SUPPORTING INFORMATION

EPR Spectroscopy of Cu(II) Complexes: Prediction of g-Tensors Using Double-Hybrid Density Functional Theory

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Table S1. Calculated Δg-values (ppt), $\Delta g^{\mathrm{calc}} = (g^{\mathrm{calc}} - g_{\mathrm{e}}) \cdot 1000$ with g_{e} = 2.0023, obtained with the **PBE0** functional, differences (D), $\mathrm{D}(\Delta g) = \Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}$, and percent differences (PD), $\mathrm{PD}(\Delta g) = \frac{\Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}}{\Delta g^{\mathrm{exp}}} \cdot 100$, from the experimental values of the Δg parameter for the set of 18 Cu(II) complexes.

	Δg_{xx}	Δg_{yy}	Δg_{zz}	$\mathrm{D}(\Delta g_{\perp})$	$\mathrm{D}(\Delta g_{\parallel})$	$\mathrm{D}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\parallel})$	$\mathrm{PD}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$
1	45	45	166	1	-72	-73	1	-30	-38
2	43	43	163	-8	-97	-89	-16	-37	-43
3	45	46	174	1	-85	-86	2	-33	-40
4	40	40	145	1	-57	-58	3	-28	-36
5	33	52	156	-7	-109	-102	-14	-41	-47
6	39	53	158	-4	-42	-38	-7	-21	-25
7	39	49	155	-4	-83	-78	-9	-35	-41
8	43	46	158	-6	-93	-86	-13	-37	-43
9	52	56	183	-6	-69	-64	-9	-27	-33
10	48	51	185	-8	-97	-90	-14	-34	-40
11	28	52	149	-8	-53	-46	-16	-26	-29
12	41	50	156	-8	-9	-1	-15	-5	-1
13	30	65	160	8	-41	-48	19	-20	-30
14	28	52	135	-17	23	41	-30	21	74
15	30	32	111	-5	-13	-7	-15	-10	-8
16	30	48	130	-3	-5	-2	-7	-4	-3
17	22	27	87	2	5	2	10	6	4
18	37	40	126	14	15	1	56	13	1

Table S2. Calculated Δg-values (ppt), $\Delta g^{\mathrm{calc}} = (g^{\mathrm{calc}} - g_{\mathrm{e}}) \cdot 1000$ with g_{e} = 2.0023, obtained with the **BHandHLYP** functional, differences (D), $\mathrm{D}(\Delta g) = \Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}$, and percent differences (PD), $\mathrm{PD}(\Delta g) = \frac{\Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}}{\Delta g^{\mathrm{exp}}} \cdot 100$, from the experimental values of the Δg parameter for the set of 18 Cu(II) complexes.

	Δg_{xx}	Δg_{yy}	Δg_{zz}	$\mathrm{D}(\Delta g_{\perp})$	$\mathrm{D}(\Delta g_{\parallel})$	$\mathrm{D}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\parallel})$	$\mathrm{PD}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$
1	64	64	245	19	6	-13	43	2	-7
2	60	61	242	10	-18	-28	19	-7	-13
3	62	64	250	18	-10	-28	41	-4	-13
4	58	58	223	19	20	1	50	10	0
5	44	77	229	11	-35	-46	22	-13	-22
6	53	75	231	14	31	17	29	16	11
7	55	66	225	13	-13	-26	28	-5	-14
8	63	65	235	12	-16	-28	24	-6	-14
9	75	80	270	18	18	0	30	7	0
10	69	71	268	12	-15	-27	21	-5	-12
11	40	86	232	15	29	14	32	14	9
12	64	75	242	16	77	62	29	47	56
13	46	107	269	36	69	32	90	34	20
14	45	85	221	8	110	102	14	98	187
15	57	59	212	21	88	66	58	71	76
16	50	76	217	21	81	60	50	60	64
17	45	46	175	23	92	69	101	111	115
18	73	75	241	49	129	80	199	116	92

Table S3. Calculated Δg-values (ppt), $\Delta g^{\mathrm{calc}} = (g^{\mathrm{calc}} - g_{\mathrm{e}}) \cdot 1000$ with g_{e} = 2.0023, obtained with the **B3LYP** functional, differences (D), $\mathrm{D}(\Delta g) = \Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}$, and percent differences (PD), $\mathrm{PD}(\Delta g) = \frac{\Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}}{\Delta g^{\mathrm{exp}}} \cdot 100$, from the experimental values of the Δg parameter for the set of 18 Cu(II) complexes.

	Δg_{xx}	Δg_{yy}	Δg_{zz}	$\mathrm{D}(\Delta g_{\perp})$	$\mathrm{D}(\Delta g_{\parallel})$	$\mathrm{D}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\parallel})$	$\mathrm{PD}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$
1	41	41	149	-4	-89	-86	-9	-37	-44
2	38	38	146	-12	-115	-102	-24	-44	-49
3	40	41	157	-4	-103	-99	-8	-40	-46
4	36	36	129	-3	-73	-70	-8	-36	-43
5	30	46	140	-12	-125	-113	-23	-47	-53
6	35	48	142	-8	-58	-49	-17	-29	-33
7	34	44	140	-8	-98	-89	-17	-41	-47
8	39	42	142	-11	-109	-98	-21	-44	-49
9	46	50	163	-11	-89	-78	-19	-35	-40
10	43	47	166	-13	-117	-104	-22	-41	-46
11	26	44	132	-13	-71	-58	-27	-35	-37
12	36	44	138	-13	-27	-13	-25	-16	-12
13	27	56	138	1	-63	-64	3	-31	-40
14	24	45	118	-22	6	29	-39	6	53
15	26	28	94	-10	-30	-20	-26	-24	-23
16	26	42	114	-8	-22	-14	-18	-16	-15
17	19	25	73	-1	-10	-9	-4	-12	-15
18	30	34	106	7	-5	-13	30	-5	-15

Table S4. Calculated Δg-values (ppt), $\Delta g^{\mathrm{calc}} = (g^{\mathrm{calc}} - g_{\mathrm{e}}) \cdot 1000$ with g_{e} = 2.0023, obtained with the **B2PLYP** functional, differences (D), $\mathrm{D}(\Delta g) = \Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}$, and percent differences (PD), $\mathrm{PD}(\Delta g) = \frac{\Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}}{\Delta g^{\mathrm{exp}}} \cdot 100$, from the experimental values of the Δg parameter for the set of 18 Cu(II) complexes.

	Δg_{xx}	Δg_{yy}	Δg_{zz}	$\mathrm{D}(\Delta g_{\perp})$	$\mathrm{D}(\Delta g_{\parallel})$	$\mathrm{D}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\parallel})$	$\mathrm{PD}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$
1	42	42	173	-3	-65	-62	-7	-27	-32
2	38	38	166	-12	-95	-83	-24	-36	-39
3	42	43	183	-2	-76	-74	-5	-29	-34
4	34	35	142	-4	-60	-56	-11	-30	-34
5	32	49	165	-10	-100	-91	-19	-38	-42
6	37	51	167	-6	-33	-27	-12	-17	-18
7	36	47	164	-6	-74	-68	-13	-31	-36
8	41	44	168	-9	-83	-74	-17	-33	-37
9	51	55	201	-7	-50	-44	-11	-20	-23
10	49	52	208	-8	-75	-68	-13	-27	-30
11	23	38	137	-17	-65	-48	-36	-32	-31
12	36	43	157	-14	-7	6	-26	-5	6
13	27	59	169	3	-32	-35	7	-16	-22
14	20	33	115	-31	3	34	-54	3	63
15	1	8	51	-32	-72	-40	-88	-58	-46
16	19	32	109	-16	-27	-11	-39	-20	-12
17	-8	-3	6	-28	-77	-49	-124	-93	-81
18	11	15	75	-12	-37	-25	-48	-33	-28

Table S5. Calculated Δg-values (ppt), $\Delta g^{\mathrm{calc}} = (g^{\mathrm{calc}} - g_{\mathrm{e}}) \cdot 1000$ with g_{e} = 2.0023, obtained with the **mPW2PLYP** functional, differences (D), $\mathrm{D}(\Delta g) = \Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}$, and percent differences (PD), $\mathrm{PD}(\Delta g) = \frac{\Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}}{\Delta g^{\mathrm{exp}}} \cdot 100$, from the experimental values of the Δg parameter for the set of 18 Cu(II) complexes.

	Δg_{xx}	Δg_{yy}	Δg_{zz}	$\mathrm{D}(\Delta g_{\perp})$	$\mathrm{D}(\Delta g_{\parallel})$	$\mathrm{D}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\parallel})$	$\mathrm{PD}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$
1	46	46	189	1	-50	-51	2	-21	-26
2	43	43	182	-8	-79	-70	-16	-30	-34
3	46	47	198	2	-61	-63	3	-24	-29
4	39	39	159	0	-44	-44	0	-22	-27
5	34	54	179	-6	-86	-80	-11	-32	-37
6	40	56	181	-2	-19	-17	-4	-9	-11
7	40	51	177	-2	-60	-58	-5	-25	-30
8	45	48	183	-4	-68	-63	-9	-27	-32
9	56	60	218	-2	-34	-32	-3	-13	-17
10	53	55	223	-3	-60	-56	-6	-21	-25
11	26	46	156	-11	-46	-35	-24	-23	-22
12	42	49	175	-8	11	19	-15	7	17
13	31	69	192	10	-8	-18	24	-4	-11
14	24	42	136	-24	24	48	-42	22	88
15	11	16	80	-23	-44	-21	-64	-36	-24
16	24	40	129	-10	-6	3	-23	-5	4
17	-1	4	32	-21	-51	-29	-93	-61	-49
18	22	25	107	-1	-5	-4	-5	-5	-4

Table S6. Calculated Δg-values (ppt), $\Delta g^{\mathrm{calc}} = (g^{\mathrm{calc}} - g_{\mathrm{e}}) \cdot 1000$ with g_{e} = 2.0023, obtained with the **B2GP-PLYP** functional, differences (D), $\mathrm{D}(\Delta g) = \Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}$, and percent differences (PD), $\mathrm{PD}(\Delta g) = \frac{\Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}}{\Delta g^{\mathrm{exp}}} \cdot 100$, from the experimental values of the Δg parameter for the set of 18 Cu(II) complexes.

	Δg_{xx}	Δg_{yy}	Δg_{zz}	$D(\Delta g_{\perp})$	$D(\Delta g_{\parallel})$	$D(\Delta g_{\parallel}-\Delta g_{\perp})$	$PD(\Delta g_{\perp})$	$PD(\Delta g_{\parallel})$	$PD(\Delta g_{\parallel}-\Delta g_{\perp})$
1	50	50	213	5	-26	-30	11	-11	-16
2	47	47	207	-4	-53	-49	-8	-21	-24
3	49	51	223	5	-37	-42	12	-14	-20
4	42	43	181	4	-22	-26	10	-11	-16
5	37	59	202	-2	-63	-61	-3	-24	-29
6	43	61	205	2	5	3	5	3	2
7	44	55	199	2	-39	-40	3	-16	-21
8	50	52	208	0	-43	-43	0	-17	-21
9	62	67	249	4	-3	-7	7	-1	-4
10	58	60	253	2	-30	-31	3	-10	-14
11	30	54	186	-6	-16	-10	-12	-8	-7
12	48	56	204	-2	40	42	-4	24	38
13	36	82	235	19	34	15	47	17	10
14	30	50	165	-17	53	71	-30	48	130
15	21	24	116	-14	-8	6	-39	-6	7
16	30	46	158	-4	22	26	-9	16	28
17	3	4	53	-19	-30	-10	-86	-36	-17
18	34	36	152	10	40	30	42	36	34

Table S7. Calculated Δg-values (ppt), $\Delta g^{\mathrm{calc}} = (g^{\mathrm{calc}} - g_{\mathrm{e}}) \cdot 1000$ with g_{e} = 2.0023, obtained with the **B2K-PLYP** functional, differences (D), $\mathrm{D}(\Delta g) = \Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}$, and percent differences (PD), $\mathrm{PD}(\Delta g) = \frac{\Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}}{\Delta g^{\mathrm{exp}}} \cdot 100$, from the experimental values of the Δg parameter for the set of 18 Cu(II) complexes.

	Δg_{xx}	Δg_{yy}	Δg_{zz}	$\mathrm{D}(\Delta g_{\perp})$	$\mathrm{D}(\Delta g_{\parallel})$	$\mathrm{D}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\parallel})$	$\mathrm{PD}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$
1	54	54	240	10	1	-8	22	1	-4
2	52	52	235	1	-26	-27	2	-10	-13
3	54	55	249	10	-11	-21	22	-4	-10
4	47	48	207	9	4	-5	23	2	-3
5	40	65	226	3	-39	-42	6	-15	-19
6	46	67	235	7	35	28	14	18	19
7	48	59	221	6	-16	-22	12	-7	-12
8	55	57	233	5	-17	-22	9	-7	-11
9	67	73	280	11	28	18	18	11	9
10	63	65	282	7	-1	-7	11	0	-3
11	34	63	223	0	21	20	1	10	13
12	54	63	236	5	71	66	9	43	59
13	42	95	276	28	76	48	70	38	30
14	33	69	209	-6	97	103	-11	87	190
15	34	35	163	-2	39	41	-5	31	47
16	35	53	208	2	73	71	5	54	75
17	14	14	97	-9	14	23	-38	17	38
18	49	51	205	25	93	68	102	83	78

Table S8. Calculated Δg-values (ppt), $\Delta g^{\mathrm{calc}} = (g^{\mathrm{calc}} - g_{\mathrm{e}}) \cdot 1000$ with g_{e} = 2.0023, obtained with the **B2T-PLYP** functional, differences (D), $\mathrm{D}(\Delta g) = \Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}$, and percent differences (PD), $\mathrm{PD}(\Delta g) = \frac{\Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}}{\Delta g^{\mathrm{exp}}} \cdot 100$, from the experimental values of the Δg parameter for the set of 18 Cu(II) complexes.

	Δg_{xx}	Δg_{yy}	Δg_{zz}	$\mathrm{D}(\Delta g_{\perp})$	$\mathrm{D}(\Delta g_{\parallel})$	$\mathrm{D}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\parallel})$	$\mathrm{PD}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$
1	47	47	198	2	-40	-43	5	-17	-22
2	44	44	192	-7	-69	-62	-13	-26	-30
3	47	48	208	3	-51	-54	7	-20	-25
4	40	40	167	1	-36	-37	3	-18	-23
5	35	56	188	-4	-77	-72	-8	-29	-34
6	41	57	191	0	-9	-9	-1	-5	-6
7	41	52	186	-1	-52	-51	-2	-22	-27
8	47	50	193	-3	-58	-55	-5	-23	-27
9	58	63	231	1	-21	-21	1	-8	-11
10	55	57	236	-1	-47	-45	-3	-17	-20
11	28	49	167	-10	-35	-26	-20	-17	-17
12	44	51	187	-6	22	28	-11	13	25
13	33	74	210	13	10	-4	34	5	-2
14	26	44	146	-22	34	56	-39	31	104
15	13	18	91	-21	-33	-12	-57	-26	-13
16	26	41	139	-8	3	11	-19	3	12
17	-2	1	34	-23	-49	-26	-102	-59	-43
18	26	28	123	2	11	9	10	10	10

Table S9. Calculated Δg-values (ppt), $\Delta g^{\mathrm{calc}} = (g^{\mathrm{calc}} - g_{\mathrm{e}}) \cdot 1000$ with g_{e} = 2.0023, obtained with the **PBE-QIDH** functional, differences (D), $\mathrm{D}(\Delta g) = \Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}$, and percent differences (PD), $\mathrm{PD}(\Delta g) = \frac{\Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}}{\Delta g^{\mathrm{exp}}} \cdot 100$, from the experimental values of the Δg parameter for the set of 18 Cu(II) complexes.

	Δg_{xx}	Δg_{yy}	Δg_{zz}	$\mathrm{D}(\Delta g_{\perp})$	$\mathrm{D}(\Delta g_{\parallel})$	$\mathrm{D}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\parallel})$	$\mathrm{PD}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$
1	57	57	247	12	8	-4	27	3	-2
2	54	54	242	3	-19	-22	6	-7	-10
3	56	58	256	12	-4	-16	27	-2	-8
4	50	50	215	11	12	1	29	6	1
5	41	68	232	5	-33	-38	10	-13	-18
6	48	69	237	9	37	28	18	19	19
7	50	61	226	8	-12	-19	16	-5	-10
8	57	59	239	7	-12	-19	13	-5	-9
9	70	75	285	13	33	21	21	13	11
10	65	67	286	8	4	-4	14	1	-2
11	35	68	230	4	28	24	8	14	16
12	57	66	242	8	77	69	14	47	62
13	42	99	282	30	81	51	75	40	32
14	37	69	210	-4	99	103	-7	88	188
15	39	40	175	3	52	49	8	42	56
16	39	58	207	7	72	64	17	53	69
17	20	20	112	-3	29	32	-13	36	54
18	54	56	218	30	106	76	123	95	87

Table S10. Calculated Δg-values (ppt), $\Delta g^{\mathrm{calc}} = (g^{\mathrm{calc}} - g_{\mathrm{e}}) \cdot 1000$ with $g_{\mathrm{e}} = 2.0023$, obtained with the **PBE0-DH** functional, differences (D), $\mathrm{D}(\Delta g) = \Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}$, and percent differences (PD), $\mathrm{PD}(\Delta g) = \frac{\Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}}{\Delta g^{\mathrm{exp}}} \cdot 100$, from the experimental values of the Δg parameter for the set of 18 Cu(II) complexes.

	Δg_{xx}	Δg_{yy}	Δg_{zz}	$\mathrm{D}(\Delta g_{\perp})$	$\mathrm{D}(\Delta g_{\parallel})$	$\mathrm{D}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\parallel})$	$\mathrm{PD}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$
1	52	53	209	8	-29	-37	18	-12	-19
2	49	49	204	-1	-57	-55	-3	-22	-26
3	52	53	209	8	-50	-58	18	-19	-27
4	46	46	183	7	-20	-28	19	-10	-17
5	38	62	197	0	-68	-68	1	-26	-32
6	45	63	198	4	-1	-5	8	-1	-4
7	46	56	194	3	-44	-47	7	-19	-25
8	57	59	239	7	-12	-19	13	-5	-9
9	63	67	236	5	-16	-21	9	-6	-11
10	59	61	238	2	-44	-46	3	-16	-21
11	31	61	184	-1	-18	-17	-3	-9	-11
12	49	59	199	0	34	33	1	21	30
13	36	82	217	19	16	-3	47	8	-2
14	32	59	167	-12	55	67	-21	49	123
15	31	33	130	-5	7	12	-14	6	14
16	34	54	162	2	26	24	6	19	25
17	20	23	92	-1	9	11	-6	11	18
18	41	44	157	18	45	27	73	41	31

Table S11. Calculated Δg-values (ppt), $\Delta g^{\mathrm{calc}} = (g^{\mathrm{calc}} - g_{\mathrm{e}}) \cdot 1000$ with $g_{\mathrm{e}} = 2.0023$, obtained with the **DSD-BLYP** functional, differences (D), $\mathrm{D}(\Delta g) = \Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}$, and percent differences (PD), $\mathrm{PD}(\Delta g) = \frac{\Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}}{\Delta g^{\mathrm{exp}}} \cdot 100$, from the experimental values of the Δg parameter for the set of 18 Cu(II) complexes.

	Δg_{xx}	Δg_{yy}	Δg_{zz}	$\mathrm{D}(\Delta g_{\perp})$	$\mathrm{D}(\Delta g_{\parallel})$	$\mathrm{D}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\parallel})$	$\mathrm{PD}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$
1	53	53	242	8	3	-5	19	1	-3
2	50	50	237	0	-24	-23	-1	-9	-11
3	53	54	252	9	-8	-17	20	-3	-8
4	46	46	206	7	3	-4	18	2	-2
5	40	63	228	2	-37	-39	4	-14	-18
6	44	68	252	6	52	46	13	26	31
7	46	59	223	5	-15	-20	10	-6	-10
8	54	56	236	4	-15	-19	8	-6	-9
9	67	73	286	10	35	25	17	14	13
10	63	64	288	6	6	0	10	2	0
11	34	60	223	-1	20	21	-1	10	13
12	54	62	240	4	75	71	8	45	64
13	43	94	285	28	84	56	70	42	35
14	28	75	217	-6	106	111	-10	95	205
15	32	33	160	-4	37	41	-12	30	47
16	33	51	216	0	80	80	1	59	85
17	9	10	88	-13	5	19	-58	7	31
18	46	48	206	23	94	72	92	84	82

Table S12. Calculated Δg-values (ppt), $\Delta g^{\mathrm{calc}} = (g^{\mathrm{calc}} - g_{\mathrm{e}}) \cdot 1000$ with $g_{\mathrm{e}} = 2.0023$, obtained with the **DSD-PBEP86** functional, differences (D), $\mathrm{D}(\Delta g) = \Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}$, and percent differences (PD), $\mathrm{PD}(\Delta g) = \frac{\Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}}{\Delta g^{\mathrm{exp}}} \cdot 100$, from the experimental values of the Δg parameter for the set of 18 Cu(II) complexes.

	Δg_{xx}	Δg_{yy}	Δg_{zz}	$D(\Delta g_{\perp})$	$D(\Delta g_{\parallel})$	$D(\Delta g_{\parallel}-\Delta g_{\perp})$	$PD(\Delta g_{\perp})$	$PD(\Delta g_{\parallel})$	$PD(\Delta g_{\parallel}-\Delta g_{\perp})$
1	53	53	235	9	-4	-13	19	-2	-7
2	51	51	231	0	-30	-30	0	-11	-14
3	53	54	244	9	-15	-24	20	-6	-11
4	46	46	201	8	-2	-9	20	-1	-6
5	40	63	221	2	-43	-45	4	-16	-21
6	45	68	247	7	47	41	13	24	27
7	47	58	217	5	-21	-26	10	-9	-14
8	54	56	229	4	-22	-26	8	-9	-13
9	66	72	275	10	24	14	16	9	7
10	62	64	278	6	-5	-11	10	-2	-5
11	34	60	216	0	13	14	0	7	9
12	54	62	233	5	68	64	8	42	58
13	42	93	273	28	73	45	68	36	28
14	29	75	212	-5	101	106	-9	90	194
15	33	34	156	-3	32	36	-9	26	41
16	34	54	208	2	73	71	5	54	75
17	12	12	89	-11	6	17	-46	8	28
18	48	50	199	24	87	63	97	78	73

Table S13. Calculated Δg-values (ppt), $\Delta g^{\mathrm{calc}} = (g^{\mathrm{calc}} - g_{\mathrm{e}}) \cdot 1000$ with $g_{\mathrm{e}} = 2.0023$, obtained with the **ωB2PLYP** functional, differences (D), $\mathrm{D}(\Delta g) = \Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}$, and percent differences (PD), $\mathrm{PD}(\Delta g) = \frac{\Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}}{\Delta g^{\mathrm{exp}}} \cdot 100$, from the experimental values of the Δg parameter for the set of 18 Cu(II) complexes.

	Δg_{xx}	Δg_{yy}	Δg_{zz}	$\mathrm{D}(\Delta g_{\perp})$	$\mathrm{D}(\Delta g_{\parallel})$	$\mathrm{D}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\parallel})$	$\mathrm{PD}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$
1	49	49	203	5	-36	-40	10	-15	-21
2	46	46	197	-5	-64	-59	-9	-25	-28
3	49	50	211	5	-49	-53	10	-19	-25
4	42	43	174	4	-29	-33	10	-14	-20
5	36	59	193	-2	-72	-70	-4	-27	-32
6	43	60	195	2	-4	-6	4	-2	-4
7	43	54	190	1	-48	-49	2	-20	-26
8	50	52	198	0	-52	-52	-1	-21	-26
9	61	66	236	4	-16	-19	6	-6	-10
10	58	60	240	1	-42	-44	2	-15	-19
11	29	52	173	-7	-30	-23	-14	-15	-15
12	47	55	193	-3	28	32	-6	17	28
13	35	79	219	17	18	2	42	9	1
14	29	50	156	-18	45	63	-31	40	115
15	20	24	109	-15	-15	0	-41	-12	0
16	30	46	150	-4	14	18	-9	11	20
17	8	10	63	-14	-20	-6	-60	-24	-11
18	33	36	143	10	31	21	39	28	25

Table S14. Calculated Δg-values (ppt), $\Delta g^{\mathrm{calc}} = (g^{\mathrm{calc}} - g_{\mathrm{e}}) \cdot 1000$ with $g_{\mathrm{e}} = 2.0023$, obtained with the **ωB2GP-PLYP** functional, differences (D), $\mathrm{D}(\Delta g) = \Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}$, and percent differences (PD), $\mathrm{PD}(\Delta g) = \frac{\Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}}{\Delta g^{\mathrm{exp}}} \cdot 100$, from the experimental values of the Δg parameter for the set of 18 Cu(II) complexes.

	Δg_{xx}	Δg_{yy}	Δg_{zz}	$\mathrm{D}(\Delta g_{\perp})$	$\mathrm{D}(\Delta g_{\parallel})$	$\mathrm{D}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\parallel})$	$\mathrm{PD}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$
1	54	54	233	10	-6	-15	21	-2	-8
2	51	51	227	0	-33	-34	1	-13	-16
3	54	55	241	10	-18	-28	21	-7	-13
4	47	47	201	9	-1	-10	22	-1	-6
5	40	65	220	3	-45	-47	6	-17	-22
6	46	67	226	7	26	19	14	13	13
7	48	59	215	6	-22	-28	12	-9	-15
8	55	57	227	5	-23	-28	9	-9	-14
9	67	73	272	10	20	9	17	8	5
10	63	65	274	6	-9	-15	11	-3	-7
11	33	62	213	0	10	10	0	5	7
12	54	62	227	4	63	58	8	38	53
13	54	54	233	14	32	18	35	16	11
14	34	64	196	-8	84	92	-15	75	169
15	33	34	154	-3	30	34	-9	24	39
16	36	53	193	3	57	55	6	42	58
17	15	15	95	-8	13	20	-34	15	34
18	47	49	195	23	83	59	95	74	68

Table S15. Calculated Δg-values (ppt), $\Delta g^{\mathrm{calc}} = (g^{\mathrm{calc}} - g_{\mathrm{e}}) \cdot 1000$ with $g_{\mathrm{e}} = 2.0023$, obtained with the **RSX-QIDH** functional, differences (D), $\mathrm{D}(\Delta g) = \Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}$, and percent differences (PD), $\mathrm{PD}(\Delta g) = \frac{\Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}}{\Delta g^{\mathrm{exp}}} \cdot 100$, from the experimental values of the Δg parameter for the set of 18 Cu(II) complexes.

	Δg_{xx}	Δg_{yy}	Δg_{zz}	$\mathrm{D}(\Delta g_{\perp})$	$\mathrm{D}(\Delta g_{\parallel})$	$\mathrm{D}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\parallel})$	$\mathrm{PD}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$
1	61	61	264	16	26	10	36	11	5
2	57	57	259	7	-1	-8	13	0	-4
3	60	61	272	16	12	-4	35	5	-2
4	54	54	233	15	30	15	39	15	9
5	43	73	247	9	-17	-26	17	-7	-12
6	50	75	263	13	64	50	27	32	34
7	53	65	240	11	3	-8	23	1	-4
8	61	63	255	11	5	-6	21	2	-3
9	74	80	305	18	53	35	30	21	18
10	69	70	305	12	22	10	21	8	4
11	39	75	246	10	43	34	20	21	22
12	62	71	262	13	97	84	24	59	76
13	46	108	308	36	107	71	91	53	44
14	39	83	239	4	128	124	7	114	227
15	47	49	207	11	83	72	31	67	83
16	45	66	235	14	100	86	32	74	92
17	29	29	146	6	64	57	28	77	96
18	64	66	254	41	142	101	165	127	116

Table S16. Calculated Δg-values (ppt), $\Delta g^{\mathrm{calc}} = (g^{\mathrm{calc}} - g_{\mathrm{e}}) \cdot 1000$ with $g_{\mathrm{e}} = 2.0023$, obtained with the **RSX-0DH** functional, differences (D), $\mathrm{D}(\Delta g) = \Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}$, and percent differences (PD), $\mathrm{PD}(\Delta g) = \frac{\Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}}{\Delta g^{\mathrm{exp}}} \cdot 100$, from the experimental values of the Δg parameter for the set of 18 Cu(II) complexes.

	Δg_{xx}	Δg_{yy}	Δg_{zz}	$\mathrm{D}(\Delta g_{\perp})$	$\mathrm{D}(\Delta g_{\parallel})$	$\mathrm{D}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\parallel})$	$\mathrm{PD}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$
1	60	60	240	15	1	-14	34	1	-7
2	57	57	235	6	-25	-31	12	-10	-15
3	59	60	246	15	-14	-28	33	-5	-13
4	54	54	214	15	11	-4	39	6	-2
5	42	73	226	8	-39	-47	16	-15	-22
6	51	72	227	12	27	16	24	14	10
7	52	63	220	10	-18	-28	21	-8	-15
8	60	62	232	10	-19	-29	19	-8	-14
9	73	78	272	16	20	4	27	8	2
10	68	69	272	11	-11	-21	18	-4	-9
11	38	75	219	9	16	7	18	8	5
12	59	70	234	11	69	59	20	42	53
13	43	102	267	32	66	34	81	33	21
14	41	74	206	0	94	94	0	84	172
15	47	47	185	10	61	50	28	49	58
16	45	66	201	14	65	51	33	48	55
17	33	34	142	11	59	48	50	72	80
18	62	64	221	39	110	71	156	98	82

Table S17. Calculated Δg-values (ppt), $\Delta g^{\mathrm{calc}} = (g^{\mathrm{calc}} - g_{\mathrm{e}}) \cdot 1000$ with $g_{\mathrm{e}} = 2.0023$, obtained with the **ωB88PP86** functional, differences (D), $\mathrm{D}(\Delta g) = \Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}$, and percent differences (PD), $\mathrm{PD}(\Delta g) = \frac{\Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}}{\Delta g^{\mathrm{exp}}} \cdot 100$, from the experimental values of the Δg parameter for the set of 18 Cu(II) complexes.

	Δg_{xx}	Δg_{yy}	Δg_{zz}	$\mathrm{D}(\Delta g_{\perp})$	$\mathrm{D}(\Delta g_{\parallel})$	$\mathrm{D}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\parallel})$	$\mathrm{PD}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$
1	49	49	213	4	-26	-30	9	-11	-15
2	46	46	207	-5	-53	-49	-9	-21	-23
3	49	50	224	5	-36	-41	11	-14	-19
4	41	42	179	3	-24	-26	7	-12	-16
5	37	58	202	-2	-62	-60	-4	-24	-28
6	42	61	211	2	11	9	4	6	6
7	43	54	199	1	-39	-40	2	-16	-21
8	50	52	209	0	-42	-41	0	-17	-21
9	62	67	253	5	1	-3	8	1	-2
10	59	60	258	2	-25	-27	3	-9	-12
11	29	51	190	-8	-12	-4	-16	-6	-3
12	47	55	206	-2	41	43	-5	25	39
13	37	83	241	20	41	21	49	20	13
14	27	54	172	-16	60	76	-29	54	140
15	20	23	114	-16	-10	6	-42	-8	7
16	28	42	172	-6	36	43	-15	27	46
17	1	2	49	-21	-34	-13	-95	-41	-21
18	33	36	154	10	42	33	40	38	37

Table S18. Calculated Δg-values (ppt), $\Delta g^{\mathrm{calc}} = (g^{\mathrm{calc}} - g_{\mathrm{e}}) \cdot 1000$ with $g_{\mathrm{e}} = 2.0023$, obtained with the **ωPBEPP86** functional, differences (D), $\mathrm{D}(\Delta g) = \Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}$, and percent differences (PD), $\mathrm{PD}(\Delta g) = \frac{\Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}}{\Delta g^{\mathrm{exp}}} \cdot 100$, from the experimental values of the Δg parameter for the set of 18 Cu(II) complexes.

	Δg_{xx}	Δg_{yy}	Δg_{zz}	$\mathrm{D}(\Delta g_{\perp})$	$\mathrm{D}(\Delta g_{\parallel})$	$\mathrm{D}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\parallel})$	$\mathrm{PD}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$
1	51	51	227	6	-12	-18	13	-5	-9
2	48	48	222	-3	-39	-36	-5	-15	-17
3	51	52	239	7	-21	-28	15	-8	-13
4	43	44	191	5	-11	-16	12	-6	-10
5	38	61	215	0	-49	-49	0	-19	-23
6	44	65	230	5	30	26	9	15	17
7	45	56	211	3	-27	-30	6	-11	-16
8	52	54	223	2	-27	-29	4	-11	-15
9	65	70	272	8	21	13	13	8	7
10	61	63	276	4	-6	-11	7	-2	-5
11	31	54	206	-5	4	8	-10	2	5
12	50	58	222	1	57	57	1	35	51
13	39	89	265	24	64	40	60	32	25
14	28	63	192	-12	80	92	-21	72	169
15	24	26	131	-11	8	19	-31	6	22
16	30	45	196	-4	60	64	-10	44	68
17	3	3	59	-20	-24	-4	-88	-29	-6
18	39	41	176	15	65	50	61	58	57

Table S19. Calculated Δg-values (ppt), $\Delta g^{\mathrm{calc}} = (g^{\mathrm{calc}} - g_{\mathrm{e}}) \cdot 1000$ with $g_{\mathrm{e}} = 2.0023$, obtained with the **ωB97X-2** functional, differences (D), $\mathrm{D}(\Delta g) = \Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}$, and percent differences (PD), $\mathrm{PD}(\Delta g) = \frac{\Delta g^{\mathrm{calc}} - \Delta g^{\mathrm{exp}}}{\Delta g^{\mathrm{exp}}} \cdot 100$, from the experimental values of the Δg parameter for the set of 18 Cu(II) complexes.

	Δg_{xx}	Δg_{yy}	Δg_{zz}	$\mathrm{D}(\Delta g_{\perp})$	$\mathrm{D}(\Delta g_{\parallel})$	$\mathrm{D}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\perp})$	$\mathrm{PD}(\Delta g_{\parallel})$	$\mathrm{PD}(\Delta g_{\parallel}\text{-}\Delta g_{\perp})$
1	47	47	199	2	-40	-41	4	-17	-21
2	44	44	194	-7	-67	-60	-13	-26	-28
3	46	47	207	2	-53	-55	4	-20	-26
4	40	40	170	1	-33	-34	3	-16	-21
5	35	55	189	-4	-76	-72	-9	-29	-33
6	35	55	189	-4	-11	-7	-9	-6	-4
7	40	52	185	-1	-53	-51	-3	-22	-27
8	47	49	194	-3	-56	-53	-6	-22	-27
9	57	63	232	1	-20	-20	1	-8	-11
10	55	57	237	-2	-46	-44	-3	-16	-20
11	28	48	183	-10	-19	-10	-20	-10	-6
12	47	55	196	-2	31	33	-5	19	30
13	36	78	226	17	25	8	42	12	5
14	27	53	166	-18	54	72	-31	49	132
15	24	26	125	-12	2	14	-33	1	16
16	27	41	167	-8	31	39	-18	23	42
17	5	6	67	-17	-15	2	-76	-19	3
18	36	40	161	13	49	36	54	44	42

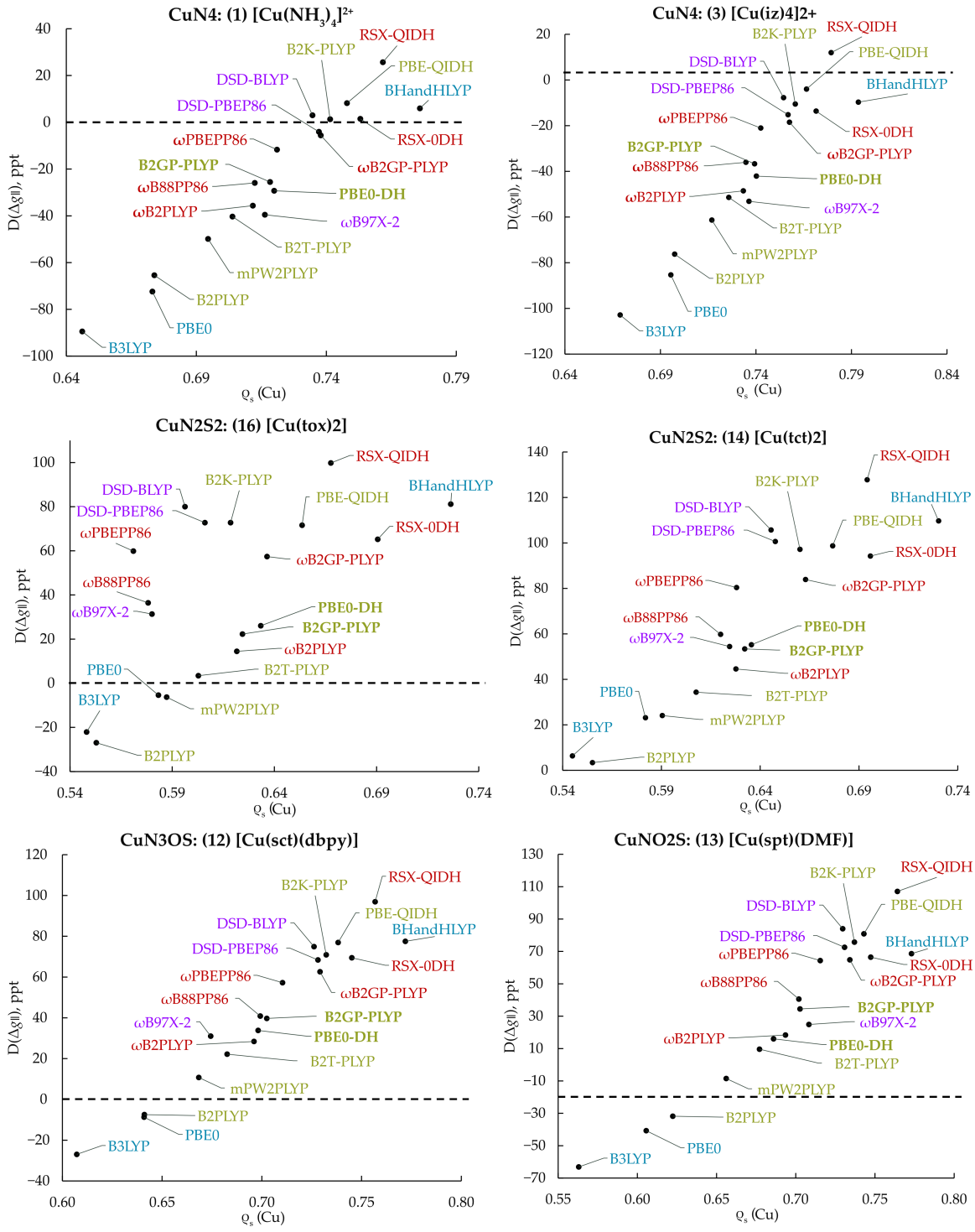

Figure S1. Correlation of the differences, $D(\Delta g_{\parallel})$, of the calculated g-tensor from the experimental value of the parallel g-shift with the Cu spin populations computed with the respective functional for pairs of complexes with the same copper-coordinating atoms **1** and **3**, **16** and **14**, and with similar coordination spheres **12** and **13**.

Cu(II) Complexes Set Optimized Structures Coordinates

(1) $[Cu(NH_3)_4]^{2+}$

Cu	0.00006419199069	-0.00003340568689	-0.00022217666782
N	2.06848435125770	0.00010161567862	0.00708711104760
H	2.50353403337608	0.92206255017040	0.01099143938875
H	2.45240522847896	-0.47709423764054	-0.81022241731436
H	2.44658665114581	-0.48121730588988	0.82470182355239
N	0.00017210694298	-2.06817901727768	-0.00703110959095
H	-0.48015601721747	-2.44633662488226	-0.82520902101680
H	-0.47799488839448	-2.45211469025323	0.80970371809922
H	0.92214716018829	-2.50321055717668	-0.00976606755074
N	-2.06837744747900	-0.00016232631948	0.00624217373816
H	-2.50344437695778	-0.92211693127714	0.00954348028378
H	-2.44672945419513	0.48078282865023	0.82396108289575
H	-2.45201109269431	0.47742545237280	-0.81097179352883
N	-0.00006737492988	2.06811092911312	-0.00647668527445
H	0.47703143664634	2.45152402711104	0.81113155825011
H	0.48134416636775	2.44676757465875	-0.82378269324413
H	-0.92202980552656	2.50316146164882	-0.01020316506768

(2) $[Cu(py)_4]^{2+}$

Cu	0.00064871054963	0.00055364112791	0.00050606191850
C	-0.62613643534546	2.72806230228956	-0.97103874156407
H	-1.13178451821264	2.14924080657570	-1.73273223452910
C	0.62818267485747	2.72758620736162	0.97276422793275
H	1.13364097332214	2.14838220946754	1.73429918701266
C	0.64123351269850	4.11093425742313	1.01169666841525
H	1.14953662101276	4.61842213520206	1.82019832789757
C	0.00135448999117	4.81853946698848	0.00116573001538
H	0.00152630808858	5.90098619691840	0.00131965963620
C	-0.63874980131543	4.11142514703775	-1.00956934786879
H	-1.14690250461267	4.61931487040205	-1.81791361997104
C	-2.72807753920898	0.63013558657336	0.96724950210857
H	-2.15014264586219	1.13757250817281	1.72843670121082
C	-4.11148738924266	0.64295921532839	1.00403531132701
H	-4.62033008779108	1.15309403121932	1.81052980822897
C	-4.81740493525664	0.00048235765528	-0.00602959798156
H	-5.89985057163160	0.00040174957786	-0.00752359769460
C	-4.10860600491109	-0.64187905025481	-1.01414993726496
H	-4.61514144278381	-1.15210049855616	-1.82204068340216
C	-2.72530638231224	-0.62882491836117	-0.97354869349491
H	-2.14520411208653	-1.13617224650530	-1.73314650006357
N	0.00091960930853	2.04128785468445	0.00076351423442
N	-2.04016214797721	0.00072076451285	-0.00220886350020
C	2.72804538074231	-0.62599434107569	0.97257489215159
H	2.14913292406489	-1.13084460159194	1.73472380818393
C	2.72780200978536	0.62665390869062	-0.97230567545531
H	2.14869535762960	1.13156800801700	-1.73426806791342
C	4.11115243388362	0.63938898424997	-1.01126768153252

H	4.61873458495279	1.14689252009011	-1.82021232820699
C	4.81863864730132	0.00024276258519	-0.00019006052434
H	5.90108551884253	0.00018120744390	-0.00036375969983
C	4.11140580814979	-0.63883415982520	1.01111066875217
H	4.61920200811367	-1.14636351252084	1.81990495893397
C	0.62869926131348	-2.72786818960170	-0.96803617311464
H	1.13559972283275	-2.14969708092376	-1.72939426660448
C	0.64114285707334	-4.11126349030151	-1.00550068567399
H	1.15044166234404	-4.61984591471691	-1.81268736268536
C	-0.00063425114495	-4.81750559454211	0.00478212580682
H	-0.00101487598637	-5.89995188341259	0.00573807367462
C	-0.64194931238644	-4.10903073186325	1.01379433144445
H	-1.15159424864755	-4.61582760836235	1.82188473664532
C	-0.62860376070508	-2.72571504053564	0.97383708995082
H	-1.13515589465627	-2.14585494837692	1.73414521786001
N	2.04138437161123	0.00034420966912	0.00022850067436
N	0.00029577160737	-2.04025841793653	0.00229805572963

(3) $[Cu(iz)_4]^{2+}$

Cu	0.00063373514287	0.00013749392920	0.00114343311217
N	-0.00427530592122	1.99919361218418	-0.27698133854338
N	0.01865980908615	-2.01295892584394	-0.14380293020921
N	-2.01228972261443	-0.00051184532441	0.14898754124251
N	1.99989197733047	0.01418829883767	0.27745970449316
C	-0.65858239570237	2.65129063737698	-1.22925220236971
N	-0.43762124311890	3.97021073912689	-1.11317233133061
C	0.38857194760509	4.18553167969414	-0.03673566506116
C	0.65521071012798	2.95348178289080	0.47639517177857
C	0.73142930699296	-2.72594659168801	-1.00620452900947
N	0.49980019651869	-4.03455667244719	-0.81716391579167
C	-0.39497873279143	-4.17904671725604	0.21539985105194
C	-0.69084079970746	-2.91598228925233	0.62708074798455
H	-1.28097077290903	2.21321308089280	-1.99103192926683
H	-0.81119610330821	4.68230883668093	-1.72387329846054
H	0.70519545631364	5.16909584943211	0.26307328023964
H	1.26841741205636	2.69573701167392	1.32118319085299
H	1.40305578469015	-2.33859500524890	-1.75350611322401
H	0.91013035155573	-4.78515154266637	-1.35366829190548
H	-0.73308460369568	-5.14096948944240	0.55881003465167
H	-1.35669603590650	-2.60345066714186	1.41135902372309
C	-2.73065193250235	0.70600570371529	1.01207219964728
C	-2.90977385172835	-0.71835975921136	-0.62062293257349
C	2.65901946254755	-0.63352826802659	1.22939594916818
C	2.94728650172290	0.68148556717359	-0.47772219074114
N	-4.03735449670527	0.46269833141679	0.82448465491760
H	-2.34848235288431	1.38116665252699	1.75885660537031
C	-4.17499231007573	-0.43350489121345	-0.20777555540587
H	-2.59215332145409	-1.38170975391346	-1.40498496642145
N	3.97578087188399	-0.40100658691058	1.11134935270394
H	2.22747407100055	-1.25905641836600	1.99233123994806

C	4.18235610660086	0.42601429745266	0.03383743526066
H	2.68298198509846	1.29175227017497	-1.32261586402748
H	-4.79099476342635	0.86642833340329	1.36172735154627
H	-5.13423919265935	-0.78022421978456	-0.55008133554670
H	4.69196456993924	-0.76765929925224	1.72146831108205
H	5.16268651389740	0.75099865940646	-0.26761315988643

(4) $[Cu(en)_2]^{2+}$

Cu	-0.00015331540197	-0.00014261966126	0.00130599187129
N	0.01888040826412	-2.05628794825318	-0.01285107026608
H	-0.23364899140073	-2.40061267060284	0.91432221304464
H	-0.65965637545835	-2.47127917104865	-0.64897001809117
N	2.04553447125029	-0.20826572185295	-0.00625176921902
H	2.40374790944715	0.02580068847256	-0.93298215161064
H	2.52519827322676	0.42058511059595	0.63540668422816
C	1.39505586446807	-2.53178094991821	-0.36465489149023
H	1.49739693819759	-2.47730900918716	-1.44961838531218
H	1.53700790937467	-3.57143567702613	-0.06750913289078
C	2.39678148529083	-1.62686650652761	0.32196070889380
H	2.34694662725292	-1.73851045698825	1.40621478410602
H	3.41510357465003	-1.85960107679818	0.00865494288315
N	-0.01919000581116	2.05602044834685	0.01290199998721
H	0.23383413033624	2.39915266058683	-0.91458674460682
H	0.65898770922794	2.47184315698049	0.64885771947717
C	-1.39556588059462	2.53190360429073	0.36334469067398
H	-1.49864731253624	2.47850101015915	1.44828688795324
H	-1.53728844189629	3.57125784446652	0.06506528340386
C	-2.39680511854110	1.62633974433174	-0.32312636704419
N	-2.04584339296127	0.20801195237866	0.00661047752892
H	-2.40489633586304	-0.02525702094040	0.93321141576271
H	-2.52495131025669	-0.42138346403964	-0.63493235170172
H	-2.34614767184780	1.73698410678809	-1.40744982870310
H	-3.41537052641735	1.85938416744688	-0.01081958887825

(5) $[Cu(gly)_2]$

Cu	-0.00019902689836	-0.00010991606501	0.00191697959717
O	0.00065892132777	-1.89504463421948	-0.02051506672269
N	-2.02935875839704	-0.16156062390687	0.00502268995214
C	-2.36892449399920	-1.57274546218537	-0.30321393112278
H	-2.34801406721589	0.11132733926863	0.92911222810248
O	-1.31580256064245	-3.70054325751094	-0.17488430622873
C	-1.14632360979321	-2.50181168212180	-0.14593162692259
H	-2.43476450549415	0.50110715023905	-0.64713762439425
H	-3.17951821204974	-1.94113338232926	0.32417713660353
O	-0.00107175784885	1.89491111406006	0.02476987750451
N	2.02893185094753	0.16166670863894	-0.00087680127971
C	1.14579235814648	2.50150211946395	0.15223682727138
C	2.36782796434397	1.57205095214539	0.31157152941100

H	2.34739605677431	-0.10794540528992	-0.92600380998595
H	2.43497929700576	-0.50287189174769	0.64898472639066
O	1.31534250123555	3.70019499990915	0.18227399960844
H	3.18077653631439	1.94178541614900	-0.31196741654389
H	2.69352291419467	1.63866775558675	1.35003239510448
H	-2.69847230895154	-1.64197472908456	-1.34026899434521

(6) [Cu(ox)$_2$]

Cu	-0.00000801612025	-0.00002405653605	-0.00018206991628
O	-0.02117161329831	1.93627776959757	-0.00194450121767
N	-1.97981024889942	0.17550198270883	-0.00118671072030
C	-2.90397404828866	-0.76533308000362	-0.00069579709856
C	-4.27185371721407	-0.44293313893140	-0.00188712928896
C	-4.65764361664131	0.87658727326228	-0.00366561283899
C	-3.68781317371574	1.90441208068080	-0.00426619573580
C	-3.96422629820857	3.28979277497971	-0.00615066250969
C	-2.91213933949776	4.17955037191731	-0.00659498641498
C	-1.56732614185677	3.76707929126945	-0.00522179574968
C	-1.23943998089412	2.41518829054763	-0.00327833519467
C	-2.33236062465255	1.48773475961889	-0.00286702783323
H	-2.54839235883358	-1.78795458415159	0.00063119546867
H	-5.00327512061875	-1.23974913657229	-0.00141410170342
H	-5.70923134115544	1.14006743980086	-0.00464764525228
H	-4.99000582272723	3.63500007156538	-0.00724443183030
H	-3.12183828988028	5.24298697874960	-0.00807241743295
H	-0.77039575598177	4.49954272031364	-0.00563986216237
O	0.02115283708314	-1.93632767045601	0.00157351879941
N	1.97979225955900	-0.17555469920370	0.00083042030685
C	1.23942031691348	-2.41524007073008	0.00292507135939
C	2.90395701046036	0.76527990172865	0.00033919722634
C	2.33234180431108	-1.48778745717406	0.00251982326454
C	1.56730537979381	-3.76713131874267	0.00489224773972
C	4.27183620261543	0.44287916196174	0.00154155011244
H	2.54837549457160	1.78790147685948	-0.00099446898386
C	3.68779414807796	-1.90446571131034	0.00393775080116
C	2.91211836828423	-4.17960328671864	0.00628668840439
H	0.77037462429662	-4.49959429294586	0.00530683404630
C	4.65762530720293	-0.87664152346814	0.00333522827837
H	5.00325885949694	1.23969402835115	0.00106646911722
C	3.96420613704625	-3.28984672901765	0.00584145572170
H	3.12181668213735	-5.24304000617309	0.00778125474489
H	5.70921204624249	-1.14012549507007	0.00432809738272
H	4.98998551339191	-3.63505439070773	0.00695379910987

(7) [Cu(sac)$_2$]

Cu	-0.00000316791655	-0.00000293538656	-0.00095429325206
O	-0.02234388292928	1.94074737339228	-0.00116985550733
C	-1.04540595716471	2.73408791974294	-0.00104717009544

C	-2.41069190140790	2.29313309646638	-0.00047478278778
C	-3.45575349070688	3.24493958403794	-0.00040434858539
H	-4.47859661075680	2.88298289060394	0.00000885462044
C	-3.20547539661539	4.59442163853088	-0.00083572333995
C	-1.86864861202310	5.03109417464890	-0.00136405653210
H	-1.65553025266125	6.09410712951882	-0.00170240073282
C	-0.82442588066406	4.13749309453469	-0.00145683301341
H	0.20336878416319	4.47737994575792	-0.00186396915290
C	-2.76385572302839	0.91061519372130	-0.00003120602274
N	-1.93282720449472	-0.07764826861816	-0.00007233411027
O	0.02233781847774	-1.94075313825274	-0.00019523570603
C	1.04539986025716	-2.73409334330351	0.00061002034657
C	2.41068568860077	-2.29313824795311	0.00126756128986
C	3.45574716824698	-3.24494441885955	0.00210419394759
H	4.47859015137646	-2.88298744721533	0.00255730582456
C	3.20546914257534	-4.59442646379640	0.00234956830655
C	1.86864255013118	-5.03109928011670	0.00174808161270
H	1.65552426691203	-6.09411228748074	0.00194037754829
C	0.82441995898270	-4.13749848644412	0.00091997392235
H	-0.20337454027480	-4.47738575912318	0.00046278017002
C	2.76384928014775	-0.91062027667018	0.00106440866770
N	1.93282067060372	0.07764274882707	0.00028865154031
H	2.34973810177148	1.00115238393758	0.00026303530863
H	-2.34974482230651	-1.00115776847171	0.00027450321319
H	-3.83389336015788	0.69322238660675	0.00034020939313
H	-4.01736900268455	5.30908751133508	-0.00078908098711
H	4.01736270064112	-5.30909211376502	0.00298774113960
H	3.83388679890514	-0.69322713520545	0.00160043197385

(8) [Cu(acac)(bpy)]⁺

Cu	-3.88792387802829	4.00094717478966	14.31020874229040
C	-4.61332108315892	1.91953655177168	16.33200306037300
H	-4.28706828533027	1.25544990373674	15.54343942505772
C	-5.07506424046352	1.45380447264498	17.55403841838232
H	-5.11846206396952	0.39057525620617	17.74390175132518
C	-5.47280645924605	2.37802218121854	18.50905358841311
H	-5.83818511667751	2.05067308361509	19.47369109322342
C	-5.39835985703783	3.73367750812824	18.21752616017038
H	-5.70508497475895	4.46283106913968	18.95276413866581
C	-4.92615254724380	4.13393523460621	16.97327206350870
C	-4.79805115102216	5.54333034396589	16.54236157105507
C	-5.13605717219724	6.63852633829692	17.32842278727206
H	-5.52332546762982	6.50335876771276	18.32744813056300
C	-4.97006350074634	7.91762735751546	16.81399907457995
H	-5.22861518110196	8.78049182258739	17.41387180528742
C	-4.47175238157893	8.07505847620502	15.52897755424017
H	-4.32841975794579	9.05435582445068	15.09439832873821
C	-4.15497154954355	6.94055306205386	14.79679351701093
H	-3.76459120358575	6.99006340510197	13.78960842766539

C	-2.90040927961589	0.59358789923410	12.06498363229286
H	-2.19280477050873	0.14971041530907	12.76895191529334
H	-2.53538262865347	0.44634115517994	11.05142354876295
H	-3.85050680238780	0.06865404982234	12.18555118179482
C	-3.08709764067838	2.04616265738159	12.39771733973431
C	-2.77795077817358	3.02686810793971	11.45288725130690
H	-2.40993751813548	2.70014262623372	10.49272522423630
C	-2.91043868946141	4.40068794636755	11.66415077106174
C	-2.54580475523584	5.36990918463979	10.57641542677089
H	-3.41465037425169	5.98587325486589	10.33410508283118
H	-2.19978872934550	4.86843735705167	9.67587240574483
H	-1.76309001055910	6.04104654012220	10.93711043778344
N	-4.54337100184769	3.22333747175374	16.05578798381459
N	-4.31570966634621	5.71297270856114	15.29508514165765
O	-3.53430813057193	2.28005591013316	13.57559585408074
O	-3.33259535296099	4.93632088165731	12.74912216501084

(9) [Cu(dpa)(dpc)]

C	1.24078335434200	5.20720171362216	6.09620016296268
H	0.71241103973380	5.65812978584819	5.26443660726232
C	1.15287447123185	5.73780901650568	7.36838058887060
H	0.55066626097864	6.61522444376807	7.55721152768347
C	1.87380732692411	5.11270884288460	8.38497314483606
H	1.84934880251084	5.49815229117534	9.39640792695307
C	2.61716949403242	3.98830917389577	8.09524601452686
H	3.17517967619053	3.47548168485073	8.86884132304962
C	2.63224564539672	3.51348324591432	6.77409059732877
C	3.32739664095597	1.48814989019179	5.42919632980825
C	3.69550618482269	0.14905496751062	5.64689533623336
H	3.99403505148263	-0.17142911134572	6.63690126901284
C	3.64547679794389	-0.74346920388493	4.59969315139464
H	3.92456846548699	-1.77754209127395	4.75790748928150
C	3.20878311009849	-0.30826052885769	3.34844888299263
H	3.13020598460712	-0.98150518372182	2.50710115120412
C	2.88041759816149	1.02191688915150	3.20605075108068
H	2.52942381138015	1.42681013632371	2.26580011570249
C	1.09638379159902	4.73650591721100	1.68239269428309
C	2.18116510479685	5.80586636148633	1.81226583348287
C	2.32078587020877	6.97498622820130	1.07887282512590
H	1.58057653061594	7.22677936202934	0.33208868860665
C	3.43258226585300	7.77850626808794	1.33213401956735
H	3.56778572171505	8.69642744597177	0.77295183062002
C	4.38048824092901	7.40564976238031	2.28474495273935
H	5.26229824958721	7.99704396588617	2.48868599835410
C	4.17751646006420	6.22200724900234	2.98002454054161
C	5.08978121806561	5.57436634549023	4.02307853356076
N	1.97487827971098	4.12850469792849	5.79513316953405
N	2.96703230589560	1.91168261693304	4.21204538683146
N	3.09276583484692	5.49977740822360	2.72777210240762

N	3.34950615636753	2.35062064409731	6.50951081540420
H	3.80512007625429	1.96632817452738	7.32031993453726
O	1.28347713898511	3.72327924767541	2.47077690952524
O	4.66021516300577	4.42360979979593	4.42956131034368
O	0.19005292706935	4.89138682322461	0.88409940504669
O	6.10560881726333	6.15101473498054	4.37198167348551
Cu	2.86225913088600	3.85983298430843	3.69039400581840

(10) [Cu(acac)$_2$]

Cu	0.00011269107690	-0.00010655450017	0.00021829953139
C	4.19831519117458	0.49151880183634	-0.00511544106359
C	2.73928441774978	0.87374821126072	-0.00433937371425
O	1.92869733208084	-0.10406594990687	-0.00144550880682
C	2.37677840174611	2.22597628947177	-0.00639447751561
C	1.05112707898334	2.67601612424226	-0.00533040375524
O	0.02261098291474	1.93091989856156	-0.00249962734297
C	0.76455740882183	4.15681821436628	-0.00774795882902
H	4.40990576254812	-0.11688987770145	0.87671688315270
H	4.85541869842753	1.35937195426886	-0.01169040311423
H	4.40630040245571	-0.12799976715212	-0.87997012086716
H	3.16469650522948	2.96406957440951	-0.00894171979219
H	0.16476473014326	4.40438860128202	-0.88608620889346
H	1.67317710531144	4.75630483958072	-0.00952761660877
H	0.16606037230649	4.40753720636089	0.87057062607960
O	-1.92847575822158	0.10385109174799	0.00122458640965
C	-2.73906849672132	-0.87395956772708	0.00349946547037
C	-4.19809838780682	-0.49172665046576	0.00286090122358
H	-4.40886454201954	0.11658424792632	-0.87923621834398
H	-4.85520976550225	-1.35957754903208	0.00892304945636
H	-4.40689750496381	0.12788983238031	0.87745233275547
C	-2.37656790674727	-2.22618861745747	0.00603811754606
C	-1.05091657762163	-2.67622956529414	0.00609761548197
O	-0.02239879146381	-1.93113374794975	0.00400498377149
C	-0.76434953123148	-4.15703172536041	0.00884546823453
H	-0.16535369586491	-4.40455425760109	0.88774188705204
H	-1.67297057470035	-4.75651814395016	0.00984831800922
H	-0.16505632146618	-4.40779872200275	-0.86891526911889
H	-3.16448904963916	-2.96428067459427	0.00791204859175

(11) [Cu(mpsme)(NCS)]

Cu	1.74856328805025	1.03999089699846	4.12158878487229
S	1.72858700812128	2.94225126925456	5.43429450167025
S	3.71334136505649	3.41793692422515	7.68971092054726
S	-1.86815489798471	2.87075517257520	1.95355674901700
N	2.31127052703020	-0.93901500096188	3.24059276379496
N	3.28827744263793	0.54180304078943	5.24745706804952
N	3.74896664042598	1.31895591435763	6.24277304742261
N	0.28222191540855	1.49140576388490	3.05921002565497

C	0.63447731108953	-1.13242402088255	1.46403194266083
H	0.86502838987087	-0.16575929954697	1.01641584810677
H	-0.21798925654140	-0.96587371877315	2.12229190438254
H	0.34841994583820	-1.83063717956531	0.67908015434848
C	1.80755977924960	-1.66014054996062	2.23059187204837
C	2.37018317916976	-2.89849184213266	1.88917775393689
H	1.94433686182806	-3.46025756902818	1.06927659537379
C	3.45426411394573	-3.38790703122882	2.59480961696633
H	3.89307429370770	-4.34327112750704	2.33598831571439
C	3.97047075280189	-2.63534017955757	3.63863236831673
H	4.81754669863673	-2.97632348803012	4.21859896177036
C	3.37293141689409	-1.41405565018653	3.93325100817901
C	3.87193350554411	-0.58355180221256	5.01091772477746
H	4.72117416366032	-0.89419745444831	5.61080921471088
C	3.07452714181546	2.44308042086770	6.38395567227372
C	2.65244387037158	4.88571159806162	7.69952860184508
H	3.03908448382608	5.50302986018671	8.51026437712430
H	1.61693452252059	4.62194863745339	7.90289322196410
H	2.72355000831837	5.42967793226821	6.76029169534682
C	-0.62646447129339	2.10038848309926	2.61258928912397

(12) [Cu(sct)(dbpy)]

Cu	8.04531034067529	4.86770068811631	3.25799671466181
S	10.29975583047287	5.18219369468177	3.57415211505016
O	6.12871193458282	5.11933299536894	3.13257954140568
N	7.98828546834352	4.46942885703126	5.18859803507015
N	9.14843600055993	4.38631063439863	5.91943092306330
N	11.43048897955901	4.58784850657846	5.89882602392506
N	8.11212823079986	5.35368509263443	1.21352817089516
N	8.11348789173602	2.80046873821752	2.06132782566810
C	5.23804963245765	4.79837789832554	4.01953201160422
C	3.86426452758724	4.88836333488355	3.67716193433268
H	3.62686675670434	5.22458127012952	2.67537843995991
C	2.86900791072089	4.56224550101754	4.57215002163305
H	1.83154560362621	4.64274131931490	4.26690527221155
C	3.18012919805704	4.12993433539697	5.86930470469266
H	2.39553591766612	3.87660299013986	6.57016074085172
C	4.50488475619688	4.04085251666840	6.23547802063115
H	4.76612877791753	3.71784395762747	7.23782958864807
C	5.55294372922499	4.36114351653169	5.34688179938964
C	6.89227351750895	4.26882743865634	5.84993036194130
H	7.01063019034121	4.01958502187881	6.90370626091603
C	10.23269439431270	4.68047763965294	5.25498797397534
C	11.58845383582790	4.36132403594497	7.32969877409298
H	10.81184318664945	3.64852253245316	7.61687833943928
C	11.39263172374004	5.64225377821569	8.15596259596636
H	12.10844545019075	6.39662185604718	7.80719671982947
H	10.39287946773271	6.03781825665173	7.96822401948913
C	11.60451532202463	5.38560973440400	9.65087598697100

H	11.49338192919930	6.31883397898881	10.20979140757722
H	10.82019444457720	4.71218936471858	10.01602025613494
C	12.97512504264230	4.76069486884944	9.92511866259500
H	13.08619549450156	4.53859087564278	10.99025742572172
H	13.75877584896427	5.48592458194482	9.67516587452664
C	13.18248404790082	3.48887631603307	9.09756581348371
H	12.48165470823320	2.71863285840184	9.43980193278210
H	14.18634322709533	3.08735596435759	9.26159187484256
C	12.96024621666209	3.73786700372313	7.60231836359509
H	13.74025610318172	4.41486129233007	7.22893211464626
H	13.05541022240191	2.80599446150958	7.03889250367822
C	7.99469369626236	6.62867204119276	0.84239964531682
H	7.97622078782648	7.35679137574857	1.64321696851072
C	7.89795785960463	7.02071806894207	-0.48009270238251
H	7.80395443038913	8.07169337130199	-0.72230833555736
C	7.91304407312228	6.04960520751177	-1.48072553586843
C	7.78996540697388	6.42429207179703	-2.93060288461756
H	7.85187872644012	5.54975182013807	-3.57775349683701
H	8.58018273738360	7.12047668047349	-3.22079947361681
H	6.83597149982519	6.92160818077920	-3.12182549197612
C	8.03570774755450	4.72492469627892	-1.07811765957843
H	8.03239377147148	3.94443109887608	-1.82563917936497
C	8.13856379006375	4.39715397510660	0.27473618602304
C	8.26731774755336	2.99097086842313	0.74895183242401
C	8.54400615367080	1.92824204080939	-0.11402454158824
H	8.69466474362568	2.09942372908412	-1.17093187166570
C	8.64863522207005	0.63358402753769	0.38381431832543
C	8.95326090371289	-0.53273193548416	-0.51432717663356
H	9.00720161288850	-0.23025910529450	-1.56001134805856
H	8.18751892466579	-1.30622707430172	-0.42202082452185
H	9.90823823478117	-0.99050892966018	-0.24476751216527
C	8.47047490379036	0.46058368499321	1.75614274654906
H	8.53742932571431	-0.52233322395915	2.20614429980356
C	8.21355214148708	1.56822745621078	2.54870700629944
H	8.08435991319564	1.46800604648486	3.62067822635285
H	12.22171078534971	4.94879711954222	5.39197365892865

(13) [Cu(spt)(DMF)]

Cu	2.43473070655123	1.41424201224545	1.22240092350480
S	1.44369917385587	1.79204040958748	3.38890353036064
O	2.42443574013807	0.56324947003638	-0.53400914270161
O	-2.28487569263889	-0.83179774858529	-4.36837539304272
O	-2.86415655493171	1.17116084262515	-3.78120608823848
N	0.95347625672529	2.65722274747000	0.70064871255318
N	0.11830441242472	3.17874402527508	1.44689291658834
N	-0.55382106936473	3.57907750861921	3.61499522264648
N	-2.09843592889086	0.20954703111162	-3.74646105459113
C	0.46390162401206	1.59461618999576	-1.43048078302778
C	1.37326991849744	0.50311560427680	-1.29410837996914

C	1.09810313450664	-0.66762644972527	-2.04667414787990
C	-0.01850388445056	-0.76334781751849	-2.84407804778013
C	-0.90912260650609	0.31058389637660	-2.92253725632888
C	-0.66689215758348	1.48420593331830	-2.21637072097135
C	0.78254340827203	2.89597382653586	-0.73781990781307
C	0.29228583408823	2.89018880449817	2.84776758740444
C	-0.58145559008407	3.41287436812380	5.07441784538687
C	-1.97313264030461	2.98200059237643	5.54163795465490
C	-3.05217396932247	3.95219767945480	5.05886873025571
C	-2.95590543457021	4.15754586417425	3.54665120503081
C	-1.54279748096984	4.55989334557430	3.12200135175528
O	3.99299730805056	0.73236192135424	1.89943710430168
C	5.04032291599134	0.64685391591906	1.00286052981121
N	5.43606593749106	1.96009147557776	0.48200886532052
C	6.26702166216835	1.85125882943472	-0.70451970296641
C	6.06020844312891	2.78328466994129	1.50632413411182
H	1.79340835580376	-1.49232247208937	-1.96180738871363
H	-0.22854448513374	-1.66201617181822	-3.40606001081730
H	-1.36586824388824	2.30388547497589	-2.31103481257556
H	0.00416258538130	3.64085958546099	-0.89804415314562
H	1.75133151711547	3.27727431434748	-1.07820148234455
H	-0.31272568927836	4.37789463627453	5.51775121951844
H	0.17750122643047	2.69019439045221	5.35654913764754
H	-1.96465957153803	2.91846562610036	6.63200528096900
H	-2.17549522405017	1.97495808051662	5.16506160237063
H	-4.04312101875980	3.58204407584374	5.32917293982614
H	-2.92854203752338	4.91600906456638	5.56542697423459
H	-3.23464439860582	3.23826202311452	3.02285610151702
H	-3.64763539366691	4.93521697298411	3.21463380622061
H	-1.45884986784758	4.64125167138097	2.04611914616048
H	-1.27809925488806	5.52708555432236	3.56285101258573
H	4.78027578981985	0.02579583899982	0.13600584376182
H	5.88850184214402	0.16192244942978	1.52782894353748
H	5.74368454516643	1.27662651271941	-1.47037762937091
H	7.24024674105956	1.36476432737140	-0.51203617044352
H	6.47117868081556	2.84740268042149	-1.10349216627979
H	5.41806495598269	2.81428630900935	2.38580288275043
H	6.19647980109505	3.80198658320234	1.13580552227055
H	7.04855065008146	2.39761255034001	1.81573590694415

(14) [Cu(tct)$_2$]

Cu	0.36282599706730	-0.74364017520631	0.03155959414245
S	-0.13572710035083	-1.61371668358034	-2.03101410738500
S	3.90264204786505	2.15427371378890	-2.66540140196895
N	1.93355721244675	0.14366242709152	-2.29389665288248
N	1.75966023777045	0.32177179778867	-0.95841472125766
N	1.23310831730244	-0.89471985218435	-4.18725245274870
C	1.11056015973578	-0.71265654815736	-2.84789288055195
C	2.49069293060627	1.22942767696524	-0.38966095449193

C	3.45959637461920	2.10070223580366	-0.98507949405622
C	4.17957043102872	3.04050355099619	-0.26760937769964
C	5.07090454380822	3.78965681570814	-1.05915136075660
C	5.02558298703616	3.41654945478356	-2.37721688507337
H	2.34238786686835	1.33945948728091	0.67754880993497
H	0.75872325308198	-1.66732846787100	-4.61781699464442
H	2.04197327190342	-0.50768598520576	-4.64502579388392
H	4.05568494373590	3.17212010898012	0.79881438278259
H	5.71595789238731	4.56738319399327	-0.67582543969568
H	5.60114643555542	3.82380614605592	-3.19406067144999
S	1.27971080072875	-0.71278601575652	2.13400508019883
S	-4.18664591263859	-1.59224141353096	2.63585825243617
N	-1.38089640059087	-1.27942392979548	2.34058670631735
N	-1.36700976307411	-1.13756230084554	0.98962735445071
N	-0.18548411341091	-1.28614823026605	4.26936396836850
C	-0.21987076094556	-1.11175309282284	2.92528391083152
C	-2.51148581490747	-1.20492963558518	0.38330166293780
C	-3.81401060223380	-1.39561317889017	0.94898769848310
C	-4.97214178490574	-1.44354815918285	0.19217129902664
C	-6.13743886315851	-1.63375997045412	0.95919925498508
C	-5.86133186912376	-1.73012063212206	2.29820888468809
H	-2.47004817736834	-1.09894621448702	-0.69379316815958
H	0.63421932738079	-1.01532254928643	4.78033356270251
H	-1.05619544340977	-1.39904616686034	4.76112094653762
H	-4.96294991226307	-1.34329563147547	-0.88475384579263
H	-7.13326155812289	-1.69718146452637	0.54420610231047
H	-6.56400695442407	-1.87789031114359	3.10368873136435

(15) [Cu(eLys)]

Cu	0.09129697125933	-0.00930005588848	0.10001620876379
S	-0.33135873055643	-1.30659893869216	-1.67548935059201
S	-1.34864882645196	1.70499307054998	0.00253757529759
N	1.13030187941693	-1.64797892243202	1.00288756904337
N	1.29156888167646	1.12224478818423	1.46009506269159
C	0.21953664123259	-2.87837371674802	-0.91799354892453
C	1.43948325725544	-2.67504533507998	-0.00194715016882
C	2.27962225404060	-1.09577239371358	1.74402349712340
C	1.85126536069547	0.18411155456365	2.45132521634043
C	0.52519168856798	2.25419667293755	2.00006528520118
C	-0.28170373463716	2.91337801293231	0.86729276660086
C	1.81706451176761	-3.99023347184114	0.67054858957310
C	1.45441893601328	3.27466254391707	2.64807365743979
C	2.84352452014090	-6.09325677440658	0.35057498441667
C	1.55973940564762	5.12986196675972	4.10639034139492
O	2.50628912219570	-4.78659871109270	-0.15525814163333
O	0.79440756707888	4.07261339599861	3.49558228347767
H	0.48432807499909	-3.57554819119541	-1.71334051941365
H	-0.59265277233435	-3.32994907653738	-0.34032828200241
H	2.27154621116249	-2.32239094173526	-0.61220316512320

H	2.68576265101454	-1.80961858184309	2.46717529284131
H	3.06682691525662	-0.87227232468653	1.01959532188326
H	1.06621928780989	-0.04013344007964	3.17783887870266
H	2.69604036306825	0.61600360734612	2.99640333628644
H	-0.17639681827114	1.87377917944297	2.74311816672542
H	-0.91094799141019	3.69741696658608	1.28912633053646
H	0.40829391702147	3.38754510669741	0.16276890378953
H	3.38573651436997	-6.58341936344621	-0.45285390450267
H	1.93929125840442	-6.64735593860769	0.59904341994076
H	3.46743511743381	-6.00589871149050	1.23924164048217
H	0.85955338531753	5.66301067492962	4.74299077651342
H	1.96669565225711	5.79157887624735	3.34290055404003
H	2.37657260437307	4.71442164652651	4.69514365937844
O	1.50065436349498	-4.28993310616652	1.79716566506204
O	2.63248164113682	3.37254537098916	2.39938303172754
H	0.48669141799621	-2.06764779855925	1.67266222533205
H	2.06053174455608	1.51237726663380	0.91653457475465

(16) [Cu(tox)$_2$]

Cu	-0.00000944068715	-0.00002652518529	-0.00030541958077
S	0.24315167447678	2.27143115427292	-0.00280858400209
N	-2.04825082280024	0.38825064690839	-0.00162183460920
C	-2.96377960177276	-0.56295490967432	-0.00086461094839
C	-4.34187875008024	-0.29849420788908	-0.00184601129056
C	-4.76716659560250	1.00314644590706	-0.00367412971036
C	-3.82315563237510	2.05111241431052	-0.00452355585244
C	-4.19389014217072	3.41462895751912	-0.00639426472800
C	-3.21761489362566	4.37928774058270	-0.00711957110220
C	-1.85616237379611	4.03375267385533	-0.00602396916898
C	-1.44062422698767	2.71186833201635	-0.00416949618117
C	-2.44137820057974	1.69776486321447	-0.00341558801052
H	-2.60874534941296	-1.58440852172295	0.00058645142682
H	-5.03885397787174	-1.12535684100918	-0.00114357698410
H	-5.82413524192371	1.24363283895998	-0.00448050053468
H	-5.24425853965548	3.67746874906036	-0.00722380421693
H	-3.49248418294903	5.42712339403874	-0.00855413219558
H	-1.10737492644386	4.81547177226534	-0.00662077666342
S	-0.24317029310283	-2.27148502756211	0.00176249117180
N	2.04823180063889	-0.38830360049584	0.00134441643872
C	1.44060552843880	-2.71192182899080	0.00338400094912
C	2.96376049870850	0.56290225279051	0.00094827861144
C	2.44135929882386	-1.69781801820150	0.00297513656949
C	1.85614355922968	-4.03380643053803	0.00512166553734
C	4.34185951155991	0.29844163225469	0.00212594465587
H	2.60872632757877	1.58435610344511	-0.00034605172888
C	3.82313659654488	-2.05116552696159	0.00427042649430
C	3.21759596356352	-4.37934140346230	0.00639474522665
H	1.10735627222576	-4.81552580632982	0.00547320698014
C	4.76714741510999	-1.00319923498397	0.00378062369913

H	5.03883462278960	1.12530455083663	0.00171232175454
C	4.19387102960524	-3.41468230837555	0.00598529476421
H	3.49246521143211	-5.42717720707546	0.00771776595519
H	5.82411595796436	-1.24368562277294	0.00473347093966
H	5.24423940414685	-3.67752177300749	0.00695648433385

(17) [Cu(dtc)$_2$]

Cu	-0.00003745870713	0.00031455500636	0.00043544654246
C	-4.90231782536811	-1.22350319913538	0.06822406053126
C	-4.90202428492746	1.22444435898848	-0.08258478608238
S	-1.84343944651585	-1.44552666600049	0.04828926302153
S	-1.84322212369754	1.44634468667883	-0.05295022073736
S	1.84342349082921	1.44610297835482	-0.04695819872895
S	1.84311816044093	-1.44578448957738	0.05377999448697
C	2.77858039520616	0.00009853367474	0.00465007669769
C	4.90230409755461	1.22396776193489	-0.06724035117535
C	4.90192470244243	-1.22400948113229	0.08306082240975
H	5.41071583180377	1.40510135002642	0.88394772273930
H	-5.41360575444383	1.40574554069459	0.86686839906188
H	4.26052644063251	2.06896090784648	-0.29515928748891
H	-4.25942429763398	2.06935965582643	-0.30846773506714
H	-5.65311730212538	1.12093783582118	-0.86913897873041
H	5.65602075597388	1.12051164731753	-0.85128448174547
H	-5.41049952592437	-1.40493474727916	-0.88303086914093
H	-4.26054884094923	-2.06839970411036	0.29652895452400
H	-5.65622004884298	-1.11986093757024	0.85206365208736
H	5.41329385065707	-1.40519689641353	-0.86652925651437
H	4.25933074003118	-2.06892725549871	0.30895492871705
H	5.65319090070810	-1.12065334163126	0.86946812582482
N	4.11446959994680	0.00002490916533	0.00667810068510
C	-2.77863883827080	0.00043398031289	-0.00369862024338
N	-4.11452760082000	0.00045870569982	-0.00584596967453

(18) [Cu(ttcn)$_2$]$^{2+}$

C	13.39618716119780	-1.40773209973671	4.58757371520757
C	13.65018547302069	0.04723429787833	4.97216103270781
C	11.35293744880155	-2.81258161376113	3.12597916256775
C	11.51137638228967	-1.94989925700434	1.88228768999857
Cu	10.28710417015302	0.00000089896149	4.34158115048898
S	10.54981755790392	-0.38413149346065	1.97007131065877
S	12.66401383434905	1.33320850484186	4.12950835265486
S	11.64466628801289	-1.95888242817653	4.71886003834683
C	11.76178521854994	0.90043719693084	1.48548752973081
C	13.01092557919842	1.05763929252424	2.35054426609452
S	10.02438998584242	0.38413272589856	6.71309031220632
S	7.91019694161065	-1.33320771710912	4.55365033446879
S	8.92954194558863	1.95888454364162	3.96430163688539
C	9.06282909689783	1.94989906837657	6.80087421696232

C	8.81242333335529	-0.90043774471878	7.19767199807188
C	6.92402505373195	-0.04723411424282	3.71099702885456
C	7.56328362903203	-1.05764016487808	6.33261437317666
C	7.17802148008021	1.40773238838573	4.09558515681241
C	9.22126767943664	2.81258271023359	5.55718361644398
H	13.73130002864985	-1.61742556912040	3.57409680463020
H	13.96611787557957	-2.05403266593653	5.25675415139902
H	13.44530203512588	0.21856605697827	6.03008115622932
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H	13.56137416764481	1.92652221344748	1.98699611638219
H	13.67739405270437	0.20252828508202	2.25531142616491
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H	8.52753666713090	-0.69642146972373	8.23168041743926
H	7.12890990222218	-0.21856533525589	2.65307706287609
H	5.86563789808398	-0.26360934128889	3.86527393124294
H	7.01283558883804	-1.92652389491903	6.69616136899285
H	6.89681424774645	-0.20252990817289	6.42784745717303
H	6.84290685097549	1.61742516006506	5.10906162270864
H	6.60809106291441	2.05403253137281	3.42640404227506
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H	10.23663577422608	3.19930718702332	5.46341476791707