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Structure and photophysical and electrochemical properties of a copper porphyrin complex with a three-dimensional framework

Dedicated to Professor Jin-Shun Huang on the occasion of his 80th birthday.

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Table S1 Bond lengths (Å) and angles (°).

Cu(1)-N(4)	1.992(6)
Cu(1)-N(1)	1.994(6)
Cu(1)-N(3)	1.997(6)
Cu(1)-N(2)	2.003(6)
Cu(2)-N(7)	1.991(7)
Cu(2)-N(8)#1	2.017(6)
Cu(2)-Cl(1)	2.182(3)
Cu(3)-N(5)	1.988(6)
Cu(3)-N(6)#2	2.005(6)
Cu(3)-Cl(1)#3	2.247(3)
Cu(3)-Cu(3)#4	2.593(3)
Cu(4)-Cu(4B)	0.983(5)
Cu(4)-Cl(3)	2.048(14)
Cu(4)-O(1W)	2.074(15)
Cu(4)-Cl(2)	2.418(7)
Cu(4B)-Cl(2)	1.773(7)
Cu(4B)-O(1W)	2.088(14)
Cl(1)-Cu(3)#5	2.247(3)
N(1)-C(5)	1.389(9)
N(1)-C(2)	1.391(9)
N(2)-C(10)	1.373(9)
N(2)-C(7)	1.383(9)
N(3)-C(12)	1.379(10)
N(3)-C(15)	1.380(9)
N(4)-C(20)	1.382(9)
N(4)-C(17)	1.387(9)
N(5)-C(25)	1.330(11)
N(5)-C(21)	1.331(11)
N(6)-C(26)	1.326(10)
N(6)-C(30)	1.334(10)
N(6)-Cu(3)#6	2.005(6)
N(7)-C(35)	1.328(10)
N(7)-C(31)	1.333(11)
N(8)-C(40)	1.325(10)
N(8)-C(36)	1.341(10)
N(8)-Cu(2)#7	2.017(6)
C(1)-C(20)	1.382(10)
C(1)-C(2)	1.383(10)
C(1)-C(23)	1.498(11)
C(2)-C(3)	1.421(10)
C(3)-C(4)	1.347(11)
C(3)-H(3A)	0.9300
C(4)-C(5)	1.431(11)
C(4)-H(4A)	0.9300
C(5)-C(6)	1.400(10)
C(6)-C(7)	1.390(11)
C(6)-C(28)	1.492(9)
C(7)-C(8)	1.427(11)
C(8)-C(9)	1.329(11)
C(8)-H(8A)	0.9300
C(9)-C(10)	1.431(10)
C(9)-H(9A)	0.9300
C(10)-C(11)	1.391(10)
C(11)-C(12)	1.395(10)
C(11)-C(33)	1.482(11)

C(12)-C(13)	1.435(10)
C(13)-C(14)	1.350(11)
C(13)-H(13A)	0.9300
C(14)-C(15)	1.449(10)
C(14)-H(14A)	0.9300
C(15)-C(16)	1.392(10)
C(16)-C(17)	1.392(11)
C(16)-C(38)	1.480(10)
C(17)-C(18)	1.440(11)
C(18)-C(19)	1.346(11)
C(18)-H(18A)	0.9300
C(19)-C(20)	1.441(10)
C(19)-H(19A)	0.9300
C(21)-C(22)	1.358(12)
C(21)-H(21A)	0.9300
C(22)-C(23)	1.388(11)
C(22)-H(22A)	0.9300
C(23)-C(24)	1.397(11)
C(24)-C(25)	1.368(12)
C(24)-H(24A)	0.9300
C(25)-H(25A)	0.9300
C(26)-C(27)	1.394(10)
C(26)-H(26A)	0.9300
C(27)-C(28)	1.387(10)
C(27)-H(27A)	0.9300
C(28)-C(29)	1.399(11)
C(29)-C(30)	1.370(11)
C(29)-H(29A)	0.9300
C(30)-H(30A)	0.9300
C(31)-C(32)	1.367(11)
C(31)-H(31A)	0.9300
C(32)-C(33)	1.382(10)
C(32)-H(32A)	0.9300
C(33)-C(34)	1.408(12)
C(34)-C(35)	1.374(12)
C(34)-H(34A)	0.9300
C(35)-H(35A)	0.9300
C(36)-C(37)	1.383(10)
C(36)-H(36A)	0.9300
C(37)-C(38)	1.399(11)
C(37)-H(37A)	0.9300
C(38)-C(39)	1.404(11)
C(39)-C(40)	1.375(11)
C(39)-H(39A)	0.9300
C(40)-H(40A)	0.9300
N(4)-Cu(1)-N(1)	90.3(2)
N(4)-Cu(1)-N(3)	89.9(2)
N(1)-Cu(1)-N(3)	175.7(2)
N(4)-Cu(1)-N(2)	175.6(2)
N(1)-Cu(1)-N(2)	89.8(2)
N(3)-Cu(1)-N(2)	90.4(2)
N(7)-Cu(2)-N(8)#1	115.9(3)
N(7)-Cu(2)-Cl(1)	127.0(2)
N(8)#1-Cu(2)-Cl(1)	116.9(2)
N(5)-Cu(3)-N(6)#2	120.4(3)
N(5)-Cu(3)-Cl(1)#3	109.3(2)
N(6)#2-Cu(3)-Cl(1)#3	111.5(2)
N(5)-Cu(3)-Cu(3)#4	119.5(2)
N(6)#2-Cu(3)-Cu(3)#4	70.0(2)

Cl(1)#3-Cu(3)-Cu(3)#4	121.31(11)
Cu(4B)-Cu(4)-Cl(3)	145.3(6)
Cu(4B)-Cu(4)-O(1W)	77.2(6)
Cl(3)-Cu(4)-O(1W)	68.2(5)
Cu(4B)-Cu(4)-Cl(2)	39.5(4)
Cl(3)-Cu(4)-Cl(2)	174.3(4)
O(1W)-Cu(4)-Cl(2)	116.6(5)
Cu(4)-Cu(4B)-Cl(2)	119.8(5)
Cu(4)-Cu(4B)-O(1W)	75.5(7)
Cl(2)-Cu(4B)-O(1W)	164.5(6)
Cu(2)-Cl(1)-Cu(3)#5	124.26(14)
Cu(4B)-Cl(2)-Cu(4)	20.65(16)
C(5)-N(1)-C(2)	104.9(6)
C(5)-N(1)-Cu(1)	127.5(5)
C(2)-N(1)-Cu(1)	127.1(5)
C(10)-N(2)-C(7)	105.8(6)
C(10)-N(2)-Cu(1)	126.6(5)
C(7)-N(2)-Cu(1)	127.4(5)
C(12)-N(3)-C(15)	106.2(6)
C(12)-N(3)-Cu(1)	126.9(5)
C(15)-N(3)-Cu(1)	126.6(5)
C(20)-N(4)-C(17)	106.1(6)
C(20)-N(4)-Cu(1)	126.4(5)
C(17)-N(4)-Cu(1)	127.0(5)
C(25)-N(5)-C(21)	117.3(7)
C(25)-N(5)-Cu(3)	120.8(6)
C(21)-N(5)-Cu(3)	120.1(6)
C(26)-N(6)-C(30)	118.2(7)
C(26)-N(6)-Cu(3)#6	119.0(5)
C(30)-N(6)-Cu(3)#6	120.7(5)
C(35)-N(7)-C(31)	117.3(7)
C(35)-N(7)-Cu(2)	123.2(6)
C(31)-N(7)-Cu(2)	119.2(6)
C(40)-N(8)-C(36)	116.7(6)
C(40)-N(8)-Cu(2)#7	125.2(5)
C(36)-N(8)-Cu(2)#7	118.1(5)
C(20)-C(1)-C(2)	125.4(7)
C(20)-C(1)-C(23)	117.3(6)
C(2)-C(1)-C(23)	117.2(7)
C(1)-C(2)-N(1)	123.7(7)
C(1)-C(2)-C(3)	125.8(7)
N(1)-C(2)-C(3)	110.3(6)
C(4)-C(3)-C(2)	107.4(7)
C(4)-C(3)-H(3A)	126.3
C(2)-C(3)-H(3A)	126.3
C(3)-C(4)-C(5)	107.5(7)
C(3)-C(4)-H(4A)	126.2
C(5)-C(4)-H(4A)	126.2
N(1)-C(5)-C(6)	124.4(7)
N(1)-C(5)-C(4)	109.8(7)
C(6)-C(5)-C(4)	125.7(7)
C(7)-C(6)-C(5)	124.5(7)
C(7)-C(6)-C(28)	117.2(7)
C(5)-C(6)-C(28)	118.1(7)
N(2)-C(7)-C(6)	124.8(7)
N(2)-C(7)-C(8)	109.2(7)
C(6)-C(7)-C(8)	125.8(7)
C(9)-C(8)-C(7)	107.9(7)
C(9)-C(8)-H(8A)	126.1
C(7)-C(8)-H(8A)	126.1

C(8)-C(9)-C(10)	107.5(7)
C(8)-C(9)-H(9A)	126.2
C(10)-C(9)-H(9A)	126.2
N(2)-C(10)-C(11)	125.5(6)
N(2)-C(10)-C(9)	109.5(6)
C(11)-C(10)-C(9)	124.9(7)
C(10)-C(11)-C(12)	124.5(7)
C(10)-C(11)-C(33)	116.7(6)
C(12)-C(11)-C(33)	118.8(6)
N(3)-C(12)-C(11)	125.0(7)
N(3)-C(12)-C(13)	109.8(6)
C(11)-C(12)-C(13)	125.2(7)
C(14)-C(13)-C(12)	107.4(7)
C(14)-C(13)-H(13A)	126.3
C(12)-C(13)-H(13A)	126.3
C(13)-C(14)-C(15)	107.2(7)
C(13)-C(14)-H(14A)	126.4
C(15)-C(14)-H(14A)	126.4
N(3)-C(15)-C(16)	126.1(7)
N(3)-C(15)-C(14)	109.2(6)
C(16)-C(15)-C(14)	124.7(7)
C(17)-C(16)-C(15)	123.0(7)
C(17)-C(16)-C(38)	118.4(7)
C(15)-C(16)-C(38)	118.7(7)
N(4)-C(17)-C(16)	125.4(7)
N(4)-C(17)-C(18)	108.7(7)
C(16)-C(17)-C(18)	125.9(7)
C(19)-C(18)-C(17)	108.3(7)
C(19)-C(18)-H(18A)	125.8
C(17)-C(18)-H(18A)	125.8
C(18)-C(19)-C(20)	106.8(7)
C(18)-C(19)-H(19A)	126.6
C(20)-C(19)-H(19A)	126.6
C(1)-C(20)-N(4)	125.2(6)
C(1)-C(20)-C(19)	124.9(7)
N(4)-C(20)-C(19)	109.8(6)
N(5)-C(21)-C(22)	122.9(8)
N(5)-C(21)-H(21A)	118.5
C(22)-C(21)-H(21A)	118.5
C(21)-C(22)-C(23)	120.7(8)
C(21)-C(22)-H(22A)	119.6
C(23)-C(22)-H(22A)	119.6
C(22)-C(23)-C(24)	115.9(8)
C(22)-C(23)-C(1)	121.0(7)
C(24)-C(23)-C(1)	123.1(7)
C(25)-C(24)-C(23)	119.5(8)
C(25)-C(24)-H(24A)	120.2
C(23)-C(24)-H(24A)	120.2
N(5)-C(25)-C(24)	123.5(8)
N(5)-C(25)-H(25A)	118.2
C(24)-C(25)-H(25A)	118.2
N(6)-C(26)-C(27)	122.7(7)
N(6)-C(26)-H(26A)	118.7
C(27)-C(26)-H(26A)	118.7
C(28)-C(27)-C(26)	119.4(7)
C(28)-C(27)-H(27A)	120.3
C(26)-C(27)-H(27A)	120.3
C(27)-C(28)-C(29)	116.8(7)
C(27)-C(28)-C(6)	119.5(7)
C(29)-C(28)-C(6)	123.7(7)

C(30)-C(29)-C(28)	119.9(7)
C(30)-C(29)-H(29A)	120.0
C(28)-C(29)-H(29A)	120.0
N(6)-C(30)-C(29)	122.9(8)
N(6)-C(30)-H(30A)	118.6
C(29)-C(30)-H(30A)	118.6
N(7)-C(31)-C(32)	123.1(8)
N(7)-C(31)-H(31A)	118.4
C(32)-C(31)-H(31A)	118.4
C(31)-C(32)-C(33)	120.9(8)
C(31)-C(32)-H(32A)	119.6
C(33)-C(32)-H(32A)	119.6
C(32)-C(33)-C(34)	115.6(8)
C(32)-C(33)-C(11)	122.0(7)
C(34)-C(33)-C(11)	122.3(7)
C(35)-C(34)-C(33)	119.8(8)
C(35)-C(34)-H(34A)	120.1
C(33)-C(34)-H(34A)	120.1
N(7)-C(35)-C(34)	123.3(8)
N(7)-C(35)-H(35A)	118.3
C(34)-C(35)-H(35A)	118.3
N(8)-C(36)-C(37)	122.9(8)
N(8)-C(36)-H(36A)	118.6
C(37)-C(36)-H(36A)	118.6
C(36)-C(37)-C(38)	120.1(8)
C(36)-C(37)-H(37A)	120.0
C(38)-C(37)-H(37A)	120.0
C(37)-C(38)-C(39)	116.6(7)
C(37)-C(38)-C(16)	119.6(7)
C(39)-C(38)-C(16)	123.7(7)
C(40)-C(39)-C(38)	118.5(8)
C(40)-C(39)-H(39A)	120.7
C(38)-C(39)-H(39A)	120.7
N(8)-C(40)-C(39)	125.2(8)
N(8)-C(40)-H(40A)	117.4
C(39)-C(40)-H(40A)	117.4
Cu(4)-O(1W)-Cu(4B)	27.3(2)

Symmetry transformations used to generate equivalent atoms: #1 *x*+1/2, -*y*+3/2, *z*+1/2; #2 *x*-1/2, -*y*+1/2, *z*-1/2; #3 *x*-1, *y*-1, *z*; #4 -*x*+1, -*y*, -*z*+1; #5 *x*+1, *y*+1, *z*; #6 *x*+1/2, -*y*+1/2, *z*+1/2; #7 *x*-1/2, -*y*+3/2, *z*-1/2.

Table S2 Atomic coordinates and equivalent isotropic displacement parameters (Å^2).

atom	x	y	z	U(eq)
Cu(1)	0.76891(10)	0.49705(4)	0.56838(4)	0.0327(3)
Cu(2)	1.12266(14)	0.94928(6)	0.62290(5)	0.0508(3)
Cu(3)	0.40412(17)	0.04857(7)	0.51300(5)	0.0700(4)
Cu(4)	-0.0074(5)	0.2190(2)	0.7403(2)	0.1048(12)
Cu(4B)	0.0510(5)	0.2390(2)	0.7758(2)	0.1048(12)
Cl(1)	1.1677(3)	1.03123(15)	0.56000(13)	0.0763(8)
Cl(2)	-0.0584(5)	0.2674(2)	0.8402(2)	0.1322(17)
Cl(3)	0.0137(12)	0.1815(5)	0.6529(6)	0.335(7)
N(1)	0.7359(7)	0.4246(3)	0.6294(2)	0.0325(14)
N(2)	0.8265(7)	0.5588(3)	0.6379(3)	0.0355(15)
N(3)	0.8190(7)	0.5673(3)	0.5069(3)	0.0355(14)
N(4)	0.6941(7)	0.4378(3)	0.4999(3)	0.0346(14)
N(5)	0.4979(9)	0.1341(3)	0.5416(3)	0.0431(16)
N(6)	0.8867(8)	0.4723(4)	0.9224(3)	0.0445(17)
N(7)	1.0605(9)	0.8572(4)	0.5999(3)	0.0475(17)

N(8)	0.6627(8)	0.5338(3)	0.2140(3)	0.0391(15)
C(1)	0.6404(9)	0.3372(4)	0.5594(3)	0.0370(18)
C(2)	0.6960(9)	0.3592(4)	0.6166(3)	0.0369(18)
C(3)	0.7077(9)	0.3206(4)	0.6715(3)	0.0401(18)
C(4)	0.7516(10)	0.3614(4)	0.7182(3)	0.042(2)
C(5)	0.7676(9)	0.4263(4)	0.6928(3)	0.0356(17)
C(6)	0.7989(9)	0.4841(4)	0.7266(3)	0.0341(17)
C(7)	0.8187(9)	0.5464(4)	0.7007(3)	0.0349(17)
C(8)	0.8495(10)	0.6061(4)	0.7340(4)	0.045(2)
C(9)	0.8787(10)	0.6534(4)	0.6931(3)	0.045(2)
C(10)	0.8677(9)	0.6243(4)	0.6328(3)	0.0342(17)
C(11)	0.9013(9)	0.6568(4)	0.5779(3)	0.0346(17)
C(12)	0.8840(9)	0.6288(4)	0.5192(3)	0.0364(17)
C(13)	0.9284(9)	0.6601(4)	0.4624(4)	0.044(2)
C(14)	0.8863(9)	0.6187(4)	0.4158(3)	0.0413(19)
C(15)	0.8110(9)	0.5614(4)	0.4433(3)	0.0331(16)
C(16)	0.7355(9)	0.5107(4)	0.4100(3)	0.0360(17)
C(17)	0.6743(9)	0.4542(4)	0.4378(3)	0.0351(17)
C(18)	0.5861(9)	0.4019(4)	0.4068(3)	0.043(2)
C(19)	0.5614(10)	0.3532(4)	0.4478(4)	0.043(2)
C(20)	0.6320(9)	0.3748(4)	0.5060(3)	0.0360(17)
C(21)	0.6333(11)	0.1569(5)	0.5171(4)	0.051(2)
C(22)	0.6830(10)	0.2206(4)	0.5234(4)	0.048(2)
C(23)	0.5895(10)	0.2663(4)	0.5544(3)	0.0409(19)
C(24)	0.4509(10)	0.2414(4)	0.5821(4)	0.047(2)
C(25)	0.4103(11)	0.1764(5)	0.5740(4)	0.048(2)
C(26)	0.9740(10)	0.4377(4)	0.8832(3)	0.045(2)
C(27)	0.9462(9)	0.4395(4)	0.8193(3)	0.0391(18)
C(28)	0.8216(9)	0.4784(4)	0.7951(3)	0.0346(17)
C(29)	0.7263(9)	0.5121(4)	0.8376(3)	0.0417(19)
C(30)	0.7627(10)	0.5079(4)	0.8996(4)	0.0423(19)
C(31)	1.1434(10)	0.8069(4)	0.6248(3)	0.044(2)
C(32)	1.0978(9)	0.7424(4)	0.6174(3)	0.0423(19)
C(33)	0.9594(9)	0.7259(4)	0.5834(3)	0.0397(19)
C(34)	0.8755(11)	0.7793(4)	0.5558(4)	0.050(2)
C(35)	0.9303(11)	0.8427(4)	0.5652(4)	0.049(2)
C(36)	0.6198(9)	0.5809(5)	0.2541(3)	0.044(2)
C(37)	0.6422(9)	0.5745(4)	0.3174(3)	0.0393(18)
C(38)	0.7155(9)	0.5177(4)	0.3421(3)	0.0360(17)
C(39)	0.7622(10)	0.4691(4)	0.2997(3)	0.0426(19)
C(40)	0.7306(10)	0.4798(4)	0.2378(3)	0.043(2)
O(1W)	0.2318(19)	0.2180(10)	0.7127(6)	0.207(7)

Table S3 Anisotropic displacement parameters ($Å^2$).

atom	U11	U22	U33	U23	U13	U12
Cu(1)	0.0469(5)	0.0240(6)	0.0271(4)	-0.0003(4)	-0.0038(3)	-0.0040(4)
Cu(2)	0.0735(8)	0.0379(7)	0.0411(6)	-0.0008(5)	0.0008(5)	-0.0070(5)
Cu(3)	0.0962(10)	0.0641(10)	0.0500(7)	-0.0105(6)	0.0053(6)	-0.0271(7)
Cu(4)	0.078(2)	0.090(2)	0.146(4)	0.016(2)	-0.0043(16)	0.0080(15)
Cu(4B)	0.078(2)	0.090(2)	0.146(4)	0.016(2)	-0.0043(16)	0.0080(15)
Cl(1)	0.0710(16)	0.078(2)	0.0802(17)	0.0376(15)	0.0092(13)	-0.0115(14)
Cl(2)	0.141(3)	0.105(3)	0.147(4)	0.059(3)	-0.065(3)	-0.024(2)

Cl(3)	0.278(10)	0.224(9)	0.515(18)	0.117(10)	0.242(12)	0.099(8)
N(1)	0.044(4)	0.027(4)	0.026(3)	0.000(3)	-0.001(2)	-0.006(3)
N(2)	0.045(4)	0.028(4)	0.034(3)	0.001(3)	-0.005(3)	-0.005(3)
N(3)	0.043(4)	0.031(4)	0.032(3)	0.002(3)	-0.003(3)	-0.003(3)
N(4)	0.048(4)	0.028(4)	0.028(3)	0.000(3)	-0.003(3)	-0.007(3)
N(5)	0.063(4)	0.025(4)	0.041(4)	-0.008(3)	-0.006(3)	-0.009(3)
N(6)	0.069(5)	0.034(4)	0.030(3)	0.002(3)	-0.009(3)	0.008(3)
N(7)	0.066(5)	0.038(5)	0.038(4)	0.003(3)	-0.003(3)	-0.004(3)
N(8)	0.052(4)	0.038(4)	0.027(3)	0.002(3)	0.000(3)	0.007(3)
C(1)	0.051(5)	0.026(5)	0.034(4)	-0.003(3)	-0.002(3)	0.000(3)
C(2)	0.042(4)	0.027(5)	0.041(4)	-0.002(3)	-0.001(3)	-0.007(3)
C(3)	0.055(5)	0.031(5)	0.034(4)	0.002(3)	-0.002(3)	-0.002(4)
C(4)	0.058(5)	0.034(5)	0.034(4)	0.009(4)	-0.008(3)	-0.001(4)
C(5)	0.042(4)	0.033(5)	0.031(4)	0.002(3)	-0.004(3)	-0.005(3)
C(6)	0.052(4)	0.026(5)	0.025(3)	-0.003(3)	-0.005(3)	-0.004(3)
C(7)	0.038(4)	0.033(5)	0.034(4)	-0.003(3)	-0.003(3)	-0.003(3)
C(8)	0.068(6)	0.035(5)	0.032(4)	-0.010(4)	-0.002(4)	-0.003(4)
C(9)	0.076(6)	0.022(5)	0.037(4)	0.000(3)	-0.004(4)	-0.005(4)
C(10)	0.048(4)	0.019(4)	0.035(4)	0.000(3)	-0.006(3)	-0.002(3)
C(11)	0.047(4)	0.023(4)	0.034(4)	0.003(3)	-0.006(3)	-0.002(3)
C(12)	0.043(4)	0.033(5)	0.034(4)	0.001(3)	0.000(3)	-0.004(3)
C(13)	0.050(5)	0.042(6)	0.041(4)	0.005(4)	-0.003(3)	-0.011(4)
C(14)	0.055(5)	0.038(5)	0.031(4)	-0.001(3)	0.004(3)	-0.003(4)
C(15)	0.044(4)	0.022(4)	0.033(4)	0.001(3)	-0.002(3)	-0.001(3)
C(16)	0.045(4)	0.030(5)	0.032(4)	0.000(3)	0.000(3)	0.004(3)
C(17)	0.045(4)	0.028(5)	0.032(4)	-0.001(3)	0.000(3)	0.000(3)
C(18)	0.053(5)	0.047(6)	0.027(4)	-0.004(4)	-0.008(3)	-0.006(4)
C(19)	0.054(5)	0.031(5)	0.045(5)	-0.003(4)	-0.008(4)	-0.008(4)
C(20)	0.050(5)	0.028(5)	0.030(4)	-0.009(3)	0.000(3)	-0.004(3)
C(21)	0.068(6)	0.036(6)	0.050(5)	-0.010(4)	0.010(4)	0.000(4)
C(22)	0.056(5)	0.041(6)	0.049(5)	-0.002(4)	0.012(4)	-0.008(4)
C(23)	0.056(5)	0.033(5)	0.033(4)	-0.001(3)	-0.003(3)	-0.007(4)
C(24)	0.064(6)	0.033(5)	0.044(5)	-0.010(4)	0.005(4)	-0.002(4)
C(25)	0.057(5)	0.038(6)	0.049(5)	0.004(4)	0.000(4)	-0.010(4)
C(26)	0.057(5)	0.041(6)	0.035(4)	0.001(4)	-0.005(3)	0.014(4)
C(27)	0.046(4)	0.036(5)	0.035(4)	-0.006(3)	-0.004(3)	0.000(3)
C(28)	0.042(4)	0.029(5)	0.032(4)	0.003(3)	-0.006(3)	-0.005(3)
C(29)	0.048(5)	0.038(5)	0.038(4)	0.000(4)	-0.007(3)	-0.001(4)
C(30)	0.056(5)	0.034(5)	0.037(4)	-0.004(4)	-0.001(3)	0.000(4)
C(31)	0.052(5)	0.040(6)	0.040(4)	-0.001(4)	0.000(3)	-0.010(4)
C(32)	0.050(5)	0.036(5)	0.040(4)	0.002(4)	-0.008(3)	0.000(4)
C(33)	0.055(5)	0.037(5)	0.028(4)	-0.002(3)	0.000(3)	-0.008(4)
C(34)	0.063(6)	0.037(6)	0.049(5)	0.002(4)	-0.014(4)	-0.002(4)
C(35)	0.073(6)	0.025(5)	0.048(5)	0.002(4)	-0.014(4)	0.007(4)
C(36)	0.051(5)	0.045(6)	0.037(4)	0.007(4)	-0.005(3)	0.005(4)
C(37)	0.050(5)	0.033(5)	0.034(4)	-0.003(3)	0.000(3)	0.001(4)
C(38)	0.043(4)	0.035(5)	0.030(4)	0.001(3)	0.002(3)	-0.004(3)
C(39)	0.054(5)	0.033(5)	0.041(4)	0.000(4)	0.000(3)	0.008(4)
C(40)	0.063(5)	0.033(5)	0.034(4)	-0.008(4)	0.003(4)	0.002(4)
O(1W)	0.186(14)	0.31(2)	0.129(11)	-0.001(12)	0.047(9)	0.037(14)

Table S4 Hydrogen coordinates and isotropic displacement parameters ($Å^2$).

	x	y	z	U(eq)
H(3A)	0.6886	0.2754	0.6746	0.048
H(4A)	0.7683	0.3496	0.7594	0.051

H(8A)	0.8492	0.6111	0.7767	0.054
H(9A)	0.9020	0.6974	0.7020	0.054
H(13A)	0.9773	0.7012	0.4585	0.053
H(14A)	0.9026	0.6256	0.3739	0.050
H(18A)	0.5521	0.4019	0.3655	0.051
H(19A)	0.5089	0.3133	0.4401	0.052
H(21A)	0.6967	0.1280	0.4946	0.061
H(22A)	0.7809	0.2337	0.5067	0.058
H(24A)	0.3868	0.2688	0.6059	0.056
H(25A)	0.3163	0.1609	0.5921	0.058
H(26A)	1.0571	0.4110	0.8989	0.053
H(27A)	1.0108	0.4149	0.7932	0.047
H(29A)	0.6384	0.5372	0.8237	0.050
H(30A)	0.6982	0.5308	0.9271	0.051
H(31A)	1.2367	0.8160	0.6483	0.053
H(32A)	1.1607	0.7091	0.6355	0.051
H(34A)	0.7833	0.7716	0.5312	0.060
H(35A)	0.8733	0.8772	0.5463	0.059
H(36A)	0.5729	0.6195	0.2386	0.053
H(37A)	0.6086	0.6081	0.3435	0.047
H(39A)	0.8133	0.4306	0.3132	0.051
H(40A)	0.7592	0.4466	0.2104	0.052