

-- Supporting Information --

Aromaticity Introduced by Antiferromagnetic Ligand Mediated Metal-Metal Interactions. Insights from the Induced Magnetic Response in $[\text{Cu}_6(\text{dmPz})_6(\text{OH})_6]$

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Content.

Table S1. Coordinates for the optimized structure of $[\text{trans-Cu}_6(\text{dmPz})_6(\text{OH})_6]$ (Å).

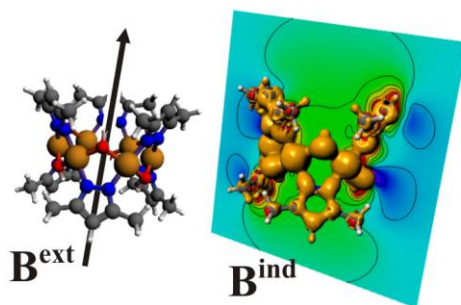


Table S1. Coordinates for the optimized structure of [*trans*-Cu₆(dmPz)₆(OH)₆] (Å).

Cu	-1.595036000	2.762684000	0.000000000
Cu	1.595036000	2.762684000	0.000000000
Cu	3.190073000	0.000000000	0.000000000
H	1.412113000	-4.152051000	3.833010000
H	2.972442000	-4.932672000	3.535532000
H	1.805214000	-4.725716000	2.200334000
H	-2.889725000	3.298952000	3.833010000
H	-3.189983000	3.926219000	2.200334000
H	-2.785598000	5.040546000	3.535532000
H	3.189983000	3.926219000	2.200334000
H	2.889725000	3.298952000	3.833010000
H	2.785598000	5.040546000	3.535532000
H	1.805214000	4.725716000	-2.200334000
H	1.412113000	4.152051000	-3.833010000
H	2.972442000	4.932672000	-3.535532000
H	4.301839000	-0.853100000	-3.833010000
H	5.758040000	0.107875000	-3.535532000
H	4.995197000	-0.799497000	-2.200334000
H	5.758040000	-0.107875000	3.535532000
H	4.995197000	0.799497000	2.200334000
H	4.301839000	0.853100000	3.833010000
O	-2.853803000	1.647644000	0.983617000
O	0.000000000	3.295288000	-0.983617000
O	2.853803000	1.647644000	0.983617000
N	2.626471000	-2.300536000	1.591079000
N	-0.679087000	3.424858000	1.591079000
N	0.679087000	3.424858000	1.591079000
N	2.626471000	2.300536000	-1.591079000
N	3.305558000	1.124322000	-1.591079000
N	3.305558000	-1.124322000	1.591079000
C	2.836163000	-2.930065000	2.774120000
C	2.225253000	-4.257099000	3.098577000
C	-1.119429000	3.921222000	2.774120000
C	0.000000000	4.254231000	3.551983000
H	0.000000000	4.691986000	4.547187000
C	1.119429000	3.921222000	2.774120000
C	-2.574129000	4.055675000	3.098577000
C	2.574129000	4.055675000	3.098577000
C	2.836163000	2.930065000	-2.774120000
C	3.684272000	2.127115000	-3.551983000
H	4.063379000	2.345993000	-4.547187000
C	3.955592000	0.991157000	-2.774120000
C	2.225253000	4.257099000	-3.098577000
C	4.799382000	-0.201424000	-3.098577000
C	3.955592000	-0.991157000	2.774120000
C	3.684272000	-2.127115000	3.551983000
H	4.063379000	-2.345993000	4.547187000
C	4.799382000	0.201424000	3.098577000
Cu	1.595036000	-2.762684000	0.000000000
Cu	-1.595036000	-2.762684000	0.000000000
Cu	-3.190073000	0.000000000	0.000000000
H	-1.412113000	4.152051000	-3.833010000
H	-2.972442000	4.932672000	-3.535532000
H	-1.805214000	4.725716000	-2.200334000
H	2.889725000	-3.298952000	-3.833010000
H	3.189983000	-3.926219000	-2.200334000
H	2.785598000	-5.040546000	-3.535532000
H	-3.189983000	-3.926219000	-2.200334000
H	-2.889725000	-3.298952000	-3.833010000
H	-2.785598000	-5.040546000	-3.535532000
H	-1.805214000	-4.725716000	2.200334000
H	-1.412113000	-4.152051000	3.833010000
H	-2.972442000	-4.932672000	3.535532000
H	-4.301839000	0.853100000	3.833010000
H	-5.758040000	-0.107875000	3.535532000
H	-4.995197000	0.799497000	2.200334000
H	-5.758040000	0.107875000	-3.535532000
H	-4.995197000	-0.799497000	-2.200334000

H	-4.301839000	-0.853100000	-3.833010000
O	2.853803000	-1.647644000	-0.983617000
O	0.000000000	-3.295288000	0.983617000
O	-2.853803000	-1.647644000	-0.983617000
N	-2.626471000	2.300536000	-1.591079000
N	0.679087000	-3.424858000	-1.591079000
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N	-2.626471000	-2.300536000	1.591079000
N	-3.305558000	-1.124322000	1.591079000
N	-3.305558000	1.124322000	-1.591079000
C	-2.836163000	2.930065000	-2.774120000
C	-2.225253000	4.257099000	-3.098577000
C	1.119429000	-3.921222000	-2.774120000
C	0.000000000	-4.254231000	-3.551983000
H	0.000000000	-4.691986000	-4.547187000
C	-1.119429000	-3.921222000	-2.774120000
C	2.574129000	-4.055675000	-3.098577000
C	-2.574129000	-4.055675000	-3.098577000
C	-2.836163000	-2.930065000	2.774120000
C	-3.684272000	-2.127115000	3.551983000
H	-4.063379000	-2.345993000	4.547187000
C	-3.955592000	-0.991157000	2.774120000
C	-2.225253000	-4.257099000	3.098577000
C	-4.799382000	0.201424000	3.098577000
C	-3.955592000	0.991157000	-2.774120000
C	-3.684272000	2.127115000	-3.551983000
H	-4.063379000	2.345993000	-4.547187000
C	-4.799382000	-0.201424000	-3.098577000
H	0.000000000	-2.892569000	1.876141000
H	2.505039000	1.446285000	1.876141000
H	-2.505039000	1.446285000	1.876141000
H	-2.505039000	-1.446285000	-1.876141000
H	0.000000000	2.892569000	-1.876141000
H	2.505039000	-1.446285000	-1.876141000