Electronic Supplementary Material (ESI) for Dalton Transactions.

Dinuclear Copper Complexes: Coordination of Group 14 Heteroborates

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Supporting Information

SI Table 1. Results of the Crystal Structure Determination

Compound	**1a** · CH_3CN	**2**	**3**	**4** · 0.5 C_6H_6 · 3 CH_2Cl_2	**5** · Et_2O	**6** · CH_3CN
Empirical formula	$C_{41}H_{73}B_{20}Cu_2N_7P_2Sn_2$	$C_{33}H_{53}B_{11}Cu_2GeN_4P_2$	$C_{33}H_{53}B_{11}Cu_2N_4P_2Sn$	$C_{44}H_{62}B_{11}Cl_6Cu_2MoN_4O_5P_2Sn$	$C_{37}H_{62}B_{10}Cu_2Ge_2N_4OP_2$	$C_{35}H_{55}B_{10}Cu_2N_5P_2$
M_r [g mol^{-1}]	1306.66	886.31	932.41	1462.24	1021.21	842.96
Temperature [K]	100(2)	120(2)	120(2)	100(2)	100(2)	120(2)
Wavelength [Å]	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	triclinic	orthorhombic	monoclinic	monoclinic	monoclinic	monoclinic
Space group	*P*–1	$P2_12_12_1$	$P2_1/n$	$P2_1/c$	$P2_1/n$	$P2_1/c$
Z	2	4	4	4	4	8
a [Å]	10.5306(3)	13.1755(4)	11.3130(2)	19.8799(4)	11.4078(3)	35.9745(11)
b [Å]	14.5334(4)	16.9103(4)	20.9852(4)	11.6874(2)	21.7301(5)	11.7365(4)
c [Å]	20.3679(6)	19.1784(5)	17.6376(3)	26.0583(5)	18.9365(4)	20.8392(6)
α [deg]	92.217(2)	90	90	90	90	90
β [deg]	95.158(2)	90	97.3290(10)	92.8580(10)	95.2350(10)	106.497(2)
γ [deg]	107.583(2)	90	90	90	90	90
V [Å^3]	2952.42(15)	4273.0(2)	4153.05(13)	6047.0(2)	4674.64(19)	8436.4(5)
Density ρ_{calc} [g/cm^3]	1.47	1.38	1.49	1.61	1.45	1.33
Abs. coeff. μ [mm^{-1}]	1.6	1.8	1.7	1.7	2.3	1.1

F(000)	1312	1816	1888	2924	2088	3504
Cryst. size [mm^3]	0.140 × 0.120 × 0.060	0.440 × 0.160 × 0.060	0.210 × 0.150 × 0.120	0.270 × 0.190 × 0.110	0.760 × 0.088 × 0.080	0.165 × 0.135 × 0.118
θ range [deg]	1.47–27.92	1.61–27.51	2.03–28.06	1.56–27.90	1.87–27.33	1.83–27.89
Limiting indices	–13 ≤ h ≤ 13, –19 ≤ k ≤ 19, –26 ≤ l ≤ 26	–16 ≤ h ≤ 17, –21 ≤ k ≤ 21, –24 ≤ l ≤ 24	–14 ≤ h ≤ 14, –27 ≤ k ≤ 27, –23 ≤ l ≤ 23	–26≤ h ≤ 25, –15 ≤ k ≤ 15, –34 ≤ l ≤ 31	–14 ≤ h ≤ 14, –27 ≤ k ≤ 27, –24 ≤ l ≤ 24	–43 ≤ h ≤ 47, –10 ≤ k ≤ 15, –27 ≤ l ≤ 27
Reflections collected	51583	51437	70853	81077	109106	75073
Indep reflns/ R_{int}	13950/0.0554	9596/0.0595	10020/0.0177	14434/0.0363	10502/0.0400	20029/0.0615
Completeness [%]	98.7	98.1	99.4	99.8	99.4	99.4
Absorp corr	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan
Max./min. transmn	0.976 / 0.884	0.900 / 0.740	0.746 / 0.669	0.840 / 0.720	0.746 / 0.611	0.900 / 0.777
Params/ restraints	670/0	472/0	488/32	685/0	544/75	975/0
R_1/wR_2 [$I > 2\sigma(I)$]	0.0354/0.0699	0.0445/0.1052	0.0208/0.0532	0.0439/0.1112	0.0388/0.0987	0.0448/0.1024
R_1/wR_2 all data	0.0727/0.0757	0.0721/0.1170	0.0252/0.0557	0.0572/0.1189	0.0530/0.1077	0.0892/0.1156
Goodness-of-fit on F^2	0.902	1.028	1.047	1.048	1.059	0.988
Largest diff. peak/hole [e·A^{-3}]	1.01 and –1.16	0.90 and –0.81	0.81 and –0.39	2.12 and –1.61	1.18 and –0.87	2.89 and –0.69
CCDC	992555	992552	992554	992553	992551	992550

SI ^{31}P VACP/MAS NMR spectrum of [Cu_2(dmapm)($SnB_{11}H_{11}$)], 3

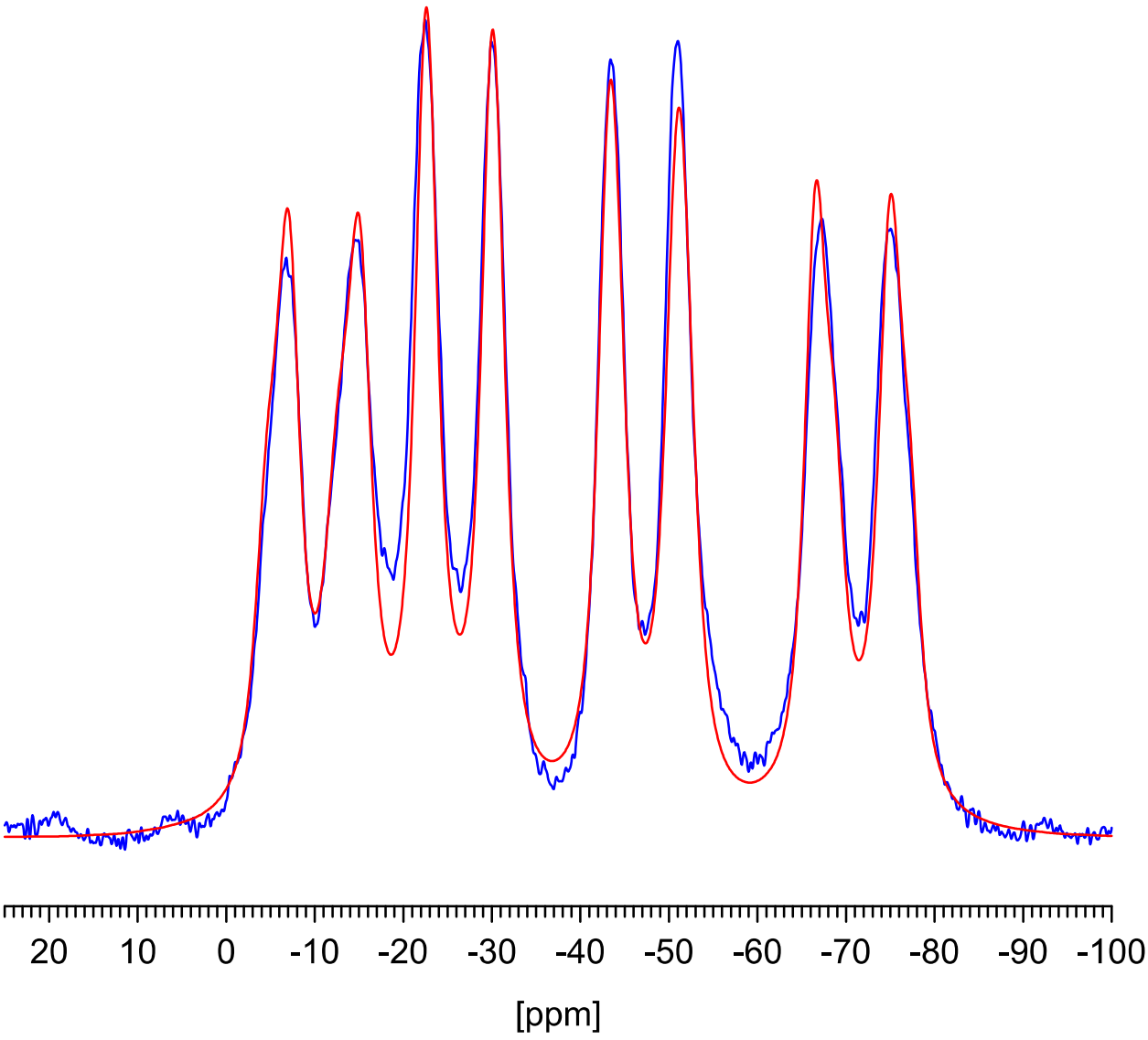

Fig. S1 Experimental (blue) and calculated (red) ^{31}P VACP/MAS NMR spectrum of [Cu_2(dmapm)($SnB_{11}H_{11}$)], **3**, obtained at 4.7 T.

The ^{31}P VACP/MAS spectrum of **3** has been calculated using the "MAS: Spin-1/2 -- Spin-S (Diag.)" model of WSolids1.[1] This model follows the theory outlined by Olivieri and coworkers and its application has been demonstrated for the ^{13}C-^{35,37}Cl spin pair.[2, 3] It is not expected that the parameters reported here constitute a unique solution.

For the ^{31}P,^{63}Cu spin pair, the following parameters have been used:

	Site 1	Site 2
δ_{iso}	-34.9 ppm	-42.8 ppm
$r_{Cu,P}$ / D	2.2287 Å / 1169 Hz	2.1932 Å / 1226 Hz
α^D, β^D	0°, 90°	0°, 90°
J, ΔJ	1650 Hz, 600 Hz	1670 Hz, 600 Hz
χ, η	-55 MHz, 0	-60 MHz, 0

The parameters of the $^{31}P,^{65}Cu$ isotopomer are related to those of the $^{31}P,^{63}Cu$ isotopomer by the ratio of the magnetogyric ratios, $\gamma(^{65}Cu) / \gamma(^{63}Cu) = 1.0693$, for D, J, ΔJ, or the ratio of the nuclear quadrupole moments, $Q(^{65}Cu) / Q(^{63}Cu) = 0.9273$, for χ.

References

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