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Notes

SUPPORTING INFORMATION

Photo-Control of Adsorption of Dye Metal Complexes Incorporating Chiral Schiff Base Ligands Containing Azo-Groups on TiO_2

Shinnosuke Tanaka[†], Hiroki Sato[†], Yota Ishida[†], Yanyang Deng[†], Tomoyuki Haraguchi[†], Takashiro Akitsu[†,*], Mutsumi Sugiyama[‡], Michikazu Hara[§], and Dohyun Moon[#,*]

[†]*Department of Chemistry, Faculty of Science, Tokyo University of Science, Tokyo, Japan.*
[*]*E-mail: akitsu@rs.kagu.tus.ac.jp*
[‡]*Department of Electrical Engineering, Faculty of Science and Technology, Tokyo University of Science, Chiba, Japan*
[§]*Materials and Structures Laboratory, Tokyo Institute of Technology, Kanagawa, Japan*
[#]*Beamline Department, Pohang Accelerator Laboratory, Korea*

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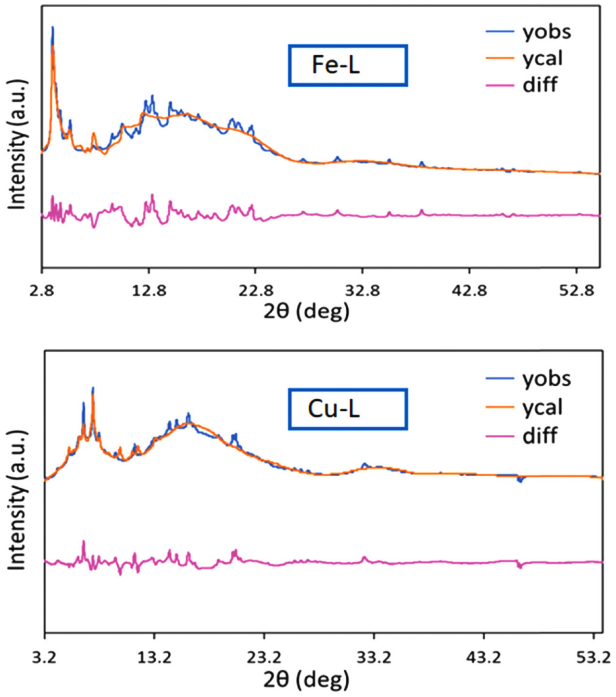

***Figure* S1.** Rietveld refinement profiles for **Fe-L.2H$_2$O** (above) and **Cu-L.2H$_2$O** (below) during analyzing their structures.

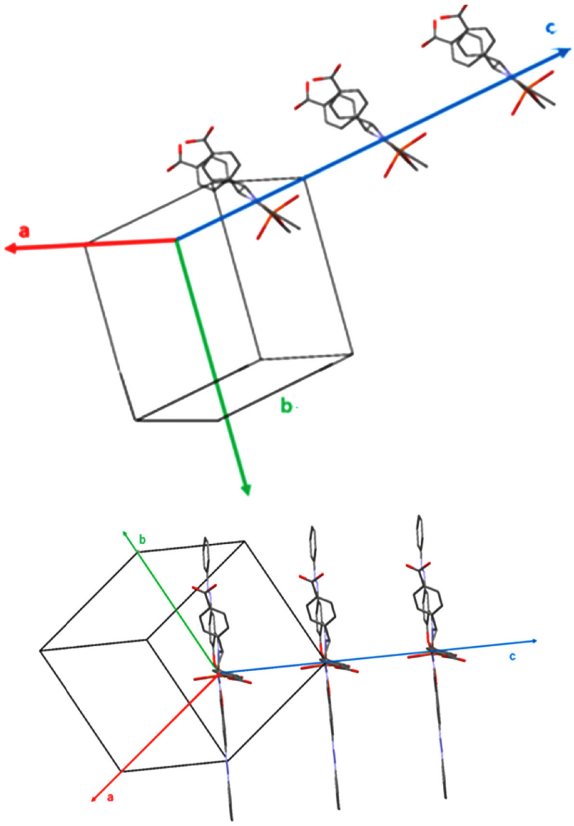

***Figure* S2.** Crystal packing (alignment of molecules) for **Fe-L.2H$_2$O** (above) and **Cu-L.2H$_2$O** (below) along the *c* axis.

ENTER FIGURE CAPTIONS
(Indexing#1)
Crystal data

$C_{10.51}Fe_{0.26}H_{8.51}N_{1.50}O_2$	V = 1786 (7) Å^3
M_r = 201.65	Z = 4
Triclinic, P1	F(000) = 418.00
a = 10.93 (2) Å	D_x = 0.75 Mg m^{-3}
b = 14.66 (2) Å	Synchrotron radiation, λ = 1 Å
c = 11.71 (3) Å	T = 298 K
α = 94.18 (14)°	brownish-brown
β = 107.1 (2)°	
γ = 86.35 (18)°	

Data collection

ENTER THE MEASUREMENT DEVICE NAME diffractometer	$2\theta_{min}$ = 2.79°, $2\theta_{max}$ = 54.97°, $2\theta_{step}$ = 0.01°

Refinement

Refinement on F^2	3811 data points
Least-squares matrix: full	31 parameters
R_p = 0.035	0 restraints
R_{wp} = 0.050	0 constraints
R_{exp} = 0.013	Weighting scheme based on measured s.u.'s
χ^2 = 14.860	$(\Delta/\sigma)_{max}$ = 0.014

Special details
Geometry. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY
Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Fe1	0.026615	0.105602	0.730398	0*
O1	0.117777	0.199457	0.875811	0*
O2	0.678220	-0.338595	0.900651	0*
O3	-0.155857	0.150604	0.660623	0*
O4	0.691630	-0.325522	0.702064	0*
O5	0.001763	0.077626	0.924222	0*
O6	-0.020369	-0.369642	0.059206	0*
O7	0.017094	-0.460076	0.215643	0*
O8	0.010957	0.195166	0.570125	0*
N1	-0.025848	-0.017554	0.607227	0*
N2	-0.586748	-0.006913	0.328991	0*
N3	0.205420	0.036629	0.748897	0*
N4	-0.690507	0.040153	0.307487	0*
N5	0.619272	0.249596	1.148983	0*
N6	0.646479	0.318940	1.233913	0*

C1	0.312076	0.066358	0.822026	0*
C2	-0.375455	0.162959	0.554176	0*
C3	-0.484449	0.126666	0.472856	0*
C4	-0.481313	0.036746	0.413202	0*
C5	-0.365999	-0.013516	0.438572	0*
C6	0.458551	0.164917	0.989658	0*
C7	0.491059	0.240577	1.083637	0*
C8	0.271698	0.286971	1.036690	0*
C9	0.394606	0.302106	1.106481	0*
C10	0.080296	-0.087536	0.624681	0*
C11	0.198598	-0.044424	0.649151	0*
C12	0.314583	-0.111469	0.687511	0*
C13	0.359150	-0.148091	0.811177	0*
C14	0.463764	-0.210526	0.844531	0*
C15	0.526468	-0.237647	0.754917	0*
C16	0.483308	-0.201163	0.631902	0*
C17	0.378331	-0.138535	0.599180	0*
C18	0.058758	-0.164118	0.508075	0*
C19	0.028765	-0.149658	0.372334	0*
C20	0.069750	-0.250709	0.534481	0*
C21	0.011469	-0.220007	0.266633	0*
C22	0.023521	-0.306565	0.294309	0*
C23	0.052591	-0.321622	0.428998	0*
C24	0.004275	-0.379381	0.177471	0*
C25	-0.796312	-0.004321	0.222452	0*
C26	-0.791731	-0.093387	0.163377	0*
C27	-0.902097	-0.129925	0.081428	0*
C28	-1.017758	-0.078661	0.057324	0*
C29	-1.022541	0.009789	0.115848	0*
C30	-0.912199	0.046809	0.198090	0*
C31	0.637722	-0.304745	0.795523	0*
C32	0.870531	0.265707	1.276284	0*
C33	0.994681	0.281283	1.346820	0*
C34	1.026130	0.358076	1.440697	0*
C35	0.932329	0.419533	1.463826	0*
C36	0.807674	0.404280	1.393434	0*
C37	-0.139035	-0.037354	0.539517	0*
C38	-0.252611	0.021700	0.521034	0*
C39	-0.255868	0.112721	0.581947	0*
C40	0.235858	0.209858	0.939531	0*
C41	0.333598	0.147291	0.916771	0*
C42	0.775890	0.327513	1.299397	0*
H1	1.067813	0.233478	1.328963	0*
H2	1.123404	0.369711	1.495383	0*
H3	-0.701402	-0.132039	0.183130	0*
H4	0.844452	0.206656	1.203297	0*

H5	0.098931	-0.113515	0.720151	0*
H6	-0.898537	-0.198763	0.035737	0*
H7	-1.103559	-0.107756	-0.006881	0*
H8	0.396813	0.028043	0.814015	0*
H9	0.092704	-0.262909	0.638893	0*
H10	-0.086411	0.099661	0.895642	0*
H11	0.044724	0.129786	0.972801	0*
H12	-0.011646	-0.209372	0.161607	0*
H13	-0.076417	0.210523	0.558346	0*
H14	0.312322	-0.126866	0.882323	0*
H15	-0.365030	-0.082283	0.392099	0*
H16	0.345094	-0.110694	0.503280	0*
H17	0.533439	0.118328	0.973289	0*
H18	0.197105	0.333766	1.053102	0*
H19	0.053260	0.242878	0.636725	0*
H20	-0.153967	-0.105193	0.489698	0*
H21	-0.376806	0.231657	0.600671	0*
H22	-0.913074	0.115396	0.244907	0*
H23	0.061619	-0.388403	0.450818	0*
H24	0.420480	0.361055	1.179908	0*
H25	0.732788	0.450888	1.409376	0*
H26	-0.574684	0.165589	0.452754	0*
H27	0.498690	-0.239121	0.939771	0*
H28	0.002636	-0.502008	0.131706	0*
H29	0.017658	-0.082799	0.349176	0*
H30	0.531714	-0.221722	0.562495	0*
H31	-1.111993	0.049830	0.097450	0*
H32	0.956227	0.479179	1.536538	0*
H33	0.183020	-0.023096	0.551147	0*
H34	0.762579	-0.369495	0.739196	0*

Geometric parameters (Å, º)

Fe1—O1	2.149 (5)	C18—C19	1.553 (5)
Fe1—O3	2.008 (5)	C12—C13	1.512 (4)
Fe1—O8	2.327 (5)	C12—C17	1.429 (3)
Fe1—N1	2.221 (5)	C13—C14	1.398 (3)
Fe1—N3	2.103 (5)	C14—C15	1.434 (3)
O1—C40	1.299 (4)	C15—C16	1.504 (4)
O2—C31	1.302 (4)	C15—C31	1.499 (4)
O3—C39	1.327 (4)	C16—C17	1.402 (3)
O4—C31	1.395 (3)	C18—C20	1.318 (2)
O6—C24	1.347 (4)	C19—C21	1.527 (3)
O7—C24	1.280 (2)	C20—C23	1.530 (3)
N5—N6	1.352 (3)	C21—C22	1.321 (2)
N2—N4	1.258 (3)	C22—C23	1.543 (4)

N3—C1	1.305 (4)	C22—C24	1.643 (4)
N3—C11	1.593 (3)	C25—C26	1.437 (3)
N4—C25	1.441 (4)	O4—H34	0.992 (2)
N5—C7	1.394 (4)	O5—H10	0.965 (2)
N6—C42	1.405 (4)	O5—H11	0.976 (2)
N1—C10	1.476 (3)	O7—H28	1.096 (3)
N1—C37	1.295 (4)	O8—H13	0.939 (2)
N2—C4	1.429 (4)	O8—H19	1.029 (3)
C25—C30	1.395 (3)	C1—H8	1.077 (2)
C26—C27	1.410 (4)	C2—H21	1.111 (2)
C27—C28	1.394 (3)	C3—H26	1.079 (3)
C28—C29	1.427 (3)	C5—H15	1.111 (2)
C29—C30	1.414 (4)	C6—H17	1.084 (2)
C32—C33	1.388 (4)	C8—H18	1.084 (2)
C1—C41	1.544 (3)	C9—H24	1.160 (3)
C32—C42	1.405 (3)	C10—H5	1.163 (3)
C2—C3	1.395 (4)	C17—H16	1.169 (3)
C2—C39	1.421 (3)	C28—H7	1.102 (3)
C40—C41	1.436 (3)	C21—H12	1.200 (3)
C3—C4	1.449 (3)	C29—H31	1.081 (3)
C33—C34	1.496 (3)	C30—H22	1.110 (2)
C4—C5	1.383 (3)	C11—H33	1.172 (3)
C5—C38	1.428 (4)	C14—H27	1.167 (3)
C34—C35	1.395 (3)	C23—H23	1.0210 (17)
C6—C7	1.486 (3)	C13—H14	1.116 (3)
C6—C41	1.409 (4)	C33—H1	1.086 (2)
C35—C36	1.391 (4)	C19—H29	1.0261 (18)
C7—C9	1.417 (3)	C34—H2	1.084 (3)
C8—C9	1.373 (4)	C16—H30	1.108 (3)
C8—C40	1.527 (3)	C35—H32	1.160 (3)
C36—C42	1.497 (3)	C26—H3	1.078 (3)
C37—C38	1.439 (3)	C36—H25	1.083 (2)
C10—C11	1.419 (3)	C20—H9	1.198 (3)
C10—C18	1.673 (4)	C37—H20	1.112 (2)
C38—C39	1.470 (3)	C27—H6	1.111 (2)
C11—C12	1.531 (4)	C32—H4	1.158 (3)
Fe1—O1—C40	133.70 (16)	C32—C42—C36	122.06 (17)
Fe1—O3—C39	132.43 (14)	C12—C17—C16	117.06 (17)
Fe1—N3—C1	122.92 (16)	C10—C18—C19	130.22 (14)
Fe1—N1—C10	112.27 (19)	C10—C18—C20	115.63 (16)
Fe1—N1—C37	127.08 (17)	C19—C18—C20	114.15 (14)
Fe1—N3—C11	112.3 (2)	C18—C19—C21	129.89 (14)
O1—Fe1—O8	99.5 (2)	C18—C20—C23	116.26 (16)
O3—Fe1—O8	70.11 (19)	C19—C21—C22	115.40 (16)
O1—Fe1—O3	108.4 (2)	C21—C22—C23	115.09 (14)
O1—Fe1—N1	164.34 (5)	C21—C22—C24	113.43 (17)

O1—Fe1—N3	88.8 (2)	C23—C22—C24	131.48 (14)
O3—Fe1—N3	161.57 (7)	C26—C25—C30	119.28 (18)
O8—Fe1—N1	91.04 (19)	C25—C26—C27	121.23 (17)
O8—Fe1—N3	101.32 (19)	C26—C27—C28	119.34 (16)
O3—Fe1—N1	86.0 (2)	C27—C28—C29	119.54 (18)
O6—C24—O7	118.98 (13)	C28—C29—C30	121.39 (17)
O2—C31—O4	125.10 (17)	Fe1—O8—H13	93.8 (2)
O4—C31—C15	108.91 (18)	Fe1—O8—H19	83.4 (2)
O7—C24—C22	107.41 (18)	N1—C37—H20	119.71 (18)
O1—C40—C41	118.69 (17)	N1—C10—H5	107.22 (18)
O1—C40—C8	121.29 (18)	N3—C1—H8	114.17 (17)
O3—C39—C2	118.21 (17)	N3—C11—H33	116.59 (16)
O3—C39—C38	124.75 (16)	C31—O4—H34	101.32 (19)
O2—C31—C15	125.99 (16)	C24—O7—H28	101.06 (18)
O6—C24—C22	133.60 (13)	C41—C1—H8	116.19 (18)
N1—Fe1—N3	77.7 (2)	C3—C2—H21	122.56 (17)
N6—N5—C7	117.18 (19)	C39—C2—H21	116.43 (19)
N5—N6—C42	116.81 (19)	C2—C3—H26	120.17 (16)
N4—N2—C4	114.03 (17)	C4—C3—H26	117.89 (19)
N2—N4—C25	113.69 (17)	C4—C5—H15	117.39 (19)
N1—C10—C11	109.79 (16)	C38—C5—H15	121.31 (17)
N1—C10—C18	112.1 (2)	C25—C26—H3	118.38 (18)
N1—C37—C38	125.72 (15)	C27—C26—H3	120.39 (16)
N4—C25—C30	114.39 (17)	C23—C20—H9	128.85 (14)
N5—C7—C9	120.69 (16)	C26—C27—H6	121.22 (17)
N2—C4—C3	126.54 (16)	C28—C27—H6	119.44 (18)
N2—C4—C5	115.26 (17)	C16—C17—H16	120.69 (17)
N5—C7—C6	118.26 (19)	C27—C28—H7	118.85 (16)
N3—C11—C10	109.44 (18)	C29—C28—H7	121.62 (17)
N3—C11—C12	110.6 (2)	C19—C21—H12	130.27 (14)
N3—C1—C41	129.64 (16)	C22—C21—H12	114.34 (14)
N4—C25—C26	126.33 (16)	C30—C29—H31	118.78 (16)
N6—C42—C36	117.46 (19)	C17—C16—H30	116.33 (18)
N6—C42—C32	120.48 (16)	C25—C30—H22	117.82 (18)
C1—N3—C11	124.00 (17)	C29—C30—H22	122.96 (17)
C10—N1—C37	119.79 (16)	C10—C11—H33	95.7 (2)
C35—C36—C42	122.60 (18)	C11—C10—H5	95.8 (2)
C25—C30—C29	119.22 (16)	C18—C19—H29	115.70 (14)
C33—C32—C42	115.06 (17)	C33—C32—H4	123.68 (18)
C32—C33—C34	122.75 (18)	C42—C32—H4	121.26 (17)
C33—C34—C35	122.30 (17)	C21—C19—H29	114.41 (17)
C34—C35—C36	115.23 (17)	C32—C33—H1	115.04 (17)
C5—C38—C37	115.80 (17)	C34—C33—H1	122.21 (17)
C5—C38—C39	120.53 (17)	C15—C16—H30	122.59 (17)
C3—C2—C39	121.01 (16)	C33—C34—H2	122.23 (18)
C37—C38—C39	123.67 (17)	C35—C34—H2	115.47 (17)

C2—C39—C38	117.04 (19)	C20—C23—H23	115.40 (17)
C2—C3—C4	121.93 (17)	C34—C35—H32	122.56 (17)
C8—C40—C41	120.02 (17)	C36—C35—H32	122.21 (18)
C1—C41—C6	119.78 (18)	C18—C10—H5	118.93 (17)
C3—C4—C5	118.20 (18)	C35—C36—H25	116.91 (17)
C4—C5—C38	121.29 (16)	C42—C36—H25	120.49 (17)
C1—C41—C40	125.88 (16)	C38—C37—H20	114.58 (18)
C6—C41—C40	114.33 (17)	C22—C23—H23	115.39 (14)
C7—C6—C41	124.65 (18)	C15—C14—H27	121.57 (18)
C6—C7—C9	121.05 (17)	C13—C14—H27	122.21 (17)
C9—C8—C40	124.18 (18)	C8—C9—H24	123.45 (18)
C7—C9—C8	115.78 (17)	C7—C9—H24	120.78 (17)
C11—C10—C18	111.76 (19)	C14—C13—H14	115.34 (18)
C20—C23—C22	129.21 (14)	C40—C8—H18	119.37 (17)
C10—C11—C12	112.72 (16)	C9—C8—H18	116.46 (17)
C11—C12—C13	122.30 (17)	C12—C13—H14	122.84 (17)
C11—C12—C17	116.22 (18)	C12—C11—H33	111.01 (18)
C13—C12—C17	121.48 (18)	C12—C17—H16	122.24 (17)
C12—C13—C14	121.81 (17)	C18—C20—H9	114.89 (14)
C13—C14—C15	116.22 (18)	C41—C6—H17	115.17 (17)
C14—C15—C16	122.35 (17)	C7—C6—H17	120.18 (17)
C14—C15—C31	113.90 (18)	C28—C29—H31	119.83 (18)
C16—C15—C31	123.75 (16)	H13—O8—H19	101.6 (2)
C15—C16—C17	121.08 (17)	H10—O5—H11	103.5 (2)

ENTER FIGURE CAPTIONS

(Indexing#1)

Crystal data

$C_{42}CuH_{34}N_6O_8$	V = 1881 (7) Å^3
M_r = 814.30	Z = 1
Triclinic, $P1$	$F(000)$ = 421.00
a = 13.18 (2) Å	D_x = 0.72 Mg m^{-3}
b = 13.21 (3) Å	Synchrotron radiation, λ = 1.2 Å
c = 12.18 (2) Å	T = 298 K
α = 103.12 (11)°	brownish-green
β = 114.10 (6)°	
γ = 81.04 (9)°	

Data collection

ENTER THE MEASUREMENT DEVICE NAME diffractometer	$2\theta_{min}$ = 2.95°, $2\theta_{max}$ = 54.97°, $2\theta_{step}$ = 0.01°

Refinement

Refinement on F^2	3799 data points
Least-squares matrix: full	32 parameters
R_p = 0.006	0 restraints
R_{wp} = 0.010	0 constraints
R_{exp} = 0.008	Weighting scheme based on measured s.u.'s
χ^2 = 1.860	$(\Delta/\sigma)_{max}$ = 0.019

Special details

Geometry. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cu1	0.187224	0.110257	0.250863	0*
O1	0.236501	0.245419	0.359127	0*
O2	0.312417	0.000475	0.312432	0*
O3	0.161298	0.060781	0.410173	0*
O4	-0.436138	0.386756	-0.349486	0*
O5	-0.337752	-0.275541	-0.430993	0*
O6	-0.540334	0.313834	-0.286424	0*
O7	0.290543	0.170986	0.166877	0*
O8	-0.344738	-0.334321	-0.273314	0*
N1	0.105645	-0.004224	0.100191	0*
N2	0.027387	0.189618	0.166549	0*
N3	0.017197	0.631875	0.415969	0*
N4	0.396823	-0.405596	0.124250	0*
N5	0.487525	-0.454137	0.185414	0*
N6	0.072772	0.701696	0.497180	0*
C1	-0.002487	0.283671	0.202097	0*
C2	0.281103	-0.248299	0.111376	0*
C3	0.380179	-0.303459	0.176804	0*
C4	0.455968	-0.253847	0.289617	0*
C5	0.431613	-0.153242	0.332797	0*
C6	0.018210	0.457887	0.317203	0*
C7	0.077362	0.536067	0.405783	0*
C8	0.191866	0.514135	0.478204	0*
C9	0.242808	0.417399	0.460901	0*
C10	0.000054	0.037179	0.007981	0*
C11	-0.056809	0.120604	0.074036	0*
C12	-0.157913	0.176701	-0.017723	0*
C13	-0.146979	0.240951	-0.092068	0*
C14	-0.239745	0.290456	-0.177311	0*
C15	-0.345741	0.276984	-0.189952	0*
C16	-0.357482	0.213688	-0.115814	0*
C17	-0.264029	0.164321	-0.030470	0*
C18	-0.079313	-0.045172	-0.075927	0*

C19	-0.118094	-0.113474	-0.028686	0*
C20	-0.116013	-0.053569	-0.202186	0*
C21	-0.192179	-0.187252	-0.105843	0*
C22	-0.229028	-0.194563	-0.232238	0*
C23	-0.190363	-0.127350	-0.280171	0*
C24	-0.308442	-0.274745	-0.310598	0*
C25	0.503642	-0.557046	0.131864	0*
C26	0.427457	-0.605427	0.020255	0*
C27	0.452421	-0.707070	-0.023257	0*
C28	0.552882	-0.761584	0.043267	0*
C29	0.628646	-0.713717	0.154113	0*
C30	0.604081	-0.611823	0.198236	0*
C31	-0.442138	0.331588	-0.282714	0*
C32	-0.101845	0.818855	0.433901	0*
C33	-0.153144	0.916669	0.451774	0*
C34	-0.092693	0.994593	0.541870	0*
C35	0.019904	0.974119	0.614372	0*
C36	0.071815	0.876201	0.596874	0*
C37	0.183885	0.335752	0.370671	0*
C38	0.067945	0.358077	0.296894	0*
C39	0.330511	-0.094876	0.267271	0*
C40	0.253464	-0.145276	0.153200	0*
C41	0.148000	-0.096459	0.076785	0*
C42	0.011550	0.798046	0.506820	0*
H1	0.393508	-0.744467	-0.109508	0*
H2	-0.240787	0.932737	0.395364	0*
H3	0.571707	-0.841012	0.008580	0*
H4	-0.133453	1.070822	0.555202	0*
H5	-0.084190	0.077565	0.123981	0*
H6	0.021591	0.079368	-0.047652	0*
H7	0.101546	-0.144776	-0.008870	0*
H8	-0.089417	0.312585	0.157917	0*
H9	0.307507	0.228587	0.233391	0*
H10	0.223799	-0.287332	0.025155	0*
H11	0.330349	0.399681	0.516078	0*
H12	-0.065221	0.253071	-0.082189	0*
H13	-0.273782	0.115012	0.026521	0*
H14	0.185724	0.124340	0.466441	0*
H15	0.229190	0.015521	0.426232	0*
H16	0.067157	1.034286	0.684345	0*
H17	0.706656	-0.755661	0.206061	0*
H18	0.489185	-0.114416	0.418879	0*
H19	0.353772	0.120183	0.195910	0*
H20	-0.389327	-0.330454	-0.472783	0*
H21	-0.147292	0.757627	0.364621	0*
H22	-0.086612	-0.001404	-0.240046	0*

H23	0.661400	-0.572650	0.284136	0*
H24	-0.069433	0.475835	0.262335	0*
H25	0.237642	0.575414	0.547226	0*
H26	-0.231972	0.340133	-0.235060	0*
H27	-0.218351	-0.132931	-0.377812	0*
H28	0.350134	-0.562061	-0.029960	0*
H29	0.533175	-0.297233	0.340297	0*
H30	-0.089163	-0.109498	0.069167	0*
H31	-0.439242	0.203303	-0.124993	0*
H32	-0.222521	-0.240213	-0.070061	0*
H33	0.159250	0.858080	0.651863	0*
H34	-0.505778	0.418924	-0.407529	0*

Geometric parameters (Å, º)

Cu1—O1	1.985 (4)	C18—C20	1.394 (2)
Cu1—O2	2.031 (4)	C19—C21	1.385 (3)
Cu1—O3	2.345 (3)	C20—C23	1.389 (3)
Cu1—O7	2.323 (3)	C21—C22	1.398 (2)
Cu1—N1	2.109 (4)	C22—C23	1.417 (2)
Cu1—N2	2.151 (3)	C22—C24	1.483 (3)
O1—C37	1.292 (3)	C25—C26	1.399 (2)
O2—C39	1.282 (3)	C25—C30	1.422 (2)
O4—C31	1.240 (2)	C26—C27	1.369 (3)
O5—C24	1.354 (2)	C27—C28	1.421 (2)
O6—C31	1.332 (2)	C28—C29	1.389 (2)
O8—C24	1.2294 (18)	C29—C30	1.372 (3)
N3—N6	1.253 (2)	C32—C42	1.413 (2)
N4—N5	1.283 (2)	C33—C34	1.388 (3)
N3—C7	1.393 (3)	C34—C35	1.403 (2)
N4—C3	1.381 (3)	O3—H15	0.9694 (16)
N5—C25	1.392 (3)	O4—H34	1.0040 (15)
N6—C42	1.405 (3)	O5—H20	0.9750 (18)
N1—C10	1.504 (2)	O7—H9	0.9543 (19)
N1—C41	1.280 (3)	O7—H19	0.9811 (17)
N2—C1	1.276 (3)	O3—H14	0.960 (2)
N2—C11	1.470 (3)	C6—H24	1.0925 (18)
C9—C37	1.414 (3)	C23—H27	1.0804 (19)
C35—C36	1.380 (3)	C14—H26	1.1070 (17)
C36—C42	1.389 (3)	C8—H25	1.075 (2)
C37—C38	1.445 (2)	C9—H11	1.0917 (18)
C39—C40	1.430 (2)	C26—H28	1.0996 (17)
C40—C41	1.467 (2)	C10—H6	1.1084 (15)
C1—C38	1.433 (3)	C27—H1	1.0811 (17)
C8—C9	1.361 (3)	C16—H31	1.0645 (19)
C2—C3	1.410 (2)	C28—H3	1.070 (2)

C2—C40	1.388 (3)	C17—H13	1.1078 (17)
C10—C11	1.502 (2)	C29—H17	1.1022 (17)
C3—C4	1.411 (2)	C30—H23	1.0789 (17)
C4—C5	1.354 (3)	C5—H18	1.0798 (17)
C32—C33	1.376 (3)	C11—H5	1.1064 (15)
C5—C39	1.448 (2)	C32—H21	1.074 (2)
C11—C12	1.558 (2)	C1—H8	1.0962 (18)
C6—C7	1.377 (3)	C33—H2	1.0924 (18)
C6—C38	1.394 (3)	C19—H30	1.0845 (19)
C10—C18	1.516 (3)	C34—H4	1.076 (2)
C7—C8	1.426 (2)	C2—H10	1.0804 (18)
C12—C13	1.434 (2)	C35—H16	1.077 (2)
C12—C17	1.375 (2)	C20—H22	1.1005 (16)
C13—C14	1.422 (2)	C36—H33	1.0911 (18)
C14—C15	1.377 (2)	C4—H29	1.1004 (17)
C15—C16	1.427 (2)	C21—H32	1.0988 (16)
C15—C31	1.524 (2)	C13—H12	1.0679 (19)
C16—C17	1.427 (2)	C41—H7	1.0811 (19)
C18—C19	1.423 (2)		
Cu1—O1—C37	131.95 (12)	C14—C15—C31	117.03 (11)
Cu1—O2—C39	132.51 (10)	C16—C15—C31	124.89 (12)
Cu1—N2—C11	113.87 (15)	C15—C16—C17	122.42 (12)
Cu1—N2—C1	125.88 (10)	C12—C17—C16	119.96 (11)
Cu1—N1—C10	113.68 (14)	C10—C18—C19	121.46 (13)
Cu1—N1—C41	124.43 (13)	C10—C18—C20	119.30 (9)
O1—Cu1—O2	106.90 (15)	C19—C18—C20	119.24 (11)
O1—Cu1—O3	88.90 (14)	C18—C19—C21	121.16 (13)
O1—Cu1—O7	75.71 (13)	C18—C20—C23	119.94 (9)
O2—Cu1—O3	74.21 (11)	C19—C21—C22	119.15 (9)
O2—Cu1—O7	89.83 (15)	C21—C22—C23	120.11 (11)
O3—Cu1—O7	153.73 (4)	C21—C22—C24	116.92 (9)
O1—Cu1—N1	163.24 (4)	C23—C22—C24	122.97 (13)
O1—Cu1—N2	87.62 (14)	C20—C23—C22	120.40 (13)
O2—Cu1—N1	88.47 (15)	C26—C25—C30	121.01 (13)
O2—Cu1—N2	164.07 (3)	C25—C26—C27	118.03 (12)
O3—Cu1—N1	102.00 (14)	C26—C27—C28	120.82 (12)
O3—Cu1—N2	100.14 (12)	Cu1—O3—H14	94.26 (15)
O7—Cu1—N1	98.20 (14)	Cu1—O3—H15	90.40 (11)
O7—Cu1—N2	100.34 (14)	Cu1—O7—H9	88.62 (14)
O4—C31—O6	120.98 (6)	Cu1—O7—H19	93.21 (15)
O5—C24—O8	122.78 (10)	N1—C10—H6	109.11 (13)
O6—C31—C15	111.80 (12)	N2—C1—H8	118.97 (10)
O4—C31—C15	127.22 (11)	N2—C11—H5	106.88 (14)
O5—C24—C22	111.91 (10)	N1—C41—H7	117.12 (13)
O2—C39—C5	119.44 (12)	C24—O5—H20	104.55 (10)
O8—C24—C22	125.31 (12)	C31—O4—H34	120.22 (12)

O2—C39—C40	121.65 (12)	C3—C2—H10	119.13 (13)
O1—C37—C38	123.72 (11)	C40—C2—H10	118.15 (12)
O1—C37—C9	118.25 (14)	C3—C4—H29	119.67 (13)
N1—Cu1—N2	78.03 (14)	C5—C4—H29	121.54 (11)
N4—N5—C25	114.95 (12)	C4—C5—H18	119.41 (12)
N3—N6—C42	113.73 (15)	C39—C5—H18	118.29 (13)
N6—N3—C7	114.08 (15)	C7—C6—H24	118.33 (12)
N5—N4—C3	115.31 (12)	C25—C26—H28	120.16 (13)
N6—C42—C36	114.46 (15)	C27—C26—H28	121.81 (11)
N3—C7—C8	125.60 (11)	C23—C20—H22	120.00 (13)
N2—C1—C38	125.96 (13)	C26—C27—H1	118.02 (12)
N1—C41—C40	127.46 (11)	C28—C27—H1	121.15 (13)
N5—C25—C30	115.66 (12)	C15—C16—H31	118.35 (7)
N1—C10—C11	108.93 (14)	C27—C28—H3	120.32 (12)
N1—C10—C18	114.48 (15)	C29—C28—H3	118.43 (12)
N4—C3—C2	116.45 (12)	C19—C21—H32	121.58 (13)
N4—C3—C4	123.59 (12)	C22—C21—H32	119.27 (11)
N6—C42—C32	125.35 (11)	C30—C29—H17	120.27 (12)
N5—C25—C26	123.33 (12)	C12—C17—H13	118.00 (7)
N2—C11—C10	108.37 (15)	C25—C30—H23	119.49 (13)
N2—C11—C12	114.88 (15)	C29—C30—H23	119.82 (12)
N3—C7—C6	115.27 (15)	C10—C11—H5	103.75 (16)
C10—N1—C41	121.03 (12)	C18—C10—H6	109.39 (14)
C1—N2—C11	119.37 (14)	C16—C17—H13	122.04 (12)
C27—C28—C29	121.25 (13)	C33—C32—H21	120.55 (14)
C28—C29—C30	118.20 (12)	C42—C32—H21	119.30 (12)
C35—C36—C42	119.39 (14)	C18—C19—H30	120.47 (11)
C14—C15—C16	118.08 (7)	C32—C33—H2	120.14 (11)
C25—C30—C29	120.68 (12)	C34—C33—H2	120.35 (12)
C33—C32—C42	120.16 (11)	C21—C19—H30	118.37 (10)
C32—C33—C34	119.52 (14)	C33—C34—H4	119.02 (14)
C33—C34—C35	120.43 (12)	C35—C34—H4	120.55 (11)
C34—C35—C36	120.33 (11)	C20—C23—H27	119.23 (9)
C9—C37—C38	118.04 (12)	C34—C35—H16	120.72 (12)
C3—C2—C40	122.71 (11)	C36—C35—H16	118.96 (14)
C1—C38—C6	116.04 (14)	C35—C36—H33	121.90 (11)
C1—C38—C37	124.51 (11)	C42—C36—H33	118.71 (12)
C2—C3—C4	119.96 (13)	C11—C10—H6	103.68 (16)
C3—C4—C5	118.79 (12)	C22—C23—H27	120.38 (11)
C6—C38—C37	119.44 (11)	C15—C14—H26	117.23 (7)
C5—C39—C40	118.91 (13)	C13—C14—H26	123.59 (12)
C4—C5—C39	122.30 (11)	C14—C13—H12	118.36 (11)
C2—C40—C39	117.32 (13)	C37—C9—H11	117.42 (12)
C2—C40—C41	117.56 (12)	C8—C9—H11	121.50 (11)
C7—C6—C38	121.42 (14)	C12—C13—H12	118.45 (7)
C39—C40—C41	125.12 (12)	C12—C11—H5	111.25 (14)

C6—C7—C8	119.12 (12)	C17—C16—H31	119.22 (11)
C7—C8—C9	120.90 (11)	C18—C20—H22	120.05 (11)
C8—C9—C37	121.08 (14)	C9—C8—H25	120.27 (14)
C11—C10—C18	110.68 (15)	C38—C1—H8	115.07 (13)
C10—C11—C12	111.04 (14)	C40—C41—H7	115.42 (13)
C11—C12—C13	123.44 (12)	C7—C8—H25	118.83 (12)
C11—C12—C17	119.38 (11)	C38—C6—H24	120.25 (11)
C13—C12—C17	117.18 (7)	C28—C29—H17	121.52 (13)
C12—C13—C14	123.18 (12)	H9—O7—H19	102.82 (14)
C13—C14—C15	119.17 (11)	H14—O3—H15	103.24 (14)
C32—C42—C36	120.19 (12)		