Electronic Supplementary Material (ESI) for Nanoscale.

Supporting information for: ^{1}H NMR Global Diatropicity in Copper Hydride Complexes

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Supplementary Tables

Table SI-1. Experimental Cu-μ_3-H distances (d_n) on top and bottom of the triangular cupola, average distance and standard deviation in Å for the Cu_{20} and Cu_{32} clusters.

		Cu1	Cu2	Cu3	Average	STD
Cu20[a]	Top					
	d_1	1.62	1.58	1.63	1.61	0.03
	d_2	1.69	1.70	1.70	1.70	0.01
	d_3	1.75	1.73	1.70	1.73	0.02
	Bottom					
	d_1	1.64	1.59	1.54	1.59	0.05
	d_2	1.75	1.75	1.73	1.75	0.01
	d_3	1.77	1.81	1.80	1.79	0.02
	Top					
Cu32[b]	d_1	1.65	1.58	1.66	1.63	0.04
	d_2	1.73	1.75	1.68	1.72	0.04
	d_3	1.77	1.87	1.71	1.78	0.08
	Bottom					
	d_1	1.65	1.58	1.66	1.63	0.04
	d_2	1.73	1.75	1.68	1.72	0.04
	d_3	1.77	1.87	1.71	1.78	0.08

[a] Ref;[1] [b] Ref.[2] .

Supplementary Figures

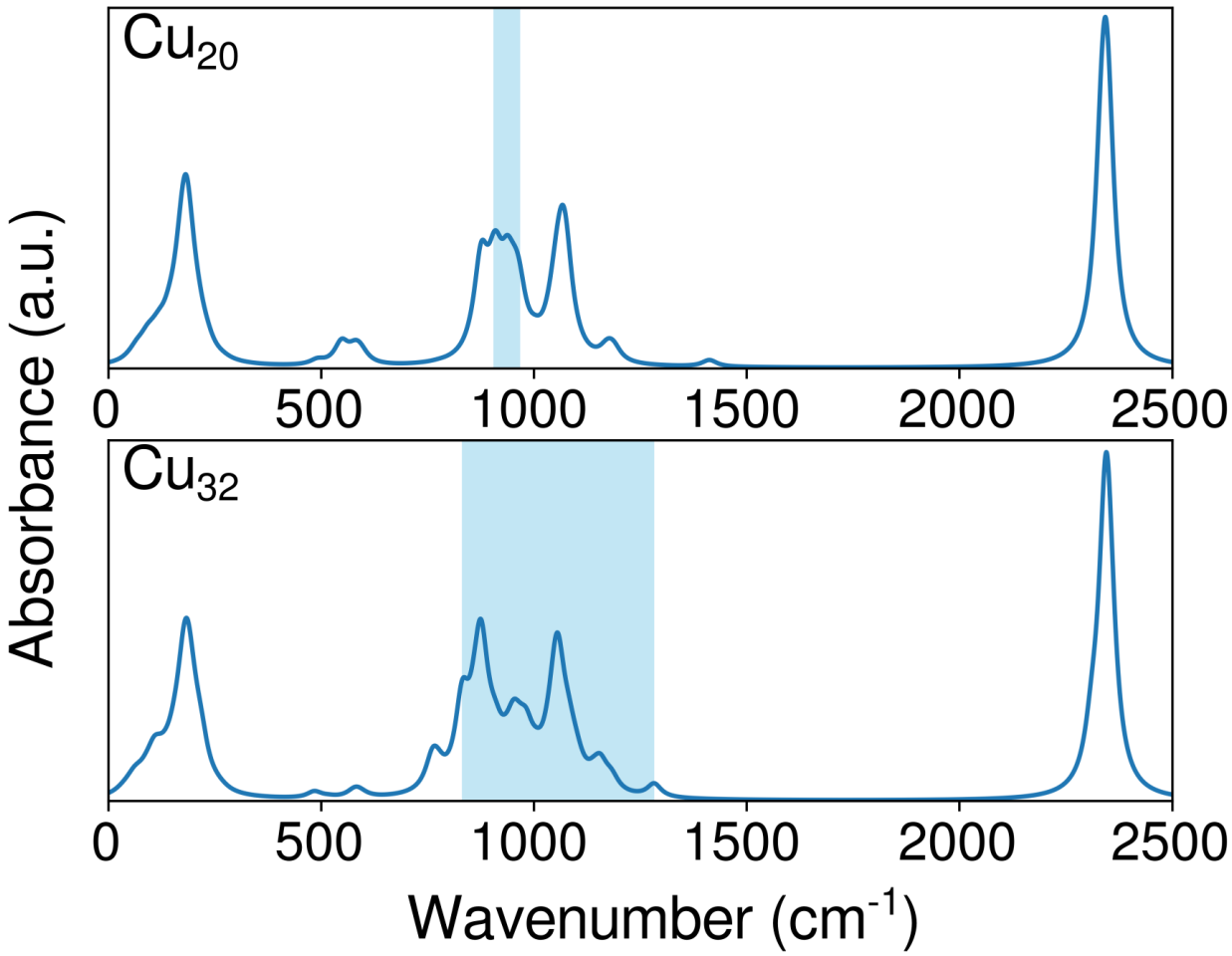

Fig. SI-1. IR spectra for $Cu_{20}H_{11}(S_2PH_2)_9$ (top row) and $Cu_{32}H_{20}(S_2PH_2)_{12}$ (bottom row). The blue shadow area indicates the range of the hydrides normal modes.

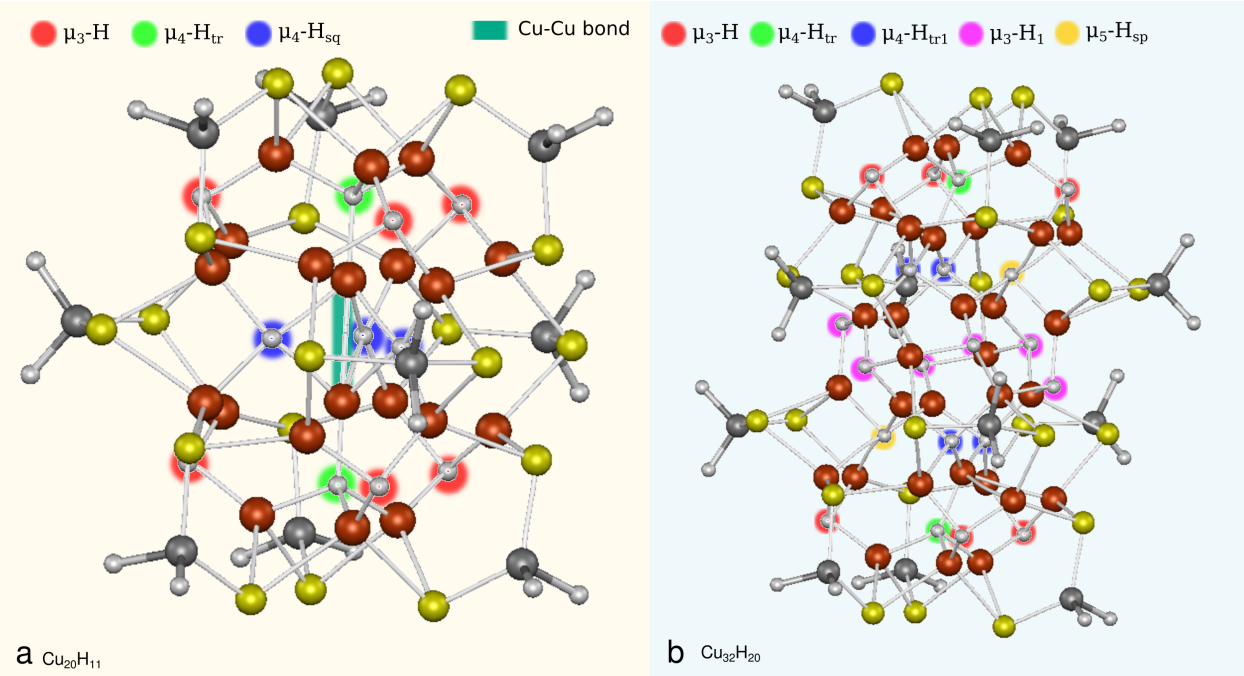

Fig. SI-2. Molecular graphs of **1** (left) and **2** (right). Bond path analyses shows that Cu-Cu bonds are absent with the exception of a Cu-Cu dimer at the centre of **1**. The different hydrides are highlighted.

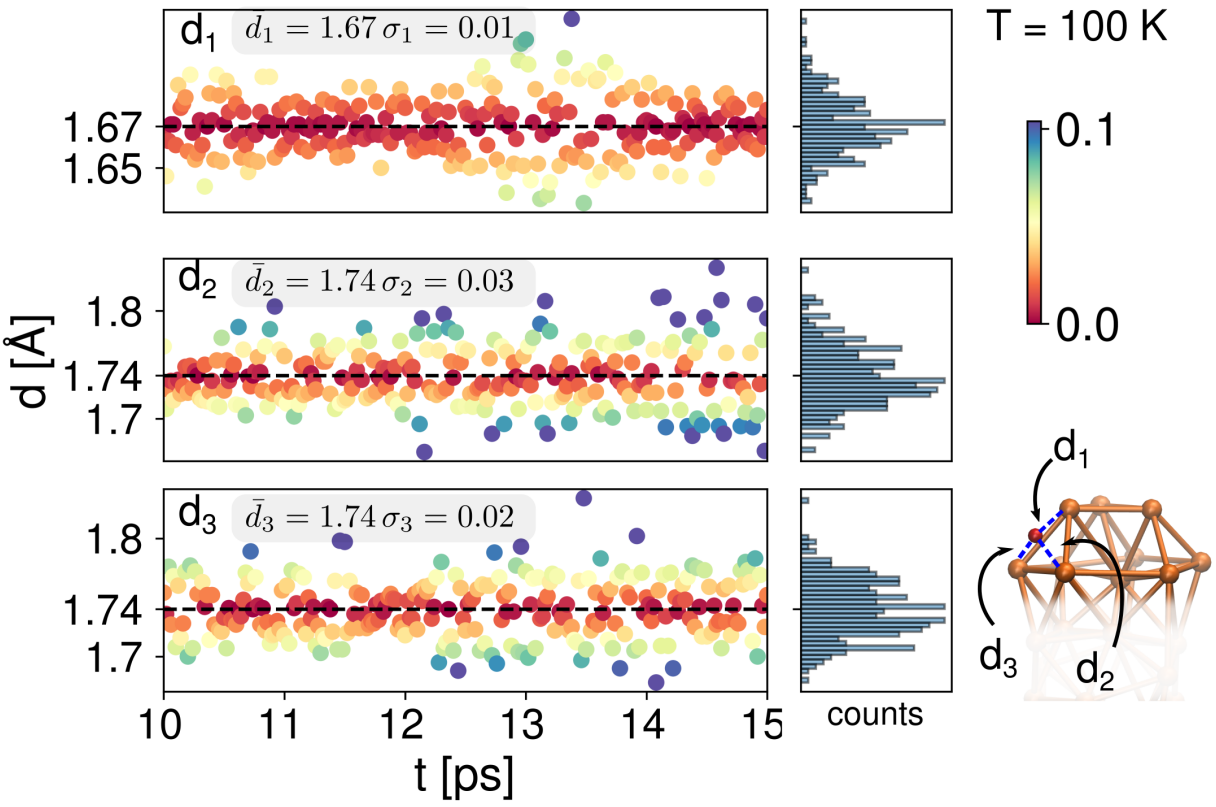

Fig. SI-3. Bond lengths analysis between the μ_3-H hydride and the three coordinated neighbor Cu atoms for the BOMD trajectory during 10 –15 ps for the cluster **2** at 100 K.

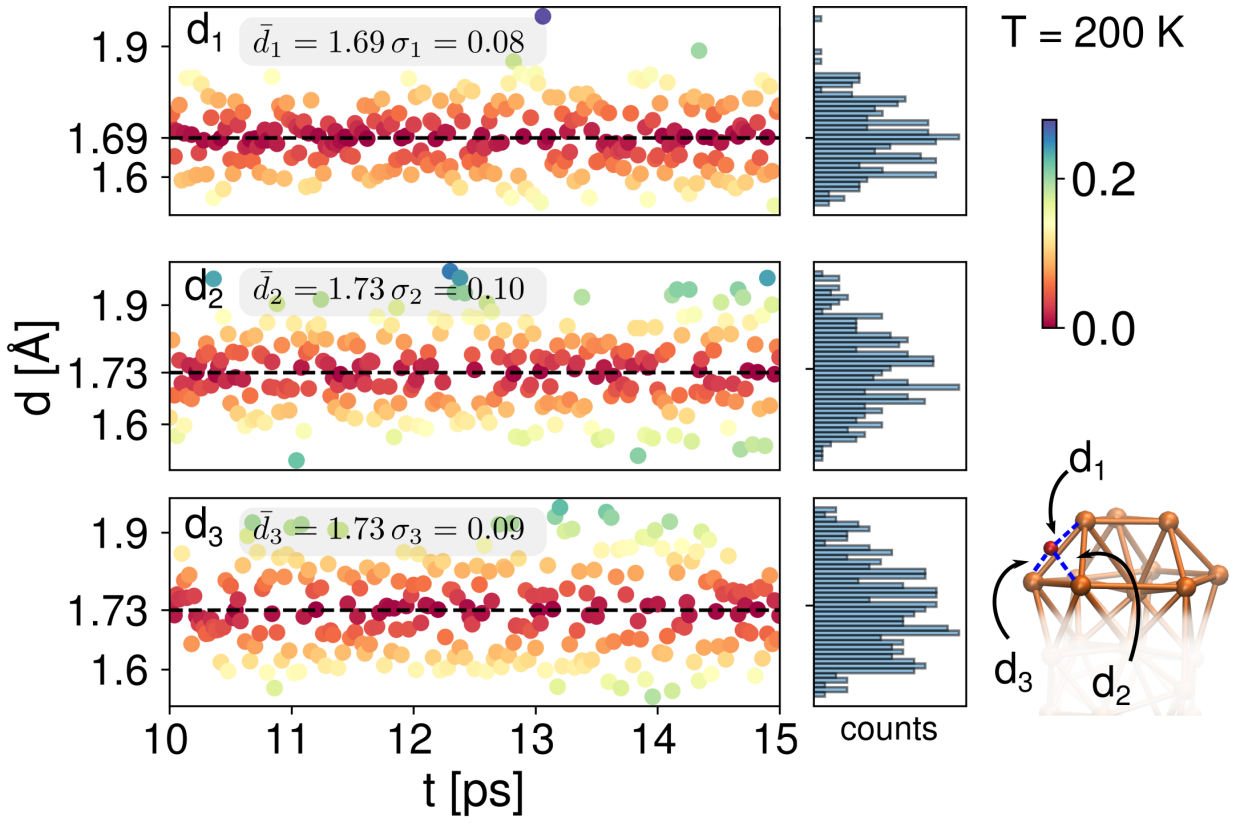

Fig. SI-4. Bond lengths analysis between the μ_3-H hydride and the three coordinated neighbor Cu atoms for the BOMD trajectory during 10 –15 ps for the cluster **2** at 200 K.

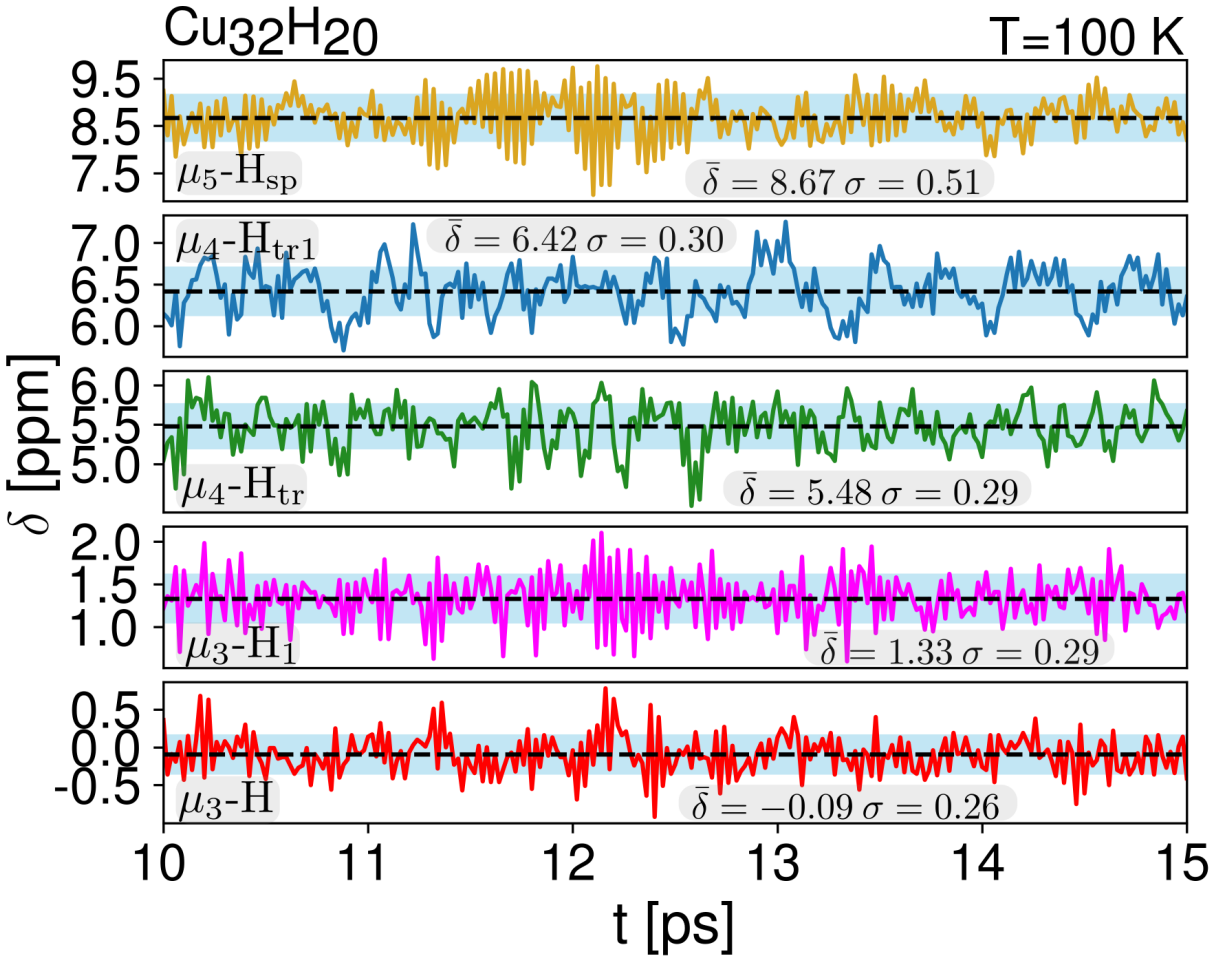

Fig. SI-5. ^{1}H NMR dynamics of one sample of each ot the μ_3-H, μ_3-H$_1$, μ_4-H$_{tr}$, μ_4-H$_{tr1}$ and μ_5-H$_{sp}$ hydride types for cluster **2** during 10 – 15 ps at 100 K. The average shifts are given by the dashed lines while the standard deviations are shown with the blue shading.

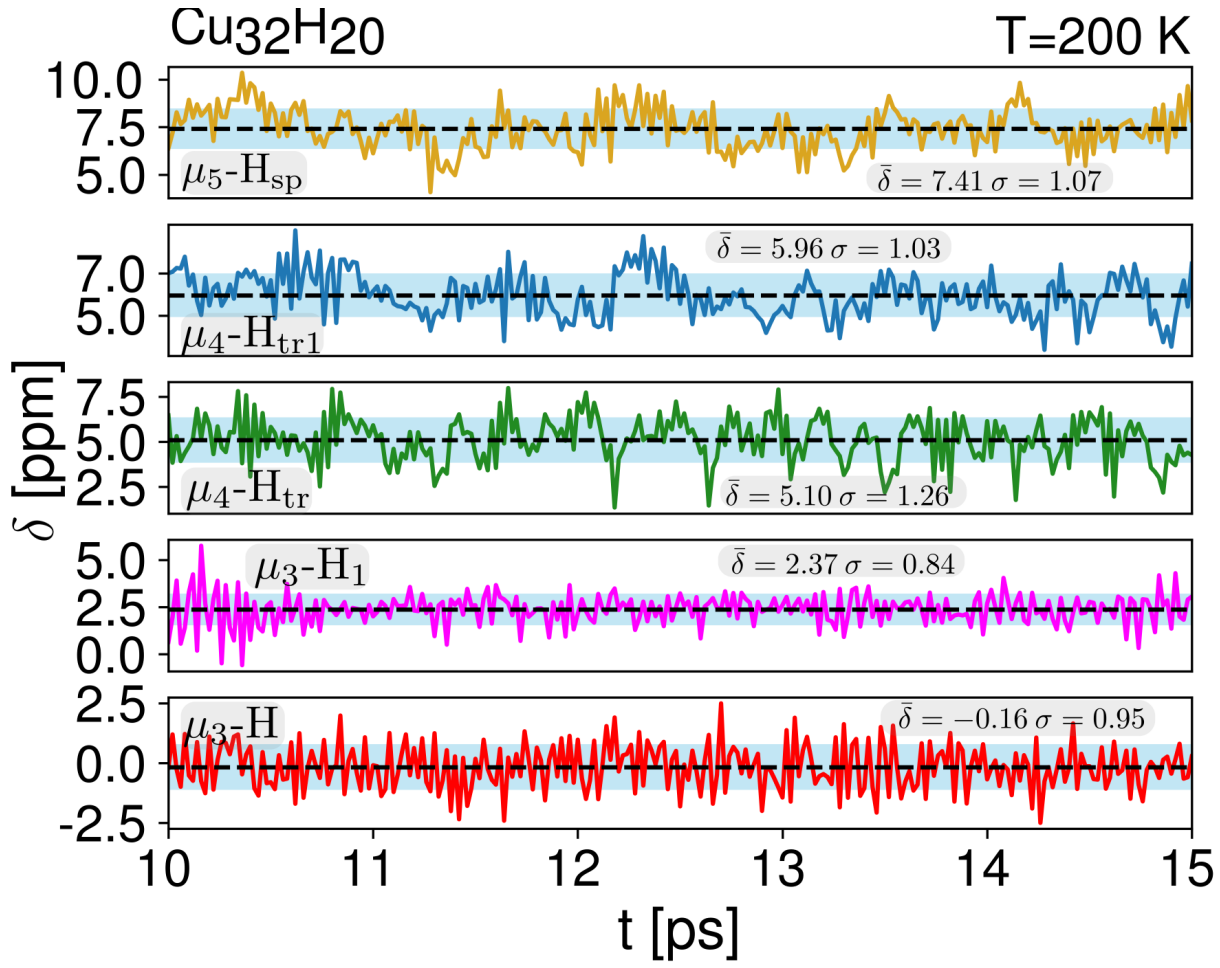

Fig. SI-6. ^{1}H NMR dynamics of one sample of each ot the μ_3-H, μ_3-H$_1$, μ_4-H$_{tr}$, μ_4-H$_{tr1}$ and μ_5-H$_{sp}$ hydride types for cluster **2** during 10 – 15 ps at 200 K. The average shifts are given by the dashed lines while the standard deviations are shown with the blue shading.

References

(1) Dhayal, R. S.; Liao, J.-H.; Lin, Y.-R.; Liao, P.-K.; Kahlal, S.; Saillard, J.-Y.; Liu, C. W. A Nanospheric Polyhydrido Copper Cluster of Elongated Triangular Orthobicupola Array: Liberation of H2 from Solar Energy. *Journal of the American Chemical Society* **2013**, *135*, 4704–4707.

(2) Dhayal, R. S.; Liao, J.-H.; Kahlal, S.; Wang, X.; Liu, Y.-C.; Chiang, M.-H.; vanZyl, W. E.; Saillard, J.-Y.; Liu, C. W. [Cu32(H)20S2P(OiPr)212]: The Largest Number of Hydrides Recorded in a Molecular Nanocluster by Neutron Diffraction. *Chemistry – A European Journal* **2015**, *21*, 8369–8374.