
O(4B)-K(2)-O(3)	75.5(3)	N(7)-C(46)-K(4)	52.6(3)
O(4B)-K(2)-O(5)	95.2(3)	N(7)-C(46)-N(5)	117.5(4)
O(4B)-K(2)-N(3)	95.8(3)	N(7)-C(46)-C(47)	125.7(4)
O(4B)-K(2)-N(4)	153.2(3)	C(47)-C(46)-K(3)	81.6(3)
O(5)-K(3)-N(7)	88.39(11)	C(47)-C(46)-K(4)	77.9(3)
O(5)-K(3)-N(8)	91.20(11)	K(2)-C(47)-K(3)	81.27(11)
O(7)-K(3)-O(5)	160.76(11)	K(2)-C(47)-K(4)	141.97(15)
O(7)-K(3)-N(7)	77.72(11)	K(3)-C(47)-K(4)	67.21(9)
O(7)-K(3)-N(8)	92.99(11)	N(6)-C(47)-K(2)	63.4(2)
N(7)-K(3)-N(8)	59.27(12)	N(6)-C(47)-K(3)	143.2(3)
O(6A)-K(3)-O(5)	78.56(18)	N(6)-C(47)-K(4)	149.2(3)
O(6A)-K(3)-O(7)	89.24(18)	N(6)-C(47)-C(46)	111.4(4)
O(6A)-K(3)-N(7)	94.62(15)	N(8)-C(47)-K(2)	94.6(3)
O(6A)-K(3)-N(8)	152.47(16)	N(8)-C(47)-K(3)	58.5(3)
O(6B)-K(3)-O(5)	87(2)	N(8)-C(47)-K(4)	51.2(3)
O(6B)-K(3)-O(7)	80(2)	N(8)-C(47)-N(6)	130.4(5)
O(6B)-K(3)-N(7)	88.9(18)	N(8)-C(47)-C(46)	118.1(4)
O(6B)-K(3)-N(8)	148.2(18)	C(46)-C(47)-K(2)	114.2(3)
O(7)-K(4)-N(7)	80.16(11)	C(46)-C(47)-K(3)	72.8(3)
N(8)-K(4)-O(7)	97.18(12)	C(46)-C(47)-K(4)	77.1(3)
N(8)-K(4)-N(7)	61.68(12)	N(6)-C(48)-K(2)	77.6(3)
O(8A)-K(4)-O(7)	131.7(7)	C(49)-C(48)-K(2)	92.7(3)
O(8A)-K(4)-N(7)	133.6(6)	C(49)-C(48)-N(6)	123.5(5)
O(8A)-K(4)-N(8)	79.3(6)	C(48)-C(49)-K(2)	63.9(3)
O(8B)-K(4)-O(7)	147.2(3)	C(48)-C(49)-C(50)	122.6(5)
O(8B)-K(4)-N(7)	122.8(2)	C(50)-C(49)-K(2)	96.1(3)
O(8B)-K(4)-N(8)	77.9(2)	N(8)-C(50)-C(5)	111.6(4)
C(15)-O(1)-K(1)	125.8(4)	N(8)-C(50)-C(49)	111.1(4)

C(15)-O(1)-C(17)	105.4(5)	C(49)-C(50)-C(5)	113.0(4)
C(17)-O(1)-K(1)	127.7(4)	N(7)-C(51)-C(52)	129.7(5)
K(1)-O(3)-K(2)	88.05(11)	N(7)-C(51)-C(56)	110.2(4)
C(22)-O(3)-K(1)	120.3(4)	C(52)-C(51)-C(56)	120.0(5)
C(22)-O(3)-K(2)	118.1(3)	C(53)-C(52)-C(51)	118.0(5)
C(22)-O(3)-C(25)	109.1(4)	C(52)-C(53)-C(54)	121.6(6)
C(25)-O(3)-K(1)	103.6(3)	C(55)-C(54)-C(53)	121.5(6)
C(25)-O(3)-K(2)	115.9(4)	C(54)-C(55)-C(56)	117.7(5)
K(3)-O(5)-K(2)	99.25(11)	N(5)-C(56)-C(51)	107.0(4)
C(30)-O(5)-K(2)	109.1(3)	C(55)-C(56)-N(5)	131.8(5)
C(30)-O(5)-K(3)	109.1(3)	C(55)-C(56)-C(51)	121.1(5)
C(30)-O(5)-C(33)	109.0(4)	Ni(2)-C(57)-K(1) ²	81.2(2)
C(33)-O(5)-K(2)	121.1(3)	Ni(2)-C(58)-K(1) ²	80.30(18)
C(33)-O(5)-K(3)	108.5(3)	C(18A)-O(2A)-K(1)	122.3(17)
K(4)-O(7)-K(3)	83.39(10)	C(18A)-O(2A)-C(21A)	107(3)
C(38)-O(7)-K(3)	112.4(3)	C(21A)-O(2A)-K(1)	128(2)
C(38)-O(7)-K(4)	102.3(3)	C(26A)-O(4A)-K(2)	130.8(9)
C(41)-O(7)-K(3)	133.2(3)	C(26A)-O(4A)-C(29A)	106.0(11)
C(41)-O(7)-K(4)	112.8(3)	C(29A)-O(4A)-K(2)	119.3(9)
C(41)-O(7)-C(38)	106.6(4)	C(34A)-O(6A)-K(3)	136.3(5)
C(1)-N(1)-Ni(1)	111.8(3)	C(34A)-O(6A)-C(37A)	105.8(8)
C(1)-N(1)-C(11)	103.1(4)	C(37A)-O(6A)-K(3)	115.3(5)
C(11)-N(1)-Ni(1)	144.8(3)	C(42A)-O(8A)-K(4)	117.9(19)
Ni(1)-N(2)-K(3)	90.19(14)	C(42A)-O(8A)-C(45A)	99(3)
C(2)-N(2)-Ni(1)	114.5(3)	C(45A)-O(8A)-K(4)	141.8(18)
C(2)-N(2)-K(3)	93.4(3)	O(2A)-C(18A)-C(19A)	109.8(19)
C(2)-N(2)-C(3)	113.2(4)	C(18A)-C(19A)-C(20A)	103.3(13)
C(3)-N(2)-Ni(1)	131.7(3)	C(21A)-C(20A)-C(19A)	105.3(14)
C(3)-N(2)-K(3)	79.7(3)	O(2A)-C(21A)-C(20A)	108.6(19)
K(2)-N(3)-K(1)	86.44(12)	O(4A)-C(26A)-C(27A)	103.6(10)
C(1)-N(3)-K(1)	103.2(3)	C(28A)-C(27A)-C(26A)	107.9(10)
C(1)-N(3)-K(2)	96.0(3)	C(27A)-C(28A)-C(29A)	105.8(12)
C(1)-N(3)-C(6)	102.7(4)	O(4A)-C(29A)-C(28A)	105.1(11)
C(6)-N(3)-K(1)	136.0(3)	O(6A)-C(34A)-C(35A)	104.4(7)
C(6)-N(3)-K(2)	125.2(3)	C(36A)-C(35A)-C(34A)	103.9(7)
K(1)-N(4)-K(2)	85.87(11)	C(37A)-C(36A)-C(35A)	102.5(7)
C(2)-N(4)-K(1)	107.0(3)	O(6A)-C(37A)-C(36A)	102.9(7)
C(2)-N(4)-K(2)	98.6(3)	O(8A)-C(42A)-C(43A)	111(2)
C(2)-N(4)-C(5)	118.8(4)	C(42A)-C(43A)-C(44A)	104.1(15)
C(5)-N(4)-K(1)	116.8(3)	C(45A)-C(44A)-C(43A)	105.1(16)

C(5)-N(4)-K(2)	124.1(3)	C(44A)-C(45A)-O(8A)	110(2)
C(46)-N(5)-Ni(2)	113.5(3)	C(18B)-O(2B)-K(1)	120(3)
C(46)-N(5)-C(56)	103.5(4)	C(18B)-O(2B)-C(21B)	103(3)
C(56)-N(5)-Ni(2)	143.0(3)	C(21B)-O(2B)-K(1)	130(3)
Ni(2)-N(6)-K(2)	95.31(15)	C(26B)-O(4B)-K(2)	129.4(11)
C(47)-N(6)-Ni(2)	115.4(3)	C(29B)-O(4B)-K(2)	110.5(15)
C(47)-N(6)-K(2)	93.0(3)	C(29B)-O(4B)-C(26B)	107.1(14)
C(47)-N(6)-C(48)	113.1(4)	C(34B)-O(6B)-K(3)	149(6)
C(48)-N(6)-Ni(2)	131.0(3)	C(34B)-O(6B)-C(37B)	89(9)
C(48)-N(6)-K(2)	75.7(3)	C(37B)-O(6B)-K(3)	118(6)
K(4)-N(7)-K(3)	82.69(11)	C(42B)-O(8B)-K(4)	119.7(7)
C(46)-N(7)-K(3)	94.0(3)	C(42B)-O(8B)-C(45B)	111.5(10)
C(46)-N(7)-K(4)	105.3(3)	C(45B)-O(8B)-K(4)	127.8(8)
C(46)-N(7)-C(51)	101.8(4)	C(19B)-C(18B)-O(2B)	103(3)
C(51)-N(7)-K(3)	125.9(3)	C(20B)-C(19B)-C(18B)	105.8(19)
C(51)-N(7)-K(4)	138.8(3)	C(21B)-C(20B)-C(19B)	108(2)
K(4)-N(8)-K(3)	82.38(11)	C(20B)-C(21B)-O(2B)	106(3)
C(47)-N(8)-K(3)	99.1(3)	O(4B)-C(26B)-C(27B)	108.2(14)
C(47)-N(8)-K(4)	107.5(3)	C(26B)-C(27B)-C(28B)	103.3(13)
C(47)-N(8)-C(50)	118.9(4)	C(27B)-C(28B)-C(29B)	105.0(12)
C(50)-N(8)-K(3)	126.6(3)	O(4B)-C(29B)-C(28B)	105.1(15)
C(50)-N(8)-K(4)	115.8(3)	C(35B)-C(34B)-O(6B)	104(6)
K(2)-C(1)-K(1)	71.46(10)	C(36B)-C(35B)-C(34B)	103(4)
N(1)-C(1)-K(1)	148.1(3)	C(35B)-C(36B)-C(37B)	102(4)
N(1)-C(1)-K(2)	134.7(3)	C(36B)-C(37B)-O(6B)	102(6)
N(1)-C(1)-C(2)	118.1(4)	O(8B)-C(42B)-C(43B)	104.7(9)
N(3)-C(1)-K(1)	54.6(2)	C(44B)-C(43B)-C(42B)	109.7(9)
N(3)-C(1)-K(2)	60.0(2)	C(43B)-C(44B)-C(45B)	103.4(10)
N(3)-C(1)-N(1)	116.6(4)	O(8B)-C(45B)-C(44B)	106.5(10)
N(3)-C(1)-C(2)	125.3(4)	C(62A)-O(9A)-C(59A)	102.9(15)
C(2)-C(1)-K(1)	78.1(3)	C(60A)-C(59A)-O(9A)	109.7(12)
C(2)-C(1)-K(2)	81.7(3)	C(59A)-C(60A)-C(61A)	107.5(13)
C(15)-C(01U)-C(16)	103.1(6)	C(62A)-C(61A)-C(60A)	104.2(12)
K(2)-C(2)-K(1)	70.11(9)	C(61A)-C(62A)-O(9A)	110.3(18)
K(3)-C(2)-K(1)	146.34(15)	C(59B)-O(9B)-C(62B)	121(4)
K(3)-C(2)-K(2)	81.27(11)	O(9B)-C(59B)-C(60B)	105(2)
N(2)-C(2)-K(1)	146.0(3)	C(61B)-C(60B)-C(59B)	97.2(16)
N(2)-C(2)-K(2)	143.5(3)	C(60B)-C(61B)-C(62B)	98.7(16)
N(2)-C(2)-K(3)	63.0(2)	O(9B)-C(62B)-C(61B)	104(3)

¹1/2-X,-1/2+Y,1/2-Z; ²3/2-X,1/2+Y,1/2-Z