The Jahn-Teller Effect in Cu(II) Complexes: Comprehensive Molecular Modelling for Elongations, Compressions and All Points Inbetween
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Supporting Information

Table S1: rms and individual bond length deviations (LFMM-X-ray)

Refcode	rms	Cu-N1	Cu-N2	Cu-N3	Cu-N4	Cu-N5	Cu-N6
TERPYC01	0.027	-0.007	-0.041	-0.043	-0.022	-0.007	-0.021
DEQSOH	0.036	0.006	-0.030	0.070	0.021	-0.022	0.029
XUTYOA	0.090	0.008	0.108	0.048	**0.160**	0.093	-0.002
JUNDAX	0.076	**-0.124**	**-0.124**	0.032	0.032	-0.026	-0.026
LOYSAT	0.079	0.049	0.049	0.064	0.063	-0.112	-0.112
WOHSAN	0.077	-0.104	0.100	-0.010	0.004	0.019	**-0.121**
KAYTOT	0.043	0.056	0.056	0.038	0.037	-0.030	-0.031
SAFLEQ	0.049	0.050	0.047	-0.065	0.032	-0.056	-0.039
LABJEE	0.069	**0.121**	0.005	0.027	-0.052	-0.019	-0.102
Cu(AM)6	0.051	-0.088	-0.005	-0.005	-0.088	-0.006	-0.006
KIQNAZ	0.018	-0.014	-0.008	-0.027	-0.013	-0.008	-0.028
FUPJEF	0.033	-0.057	0.006	0.010	-0.057	0.006	0.010
TACCUP	0.025	-0.034	-0.035	0.017	0.019	0.018	0.020
LOMREK	0.071	0.019	0.037	0.116	0.036	0.019	0.116
NIJYAG	0.068	-0.039	-0.072	0.083	-0.031	-0.080	0.084
LUBXAH01	0.023	-0.023	0.025	-0.020	0.025	-0.024	-0.019
SOFPAE	0.064	0.026	-0.099	0.045	0.026	-0.099	0.045
PEFQIA01	0.053	-0.008	0.004	0.011	0.043	-0.100	-0.071
PEFQEW01	0.054	0.072	-0.009	0.035	-0.019	-0.066	-0.079
XAJBAL	0.056	-0.026	-0.001	0.095	-0.059	-0.048	-0.056
XAHZUB	0.054	-0.083	-0.044	-0.022	-0.054	-0.054	-0.049

Table S2: terpy data

Refcode	Structure
BEJPUB	compressed
KOFQAX	elongated
NELKEU	compressed
NIQTAI	compressed
PULCAA	elongated
SIBWEF	rhombic compressed
SIMJAZ	rhombic compressed
TERPYC01	elongated

Table S3: phen data

Refcode	Structure
AGOJIP	rhombic compressed
CAJSUC	rhombic
DEQSOH	elongated
EGAXUF	elongated
IKUCIA	elongated
IVUPIY	elongated
JANLIT	compressed
NILTEH	elongated
PENCUC	elongated
UKEVAH	compressed

WUTXAK   elongated