Table S2. The ^{1}H and Cu shielding tensor elements (σ, ppm along with the chemical shifts (δ, ppm) for the cyclic Cu_nH_n clusters computed at the GIAO/B3LYP/6-311+G(*d,p*)//B3LYP/6-311+G(*d,p*) and GIAO/B3LYP/6-31G(*d,p*)//B3LYP/LANL2DZ (figures in parentheses).[a]

	^{63}Cu			^{1}H		
Cluster	σ^{iso}	σ^{aniso}	(δ,ppm)	σ^{iso}	σ^{aniso}	(δ,ppm)
$Cu_3H_3(D_{3h})$	1459.7 (1411.0)	776.5 (1197.0)		29.0 (29.8)	15.9 (17.4)	2.9 (2.0)
$Cu_4H_4(D_{4h})$	1455.6 (1540.9)	1054.0 (1395.7)		31.6 (32.4)	11.6 (11.9)	0.3 (-0.6)
	(1516.0)	(1288.2)		(32.3)	(12.1)	(-0.5)
$Cu_4H_4(T_d)$	1674.7	21.8		30.3	11.8	1.6
$Cu_5H_5(D_{5h})$	1491.5 (1581.2)	1185.5 (1527.4)		32.5 (33.9)	10.4 (7.0)	-0.6 (-2.1)
	(1582.5)	(1527.5)				
$Cu_5H_5(C_{2v})$	1291.8	1058.6		32.0	14.1	-0.1
	1344.6	1173.1		31.4	9.0	0.5
	1263.3	657.5		30.9	16.8	1.0
	849.0	361.4		28.6	16.1	3.3
	1262.7	644.2				
$Cu_6H_6(D_{6h})$	1539.7 (1617.0)	1205.0 (1401.3)		32.8 (34.1)	15.0 (9.0)	-0.9 (-2.3)
	(1614.5)	(1451.9)				
$Cu_6H_6(D_{2h})$	1625.0 (1635.9)	411.0 (418.7)		30.0 (29.9)	11.6 (14.8)	1.9 (2.0)
	(1763.2)	(648.0)				

[a] The calculated absolute ^{63}Cu, and ^{1}H shielding tensor elements $\sigma^{iso}(\sigma^{aniso})$ for TMS(Tetramethylsilane) external reference standards at the same level of theory are 31.9 (9.9) ppm.