Fig. S1. Structure of second cluster with numbering scheme.

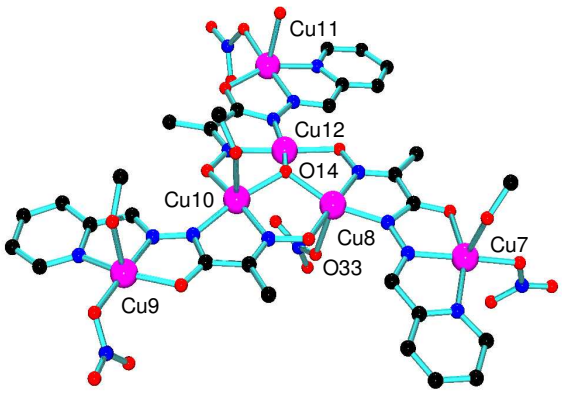

Table S1. Bond lengths (Å) and angles (◦) for **1**.

Cu1	N2	1.928(6)
Cu1	O15	1.954(6)
Cu1	N1	1.999(9)
Cu1	O1	2.003(6)
Cu1	O42	2.240(8)
Cu2	O6	1.937(6)
Cu2	O13	1.966(5)
Cu2	N3	1.973(6)
Cu2	N4	1.973(7)
Cu2	O43	2.317(8)
Cu3	N6	1.917(6)
Cu3	O18	1.963(6)
Cu3	N5	2.006(6)
Cu3	O3	2.008(5)
Cu3	O44	2.217(7)
Cu4	O2	1.932(5)
Cu4	O13	1.964(6)
Cu4	N7	1.983(6)
Cu4	N8	1.998(6)
Cu4	O21	2.365(6)
Cu5	N10	1.946(6)
Cu5	O24	1.956(5)
Cu5	O5	1.992(5)
Cu5	N9	2.025(6)
Cu5	O27	2.265(6)
Cu6	O4	1.928(5)
Cu6	O13	1.969(5)
Cu6	N12	1.974(6)
Cu6	N11	1.982(6)
Cu6	O22	2.375(7)
Cu7	O30	1.938(7)
Cu7	N14	1.943(7)
Cu7	O7	2.014(5)
Cu7	N13	2.033(7)
Cu7	O45	2.190(8)
Cu8	O14	1.951(6)
Cu8	O10	1.953(5)
Cu8	N15	1.954(7)
Cu8	N16	1.965(6)
Cu8	O33	2.331(6)
Cu9	N18	1.941(6)
Cu9	O36	1.969(7)
Cu9	O9	1.978(7)
Cu9	N17	1.986(8)
Cu9	O46	2.181(6)
Cu10	O12	1.909(7)
Cu10	O14	1.949(5)
Cu10	N19	1.992(6)
Cu10	N20	1.998(7)
Cu10	O47	2.381(9)
Cu11	O39	1.940(5)
Cu11	N22	1.946(6)
Cu11	N21	2.019(6)
Cu11	O11	2.030(5)
Cu11	O48	2.264(7)
Cu12	O8	1.925(5)
Cu12	N24	1.960(6)
Cu12	O14	1.963(6)
Cu12	N23	1.985(6)

N2	Cu1	O15	176.3(3)
N2	Cu1	N1	80.6(3)
O15	Cu1	N1	97.8(3)
N2	Cu1	O1	79.7(3)
O15	Cu1	O1	102.2(3)
N1	Cu1	O1	159.2(2)
N2	Cu1	O42	92.6(3)
O15	Cu1	O42	83.8(4)
N1	Cu1	O42	85.8(3)
O1	Cu1	O42	101.8(3)
O6	Cu2	O13	95.2(2)
O6	Cu2	N3	98.0(2)
O13	Cu2	N3	166.6(3)
O6	Cu2	N4	168.3(3)
O13	Cu2	N4	88.3(2)
N3	Cu2	N4	79.3(3)
O6	Cu2	O43	86.8(3)
O13	Cu2	O43	88.2(3)
N3	Cu2	O43	90.1(3)
N4	Cu2	O43	104.5(3)
N6	Cu3	O18	173.0(3)
N6	Cu3	N5	80.7(3)
O18	Cu3	N5	100.5(3)
N6	Cu3	O3	79.4(2)
O18	Cu3	O3	98.0(2)
N5	Cu3	O3	157.8(2)
N6	Cu3	O44	93.5(3)
O18	Cu3	O44	93.3(3)
N5	Cu3	O44	97.1(3)
O3	Cu3	O44	93.9(3)
O2	Cu4	O13	93.0(2)
O2	Cu4	N7	99.0(2)
O13	Cu4	N7	164.3(2)
O2	Cu4	N8	177.3(2)

O13	Cu4	N8	88.7(2)
N7	Cu4	N8	78.9(2)
O2	Cu4	O21	86.0(2)
O13	Cu4	O21	89.6(2)
N7	Cu4	O21	101.1(2)
N8	Cu4	O21	96.2(2)
N10	Cu5	O24	177.9(2)
N10	Cu5	O5	79.5(2)
O24	Cu5	O5	98.4(2)
N10	Cu5	N9	79.8(2)
O24	Cu5	N9	102.3(2)
O5	Cu5	N9	155.2(2)
N10	Cu5	O27	93.9(3)
O24	Cu5	O27	86.1(2)
O5	Cu5	O27	104.4(2)
N9	Cu5	O27	90.6(2)
O4	Cu6	O13	93.0(2)
O4	Cu6	N12	176.7(2)
O13	Cu6	N12	89.4(3)
O4	Cu6	N11	97.3(2)
O13	Cu6	N11	158.3(2)
N12	Cu6	N11	79.7(3)
O4	Cu6	O22	93.4(3)
O13	Cu6	O22	92.0(3)
N12	Cu6	O22	88.8(3)
N11	Cu6	O22	106.4(3)
O30	Cu7	N14	172.3(3)
O30	Cu7	O7	96.4(2)
N14	Cu7	O7	79.3(2)
O30	Cu7	N13	103.1(3)
N14	Cu7	N13	79.9(3)
O7	Cu7	N13	157.1(2)
O30	Cu7	O45	88.4(4)
N14	Cu7	O45	98.5(3)
O7	Cu7	O45	98.8(3)
N13	Cu7	O45	93.7(3)
O14	Cu8	O10	92.6(2)
O14	Cu8	N15	162.8(2)
O10	Cu8	N15	98.4(2)
O14	Cu8	N16	89.2(2)
O10	Cu8	N16	177.6(3)
N15	Cu8	N16	79.5(3)
O14	Cu8	O33	95.1(2)
O10	Cu8	O33	90.5(3)
N15	Cu8	O33	98.1(3)
N16	Cu8	O33	90.9(3)
N18	Cu9	O36	178.5(4)
N18	Cu9	O9	79.7(3)
O36	Cu9	O9	99.4(3)
N18	Cu9	N17	80.6(3)
O36	Cu9	N17	100.1(3)
O9	Cu9	N17	158.6(2)
N18	Cu9	O46	95.4(3)
O36	Cu9	O46	85.9(3)
O9	Cu9	O46	96.2(3)
N17	Cu9	O46	93.9(3)
O12	Cu10	O14	94.2(2)
O12	Cu10	N19	98.2(3)
O14	Cu10	N19	167.6(3)
O12	Cu10	N20	170.4(3)
O14	Cu10	N20	87.8(2)
N19	Cu10	N20	80.0(3)
O12	Cu10	O47	103.7(3)
O14	Cu10	O47	85.0(3)
N19	Cu10	O47	91.8(3)
N20	Cu10	O47	85.8(3)
O39	Cu11	N22	177.2(2)
O39	Cu11	N21	99.8(2)
N22	Cu11	N21	79.9(2)
O39	Cu11	O11	102.2(2)
N22	Cu11	O11	78.7(2)
N21	Cu11	O11	155.8(2)
O39	Cu11	O48	84.6(3)
N22	Cu11	O48	92.7(3)
N21	Cu11	O48	94.2(4)
O11	Cu11	O48	97.9(4)
O8	Cu12	N24	177.4(2)
O8	Cu12	O14	93.4(2)
N24	Cu12	O14	89.0(3)
O8	Cu12	N23	97.3(2)
N24	Cu12	N23	80.2(3)
O14	Cu12	N23	163.9(2)