Inorganic Chemistry
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Supplementary Material

AF50

Experimental. A prismatic crystal (0.1x0.1x0.2 mm) was selected and mounted on a Enraf-Nonius CAD4 four-circle diffractometer. Unit-cell parameters were determined from automatic centering of 25 reflections ($12 < \theta < 21^{\circ}$) and refined by least-squares method. Intensities were collected with graphite monochromatized Mo Kα radiation, using $\omega/2\theta$ scan-technique. 6769 reflections were measured in the range $1.61 \leq \theta \leq 30.02$. 5049 reflections were assumed as observed applying the condition $I > 2\sigma(I)$. Three reflections were measured every two hours as orientation and intensity control, significant intensity decay was not observed. Lorentz-polarization and absorption corrections were made.

The structure was solved by Patterson synthesis, using SHELXS computer program (Sheldrick, G.M., (1990), Acta Cryst., A46, 467-473) and refined by full-matrix least-squares method with SHELX93 computer program (Sheldrick, G.M., (1994), in preparation), using 6719 reflections, (very negative intensities were not assumed). The function minimized was $\Sigma\ w\ |\ |Fo|^2 - |Fc|^2|^2$, where $w = [\sigma^2(I) + (0.0820\ P)^2]^{-1}$, and $P = (|Fo|^2 + 2\ |Fc|^2)/3$, f, f' and f" were taken from International Tables of X-Ray Crystallography (International Tables of X-Ray Crystallography, (1974), Ed. Kynoch press, Vol. IV, pp 99-100 and 149). Refinement gave that the crystal was a twin with twin law (-1,0,0/0,1,0/0,0,-1). Refinement lead a proportion of every crystal of 0.92 and 0.08. The extinction coefficient was 0.00043. The chyrality of structure was define from the Flack coefficient, which it is equal to 0.01(4) for the given results (Flack, H.D., (1983), Acta Cryst., A39, 876-881). 0.044, wR(on $|F|^2$) = 0.119 and goodness of fit = 1.158 for all observed reflections. Number of refined parameters was 468. Max. shift/esd = 3.9, Mean shift/esd = 0.31. Max. and min. peaks in final difference synthesis was 1.138 and -0.916 eÅ^{-3}, respectively.

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Table S1. Crystal data and structure refinement for 1.

Identification code	af50
Empirical formula	$C_{22}H_{57}Cl_4Cu_3N_9O_{19}$
Formula weight	1084.20
Temperature	293(2) K
Wavelength	0.71069Å
Crystal system	monoclinic
Space group	Cc
Unit cell dimensions	a = 16.849(5)Å α = 90°. b = 20.907(4)Å β = 109.69(4)°. c = 13.501(7)Å γ = 90°.
Volume	4478(3) Å³
Z	4
Density (calculated)	1.608 Mg/m³
Absorption coefficient	1.782 mm⁻¹
F(000)	2236
Crystal size	0.1 x 0.1 x 0.2 mm
Theta range for data collection	1.61 to 30.02°.
Index ranges	-23<=h<=22, 0<=k<=29, 0<=l<=18
Reflections collected	6769
Independent reflections	6769
Refinement method	Full-matrix least-squares on F^2
Data / parameters	6719 / 468
Goodness-of-fit on F^2	1.078
Final R indices [I>2σ(I)]	R1 = 0.0444, wR2 = 0.1191
R indices (all data)	R1 = 0.0647, wR2 = 0.1418
Absolute structure parameter	0.01(4)
Extinction coefficient	0.0004(3)
Largest diff. peak and hole	1.138 and -0.916 e.Å⁻³

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Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cu(1)	7830(1)	1367(1)	5456(1)	41(1)
Cu(2)	6640(1)	2440(1)	7841(1)	41(1)
Cu(3)	7775(1)	3692(1)	5579(1)	41(1)
O(1)	7286(7)	1885(4)	6258(7)	48(2)
O(2)	7017(6)	2855(4)	6758(6)	45(2)
O(3)	7624(7)	2756(3)	5544(8)	49(2)
Cl(1)	6430(4)	247(2)	5669(5)	86(2)
O(11)	7060(10)	354(8)	5200(14)	99(5)
O(12)	5971(22)	-273(16)	5355(29)	104(10)
O(13)	5960(36)	817(23)	5580(54)	105(37)
O(14)	7001(22)	312(17)	6838(21)	90(9)
O(12′)	6340(17)	-428(11)	5796(23)	77(6)
O(13′)	5687(33)	549(30)	5084(52)	269(36)
O(14′)	6663(25)	504(18)	6680(26)	108(11)
Cl(2)	5477(4)	3805(2)	7561(5)	85(2)
O(21)	5625(9)	3216(7)	8091(13)	88(4)
O(22)	4781(21)	3954(18)	7333(34)	152(12)
O(23)	6254(18)	4111(19)	7884(33)	113(10)
O(24)	5189(14)	4258(11)	8181(19)	72(5)
O(22′)	5173(58)	3535(38)	6605(38)	274(48)
O(23′)	5598(26)	3792(24)	6591(43)	141(15)
O(24′)	5728(14)	4190(11)	8214(19)	72(5)
Cl(3)	7736(5)	3449(2)	3057(4)	87(2)
O(31)	7786(10)	3921(8)	3772(14)	103(5)
O(32)	8536(19)	3098(14)	3589(23)	91(8)
O(33)	7252(26)	3619(24)	2257(29)	212(18)
O(34)	8116(15)	3667(12)	2321(19)	142(7)
O(32′)	8204(21)	2972(15)	3622(27)	103(9)
O(33′)	6909(21)	3294(21)	3311(40)	168(14)
O(34′)	7319(28)	2876(20)	2810(45)	190(19)
Cl(4)	4716(3)	2496(2)	3592(5)	77(1)
O(41)	5500(18)	2503(10)	4371(25)	133(8)
O(42)	4150(24)	2898(22)	3765(36)	214(15)
O(43)	4349(18)	1906(15)	3361(26)	164(10)
O(44)	4754(26)	2713(20)	2604(31)	200(14)
N(1)	7031(11)	1713(7)	4106(10)	69(4)
N(2)	8686(8)	1053(6)	4804(10)	55(3)
N(3)	8485(12)	1053(7)	6914(11)	80(5)
N(4)	5732(10)	2007(8)	6707(12)	71(3)
N(5)	6580(9)	1838(5)	9010(9)	57(3)
N(6)	7526(11)	3000(8)	8794(12)	75(4)
N(7)	6536(9)	3791(7)	5110(12)	65(3)
N(8)	8024(9)	4615(5)	6114(11)	56(3)
N(9)	8974(10)	3442(7)	5893(15)	77(4)
C(1)	7304(8)	2507(4)	6178(9)	36(2)
C(2)	6880(15)	1380(9)	3112(13)	78(6)
C(3)	7773(18)	1260(12)	2945(19)	90(6)
C(4)	8275(18)	818(9)	3658(18)	94(7)

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C(5)	9243(19)	493(13)	5361(25)	105(8)
C(6)	9678(15)	572(15)	6520(28)	104(9)
C(7)	9031(17)	494(10)	7137(20)	95(7)
C(8)	9223(13)	1611(10)	4823(17)	76(5)
C(9)	4997(12)	1745(12)	6908(17)	80(6)
C(10)	5302(18)	1283(11)	7898(28)	98(8)
C(11)	5695(16)	1613(10)	8827(20)	90(6)
C(12)	6861(26)	2134(12)	10112(18)	123(11)
C(13)	7735(29)	2456(10)	10506(19)	98(9)
C(14)	7655(17)	3093(10)	9927(16)	91(7)
C(15)	7137(13)	1302(8)	8972(17)	75(5)
C(16)	6119(15)	4412(11)	4679(18)	86(6)
C(17)	6503(16)	4944(10)	5380(21)	89(7)
C(18)	7336(18)	5072(8)	5435(22)	99(7)
C(19)	8826(23)	4880(11)	6088(26)	114(11)
C(20)	9625(18)	4497(14)	6617(25)	100(8)
C(21)	9628(17)	3897(14)	5934(22)	103(7)
C(22)	7997(13)	4573(9)	7218(14)	73(4)

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Table S3. Bond lengths [Å] and angles [°] for 1.

Cu(1)-O(1)	1.963(9)
Cu(1)-N(1)	2.001(13)
Cu(1)-N(3)	2.016(14)
Cu(1)-N(2)	2.035(11)
Cu(1)-O(11)	2.45(2)
Cu(2)-N(4)	1.98(2)
Cu(2)-O(2)	1.980(8)
Cu(2)-N(6)	1.991(14)
Cu(2)-N(5)	2.048(11)
Cu(2)-O(21)	2.46(2)
Cu(3)-N(7)	1.977(14)
Cu(3)-O(3)	1.973(7)
Cu(3)-N(9)	1.99(2)
Cu(3)-N(8)	2.053(11)
Cu(3)-O(31)	2.49(2)
O(1)-C(1)	1.306(11)
O(2)-C(1)	1.277(12)
O(3)-C(1)	1.267(13)
Cl(1)-O(13′)	1.39(4)
Cl(1)-O(14′)	1.39(3)
Cl(1)-O(13)	1.41(4)
Cl(1)-O(12)	1.32(3)
Cl(1)-O(11)	1.42(2)
Cl(1)-O(12′)	1.44(2)
Cl(1)-O(14)	1.55(3)
Cl(2)-O(23′)	1.39(4)
Cl(2)-O(22′)	1.15(3)
Cl(2)-O(24)	1.45(2)
Cl(2)-O(24′)	1.16(2)
Cl(2)-O(22)	1.34(5)
Cl(2)-O(21)	1.40(2)
Cl(2)-O(23)	1.39(3)
Cl(3)-O(32′)	1.34(3)
Cl(3)-O(34′)	1.37(4)
Cl(3)-O(33)	1.17(3)
Cl(3)-O(34)	1.43(2)
Cl(3)-O(31)	1.36(2)
Cl(3)-O(33′)	1.58(4)
Cl(3)-O(32)	1.49(3)
Cl(4)-O(41)	1.38(3)
Cl(4)-O(43)	1.37(3)
Cl(4)-O(42)	1.35(4)
Cl(4)-O(44)	1.43(4)
N(1)-C(2)	1.46(2)
N(2)-C(8)	1.47(2)
N(2)-C(4)	1.55(2)
N(2)-C(5)	1.53(3)
N(3)-C(7)	1.46(2)
N(4)-C(9)	1.46(2)
N(5)-C(11)	1.50(3)
N(5)-C(15)	1.47(2)
N(5)-C(12)	1.53(3)
N(6)-C(14)	1.48(2)
N(7)-C(16)	1.50(2)

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N(8)-C(19)	1.47(3)
N(8)-C(22)	1.51(2)
N(8)-C(18)	1.54(3)
N(9)-C(21)	1.44(3)
C(2)-C(3)	1.61(4)
C(3)-C(4)	1.40(4)
C(5)-C(6)	1.50(5)
C(6)-C(7)	1.59(4)
C(9)-C(10)	1.59(4)
C(10)-C(11)	1.39(4)
C(12)-C(13)	1.54(5)
C(13)-C(14)	1.53(3)
C(16)-C(17)	1.46(4)
C(17)-C(18)	1.41(4)
C(19)-C(20)	1.52(5)
C(20)-C(21)	1.56(4)

O(1)-Cu(1)-N(1)	90.4(5)
O(1)-Cu(1)-N(3)	81.0(5)
N(1)-Cu(1)-N(3)	170.6(7)
O(1)-Cu(1)-N(2)	161.3(5)
N(1)-Cu(1)-N(2)	94.6(6)
N(3)-Cu(1)-N(2)	94.8(6)
O(11)-Cu(1)-N(1)	91.3(7)
O(11)-Cu(1)-N(2)	94.5(7)
O(11)-Cu(1)-N(3)	86.9(7)
O(11)-Cu(1)-O(1)	103.4(7)
N(4)-Cu(2)-O(2)	89.2(5)
N(4)-Cu(2)-N(6)	169.8(7)
O(2)-Cu(2)-N(6)	82.1(5)
N(4)-Cu(2)-N(5)	95.1(6)
O(2)-Cu(2)-N(5)	161.8(5)
N(6)-Cu(2)-N(5)	94.8(6)
N(4)-Cu(2)-O(21)	90.9(6)
O(2)-Cu(2)-O(21)	102.9(4)
N(6)-Cu(2)-O(21)	85.9(6)
N(5)-Cu(2)-O(21)	94.8(5)
N(7)-Cu(3)-O(3)	89.0(5)
N(7)-Cu(3)-N(9)	169.2(7)
O(3)-Cu(3)-N(9)	81.8(5)
N(7)-Cu(3)-N(8)	94.8(6)
O(3)-Cu(3)-N(8)	161.9(5)
N(9)-Cu(3)-N(8)	95.7(6)
O(31)-Cu(3)-N(7)	91.3(7)
O(31)-Cu(3)-N(8)	95.5(7)
O(31)-Cu(3)-N(9)	85.2(7)
O(31)-Cu(3)-O(3)	102.1(7)
C(1)-O(1)-Cu(1)	118.4(7)
C(1)-O(2)-Cu(2)	119.1(6)
C(1)-O(3)-Cu(3)	118.1(7)
O(13')-Cl(1)-O(14')	107(3)
O(13)-Cl(1)-O(12)	115(3)
O(13)-Cl(1)-O(11)	108(3)
O(12)-Cl(1)-O(11)	116(2)
O(13')-Cl(1)-O(12')	114(3)
O(14')-Cl(1)-O(12')	106(2)
O(13)-Cl(1)-O(12')	139(3)
O(13)-Cl(1)-O(14)	99(3)

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O(12)-Cl(1)-O(14)	120(2)
O(11)-Cl(1)-O(14)	98.0(14)
O(21)-Cl(2)-O(22′)	93.8(4)
O(21)-Cl(2)-O(23)	104.8(12)
O(21)-Cl(2)-O(24)	108.4(12)
O(21)-Cl(2)-O(22)	111.4(12)
O(21)-Cl(2)-O(23′)	113.9(14)
O(21)-Cl(2)-O(24′)	105.3(14)
O(22′)-Cl(2)-O(23)	121(2)
O(22′)-Cl(2)-O(24)	137(3)
O(23)-Cl(2)-O(24)	89(5)
O(22)-Cl(2)-O(23′)	102(2)
O(22)-Cl(2)-O(24′)	95(3)
O(23′)-Cl(2)-O(24′)	127(3)
Cl(2)-O(21)-Cu(2)	121.4(9)
O(33)-Cl(3)-O(31)	107(2)
O(34)-Cl(3)-O(31)	109.0(12)
O(32′)-Cl(3)-O(33′)	97(2)
O(34)-Cl(3)-O(32)	87(2)
O(31)-Cl(3)-O(32)	100.7(14)
O(41)-Cl(4)-O(43)	115(2)
O(41)-Cl(4)-O(42)	114(2)
O(43)-Cl(4)-O(42)	108(2)
O(41)-Cl(4)-O(44)	112(2)
O(43)-Cl(4)-O(44)	103(2)
O(42)-Cl(4)-O(44)	103(3)
C(2)-N(1)-Cu(1)	121.5(11)
C(8)-N(2)-C(4)	109.6(13)
C(8)-N(2)-C(5)	109(2)
C(4)-N(2)-C(5)	104(2)
C(8)-N(2)-Cu(1)	104.9(9)
C(4)-N(2)-Cu(1)	113.0(12)
C(5)-N(2)-Cu(1)	116.1(11)
C(7)-N(3)-Cu(1)	124.3(14)
C(9)-N(4)-Cu(2)	120.6(12)
C(11)-N(5)-C(15)	111.4(14)
C(11)-N(5)-C(12)	105(2)
C(15)-N(5)-C(12)	110(2)
C(11)-N(5)-Cu(2)	111.7(12)
C(15)-N(5)-Cu(2)	104.1(10)
C(12)-N(5)-Cu(2)	114.9(11)
C(14)-N(6)-Cu(2)	124.1(13)
C(16)-N(7)-Cu(3)	121.4(13)
C(19)-N(8)-C(22)	112(2)
C(19)-N(8)-C(18)	105(2)
C(22)-N(8)-C(18)	110.8(14)
C(19)-N(8)-Cu(3)	115.3(11)
C(22)-N(8)-Cu(3)	102.9(10)
C(18)-N(8)-Cu(3)	110.4(12)
C(21)-N(9)-Cu(3)	123(2)
O(3)-C(1)-O(2)	121.1(8)
O(3)-C(1)-O(1)	119.4(9)
O(2)-C(1)-O(1)	119.5(9)
N(1)-C(2)-C(3)	109(2)
C(4)-C(3)-C(2)	113(2)
C(3)-C(4)-N(2)	116(2)
C(6)-C(5)-N(2)	116(2)
C(5)-C(6)-C(7)	111(2)

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N(3)-C(7)-C(6)	108(2)
N(4)-C(9)-C(10)	109(2)
C(11)-C(10)-C(9)	112(2)
C(10)-C(11)-N(5)	117(2)
C(13)-C(12)-N(5)	117(2)
C(12)-C(13)-C(14)	107(3)
N(6)-C(14)-C(13)	112(2)
C(17)-C(16)-N(7)	111(2)
C(18)-C(17)-C(16)	113(2)
C(17)-C(18)-N(8)	117(2)
C(20)-C(19)-N(8)	118(2)
C(19)-C(20)-C(21)	109(2)
N(9)-C(21)-C(20)	114(2)

Symmetry transformations used to generate equivalent atoms:

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Table 5. Anisotropic displacement parameters (Å² x 10³) for 1. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cu(1)	62(1)	29(1)	40(1)	0(1)	27(1)	3(1)
Cu(2)	61(1)	34(1)	36(1)	-1(1)	27(1)	-1(1)
Cu(3)	61(1)	29(1)	42(1)	2(1)	27(1)	-3(1)
O(1)	84(6)	26(3)	49(4)	2(3)	43(5)	-1(4)
O(2)	83(6)	28(3)	36(4)	3(3)	36(4)	2(3)
O(3)	84(6)	26(3)	52(5)	-7(3)	44(5)	-11(4)
Cl(1)	119(4)	47(2)	124(4)	-17(2)	82(3)	-19(2)
Cl(2)	129(4)	64(2)	95(3)	25(2)	79(3)	39(3)
Cl(3)	166(5)	57(2)	60(2)	-3(2)	67(3)	-17(3)
Cl(4)	75(3)	83(3)	63(2)	-1(2)	8(2)	-1(2)
N(1)	94(10)	60(7)	41(6)	-8(5)	7(6)	15(7)
N(2)	72(7)	50(6)	55(6)	-3(5)	39(6)	4(5)
N(3)	121(12)	61(8)	45(6)	4(6)	11(7)	36(8)
N(4)	79(8)	75(9)	66(8)	-10(7)	32(7)	-17(7)
N(5)	93(8)	45(5)	42(5)	7(4)	35(6)	-3(5)
N(6)	102(10)	77(9)	59(8)	-29(7)	42(8)	-35(8)
N(7)	70(8)	62(7)	55(7)	20(6)	10(6)	13(6)
N(8)	88(8)	36(5)	58(6)	-8(4)	41(6)	-9(5)
N(9)	85(10)	52(7)	103(12)	21(7)	42(9)	10(7)
C(1)	58(6)	23(4)	36(5)	3(4)	26(5)	7(4)
C(2)	111(15)	57(9)	41(7)	-9(7)	-6(9)	-2(9)
C(3)	120(16)	92(15)	59(11)	-15(10)	30(11)	7(12)
C(4)	165(19)	67(10)	89(12)	-41(10)	95(14)	-31(12)
C(5)	137(21)	82(15)	126(21)	0(14)	85(19)	28(14)
C(6)	63(10)	113(16)	135(24)	57(17)	35(13)	41(11)
C(7)	118(17)	61(10)	90(15)	29(10)	16(13)	29(11)
C(8)	86(11)	77(11)	78(11)	-18(9)	48(10)	-12(9)
C(9)	61(9)	106(15)	78(12)	-30(11)	29(9)	-34(10)
C(10)	98(14)	78(13)	141(23)	15(15)	70(16)	-24(12)
C(11)	124(16)	72(10)	115(16)	-6(11)	94(14)	-24(11)
C(12)	255(37)	82(14)	60(11)	5(10)	90(18)	-8(19)
C(13)	173(27)	71(11)	43(8)	-3(7)	26(11)	19(14)
C(14)	139(19)	65(10)	64(10)	-30(9)	28(12)	-20(12)
C(15)	91(12)	56(8)	82(11)	18(8)	35(10)	15(8)
C(16)	88(14)	85(13)	79(13)	32(11)	20(11)	34(11)
C(17)	109(15)	60(10)	103(16)	31(11)	42(13)	40(11)
C(18)	157(20)	35(7)	137(18)	30(9)	93(17)	27(10)
C(19)	166(28)	61(12)	160(24)	-44(14)	115(23)	-50(16)
C(20)	97(15)	104(17)	110(16)	-54(14)	49(13)	-56(14)
C(21)	111(17)	117(18)	109(16)	-15(14)	74(15)	-22(14)
C(22)	104(13)	65(9)	54(8)	-13(7)	31(9)	-1(8)

P-251-10

1	Cu1	Cu2	4.875606	.387192	-.460111	-.798987	143.0335	310.0812
2	Cu1	Cu3	4.865662	.017932	-.999017	-.040546	92.3238	271.0283
3	Cu2	Cu3	4.875519	-.369303	-.536877	.758537	40.6646	235.4770

ANGLES

1	Cu1	Cu2	Cu3	120.134305
2	Cu2	Cu3	Cu1	119.931956
3	Cu2	Cu1	Cu3	119.933729

Main planes equations

PIANI QUADRATICI MEDI

```
      1              PIANO       4        7
O1    O2    O3    C1    Cu1   Cu2   Cu3
      12.325       .90002   .01160   .43569
.003 .003 .003-.008 .160 .185 .224

      2              PIANO       7        7
O1    O2    O3    C1    Cu1   Cu2   Cu3
      12.349       .89965   .00076   .43662
.065-.086-.086-.090 .103 .108 .115

      3              PIANO       5        5
Cu1   O1    N1    N2    N3
      -9.266      -.56070  -.82603   .05741
.108-.222 .143-.189 .160

      4              PIANO       5        5
Cu2   O2    N4    N5    N6
       1.732       .67622  -.67171  -.30254
.098 .231-.157 .195-.171

      5              PIANO       5        5
Cu3   O3    N7    N8    N9
       2.596       .05080  -.15599   .98645
.097 .234-.160 .195-.172
```

PIANO		ANGOLO
1	2	.624
1	3	60.711
1	4	62.030
1	5	61.725
2	3	61.315
2	4	61.592
2	5	61.557
3	4	80.890
3	5	80.968
4	5	80.833

Stop - Program terminated.

P-251-11

CNRS/LCC Service de Mesures Magnetiques 14-02-95

*** Juan RIBAS ***

Reference echantillon : AE294
Nom du fichier : 95qd068.SUS
Nombre de points : 32
Masse molaire : 1084.20
Correction pour ligands : -5.450000e-004
Masse de compose (g) : 0.05490

Temp(K)	H(Gauss)	Aimant/g	Khi/g	Khi/a	(M.B.)
2.00	250.00	1.3843e-001	5.5373e-004	6.0090e-001	3.100
2.00	493.14	2.8913e-001	5.8630e-004	6.3621e-001	3.190
2.00	744.13	4.4026e-001	5.9164e-004	6.4200e-001	3.205
2.00	994.01	5.8962e-001	5.9317e-004	6.4366e-001	3.209
2.00	1492.68	8.8661e-001	5.9397e-004	6.4453e-001	3.211
2.00	1995.77	1.1845e+000	5.9349e-004	6.4400e-001	3.210
2.00	2496.65	1.4833e+000	5.9411e-004	6.4468e-001	3.211
2.00	2999.73	1.7799e+000	5.9336e-004	6.4386e-001	3.209
2.00	3502.82	2.0801e+000	5.9385e-004	6.4440e-001	3.210
2.00	4002.59	2.3658e+000	5.9106e-004	6.4137e-001	3.203
2.00	5005.45	2.9539e+000	5.9014e-004	6.4037e-001	3.200
2.00	6006.10	3.5337e+000	5.8835e-004	6.3844e-001	3.196
2.00	7011.17	4.1098e+000	5.8618e-004	6.3609e-001	3.190
2.00	8014.04	4.6780e+000	5.8372e-004	6.3341e-001	3.183
2.00	9016.89	5.2355e+000	5.8063e-004	6.3007e-001	3.175
2.00	10018.65	5.7832e+000	5.7725e-004	6.2640e-001	3.165
2.00	12526.35	7.0951e+000	5.6641e-004	6.1465e-001	3.136
2.00	15031.84	8.3217e+000	5.5360e-004	6.0076e-001	3.100
2.00	17539.55	9.4463e+000	5.3857e-004	5.8446e-001	3.058
2.00	20045.04	1.0455e+001	5.2158e-004	5.6604e-001	3.009
2.00	22550.53	1.1340e+001	5.0288e-004	5.4577e-001	2.955
2.00	25057.12	1.2119e+001	4.8364e-004	5.2491e-001	2.898
2.00	27561.51	1.2762e+001	4.6302e-004	5.0255e-001	2.835
2.00	30070.33	1.3348e+001	4.4389e-004	4.8181e-001	2.776
2.00	32575.81	1.3802e+001	4.2368e-004	4.5990e-001	2.712
2.00	35083.52	1.3999e+001	3.9902e-004	4.3316e-001	2.632
2.00	37590.11	1.4513e+001	3.8610e-004	4.1915e-001	2.589
2.00	40094.49	1.4872e+001	3.7091e-004	4.0269e-001	2.538
2.00	42604.41	1.5024e+001	3.5264e-004	3.8287e-001	2.475
2.00	45107.69	1.5236e+001	3.3777e-004	3.6675e-001	2.422
2.00	47614.29	1.5328e+001	3.2191e-004	3.4956e-001	2.365
2.00	50125.30	1.5691e+001	3.1304e-004	3.3994e-001	2.332