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Supplementary Material

E. Müller, G. Bernardinelli & J. Reedijk

$[Cu^{I}(C_{28}H_{22}N_{8})](ClO_4)(CH_3CN)$, TriClinic, $P\ \bar{1}$

a = 11.6178(9) , b = 14.9054(12) , c = 19.390(3) Å; α = 67.793(8) , β = 81.557(8) , γ = 78.356(6) °.

Non-Hydrogen Positional, Isotropic Displacement and Occupation Parameters

	x/a	y/b	z/c	U_{eq}	PP (if ≠ 1)
Cu(1)	0.7609(1)	0.42430(9)	0.17032(8)	0.0661(7)	
N(1)	0.9099(8)	0.4973(7)	0.1476(5)	0.061(5)	
N(2)	0.8697(8)	0.3423(7)	0.1200(5)	0.059(5)	
N(3)	1.0476(8)	0.3226(8)	0.0617(5)	0.078(6)	
N(4)	0.983(1)	0.2518(7)	0.0649(5)	0.073(6)	
N(5)	0.6643(7)	0.3331(6)	0.2572(4)	0.046(4)	
N(6)	0.5511(9)	0.2320(6)	0.3346(5)	0.057(5)	
N(7)	0.4784(7)	0.3220(7)	0.3099(5)	0.064(5)	
N(8)	0.6082(7)	0.5183(6)	0.1654(5)	0.050(5)	
C(1)	0.923(1)	0.576(1)	0.1628(7)	0.080(7)	
C(2)	1.026(2)	0.614(1)	0.1411(9)	0.10(1)	
C(3)	1.118(1)	0.573(1)	0.1041(9)	0.11(1)	
C(4)	1.106(1)	0.496(1)	0.0876(7)	0.083(8)	
C(5)	1.000(1)	0.4611(8)	0.1113(7)	0.061(7)	
C(6)	0.973(1)	0.3757(9)	0.0969(6)	0.068(7)	
C(7)	0.879(1)	0.2623(9)	0.1012(6)	0.059(7)	
C(8)	0.788(1)	0.2025(8)	0.1144(8)	0.057(6)	
C(9)	0.737(1)	0.1994(9)	0.0547(6)	0.077(7)	
C(10)	0.649(1)	0.146(1)	0.0690(8)	0.083(8)	
C(11)	0.605(1)	0.1013(8)	0.1389(9)	0.077(7)	
C(12)	0.653(1)	0.1036(8)	0.1999(6)	0.062(6)	
C(13)	0.750(1)	0.1527(7)	0.1871(7)	0.047(6)	
C(14)	0.8134(9)	0.1305(7)	0.2562(7)	0.047(6)	
C(15)	0.918(1)	0.0675(8)	0.2656(7)	0.062(7)	
C(16)	0.970(1)	0.0297(8)	0.3358(9)	0.074(7)	
C(17)	0.915(1)	0.0529(9)	0.3913(7)	0.074(7)	
C(18)	0.812(1)	0.1181(8)	0.3837(6)	0.066(7)	
C(19)	0.7608(9)	0.1575(7)	0.3143(7)	0.046(6)	
C(20)	0.661(1)	0.2379(9)	0.3030(6)	0.049(6)	
C(21)	0.552(1)	0.3785(8)	0.2639(6)	0.047(6)	
C(22)	0.524(1)	0.4841(8)	0.2168(6)	0.052(6)	
C(23)	0.4156(9)	0.5371(9)	0.2284(6)	0.063(6)	
C(24)	0.396(1)	0.635(1)	0.1821(8)	0.080(8)	
C(25)	0.480(1)	0.6726(8)	0.1288(7)	0.072(7)	
C(26)	0.588(1)	0.6131(9)	0.1216(6)	0.063(6)	
C(27)	1.041(1)	0.1763(9)	0.0315(7)	0.099(8)	
C(28)	0.4990(9)	0.1473(7)	0.3865(6)	0.077(6)	
Cu(01)	0.2070(1)	0.4857(1)	0.63753(8)	0.0691(8)	
N(01)	0.3465(7)	0.5641(6)	0.5766(5)	0.055(5)	
N(02)	0.3481(7)	0.3778(6)	0.6750(5)	0.049(5)	
N(03)	0.5462(7)	0.3362(7)	0.6593(5)	0.054(5)	
N(04)	0.4961(8)	0.2577(6)	0.7054(5)	0.048(5)	
N(05)	0.0692(7)	0.4211(7)	0.6315(4)	0.048(5)	

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N(06)	-0.0731(8)	0.3415(6)	0.6434(5)	0.053(5)	
N(07)	-0.1263(7)	0.4215(7)	0.6590(5)	0.059(5)	
N(08)	0.0643(7)	0.5802(6)	0.6636(4)	0.053(5)	
C(01)	0.348(1)	0.6588(9)	0.5314(7)	0.071(7)	
C(02)	0.449(1)	0.6996(8)	0.5016(6)	0.072(7)	
C(03)	0.555(1)	0.6431(9)	0.5178(6)	0.068(7)	
C(04)	0.5602(9)	0.5448(8)	0.5645(6)	0.054(6)	
C(05)	0.455(1)	0.5095(8)	0.5924(5)	0.048(6)	
C(06)	0.453(1)	0.4062(7)	0.6432(5)	0.043(6)	
C(07)	0.380(1)	0.2826(8)	0.7143(5)	0.044(6)	
C(08)	0.2982(9)	0.2174(7)	0.7630(6)	0.045(6)	
C(09)	0.3045(9)	0.1838(8)	0.8398(7)	0.057(6)	
C(010)	0.226(1)	0.1262(8)	0.8871(6)	0.064(6)	
C(011)	0.1364(9)	0.1046(7)	0.8604(7)	0.058(6)	
C(012)	0.1304(8)	0.1375(7)	0.7838(7)	0.048(6)	
C(013)	0.2106(8)	0.1910(6)	0.7335(6)	0.038(5)	
C(014)	0.2153(9)	0.2022(7)	0.6544(6)	0.041(5)	
C(015)	0.2989(8)	0.1404(7)	0.6268(6)	0.050(6)	
C(016)	0.2958(9)	0.1355(7)	0.5593(7)	0.054(6)	
C(017)	0.206(1)	0.1915(9)	0.5146(6)	0.070(7)	
C(018)	0.1249(9)	0.2567(8)	0.5377(6)	0.062(6)	
C(019)	0.1266(9)	0.2656(7)	0.6067(6)	0.045(6)	
C(020)	0.041(1)	0.3413(8)	0.6287(5)	0.045(6)	
C(021)	-0.034(1)	0.4661(8)	0.6502(5)	0.048(6)	
C(022)	-0.043(1)	0.5579(7)	0.6638(5)	0.047(5)	
C(023)	-0.1477(9)	0.6153(8)	0.6763(6)	0.061(6)	
C(024)	-0.143(1)	0.6984(8)	0.6893(6)	0.071(7)	
C(025)	-0.033(1)	0.7224(8)	0.6905(6)	0.072(7)	
C(026)	0.066(1)	0.6627(9)	0.6764(6)	0.068(7)	
C(027)	0.5697(8)	0.1647(7)	0.7368(6)	0.071(6)	
C(028)	-0.1452(9)	0.2685(8)	0.6490(6)	0.080(7)	
CL(1)	0.7011(3)	0.0192(2)	0.6029(2)	0.074(2)	
O(1)	0.7596(7)	0.0994(6)	0.5896(5)	0.126(6)	
O(2)	0.7766(9)	-0.0558(8)	0.5925(9)	0.23(1)	
O(3)	0.621(1)	0.0428(7)	0.5535(7)	0.214(9)	
O(4)	0.639(2)	-0.005(1)	0.6668(7)	0.31(1)	
CL(01)	0.8148(3)	0.1042(2)	0.8853(2)	0.068(2)	
O(01)	0.8431(7)	0.2003(6)	0.8612(5)	0.131(6)	
O(02)	0.8615(7)	0.0644(6)	0.8300(4)	0.108(5)	
O(03)	0.6919(7)	0.1077(6)	0.8996(5)	0.104(5)	
O(04)	0.8700(7)	0.0433(6)	0.9529(4)	0.103(5)	
N(001)	0.358(2)	0.174(2)	0.022(1)	0.09(1)	0.5
C(001)	0.259(2)	0.129(1)	0.167(1)	0.06(1)	0.5
C(002)	0.316(2)	0.161(2)	0.081(1)	0.06(1)	0.5
N(002)	0.449(2)	0.491(3)	0.025(3)	0.12(2)	0.5
C(003)	0.478(5)	0.415(3)	0.055(2)	0.14(4)	0.5
C(004)	0.421(4)	0.351(3)	0.120(2)	0.25(4)	0.5

Hydrogen Positional and Isotropic Displacement Parameters

	x/a	y/b	z/c	U
H(1)	0.8491	0.6076	0.1936	0.050
H(2)	1.0338	0.6771	0.1538	0.050
H(3)	1.1993	0.6027	0.0875	0.050

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H(4)	1.1764	0.4616	0.0567	0.050
H(9)	0.7652	0.2363	-0.0026	0.050
H(10)	0.6098	0.1388	0.0235	0.050
H(11)	0.5293	0.0630	0.1494	0.050
H(12)	0.6165	0.0682	0.2577	0.050
H(15)	0.9620	0.0456	0.2187	0.050
H(16)	1.0554	-0.0183	0.3413	0.050
H(17)	0.9515	0.0181	0.4457	0.050
H(18)	0.7708	0.1420	0.4287	0.050
H(23)	0.3489	0.5048	0.2720	0.050
H(24)	0.3121	0.6806	0.1876	0.050
H(25)	0.4653	0.7496	0.0925	0.050
H(26)	0.6583	0.6454	0.0793	0.050
H(271)	1.0406	0.1069	0.0776	0.050
H(272)	0.9787	0.1826	-0.0083	0.050
H(273)	1.1267	0.1671	0.0008	0.050
H(281)	0.5125	0.0958	0.3571	0.050
H(282)	0.5509	0.1179	0.4342	0.050
H(283)	0.4072	0.1413	0.4126	0.050
H(01)	0.2619	0.7057	0.5180	0.050
H(02)	0.4413	0.7760	0.4654	0.050
H(03)	0.6353	0.6740	0.4947	0.050
H(04)	0.6444	0.4967	0.5788	0.050
H(09)	0.3728	0.2026	0.8629	0.050
H(010)	0.2347	0.0974	0.9470	0.050
H(011)	0.0711	0.0623	0.8988	0.050
H(012)	0.0588	0.1196	0.7624	0.050
H(015)	0.3699	0.0936	0.6613	0.050
H(016)	0.3647	0.0871	0.5395	0.050
H(017)	0.1994	0.1839	0.4610	0.050
H(018)	0.0559	0.3039	0.5008	0.050
H(023)	-0.2323	0.5953	0.6760	0.050
H(024)	-0.2243	0.7464	0.6988	0.050
H(025)	-0.0278	0.7874	0.7023	0.050
H(026)	0.1516	0.6838	0.6759	0.050
H(0271)	0.5512	0.1458	0.7972	0.050
H(0272)	0.5342	0.1146	0.7196	0.050
H(0273)	0.6648	0.1438	0.7299	0.050
H(0281)	-0.1273	0.2596	0.5947	0.050
H(0282)	-0.1067	0.2014	0.6918	0.050
H(0283)	-0.2402	0.2681	0.6610	0.050

Atomic Anisotropic Displacement Parameters

	U11	U22	U33	U12	U13	U23
Cu(1)	.065(1)	.0474(9)	.080(1)	-.0044(8)	.0024(8)	-.0217(8)
N(1)	.083(8)	.033(7)	.060(7)	-.002(6)	-.015(6)	-.008(5)
N(2)	.064(7)	.056(7)	.050(6)	-.013(6)	.010(5)	-.017(5)
N(3)	.063(7)	.058(8)	.092(8)	-.012(7)	-.007(6)	-.002(7)
N(4)	.082(8)	.046(7)	.077(8)	.007(7)	-.003(7)	-.018(6)
N(5)	.037(6)	.039(6)	.054(6)	.007(5)	-.013(5)	-.012(5)
N(6)	.062(7)	.038(7)	.064(7)	-.000(6)	-.014(6)	-.010(5)
N(7)	.062(7)	.053(7)	.073(7)	-.007(6)	-.006(6)	-.019(6)
N(8)	.053(6)	.036(7)	.053(7)	.000(5)	-.010(5)	-.010(5)

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C(1)	.11(1)	.045(9)	.08(1)	-.010(8)	-.031(9)	-.013(8)
C(2)	.14(2)	.06(1)	.11(1)	-.04(1)	-.06(1)	-.008(9)
C(3)	.11(1)	.07(1)	.13(2)	-.05(1)	-.06(1)	.03(1)
C(4)	.06(1)	.07(1)	.09(1)	-.026(8)	-.010(8)	.007(9)
C(5)	.08(1)	.022(8)	.067(9)	-.003(8)	-.024(8)	.001(7)
C(6)	.060(9)	.051(9)	.054(9)	.033(9)	.012(7)	-.001(7)
C(7)	.07(1)	.048(9)	.056(9)	.008(8)	.005(7)	-.022(7)
C(8)	.072(9)	.032(8)	.06(1)	-.010(7)	.004(8)	-.014(7)
C(9)	.13(1)	.07(1)	.034(8)	-.007(9)	-.030(8)	-.011(7)
C(10)	.11(1)	.06(1)	.09(1)	-.017(8)	-.05(1)	-.028(9)
C(11)	.075(9)	.054(9)	.10(1)	-.011(7)	-.03(1)	-.015(9)
C(12)	.08(1)	.041(8)	.061(9)	.003(7)	-.034(8)	-.011(7)
C(13)	.057(8)	.024(7)	.06(1)	.005(6)	-.014(8)	-.020(7)
C(14)	.043(8)	.026(7)	.07(1)	.004(6)	-.008(7)	-.017(7)
C(15)	.061(9)	.033(8)	.10(1)	-.010(7)	-.000(8)	-.029(7)
C(16)	.065(9)	.034(8)	.11(1)	.011(7)	-.05(1)	-.009(9)
C(17)	.09(1)	.052(9)	.07(1)	.015(8)	-.042(9)	-.010(8)
C(18)	.10(1)	.041(8)	.055(9)	-.015(7)	-.023(8)	-.007(7)
C(19)	.042(8)	.028(7)	.059(9)	.003(6)	-.012(7)	-.005(7)
C(20)	.043(8)	.06(1)	.048(8)	-.024(8)	.001(7)	-.019(7)
C(21)	.051(8)	.042(8)	.054(8)	-.008(7)	-.012(7)	-.021(7)
C(22)	.065(9)	.034(8)	.064(9)	.012(7)	-.032(7)	-.026(7)
C(23)	.051(8)	.047(8)	.09(1)	-.000(7)	-.007(7)	-.027(8)
C(24)	.07(1)	.06(1)	.12(1)	.019(8)	-.039(9)	-.05(1)
C(25)	.10(1)	.035(8)	.08(1)	.013(9)	-.060(9)	-.013(8)
C(26)	.09(1)	.043(9)	.056(8)	-.004(7)	-.027(7)	-.011(7)
C(27)	.10(1)	.09(1)	.11(1)	.019(8)	.003(8)	-.059(9)
C(28)	.090(9)	.052(8)	.075(9)	-.040(7)	.009(7)	.004(7)
Cu(01)	.0452(9)	.061(1)	.098(1)	-.0028(7)	-.0137(8)	-.0260(9)
N(01)	.055(7)	.040(6)	.062(7)	.010(5)	-.027(5)	-.010(5)
N(02)	.043(6)	.037(7)	.070(7)	-.009(5)	-.012(5)	-.017(5)
N(03)	.036(6)	.046(6)	.083(7)	.002(6)	-.020(5)	-.027(6)
N(04)	.032(6)	.043(7)	.071(7)	-.012(6)	-.005(5)	-.019(5)
N(05)	.034(6)	.038(6)	.073(7)	.003(5)	-.016(5)	-.021(5)
N(06)	.039(7)	.039(7)	.079(7)	-.004(6)	-.012(5)	-.017(5)
N(07)	.046(6)	.039(6)	.093(8)	.007(6)	-.021(5)	-.025(6)
N(08)	.054(7)	.041(6)	.061(6)	-.008(5)	-.012(5)	-.012(5)
C(01)	.09(1)	.041(9)	.08(1)	.016(7)	-.036(8)	-.011(7)
C(02)	.09(1)	.055(9)	.070(9)	-.018(9)	-.001(8)	-.018(7)
C(03)	.070(9)	.06(1)	.08(1)	-.032(8)	.001(8)	-.025(8)
C(04)	.057(8)	.039(8)	.071(9)	-.014(6)	-.007(6)	-.021(7)
C(05)	.060(8)	.050(8)	.046(8)	-.018(8)	-.005(7)	-.026(7)
C(06)	.050(8)	.036(8)	.053(8)	-.020(7)	-.008(7)	-.019(6)
C(07)	.055(9)	.033(8)	.047(8)	-.018(7)	-.013(7)	-.009(6)
C(08)	.047(8)	.030(7)	.052(9)	.005(6)	-.015(7)	-.011(6)
C(09)	.058(8)	.062(8)	.053(9)	-.013(6)	-.014(7)	-.019(7)
C(010)	.09(1)	.058(9)	.040(8)	-.013(7)	.007(8)	-.015(7)
C(011)	.056(8)	.046(8)	.07(1)	-.014(6)	.002(7)	-.015(7)
C(012)	.053(8)	.038(7)	.055(8)	-.012(6)	-.012(7)	-.014(6)
C(013)	.032(7)	.023(6)	.052(8)	-.000(5)	-.004(6)	-.008(6)
C(014)	.047(7)	.029(7)	.044(8)	-.013(6)	.001(7)	-.007(6)
C(015)	.057(8)	.043(7)	.042(8)	-.001(6)	.003(6)	-.013(6)
C(016)	.063(9)	.033(7)	.056(9)	.003(6)	.003(7)	-.013(7)
C(017)	.10(1)	.063(9)	.060(9)	-.022(8)	.010(8)	-.041(8)
C(018)	.062(8)	.068(9)	.054(9)	-.004(7)	-.025(7)	-.013(7)
C(019)	.050(8)	.042(8)	.047(8)	-.013(6)	-.007(7)	-.016(7)

C(020)	.038(8)	.042(8)	.051(8)	-.003(7)	-.020(6)	-.006(6)
C(021)	.042(8)	.041(8)	.058(8)	-.004(7)	-.022(6)	-.009(6)
C(022)	.036(7)	.035(8)	.063(8)	-.001(7)	-.010(6)	-.010(6)
C(023)	.054(8)	.040(8)	.088(9)	-.006(7)	-.012(7)	-.021(7)
C(024)	.068(9)	.043(9)	.09(1)	.014(7)	-.004(8)	-.025(7)
C(025)	.09(1)	.037(8)	.10(1)	-.004(8)	-.022(8)	-.029(7)
C(026)	.071(9)	.047(8)	.09(1)	-.008(7)	-.035(7)	-.021(8)
C(027)	.053(7)	.031(7)	.11(1)	.028(6)	-.026(7)	-.019(7)
C(028)	.060(8)	.053(8)	.13(1)	-.022(7)	-.015(7)	-.024(8)
CL(1)	.094(3)	.049(2)	.079(3)	.002(2)	-.029(2)	-.020(2)
O(1)	.131(8)	.053(6)	.20(1)	-.019(6)	-.081(7)	-.026(6)
O(2)	.14(1)	.12(1)	.49(2)	.040(8)	-.10(1)	-.19(1)
O(3)	.22(1)	.13(1)	.25(1)	-.089(8)	-.18(1)	.074(9)
O(4)	.67(3)	.26(2)	.11(1)	-.31(2)	.13(2)	-.11(1)
CL(01)	.060(2)	.057(2)	.078(3)	.004(2)	-.010(2)	-.019(2)
O(01)	.119(8)	.039(6)	.21(1)	.003(5)	-.038(7)	-.015(6)
O(02)	.117(7)	.139(8)	.094(7)	-.015(6)	.012(6)	-.080(7)
O(03)	.063(6)	.122(8)	.130(8)	-.012(5)	.001(5)	-.053(6)
O(04)	.107(7)	.081(6)	.098(7)	.016(5)	-.050(6)	-.006(6)
N(001)	.07(2)	.14(2)	.05(1)	-.08(1)	-.03(1)	.03(1)
C(001)	.05(1)	.09(2)	.04(1)	.02(1)	-.03(1)	-.01(1)
C(002)	.02(1)	.05(2)	.09(2)	.01(1)	-.05(1)	-.02(2)
N(002)	.09(2)	.11(3)	.22(4)	.06(2)	-.08(2)	-.15(3)
C(003)	.17(4)	.22(7)	.13(5)	-.06(5)	-.00(4)	-.16(5)
C(004)	.39(6)	.12(4)	.30(5)	.21(4)	-.34(5)	-.18(4)

Bond Distances (Angstroms)

	Molécule 1	Molécule 2
Cu1-N2	1.99(1)	2.050(7)
Cu1-N5	2.068(7)	2.07(1)
Cu1-N8	2.016(8)	2.082(8)
N1-C1	1.35(2)	1.35(1)
N1-C5	1.32(2)	1.36(1)
N2-C6	1.34(2)	1.35(1)
N2-C7	1.36(2)	1.34(1)
N3-N4	1.39(2)	1.35(1)
N3-C6	1.34(2)	1.33(1)
N4-C7	1.32(2)	1.33(1)
N4-C27	1.50(2)	1.44(1)
N5-C20	1.37(1)	1.32(2)
N5-C21	1.35(1)	1.33(1)
N6-N7	1.38(1)	1.35(1)
N6-C20	1.34(1)	1.32(1)
N6-C28	1.46(1)	1.47(2)
N7-C21	1.32(1)	1.33(2)
N8-C22	1.32(1)	1.35(2)
N8-C26	1.34(1)	1.35(2)
C1-C2	1.36(2)	1.38(2)
C2-C3	1.37(2)	1.35(2)
C3-C4	1.34(3)	1.39(2)
C4-C5	1.38(2)	1.38(2)
C5-C6	1.50(2)	1.49(1)
C7-C8	1.45(2)	1.47(1)

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C8-C9	1.39(2)	1.39(2)
C8-C13	1.37(2)	1.42(2)
C9-C10	1.35(2)	1.37(2)
C10-C11	1.34(2)	1.37(2)
C11-C12	1.40(2)	1.38(2)
C12-C13	1.41(2)	1.38(1)
C13-C14	1.52(2)	1.47(2)
C14-C15	1.37(1)	1.39(1)
C14-C19	1.36(2)	1.43(1)
C15-C16	1.43(2)	1.34(2)
C16-C17	1.29(2)	1.38(2)
C17-C18	1.37(2)	1.37(2)
C18-C19	1.42(2)	1.40(2)
C19-C20	1.46(1)	1.49(2)
C21-C22	1.49(1)	1.47(2)
C22-C23	1.38(2)	1.39(1)
C23-C24	1.38(2)	1.37(2)
C24-C25	1.36(2)	1.40(2)
C25-C26	1.40(2)	1.37(2)
CL1-O1	1.41(1)	1.421(9)
CL1-O2	1.34(1)	1.41(1)
CL1-O3	1.34(1)	1.408(8)
CL1-O4	1.30(1)	1.437(8)
N001-C002	1.14(3)	1.07(6)
C001-C002	1.63(3)	1.43(6)

Bond Angles (degrees)

	Molécule 1	Molécule 2
N2-Cu1-N5	108.1(4)	108.6(4)
N2-Cu1-N8	145.4(4)	147.2(4)
N5-Cu1-N8	81.5(3)	79.7(4)
C1-N1-C5	116(1)	114.7(9)
Cu1-N2-C6	110.7(9)	113.0(6)
Cu1-N2-C7	142.6(8)	144.3(8)
C6-N2-C7	107(1)	102.2(8)
N4-N3-C6	103(1)	101.5(8)
N3-N4-C7	111(1)	110.7(8)
N3-N4-C27	118(1)	119.3(8)
C7-N4-C27	131(1)	129.9(8)
Cu1-N5-C20	144.0(7)	144.4(7)
Cu1-N5-C21	110.6(6)	112.1(9)
C20-N5-C21	103.9(8)	102.1(9)
N7-N6-C20	111.5(8)	111(1)
N7-N6-C28	118.1(8)	118.3(8)
C20-N6-C28	130.4(9)	131(1)
N6-N7-C21	101.6(8)	100.2(8)
Cu1-N8-C22	115.2(6)	115.3(8)
Cu1-N8-C26	127.1(7)	127.7(7)
C22-N8-C26	117.2(9)	116.9(9)
N1-C1-C2	121(1)	124(1)
C1-C2-C3	121(2)	119(1)

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C2-C3-C4	119(2)	119(1)
C3-C4-C5	117(1)	117.9(9)
N1-C5-C4	126(1)	124.3(9)
N1-C5-C6	111(1)	114(1)
C4-C5-C6	123(1)	121.3(9)
N2-C6-N3	112(1)	115.6(8)
N2-C6-C5	123(1)	119.1(9)
N3-C6-C5	125(1)	125(1)
N2-C7-N4	107(1)	110.0(9)
N2-C7-C8	126(1)	124.3(9)
N4-C7-C8	126(1)	125.6(8)
C7-C8-C9	121(1)	119(1)
C7-C8-C13	118(1)	122(1)
C9-C8-C13	121(1)	119.6(9)
C8-C9-C10	119(1)	120(1)
C9-C10-C11	122(2)	121(1)
C10-C11-C12	121(1)	118(1)
C11-C12-C13	119(1)	123(1)
C8-C13-C12	118(1)	117(1)
C8-C13-C14	127(1)	122.9(9)
C12-C13-C14	114.3(9)	119(1)
C13-C14-C15	118(1)	119.8(8)
C13-C14-C19	122.1(9)	122.0(9)
C15-C14-C19	119(1)	118(1)
C14-C15-C16	120(1)	122.7(9)
C15-C16-C17	120(1)	120(1)
C16-C17-C18	122(1)	119(1)
C17-C18-C19	119(1)	122(1)
C14-C19-C18	120.1(9)	118(1)
C14-C19-C20	120(1)	121(1)
C18-C19-C20	119(1)	121.1(9)
N5-C20-N6	107.7(9)	110(1)
N5-C20-C19	125.4(9)	124(1)
N6-C20-C19	126.9(9)	125(1)
N5-C21-N7	115.4(9)	116(1)
N5-C21-C22	117.5(9)	121(1)
N7-C21-C22	127(1)	123(1)
N8-C22-C21	114.6(9)	112.0(9)
N8-C22-C23	125.7(9)	123(1)
C21-C22-C23	120(1)	125(1)
C22-C23-C24	116(1)	119(1)
C23-C24-C25	120(1)	119(1)
C24-C25-C26	120(1)	119(1)
N8-C26-C25	121(1)	123(1)
O1-CL1-O2	110.6(6)	108.0(6)
O1-CL1-O3	110.8(6)	109.9(5)
O1-CL1-O4	113(1)	109.7(6)
O2-CL1-O3	105.1(9)	112.6(6)
O2-CL1-O4	113.4(9)	107.8(5)
O3-CL1-O4	103(1)	108.8(5)
N001-C002-C001	174(2)	127(5)

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Dihedral Angles (degrees)

	Molécule 1	Molécule 2
N5-Cu1-N2-C6	-144.0(7)	144.3(8)
N5-Cu1-N2-C7	34(1)	-25(2)
N8-Cu1-N2-C6	114.5(9)	-115.8(9)
N8-Cu1-N2-C7	-67(1)	75(2)
N2-Cu1-N5-C20	19(2)	-19(1)
N2-Cu1-N5-C21	-142.9(9)	143.8(6)
N8-Cu1-N5-C20	165(2)	-166(1)
N8-Cu1-N5-C21	2.9(9)	-3.3(6)
N2-Cu1-N8-C22	112(1)	-108.9(9)
N2-Cu1-N8-C26	-76(1)	75(1)
N5-Cu1-N8-C22	2(1)	-.5(6)
N5-Cu1-N8-C26	174(1)	-176.9(8)
C5-N1-C1-C2	0(2)	0(2)
C1-N1-C5-C4	0(2)	-1(2)
C1-N1-C5-C6	-178.9(9)	179(1)
Cu1-N2-C6-N3	-179.1(7)	-173.1(9)
Cu1-N2-C6-C5	2(1)	5(1)
C7-N2-C6-N3	2(1)	0(1)
C7-N2-C6-C5	-177(1)	179(1)
Cu1-N2-C7-N4	178.9(8)	170(1)
Cu1-N2-C7-C8	2(2)	-13(2)
C6-N2-C7-N4	-3(1)	0(1)
C6-N2-C7-C8	-179(1)	177(1)
C6-N3-N4-C7	-1(1)	0(1)
C6-N3-N4-C27	-178.9(9)	-179(1)
N4-N3-C6-N2	0(1)	0(1)
N4-N3-C6-C5	178(1)	-178(1)
N3-N4-C7-N2	2(1)	0(1)
N3-N4-C7-C8	179(1)	-177(1)
C27-N4-C7-N2	180(1)	179(1)
C27-N4-C7-C8	-4(2)	2(2)
Cu1-N5-C20-N6	-164(1)	164.8(8)
Cu1-N5-C20-C19	16(2)	-19(2)
C21-N5-C20-N6	0(1)	1(1)
C21-N5-C20-C19	179(1)	177.4(9)
Cu1-N5-C21-N7	170.1(9)	-170.1(7)
Cu1-N5-C21-C22	-7(1)	7(1)
C20-N5-C21-N7	0(2)	0(1)
C20-N5-C21-C22	-177(1)	176.5(8)
C20-N6-N7-C21	0(1)	1(1)
C28-N6-N7-C21	-178(1)	178.2(8)
N7-N6-C20-N5	0(1)	-2(1)
N7-N6-C20-C19	-179(1)	-177.8(9)
C28-N6-C20-N5	178(1)	-178.1(9)
C28-N6-C20-C19	-1(2)	6(2)
N6-N7-C21-N5	0(1)	0(1)
N6-N7-C21-C22	177(1)	-177.4(9)
Cu1-N8-C22-C21	-7(2)	3.9(9)
Cu1-N8-C22-C23	175(1)	-176.7(7)
C26-N8-C22-C21	-180(1)	-179.4(8)
C26-N8-C22-C23	2(2)	0(1)

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Cu1-N8-C26-C25	-174(1)	177.4(8)
C22-N8-C26-C25	-2(2)	1(1)
N1-C1-C2-C3	0(2)	0(2)
C1-C2-C3-C4	1(2)	0(2)
C2-C3-C4-C5	-2(2)	0(2)
C3-C4-C5-N1	1(2)	0(2)
C3-C4-C5-C6	180(1)	-179(1)
N1-C5-C6-N2	-1(1)	-7(2)
N1-C5-C6-N3	-179(1)	171(1)
C4-C5-C6-N2	-180(1)	173(1)
C4-C5-C6-N3	2(2)	-9(2)
N2-C7-C8-C9	114(1)	-110(1)
N2-C7-C8-C13	-63(1)	68(2)
N4-C7-C8-C9	-62(2)	67(2)
N4-C7-C8-C13	121(1)	-116(1)
C7-C8-C9-C10	-177(1)	177(1)
C13-C8-C9-C10	0(2)	0(2)
C7-C8-C13-C12	173(1)	-173.7(9)
C7-C8-C13-C14	-18(2)	18(1)
C9-C8-C13-C12	-4(2)	4(1)
C9-C8-C13-C14	165(1)	-164.5(9)
C8-C9-C10-C11	4(2)	-3(2)
C9-C10-C11-C12	-4(2)	4(2)
C10-C11-C12-C13	0(2)	0(2)
C11-C12-C13-C8	5(2)	-4(1)
C11-C12-C13-C14	-166(1)	165.2(9)
C8-C13-C14-C15	-67(2)	71(1)
C8-C13-C14-C19	125(1)	-118(1)
C12-C13-C14-C15	103(1)	-97(1)
C12-C13-C14-C19	-66(1)	74(1)
C13-C14-C15-C16	-168(1)	169(1)
C19-C14-C15-C16	1(2)	-3(2)
C13-C14-C19-C18	167(1)	-167(1)
C13-C14-C19-C20	-23(2)	15(2)
C15-C14-C19-C18	-2(2)	4(1)
C15-C14-C19-C20	169(1)	-174(1)
C14-C15-C16-C17	2(2)	-2(2)
C15-C16-C17-C18	-4(2)	5(2)
C16-C17-C18-C19	3(2)	-3(2)
C17-C18-C19-C14	0(2)	-1(2)
C17-C18-C19-C20	-171(1)	177(1)
C14-C19-C20-N5	-62(2)	71(1)
C14-C19-C20-N6	117(1)	-114(1)
C18-C19-C20-N5	109(1)	-107(1)
C18-C19-C20-N6	-72(2)	68(1)
N5-C21-C22-N8	10(2)	-7(1)
N5-C21-C22-C23	-172(1)	173.4(9)
N7-C21-C22-N8	-167(1)	169.4(9)
N7-C21-C22-C23	11(2)	-10(1)
N8-C22-C23-C24	0(2)	0(1)
C21-C22-C23-C24	-180(1)	179.2(9)
C22-C23-C24-C25	0(2)	0(1)
C23-C24-C25-C26	0(3)	2(2)
C24-C25-C26-N8	2(2)	-2(2)

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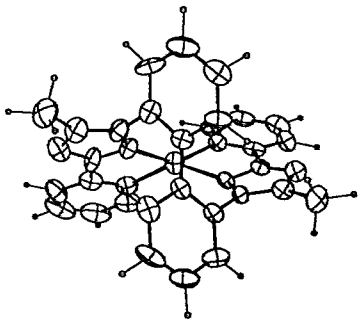

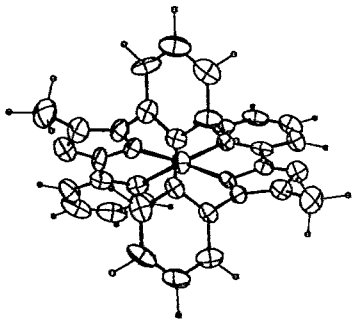

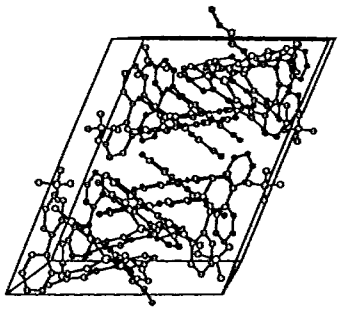

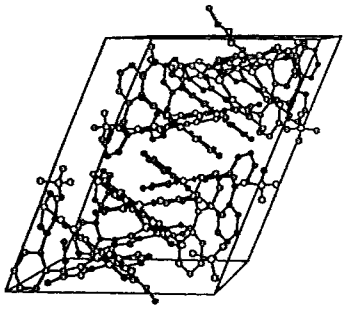

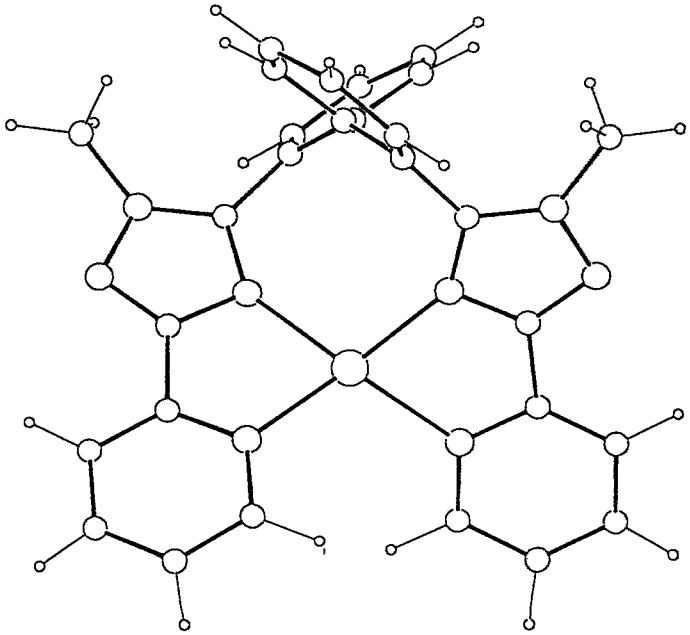

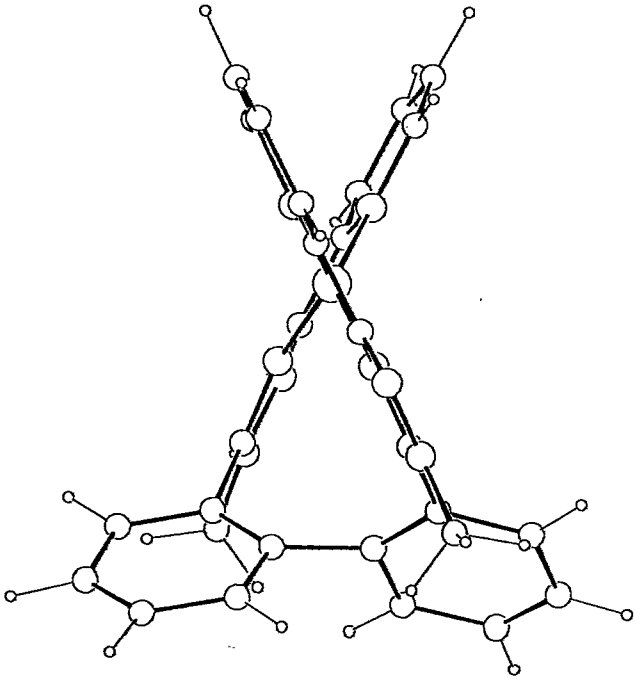

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$[Cu^{II}(C_{28}H_{22}N_8)](ClO_4)_2(CH_3CN)$, Orthorhombic , *Cmca*

a = 28.571(6) , b = 16.559(9) , c = 14.077(6) Å.

Non-Hydrogen Positional, Isotropic Displacement and Occupation Parameters

	x/a	y/b	z/c	U_{eq}	PP (if ≠ 1)
Cu	0.23849(6)	0	1/2	0.0481(6)	
N(1)	0.2820(3)	0.0940(5)	0.5197(5)	0.046(3)	
N(2)	0.1963(3)	0.0680(4)	0.5754(5)	0.037(3)	
N(3)	0.1920(3)	0.1774(5)	0.6659(6)	0.059(3)	
N(4)	0.1525(3)	0.1307(5)	0.6750(6)	0.051(3)	
C(1)	0.3250(4)	0.1044(7)	0.4828(8)	0.060(4)	
C(2)	0.3503(5)	0.173(1)	0.501(1)	0.080(5)	
C(3)	0.3315(6)	0.233(1)	0.553(1)	0.087(7)	
C(4)	0.2885(5)	0.2232(7)	0.5921(9)	0.060(5)	
C(5)	0.2640(4)	0.1534(6)	0.5723(7)	0.051(4)	
C(6)	0.2176(4)	0.1363(6)	0.6052(7)	0.043(3)	
C(7)	0.1556(4)	0.0645(6)	0.6217(7)	0.046(4)	
C(8)	0.1219(3)	-0.0018(7)	0.6242(7)	0.045(3)	
C(9)	0.1159(4)	-0.0449(7)	0.7084(8)	0.059(4)	
C(10)	0.0877(4)	-0.1096(8)	0.712(1)	0.064(5)	
C(11)	0.0646(4)	-0.1356(8)	0.633(1)	0.067(5)	
C(12)	0.0696(4)	-0.0921(9)	0.550(1)	0.067(5)	
C(13)	0.0977(3)	-0.0244(5)	0.5431(7)	0.043(3)	
C(14)	0.1144(4)	0.1575(8)	0.738(1)	0.090(6)	
Cl(1)	1/4	0.0496(2)	1/4	0.056(1)	
O(1)	0.2739(3)	0.0948(5)	0.1807(7)	0.102(4)	
O(2)	0.2168(3)	-0.0020(6)	0.2025(5)	0.082(3)	
Cl(2)	1/2	0.2447(6)	0.3850(6)	0.128(4)	
O(3)	0.4592(5)	0.2327(9)	0.426(1)	0.197(9)	
O(4)	1/2	0.337(2)	0.369(2)	0.19(1)	
O(5)	1/2	0.231(2)	0.283(2)	0.17(1)	0.75
O(6)	1/2	0.156(5)	0.364(5)	0.14(4)	0.25
N(01)	0	0.048(4)	0.855(3)	0.19(3)	0.50
C(01)	0.041(2)	0.030(3)	0.908(2)	0.14(2)	0.50
C(02)	0.078(1)	0.020(2)	0.947(3)	0.12(2)	0.50

Hydrogen Positional and Isotropic Displacement Parameters

	x/a	y/b	z/c	U
H(1)	0.330(3)	0.051(5)	0.448(6)	0.050
H(2)	0.378(3)	0.167(6)	0.472(7)	0.050
H(3)	0.346(3)	0.276(6)	0.558(7)	0.050
H(4)	0.272(3)	0.256(6)	0.627(7)	0.050
H(9)	0.135(3)	-0.016(5)	0.761(7)	0.050
H(10)	0.084(3)	-0.141(5)	0.771(7)	0.050
H(11)	0.044(3)	-0.181(5)	0.636(7)	0.050
H(12)	0.058(4)	-0.102(6)	0.504(7)	0.050
H(141)	0.0850	0.1632	0.6884	0.050
H(142)	0.1099	0.1097	0.7858	0.050
H(143)	0.1127	0.2132	0.7794	0.050

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Atomic Anisotropic Displacement Parameters

	U11	U22	U33	U12	U13	U23
Cu	.0424(9)	.0453(9)	.057(1)	0	0	-.012(1)
N(1)	.051(5)	.053(5)	.036(5)	-.007(4)	-.008(4)	.006(4)
N(2)	.046(5)	.025(4)	.039(5)	.004(4)	.005(4)	-.007(3)
N(3)	.071(6)	.045(5)	.062(6)	-.003(5)	-.019(5)	-.012(5)
N(4)	.052(5)	.062(6)	.040(5)	.010(5)	-.011(4)	-.013(5)
C(1)	.061(7)	.071(8)	.049(8)	-.022(6)	-.009(6)	-.001(6)
C(2)	.068(8)	.10(1)	.072(9)	-.020(9)	.000(9)	.03(1)
C(3)	.10(1)	.07(1)	.10(1)	-.050(9)	-.05(1)	.038(9)
C(4)	.07(1)	.050(7)	.060(8)	-.010(7)	-.025(7)	.013(6)
C(5)	.063(7)	.043(6)	.048(6)	-.019(6)	-.027(6)	.005(5)
C(6)	.055(7)	.022(5)	.052(7)	-.006(5)	-.018(6)	-.002(5)
C(7)	.060(7)	.048(6)	.031(6)	.009(6)	-.009(5)	-.013(5)
C(8)	.045(5)	.039(5)	.053(6)	.000(6)	.009(5)	-.013(6)
C(9)	.057(7)	.066(8)	.054(7)	-.006(6)	.005(6)	-.002(6)
C(10)	.060(8)	.066(8)	.065(8)	-.010(7)	.012(7)	.014(7)
C(11)	.057(8)	.064(8)	.08(1)	-.017(7)	.010(7)	.014(8)
C(12)	.053(8)	.079(9)	.07(1)	-.005(7)	-.005(6)	-.016(9)
C(13)	.039(5)	.034(6)	.056(6)	.000(4)	.006(5)	-.008(4)
C(14)	.08(1)	.087(9)	.10(1)	.020(8)	.004(8)	-.065(9)
Cl(1)	.061(3)	.053(2)	.054(2)	0	.008(2)	0
O(1)	.106(7)	.088(6)	.114(7)	.012(5)	.028(6)	.058(6)
O(2)	.077(5)	.092(6)	.077(5)	-.003(6)	-.009(4)	-.034(6)
Cl(2)	.049(3)	.174(8)	.161(7)	0	0	-.103(6)
O(3)	.14(1)	.16(1)	.29(2)	-.00(1)	.12(1)	.01(1)
O(4)	.15(2)	.27(3)	.16(2)	0	0	-.02(2)
O(5)	.13(2)	.25(3)	.12(2)	0	0	-.10(2)
O(6)	.13(6)	.16(7)	.12(5)	0	0	-.07(6)
N(01)	.03(2)	.39(9)	.14(4)	0	0	.13(5)
C(01)	.17(4)	.18(4)	.08(2)	-.08(4)	.06(3)	-.01(2)
C(02)	.05(2)	.12(4)	.18(4)	.00(2)	-.03(2)	-.02(3)

Bond Distances (Angstroms)

Cu-N1	2.011(8)	C5-C6	1.43(2)
Cu-N2	1.962(7)	C7-C8	1.46(1)
N1-C1	1.35(1)	C8-C9	1.39(2)
N1-C5	1.33(1)	C8-C13	1.39(1)
N2-C6	1.35(1)	C9-C10	1.34(2)
N2-C7	1.33(1)	C10-C11	1.37(2)
N3-N4	1.37(1)	C11-C12	1.38(2)
N3-C6	1.32(1)	C12-C13	1.38(2)
N4-C7	1.33(1)	C13-C13	1.46(1)
N4-C14	1.47(2)	Cl1-O1	1.407(9)
C1-C2	1.37(2)	Cl1-O2	1.441(9)
C2-C3	1.34(2)	Cl1-O1	1.407(9)
C3-C4	1.35(2)	Cl1-O2	1.441(9)
C4-C5	1.38(2)		

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Bond Angles (degrees)

N1-Cu-N2	82.0(3)	N3-C6-C5	128.6(9)
N1-Cu-N1	103.7(3)	N2-C7-N4	107.3(9)
N1-Cu-N2	154.0(3)	N2-C7-C8	128.2(9)
N2-Cu-N2	104.1(3)	N4-C7-C8	124.2(9)
N1-Cu-N2	82.0(3)	C7-C8-C9	119.1(9)
C1-N1-C5	118.2(9)	C7-C8-C13	120.8(9)
C6-N2-C7	106.1(8)	C9-C8-C13	120(1)
N4-N3-C6	103.1(8)	C8-C9-C10	121(1)
N3-N4-C7	110.9(8)	C9-C10-C11	121(1)
N3-N4-C14	119.6(9)	C10-C11-C12	119(1)
C7-N4-C14	129.5(9)	C11-C12-C13	123(1)
N1-C1-C2	121(1)	C8-C13-C12	117(1)
C1-C2-C3	120(1)	C8-C13-C13	122.4(8)
C2-C3-C4	120(1)	C12-C13-C13	120(1)
C3-C4-C5	118(1)	O1-Cl1-O2	108.3(5)
N1-C5-C4	122(1)	O1-Cl1-O1	115.7(6)
N1-C5-C6	113.0(9)	O1-Cl1-O2	108.5(5)
C4-C5-C6	125(1)	O2-Cl1-O1	108.5(5)
N2-C6-N3	112.5(9)	O2-Cl1-O2	107.3(6)
N2-C6-C5	118.9(9)	O1-Cl1-O2	108.3(5)

Dihedral Angles (degrees)

C5-N1-C1-C2	2(2)	N1-C5-C6-N2	-5(1)
C1-N1-C5-C4	-2(1)	N1-C5-C6-N3	172(1)
C1-N1-C5-C6	178.3(9)	C4-C5-C6-N2	176(1)
C7-N2-C6-N3	-2(1)	C4-C5-C6-N3	-8(2)
C7-N2-C6-C5	175.6(9)	N2-C7-C8-C9	111(1)
C6-N2-C7-N4	2(1)	N2-C7-C8-C13	-66(1)
C6-N2-C7-C8	-172(1)	N4-C7-C8-C9	-62(1)
C6-N3-N4-C7	0(1)	N4-C7-C8-C13	121(1)
C6-N3-N4-C14	-179.2(9)	C7-C8-C9-C10	-175(1)
N4-N3-C6-N2	0(1)	C13-C8-C9-C10	2(2)
N4-N3-C6-C5	-176(1)	C7-C8-C13-C12	175(1)
N3-N4-C7-N2	-2(1)	C7-C8-C13-C13	-11(1)
N3-N4-C7-C8	172.5(9)	C9-C8-C13-C12	-2(1)
C14-N4-C7-N2	178(1)	C9-C8-C13-C13	171.6(9)
C14-N4-C7-C8	-8(2)	C8-C9-C10-C11	0(2)
N1-C1-C2-C3	-2(2)	C9-C10-C11-C12	-2(2)
C1-C2-C3-C4	3(2)	C10-C11-C12-C13	1(2)
C2-C3-C4-C5	-3(2)	C11-C12-C13-C8	0(2)
C3-C4-C5-N1	3(2)	C11-C12-C13-C13	-173(1)
C3-C4-C5-C6	-178(1)		

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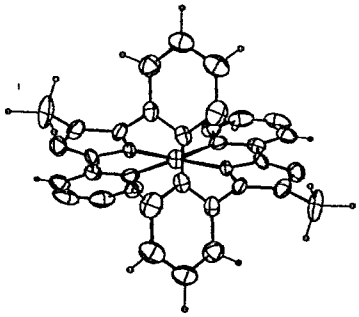

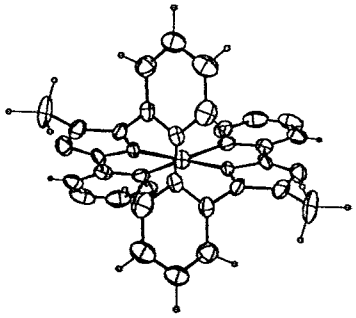

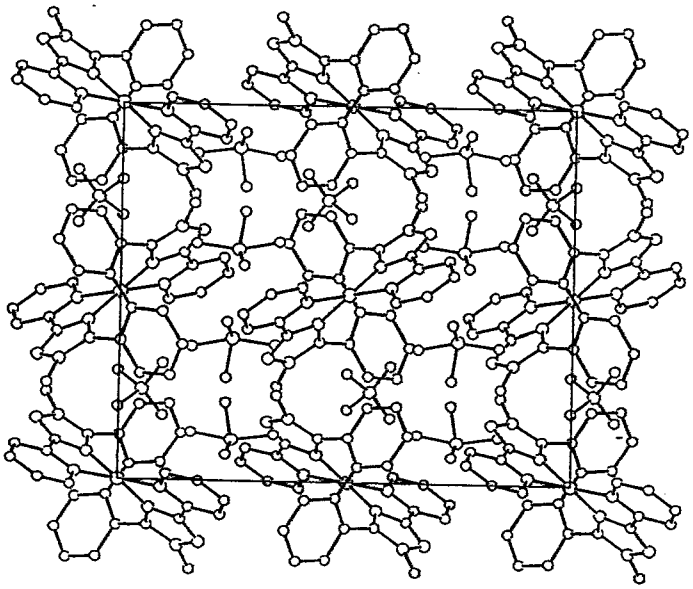

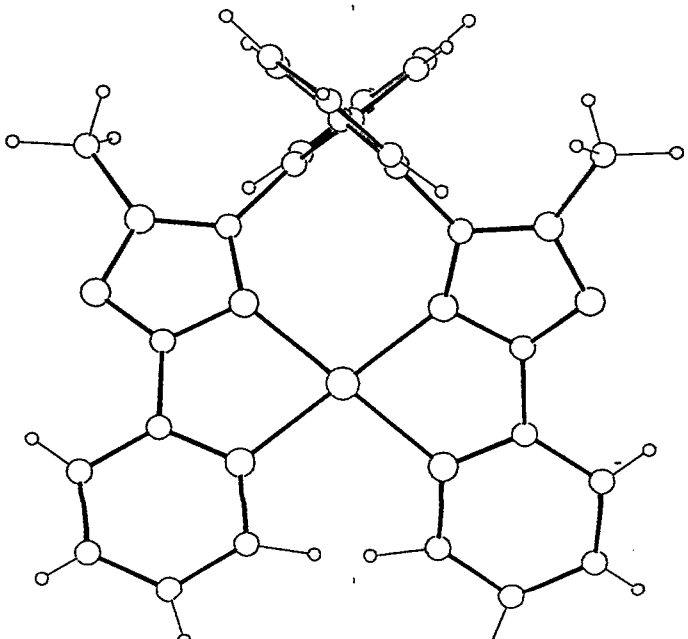

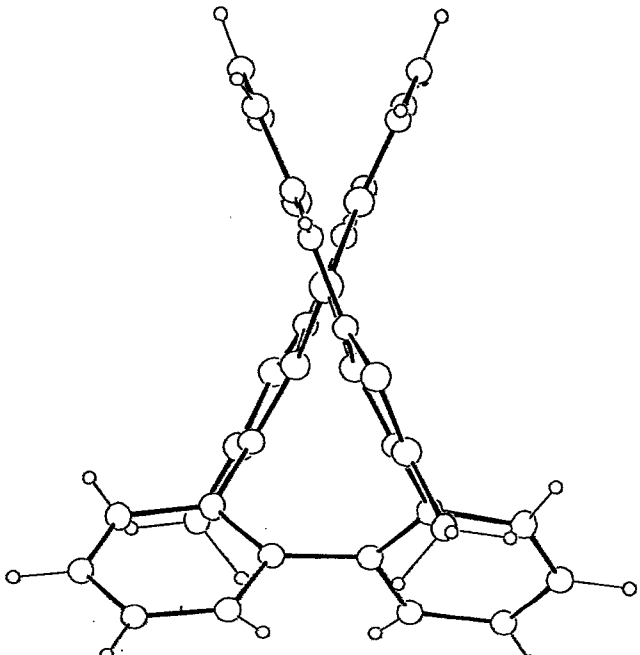

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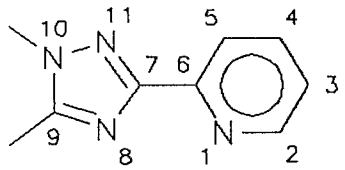
Hueckel Calculation: Pyridyltriazole



Interaction matrix (eV):

	N 1	C 2	C 3	C 4	C 5	C 6	C 7	N 8	C 9	N10	N11
N 1	-12.582	-2.705	0.000	0.000	0.000	-2.646	0.000	0.000	0.000	0.000	0.000
C 2	-2.705	-11.459	-2.830	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C 3	0.000	-2.830	-11.180	-2.795	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C 4	0.000	0.000	-2.795	-11.180	-2.795	0.000	0.000	0.000	0.000	0.000	0.000
C 5	0.000	0.000	0.000	-2.795	-11.180	-2.765	0.000	0.000	0.000	0.000	0.000
C 6	-2.646	0.000	0.000	0.000	-2.765	-10.939	-2.770	0.000	0.000	0.000	0.000
C 7	0.000	0.000	0.000	0.000	0.000	-2.770	-11.218	-2.678	0.000	0.000	-2.709
N 8	0.000	0.000	0.000	0.000	0.000	0.000	-2.678	-12.582	-2.678	0.000	0.000
C 9	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-2.678	-11.218	-2.678	0.000
N10	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-2.678	-12.582	-2.576
N11	0.000	0.000	0.000	0.000	0.000	0.000	-2.709	0.000	0.000	-2.576	-12.861

	1(2)	2(2)	3(2)	4(2)	5(2)	6(2)	7(0)	8(0)	9(0)	10(0)	11(0)
Energies	-17.960	-16.871	-14.711	-14.372	-14.090	-12.954	-9.281	-8.741	-7.752	-6.931	-5.318

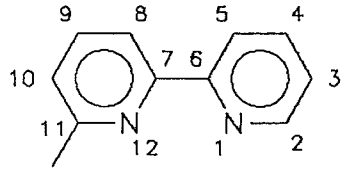
The total energy is -181.915 eV

MO-coefficients:

	1(2)	2(2)	3(2)	4(2)	5(2)	6(2) χ HOMO	7(0) ψ LUMO	8(0) χ SLUMO	9(0)	10(0)	11(0)
N 1	0.255	0.419	0.162	-0.527	-0.013	0.253	-0.463	0.299	-0.018	0.058	0.289
C 2	0.158	0.392	-0.279	-0.415	0.113	-0.195	0.145	-0.562	-0.075	-0.336	-0.257
C 3	0.120	0.349	-0.476	0.077	0.117	-0.345	0.331	0.254	0.116	0.482	0.280
C 4	0.132	0.314	-0.318	0.507	0.008	-0.022	-0.372	0.347	-0.066	-0.393	-0.328
C 5	0.199	0.290	0.074	0.503	-0.109	0.331	-0.079	-0.557	-0.035	0.115	0.407
C 6	0.356	0.279	0.416	0.067	-0.122	0.235	0.430	0.140	0.110	0.220	-0.532
C 7	0.459	-0.092	0.338	0.085	-0.018	-0.402	0.264	0.159	-0.074	-0.489	0.397
N 8	0.368	-0.214	0.125	0.077	0.660	-0.165	-0.273	-0.118	-0.333	0.324	-0.170
C 9	0.281	-0.251	-0.239	-0.033	0.390	0.379	0.073	0.010	0.676	-0.195	0.063
N10	0.339	-0.316	-0.436	-0.117	-0.242	0.411	0.220	0.108	-0.541	-0.012	0.031
N11	0.415	-0.266	-0.113	-0.046	-0.547	-0.335	-0.358	-0.172	0.312	0.228	-0.153

	N 1	C 2	C 3	C 4	C 5	C 6	C 7	N 8	C 9	N10	N11
Charges	1.218	0.959	1.003	0.950	1.007	0.903	1.006	1.333	0.992	1.292	1.338

Hueckel Calculation: Bipyridine



Interaction matrix (eV):

	N 1	C 2	C 3	C 4	C 5	C 6	C 7	C 8	C 9	C10	C11	N12
N 1	-12.582	-2.705	0.000	0.000	0.000	-2.646	0.000	0.000	0.000	0.000	0.000	0.000
C 2	-2.705	-11.459	-2.830	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C 3	0.000	-2.830	-11.180	-2.795	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C 4	0.000	0.000	-2.795	-11.180	-2.795	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C 5	0.000	0.000	0.000	-2.795	-11.180	-2.765	0.000	0.000	0.000	0.000	0.000	0.000
C 6	-2.646	0.000	0.000	0.000	-2.765	-10.939	-2.735	0.000	0.000	0.000	0.000	0.000
C 7	0.000	0.000	0.000	0.000	0.000	-2.735	-10.939	-2.765	0.000	0.000	0.000	-2.646
C 8	0.000	0.000	0.000	0.000	0.000	0.000	-2.765	-11.180	-2.795	0.000	0.000	0.000
C 9	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-2.795	-11.180	-2.795	0.000	0.000
C10	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-2.795	-11.180	-2.765	0.000
C11	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-2.765	-10.939	-2.646
N12	0.000	0.000	0.000	0.000	0.000	0.000	-2.646	0.000	0.000	0.000	-2.646	-12.582

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	1(2)	2(2)	3(2)	4(2)	5(2)	6(2)	7(0)	8(0)	9(0)	10(0)	11(0)	12(0)
Energies	-17.590	-16.631	-14.801	-14.381	-14.265	-13.254	-9.565	-8.811	-8.633	-7.461	-6.088	-5.039

The total energy is -181.844 eV

MO-coefficients:

	1(2)	2(2)	3(2)	4(2)	5(2)	6(2) χ HOMO	7(0) ψ LUMO	8(0) χ SLUMO	9(0)	10(0)	11(0)	12(0)
N 1	0.368	0.323	-0.106	-0.539	-0.061	0.237	0.394	0.385	-0.062	-0.035	-0.196	-0.228
C 2	0.257	0.342	0.272	-0.366	-0.181	-0.235	-0.079	-0.511	0.239	-0.287	0.287	0.178
C 3	0.206	0.316	0.422	0.137	-0.121	-0.375	-0.324	0.111	-0.179	0.440	-0.357	-0.186
C 4	0.211	0.271	0.272	0.528	0.049	-0.041	0.267	0.424	-0.078	-0.294	0.360	0.228
C 5	0.279	0.212	-0.070	0.468	0.176	0.345	0.170	-0.470	0.251	-0.048	-0.299	-0.315
C 6	0.433	0.144	-0.367	0.008	0.146	0.300	-0.369	-0.025	-0.152	0.362	0.187	0.469
C 7	0.415	-0.226	-0.345	0.059	0.059	-0.324	-0.368	0.123	-0.066	-0.378	0.160	-0.472
C 8	0.260	-0.268	0.014	-0.072	0.458	-0.387	0.183	0.138	0.504	0.088	-0.281	0.319
C 9	0.186	-0.299	0.360	-0.141	0.447	0.033	0.259	-0.239	-0.394	0.257	0.354	-0.234
C10	0.167	-0.315	0.452	-0.089	0.036	0.412	-0.332	0.064	-0.145	-0.430	-0.364	0.195
C11	0.198	-0.318	0.228	0.039	-0.413	0.276	-0.067	0.186	0.532	0.318	0.313	-0.197
N12	0.324	-0.356	-0.139	0.144	-0.556	-0.189	0.382	-0.217	-0.312	0.031	-0.193	0.235

	N 1	C 2	C 3	C 4	C 5	C 6	C 7	C 8	C 9	C10	C11	N12
Charges	1.202	0.958	0.990	0.950	0.992	0.908	0.908	1.010	0.949	1.019	0.881	1.233
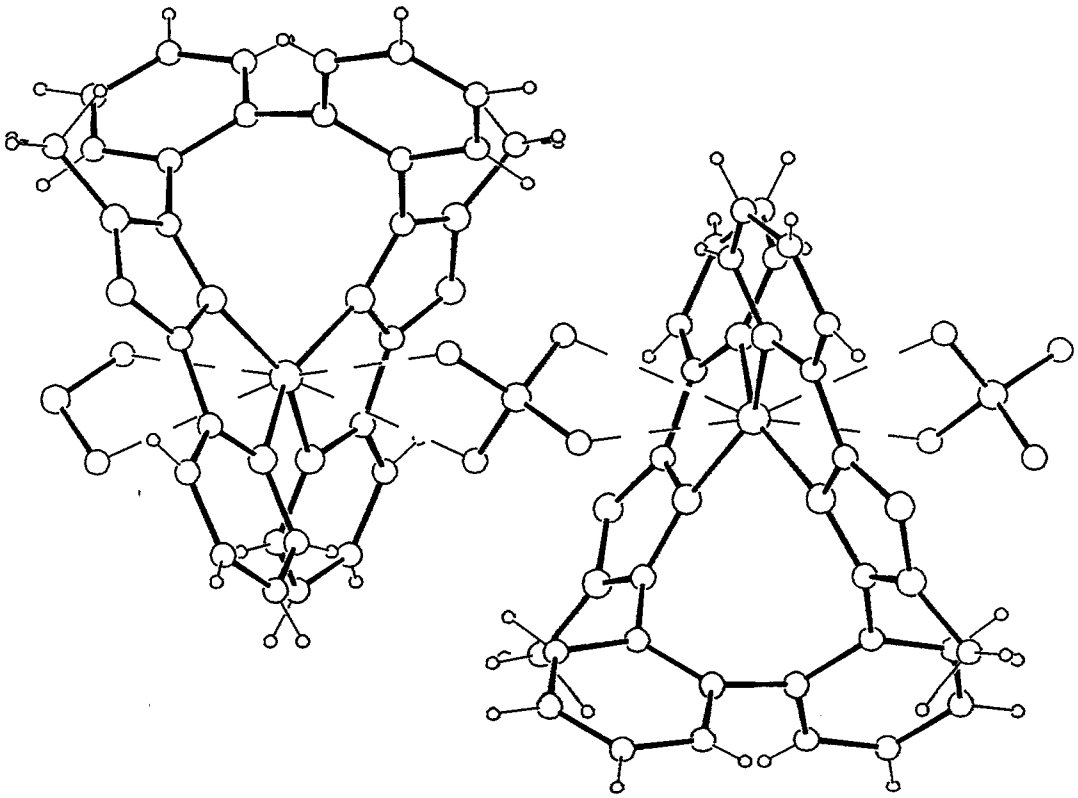
Figure 7: The axial contacts of $[Cu^{II}(\mathbf{mbptb})]^{2+}$ with one of the perchlorate anions.