Supporting Information for:

Solid-state NMR Fermi Contact and Dipolar Shifts in Organometallic Complexes and Metalloporphyrins

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Computational Details:

The details of computational aspects are basically the same as we used before (see Refs.9 and 11-12), except that for **1**, a cluster approach was used due to its polymeric structure nature as revealed by the x-ray crystallography. The basis set schemes used for different cluster models for **1** were described in Ref.15. As before, SGI O300 workstations were employed in our calculations using up to 8 CPUs. The most important aspect of these calculations lies in the design of an appropriate structural model of the x-ray structure to mimic the real metal complex system. The 5-coordinate Cu-1 model contains one Cu(DL-ala)$_2$ unit with one axially coordinated water, as expected in previous studies. The other axially coordinated water was incorporated in the 6-coordinate Cu-1 model. So, in this 6-coordinate Cu-1 model, the copper coordination is complete. To consider copper-copper interactions along the polymer chain, a 6-coordinate Cu-3 model was used. Two Cu(DL-ala)$_2$ units coordinated to the two axial water molecules in the central unit (H_2O–Cu–H_2O) of the 6-coordinate Cu-1 model were included in the calculation, forming a Cu–H_2O–Cu–H_2O–Cu structure. However, as shown in Figure 2A, the shift deviation is still large, especially for the methyl carbon, which suggests that the inter-chain interaction is not negligible. In fact, the x-ray structure shows that the central unit (H_2O–Cu–H_2O) has 14 hydrogen bonds between eight neighboring Cu(DL-ala)$_2$ and two water molecules. Therefore, this central unit, together with the hydrogen bonded neighboring Cu(DL-ala)$_2$ and water molecules, were considered in the Cu-9 cluster. In the following Table, we present the results of spin densities of both carbon and hydrogen atoms of interest, calculated in the different models. It is clear that the ^{13}C spin densities (and hyperfine shifts) suffer most from the incomplete consideration of metal-metal interactions, which is graphically demonstrated in Figure 2A.

Table S1. Computed Spin Densities of **1** in Different Models (unit: au)

Nucleus [a]	5-coordinate Cu-1	6-coordinate Cu-1	6-coordinate Cu-3	6-coordinate Cu-9
1 ^{13}**C**H	-0.00349	-0.00329	-0.00333	-0.00323
1 ^{13}**C**O_2^-	-0.00511	-0.00483	-0.00457	-0.00400
1 ^{13}**C**H_3	0.00069	0.00073	0.00096	0.00138
1 N^1**H**$_2$	-0.00137	-0.00134	-0.00138	-0.00142
1 C^1**H**	-0.00001	0.00000	0.00000	0.00000
1 C^1**H**$_3$	0.00032	0.00030	0.00030	0.00026

[a] The nucleus of interest is in bold.

The largest structure (Cu-9) investigated has 1628 basis functions and the DFT calculation took approximately 130 CPU hours. For the convenience of the reader, the Gaussian input file of the Cu-9 cluster calculation is provided below:

```
%chk=Cu-bigcluster
%mem=900MB
%nproc=4
# b3lyp/gen scf=(conver=5,diis,maxcyc=918) iop(6/82=1)

Cu-9 model of the x-ray structure of complex (1)

0 10
 C      1.22200      0.19900      4.42800
 H      1.41800      0.67900      3.57300
 C      0.56100      1.22500      5.36700
 C      2.53000     -0.30900      4.93800
 H      3.15200      0.44000      5.04700
 H      2.39500     -0.75000      5.80300
 H      2.90300     -0.95300      4.29900
 N      0.21800     -0.84400      4.10600
 H      0.38700     -1.21100      3.27400
 H      0.22600     -1.50900      4.71100
 O     -0.71100      1.26300      5.38300
 O      1.27100      1.99700      6.03600
 Cu    -1.56900      0.00000      4.15700
 N     -3.35700      0.84400      4.20900
 O     -2.42800     -1.26300      2.93200
 C     -4.36100     -0.19900      3.88700
 H     -4.55700     -0.67900      4.74100
 C     -3.70000     -1.22500      2.94800
 C     -5.66900      0.30900      3.37700
 H     -6.29100     -0.44000      3.26800
 H     -5.53400      0.75000      2.51200
 H     -6.04200      0.95300      4.01600
 H     -3.52600      1.21100      5.04000
 H     -3.36500      1.50900      3.60400
 O     -4.41000     -1.99700      2.27800
 O     -0.78500      1.45000      2.07900
 H     -1.41100      1.94200      1.91700
 H     -0.15800      1.94200      2.24000
 C      2.79200     -0.19900      0.27100
 H      2.98700     -0.67900     -0.58400
 C      2.13100     -1.22500      1.21000
 C      4.10000      0.30900      0.78100
 H      4.72200     -0.44000      0.88900
 H      3.96400      0.75000      1.64600
 H      4.47200      0.95300      0.14200
 N      1.78800      0.84400     -0.05200
 H      1.95600      1.21100     -0.88300
 H      1.79500      1.50900      0.55400
 O      0.85800     -1.26300      1.22500
 O      2.84100     -1.99700      1.87900
 Cu     0.00000      0.00000      0.00000
 N     -1.78800     -0.84400      0.05200
```

O	-0.85800	1.26300	-1.22500
C	-2.79200	0.19900	-0.27100
H	-2.98700	0.67900	0.58400
C	-2.13100	1.22500	-1.21000
C	-4.10000	-0.30900	-0.78100
H	-4.72200	0.44000	-0.88900
H	-3.96400	-0.75000	-1.64600
H	-4.47200	-0.95300	-0.14200
H	-1.95600	-1.21100	0.88300
H	-1.79500	-1.50900	-0.55400
O	-2.84100	1.99700	-1.87900
C	11.71400	-0.19900	8.58500
H	11.90900	-0.67900	7.73000
C	11.05300	-1.22500	9.52400
C	13.02200	0.30900	9.09500
H	13.64400	-0.44000	9.20400
H	12.88600	0.75000	9.96000
H	13.39400	0.95300	8.45600
N	10.71000	0.84400	8.26300
H	10.87900	1.21100	7.43200
H	10.71700	1.50900	8.86800
O	9.78000	-1.26300	9.54000
O	11.76300	-1.99700	10.19300
Cu	8.92200	0.00000	8.31500
N	7.13400	-0.84400	8.36600
O	8.06400	1.26300	7.08900
C	6.13000	0.19900	8.04400
H	5.93500	0.67900	8.89900
C	6.79100	1.22500	7.10500
C	4.82200	-0.30900	7.53400
H	4.20000	0.44000	7.42500
H	4.95800	-0.75000	6.66900
H	4.45000	-0.95300	8.17300
H	6.96600	-1.21100	9.19700
H	7.12700	-1.50900	7.76100
O	6.08100	1.99700	6.43600
C	2.79200	9.36600	0.27100
H	2.98700	8.88500	-0.58400
C	2.13100	8.33900	1.21000
C	4.10000	9.87400	0.78100
H	4.72200	9.12400	0.88900
H	3.96400	10.31400	1.64600
H	4.47200	10.51700	0.14200
N	1.78800	10.40800	-0.05200
H	1.95600	10.77500	-0.88300
H	1.79500	11.07300	0.55400
O	0.85800	8.30100	1.22500
O	2.84100	7.56700	1.87900
Cu	0.00000	9.56400	0.00000
N	-1.78800	8.72000	0.05200
O	-0.85800	10.82700	-1.22500
C	-2.79200	9.76300	-0.27100
H	-2.98700	10.24400	0.58400
C	-2.13100	10.78900	-1.21000
C	-4.10000	9.25500	-0.78100
H	-4.72200	10.00400	-0.88900

H	-3.96400	8.81500	-1.64600
H	-4.47200	8.61200	-0.14200
H	-1.95600	8.35300	0.88300
H	-1.79500	8.05500	-0.55400
O	-2.84100	11.56100	-1.87900
C	8.82200	4.58400	0.27100
H	9.01800	4.10300	-0.58400
C	8.16100	3.55700	1.21000
C	10.13000	5.09200	0.78100
H	10.75200	4.34200	0.88900
H	9.99500	5.53200	1.64600
H	10.50300	5.73500	0.14200
N	7.81800	5.62600	-0.05200
H	7.98700	5.99300	-0.88300
H	7.82600	6.29100	0.55400
O	6.88900	3.51900	1.22500
O	8.87100	2.78500	1.87900
Cu	6.03100	4.78200	0.00000
N	4.24300	3.93800	0.05200
O	5.17200	6.04500	-1.22500
C	3.23900	4.98100	-0.27100
H	3.04300	5.46100	0.58400
C	3.90000	6.00700	-1.21000
C	1.93100	4.47300	-0.78100
H	1.30900	5.22200	-0.88900
H	2.06600	4.03300	-1.64600
H	1.55800	3.83000	-0.14200
H	4.07400	3.57100	0.88300
H	4.23500	3.27300	-0.55400
O	3.19000	6.77900	-1.87900
O	3.67600	3.33200	6.23600
H	4.30300	2.84000	6.39700
H	3.05000	2.84000	6.07400
C	1.66900	4.58400	3.88700
H	1.47400	4.10300	4.74100
C	2.33000	3.55700	2.94800
C	0.36100	5.09200	3.37700
H	-0.26100	4.34200	3.26800
H	0.49700	5.53200	2.51200
H	-0.01100	5.73500	4.01600
N	2.67300	5.62600	4.20900
H	2.50500	5.99300	5.04000
H	2.66600	6.29100	3.60400
O	3.60300	3.51900	2.93200
O	1.62000	2.78500	2.27800
Cu	4.46100	4.78200	4.15700
N	6.24900	3.93800	4.10600
O	5.31900	6.04500	5.38300
C	7.25300	4.98100	4.42800
H	7.44800	5.46100	3.57300
C	6.59200	6.00700	5.36700
C	8.56100	4.47300	4.93800
H	9.18300	5.22200	5.04700
H	8.42500	4.03300	5.80300
H	8.93300	3.83000	4.29900
H	6.41800	3.57100	3.27400

H	6.25600	3.27300	4.71100
O	7.30200	6.77900	6.03600
O	5.24600	6.23300	2.07900
H	4.61900	6.72500	1.91700
H	5.87200	6.72500	2.24000
C	5.68300	4.58400	8.58500
H	5.87900	4.10300	7.73000
C	5.02200	3.55700	9.52400
C	6.99100	5.09200	9.09500
H	7.61300	4.34200	9.20400
H	6.85600	5.53200	9.96000
H	7.36400	5.73500	8.45600
N	4.67900	5.62600	8.26300
H	4.84800	5.99300	7.43200
H	4.68700	6.29100	8.86800
O	3.75000	3.51900	9.54000
O	5.73200	2.78500	10.19300
Cu	2.89200	4.78200	8.31500
N	1.10400	3.93800	8.36600
O	2.03300	6.04500	7.08900
C	0.10000	4.98100	8.04400
H	-0.09600	5.46100	8.89900
C	0.76100	6.00700	7.10500
C	-1.20800	4.47300	7.53400
H	-1.83000	5.22200	7.42500
H	-1.07300	4.03300	6.66900
H	-1.58100	3.83000	8.17300
H	0.93500	3.57100	9.19700
H	1.09600	3.27300	7.76100
O	0.05100	6.77900	6.43600
O	9.70700	8.11400	6.23600
H	10.33300	7.62200	6.39700
H	9.08100	7.62200	6.07400
C	7.70000	9.36600	3.88700
H	7.50400	8.88500	4.74100
C	8.36100	8.33900	2.94800
C	6.39200	9.87400	3.37700
H	5.77000	9.12400	3.26800
H	6.52700	10.31400	2.51200
H	6.01900	10.51700	4.01600
N	8.70400	10.40800	4.20900
H	8.53500	10.77500	5.04000
H	8.69600	11.07300	3.60400
O	9.63300	8.30100	2.93200
O	7.65100	7.56700	2.27800
Cu	10.49200	9.56400	4.15700
N	12.27900	8.72000	4.10600
O	11.35000	10.82700	5.38300
C	13.28300	9.76300	4.42800
H	13.47900	10.24400	3.57300
C	12.62200	10.78900	5.36700
C	14.59100	9.25500	4.93800
H	15.21300	10.00400	5.04700
H	14.45600	8.81500	5.80300
H	14.96400	8.61200	4.29900
H	12.44800	8.35300	3.27400

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 H      12.28700      8.05500      4.71100
 O      13.33200     11.56100      6.03600
 C      11.71400      9.36600      8.58500
 H      11.90900      8.88500      7.73000
 C      11.05300      8.33900      9.52400
 C      13.02200      9.87400      9.09500
 H      13.64400      9.12400      9.20400
 H      12.88600     10.31400      9.96000
 H      13.39400     10.51700      8.45600
 N      10.71000     10.40800      8.26300
 H      10.87900     10.77500      7.43200
 H      10.71700     11.07300      8.86800
 O       9.78000      8.30100      9.54000
 O      11.76300      7.56700     10.19300
Cu       8.92200      9.56400      8.31500
 N       7.13400      8.72000      8.36600
 O       8.06400     10.82700      7.08900
 C       6.13000      9.76300      8.04400
 H       5.93500     10.24400      8.89900
 C       6.79100     10.78900      7.10500
 C       4.82200      9.25500      7.53400
 H       4.20000     10.00400      7.42500
 H       4.95800      8.81500      6.66900
 H       4.45000      8.61200      8.17300
 H       6.96600      8.35300      9.19700
 H       7.12700      8.05500      7.76100
 O       6.08100     11.56100      6.43600

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6-31g*
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      50072.9000        0.217000000E-02
      11373.4000        0.112200000E-01
      3239.82000        0.446210000E-01
      1071.97000        0.138360000
      395.099000        0.312550000
 S   2  1.00
      158.399000        0.410600000
      67.3591000        0.214530000
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 S   1  1.00
      9.39357000         1.00000000
 S   1  1.00
      2.57848000         1.00000000
 S   1  1.00
     0.964080000         1.00000000
 S   1  1.00
     0.113303000         1.00000000
 S   1  1.00
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    0.407910000E-01      1.00000000
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     532.106000        0.184100000E-01
     172.195000        0.864600000E-01
P   3  1.00
     65.3239000        0.254500000
     27.0551000        0.434190000
     11.7435000        0.333900000
P   1  1.00
     4.69382000         1.00000000
P   2  1.00
     1.90667000        0.569360000
    0.711445000        0.247020000
P   1  1.00
    0.232598000         1.00000000
P   1  1.00
    0.692990000E-01      1.00000000
D   3  1.00
     48.5439000        0.309700000E-01
     13.5490000        0.161960000
     4.51628000        0.378120000
D   1  1.00
     1.47329000         1.00000000
D   1  1.00
    0.414875000         1.00000000
D   1  1.00
    0.149100000         1.00000000
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3-21G*
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3-21G*
****
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3-21G*
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Table S2. Crystal data and structure refinement for p05yas.

Identification code	p05yas	
Empirical formula	C6 H14 Cu N2 O5	
Formula weight	257.73	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 12.061(5) Å	α= 90°.
	b = 9.564(4) Å	β= 110.683(7)°.
	c = 8.887(4) Å	γ = 90°.
Volume	959.1(7) $Å^3$	
Z	4	
Density (calculated)	1.785 Mg/m^3	
Absorption coefficient	2.277 mm^{-1}	
F(000)	532	
Crystal size	0.22 x 0.08 x 0.08 mm^3	
Theta range for data collection	2.79 to 25.47°.	
Index ranges	-14<=h<=13, 0<=k<=11, 0<=l<=10	
Reflections collected	2938	
Independent reflections	2738 [R(int) = 0.0000]	
Completeness to theta = 25.47°	98.8 %	
Absorption correction	Integration	
Max. and min. transmission	0.8565 and 0.6545	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2738 / 3 / 78	
Goodness-of-fit on F^2	0.965	
Final R indices [I>2sigma(I)]	R1 = 0.0526, wR2 = 0.1429	
R indices (all data)	R1 = 0.0796, wR2 = 0.1562	
Largest diff. peak and hole	0.863 and -0.501 $e.Å^{-3}$	

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for p05yas. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	7400(4)	4792(4)	325(5)	29(1)
C(2)	7145(3)	3719(4)	1455(4)	21(1)
C(3)	8644(4)	5324(5)	939(6)	41(1)
N(1)	6466(3)	5882(3)	-62(3)	20(1)
O(1)	6095(2)	3679(2)	1474(3)	22(1)
O(2)	7943(2)	2912(3)	2260(3)	28(1)
O(3)	5000	6517(4)	2500	27(1)
Cu(1)	5000	5000	0	19(1)

Table S4. Bond lengths [Å] and angles [°] for p05yas.

C(1)-N(1)	1.483(5)
C(1)-C(3)	1.493(7)
C(1)-C(2)	1.540(5)
C(1)-H(1)	1.0000
C(2)-O(2)	1.244(4)
C(2)-O(1)	1.273(4)
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
N(1)-Cu(1)	1.977(3)
N(1)-H(1A)	0.92(3)
N(1)-H(1B)	0.899(19)
O(1)-Cu(1)	1.958(2)
O(3)-H(3)	0.81(2)
Cu(1)-O(1)#1	1.958(2)
Cu(1)-N(1)#1	1.977(3)
N(1)-C(1)-C(3)	115.4(3)
N(1)-C(1)-C(2)	108.1(3)
C(3)-C(1)-C(2)	113.2(3)
N(1)-C(1)-H(1)	106.5
C(3)-C(1)-H(1)	106.5
C(2)-C(1)-H(1)	106.5
O(2)-C(2)-O(1)	123.0(3)
O(2)-C(2)-C(1)	119.8(3)
O(1)-C(2)-C(1)	117.2(3)
C(1)-C(3)-H(3A)	109.5
C(1)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(1)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(1)-N(1)-Cu(1)	107.9(2)
C(1)-N(1)-H(1A)	111(2)

Cu(1)-N(1)-H(1A)	111(2)
C(1)-N(1)-H(1B)	112(2)
Cu(1)-N(1)-H(1B)	108(2)
H(1A)-N(1)-H(1B)	108(3)
C(2)-O(1)-Cu(1)	114.3(2)
O(1)-Cu(1)-O(1)#1	180.0
O(1)-Cu(1)-N(1)	84.00(11)
O(1)#1-Cu(1)-N(1)	96.00(11)
O(1)-Cu(1)-N(1)#1	96.00(11)
O(1)#1-Cu(1)-N(1)#1	84.00(11)
N(1)-Cu(1)-N(1)#1	180.00(15)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z

Table S5. Anisotropic displacement parameters ($Å^2 x 10^3$) for p05yas. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	23(3)	29(2)	34(2)	5(2)	9(2)	3(2)
C(2)	20(2)	21(2)	18(2)	-3(1)	3(2)	2(2)
C(3)	21(3)	42(3)	53(3)	14(2)	4(2)	1(2)
N(1)	20(2)	18(2)	19(1)	1(1)	5(1)	2(1)
O(1)	18(1)	26(1)	23(1)	6(1)	6(1)	2(1)
O(2)	20(2)	30(2)	32(1)	8(1)	7(1)	8(1)
O(3)	15(2)	25(2)	34(2)	0	2(2)	0
Cu(1)	11(1)	20(1)	23(1)	4(1)	2(1)	1(1)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for p05yas.

	x	y	z	U(eq)
H(1)	7294	4290	-703	35
H(3A)	9193	4540	1070	62
H(3B)	8802	5784	1979	62
H(3C)	8752	5996	170	62
H(1A)	6350(30)	6270(40)	-1060(40)	29
H(1B)	6660(30)	6580(30)	670(40)	29
H(3)	4430(30)	7030(30)	2310(50)	40

Table S7. Torsion angles [°] for p05yas.

N(1)-C(1)-C(2)-O(2)	-162.1(3)
C(3)-C(1)-C(2)-O(2)	-33.1(5)
N(1)-C(1)-C(2)-O(1)	20.0(4)
C(3)-C(1)-C(2)-O(1)	149.1(3)
C(3)-C(1)-N(1)-Cu(1)	-157.9(3)
C(2)-C(1)-N(1)-Cu(1)	-30.0(3)
O(2)-C(2)-O(1)-Cu(1)	-176.7(2)
C(1)-C(2)-O(1)-Cu(1)	1.1(4)
C(2)-O(1)-Cu(1)-N(1)	-15.5(2)
C(2)-O(1)-Cu(1)-N(1)#1	164.5(2)
C(1)-N(1)-Cu(1)-O(1)	25.5(2)
C(1)-N(1)-Cu(1)-O(1)#1	-154.5(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z

Table S8. Hydrogen bonds for p05yas [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...O(1)#2	0.92(3)	2.10(4)	2.980(4)	158(3)
N(1)-H(1B)...O(2)#3	0.899(19)	2.15(2)	3.037(4)	168(3)
O(3)-H(3)...O(2)#4	0.81(2)	1.97(3)	2.758(3)	164(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z #2 x,-y+1,z-1/2 #3 -x+3/2,y+1/2,-z+1/2

#4 x-1/2,y+1/2,z