Supporting information

Table S1 Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	y	z	$U_{iso}{}^*/U_{eq}$
Cu1	0.0000	0.549374 (13)	0.2500	0.0239
O2	-0.33143 (13)	0.55168 (6)	0.28700 (8)	0.0342
S3	-0.5000	0.61063 (3)	0.2500	0.0234
O4	-0.45010 (12)	0.67416 (6)	0.17315 (7)	0.0306
O5	0.09159 (12)	0.64655 (6)	0.34787 (6)	0.0279
N6	-0.07697 (15)	0.43982 (7)	0.15978 (8)	0.0255
C7	-0.04169 (15)	0.35214 (8)	0.20117 (9)	0.0241
C8	-0.08399 (18)	0.26451 (10)	0.15311 (11)	0.0331
C9	-0.1675 (2)	0.27090 (12)	0.05694 (12)	0.0434
C10	-0.2044 (2)	0.35913 (13)	0.01553 (11)	0.0455
C11	-0.1572 (2)	0.44304 (10)	0.06912 (10)	0.0354
C12	-0.0404 (2)	0.17606 (9)	0.20395 (13)	0.0418
H91	-0.1984	0.2135	0.0221	0.0504*
H101	-0.2607	0.3659	-0.0495	0.0527*
H111	-0.1832	0.5059	0.0418	0.0417*
H121	-0.0711	0.1161	0.1705	0.0492*
H52	0.2090	0.6593	0.3445	0.0425*
H53	0.0351	0.6995	0.3427	0.0414*
O2	-0.66857 (13)	0.55168 (6)	0.21300 (8)	0.0342
O4	-0.54990 (12)	0.67416 (6)	0.32685 (7)	0.0306
N6	0.07697 (15)	0.43982 (7)	0.34022 (8)	0.0255
C7	0.04169 (15)	0.35214 (8)	0.29883 (9)	0.0241
C8	0.08399 (18)	0.26451 (10)	0.34689 (11)	0.0311
C9	0.1675 (2)	0.27090 (12)	0.44306 (12)	0.0434
C10	0.2044 (2)	0.35913 (13)	0.48447 (11)	0.0455
C11	0.1577 (2)	0.44304 (10)	0.43088 (10)	0.0354
C12	0.0404 (2)	0.17606 (9)	0.29605 (13)	0.0418
H91	0.1984	0.2135	0.4779	0.0504*
H101	0.2607	0.3659	0.5495	0.0527*
H111	0.1832	0.5059	0.4582	0.0417*
H121	0.0711	0.1161	0.3295	0.0492*

O5	-0.09159 (12)	0.64655 (6)	0.15213 (6)	0.0279
H52	-0.2090	0.6593	0.1553	0.0451*
H53	-0.0351	0.6995	0.1573	0.0414*
Cu1	-1.0000	0.549374 (13)	0.2500	0.0239
O2	0.33143 (13)	0.55168 (6)	0.21300 (8)	0.0342

Table S2 Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0239	0.0168	0.0239	0.0000	-0.0004	0.0000
O2	0.0268	0.0288	0.0464	0.0065	0.0042	0.0108
S3	0.0194	0.0178	0.0323	0.0000	0.0020	0.0000
O4	0.0279	0.0267	0.0372	0.0039	0.0052	0.0064
O5	0.0263	0.0218	0.0353	-0.0003	0.0045	-0.0052
N6	0.0261	0.0248	0.0248	-0.0015	0.0014	-0.0007
C7	0.0209	0.0217	0.0306	-0.0010	0.0066	-0.0027
C8	0.0293	0.0278	0.0445	-0.0056	0.0128	-0.0107
C9	0.0424	0.0444	0.0439	-0.0098	0.0084	-0.0218
C10	0.0446	0.0604	0.0294	-0.0079	-0.0006	-0.0130
C11	0.0375	0.0405	0.0261	-0.0014	-0.0012	-0.0010
C12	0.0425	0.0218	0.0662	-0.0046	0.0239	-0.0097
O2	0.0268	0.0288	0.0464	-0.0065	0.0042	-0.0108
O4	0.0279	0.0267	0.0372	-0.0039	0.0052	-0.0064
N6	0.0261	0.0248	0.0248	0.0015	0.0014	0.0007
C7	0.0209	0.0217	0.0306	0.0010	0.0066	0.0027
C8	0.0293	0.0278	0.0445	0.0056	0.0128	0.0107
C9	0.0424	0.0444	0.0439	0.0098	0.0084	0.0218
C10	0.0446	0.0604	0.0294	0.0079	-0.0006	0.0130
C11	0.0375	0.0405	0.0261	0.0014	-0.0012	0.0010
C12	0.0425	0.0218	0.0662	0.0046	0.0239	0.0097
O5	0.0263	0.0218	0.0353	0.0003	0.0045	0.0052
Cu1	0.0239	0.0168	0.0239	0.0000	-0.0004	0.0000
O2	0.0268	0.0288	0.0464	-0.0065	0.0042	-0.0108

Table S3 Geometric parameters (Å, º)

Cu1-O2	2.464	C7-C8	1.400 (2)
Cu1-O5	1.9702	C8-C9	1.407 (2)
Cu1-N6	2.005	C8-C12	1.430 (2)
O2-S3	1.4620	C9-C10	1.362 (2)
S3-O4	1.491	C9-H91	0.943
O5-H52	0.8504	C10-C11	1.400 (2)
O5-H53	0.8296	C10-H101	0.954
N6-C7	1.354 (2)	C11-H111	0.958
N6-C11	1.327 (2)	C12-H121	0.963
O2-Cu1-O5	92.83	O2-Cu1-N6	89.00
O2-Cu1-N6	92.12	O2-Cu1-O5	86.16
O2-Cu1-O2	178.52	O5-Cu1-N6	173.76
O5-Cu1-N6	92.02	O5-Cu1-O5	94.06
O5-Cu1-O2	86.16	N6-Cu1-N6	81.94
N6-Cu1-O5	92.02	Cu1-O2-S3	131.63
O2-S3-O4	108.82	O2-S3-O2	112.27
O2-S3-O4	109.49	O4-S3-O4	107.85
Cu1-O5-H52	107.97	Cu1-O5-H53	116.22
H52-O5-H53	105.33	Cu1-N6-C7	112.57
Cu1-N6-C11	129.05	C7-N6-C11	118.4 (1)
N6-C7-C8	123.4 (1)	N6-C7-C7	116.5 (1)
C8-C7-C7	120.1 (1)	C7-C8-C9	116.5 (1)
C7-C8-C12	118.6 (1)	C9-C8-C12	124.8 (1)
C8-C9-C10	120.0 (1)	C8-C9-H91	119.1
C10-C9-H91	120.8	C9-C10-C11	119.5 (1)
C9-C10-H101	122.1	C11-C10-H101	118.4
N6-C11-C10	122.1 (1)	N6-C11-H111	116.8
C10-C11-H111	121.1	C8-C12-H121	118.1
C8-C12-C12	121.2 (1)	H121-C12-C12	120.7
Cu1-N6-C7	112.57		
O5-Cu1-O2-S3	89.68	N6-Cu1-O2-S3	-96.29
N6-Cu1-O2-S3	-178.19	O5-Cu1-O2-S3	-4.20
O2-Cu1-O2-S3	43.00	O2-Cu1-O5-H52	-176.60

O2-Cu1-O5-H52	2.32	O2-Cu1-O5-H53	-58.59
O2-Cu1-O5-H53	120.32	N6-Cu1-O5-H52	76.5
N6-Cu1-O5-H52	91.18	N6-Cu1-O5-H53	-165.5
N6-Cu1-O5-H53	-150.81	O5-Cu1-O5-H52	-90.25
O5-Cu1-O5-H53	27.75	O2-Cu1-N6-C7	-92.27
O2-Cu1-N6-C11	88.6	O2-Cu1-N6-C11	-92.4
O5-Cu1-N6-C7	14.9	O5-Cu1-N6-C7	-178.39
O5-Cu1-N6-C11	-166.2	O5-Cu1-N6-C11	0.5
N6-Cu1-N6-C7	0.01	N6-Cu1-N6-C11	178.9
O5-Cu1-N6-C7	-178.39	O5-Cu1-N6-C11	0.5
O2-Cu1-N6-C7	88.70	O2-Cu1-N6-C7	-92.27
Cu1-O2-S3-O4	3.78	Cu1-O2-S3-O4	-113.88
Cu1-O2-S3-O2	125.14	Cu1-N6-C7-C8	179.6
Cu1-N6-C7-C7	-0.0	Cu1-N6-C7-C7	-179.1 (1)
C11-N6-C7-C8	0.5 (2)	Cu1-N6-C11-C10	-179.4
Cu1-N6-C11-H111	-0.1	C7-C11-N6-C7	-0.5 (2)
C7-N6-C11-H111	178.7	N6-C7-C8-C9	-0.0 (2)
N6-C7-C8-C12	180.0 (1)	C7-C7-C8-C9	179.5 (1)
C7-C7-C8-C12	-0.5 (2)	N6-C7-C7-N6	0.0 (2)
N6-C7-C7-C8	-179.6 (1)	C8-C7-C7-C8	0.8 (2)
C7-C8-C9-C10	-0.5 (2)	C7-C8-C9-H91	-179.9
C12-C8-C9-C10	179.5 (1)	C12-C8-C9-H91	0.1
C7-C8-C12-H121	179.4	C7-C8-C12-C12	-0.3 (2)
C9-C8-C12-H121	-0.6	C9-C8-C12-C12	179.7 (1)
C8-C9-C10-C11	0.5 (2)	C8-C9-C10-H101	179.9
H91-C9-C10-C11	179.9	H91-C9-C10-H101	-0.7
C9-C10-C11-N6	-0.0 (2)	C9-C10-C11-H111	-179.2
H101-C10-C11-N6	-179.4	H101-C10-C11-H111	1.4
C8-C12-C12-C8	0.6 (2)	C8-C12-C12-H121	-179.0
H121-C12-C12-H121	1.3		