Electronic Supplementary Material (ESI) for Dalton Transactions

Resolution and Characterization of Helicate Dimer and Trimer Complexes of 1,3-bis(9-methyl-1,10-phenanthrolin-2-yl)propane with Copper(I).

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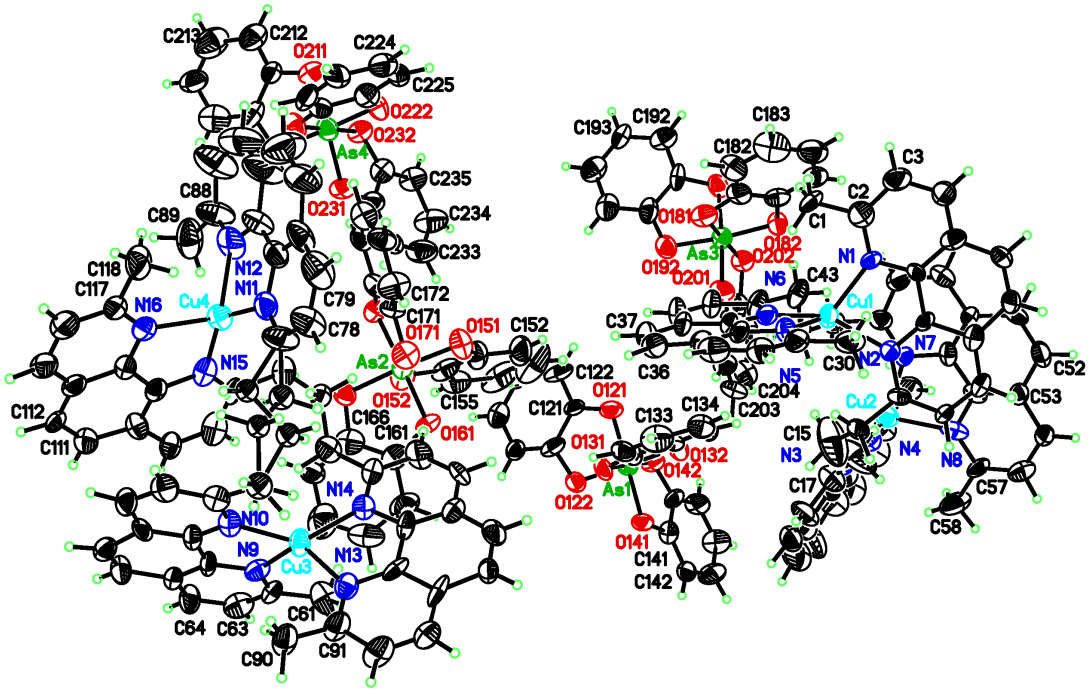
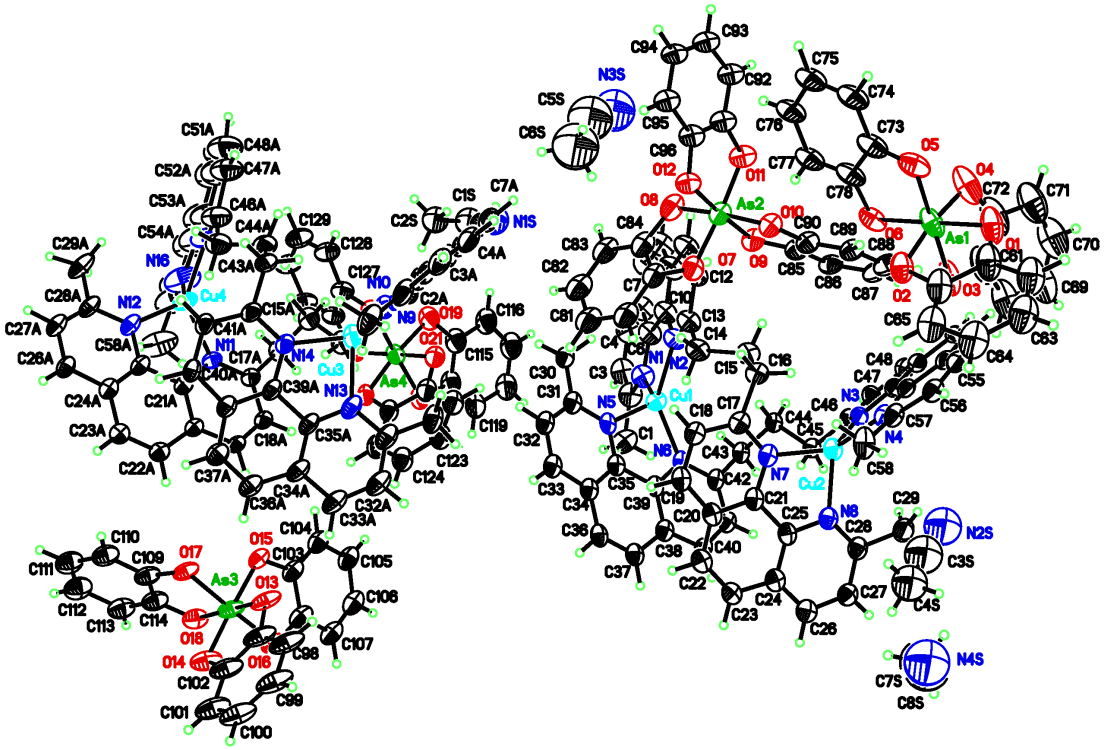
Supplementary information

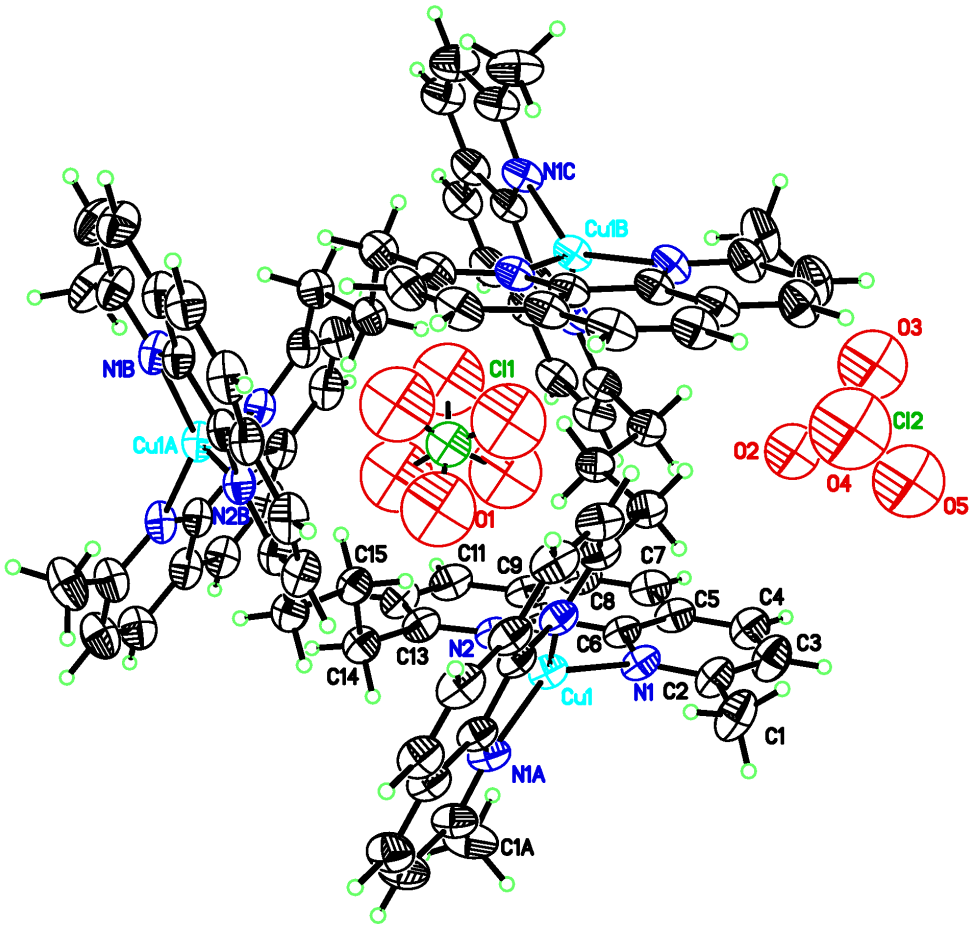
Crystal Structure CIF files for:
P-$[Cu_2(mphenpr)_2](\Delta\text{-}[As(cat)_3])_2$ **Compound 1**
P-$[Cu_2(mphenpr)_2](\Delta\text{-}[As(cat)_3])_2 \cdot 4(CH_3CN)$ **Compound 2**
$[Cu_3(mphenpr)_3](ClO_4)_3$ **Compound 3**
P-$[Cu_3(mphenpr)_3](\Delta\text{-}[As(cat)_3])_3$ **Compound 4**



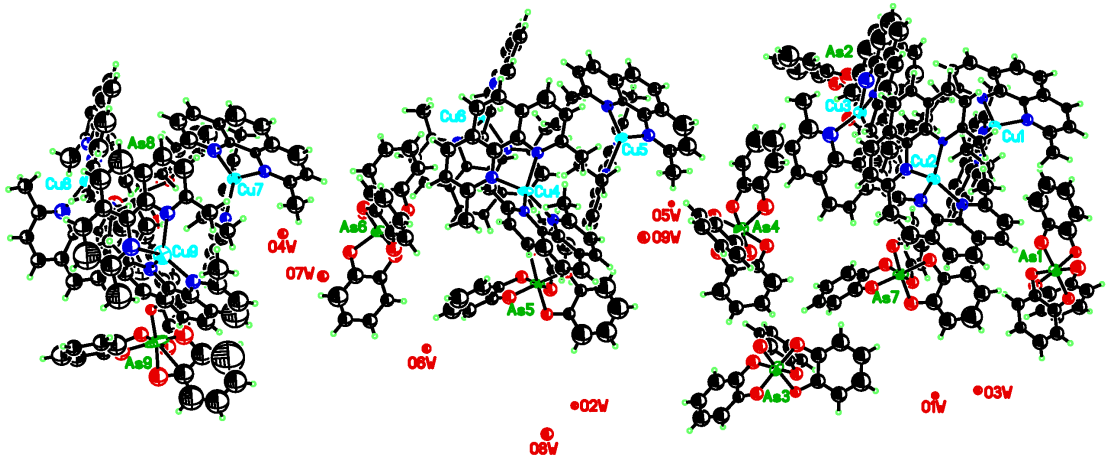
S1: Labeling for Compound 1



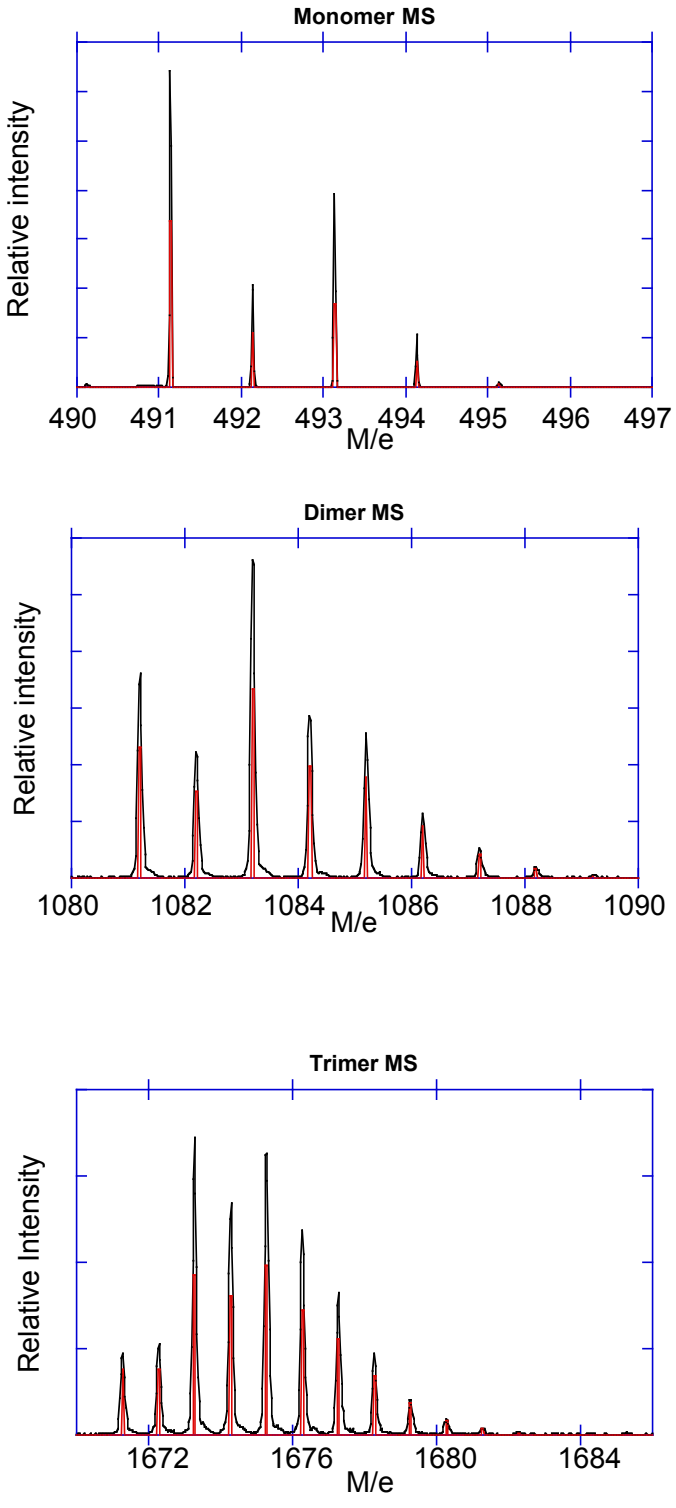
S2: Labeling for Compound 2



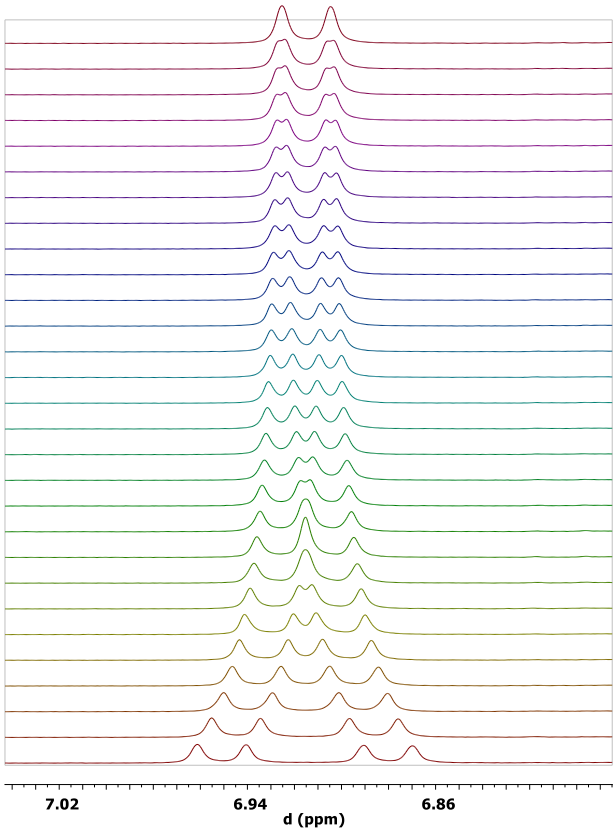
S3: Labeling for Compound 3



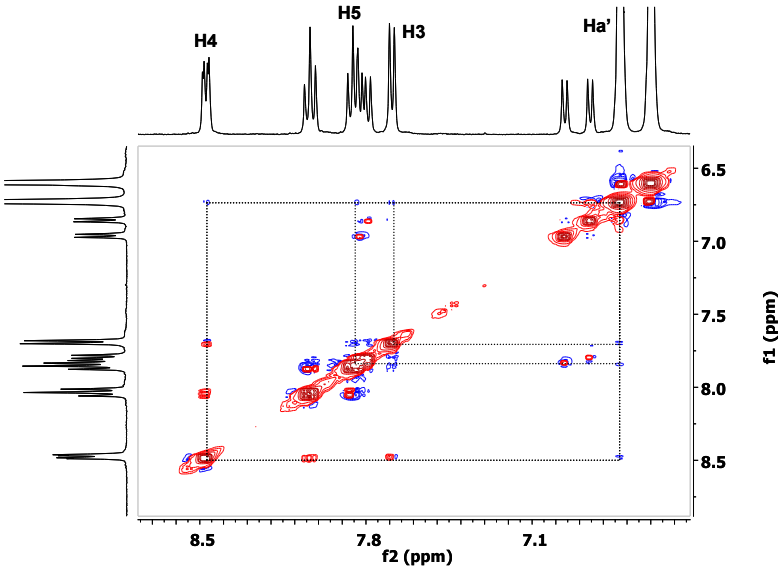
S4: Labeling for Compound 4



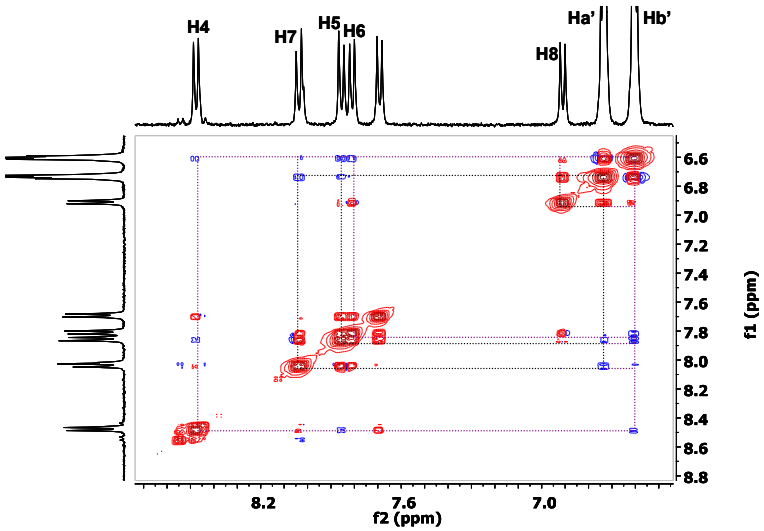
S5: Mass spectra of monomer, $[Cu(mphenpr)]^{+}$, dimer, $[Cu_2(mphenpr)_2](ClO_4)^{+}$, and trimer, $[Cu_3(mphenpr)_3](ClO_4)_2^{+}$, ions. Calculated isotope pattern in red.



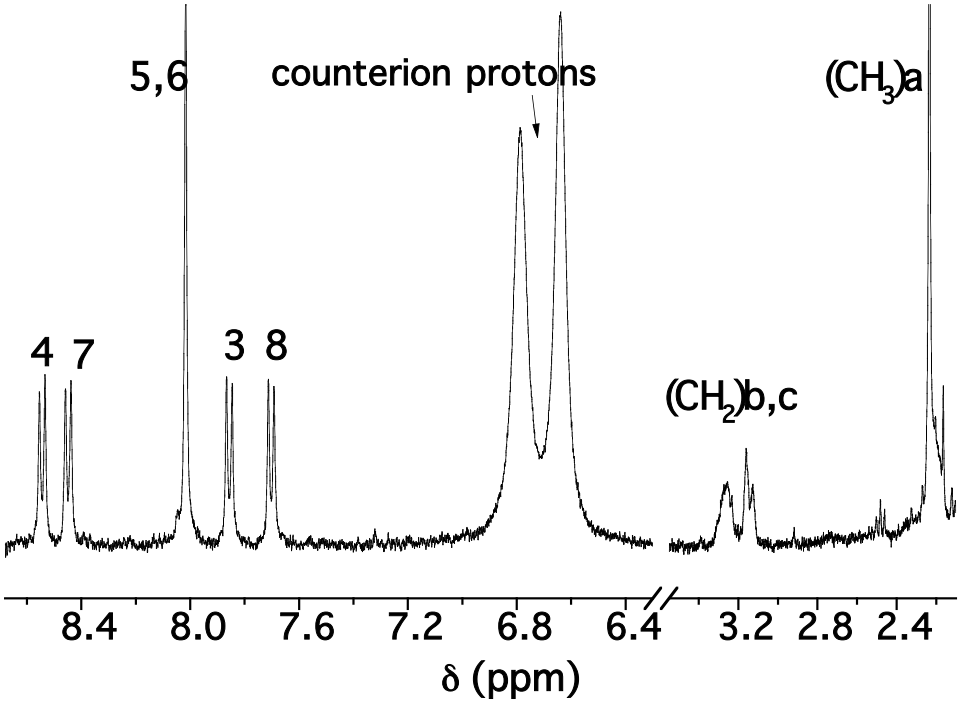
S6: Typical ^{1}H-NMR stack plot for the coalescence of the H8 protons of rac-$[Cu_2(mphenpr)_2](\Delta\text{-}[As(cat)_3])_2$ in TCE at 42 °C.



S7: NOE interactions between the Ha' protons of the chiral counterion with H3, H4 and H5 of the racemic complex, rac-$[Cu_2(mphenpr)_2](\Delta\text{-}[As(cat)_3])_2$ in TCE, indicative that the counterion is placed in a preferential position close to these group of protons of the helicate. No correlations are observed between Hb' and any phenanthroline proton. In addition, there are no significative NOE correlations of Ha' nor Hb' with H8, which is the proton closer to the aliphatic bridge.

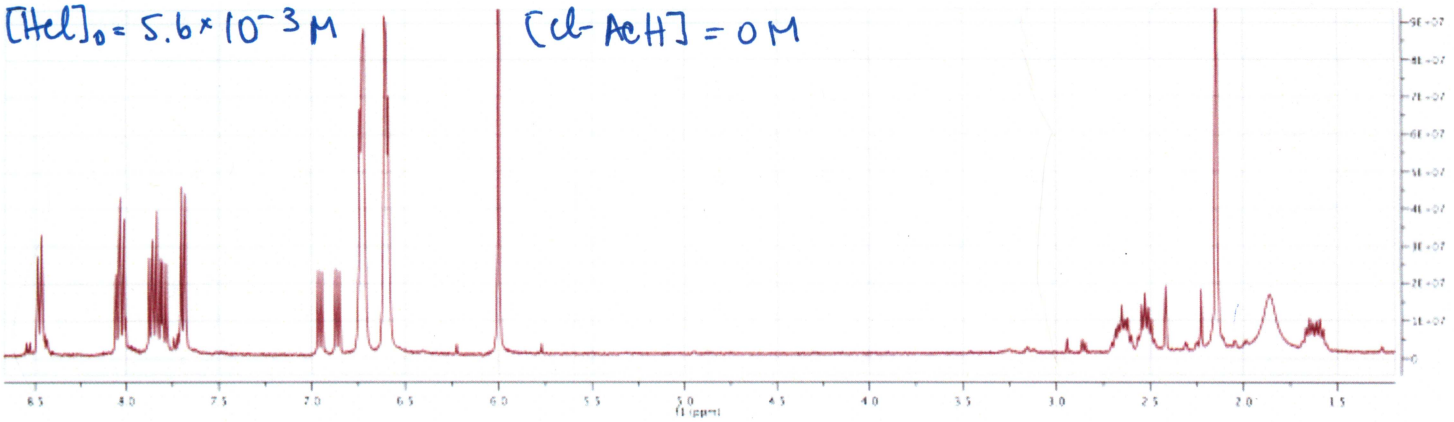


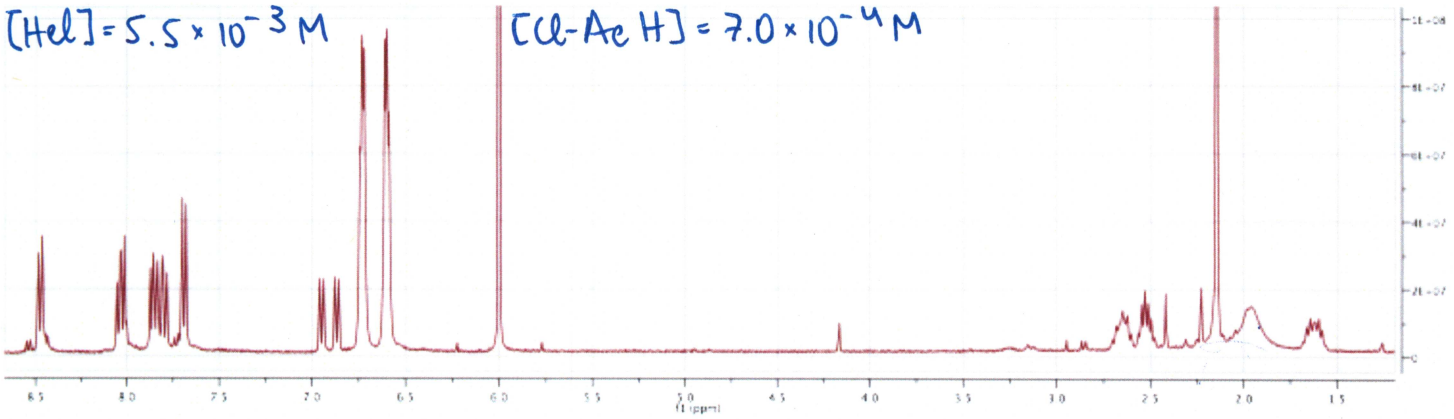
S8: NOE interactions of the coalesced spectrum of rac-$[Cu_2(mphenpr)_2](\Delta\text{-}[As(cat)_3])_2$ in TCE, showing Ha' has NOE correlations with the protons closer to the aliphatic inter-phenanthroline bridge, i.e. H5, H7, H8. In addition, several NOE correlations between Hb' and the aromatic protons of the helicate are observed: Hb'-H4 , Hb'-H5 , Hb'-H6 , Hb'-H7 and Hb'-H8.

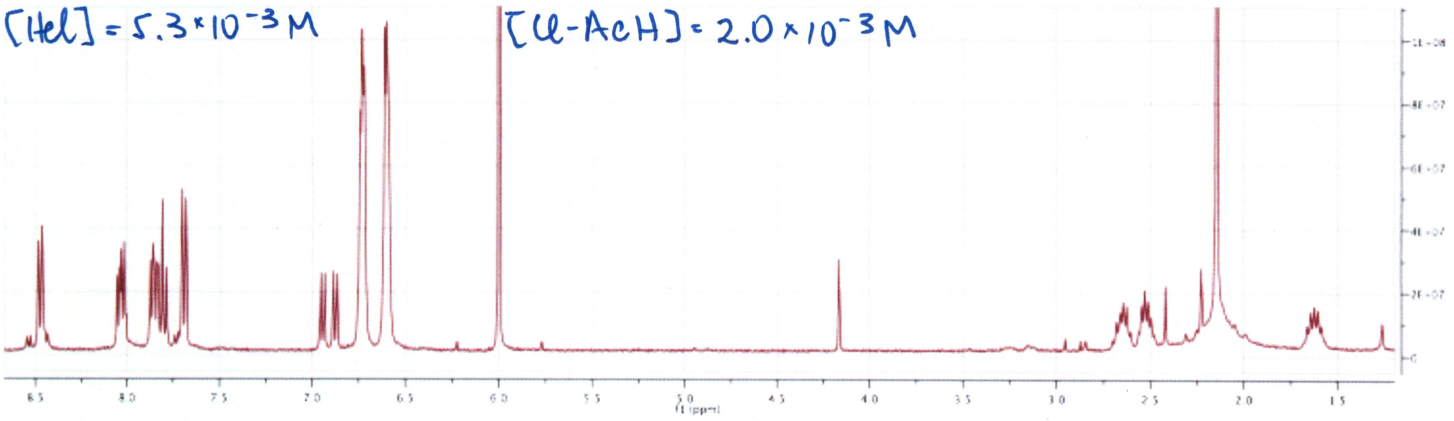


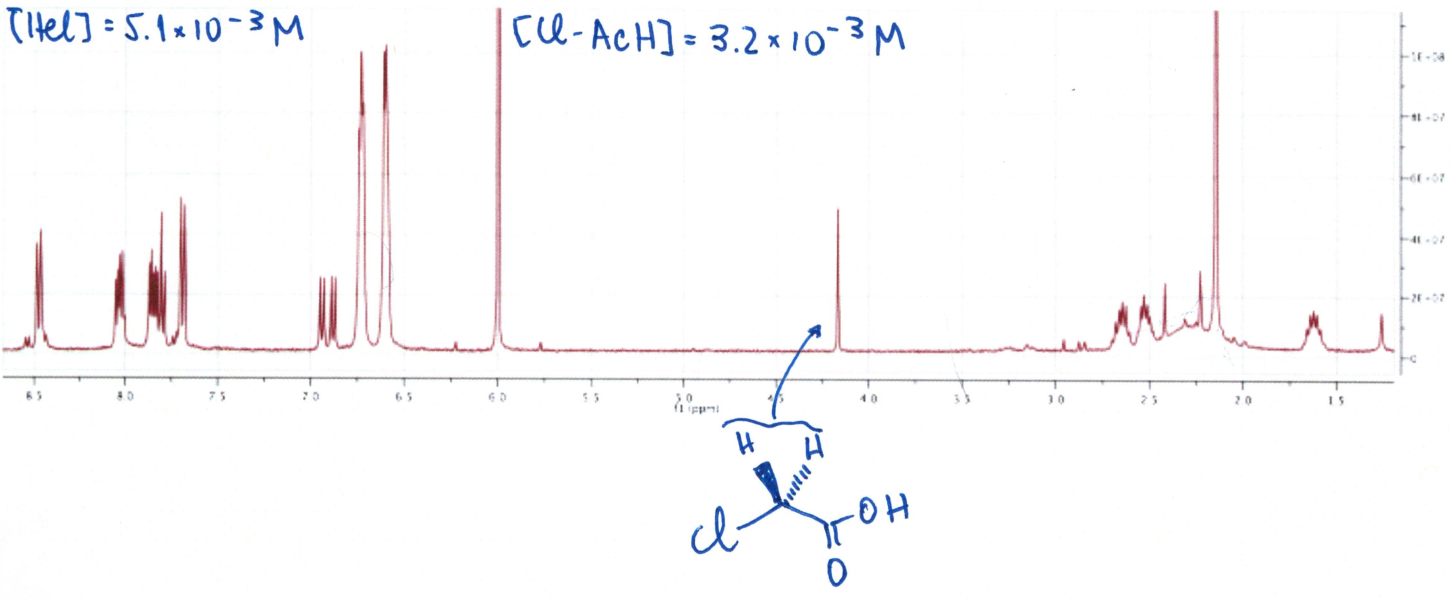
S9: ^{1}H-NMR spectrum of the monometallic complex [Cu(mphenpr)]{(Δ)[As(cat)$_3$]} in *d*$_2$-TCE, produced by heating of the racemic helicate complex, measured after 30 min at 365 K.

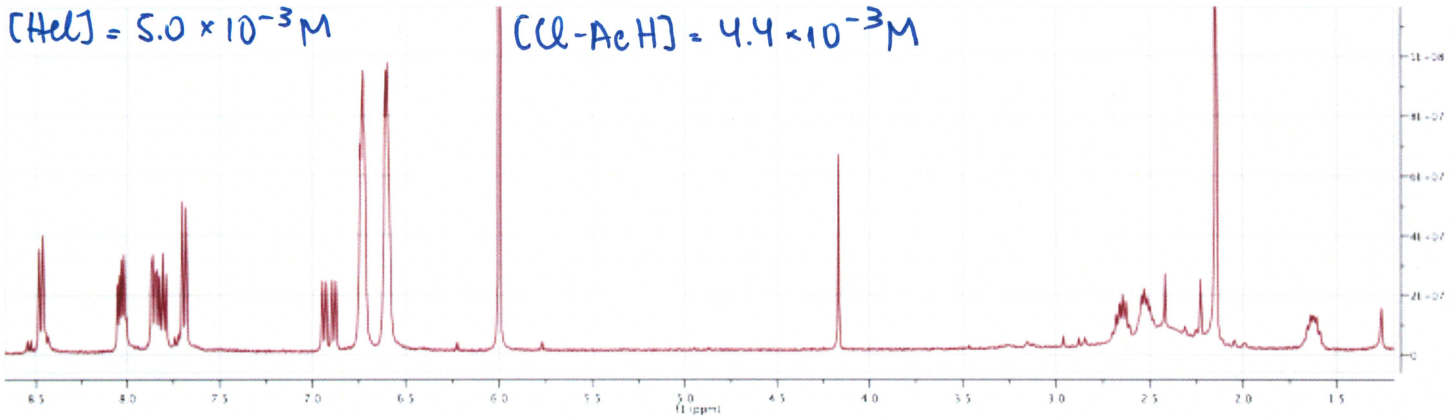
S10: ^{1}H-NMR spectrum of the coalescence of the spectra of P- and M-[Cu$_2$(mphenpr)$_2$](Δ-[As(cat)$_3$])$_2$ in TCE at 25 °C by titration with ClCH$_2$CO$_2$H.

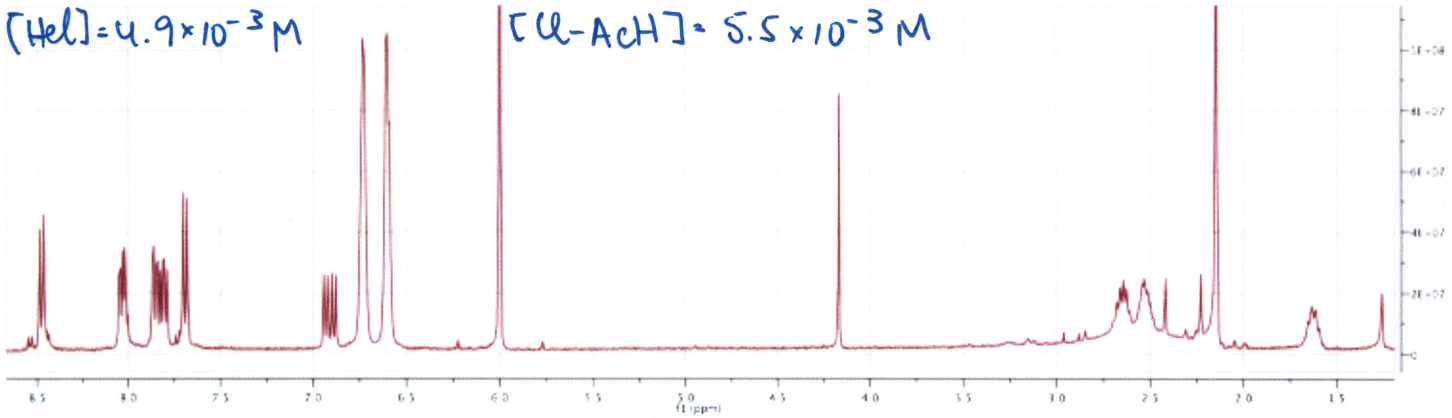


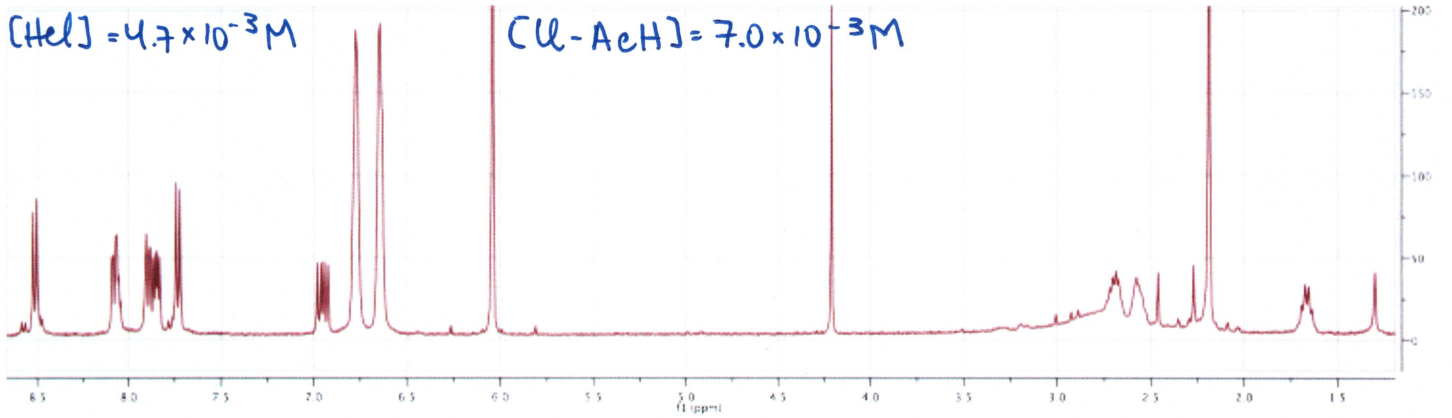


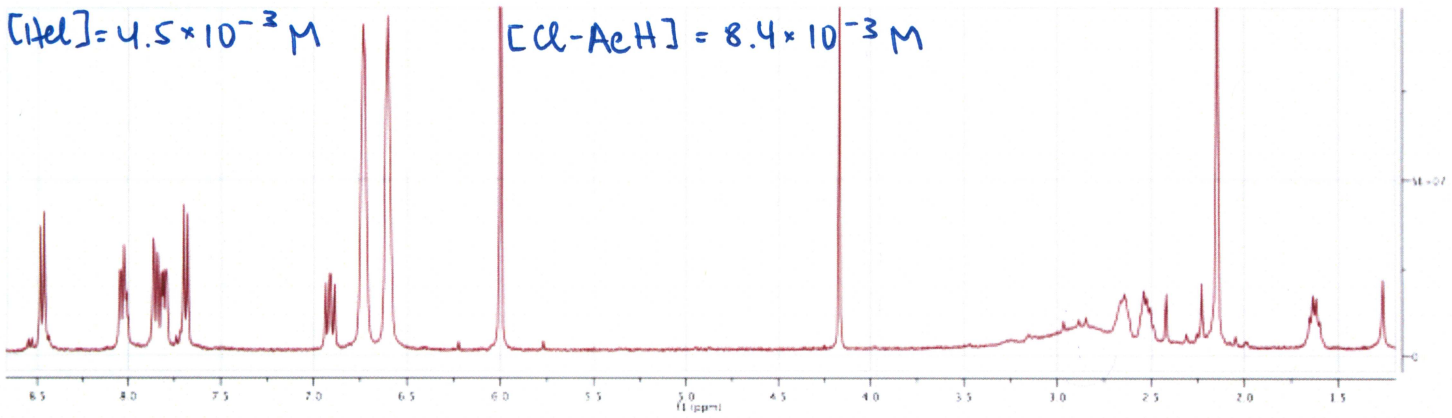


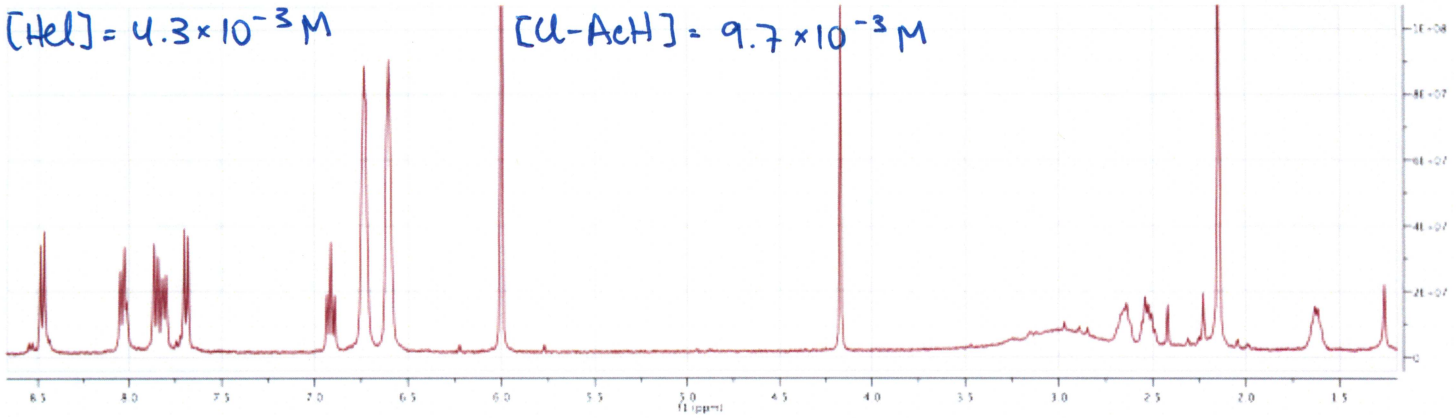


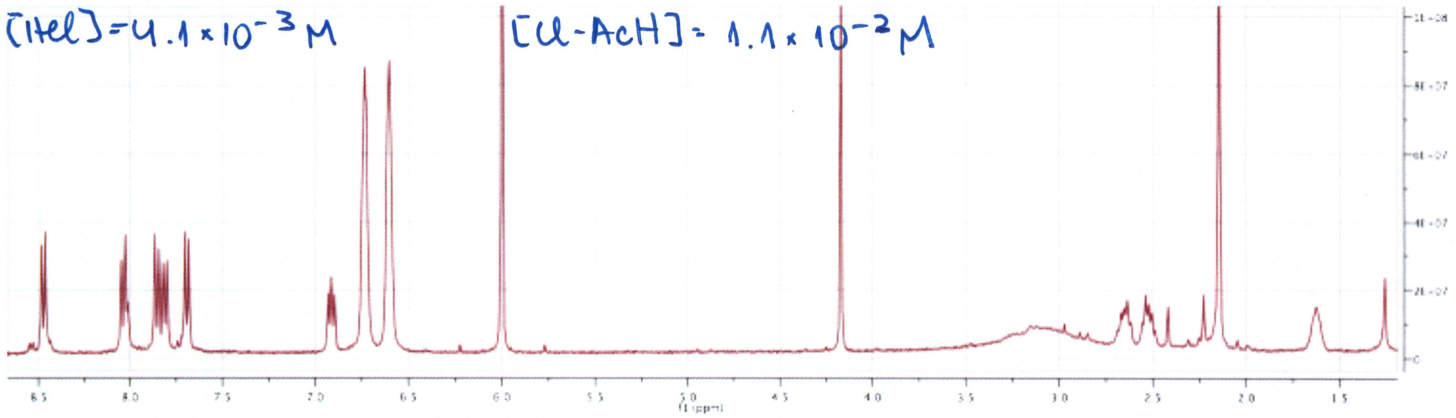


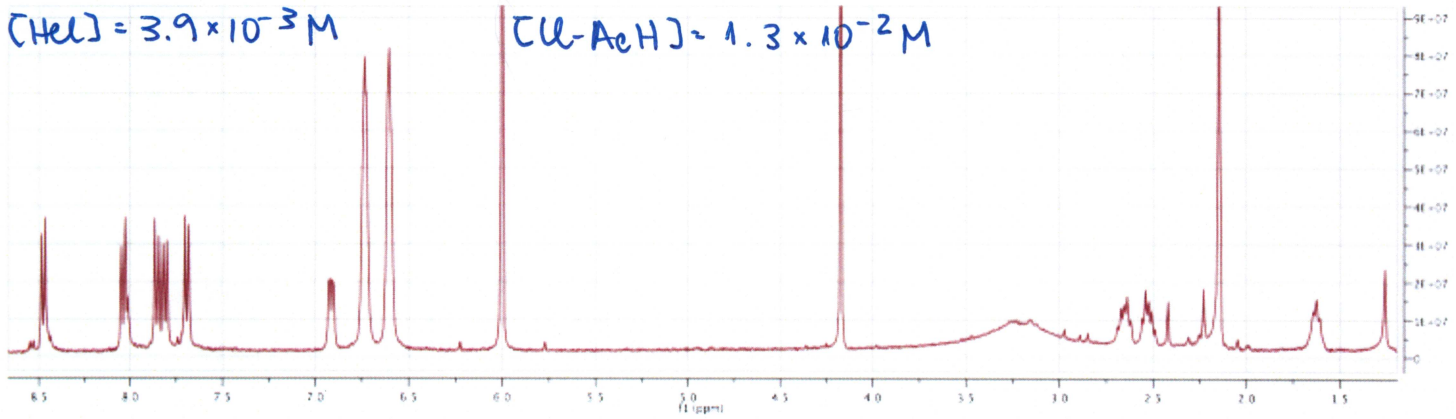


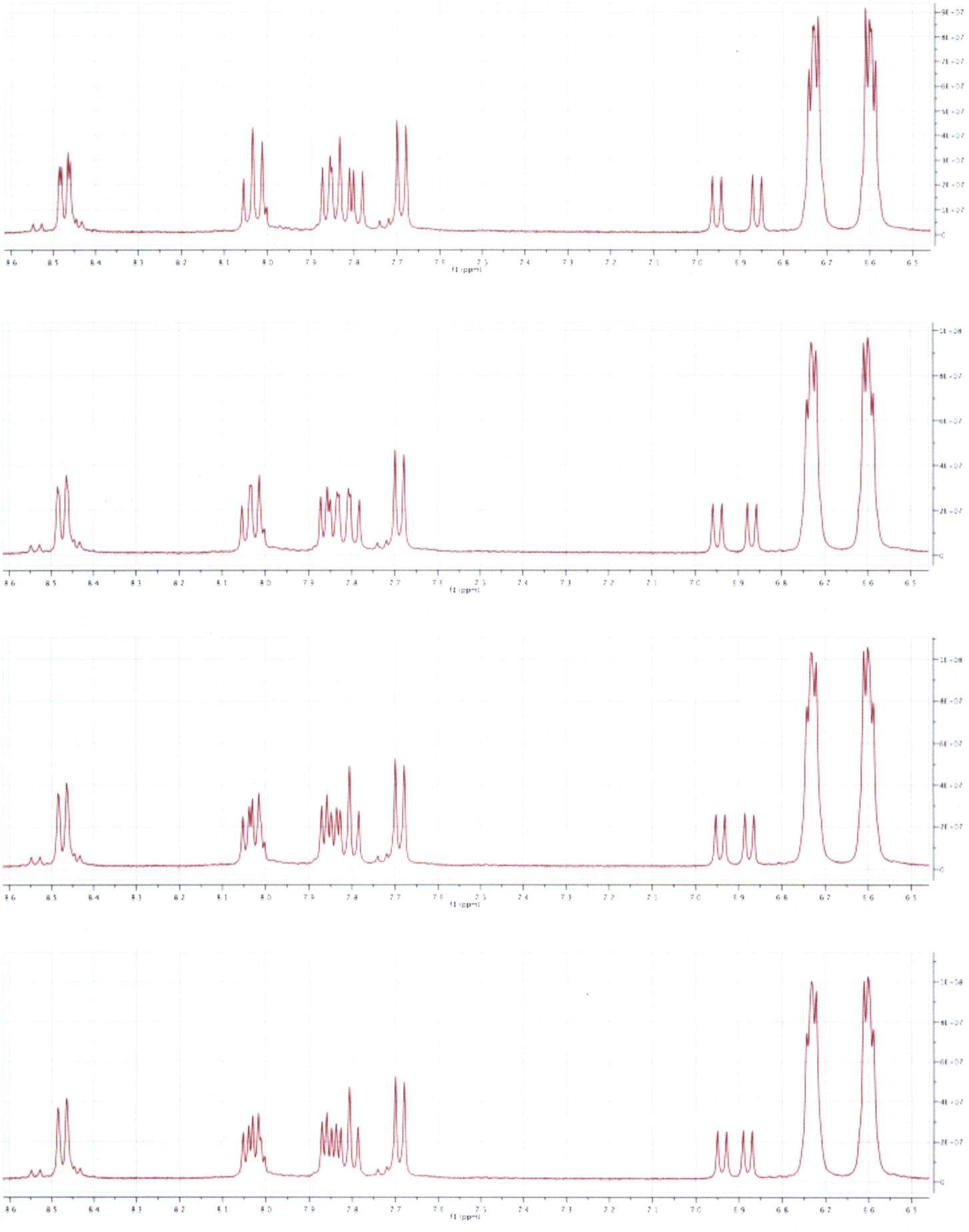


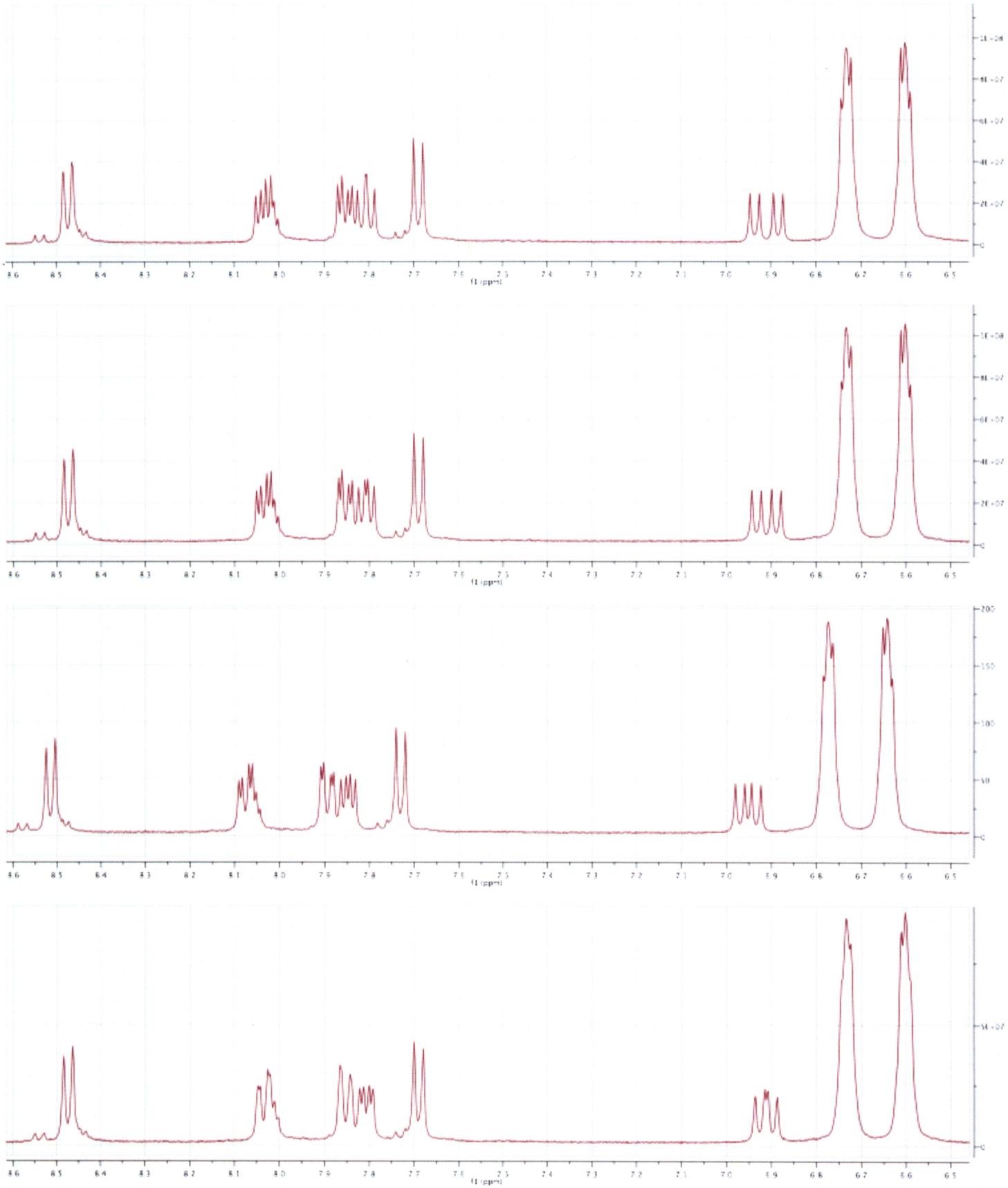


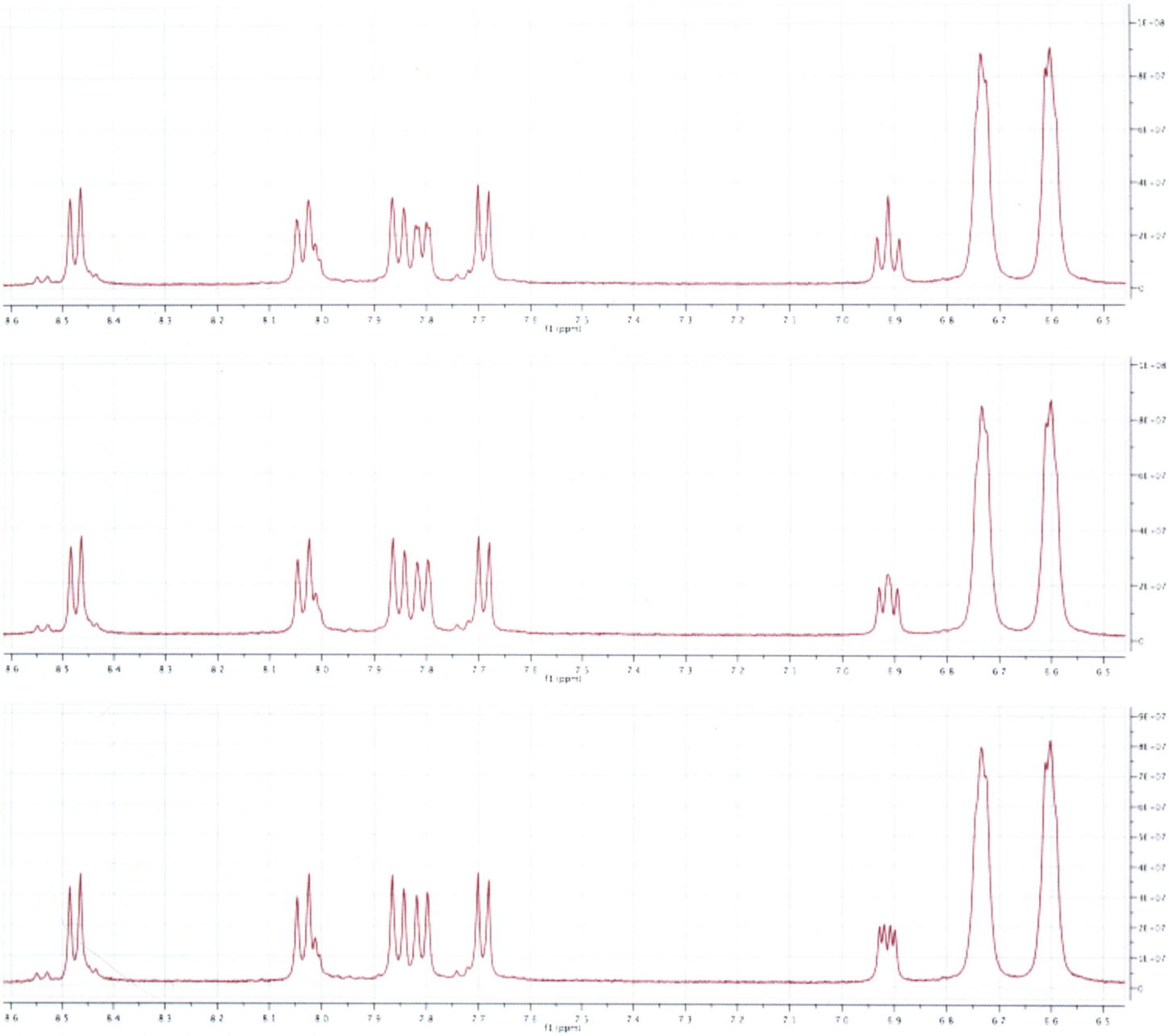


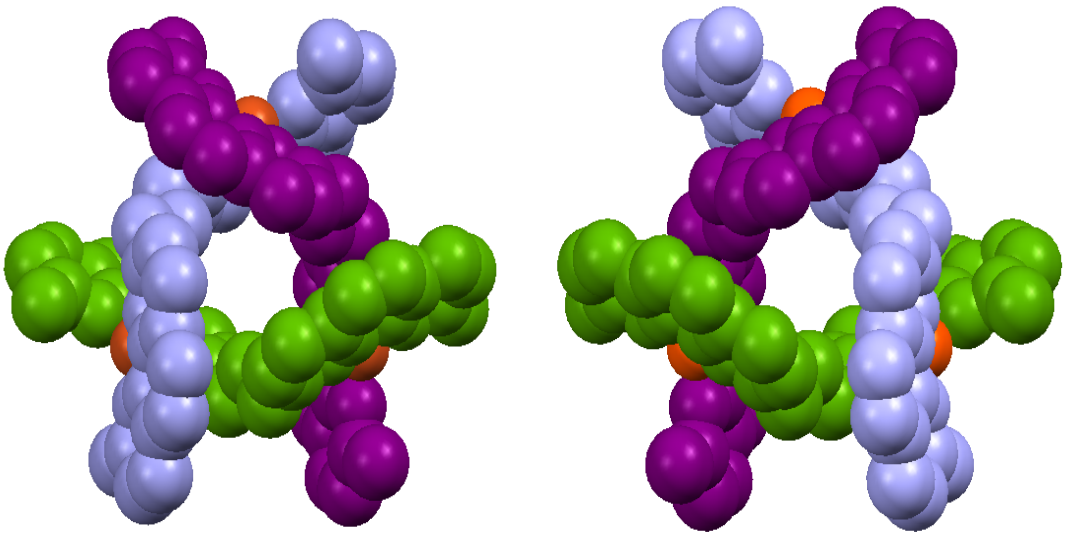












S11: Space filling models of the P- (left) and M-$[Cu_3(mphenpr)_3]^{3+}$ (right) helical trimer cations tracing the individual binucleating ligands.

Tables of X-Ray Data for Compounds 1-4

Lemus, Lappin Compound 1 (nd019)

Table 1. Crystal data and structure refinement for nd019.

Identification code	nd019	
Empirical formula	$C_{94}H_{72}As_2Cu_2N_8O_{12}$	
Formula weight	1782.52	
Temperature	150(2) K	
Wavelength	0.77490 Å	
Crystal system	monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 16.5080(5) Å	α = 90°
	b = 17.4618(5) Å	β = 90.195(2)°
	c = 28.2773(9) Å	γ = 90°
Volume	8151.1(4) $Å^3$	
Z	4	
Density (calculated)	1.453 $g.cm^{-3}$	
Absorption coefficient (μ)	1.698 mm^{-1}	
F(000)	3648	
Crystal size	0.10 × 0.05 × 0.04 mm^3	
ω range for data collection	0.79 to 27.24°	
Index ranges	$-19 \le h \le 19$, $-20 \le k \le 20$, $-32 \le l \le 33$	
Reflections collected	98832	
Independent reflections	27567 [R_{int} = 0.0936]	
Completeness to θ = 27.24°	99.7 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9352 and 0.8485	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	27567 / 25 / 2126	
Goodness-of-fit on F^2	0.971	
Final R indices [I>2σ(I)]	R_1 = 0.0865, wR_2 = 0.2182	
R indices (all data)	R_1 = 0.1722, wR_2 = 0.2786	
Absolute structure parameter	0.018(12)	
Largest diff. peak and hole	3.098 and -0.738 $e^-.Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for nd019. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cu(1)	0.10050(10)	0.43390(9)	0.87611(6)	0.040(1)
Cu(2)	0.19222(11)	0.61536(10)	1.07111(6)	0.045(1)
N(1)	-0.0116(6)	0.4754(6)	0.8657(4)	0.036(3)
N(2)	0.0543(6)	0.4094(6)	0.9410(4)	0.038(3)
N(3)	0.2944(7)	0.5507(7)	1.0663(4)	0.048(3)
N(4)	0.2667(8)	0.6869(7)	1.1054(5)	0.058(4)
N(5)	0.1505(6)	0.3497(6)	0.8361(4)	0.040(3)
N(6)	0.1967(7)	0.4933(6)	0.8524(4)	0.038(3)
N(7)	0.0958(6)	0.6329(6)	1.0290(3)	0.033(2)
N(8)	0.1040(7)	0.5716(7)	1.1166(5)	0.052(3)
C(1)	0.0083(9)	0.5153(10)	0.7852(5)	0.059(4)
C(2)	-0.0448(9)	0.5062(8)	0.8268(6)	0.054(4)
C(3)	-0.1274(11)	0.5308(10)	0.8259(6)	0.075(6)
C(4)	-0.1744(10)	0.5243(9)	0.8674(5)	0.054(4)
C(5)	-0.1404(9)	0.4930(8)	0.9061(5)	0.044(4)
C(6)	-0.0591(7)	0.4666(7)	0.9035(4)	0.033(3)
C(7)	-0.1873(8)	0.4760(8)	0.9486(5)	0.045(3)
C(8)	-0.1549(8)	0.4435(8)	0.9859(5)	0.045(4)
C(9)	-0.0698(8)	0.4172(8)	0.9862(5)	0.044(3)
C(10)	-0.0213(8)	0.4321(7)	0.9441(4)	0.032(3)
C(11)	-0.0316(8)	0.3833(7)	1.0243(4)	0.039(3)
C(12)	0.0448(8)	0.3604(8)	1.0192(4)	0.037(3)
C(13)	0.0872(8)	0.3723(7)	0.9775(5)	0.039(3)
C(14)	0.1730(8)	0.3442(7)	0.9717(5)	0.043(3)
C(15)	0.2378(12)	0.3991(17)	0.9851(9)	0.126(10)
C(16)	0.2344(12)	0.4356(15)	1.0282(9)	0.114(9)
C(17)	0.3100(10)	0.4815(10)	1.0483(6)	0.062(4)
C(18)	0.3793(9)	0.4411(10)	1.0506(7)	0.069(5)
C(19)	0.4432(10)	0.4757(11)	1.0780(6)	0.067(5)
C(20)	0.4291(10)	0.5430(12)	1.0999(6)	0.065(5)
C(21)	0.3564(9)	0.5811(9)	1.0931(6)	0.054(4)

C(22)	0.4908(12)	0.5747(15)	1.1336(9)	0.098(7)
C(23)	0.4732(11)	0.6468(17)	1.1529(9)	0.120(9)
C(24)	0.4002(12)	0.6844(11)	1.1438(7)	0.077(5)
C(25)	0.3397(10)	0.6542(9)	1.1143(5)	0.056(4)
C(26)	0.3782(14)	0.7539(14)	1.1652(8)	0.101(7)
C(27)	0.3048(14)	0.7901(12)	1.1559(8)	0.094(7)
C(28)	0.2495(10)	0.7537(9)	1.1269(6)	0.061(4)
C(29)	0.1695(11)	0.7842(10)	1.1151(6)	0.076(5)
C(30)	0.0559(9)	0.2508(9)	0.8563(6)	0.059(4)
C(31)	0.1284(9)	0.2754(9)	0.8297(5)	0.047(4)
C(32)	0.1720(10)	0.2268(9)	0.8007(5)	0.052(4)
C(33)	0.2365(11)	0.2495(9)	0.7775(6)	0.059(4)
C(34)	0.2659(9)	0.3254(9)	0.7859(5)	0.049(4)
C(35)	0.2190(8)	0.3723(8)	0.8141(4)	0.034(3)
C(36)	0.3397(10)	0.3528(9)	0.7661(5)	0.053(4)
C(37)	0.3615(9)	0.4269(10)	0.7723(5)	0.057(4)
C(38)	0.3158(9)	0.4790(9)	0.8007(5)	0.046(4)
C(39)	0.2446(8)	0.4484(9)	0.8219(4)	0.045(4)
C(40)	0.3326(9)	0.5548(9)	0.8084(6)	0.056(4)
C(41)	0.2871(9)	0.5971(9)	0.8348(5)	0.048(4)
C(42)	0.2162(9)	0.5678(8)	0.8575(5)	0.047(3)
C(43)	0.1611(9)	0.6159(8)	0.8895(5)	0.049(3)
C(44)	0.2129(9)	0.6379(8)	0.9353(5)	0.050(3)
C(45)	0.1681(9)	0.6963(8)	0.9658(5)	0.051(4)
C(46)	0.0916(8)	0.6664(7)	0.9873(5)	0.042(3)
C(47)	0.0187(10)	0.6724(9)	0.9622(5)	0.053(4)
C(48)	-0.0528(9)	0.6468(8)	0.9814(5)	0.047(4)
C(49)	-0.0497(8)	0.6113(8)	1.0273(4)	0.037(3)
C(50)	0.0255(8)	0.6054(7)	1.0476(5)	0.036(3)
C(51)	-0.1201(8)	0.5842(8)	1.0496(5)	0.041(3)
C(52)	-0.1149(8)	0.5477(8)	1.0921(5)	0.051(4)
C(53)	-0.0377(8)	0.5427(7)	1.1146(5)	0.038(3)
C(54)	0.0285(8)	0.5719(7)	1.0940(5)	0.035(3)
C(55)	-0.0310(8)	0.5047(8)	1.1597(4)	0.040(3)
C(56)	0.0450(10)	0.5073(8)	1.1813(5)	0.055(4)
C(57)	0.1099(9)	0.5429(8)	1.1609(5)	0.043(4)

C(58)	0.1899(11)	0.5512(11)	1.1845(6)	0.079(6)
Cu(3)	0.90053(10)	0.03410(9)	0.62420(6)	0.043(1)
Cu(4)	0.79632(11)	0.21027(9)	0.43551(6)	0.044(1)
N(9)	1.0137(7)	0.0807(6)	0.6334(4)	0.040(3)
N(10)	0.9471(7)	0.0085(6)	0.5592(4)	0.040(3)
N(11)	0.6951(7)	0.1413(7)	0.4403(4)	0.049(3)
N(12)	0.7204(8)	0.2805(7)	0.3983(5)	0.063(4)
N(13)	0.8560(7)	-0.0508(6)	0.6649(4)	0.042(3)
N(14)	0.8051(6)	0.0919(6)	0.6493(4)	0.037(3)
N(15)	0.8943(7)	0.2306(6)	0.4737(4)	0.040(3)
N(16)	0.8798(7)	0.1620(6)	0.3891(4)	0.039(3)
C(61)	0.9917(9)	0.1274(10)	0.7127(6)	0.065(5)
C(62)	1.0447(9)	0.1166(9)	0.6708(5)	0.043(3)
C(63)	1.1223(9)	0.1474(9)	0.6695(5)	0.053(4)
C(64)	1.1709(8)	0.1391(9)	0.6308(5)	0.048(4)
C(65)	1.1396(8)	0.0981(8)	0.5923(4)	0.035(3)
C(66)	1.0612(8)	0.0717(7)	0.5952(4)	0.035(3)
C(67)	1.1853(9)	0.0850(9)	0.5493(5)	0.049(4)
C(68)	1.1538(8)	0.0461(7)	0.5135(5)	0.042(3)
C(69)	1.0682(7)	0.0214(8)	0.5147(5)	0.039(3)
C(70)	1.0244(8)	0.0343(7)	0.5545(4)	0.036(3)
C(71)	1.0314(9)	-0.0131(8)	0.4751(5)	0.046(4)
C(72)	0.9536(10)	-0.0396(8)	0.4812(5)	0.051(4)
C(73)	0.9108(8)	-0.0300(8)	0.5221(5)	0.039(3)
C(74)	0.8278(8)	-0.0621(8)	0.5294(5)	0.045(4)
C(75)	0.7707(15)	-0.0320(14)	0.4902(9)	0.033(6)
C(76)	0.7462(16)	0.0491(16)	0.5002(10)	0.041(7)
C(74A)	0.8278(8)	-0.0621(8)	0.5294(5)	0.045(4)
C(75A)	0.7607(15)	-0.0022(15)	0.5213(9)	0.037(6)
C(76A)	0.7697(15)	0.0293(15)	0.4703(9)	0.033(6)
C(77)	0.6870(10)	0.0741(9)	0.4598(6)	0.060(5)
C(78)	0.6156(10)	0.0309(10)	0.4539(6)	0.064(5)
C(79)	0.5545(11)	0.0568(11)	0.4263(7)	0.076(5)
C(80)	0.5646(9)	0.1285(10)	0.4056(6)	0.063(5)
C(81)	0.6330(9)	0.1714(9)	0.4129(5)	0.051(4)
C(82)	0.5061(11)	0.1572(17)	0.3695(7)	0.109(9)

C(83)	0.5185(14)	0.2219(16)	0.3473(8)	0.116(9)
C(84)	0.5865(12)	0.2705(12)	0.3599(9)	0.102(8)
C(85)	0.6465(9)	0.2432(9)	0.3916(6)	0.056(4)
C(86)	0.6079(17)	0.3401(17)	0.3373(9)	0.134(10)
C(87)	0.6804(13)	0.3785(11)	0.3440(9)	0.097(7)
C(88)	0.7317(12)	0.3468(10)	0.3780(7)	0.078(6)
C(89)	0.8134(12)	0.3865(11)	0.3885(7)	0.089(7)
C(90)	0.9468(10)	-0.1463(9)	0.6446(6)	0.069(4)
C(91)	0.8813(10)	-0.1216(8)	0.6716(5)	0.057(4)
C(92)	0.8371(11)	-0.1737(8)	0.7017(5)	0.059(4)
C(93)	0.7700(9)	-0.1518(8)	0.7232(5)	0.045(4)
C(94)	0.7391(9)	-0.0763(9)	0.7164(4)	0.046(4)
C(95)	0.7864(9)	-0.0286(8)	0.6866(4)	0.039(3)
C(96)	0.6674(8)	-0.0481(9)	0.7382(5)	0.043(4)
C(97)	0.6464(8)	0.0256(10)	0.7317(5)	0.051(4)
C(98)	0.6914(9)	0.0766(8)	0.7032(5)	0.042(3)
C(99)	0.7567(8)	0.0507(7)	0.6791(5)	0.038(3)
C(100)	0.6711(8)	0.1532(9)	0.6972(5)	0.052(4)
C(101)	0.7181(9)	0.1997(8)	0.6686(6)	0.058(4)
C(102)	0.7836(8)	0.1667(8)	0.6446(4)	0.037(3)
C(103)	0.8323(8)	0.2142(8)	0.6108(5)	0.050(4)
C(104)	0.7841(8)	0.2383(8)	0.5672(4)	0.037(3)
C(105)	0.8258(9)	0.2959(9)	0.5374(5)	0.050(4)
C(106)	0.9026(9)	0.2676(7)	0.5150(4)	0.037(3)
C(107)	0.9805(10)	0.2768(8)	0.5361(5)	0.052(4)
C(108)	1.0462(9)	0.2518(8)	0.5166(5)	0.042(3)
C(109)	1.0427(8)	0.2146(8)	0.4717(5)	0.042(3)
C(110)	0.9660(8)	0.2051(7)	0.4525(4)	0.037(3)
C(111)	1.1112(9)	0.1868(9)	0.4460(5)	0.050(4)
C(112)	1.1027(8)	0.1504(7)	0.4047(4)	0.038(3)
C(113)	1.0249(9)	0.1363(8)	0.3851(4)	0.042(3)
C(114)	0.9548(8)	0.1668(7)	0.4081(4)	0.034(3)
C(115)	1.0125(10)	0.0941(9)	0.3441(5)	0.052(4)
C(116)	0.9343(10)	0.0900(10)	0.3254(6)	0.061(4)
C(117)	0.8702(8)	0.1254(8)	0.3491(5)	0.041(3)
C(118)	0.7852(9)	0.1220(12)	0.3284(6)	0.070(5)

As(1)	0.63983(9)	0.65928(8)	0.94983(5)	0.042(1)
O(121)	0.6100(6)	0.7259(5)	0.9031(3)	0.048(3)
O(122)	0.7454(5)	0.6794(5)	0.9358(3)	0.044(2)
O(131)	0.6466(5)	0.5749(5)	0.9106(3)	0.044(2)
O(132)	0.5345(6)	0.6352(6)	0.9607(4)	0.052(3)
O(141)	0.6759(5)	0.6026(5)	1.0000(3)	0.040(2)
O(142)	0.6289(6)	0.7406(5)	0.9902(3)	0.045(2)
C(121)	0.6741(8)	0.7634(8)	0.8852(4)	0.040(3)
C(122)	0.6715(11)	0.8269(8)	0.8571(5)	0.055(4)
C(123)	0.7452(12)	0.8589(11)	0.8408(6)	0.071(5)
C(124)	0.8211(10)	0.8291(9)	0.8558(5)	0.057(4)
C(125)	0.8224(9)	0.7685(8)	0.8862(5)	0.041(3)
C(126)	0.7515(10)	0.7379(8)	0.9017(5)	0.047(4)
C(131)	0.5740(8)	0.5392(8)	0.9067(5)	0.038(3)
C(132)	0.5589(9)	0.4780(8)	0.8783(5)	0.044(3)
C(133)	0.4841(12)	0.4426(10)	0.8786(6)	0.071(5)
C(134)	0.4196(10)	0.4752(9)	0.9067(6)	0.056(4)
C(135)	0.4356(9)	0.5374(9)	0.9342(5)	0.054(4)
C(136)	0.5117(9)	0.5724(9)	0.9343(5)	0.050(4)
C(141)	0.6680(8)	0.6419(7)	1.0420(5)	0.039(3)
C(142)	0.6860(8)	0.6120(8)	1.0850(5)	0.043(3)
C(143)	0.6712(10)	0.6617(10)	1.1232(5)	0.059(4)
C(144)	0.6462(10)	0.7346(9)	1.1177(6)	0.058(4)
C(145)	0.6310(9)	0.7639(8)	1.0736(5)	0.051(4)
C(146)	0.6404(8)	0.7180(8)	1.0360(5)	0.043(4)
As(2)	0.74019(9)	0.46684(7)	0.65025(5)	0.039(1)
O(151)	0.6429(6)	0.4954(6)	0.6759(4)	0.060(3)
O(152)	0.7868(6)	0.5517(5)	0.6790(3)	0.052(3)
O(161)	0.7568(6)	0.4062(5)	0.7022(3)	0.045(2)
O(162)	0.8430(5)	0.4419(5)	0.6297(3)	0.043(2)
O(171)	0.6869(5)	0.3867(5)	0.6225(3)	0.045(2)
O(172)	0.7244(5)	0.5212(5)	0.5959(3)	0.038(2)
C(151)	0.6579(10)	0.5508(9)	0.7106(6)	0.055(4)
C(152)	0.6011(12)	0.5727(11)	0.7416(6)	0.080(6)
C(153)	0.619(2)	0.6269(13)	0.7748(9)	0.135(13)
C(154)	0.6977(19)	0.6599(12)	0.7748(6)	0.103(9)

C(155)	0.7579(11)	0.6379(9)	0.7430(5)	0.063(5)
C(156)	0.7324(11)	0.5804(8)	0.7098(5)	0.052(4)
C(161)	0.8361(10)	0.3857(8)	0.7043(5)	0.048(4)
C(162)	0.8696(11)	0.3450(10)	0.7429(5)	0.069(5)
C(163)	0.9530(12)	0.3252(11)	0.7395(8)	0.083(6)
C(164)	0.9987(13)	0.3414(13)	0.7022(7)	0.092(7)
C(165)	0.9656(9)	0.3833(8)	0.6631(5)	0.051(4)
C(166)	0.8835(10)	0.4040(9)	0.6657(5)	0.054(4)
C(171)	0.6537(7)	0.4087(7)	0.5801(5)	0.036(3)
C(172)	0.6049(9)	0.3660(10)	0.5517(6)	0.062(5)
C(173)	0.5733(8)	0.3937(8)	0.5120(6)	0.050(4)
C(174)	0.5939(9)	0.4651(9)	0.4961(6)	0.055(4)
C(175)	0.6455(8)	0.5129(8)	0.5236(5)	0.045(4)
C(176)	0.6754(8)	0.4836(8)	0.5660(5)	0.040(3)
As(3)	0.26276(9)	0.86550(8)	0.85327(5)	0.039(1)
O(181)	0.2425(7)	0.8018(6)	0.8027(3)	0.052(3)
O(182)	0.1593(5)	0.8459(5)	0.8737(3)	0.042(2)
O(191)	0.2218(5)	0.9486(5)	0.8222(3)	0.047(2)
O(192)	0.3613(6)	0.8875(6)	0.8278(4)	0.053(3)
O(201)	0.3095(6)	0.7852(5)	0.8826(3)	0.047(2)
O(202)	0.2783(5)	0.9221(5)	0.9066(3)	0.044(2)
C(181)	0.1601(10)	0.7833(8)	0.8013(5)	0.050(4)
C(182)	0.1275(10)	0.7483(10)	0.7646(6)	0.060(4)
C(183)	0.0448(14)	0.7318(11)	0.7674(8)	0.087(6)
C(184)	-0.0002(12)	0.7553(11)	0.8057(7)	0.074(5)
C(185)	0.0365(10)	0.7945(9)	0.8414(6)	0.054(4)
C(186)	0.1173(9)	0.8081(8)	0.8385(5)	0.045(4)
C(191)	0.2779(9)	0.9820(8)	0.7927(5)	0.042(4)
C(192)	0.2617(11)	1.0368(8)	0.7587(5)	0.057(4)
C(193)	0.3278(10)	1.0630(10)	0.7320(5)	0.055(4)
C(194)	0.4043(11)	1.0323(9)	0.7362(6)	0.062(5)
C(195)	0.4186(10)	0.9733(10)	0.7686(5)	0.061(5)
C(196)	0.3549(9)	0.9469(9)	0.7954(5)	0.052(4)
C(201)	0.3447(8)	0.8091(9)	0.9237(5)	0.042(3)
C(202)	0.3972(9)	0.7638(9)	0.9512(5)	0.048(4)
C(203)	0.4283(8)	0.7962(9)	0.9928(5)	0.052(4)

C(204)	0.4103(8)	0.8689(8)	1.0062(5)	0.049(4)
C(205)	0.3610(8)	0.9156(9)	0.9774(5)	0.047(4)
C(206)	0.3296(8)	0.8852(7)	0.9371(5)	0.038(3)
As(4)	0.63864(9)	0.75644(8)	0.45537(5)	0.045(1)
O(211)	0.6093(6)	0.8195(6)	0.4073(3)	0.059(3)
O(212)	0.7453(6)	0.7782(6)	0.4411(3)	0.049(3)
O(221)	0.6470(5)	0.6723(6)	0.4167(3)	0.048(2)
O(222)	0.5323(5)	0.7316(5)	0.4653(4)	0.048(3)
O(231)	0.6763(6)	0.6997(5)	0.5060(3)	0.046(2)
O(232)	0.6263(6)	0.8375(5)	0.4949(3)	0.043(2)
C(211)	0.6748(10)	0.8510(9)	0.3858(5)	0.052(4)
C(212)	0.6714(11)	0.9024(10)	0.3513(6)	0.068(5)
C(213)	0.7465(14)	0.9277(13)	0.3313(7)	0.097(7)
C(214)	0.8159(12)	0.9067(11)	0.3481(6)	0.067(5)
C(215)	0.8181(12)	0.8565(10)	0.3864(6)	0.069(5)
C(216)	0.7499(11)	0.8284(10)	0.4049(5)	0.061(5)
C(221)	0.5768(8)	0.6357(8)	0.4118(5)	0.040(3)
C(222)	0.5596(10)	0.5749(9)	0.3839(5)	0.053(4)
C(223)	0.4827(9)	0.5429(10)	0.3805(5)	0.056(4)
C(224)	0.4220(10)	0.5785(9)	0.4074(5)	0.055(4)
C(225)	0.4338(9)	0.6393(8)	0.4363(5)	0.045(4)
C(226)	0.5108(9)	0.6688(8)	0.4378(5)	0.048(4)
C(231)	0.6671(8)	0.7413(8)	0.5467(5)	0.042(3)
C(232)	0.6861(8)	0.7144(9)	0.5899(5)	0.050(4)
C(233)	0.6736(11)	0.7602(10)	0.6284(6)	0.072(5)
C(234)	0.6461(11)	0.8338(9)	0.6234(6)	0.072(5)
C(235)	0.6249(9)	0.8631(9)	0.5788(5)	0.054(4)
C(236)	0.6401(9)	0.8163(8)	0.5406(5)	0.045(4)
H(1A)	0.0598	0.4888	0.7910	0.089
H(1B)	0.0186	0.5698	0.7797	0.089
H(1C)	-0.0182	0.4931	0.7573	0.089
H(3A)	-0.1504	0.5513	0.7977	0.091
H(4A)	-0.2290	0.5417	0.8679	0.065
H(7A)	-0.2432	0.4889	0.9492	0.053
H(8A)	-0.1869	0.4368	1.0135	0.054
H(11A)	-0.0591	0.3765	1.0534	0.046

H(12A)	0.0711	0.3352	1.0448	0.045
H(14A)	0.1798	0.2973	0.9910	0.052
H(14B)	0.1808	0.3296	0.9382	0.052
H(15A)	0.2900	0.3713	0.9837	0.151
H(15B)	0.2395	0.4392	0.9603	0.151
H(16A)	0.2203	0.3963	1.0520	0.137
H(16B)	0.1884	0.4719	1.0267	0.137
H(18A)	0.3856	0.3932	1.0352	0.083
H(19A)	0.4945	0.4515	1.0807	0.080
H(22A)	0.5390	0.5477	1.1414	0.117
H(23A)	0.5121	0.6708	1.1728	0.143
H(26A)	0.4149	0.7771	1.1869	0.121
H(27A)	0.2930	0.8388	1.1693	0.113
H(29A)	0.1287	0.7440	1.1191	0.114
H(29B)	0.1692	0.8018	1.0822	0.114
H(29C)	0.1570	0.8273	1.1361	0.114
H(30A)	0.0164	0.2927	0.8569	0.089
H(30B)	0.0715	0.2374	0.8887	0.089
H(30C)	0.0317	0.2061	0.8408	0.089
H(32A)	0.1547	0.1752	0.7975	0.063
H(33A)	0.2628	0.2165	0.7557	0.070
H(36A)	0.3734	0.3192	0.7486	0.063
H(37A)	0.4092	0.4449	0.7573	0.068
H(40A)	0.3788	0.5769	0.7939	0.067
H(41A)	0.3012	0.6494	0.8394	0.058
H(43A)	0.1126	0.5860	0.8986	0.059
H(43B)	0.1431	0.6627	0.8728	0.059
H(44A)	0.2237	0.5912	0.9542	0.060
H(44B)	0.2657	0.6595	0.9255	0.060
H(45A)	0.2047	0.7136	0.9915	0.061
H(45B)	0.1549	0.7415	0.9461	0.061
H(47A)	0.0185	0.6945	0.9315	0.063
H(48A)	-0.1027	0.6525	0.9649	0.057
H(51A)	-0.1714	0.5914	1.0350	0.049
H(52A)	-0.1617	0.5261	1.1063	0.061
H(55A)	-0.0757	0.4795	1.1739	0.048

H(56A)	0.0520	0.4834	1.2112	0.066
H(58A)	0.2315	0.5256	1.1656	0.118
H(58B)	0.1878	0.5279	1.2160	0.118
H(58C)	0.2032	0.6057	1.1875	0.118
H(61A)	0.9559	0.0829	0.7160	0.098
H(61B)	0.9589	0.1737	0.7084	0.098
H(61C)	1.0252	0.1326	0.7411	0.098
H(63A)	1.1420	0.1749	0.6962	0.063
H(64A)	1.2239	0.1603	0.6300	0.058
H(67A)	1.2388	0.1046	0.5468	0.059
H(68A)	1.1864	0.0340	0.4869	0.051
H(71A)	1.0588	-0.0179	0.4458	0.055
H(72A)	0.9283	-0.0659	0.4557	0.061
H(74A)	0.8071	-0.0466	0.5608	0.055
H(74B)	0.8299	-0.1188	0.5283	0.055
H(75A)	0.7985	-0.0346	0.4593	0.039
H(75B)	0.7218	-0.0647	0.4885	0.039
H(76A)	0.7945	0.0827	0.5007	0.049
H(76B)	0.7190	0.0525	0.5312	0.049
H(74C)	0.8237	-0.0822	0.5621	0.055
H(74D)	0.8194	-0.1055	0.5074	0.055
H(75C)	0.7661	0.0400	0.5445	0.044
H(75D)	0.7068	-0.0261	0.5253	0.044
H(76C)	0.7772	-0.0131	0.4475	0.039
H(76D)	0.8166	0.0644	0.4682	0.039
H(78A)	0.6104	-0.0170	0.4695	0.077
H(79A)	0.5067	0.0275	0.4213	0.091
H(82A)	0.4589	0.1281	0.3625	0.131
H(83A)	0.4827	0.2372	0.3226	0.139
H(86A)	0.5698	0.3619	0.3160	0.161
H(87A)	0.6942	0.4232	0.3267	0.117
H(89A)	0.8351	0.3678	0.4186	0.133
H(89B)	0.8052	0.4420	0.3903	0.133
H(89C)	0.8518	0.3750	0.3631	0.133
H(90A)	0.9819	-0.1026	0.6374	0.104
H(90B)	0.9269	-0.1690	0.6151	0.104

H(90C)	0.9776	-0.1847	0.6624	0.104
H(92A)	0.8565	-0.2244	0.7061	0.070
H(93A)	0.7422	-0.1865	0.7432	0.054
H(96A)	0.6349	-0.0808	0.7571	0.052
H(97A)	0.5992	0.0443	0.7469	0.061
H(10A)	0.6250	0.1738	0.7127	0.063
H(10B)	0.7062	0.2526	0.6653	0.069
H(10C)	0.8803	0.1846	0.6006	0.060
H(10D)	0.8519	0.2607	0.6273	0.060
H(10E)	0.7727	0.1923	0.5478	0.045
H(10F)	0.7314	0.2596	0.5775	0.045
H(10G)	0.8388	0.3411	0.5572	0.061
H(10H)	0.7882	0.3128	0.5122	0.061
H(10I)	0.9844	0.3023	0.5657	0.063
H(10J)	1.0968	0.2582	0.5322	0.051
H(11B)	1.1640	0.1944	0.4586	0.060
H(11C)	1.1495	0.1337	0.3882	0.046
H(11D)	1.0563	0.0686	0.3291	0.063
H(11E)	0.9246	0.0633	0.2967	0.073
H(11F)	0.7473	0.1044	0.3527	0.106
H(11G)	0.7842	0.0864	0.3016	0.106
H(11H)	0.7691	0.1732	0.3176	0.106
H(12B)	0.6211	0.8493	0.8486	0.066
H(12C)	0.7438	0.9009	0.8195	0.086
H(12D)	0.8702	0.8511	0.8449	0.069
H(12E)	0.8726	0.7477	0.8965	0.049
H(13A)	0.6003	0.4594	0.8581	0.053
H(13B)	0.4751	0.3975	0.8605	0.085
H(13C)	0.3668	0.4535	0.9059	0.068
H(13D)	0.3940	0.5575	0.9538	0.065
H(14C)	0.7068	0.5617	1.0890	0.051
H(14D)	0.6793	0.6429	1.1544	0.071
H(14E)	0.6389	0.7661	1.1447	0.070
H(14F)	0.6142	0.8155	1.0698	0.061
H(15C)	0.5486	0.5507	0.7404	0.096
H(15D)	0.5802	0.6422	0.7974	0.162

H(15E)	0.7097	0.6986	0.7973	0.124
H(15F)	0.8109	0.6591	0.7433	0.075
H(16C)	0.8381	0.3315	0.7696	0.083
H(16D)	0.9774	0.2991	0.7654	0.100
H(16E)	1.0536	0.3251	0.7015	0.110
H(16F)	0.9978	0.3964	0.6365	0.061
H(17A)	0.5932	0.3146	0.5604	0.075
H(17B)	0.5358	0.3637	0.4944	0.059
H(17C)	0.5737	0.4829	0.4665	0.066
H(17D)	0.6591	0.5631	0.5135	0.054
H(18B)	0.1586	0.7349	0.7376	0.072
H(18C)	0.0193	0.7041	0.7425	0.104
H(18D)	-0.0564	0.7441	0.8071	0.088
H(18E)	0.0062	0.8119	0.8678	0.064
H(19B)	0.2085	1.0559	0.7536	0.068
H(19C)	0.3194	1.1036	0.7101	0.066
H(19D)	0.4472	1.0511	0.7172	0.074
H(19E)	0.4712	0.9519	0.7721	0.073
H(20A)	0.4110	0.7131	0.9420	0.057
H(20B)	0.4632	0.7664	1.0122	0.062
H(20C)	0.4312	0.8885	1.0351	0.059
H(20D)	0.3499	0.9671	0.9860	0.057
H(21A)	0.6210	0.9218	0.3403	0.082
H(21B)	0.7451	0.9611	0.3048	0.116
H(21C)	0.8647	0.9252	0.3345	0.080
H(21D)	0.8689	0.8419	0.3996	0.083
H(22B)	0.6020	0.5531	0.3657	0.063
H(22C)	0.4719	0.4996	0.3611	0.068
H(22D)	0.3686	0.5583	0.4052	0.066
H(22E)	0.3910	0.6604	0.4545	0.054
H(23B)	0.7079	0.6644	0.5936	0.060
H(23C)	0.6842	0.7407	0.6592	0.086
H(23D)	0.6411	0.8655	0.6506	0.086
H(23E)	0.6015	0.9125	0.5752	0.064

Table 3. Anisotropic displacement parameters $(Å)^2$ for nd019. 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)	0.0417(11)	0.0375(10)	0.0413(10)	0.0040(8)	0.0124(8)	0.0036(8)
Cu(2)	0.0416(11)	0.0412(11)	0.0535(11)	0.0058(9)	-0.0034(9)	0.0017(8)
N(1)	0.041(7)	0.034(6)	0.034(6)	0.016(5)	0.004(5)	0.008(5)
N(2)	0.036(7)	0.040(7)	0.037(6)	0.007(5)	0.005(5)	0.008(5)
N(3)	0.053(8)	0.044(8)	0.046(7)	0.010(6)	0.006(6)	-0.003(6)
N(4)	0.050(8)	0.036(7)	0.088(10)	0.017(7)	0.005(7)	0.002(6)
N(5)	0.035(6)	0.039(7)	0.046(7)	-0.002(6)	0.006(5)	-0.004(5)
N(6)	0.043(7)	0.038(7)	0.033(6)	0.003(5)	0.002(5)	0.009(5)
N(7)	0.041(6)	0.033(6)	0.025(5)	0.000(5)	0.010(5)	0.010(5)
N(8)	0.045(8)	0.041(7)	0.070(9)	0.005(7)	-0.022(6)	0.007(6)
C(1)	0.069(11)	0.074(11)	0.035(8)	0.030(8)	0.012(7)	0.015(9)
C(2)	0.054(10)	0.038(9)	0.069(11)	0.009(8)	0.003(8)	-0.002(7)
C(3)	0.082(13)	0.081(13)	0.063(11)	0.031(10)	0.014(10)	0.047(11)
C(4)	0.056(10)	0.052(10)	0.055(10)	0.009(8)	0.013(8)	0.023(8)
C(5)	0.060(10)	0.040(8)	0.032(8)	-0.001(7)	-0.003(7)	0.010(7)
C(6)	0.024(7)	0.032(7)	0.043(8)	0.010(6)	0.005(6)	0.012(6)
C(7)	0.033(8)	0.052(9)	0.049(9)	0.002(7)	0.004(7)	0.016(7)
C(8)	0.038(8)	0.066(10)	0.032(8)	0.000(7)	0.010(6)	0.009(7)
C(9)	0.047(9)	0.039(8)	0.044(9)	-0.002(7)	0.012(7)	-0.007(7)
C(10)	0.040(8)	0.023(7)	0.032(7)	0.013(6)	0.008(6)	0.003(6)
C(11)	0.048(9)	0.038(8)	0.030(7)	0.003(6)	0.009(6)	-0.006(6)
C(12)	0.034(8)	0.047(8)	0.030(7)	0.017(7)	0.003(6)	-0.002(7)
C(13)	0.038(8)	0.032(8)	0.047(8)	0.012(7)	-0.003(6)	0.014(6)
C(14)	0.038(8)	0.032(8)	0.058(9)	0.011(7)	0.008(7)	0.017(6)
C(15)	0.065(14)	0.18(3)	0.13(2)	-0.08(2)	0.016(13)	-0.040(15)
C(16)	0.058(13)	0.14(2)	0.14(2)	-0.047(18)	-0.040(13)	0.024(13)
C(17)	0.049(10)	0.066(12)	0.073(11)	-0.007(10)	-0.001(8)	0.012(9)
C(18)	0.035(9)	0.065(12)	0.108(15)	0.013(11)	-0.005(9)	0.012(8)
C(19)	0.051(11)	0.061(12)	0.087(13)	0.019(11)	0.021(9)	0.016(9)
C(20)	0.044(10)	0.091(14)	0.058(11)	0.005(10)	-0.004(8)	-0.016(10)
C(21)	0.035(9)	0.059(11)	0.069(11)	0.023(9)	0.007(8)	-0.001(8)

C(22)	0.050(12)	0.101(18)	0.14(2)	0.018(16)	-0.006(12)	-0.028(12)
C(23)	0.034(11)	0.16(3)	0.16(2)	-0.04(2)	-0.020(13)	-0.027(14)
C(24)	0.074(14)	0.058(12)	0.100(15)	-0.009(11)	-0.007(11)	-0.008(10)
C(25)	0.058(11)	0.053(10)	0.056(10)	0.003(8)	-0.013(8)	-0.015(8)
C(26)	0.088(17)	0.102(18)	0.113(18)	-0.019(15)	-0.012(14)	-0.043(14)
C(27)	0.103(18)	0.062(13)	0.118(18)	-0.019(13)	-0.012(14)	-0.025(13)
C(28)	0.052(10)	0.044(10)	0.086(12)	-0.001(9)	-0.005(9)	-0.007(8)
C(29)	0.087(14)	0.059(11)	0.080(13)	0.011(10)	0.009(11)	0.025(10)
C(30)	0.057(10)	0.050(10)	0.070(11)	0.026(9)	-0.013(8)	-0.006(8)
C(31)	0.052(9)	0.057(10)	0.032(8)	-0.001(7)	0.000(7)	0.008(8)
C(32)	0.060(10)	0.050(10)	0.047(9)	-0.003(8)	-0.002(8)	0.003(8)
C(33)	0.076(12)	0.046(10)	0.054(10)	-0.011(8)	-0.008(9)	0.019(9)
C(34)	0.052(10)	0.055(10)	0.039(8)	0.000(8)	0.004(7)	0.010(8)
C(35)	0.040(8)	0.043(9)	0.020(7)	-0.003(6)	0.003(6)	-0.002(7)
C(36)	0.067(11)	0.048(10)	0.043(9)	-0.005(8)	0.007(8)	0.024(8)
C(37)	0.052(10)	0.073(12)	0.046(9)	-0.001(9)	0.016(7)	0.013(9)
C(38)	0.045(9)	0.057(10)	0.036(8)	0.007(7)	0.018(7)	0.008(8)
C(39)	0.037(8)	0.074(11)	0.025(7)	0.011(7)	0.008(6)	0.005(8)
C(40)	0.045(9)	0.058(11)	0.065(10)	-0.005(9)	0.027(8)	-0.008(8)
C(41)	0.048(9)	0.044(9)	0.051(9)	-0.002(7)	0.020(7)	-0.006(7)
C(42)	0.068(7)	0.032(6)	0.041(6)	-0.003(5)	0.019(5)	-0.008(5)
C(43)	0.074(7)	0.035(5)	0.040(5)	-0.007(4)	0.021(5)	-0.010(5)
C(44)	0.071(7)	0.038(6)	0.040(6)	-0.004(5)	0.021(5)	-0.009(5)
C(45)	0.051(9)	0.041(9)	0.060(10)	0.015(8)	0.006(8)	0.003(7)
C(46)	0.043(9)	0.031(8)	0.051(9)	0.008(7)	-0.003(7)	0.005(6)
C(47)	0.066(11)	0.052(10)	0.040(8)	0.005(7)	0.009(8)	0.021(8)
C(48)	0.036(8)	0.052(9)	0.054(9)	-0.013(8)	-0.009(7)	0.011(7)
C(49)	0.036(8)	0.051(9)	0.025(7)	0.007(6)	0.005(6)	0.005(7)
C(50)	0.037(8)	0.022(7)	0.049(8)	-0.005(6)	0.016(7)	0.002(6)
C(51)	0.032(8)	0.043(8)	0.048(9)	-0.003(7)	-0.007(7)	0.015(6)
C(52)	0.035(8)	0.049(9)	0.069(11)	0.004(8)	0.014(7)	0.002(7)
C(53)	0.039(8)	0.031(8)	0.044(8)	0.004(6)	0.006(6)	-0.002(6)
C(54)	0.034(8)	0.026(7)	0.043(8)	-0.014(6)	-0.009(6)	0.008(6)
C(55)	0.037(8)	0.050(9)	0.032(7)	0.003(7)	0.002(6)	-0.002(7)
C(56)	0.072(11)	0.042(9)	0.050(9)	0.014(7)	-0.009(8)	-0.001(8)
C(57)	0.053(9)	0.036(8)	0.039(8)	0.020(7)	-0.006(7)	-0.013(7)

C(58)	0.086(14)	0.090(14)	0.059(11)	0.032(10)	-0.033(10)	-0.033(11)
Cu(3)	0.0426(11)	0.0379(11)	0.0477(11)	0.0020(8)	0.0147(8)	-0.0063(8)
Cu(4)	0.0456(11)	0.0350(10)	0.0506(11)	-0.0024(8)	0.0020(8)	0.0007(8)
N(9)	0.045(7)	0.040(7)	0.036(7)	0.009(5)	-0.004(5)	-0.007(5)
N(10)	0.046(7)	0.023(6)	0.051(7)	0.000(5)	0.013(6)	0.000(5)
N(11)	0.038(7)	0.053(8)	0.056(8)	0.007(7)	0.010(6)	-0.002(6)
N(12)	0.070(10)	0.028(7)	0.091(10)	0.001(7)	0.019(8)	0.019(6)
N(13)	0.040(7)	0.044(7)	0.042(7)	0.001(6)	0.004(5)	-0.008(6)
N(14)	0.041(7)	0.024(6)	0.044(7)	-0.001(5)	0.006(5)	-0.004(5)
N(15)	0.059(8)	0.021(6)	0.042(7)	-0.007(5)	0.010(6)	-0.013(5)
N(16)	0.042(7)	0.031(6)	0.045(7)	0.014(6)	0.004(5)	-0.007(5)
C(61)	0.046(10)	0.068(11)	0.082(12)	-0.027(10)	-0.006(9)	-0.010(8)
C(62)	0.048(9)	0.053(9)	0.029(7)	0.013(7)	0.009(6)	-0.001(7)
C(63)	0.062(10)	0.048(9)	0.048(9)	-0.004(8)	-0.016(8)	-0.013(8)
C(64)	0.035(8)	0.065(10)	0.045(9)	-0.010(8)	0.007(7)	-0.012(7)
C(65)	0.033(8)	0.041(8)	0.032(7)	0.002(6)	0.007(6)	-0.001(6)
C(66)	0.037(8)	0.034(7)	0.036(8)	0.004(6)	0.019(6)	0.001(6)
C(67)	0.038(8)	0.063(10)	0.046(9)	-0.010(8)	0.009(7)	-0.001(7)
C(68)	0.056(10)	0.036(8)	0.035(8)	0.004(6)	0.007(7)	0.004(7)
C(69)	0.017(7)	0.046(8)	0.055(9)	0.014(7)	0.008(6)	0.002(6)
C(70)	0.034(8)	0.036(8)	0.039(8)	0.000(6)	0.013(6)	-0.001(6)
C(71)	0.044(9)	0.062(10)	0.032(8)	-0.014(7)	0.004(7)	0.002(7)
C(72)	0.065(11)	0.038(9)	0.050(9)	-0.011(7)	0.001(8)	0.011(8)
C(73)	0.043(8)	0.030(7)	0.045(8)	-0.007(7)	-0.005(7)	-0.006(6)
C(77)	0.054(10)	0.036(9)	0.091(13)	0.019(9)	-0.021(9)	-0.004(7)
C(78)	0.046(10)	0.048(10)	0.097(14)	0.005(10)	-0.012(9)	-0.010(8)
C(79)	0.048(11)	0.064(12)	0.114(16)	-0.002(12)	0.007(11)	-0.019(9)
C(80)	0.029(8)	0.060(11)	0.100(13)	0.014(10)	0.011(8)	-0.008(8)
C(81)	0.043(9)	0.051(10)	0.059(10)	0.002(8)	0.007(7)	0.010(8)
C(82)	0.038(11)	0.19(3)	0.098(16)	0.034(18)	-0.027(10)	-0.012(14)
C(83)	0.101(18)	0.14(2)	0.103(18)	0.066(17)	-0.025(14)	-0.033(16)
C(84)	0.063(13)	0.079(14)	0.16(2)	0.062(15)	-0.020(13)	0.004(11)
C(85)	0.042(9)	0.047(10)	0.081(12)	0.000(9)	-0.013(8)	0.010(8)
C(86)	0.12(2)	0.15(3)	0.13(2)	0.05(2)	-0.028(18)	0.04(2)
C(87)	0.073(14)	0.045(11)	0.17(2)	0.025(13)	-0.023(15)	0.001(10)
C(88)	0.082(14)	0.048(11)	0.104(15)	0.015(11)	-0.024(11)	0.021(10)

C(89)	0.093(16)	0.060(12)	0.113(16)	0.013(12)	0.052(13)	-0.002(11)
C(90)	0.097(8)	0.039(6)	0.072(7)	0.021(6)	0.043(6)	0.020(6)
C(91)	0.089(9)	0.027(7)	0.056(8)	0.011(6)	0.026(7)	0.011(7)
C(92)	0.093(13)	0.026(8)	0.057(10)	0.004(7)	0.014(9)	-0.008(8)
C(93)	0.059(10)	0.040(9)	0.035(8)	-0.003(7)	0.002(7)	-0.010(7)
C(94)	0.064(10)	0.056(10)	0.019(7)	0.001(7)	0.015(7)	-0.028(8)
C(95)	0.055(9)	0.040(8)	0.022(7)	0.013(6)	-0.005(6)	-0.020(7)
C(96)	0.030(8)	0.068(11)	0.032(7)	0.001(7)	0.004(6)	0.001(7)
C(97)	0.029(8)	0.086(13)	0.039(8)	-0.010(9)	-0.008(6)	0.005(8)
C(98)	0.046(9)	0.046(9)	0.034(8)	0.005(7)	0.003(7)	-0.009(7)
C(99)	0.044(8)	0.033(8)	0.038(8)	-0.004(6)	0.020(7)	-0.012(6)
C(100)	0.025(7)	0.073(11)	0.060(10)	0.008(9)	0.007(7)	0.021(7)
C(101)	0.063(11)	0.024(8)	0.086(12)	0.006(8)	0.016(9)	0.009(7)
C(102)	0.042(8)	0.034(8)	0.035(7)	-0.006(6)	0.006(6)	-0.009(6)
C(103)	0.042(8)	0.041(9)	0.066(10)	0.004(8)	0.001(7)	-0.007(7)
C(104)	0.035(8)	0.042(8)	0.034(7)	-0.002(6)	0.001(6)	-0.004(6)
C(105)	0.055(10)	0.050(9)	0.046(9)	-0.021(8)	0.008(7)	-0.009(8)
C(106)	0.059(10)	0.022(7)	0.030(7)	-0.006(6)	0.019(7)	0.000(6)
C(107)	0.061(11)	0.037(9)	0.059(10)	-0.016(7)	0.011(8)	-0.032(8)
C(108)	0.041(8)	0.045(9)	0.041(8)	-0.005(7)	0.007(7)	-0.011(7)
C(109)	0.036(8)	0.038(8)	0.052(9)	-0.009(7)	0.004(7)	-0.002(6)
C(110)	0.049(9)	0.027(7)	0.035(7)	0.007(6)	0.009(6)	0.000(6)
C(111)	0.047(9)	0.054(10)	0.050(9)	0.005(8)	0.007(7)	0.003(7)
C(112)	0.049(9)	0.039(8)	0.026(7)	0.012(6)	0.009(6)	0.004(7)
C(113)	0.061(10)	0.035(8)	0.030(7)	0.008(6)	0.003(7)	0.008(7)
C(114)	0.045(8)	0.021(7)	0.037(7)	-0.002(6)	0.007(6)	0.001(6)
C(115)	0.072(12)	0.047(9)	0.037(8)	-0.006(7)	-0.003(8)	0.017(8)
C(116)	0.062(11)	0.072(12)	0.050(10)	0.010(9)	0.001(8)	-0.002(9)
C(117)	0.045(8)	0.044(8)	0.033(7)	0.000(7)	0.002(6)	0.004(7)
C(118)	0.038(9)	0.114(15)	0.059(10)	-0.005(11)	0.007(8)	-0.022(10)
As(1)	0.0438(10)	0.0344(9)	0.0481(9)	0.0022(7)	0.0028(7)	0.0094(7)
O(121)	0.056(7)	0.045(6)	0.043(6)	0.009(5)	-0.003(5)	0.019(5)
O(122)	0.037(5)	0.037(5)	0.060(6)	0.014(5)	0.007(5)	0.004(4)
O(131)	0.034(5)	0.052(6)	0.047(6)	-0.010(5)	0.009(4)	0.014(5)
O(132)	0.045(6)	0.039(6)	0.071(7)	-0.010(5)	0.014(5)	0.009(5)
O(141)	0.046(6)	0.030(5)	0.044(6)	0.007(4)	-0.002(4)	0.012(4)

O(142)	0.067(7)	0.028(5)	0.040(5)	0.000(4)	-0.002(5)	0.015(5)
C(121)	0.037(8)	0.055(9)	0.028(7)	0.014(7)	-0.010(6)	-0.006(7)
C(122)	0.100(13)	0.039(9)	0.027(8)	0.001(7)	-0.014(8)	0.014(9)
C(123)	0.088(14)	0.068(12)	0.058(10)	0.026(10)	-0.002(10)	-0.022(11)
C(124)	0.059(11)	0.060(11)	0.053(10)	0.003(8)	0.009(8)	-0.011(9)
C(125)	0.045(9)	0.037(8)	0.041(8)	0.007(7)	0.007(7)	-0.001(7)
C(126)	0.078(12)	0.038(8)	0.025(7)	0.004(6)	-0.001(7)	0.009(8)
C(131)	0.031(8)	0.035(8)	0.048(8)	0.005(7)	0.002(6)	-0.003(6)
C(132)	0.046(9)	0.037(8)	0.049(9)	-0.002(7)	-0.004(7)	0.013(7)
C(133)	0.086(14)	0.062(12)	0.065(11)	-0.008(9)	-0.017(10)	0.000(10)
C(134)	0.058(11)	0.050(10)	0.061(10)	0.003(9)	-0.004(8)	0.006(8)
C(135)	0.038(9)	0.063(11)	0.060(10)	0.021(9)	0.011(7)	0.008(8)
C(136)	0.041(9)	0.063(11)	0.047(9)	0.027(8)	0.007(7)	0.023(8)
C(141)	0.045(8)	0.027(7)	0.044(8)	-0.007(6)	0.008(6)	-0.004(6)
C(142)	0.034(8)	0.042(9)	0.052(9)	0.011(7)	0.004(7)	-0.001(6)
C(143)	0.071(11)	0.069(12)	0.038(9)	0.004(9)	-0.022(8)	-0.009(9)
C(144)	0.079(12)	0.036(9)	0.059(10)	-0.015(8)	-0.011(9)	0.002(8)
C(145)	0.066(10)	0.029(8)	0.059(10)	-0.002(7)	0.000(8)	0.016(7)
C(146)	0.052(9)	0.037(8)	0.040(8)	0.018(7)	0.009(7)	0.004(7)
As(2)	0.0441(10)	0.0297(9)	0.0419(9)	-0.0029(6)	0.0072(7)	-0.0037(6)
O(151)	0.048(7)	0.059(7)	0.074(7)	-0.009(6)	0.015(5)	0.001(5)
O(152)	0.072(7)	0.035(6)	0.051(6)	-0.015(5)	0.009(5)	-0.007(5)
O(161)	0.059(7)	0.050(6)	0.028(5)	0.011(4)	-0.004(5)	-0.001(5)
O(162)	0.040(6)	0.046(6)	0.041(5)	-0.011(5)	-0.003(4)	0.009(5)
O(171)	0.053(6)	0.018(5)	0.065(6)	-0.004(4)	0.000(5)	-0.018(4)
O(172)	0.049(6)	0.023(5)	0.041(5)	0.004(4)	0.004(4)	-0.007(4)
C(151)	0.053(10)	0.042(9)	0.070(11)	0.009(8)	0.021(9)	-0.007(8)
C(152)	0.090(14)	0.071(13)	0.078(13)	0.017(11)	0.041(11)	0.036(11)
C(153)	0.26(4)	0.047(14)	0.101(19)	-0.002(13)	0.09(2)	0.062(18)
C(154)	0.22(3)	0.053(13)	0.037(10)	-0.015(10)	0.010(15)	0.042(16)
C(155)	0.094(13)	0.051(10)	0.042(9)	-0.013(8)	-0.012(9)	0.024(9)
C(156)	0.099(14)	0.030(8)	0.028(8)	-0.004(6)	-0.002(8)	0.011(8)
C(161)	0.064(11)	0.029(8)	0.050(9)	0.000(7)	0.000(8)	-0.008(7)
C(162)	0.081(13)	0.088(14)	0.038(9)	0.010(9)	-0.012(8)	-0.002(11)
C(163)	0.086(15)	0.078(14)	0.085(15)	0.010(12)	-0.031(12)	0.017(11)
C(164)	0.096(16)	0.119(19)	0.061(12)	-0.020(13)	0.004(12)	-0.007(14)

C(165)	0.051(10)	0.051(10)	0.051(9)	0.000(8)	-0.004(7)	0.015(7)
C(166)	0.070(12)	0.046(9)	0.047(10)	-0.020(8)	-0.016(9)	0.001(8)
C(171)	0.032(8)	0.032(8)	0.045(8)	0.007(6)	-0.014(6)	0.000(6)
C(172)	0.059(10)	0.058(11)	0.070(11)	0.013(9)	-0.017(9)	-0.027(9)
C(173)	0.039(9)	0.044(9)	0.066(11)	0.010(8)	-0.012(7)	-0.006(7)
C(174)	0.051(10)	0.052(10)	0.061(10)	-0.010(8)	0.001(8)	-0.003(8)
C(175)	0.028(7)	0.042(8)	0.065(10)	0.016(8)	0.007(7)	-0.003(6)
C(176)	0.031(8)	0.035(8)	0.054(9)	-0.010(7)	-0.004(7)	-0.001(6)
As(3)	0.0443(9)	0.0329(9)	0.0405(9)	-0.0038(7)	0.0053(7)	0.0058(6)
O(181)	0.070(8)	0.042(6)	0.046(6)	-0.005(5)	-0.005(5)	0.014(5)
O(182)	0.038(5)	0.052(6)	0.035(5)	-0.014(5)	0.001(4)	-0.008(5)
O(191)	0.040(6)	0.042(6)	0.060(6)	-0.002(5)	0.008(5)	0.010(4)
O(192)	0.049(6)	0.048(6)	0.061(7)	0.005(5)	0.012(5)	0.015(5)
O(201)	0.054(6)	0.033(5)	0.053(6)	-0.004(5)	-0.002(5)	0.018(4)
O(202)	0.051(6)	0.031(5)	0.048(6)	-0.002(5)	0.000(5)	0.005(4)
C(181)	0.059(11)	0.041(9)	0.051(10)	-0.006(7)	0.001(8)	0.027(8)
C(182)	0.059(11)	0.068(11)	0.054(10)	-0.028(9)	-0.007(8)	0.012(9)
C(183)	0.104(18)	0.058(12)	0.097(16)	-0.022(11)	-0.020(13)	0.005(11)
C(184)	0.066(12)	0.068(12)	0.086(14)	0.025(11)	-0.018(11)	-0.006(10)
C(185)	0.059(11)	0.046(10)	0.056(10)	0.017(8)	-0.013(8)	-0.009(8)
C(186)	0.055(10)	0.035(8)	0.044(9)	0.006(7)	-0.012(8)	0.003(7)
C(191)	0.045(9)	0.040(8)	0.040(8)	-0.011(7)	0.022(7)	-0.016(7)
C(192)	0.086(13)	0.037(9)	0.049(9)	-0.001(8)	-0.003(9)	0.013(8)
C(193)	0.065(11)	0.064(11)	0.035(8)	0.006(8)	0.015(8)	-0.006(9)
C(194)	0.074(13)	0.054(10)	0.058(11)	0.008(9)	-0.002(9)	-0.020(9)
C(195)	0.059(11)	0.079(13)	0.046(9)	-0.015(9)	0.001(8)	-0.017(9)
C(196)	0.048(10)	0.067(11)	0.040(8)	-0.011(8)	0.010(7)	-0.010(8)
C(201)	0.030(8)	0.057(10)	0.037(8)	-0.006(7)	0.002(6)	0.007(7)
C(202)	0.055(10)	0.052(9)	0.037(8)	-0.006(7)	-0.006(7)	0.006(8)
C(203)	0.043(9)	0.048(9)	0.064(10)	-0.001(8)	-0.020(7)	0.011(7)
C(204)	0.041(9)	0.048(9)	0.058(9)	-0.019(8)	-0.008(7)	-0.010(7)
C(205)	0.038(8)	0.054(9)	0.050(9)	-0.016(8)	0.002(7)	-0.010(7)
C(206)	0.031(7)	0.032(8)	0.050(9)	0.003(7)	0.011(6)	0.005(6)
As(4)	0.0434(10)	0.0403(10)	0.0504(10)	-0.0020(7)	0.0037(7)	0.0074(7)
O(211)	0.065(7)	0.070(8)	0.042(6)	0.018(6)	-0.002(5)	0.003(6)
O(212)	0.049(6)	0.048(6)	0.051(6)	0.006(5)	0.007(5)	0.008(5)

O(221)	0.036(6)	0.056(6)	0.051(6)	-0.023(5)	0.003(4)	0.004(5)
O(222)	0.037(6)	0.036(6)	0.073(7)	-0.009(5)	0.009(5)	0.002(4)
O(231)	0.066(7)	0.026(5)	0.045(6)	0.002(4)	-0.004(5)	0.019(5)
O(232)	0.061(6)	0.027(5)	0.042(6)	0.000(4)	-0.004(5)	-0.002(4)
C(211)	0.057(10)	0.063(11)	0.035(8)	0.005(8)	0.009(8)	0.018(8)
C(212)	0.078(13)	0.074(12)	0.052(10)	-0.001(10)	-0.005(9)	-0.011(10)
C(213)	0.107(18)	0.103(17)	0.081(14)	0.022(13)	-0.009(13)	-0.037(15)
C(214)	0.072(13)	0.081(13)	0.047(10)	0.005(10)	-0.015(9)	0.001(10)
C(215)	0.083(13)	0.049(10)	0.076(12)	-0.014(10)	-0.019(10)	-0.006(10)
C(216)	0.071(12)	0.080(13)	0.032(8)	-0.001(8)	0.006(8)	-0.026(10)
C(221)	0.040(8)	0.037(8)	0.042(8)	0.002(7)	-0.004(7)	0.005(7)
C(222)	0.070(12)	0.056(10)	0.031(8)	0.005(7)	0.014(7)	0.005(8)
C(223)	0.048(10)	0.073(12)	0.048(9)	-0.006(8)	-0.009(7)	0.007(9)
C(224)	0.053(10)	0.054(10)	0.057(10)	0.011(8)	-0.010(8)	-0.008(8)
C(225)	0.045(9)	0.036(8)	0.054(9)	0.015(7)	0.009(7)	0.012(7)
C(226)	0.052(10)	0.037(8)	0.055(9)	0.008(7)	0.001(7)	-0.002(7)
C(231)	0.042(8)	0.039(8)	0.045(9)	0.005(7)	-0.003(7)	0.004(7)
C(232)	0.032(8)	0.053(10)	0.065(10)	0.008(9)	0.000(7)	0.003(7)
C(233)	0.097(14)	0.057(11)	0.062(11)	-0.003(9)	-0.015(10)	0.029(10)
C(234)	0.113(15)	0.052(11)	0.051(10)	-0.018(8)	-0.026(10)	0.019(10)
C(235)	0.074(11)	0.038(9)	0.049(9)	-0.008(8)	-0.009(8)	-0.001(8)
C(236)	0.054(9)	0.037(8)	0.045(9)	-0.010(7)	-0.003(7)	-0.008(7)

Table 4. Bond lengths [Å] for nd019.

atom-atom	distance	atom-atom	distance
Cu(1)-N(1)	2.008(10)	Cu(1)-N(6)	2.014(11)
Cu(1)-N(5)	2.033(11)	Cu(1)-N(2)	2.035(10)
Cu(2)-N(4)	2.002(14)	Cu(2)-N(7)	2.009(10)
Cu(2)-N(3)	2.035(12)	Cu(2)-N(8)	2.091(13)
N(1)-C(6)	1.336(15)	N(1)-C(2)	1.340(17)
N(2)-C(10)	1.313(15)	N(2)-C(13)	1.333(15)
N(3)-C(17)	1.34(2)	N(3)-C(21)	1.378(19)
N(4)-C(28)	1.35(2)	N(4)-C(25)	1.356(19)
N(5)-C(35)	1.351(16)	N(5)-C(31)	1.360(18)
N(6)-C(42)	1.348(17)	N(6)-C(39)	1.409(17)
N(7)-C(46)	1.317(15)	N(7)-C(50)	1.364(15)
N(8)-C(57)	1.352(17)	N(8)-C(54)	1.399(16)
C(1)-C(2)	1.480(19)	C(2)-C(3)	1.43(2)
C(3)-C(4)	1.41(2)	C(4)-C(5)	1.344(19)
C(5)-C(6)	1.422(18)	C(5)-C(7)	1.463(19)
C(6)-C(10)	1.435(16)	C(7)-C(8)	1.311(18)
C(8)-C(9)	1.479(18)	C(9)-C(11)	1.379(18)
C(9)-C(10)	1.461(17)	C(11)-C(12)	1.332(17)
C(12)-C(13)	1.387(17)	C(13)-C(14)	1.509(17)
C(14)-C(15)	1.48(2)	C(15)-C(16)	1.38(3)
C(16)-C(17)	1.59(3)	C(17)-C(18)	1.34(2)
C(18)-C(19)	1.44(2)	C(19)-C(20)	1.35(2)
C(20)-C(21)	1.39(2)	C(20)-C(22)	1.50(3)
C(21)-C(25)	1.44(2)	C(22)-C(23)	1.40(3)
C(23)-C(24)	1.39(3)	C(24)-C(25)	1.40(2)
C(24)-C(26)	1.41(3)	C(26)-C(27)	1.39(3)
C(27)-C(28)	1.38(2)	C(28)-C(29)	1.46(2)
C(30)-C(31)	1.48(2)	C(31)-C(32)	1.382(19)
C(32)-C(33)	1.31(2)	C(33)-C(34)	1.43(2)
C(34)-C(35)	1.380(18)	C(34)-C(36)	1.43(2)
C(35)-C(39)	1.41(2)	C(36)-C(37)	1.35(2)
C(37)-C(38)	1.43(2)	C(38)-C(40)	1.37(2)
C(38)-C(39)	1.425(19)	C(40)-C(41)	1.295(19)
C(41)-C(42)	1.429(19)	C(42)-C(43)	1.536(19)
C(43)-C(44)	1.60(2)	C(44)-C(45)	1.527(19)
C(45)-C(46)	1.499(19)	C(46)-C(47)	1.399(19)
C(47)-C(48)	1.37(2)	C(48)-C(49)	1.438(18)
C(49)-C(50)	1.370(18)	C(49)-C(51)	1.406(18)
C(50)-C(54)	1.437(18)	C(51)-C(52)	1.363(19)
C(52)-C(53)	1.426(19)	C(53)-C(54)	1.340(18)
C(53)-C(55)	1.442(18)	C(55)-C(56)	1.394(19)
C(56)-C(57)	1.37(2)	C(57)-C(58)	1.49(2)

Cu(3)-N(14)	2.004(11)	Cu(3)-N(13)	2.016(11)
Cu(3)-N(10)	2.045(11)	Cu(3)-N(9)	2.054(11)
Cu(4)-N(15)	1.974(11)	Cu(4)-N(12)	2.042(13)
Cu(4)-N(11)	2.065(12)	Cu(4)-N(16)	2.085(11)
N(9)-C(62)	1.331(17)	N(9)-C(66)	1.345(16)
N(10)-C(70)	1.361(16)	N(10)-C(73)	1.379(16)
N(11)-C(77)	1.304(18)	N(11)-C(81)	1.385(18)
N(12)-C(88)	1.31(2)	N(12)-C(85)	1.395(19)
N(13)-C(91)	1.319(17)	N(13)-C(95)	1.361(17)
N(14)-C(102)	1.359(16)	N(14)-C(99)	1.366(15)
N(15)-C(106)	1.340(15)	N(15)-C(110)	1.402(16)
N(16)-C(117)	1.309(16)	N(16)-C(114)	1.351(16)
C(61)-C(62)	1.487(19)	C(62)-C(63)	1.389(19)
C(63)-C(64)	1.368(19)	C(64)-C(65)	1.400(18)
C(65)-C(66)	1.377(17)	C(65)-C(67)	1.451(18)
C(66)-C(70)	1.454(18)	C(67)-C(68)	1.324(18)
C(68)-C(69)	1.478(18)	C(69)-C(70)	1.358(17)
C(69)-C(71)	1.408(19)	C(71)-C(72)	1.38(2)
C(72)-C(73)	1.368(19)	C(73)-C(74)	1.495(18)
C(74)-C(75)	1.54(3)	C(75)-C(76)	1.50(4)
C(76)-C(77)	1.56(3)	C(75A)-C(76A)	1.55(3)
C(76A)-C(77)	1.60(3)	C(77)-C(78)	1.41(2)
C(78)-C(79)	1.35(2)	C(79)-C(80)	1.39(2)
C(80)-C(81)	1.37(2)	C(80)-C(82)	1.49(2)
C(81)-C(85)	1.41(2)	C(82)-C(83)	1.31(3)
C(83)-C(84)	1.45(3)	C(84)-C(85)	1.41(2)
C(84)-C(86)	1.42(3)	C(86)-C(87)	1.38(3)
C(87)-C(88)	1.39(3)	C(88)-C(89)	1.55(3)
C(90)-C(91)	1.39(2)	C(91)-C(92)	1.445(19)
C(92)-C(93)	1.32(2)	C(93)-C(94)	1.43(2)
C(94)-C(95)	1.420(17)	C(94)-C(96)	1.425(19)
C(95)-C(99)	1.484(19)	C(96)-C(97)	1.35(2)
C(97)-C(98)	1.41(2)	C(98)-C(99)	1.355(18)
C(98)-C(100)	1.39(2)	C(100)-C(101)	1.39(2)
C(101)-C(102)	1.402(19)	C(102)-C(103)	1.503(18)
C(103)-C(104)	1.523(18)	C(104)-C(105)	1.484(18)
C(105)-C(106)	1.502(18)	C(106)-C(107)	1.43(2)
C(107)-C(108)	1.293(19)	C(108)-C(109)	1.428(18)
C(109)-C(110)	1.385(18)	C(109)-C(111)	1.431(18)
C(110)-C(114)	1.433(17)	C(111)-C(112)	1.336(18)
C(112)-C(113)	1.419(19)	C(113)-C(115)	1.389(19)
C(113)-C(114)	1.432(18)	C(115)-C(116)	1.40(2)
C(116)-C(117)	1.40(2)	C(117)-C(118)	1.520(19)
As(1)-O(132)	1.815(10)	As(1)-O(122)	1.823(9)
As(1)-O(141)	1.828(8)	As(1)-O(121)	1.828(9)
As(1)-O(142)	1.830(9)	As(1)-O(131)	1.848(9)

O(121)-C(121)	1.344(16)	O(122)-C(126)	1.408(15)
O(131)-C(131)	1.356(15)	O(132)-C(136)	1.377(19)
O(141)-C(141)	1.378(15)	O(142)-C(146)	1.368(15)
C(121)-C(122)	1.366(18)	C(121)-C(126)	1.429(19)
C(122)-C(123)	1.42(2)	C(123)-C(124)	1.42(2)
C(124)-C(125)	1.364(19)	C(125)-C(126)	1.36(2)
C(131)-C(132)	1.358(18)	C(131)-C(136)	1.417(19)
C(132)-C(133)	1.38(2)	C(133)-C(134)	1.45(2)
C(134)-C(135)	1.36(2)	C(135)-C(136)	1.40(2)
C(141)-C(142)	1.356(18)	C(141)-C(146)	1.414(18)
C(142)-C(143)	1.41(2)	C(143)-C(144)	1.35(2)
C(144)-C(145)	1.37(2)	C(145)-C(146)	1.341(19)
As(2)-O(172)	1.824(8)	As(2)-O(171)	1.827(8)
As(2)-O(161)	1.832(9)	As(2)-O(151)	1.834(10)
As(2)-O(162)	1.847(9)	As(2)-O(152)	1.856(9)
O(151)-C(151)	1.400(18)	O(152)-C(156)	1.350(17)
O(161)-C(161)	1.358(17)	O(162)-C(166)	1.384(17)
O(171)-C(171)	1.372(15)	O(172)-C(176)	1.341(15)
C(151)-C(156)	1.33(2)	C(151)-C(152)	1.34(2)
C(152)-C(153)	1.37(3)	C(153)-C(154)	1.42(4)
C(154)-C(155)	1.40(3)	C(155)-C(156)	1.44(2)
C(161)-C(166)	1.38(2)	C(161)-C(162)	1.41(2)
C(162)-C(163)	1.42(2)	C(163)-C(164)	1.33(3)
C(164)-C(165)	1.43(2)	C(165)-C(166)	1.41(2)
C(171)-C(172)	1.360(19)	C(171)-C(176)	1.413(18)
C(172)-C(173)	1.33(2)	C(173)-C(174)	1.37(2)
C(174)-C(175)	1.42(2)	C(175)-C(176)	1.392(19)
As(3)-O(201)	1.802(9)	As(3)-O(202)	1.820(9)
As(3)-O(192)	1.823(10)	As(3)-O(191)	1.824(9)
As(3)-O(182)	1.837(9)	As(3)-O(181)	1.841(10)
O(181)-C(181)	1.398(18)	O(182)-C(186)	1.379(16)
O(191)-C(191)	1.379(15)	O(192)-C(196)	1.387(17)
O(201)-C(201)	1.363(16)	O(202)-C(206)	1.369(15)
C(181)-C(182)	1.32(2)	C(181)-C(186)	1.340(19)
C(182)-C(183)	1.40(2)	C(183)-C(184)	1.38(3)
C(184)-C(185)	1.36(2)	C(185)-C(186)	1.36(2)
C(191)-C(192)	1.38(2)	C(191)-C(196)	1.41(2)
C(192)-C(193)	1.41(2)	C(193)-C(194)	1.38(2)
C(194)-C(195)	1.40(2)	C(195)-C(196)	1.38(2)
C(201)-C(206)	1.404(19)	C(201)-C(202)	1.406(19)
C(202)-C(203)	1.401(19)	C(203)-C(204)	1.36(2)
C(204)-C(205)	1.41(2)	C(205)-C(206)	1.357(18)
As(4)-O(211)	1.814(10)	As(4)-O(232)	1.816(9)
As(4)-O(222)	1.831(9)	As(4)-O(221)	1.836(9)
As(4)-O(212)	1.847(10)	As(4)-O(231)	1.847(9)
O(211)-C(211)	1.359(18)	O(212)-C(216)	1.351(18)

O(221)-C(221)	1.331(16)	O(222)-C(226)	1.390(17)
O(231)-C(231)	1.369(16)	O(232)-C(236)	1.364(16)
C(211)-C(212)	1.33(2)	C(211)-C(216)	1.41(2)
C(212)-C(213)	1.43(2)	C(213)-C(214)	1.29(3)
C(214)-C(215)	1.40(2)	C(215)-C(216)	1.34(2)
C(221)-C(222)	1.352(19)	C(221)-C(226)	1.44(2)
C(222)-C(223)	1.39(2)	C(223)-C(224)	1.41(2)
C(224)-C(225)	1.35(2)	C(225)-C(226)	1.373(19)
C(231)-C(232)	1.346(19)	C(231)-C(236)	1.394(19)
C(232)-C(233)	1.37(2)	C(233)-C(234)	1.37(2)
C(234)-C(235)	1.40(2)	C(235)-C(236)	1.378(19)

Symmetry transformations used to generate equivalent atoms:

Table 5. Bond angles [°] for nd019.

atom-atom-atom	angle	atom-atom-atom	angle
N(1)-Cu(1)-N(6)	119.5(4)	N(1)-Cu(1)-N(5)	123.8(4)
N(6)-Cu(1)-N(5)	82.2(4)	N(1)-Cu(1)-N(2)	81.9(4)
N(6)-Cu(1)-N(2)	135.0(4)	N(5)-Cu(1)-N(2)	120.3(4)
N(4)-Cu(2)-N(7)	132.6(5)	N(4)-Cu(2)-N(3)	82.6(5)
N(7)-Cu(2)-N(3)	134.4(4)	N(4)-Cu(2)-N(8)	111.0(5)
N(7)-Cu(2)-N(8)	82.5(4)	N(3)-Cu(2)-N(8)	114.7(4)
C(6)-N(1)-C(2)	117.5(11)	C(6)-N(1)-Cu(1)	112.6(8)
C(2)-N(1)-Cu(1)	129.8(9)	C(10)-N(2)-C(13)	118.7(11)
C(10)-N(2)-Cu(1)	110.8(8)	C(13)-N(2)-Cu(1)	130.4(9)
C(17)-N(3)-C(21)	114.5(14)	C(17)-N(3)-Cu(2)	133.5(11)
C(21)-N(3)-Cu(2)	111.2(10)	C(28)-N(4)-C(25)	118.1(14)
C(28)-N(4)-Cu(2)	129.0(11)	C(25)-N(4)-Cu(2)	111.8(10)
C(35)-N(5)-C(31)	116.2(12)	C(35)-N(5)-Cu(1)	112.8(9)
C(31)-N(5)-Cu(1)	130.9(9)	C(42)-N(6)-C(39)	117.9(12)
C(42)-N(6)-Cu(1)	130.5(9)	C(39)-N(6)-Cu(1)	111.2(9)
C(46)-N(7)-C(50)	117.4(11)	C(46)-N(7)-Cu(2)	129.6(9)
C(50)-N(7)-Cu(2)	113.0(8)	C(57)-N(8)-C(54)	119.0(12)
C(57)-N(8)-Cu(2)	131.1(9)	C(54)-N(8)-Cu(2)	109.8(9)
N(1)-C(2)-C(3)	121.6(14)	N(1)-C(2)-C(1)	117.0(13)
C(3)-C(2)-C(1)	121.4(14)	C(4)-C(3)-C(2)	119.0(15)
C(5)-C(4)-C(3)	118.7(15)	C(4)-C(5)-C(6)	118.8(13)
C(4)-C(5)-C(7)	122.1(14)	C(6)-C(5)-C(7)	118.6(12)
N(1)-C(6)-C(5)	124.1(11)	N(1)-C(6)-C(10)	115.7(10)
C(5)-C(6)-C(10)	120.2(11)	C(8)-C(7)-C(5)	122.3(12)
C(7)-C(8)-C(9)	121.6(12)	C(11)-C(9)-C(10)	117.6(12)
C(11)-C(9)-C(8)	124.7(12)	C(10)-C(9)-C(8)	117.6(12)
N(2)-C(10)-C(6)	118.9(10)	N(2)-C(10)-C(9)	121.6(11)
C(6)-C(10)-C(9)	119.3(11)	C(12)-C(11)-C(9)	118.3(12)
C(11)-C(12)-C(13)	121.8(12)	N(2)-C(13)-C(12)	121.7(12)
N(2)-C(13)-C(14)	117.0(12)	C(12)-C(13)-C(14)	121.3(12)
C(15)-C(14)-C(13)	116.0(14)	C(16)-C(15)-C(14)	119.6(19)
C(15)-C(16)-C(17)	121.2(19)	N(3)-C(17)-C(18)	128.3(17)
N(3)-C(17)-C(16)	116.2(14)	C(18)-C(17)-C(16)	114.8(17)
C(17)-C(18)-C(19)	115.3(17)	C(20)-C(19)-C(18)	119.1(16)
C(19)-C(20)-C(21)	120.3(16)	C(19)-C(20)-C(22)	119.8(19)
C(21)-C(20)-C(22)	119.9(19)	N(3)-C(21)-C(20)	122.2(16)
N(3)-C(21)-C(25)	115.5(14)	C(20)-C(21)-C(25)	122.4(16)
C(23)-C(22)-C(20)	116(2)	C(24)-C(23)-C(22)	122(2)
C(23)-C(24)-C(25)	123.1(19)	C(23)-C(24)-C(26)	123(2)
C(25)-C(24)-C(26)	113.4(18)	N(4)-C(25)-C(24)	125.7(16)
N(4)-C(25)-C(21)	117.9(14)	C(24)-C(25)-C(21)	116.4(16)
C(27)-C(26)-C(24)	122.5(19)	C(28)-C(27)-C(26)	118.5(19)

N(4)-C(28)-C(27)	121.8(17)	N(4)-C(28)-C(29)	113.9(15)
C(27)-C(28)-C(29)	124.2(18)	N(5)-C(31)-C(32)	121.6(14)
N(5)-C(31)-C(30)	115.3(13)	C(32)-C(31)-C(30)	123.1(15)
C(33)-C(32)-C(31)	122.4(15)	C(32)-C(33)-C(34)	118.1(15)
C(35)-C(34)-C(36)	120.6(14)	C(35)-C(34)-C(33)	117.1(14)
C(36)-C(34)-C(33)	122.3(14)	N(5)-C(35)-C(34)	124.3(13)
N(5)-C(35)-C(39)	116.9(12)	C(34)-C(35)-C(39)	118.7(13)
C(37)-C(36)-C(34)	119.8(14)	C(36)-C(37)-C(38)	122.7(15)
C(40)-C(38)-C(39)	117.5(13)	C(40)-C(38)-C(37)	126.7(14)
C(39)-C(38)-C(37)	115.9(15)	N(6)-C(39)-C(35)	116.8(12)
N(6)-C(39)-C(38)	121.0(14)	C(35)-C(39)-C(38)	122.2(13)
C(41)-C(40)-C(38)	121.8(14)	C(40)-C(41)-C(42)	122.1(14)
N(6)-C(42)-C(41)	119.6(13)	N(6)-C(42)-C(43)	116.6(12)
C(41)-C(42)-C(43)	123.8(12)	C(42)-C(43)-C(44)	107.1(12)
C(45)-C(44)-C(43)	111.0(12)	C(46)-C(45)-C(44)	114.0(12)
N(7)-C(46)-C(47)	122.0(13)	N(7)-C(46)-C(45)	118.4(12)
C(47)-C(46)-C(45)	119.6(13)	C(48)-C(47)-C(46)	120.9(13)
C(47)-C(48)-C(49)	117.9(13)	C(50)-C(49)-C(51)	122.3(12)
C(50)-C(49)-C(48)	116.2(12)	C(51)-C(49)-C(48)	121.5(12)
N(7)-C(50)-C(49)	125.6(12)	N(7)-C(50)-C(54)	118.0(12)
C(49)-C(50)-C(54)	116.3(11)	C(52)-C(51)-C(49)	120.3(12)
C(51)-C(52)-C(53)	118.3(13)	C(54)-C(53)-C(52)	120.8(13)
C(54)-C(53)-C(55)	119.9(13)	C(52)-C(53)-C(55)	119.2(12)
C(53)-C(54)-N(8)	121.8(13)	C(53)-C(54)-C(50)	121.7(12)
N(8)-C(54)-C(50)	116.5(12)	C(56)-C(55)-C(53)	116.0(12)
C(57)-C(56)-C(55)	122.3(14)	N(8)-C(57)-C(56)	120.4(13)
N(8)-C(57)-C(58)	116.1(12)	C(56)-C(57)-C(58)	123.5(13)
N(14)-Cu(3)-N(13)	83.1(4)	N(14)-Cu(3)-N(10)	136.6(4)
N(13)-Cu(3)-N(10)	119.4(4)	N(14)-Cu(3)-N(9)	118.2(4)
N(13)-Cu(3)-N(9)	123.5(4)	N(10)-Cu(3)-N(9)	81.7(4)
N(15)-Cu(4)-N(12)	132.4(5)	N(15)-Cu(4)-N(11)	137.0(5)
N(12)-Cu(4)-N(11)	83.6(5)	N(15)-Cu(4)-N(16)	82.8(4)
N(12)-Cu(4)-N(16)	108.9(5)	N(11)-Cu(4)-N(16)	110.0(4)
C(62)-N(9)-C(66)	118.1(12)	C(62)-N(9)-Cu(3)	129.4(9)
C(66)-N(9)-Cu(3)	112.6(9)	C(70)-N(10)-C(73)	119.5(11)
C(70)-N(10)-Cu(3)	111.7(8)	C(73)-N(10)-Cu(3)	128.7(9)
C(77)-N(11)-C(81)	120.0(13)	C(77)-N(11)-Cu(4)	129.6(11)
C(81)-N(11)-Cu(4)	109.9(10)	C(88)-N(12)-C(85)	118.6(15)
C(88)-N(12)-Cu(4)	132.1(13)	C(85)-N(12)-Cu(4)	109.0(10)
C(91)-N(13)-C(95)	118.0(12)	C(91)-N(13)-Cu(3)	131.0(10)
C(95)-N(13)-Cu(3)	111.0(9)	C(102)-N(14)-C(99)	114.3(11)
C(102)-N(14)-Cu(3)	130.9(9)	C(99)-N(14)-Cu(3)	114.5(8)
C(106)-N(15)-C(110)	116.2(11)	C(106)-N(15)-Cu(4)	130.1(9)
C(110)-N(15)-Cu(4)	113.7(8)	C(117)-N(16)-C(114)	118.9(12)
C(117)-N(16)-Cu(4)	131.6(10)	C(114)-N(16)-Cu(4)	109.3(9)
N(9)-C(62)-C(63)	120.9(12)	N(9)-C(62)-C(61)	117.8(13)

C(63)-C(62)-C(61)	121.2(14)	C(64)-C(63)-C(62)	121.6(13)
C(63)-C(64)-C(65)	117.4(13)	C(66)-C(65)-C(64)	118.0(12)
C(66)-C(65)-C(67)	119.2(12)	C(64)-C(65)-C(67)	122.7(12)
N(9)-C(66)-C(65)	123.9(12)	N(9)-C(66)-C(70)	116.4(11)
C(65)-C(66)-C(70)	119.6(11)	C(68)-C(67)-C(65)	121.2(13)
C(67)-C(68)-C(69)	120.3(13)	C(70)-C(69)-C(71)	120.0(12)
C(70)-C(69)-C(68)	118.9(13)	C(71)-C(69)-C(68)	121.1(12)
C(69)-C(70)-N(10)	121.9(12)	C(69)-C(70)-C(66)	120.5(12)
N(10)-C(70)-C(66)	117.5(11)	C(72)-C(71)-C(69)	116.4(12)
C(73)-C(72)-C(71)	123.3(14)	C(72)-C(73)-N(10)	118.6(13)
C(72)-C(73)-C(74)	123.1(13)	N(10)-C(73)-C(74)	118.3(12)
C(73)-C(74)-C(75)	109.3(14)	C(76)-C(75)-C(74)	111(2)
C(75)-C(76)-C(77)	107(2)	C(75A)-C(76A)-C(77)	105.2(19)
N(11)-C(77)-C(78)	121.3(14)	N(11)-C(77)-C(76)	119.7(16)
C(78)-C(77)-C(76)	117.2(17)	N(11)-C(77)-C(76A)	115.5(15)
C(78)-C(77)-C(76A)	118.2(15)	C(76)-C(77)-C(76A)	36.5(12)
C(79)-C(78)-C(77)	120.7(16)	C(78)-C(79)-C(80)	117.0(16)
C(81)-C(80)-C(79)	121.8(16)	C(81)-C(80)-C(82)	116.9(17)
C(79)-C(80)-C(82)	120.8(18)	C(80)-C(81)-N(11)	119.0(14)
C(80)-C(81)-C(85)	123.5(15)	N(11)-C(81)-C(85)	117.3(14)
C(83)-C(82)-C(80)	121(2)	C(82)-C(83)-C(84)	120(2)
C(85)-C(84)-C(86)	113.5(19)	C(85)-C(84)-C(83)	119.9(18)
C(86)-C(84)-C(83)	126(2)	N(12)-C(85)-C(81)	119.7(13)
N(12)-C(85)-C(84)	122.6(16)	C(81)-C(85)-C(84)	117.3(16)
C(87)-C(86)-C(84)	125(2)	C(86)-C(87)-C(88)	115(2)
N(12)-C(88)-C(87)	124.6(19)	N(12)-C(88)-C(89)	116.1(16)
C(87)-C(88)-C(89)	118.8(18)	N(13)-C(91)-C(90)	117.2(13)
N(13)-C(91)-C(92)	121.0(14)	C(90)-C(91)-C(92)	121.5(13)
C(93)-C(92)-C(91)	121.0(14)	C(92)-C(93)-C(94)	120.4(13)
C(95)-C(94)-C(96)	120.8(15)	C(95)-C(94)-C(93)	115.2(14)
C(96)-C(94)-C(93)	124.0(13)	N(13)-C(95)-C(94)	124.5(13)
N(13)-C(95)-C(99)	118.7(11)	C(94)-C(95)-C(99)	116.8(13)
C(97)-C(96)-C(94)	119.1(14)	C(96)-C(97)-C(98)	123.1(14)
C(99)-C(98)-C(100)	116.8(13)	C(99)-C(98)-C(97)	119.8(14)
C(100)-C(98)-C(97)	123.3(14)	C(98)-C(99)-N(14)	127.0(13)
C(98)-C(99)-C(95)	120.1(12)	N(14)-C(99)-C(95)	112.7(11)
C(101)-C(100)-C(98)	120.0(13)	C(100)-C(101)-C(102)	118.4(13)
N(14)-C(102)-C(101)	123.3(12)	N(14)-C(102)-C(103)	116.9(12)
C(101)-C(102)-C(103)	119.7(12)	C(102)-C(103)-C(104)	112.8(11)
C(105)-C(104)-C(103)	113.8(11)	C(104)-C(105)-C(106)	114.2(12)
N(15)-C(106)-C(107)	120.5(12)	N(15)-C(106)-C(105)	116.3(13)
C(107)-C(106)-C(105)	123.1(12)	C(108)-C(107)-C(106)	122.7(14)
C(107)-C(108)-C(109)	120.1(14)	C(110)-C(109)-C(108)	115.9(12)
C(110)-C(109)-C(111)	118.9(13)	C(108)-C(109)-C(111)	125.2(13)
C(109)-C(110)-N(15)	124.6(12)	C(109)-C(110)-C(114)	120.9(12)
N(15)-C(110)-C(114)	114.5(12)	C(112)-C(111)-C(109)	121.6(14)

C(111)-C(112)-C(113)	121.1(13)	C(115)-C(113)-C(112)	123.3(13)
C(115)-C(113)-C(114)	117.4(14)	C(112)-C(113)-C(114)	119.3(12)
N(16)-C(114)-C(113)	122.4(12)	N(16)-C(114)-C(110)	119.6(12)
C(113)-C(114)-C(110)	118.0(12)	C(113)-C(115)-C(116)	118.4(14)
C(115)-C(116)-C(117)	119.8(15)	N(16)-C(117)-C(116)	122.7(14)
N(16)-C(117)-C(118)	117.4(13)	C(116)-C(117)-C(118)	119.9(14)
O(132)-As(1)-O(122)	176.4(5)	O(132)-As(1)-O(141)	93.0(4)
O(122)-As(1)-O(141)	88.0(4)	O(132)-As(1)-O(121)	90.8(5)
O(122)-As(1)-O(121)	88.6(4)	O(141)-As(1)-O(121)	173.0(4)
O(132)-As(1)-O(142)	88.8(4)	O(122)-As(1)-O(142)	94.7(4)
O(141)-As(1)-O(142)	88.2(4)	O(121)-As(1)-O(142)	86.0(4)
O(132)-As(1)-O(131)	88.7(4)	O(122)-As(1)-O(131)	87.9(4)
O(141)-As(1)-O(131)	90.8(4)	O(121)-As(1)-O(131)	95.2(4)
O(142)-As(1)-O(131)	177.2(4)	C(121)-O(121)-As(1)	111.7(8)
C(126)-O(122)-As(1)	111.0(8)	C(131)-O(131)-As(1)	111.1(8)
C(136)-O(132)-As(1)	110.7(8)	C(141)-O(141)-As(1)	111.5(8)
C(146)-O(142)-As(1)	110.7(8)	O(121)-C(121)-C(122)	126.2(13)
O(121)-C(121)-C(126)	115.5(12)	C(122)-C(121)-C(126)	118.0(14)
C(121)-C(122)-C(123)	118.9(15)	C(122)-C(123)-C(124)	121.1(15)
C(125)-C(124)-C(123)	118.9(15)	C(126)-C(125)-C(124)	119.8(14)
C(125)-C(126)-O(122)	124.7(13)	C(125)-C(126)-C(121)	122.8(13)
O(122)-C(126)-C(121)	112.6(13)	O(131)-C(131)-C(132)	124.7(12)
O(131)-C(131)-C(136)	114.2(13)	C(132)-C(131)-C(136)	121.1(14)
C(131)-C(132)-C(133)	120.7(14)	C(132)-C(133)-C(134)	119.1(15)
C(135)-C(134)-C(133)	119.1(15)	C(134)-C(135)-C(136)	121.5(15)
O(132)-C(136)-C(135)	126.4(13)	O(132)-C(136)-C(131)	115.2(13)
C(135)-C(136)-C(131)	118.3(16)	C(142)-C(141)-O(141)	124.1(12)
C(142)-C(141)-C(146)	122.5(13)	O(141)-C(141)-C(146)	113.4(12)
C(141)-C(142)-C(143)	114.4(13)	C(144)-C(143)-C(142)	123.2(14)
C(143)-C(144)-C(145)	120.9(15)	C(146)-C(145)-C(144)	118.5(13)
C(145)-C(146)-O(142)	124.3(12)	C(145)-C(146)-C(141)	120.3(13)
O(142)-C(146)-C(141)	115.3(13)	O(172)-As(2)-O(171)	88.3(4)
O(172)-As(2)-O(161)	176.0(4)	O(171)-As(2)-O(161)	88.4(4)
O(172)-As(2)-O(151)	94.0(4)	O(171)-As(2)-O(151)	87.5(5)
O(161)-As(2)-O(151)	88.2(5)	O(172)-As(2)-O(162)	89.2(4)
O(171)-As(2)-O(162)	97.3(4)	O(161)-As(2)-O(162)	88.9(4)
O(151)-As(2)-O(162)	174.3(5)	O(172)-As(2)-O(152)	90.6(4)
O(171)-As(2)-O(152)	175.7(4)	O(161)-As(2)-O(152)	92.9(4)
O(151)-As(2)-O(152)	88.4(5)	O(162)-As(2)-O(152)	86.9(4)
C(151)-O(151)-As(2)	108.2(9)	C(156)-O(152)-As(2)	107.7(10)
C(161)-O(161)-As(2)	109.2(8)	C(166)-O(162)-As(2)	108.9(9)
C(171)-O(171)-As(2)	110.6(7)	C(176)-O(172)-As(2)	111.1(8)
C(156)-C(151)-C(152)	123.2(18)	C(156)-C(151)-O(151)	114.6(13)
C(152)-C(151)-O(151)	122.1(17)	C(151)-C(152)-C(153)	120(2)
C(152)-C(153)-C(154)	119(2)	C(155)-C(154)-C(153)	123(2)
C(154)-C(155)-C(156)	113.9(19)	C(151)-C(156)-O(152)	118.8(14)

C(151)-C(156)-C(155)	121.8(16)	O(152)-C(156)-C(155)	119.2(16)
O(161)-C(161)-C(166)	117.0(14)	O(161)-C(161)-C(162)	122.7(14)
C(166)-C(161)-C(162)	120.3(16)	C(161)-C(162)-C(163)	116.6(16)
C(164)-C(163)-C(162)	123.5(18)	C(163)-C(164)-C(165)	120(2)
C(166)-C(165)-C(164)	117.1(16)	C(161)-C(166)-O(162)	114.7(14)
C(161)-C(166)-C(165)	122.1(15)	O(162)-C(166)-C(165)	123.2(14)
C(172)-C(171)-O(171)	126.7(12)	C(172)-C(171)-C(176)	119.4(13)
O(171)-C(171)-C(176)	113.9(11)	C(173)-C(172)-C(171)	122.0(15)
C(172)-C(173)-C(174)	120.9(15)	C(173)-C(174)-C(175)	120.2(15)
C(176)-C(175)-C(174)	117.8(13)	O(172)-C(176)-C(175)	125.0(12)
O(172)-C(176)-C(171)	115.4(12)	C(175)-C(176)-C(171)	119.6(12)
O(201)-As(3)-O(202)	89.0(4)	O(201)-As(3)-O(192)	88.0(4)
O(202)-As(3)-O(192)	95.2(4)	O(201)-As(3)-O(191)	176.4(4)
O(202)-As(3)-O(191)	91.0(4)	O(192)-As(3)-O(191)	88.4(4)
O(201)-As(3)-O(182)	96.1(4)	O(202)-As(3)-O(182)	88.3(4)
O(192)-As(3)-O(182)	174.7(4)	O(191)-As(3)-O(182)	87.5(4)
O(201)-As(3)-O(181)	87.9(4)	O(202)-As(3)-O(181)	174.8(4)
O(192)-As(3)-O(181)	88.9(5)	O(191)-As(3)-O(181)	92.4(4)
O(182)-As(3)-O(181)	88.0(4)	C(181)-O(181)-As(3)	109.6(8)
C(186)-O(182)-As(3)	109.1(8)	C(191)-O(191)-As(3)	112.3(9)
C(196)-O(192)-As(3)	110.6(8)	C(201)-O(201)-As(3)	109.5(8)
C(206)-O(202)-As(3)	110.6(8)	C(182)-C(181)-C(186)	123.5(16)
C(182)-C(181)-O(181)	121.6(14)	C(186)-C(181)-O(181)	114.8(14)
C(181)-C(182)-C(183)	116.6(16)	C(184)-C(183)-C(182)	120.8(18)
C(185)-C(184)-C(183)	119.6(18)	C(186)-C(185)-C(184)	118.5(17)
C(181)-C(186)-C(185)	120.8(15)	C(181)-C(186)-O(182)	117.1(14)
C(185)-C(186)-O(182)	122.1(14)	O(191)-C(191)-C(192)	125.9(14)
O(191)-C(191)-C(196)	112.9(13)	C(192)-C(191)-C(196)	120.7(13)
C(191)-C(192)-C(193)	116.8(15)	C(194)-C(193)-C(192)	122.7(15)
C(193)-C(194)-C(195)	119.8(16)	C(196)-C(195)-C(194)	118.7(17)
C(195)-C(196)-O(192)	123.9(15)	C(195)-C(196)-C(191)	120.8(16)
O(192)-C(196)-C(191)	115.3(12)	O(201)-C(201)-C(206)	116.4(12)
O(201)-C(201)-C(202)	124.0(13)	C(206)-C(201)-C(202)	119.5(13)
C(203)-C(202)-C(201)	117.4(14)	C(204)-C(203)-C(202)	122.1(14)
C(203)-C(204)-C(205)	120.4(13)	C(206)-C(205)-C(204)	118.5(14)
C(205)-C(206)-O(202)	125.3(13)	C(205)-C(206)-C(201)	121.9(14)
O(202)-C(206)-C(201)	112.7(12)	O(211)-As(4)-O(232)	87.6(5)
O(211)-As(4)-O(222)	90.3(5)	O(232)-As(4)-O(222)	88.9(4)
O(211)-As(4)-O(221)	93.5(5)	O(232)-As(4)-O(221)	177.3(4)
O(222)-As(4)-O(221)	88.6(4)	O(211)-As(4)-O(212)	87.9(5)
O(232)-As(4)-O(212)	94.8(4)	O(222)-As(4)-O(212)	175.9(4)
O(221)-As(4)-O(212)	87.8(4)	O(211)-As(4)-O(231)	174.1(5)
O(232)-As(4)-O(231)	88.8(4)	O(222)-As(4)-O(231)	94.3(4)
O(221)-As(4)-O(231)	90.4(4)	O(212)-As(4)-O(231)	87.8(4)
C(211)-O(211)-As(4)	111.7(9)	C(216)-O(212)-As(4)	110.8(10)
C(221)-O(221)-As(4)	112.3(8)	C(226)-O(222)-As(4)	110.1(8)

C(231)-O(231)-As(4)	109.2(7)	C(236)-O(232)-As(4)	110.7(8)
C(212)-C(211)-O(211)	124.8(15)	C(212)-C(211)-C(216)	120.5(16)
O(211)-C(211)-C(216)	114.6(14)	C(211)-C(212)-C(213)	117.7(18)
C(214)-C(213)-C(212)	122(2)	C(213)-C(214)-C(215)	119(2)
C(216)-C(215)-C(214)	121.0(18)	C(215)-C(216)-O(212)	125.8(17)
C(215)-C(216)-C(211)	119.3(17)	O(212)-C(216)-C(211)	114.9(14)
O(221)-C(221)-C(222)	128.3(13)	O(221)-C(221)-C(226)	114.5(12)
C(222)-C(221)-C(226)	117.1(14)	C(221)-C(222)-C(223)	123.1(15)
C(222)-C(223)-C(224)	116.0(15)	C(225)-C(224)-C(223)	124.9(15)
C(224)-C(225)-C(226)	116.4(14)	C(225)-C(226)-O(222)	123.2(13)
C(225)-C(226)-C(221)	122.5(14)	O(222)-C(226)-C(221)	114.3(12)
C(232)-C(231)-O(231)	123.5(13)	C(232)-C(231)-C(236)	120.8(14)
O(231)-C(231)-C(236)	115.6(12)	C(231)-C(232)-C(233)	119.0(15)
C(232)-C(233)-C(234)	121.1(16)	C(233)-C(234)-C(235)	121.1(15)
C(236)-C(235)-C(234)	116.2(14)	O(232)-C(236)-C(235)	123.4(13)
O(232)-C(236)-C(231)	115.1(12)	C(235)-C(236)-C(231)	121.4(14)

Symmetry transformations used to generate equivalent atoms:

Table 6. Torsion angles [°] for nd019.

atom-atom-atom-atom	angle	atom-atom-atom-atom	angle
N(6)-Cu(1)-N(1)-C(6)	-138.6(9)	N(5)-Cu(1)-N(1)-C(6)	120.5(9)
N(2)-Cu(1)-N(1)-C(6)	-0.7(9)	N(6)-Cu(1)-N(1)-C(2)	44.9(14)
N(5)-Cu(1)-N(1)-C(2)	-56.1(14)	N(2)-Cu(1)-N(1)-C(2)	-177.3(13)
N(1)-Cu(1)-N(2)-C(10)	-0.6(9)	N(6)-Cu(1)-N(2)-C(10)	123.6(9)
N(5)-Cu(1)-N(2)-C(10)	-125.1(9)	N(1)-Cu(1)-N(2)-C(13)	175.9(12)
N(6)-Cu(1)-N(2)-C(13)	-60.0(14)	N(5)-Cu(1)-N(2)-C(13)	51.3(13)
N(4)-Cu(2)-N(3)-C(17)	177.5(15)	N(7)-Cu(2)-N(3)-C(17)	-36.6(16)
N(8)-Cu(2)-N(3)-C(17)	67.8(15)	N(4)-Cu(2)-N(3)-C(21)	8.3(10)
N(7)-Cu(2)-N(3)-C(21)	154.2(9)	N(8)-Cu(2)-N(3)-C(21)	-101.4(10)
N(7)-Cu(2)-N(4)-C(28)	36.8(16)	N(3)-Cu(2)-N(4)-C(28)	-176.2(14)
N(8)-Cu(2)-N(4)-C(28)	-62.5(15)	N(7)-Cu(2)-N(4)-C(25)	-156.1(9)
N(3)-Cu(2)-N(4)-C(25)	-9.0(11)	N(8)-Cu(2)-N(4)-C(25)	104.6(11)
N(1)-Cu(1)-N(5)-C(35)	120.1(9)	N(6)-Cu(1)-N(5)-C(35)	-0.3(9)
N(2)-Cu(1)-N(5)-C(35)	-138.7(9)	N(1)-Cu(1)-N(5)-C(31)	-63.0(13)
N(6)-Cu(1)-N(5)-C(31)	176.6(13)	N(2)-Cu(1)-N(5)-C(31)	38.3(14)
N(1)-Cu(1)-N(6)-C(42)	49.1(14)	N(5)-Cu(1)-N(6)-C(42)	173.6(13)
N(2)-Cu(1)-N(6)-C(42)	-60.7(14)	N(1)-Cu(1)-N(6)-C(39)	-123.9(8)
N(5)-Cu(1)-N(6)-C(39)	0.7(8)	N(2)-Cu(1)-N(6)-C(39)	126.4(8)
N(4)-Cu(2)-N(7)-C(46)	64.5(13)	N(3)-Cu(2)-N(7)-C(46)	-66.5(13)
N(8)-Cu(2)-N(7)-C(46)	176.1(12)	N(4)-Cu(2)-N(7)-C(50)	-115.4(9)
N(3)-Cu(2)-N(7)-C(50)	113.7(9)	N(8)-Cu(2)-N(7)-C(50)	-3.7(8)
N(4)-Cu(2)-N(8)-C(57)	-45.2(14)	N(7)-Cu(2)-N(8)-C(57)	-178.1(13)
N(3)-Cu(2)-N(8)-C(57)	46.1(14)	N(4)-Cu(2)-N(8)-C(54)	137.0(9)
N(7)-Cu(2)-N(8)-C(54)	4.2(8)	N(3)-Cu(2)-N(8)-C(54)	-131.6(8)
C(6)-N(1)-C(2)-C(3)	2(2)	Cu(1)-N(1)-C(2)-C(3)	178.1(12)
C(6)-N(1)-C(2)-C(1)	-179.7(13)	Cu(1)-N(1)-C(2)-C(1)	-3(2)
N(1)-C(2)-C(3)-C(4)	2(3)	C(1)-C(2)-C(3)-C(4)	-176.9(16)
C(2)-C(3)-C(4)-C(5)	-2(3)	C(3)-C(4)-C(5)-C(6)	-1(2)
C(3)-C(4)-C(5)-C(7)	-172.8(15)	C(2)-N(1)-C(6)-C(5)	-5(2)
Cu(1)-N(1)-C(6)-C(5)	178.1(11)	C(2)-N(1)-C(6)-C(10)	178.9(12)
Cu(1)-N(1)-C(6)-C(10)	1.9(15)	C(4)-C(5)-C(6)-N(1)	5(2)
C(7)-C(5)-C(6)-N(1)	176.7(13)	C(4)-C(5)-C(6)-C(10)	-179.3(13)
C(7)-C(5)-C(6)-C(10)	-7(2)	C(4)-C(5)-C(7)-C(8)	178.1(15)
C(6)-C(5)-C(7)-C(8)	6(2)	C(5)-C(7)-C(8)-C(9)	-4(2)
C(7)-C(8)-C(9)-C(11)	179.3(14)	C(7)-C(8)-C(9)-C(10)	3(2)
C(13)-N(2)-C(10)-C(6)	-175.1(12)	Cu(1)-N(2)-C(10)-C(6)	1.8(15)
C(13)-N(2)-C(10)-C(9)	-0.5(19)	Cu(1)-N(2)-C(10)-C(9)	176.4(10)
N(1)-C(6)-C(10)-N(2)	-2.5(18)	C(5)-C(6)-C(10)-N(2)	-178.9(12)
N(1)-C(6)-C(10)-C(9)	-177.3(12)	C(5)-C(6)-C(10)-C(9)	6.3(19)
C(11)-C(9)-C(10)-N(2)	4.8(19)	C(8)-C(9)-C(10)-N(2)	-178.7(12)
C(11)-C(9)-C(10)-C(6)	179.4(12)	C(8)-C(9)-C(10)-C(6)	-4.1(18)
C(10)-C(9)-C(11)-C(12)	-5.6(19)	C(8)-C(9)-C(11)-C(12)	178.2(13)

C(9)-C(11)-C(12)-C(13)	2(2)	C(10)-N(2)-C(13)-C(12)	-3(2)
Cu(1)-N(2)-C(13)-C(12)	-179.2(10)	C(10)-N(2)-C(13)-C(14)	177.4(12)
Cu(1)-N(2)-C(13)-C(14)	1.2(18)	C(11)-C(12)-C(13)-N(2)	2(2)
C(11)-C(12)-C(13)-C(14)	-178.3(13)	N(2)-C(13)-C(14)-C(15)	88.3(19)
C(12)-C(13)-C(14)-C(15)	-91.3(19)	C(13)-C(14)-C(15)-C(16)	50(3)
C(14)-C(15)-C(16)-C(17)	168(2)	C(21)-N(3)-C(17)-C(18)	-5(3)
Cu(2)-N(3)-C(17)-C(18)	-173.8(14)	C(21)-N(3)-C(17)-C(16)	165.5(16)
Cu(2)-N(3)-C(17)-C(16)	-3(2)	C(15)-C(16)-C(17)-N(3)	134(2)
C(15)-C(16)-C(17)-C(18)	-54(3)	N(3)-C(17)-C(18)-C(19)	3(3)
C(16)-C(17)-C(18)-C(19)	-167.0(17)	C(17)-C(18)-C(19)-C(20)	2(2)
C(18)-C(19)-C(20)-C(21)	-5(2)	C(18)-C(19)-C(20)-C(22)	172.1(16)
C(17)-N(3)-C(21)-C(20)	1(2)	Cu(2)-N(3)-C(21)-C(20)	172.5(12)
C(17)-N(3)-C(21)-C(25)	-177.6(13)	Cu(2)-N(3)-C(21)-C(25)	-6.2(15)
C(19)-C(20)-C(21)-N(3)	4(2)	C(22)-C(20)-C(21)-N(3)	-173.4(15)
C(19)-C(20)-C(21)-C(25)	-177.8(15)	C(22)-C(20)-C(21)-C(25)	5(2)
C(19)-C(20)-C(22)-C(23)	177(2)	C(21)-C(20)-C(22)-C(23)	-6(3)
C(20)-C(22)-C(23)-C(24)	4(4)	C(22)-C(23)-C(24)-C(25)	-1(4)
C(22)-C(23)-C(24)-C(26)	175(2)	C(28)-N(4)-C(25)-C(24)	-1(2)
Cu(2)-N(4)-C(25)-C(24)	-169.7(14)	C(28)-N(4)-C(25)-C(21)	177.1(14)
Cu(2)-N(4)-C(25)-C(21)	8.4(17)	C(23)-C(24)-C(25)-N(4)	178(2)
C(26)-C(24)-C(25)-N(4)	1(3)	C(23)-C(24)-C(25)-C(21)	0(3)
C(26)-C(24)-C(25)-C(21)	-176.9(16)	N(3)-C(21)-C(25)-N(4)	-1(2)
C(20)-C(21)-C(25)-N(4)	179.9(15)	N(3)-C(21)-C(25)-C(24)	176.8(14)
C(20)-C(21)-C(25)-C(24)	-2(2)	C(23)-C(24)-C(26)-C(27)	-179(2)
C(25)-C(24)-C(26)-C(27)	-3(3)	C(24)-C(26)-C(27)-C(28)	4(3)
C(25)-N(4)-C(28)-C(27)	2(2)	Cu(2)-N(4)-C(28)-C(27)	168.7(14)
C(25)-N(4)-C(28)-C(29)	-179.9(15)	Cu(2)-N(4)-C(28)-C(29)	-13(2)
C(26)-C(27)-C(28)-N(4)	-4(3)	C(26)-C(27)-C(28)-C(29)	178.5(19)
C(35)-N(5)-C(31)-C(32)	-2.5(19)	Cu(1)-N(5)-C(31)-C(32)	-179.4(10)
C(35)-N(5)-C(31)-C(30)	176.7(11)	Cu(1)-N(5)-C(31)-C(30)	-0.2(19)
N(5)-C(31)-C(32)-C(33)	-1(2)	C(30)-C(31)-C(32)-C(33)	-179.7(15)
C(31)-C(32)-C(33)-C(34)	5(2)	C(32)-C(33)-C(34)-C(35)	-7(2)
C(32)-C(33)-C(34)-C(36)	173.7(14)	C(31)-N(5)-C(35)-C(34)	0.6(19)
Cu(1)-N(5)-C(35)-C(34)	178.0(11)	C(31)-N(5)-C(35)-C(39)	-177.5(12)
Cu(1)-N(5)-C(35)-C(39)	-0.1(15)	C(36)-C(34)-C(35)-N(5)	-176.6(13)
C(33)-C(34)-C(35)-N(5)	4(2)	C(36)-C(34)-C(35)-C(39)	2(2)
C(33)-C(34)-C(35)-C(39)	-177.8(13)	C(35)-C(34)-C(36)-C(37)	-4(2)
C(33)-C(34)-C(36)-C(37)	175.0(15)	C(34)-C(36)-C(37)-C(38)	4(2)
C(36)-C(37)-C(38)-C(40)	-179.0(16)	C(36)-C(37)-C(38)-C(39)	-1(2)
C(42)-N(6)-C(39)-C(35)	-174.9(13)	Cu(1)-N(6)-C(39)-C(35)	-1.0(14)
C(42)-N(6)-C(39)-C(38)	5.7(19)	Cu(1)-N(6)-C(39)-C(38)	179.7(10)
N(5)-C(35)-C(39)-N(6)	0.7(18)	C(34)-C(35)-C(39)-N(6)	-177.5(12)
N(5)-C(35)-C(39)-C(38)	-179.9(12)	C(34)-C(35)-C(39)-C(38)	2(2)
C(40)-C(38)-C(39)-N(6)	-4(2)	C(37)-C(38)-C(39)-N(6)	177.0(12)
C(40)-C(38)-C(39)-C(35)	176.3(14)	C(37)-C(38)-C(39)-C(35)	-2(2)
C(39)-C(38)-C(40)-C(41)	2(2)	C(37)-C(38)-C(40)-C(41)	-179.8(15)

C(38)-C(40)-C(41)-C(42)	0(3)	C(39)-N(6)-C(42)-C(41)	-4(2)
Cu(1)-N(6)-C(42)-C(41)	-176.9(10)	C(39)-N(6)-C(42)-C(43)	177.9(12)
Cu(1)-N(6)-C(42)-C(43)	5(2)	C(40)-C(41)-C(42)-N(6)	2(2)
C(40)-C(41)-C(42)-C(43)	179.4(15)	N(6)-C(42)-C(43)-C(44)	111.6(14)
C(41)-C(42)-C(43)-C(44)	-66.0(18)	C(42)-C(43)-C(44)-C(45)	170.9(11)
C(43)-C(44)-C(45)-C(46)	65.7(15)	C(50)-N(7)-C(46)-C(47)	-1.4(19)
Cu(2)-N(7)-C(46)-C(47)	178.8(10)	C(50)-N(7)-C(46)-C(45)	-179.3(11)
Cu(2)-N(7)-C(46)-C(45)	0.8(18)	C(44)-C(45)-C(46)-N(7)	89.3(16)
C(44)-C(45)-C(46)-C(47)	-88.7(16)	N(7)-C(46)-C(47)-C(48)	3(2)
C(45)-C(46)-C(47)-C(48)	-178.7(13)	C(46)-C(47)-C(48)-C(49)	-2(2)
C(47)-C(48)-C(49)-C(50)	-0.6(19)	C(47)-C(48)-C(49)-C(51)	179.4(13)
C(46)-N(7)-C(50)-C(49)	-1.8(18)	Cu(2)-N(7)-C(50)-C(49)	178.1(10)
C(46)-N(7)-C(50)-C(54)	-177.2(11)	Cu(2)-N(7)-C(50)-C(54)	2.7(13)
C(51)-C(49)-C(50)-N(7)	-177.3(12)	C(48)-C(49)-C(50)-N(7)	2.7(19)
C(51)-C(49)-C(50)-C(54)	-1.7(19)	C(48)-C(49)-C(50)-C(54)	178.3(11)
C(50)-C(49)-C(51)-C(52)	-3(2)	C(48)-C(49)-C(51)-C(52)	177.1(13)
C(49)-C(51)-C(52)-C(53)	4(2)	C(51)-C(52)-C(53)-C(54)	-1(2)
C(51)-C(52)-C(53)-C(55)	179.6(13)	C(52)-C(53)-C(54)-N(8)	176.2(12)
C(55)-C(53)-C(54)-N(8)	-4.6(19)	C(52)-C(53)-C(54)-C(50)	-4(2)
C(55)-C(53)-C(54)-C(50)	175.6(11)	C(57)-N(8)-C(54)-C(53)	-1.9(19)
Cu(2)-N(8)-C(54)-C(53)	176.2(10)	C(57)-N(8)-C(54)-C(50)	178.0(12)
Cu(2)-N(8)-C(54)-C(50)	-4.0(13)	N(7)-C(50)-C(54)-C(53)	-179.1(11)
C(49)-C(50)-C(54)-C(53)	5.0(18)	N(7)-C(50)-C(54)-N(8)	1.1(16)
C(49)-C(50)-C(54)-N(8)	-174.8(11)	C(54)-C(53)-C(55)-C(56)	5.6(19)
C(52)-C(53)-C(55)-C(56)	-175.1(13)	C(53)-C(55)-C(56)-C(57)	-1(2)
C(54)-N(8)-C(57)-C(56)	7(2)	Cu(2)-N(8)-C(57)-C(56)	-170.5(11)
C(54)-N(8)-C(57)-C(58)	-174.2(14)	Cu(2)-N(8)-C(57)-C(58)	8(2)
C(55)-C(56)-C(57)-N(8)	-6(2)	C(55)-C(56)-C(57)-C(58)	175.6(16)
N(14)-Cu(3)-N(9)-C(62)	40.6(13)	N(13)-Cu(3)-N(9)-C(62)	-60.4(13)
N(10)-Cu(3)-N(9)-C(62)	179.6(12)	N(14)-Cu(3)-N(9)-C(66)	-139.9(9)
N(13)-Cu(3)-N(9)-C(66)	119.0(9)	N(10)-Cu(3)-N(9)-C(66)	-0.9(9)
N(14)-Cu(3)-N(10)-C(70)	122.0(9)	N(13)-Cu(3)-N(10)-C(70)	-124.7(9)
N(9)-Cu(3)-N(10)-C(70)	-0.8(9)	N(14)-Cu(3)-N(10)-C(73)	-58.3(13)
N(13)-Cu(3)-N(10)-C(73)	55.0(12)	N(9)-Cu(3)-N(10)-C(73)	179.0(11)
N(15)-Cu(4)-N(11)-C(77)	-31.2(17)	N(12)-Cu(4)-N(11)-C(77)	177.9(15)
N(16)-Cu(4)-N(11)-C(77)	70.1(15)	N(15)-Cu(4)-N(11)-C(81)	157.4(9)
N(12)-Cu(4)-N(11)-C(81)	6.5(10)	N(16)-Cu(4)-N(11)-C(81)	-101.3(10)
N(15)-Cu(4)-N(12)-C(88)	27.0(19)	N(11)-Cu(4)-N(12)-C(88)	-179.7(17)
N(16)-Cu(4)-N(12)-C(88)	-70.7(17)	N(15)-Cu(4)-N(12)-C(85)	-159.4(9)
N(11)-Cu(4)-N(12)-C(85)	-6.1(11)	N(16)-Cu(4)-N(12)-C(85)	102.9(11)
N(14)-Cu(3)-N(13)-C(91)	178.6(14)	N(10)-Cu(3)-N(13)-C(91)	38.0(15)
N(9)-Cu(3)-N(13)-C(91)	-62.1(15)	N(14)-Cu(3)-N(13)-C(95)	1.7(9)
N(10)-Cu(3)-N(13)-C(95)	-138.9(8)	N(9)-Cu(3)-N(13)-C(95)	121.0(9)
N(13)-Cu(3)-N(14)-C(102)	173.0(12)	N(10)-Cu(3)-N(14)-C(102)	-60.7(14)
N(9)-Cu(3)-N(14)-C(102)	48.6(13)	N(13)-Cu(3)-N(14)-C(99)	-1.2(9)
N(10)-Cu(3)-N(14)-C(99)	125.1(9)	N(9)-Cu(3)-N(14)-C(99)	-125.7(9)

N(12)-Cu(4)-N(15)-C(106)	67.7(12)	N(11)-Cu(4)-N(15)-C(106)	-71.3(13)
N(16)-Cu(4)-N(15)-C(106)	176.9(11)	N(12)-Cu(4)-N(15)-C(110)	-108.8(9)
N(11)-Cu(4)-N(15)-C(110)	112.1(9)	N(16)-Cu(4)-N(15)-C(110)	0.3(8)
N(15)-Cu(4)-N(16)-C(117)	175.9(12)	N(12)-Cu(4)-N(16)-C(117)	-51.7(13)
N(11)-Cu(4)-N(16)-C(117)	38.3(13)	N(15)-Cu(4)-N(16)-C(114)	1.6(8)
N(12)-Cu(4)-N(16)-C(114)	134.1(8)	N(11)-Cu(4)-N(16)-C(114)	-136.0(8)
C(66)-N(9)-C(62)-C(63)	3(2)	Cu(3)-N(9)-C(62)-C(63)	-177.2(10)
C(66)-N(9)-C(62)-C(61)	179.2(13)	Cu(3)-N(9)-C(62)-C(61)	-1(2)
N(9)-C(62)-C(63)-C(64)	-3(2)	C(61)-C(62)-C(63)-C(64)	-178.7(15)
C(62)-C(63)-C(64)-C(65)	0(2)	C(63)-C(64)-C(65)-C(66)	3(2)
C(63)-C(64)-C(65)-C(67)	-179.6(14)	C(62)-N(9)-C(66)-C(65)	-1(2)
Cu(3)-N(9)-C(66)-C(65)	179.7(10)	C(62)-N(9)-C(66)-C(70)	-178.1(12)
Cu(3)-N(9)-C(66)-C(70)	2.3(14)	C(64)-C(65)-C(66)-N(9)	-2(2)
C(67)-C(65)-C(66)-N(9)	179.9(12)	C(64)-C(65)-C(66)-C(70)	175.0(12)
C(67)-C(65)-C(66)-C(70)	-2.8(19)	C(66)-C(65)-C(67)-C(68)	-2(2)
C(64)-C(65)-C(67)-C(68)	-179.8(14)	C(65)-C(67)-C(68)-C(69)	6(2)
C(67)-C(68)-C(69)-C(70)	-5(2)	C(67)-C(68)-C(69)-C(71)	173.6(14)
C(71)-C(69)-C(70)-N(10)	6(2)	C(68)-C(69)-C(70)-N(10)	-175.5(12)
C(71)-C(69)-C(70)-C(66)	-178.5(12)	C(68)-C(69)-C(70)-C(66)	-0.1(19)
C(73)-N(10)-C(70)-C(69)	-2.0(19)	Cu(3)-N(10)-C(70)-C(69)	177.8(10)
C(73)-N(10)-C(70)-C(66)	-177.5(11)	Cu(3)-N(10)-C(70)-C(66)	2.3(14)
N(9)-C(66)-C(70)-C(69)	-178.7(12)	C(65)-C(66)-C(70)-C(69)	4(2)
N(9)-C(66)-C(70)-N(10)	-3.2(18)	C(65)-C(66)-C(70)-N(10)	179.4(12)
C(70)-C(69)-C(71)-C(72)	-7(2)	C(68)-C(69)-C(71)-C(72)	174.9(12)
C(69)-C(71)-C(72)-C(73)	4(2)	C(71)-C(72)-C(73)-N(10)	0(2)
C(71)-C(72)-C(73)-C(74)	-176.9(13)	C(70)-N(10)-C(73)-C(72)	-1.2(19)
Cu(3)-N(10)-C(73)-C(72)	179.0(10)	C(70)-N(10)-C(73)-C(74)	176.1(12)
Cu(3)-N(10)-C(73)-C(74)	-3.7(18)	C(72)-C(73)-C(74)-C(75)	-57(2)
N(10)-C(73)-C(74)-C(75)	125.7(15)	C(73)-C(74)-C(75)-C(76)	-77(2)
C(74)-C(75)-C(76)-C(77)	-178.5(17)	C(81)-N(11)-C(77)-C(78)	0(2)
Cu(4)-N(11)-C(77)-C(78)	-171.1(13)	C(81)-N(11)-C(77)-C(76)	-164.8(17)
Cu(4)-N(11)-C(77)-C(76)	25(2)	C(81)-N(11)-C(77)-C(76A)	154.0(15)
Cu(4)-N(11)-C(77)-C(76A)	-17(2)	C(75)-C(76)-C(77)-N(11)	-136(2)
C(75)-C(76)-C(77)-C(78)	59(3)	C(75)-C(76)-C(77)-C(76A)	-42(2)
C(75A)-C(76A)-C(77)-N(11)	134.4(19)	C(75A)-C(76A)-C(77)-C(78)	-70(2)
C(75A)-C(76A)-C(77)-C(76)	28(2)	N(11)-C(77)-C(78)-C(79)	3(3)
C(76)-C(77)-C(78)-C(79)	167.3(19)	C(76A)-C(77)-C(78)-C(79)	-151.3(18)
C(77)-C(78)-C(79)-C(80)	-2(3)	C(78)-C(79)-C(80)-C(81)	0(3)
C(78)-C(79)-C(80)-C(82)	171.5(18)	C(79)-C(80)-C(81)-N(11)	2(2)
C(82)-C(80)-C(81)-N(11)	-169.8(16)	C(79)-C(80)-C(81)-C(85)	178.3(16)
C(82)-C(80)-C(81)-C(85)	6(3)	C(77)-N(11)-C(81)-C(80)	-2(2)
Cu(4)-N(11)-C(81)-C(80)	170.4(12)	C(77)-N(11)-C(81)-C(85)	-178.1(15)
Cu(4)-N(11)-C(81)-C(85)	-5.7(16)	C(81)-C(80)-C(82)-C(83)	-2(3)
C(79)-C(80)-C(82)-C(83)	-175(2)	C(80)-C(82)-C(83)-C(84)	-5(4)
C(82)-C(83)-C(84)-C(85)	9(4)	C(82)-C(83)-C(84)-C(86)	177(3)
C(88)-N(12)-C(85)-C(81)	179.6(16)	Cu(4)-N(12)-C(85)-C(81)	5.0(18)

C(88)-N(12)-C(85)-C(84)	7(3)	Cu(4)-N(12)-C(85)-C(84)	-168.0(16)
C(80)-C(81)-C(85)-N(12)	-175.4(15)	N(11)-C(81)-C(85)-N(12)	1(2)
C(80)-C(81)-C(85)-C(84)	-2(3)	N(11)-C(81)-C(85)-C(84)	173.9(17)
C(86)-C(84)-C(85)-N(12)	-2(3)	C(83)-C(84)-C(85)-N(12)	168(2)
C(86)-C(84)-C(85)-C(81)	-175.2(19)	C(83)-C(84)-C(85)-C(81)	-6(3)
C(85)-C(84)-C(86)-C(87)	1(4)	C(83)-C(84)-C(86)-C(87)	-168(3)
C(84)-C(86)-C(87)-C(88)	-4(4)	C(85)-N(12)-C(88)-C(87)	-10(3)
Cu(4)-N(12)-C(88)-C(87)	162.7(17)	C(85)-N(12)-C(88)-C(89)	177.6(15)
Cu(4)-N(12)-C(88)-C(89)	-9(3)	C(86)-C(87)-C(88)-N(12)	9(3)
C(86)-C(87)-C(88)-C(89)	-179(2)	C(95)-N(13)-C(91)-C(90)	172.3(14)
Cu(3)-N(13)-C(91)-C(90)	-4(2)	C(95)-N(13)-C(91)-C(92)	-1(2)
Cu(3)-N(13)-C(91)-C(92)	-177.8(11)	N(13)-C(91)-C(92)-C(93)	0(2)
C(90)-C(91)-C(92)-C(93)	-172.7(17)	C(91)-C(92)-C(93)-C(94)	1(2)
C(92)-C(93)-C(94)-C(95)	-2(2)	C(92)-C(93)-C(94)-C(96)	-179.9(14)
C(91)-N(13)-C(95)-C(94)	0(2)	Cu(3)-N(13)-C(95)-C(94)	177.8(10)
C(91)-N(13)-C(95)-C(99)	-179.3(13)	Cu(3)-N(13)-C(95)-C(99)	-2.0(15)
C(96)-C(94)-C(95)-N(13)	179.2(12)	C(93)-C(94)-C(95)-N(13)	0.8(19)
C(96)-C(94)-C(95)-C(99)	-1.0(19)	C(93)-C(94)-C(95)-C(99)	-179.4(12)
C(95)-C(94)-C(96)-C(97)	-2(2)	C(93)-C(94)-C(96)-C(97)	175.9(13)
C(94)-C(96)-C(97)-C(98)	1(2)	C(96)-C(97)-C(98)-C(99)	3(2)
C(96)-C(97)-C(98)-C(100)	-178.4(14)	C(100)-C(98)-C(99)-N(14)	0(2)
C(97)-C(98)-C(99)-N(14)	178.2(13)	C(100)-C(98)-C(99)-C(95)	174.9(13)
C(97)-C(98)-C(99)-C(95)	-7(2)	C(102)-N(14)-C(99)-C(98)	1(2)
Cu(3)-N(14)-C(99)-C(98)	175.8(12)	C(102)-N(14)-C(99)-C(95)	-174.8(11)
Cu(3)-N(14)-C(99)-C(95)	0.5(14)	N(13)-C(95)-C(99)-C(98)	-174.7(12)
C(94)-C(95)-C(99)-C(98)	5.6(19)	N(13)-C(95)-C(99)-N(14)	1.1(17)
C(94)-C(95)-C(99)-N(14)	-178.7(11)	C(99)-C(98)-C(100)-C(101)	-2(2)
C(97)-C(98)-C(100)-C(101)	-179.9(14)	C(98)-C(100)-C(101)-C(102)	3(2)
C(99)-N(14)-C(102)-C(101)	0.7(19)	Cu(3)-N(14)-C(102)-C(101)	-173.6(11)
C(99)-N(14)-C(102)-C(103)	-177.5(11)	Cu(3)-N(14)-C(102)-C(103)	8.2(18)
C(100)-C(101)-C(102)-N(14)	-2(2)	C(100)-C(101)-C(102)-C(103)	175.9(13)
N(14)-C(102)-C(103)-C(104)	111.6(14)	C(101)-C(102)-C(103)-C(104)	-66.7(17)
C(102)-C(103)-C(104)-C(105)	170.1(12)	C(103)-C(104)-C(105)-C(106)	64.9(16)
C(110)-N(15)-C(106)-C(107)	-2.4(17)	Cu(4)-N(15)-C(106)-C(107)	-178.9(9)
C(110)-N(15)-C(106)-C(105)	179.2(11)	Cu(4)-N(15)-C(106)-C(105)	2.7(17)
C(104)-C(105)-C(106)-N(15)	85.8(15)	C(104)-C(105)-C(106)-C(107)	-92.6(15)
N(15)-C(106)-C(107)-C(108)	1(2)	C(105)-C(106)-C(107)-C(108)	179.6(14)
C(106)-C(107)-C(108)-C(109)	1(2)	C(107)-C(108)-C(109)-C(110)	-2(2)
C(107)-C(108)-C(109)-C(111)	177.9(14)	C(108)-C(109)-C(110)-N(15)	1.3(19)
C(111)-C(109)-C(110)-N(15)	-179.1(12)	C(108)-C(109)-C(110)-C(114)	-178.4(12)
C(111)-C(109)-C(110)-C(114)	1.3(19)	C(106)-N(15)-C(110)-C(109)	1.1(18)
Cu(4)-N(15)-C(110)-C(109)	178.2(10)	C(106)-N(15)-C(110)-C(114)	-179.2(10)
Cu(4)-N(15)-C(110)-C(114)	-2.1(13)	C(110)-C(109)-C(111)-C(112)	-2(2)
C(108)-C(109)-C(111)-C(112)	177.9(13)	C(109)-C(111)-C(112)-C(113)	-1(2)
C(111)-C(112)-C(113)-C(115)	-175.3(13)	C(111)-C(112)-C(113)-C(114)	4.9(19)
C(117)-N(16)-C(114)-C(113)	2.9(18)	Cu(4)-N(16)-C(114)-C(113)	178.0(10)

C(117)-N(16)-C(114)-C(110)	-178.5(11)	Cu(4)-N(16)-C(114)-C(110)	-3.4(14)
C(115)-C(113)-C(114)-N(16)	-6.3(19)	C(112)-C(113)-C(114)-N(16)	173.4(11)
C(115)-C(113)-C(114)-C(110)	175.0(12)	C(112)-C(113)-C(114)-C(110)	-5.2(17)
C(109)-C(110)-C(114)-N(16)	-176.5(12)	N(15)-C(110)-C(114)-N(16)	3.8(16)
C(109)-C(110)-C(114)-C(113)	2.2(18)	N(15)-C(110)-C(114)-C(113)	-177.5(11)
C(112)-C(113)-C(115)-C(116)	-173.8(13)	C(114)-C(113)-C(115)-C(116)	6(2)
C(113)-C(115)-C(116)-C(117)	-3(2)	C(114)-N(16)-C(117)-C(116)	1(2)
Cu(4)-N(16)-C(117)-C(116)	-173.0(11)	C(114)-N(16)-C(117)-C(118)	-179.3(13)
Cu(4)-N(16)-C(117)-C(118)	6.9(19)	C(115)-C(116)-C(117)-N(16)	-1(2)
C(115)-C(116)-C(117)-C(118)	179.1(14)	O(132)-As(1)-O(121)-C(121)	176.4(9)
O(122)-As(1)-O(121)-C(121)	-7.1(9)	O(141)-As(1)-O(121)-C(121)	53(4)
O(142)-As(1)-O(121)-C(121)	87.7(9)	O(131)-As(1)-O(121)-C(121)	-94.9(9)
O(132)-As(1)-O(122)-C(126)	86(7)	O(141)-As(1)-O(122)-C(126)	-168.3(8)
O(121)-As(1)-O(122)-C(126)	5.6(8)	O(142)-As(1)-O(122)-C(126)	-80.3(8)
O(131)-As(1)-O(122)-C(126)	100.8(8)	O(132)-As(1)-O(131)-C(131)	2.8(9)
O(122)-As(1)-O(131)-C(131)	-176.3(9)	O(141)-As(1)-O(131)-C(131)	95.8(8)
O(121)-As(1)-O(131)-C(131)	-87.9(9)	O(142)-As(1)-O(131)-C(131)	26(9)
O(122)-As(1)-O(132)-C(136)	13(7)	O(141)-As(1)-O(132)-C(136)	-93.5(8)
O(121)-As(1)-O(132)-C(136)	92.4(9)	O(142)-As(1)-O(132)-C(136)	178.3(8)
O(131)-As(1)-O(132)-C(136)	-2.8(8)	O(132)-As(1)-O(141)-C(141)	-81.2(8)
O(122)-As(1)-O(141)-C(141)	102.3(8)	O(121)-As(1)-O(141)-C(141)	42(4)
O(142)-As(1)-O(141)-C(141)	7.5(8)	O(131)-As(1)-O(141)-C(141)	-169.8(8)
O(132)-As(1)-O(142)-C(146)	84.5(9)	O(122)-As(1)-O(142)-C(146)	-96.3(9)
O(141)-As(1)-O(142)-C(146)	-8.5(9)	O(121)-As(1)-O(142)-C(146)	175.4(9)
O(131)-As(1)-O(142)-C(146)	61(9)	As(1)-O(121)-C(121)-C(122)	-166.1(11)
As(1)-O(121)-C(121)-C(126)	7.1(15)	O(121)-C(121)-C(122)-C(123)	-179.3(14)
C(126)-C(121)-C(122)-C(123)	8(2)	C(121)-C(122)-C(123)-C(124)	-4(2)
C(122)-C(123)-C(124)-C(125)	0(2)	C(123)-C(124)-C(125)-C(126)	0(2)
C(124)-C(125)-C(126)-O(122)	-174.7(13)	C(124)-C(125)-C(126)-C(121)	4(2)
As(1)-O(122)-C(126)-C(125)	176.0(11)	As(1)-O(122)-C(126)-C(121)	-3.0(14)
O(121)-C(121)-C(126)-C(125)	178.3(12)	C(122)-C(121)-C(126)-C(125)	-8(2)
O(121)-C(121)-C(126)-O(122)	-2.7(17)	C(122)-C(121)-C(126)-O(122)	171.0(11)
As(1)-O(131)-C(131)-C(132)	176.2(11)	As(1)-O(131)-C(131)-C(136)	-2.1(14)
O(131)-C(131)-C(132)-C(133)	176.4(14)	C(136)-C(131)-C(132)-C(133)	-5(2)
C(131)-C(132)-C(133)-C(134)	5(2)	C(132)-C(133)-C(134)-C(135)	-4(2)
C(133)-C(134)-C(135)-C(136)	3(2)	As(1)-O(132)-C(136)-C(135)	179.2(11)
As(1)-O(132)-C(136)-C(131)	2.3(14)	C(134)-C(135)-C(136)-O(132)	-180.0(13)
C(134)-C(135)-C(136)-C(131)	-3(2)	O(131)-C(131)-C(136)-O(132)	-0.1(17)
C(132)-C(131)-C(136)-O(132)	-178.4(12)	O(131)-C(131)-C(136)-C(135)	-177.3(12)
C(132)-C(131)-C(136)-C(135)	4(2)	As(1)-O(141)-C(141)-C(142)	176.4(11)
As(1)-O(141)-C(141)-C(146)	-4.8(14)	O(141)-C(141)-C(142)-C(143)	-178.4(12)
C(146)-C(141)-C(142)-C(143)	3(2)	C(141)-C(142)-C(143)-C(144)	-4(2)
C(142)-C(143)-C(144)-C(145)	2(3)	C(143)-C(144)-C(145)-C(146)	1(3)
C(144)-C(145)-C(146)-O(142)	-178.6(14)	C(144)-C(145)-C(146)-C(141)	-2(2)
As(1)-O(142)-C(146)-C(145)	-175.5(12)	As(1)-O(142)-C(146)-C(141)	7.9(15)
C(142)-C(141)-C(146)-C(145)	0(2)	O(141)-C(141)-C(146)-C(145)	-178.9(13)

C(142)-C(141)-C(146)-O(142)	176.8(12)	O(141)-C(141)-C(146)-O(142)	-2.1(17)
O(172)-As(2)-O(151)-C(151)	-104.2(9)	O(171)-As(2)-O(151)-C(151)	167.6(9)
O(161)-As(2)-O(151)-C(151)	79.2(9)	O(162)-As(2)-O(151)-C(151)	20(5)
O(152)-As(2)-O(151)-C(151)	-13.7(9)	O(172)-As(2)-O(152)-C(156)	105.5(9)
O(171)-As(2)-O(152)-C(156)	30(6)	O(161)-As(2)-O(152)-C(156)	-76.6(9)
O(151)-As(2)-O(152)-C(156)	11.5(9)	O(162)-As(2)-O(152)-C(156)	-165.3(9)
O(172)-As(2)-O(161)-C(161)	73(6)	O(171)-As(2)-O(161)-C(161)	107.8(9)
O(151)-As(2)-O(161)-C(161)	-164.6(9)	O(162)-As(2)-O(161)-C(161)	10.5(9)
O(152)-As(2)-O(161)-C(161)	-76.3(9)	O(172)-As(2)-O(162)-C(166)	173.3(8)
O(171)-As(2)-O(162)-C(166)	-98.5(8)	O(161)-As(2)-O(162)-C(166)	-10.3(8)
O(151)-As(2)-O(162)-C(166)	49(5)	O(152)-As(2)-O(162)-C(166)	82.7(9)
O(172)-As(2)-O(171)-C(171)	-7.9(8)	O(161)-As(2)-O(171)-C(171)	174.4(8)
O(151)-As(2)-O(171)-C(171)	86.2(9)	O(162)-As(2)-O(171)-C(171)	-96.9(8)
O(152)-As(2)-O(171)-C(171)	67(6)	O(171)-As(2)-O(172)-C(176)	7.9(8)
O(161)-As(2)-O(172)-C(176)	43(6)	O(151)-As(2)-O(172)-C(176)	-79.5(9)
O(162)-As(2)-O(172)-C(176)	105.2(8)	O(152)-As(2)-O(172)-C(176)	-167.9(8)
As(2)-O(151)-C(151)-C(156)	13.4(16)	As(2)-O(151)-C(151)-C(152)	-167.6(13)
C(156)-C(151)-C(152)-C(153)	-1(3)	O(151)-C(151)-C(152)-C(153)	179.8(17)
C(151)-C(152)-C(153)-C(154)	2(3)	C(152)-C(153)-C(154)-C(155)	-2(4)
C(153)-C(154)-C(155)-C(156)	1(3)	C(152)-C(151)-C(156)-O(152)	176.5(14)
O(151)-C(151)-C(156)-O(152)	-5(2)	C(152)-C(151)-C(156)-C(155)	1(2)
O(151)-C(151)-C(156)-C(155)	-180.0(13)	As(2)-O(152)-C(156)-C(151)	-6.7(16)
As(2)-O(152)-C(156)-C(155)	168.9(10)	C(154)-C(155)-C(156)-C(151)	-1(2)
C(154)-C(155)-C(156)-O(152)	-176.5(14)	As(2)-O(161)-C(161)-C(166)	-8.6(15)
As(2)-O(161)-C(161)-C(162)	173.7(12)	O(161)-C(161)-C(162)-C(163)	178.1(14)
C(166)-C(161)-C(162)-C(163)	0(2)	C(161)-C(162)-C(163)-C(164)	-2(3)
C(162)-C(163)-C(164)-C(165)	2(3)	C(163)-C(164)-C(165)-C(166)	-2(3)
O(161)-C(161)-C(166)-O(162)	0.4(18)	C(162)-C(161)-C(166)-O(162)	178.2(13)
O(161)-C(161)-C(166)-C(165)	-177.6(12)	C(162)-C(161)-C(166)-C(165)	0(2)
As(2)-O(162)-C(166)-C(161)	7.9(14)	As(2)-O(162)-C(166)-C(165)	-174.1(11)
C(164)-C(165)-C(166)-C(161)	0(2)	C(164)-C(165)-C(166)-O(162)	-177.5(14)
As(2)-O(171)-C(171)-C(172)	-174.7(13)	As(2)-O(171)-C(171)-C(176)	6.3(13)
O(171)-C(171)-C(172)-C(173)	177.3(14)	C(176)-C(171)-C(172)-C(173)	-4(2)
C(171)-C(172)-C(173)-C(174)	5(3)	C(172)-C(173)-C(174)-C(175)	-4(2)
C(173)-C(174)-C(175)-C(176)	2(2)	As(2)-O(172)-C(176)-C(175)	173.5(11)
As(2)-O(172)-C(176)-C(171)	-6.2(14)	C(174)-C(175)-C(176)-O(172)	-179.9(13)
C(174)-C(175)-C(176)-C(171)	-0.2(19)	C(172)-C(171)-C(176)-O(172)	-179.2(13)
O(171)-C(171)-C(176)-O(172)	-0.1(17)	C(172)-C(171)-C(176)-C(175)	1(2)
O(171)-C(171)-C(176)-C(175)	-179.8(11)	O(201)-As(3)-O(181)-C(181)	106.1(9)
O(202)-As(3)-O(181)-C(181)	53(5)	O(192)-As(3)-O(181)-C(181)	-165.9(9)
O(191)-As(3)-O(181)-C(181)	-77.5(9)	O(182)-As(3)-O(181)-C(181)	9.9(9)
O(201)-As(3)-O(182)-C(186)	-98.5(9)	O(202)-As(3)-O(182)-C(186)	172.7(8)
O(192)-As(3)-O(182)-C(186)	42(5)	O(191)-As(3)-O(182)-C(186)	81.6(9)
O(181)-As(3)-O(182)-C(186)	-10.9(8)	O(201)-As(3)-O(191)-C(191)	10(7)
O(202)-As(3)-O(191)-C(191)	100.7(9)	O(192)-As(3)-O(191)-C(191)	5.6(9)
O(182)-As(3)-O(191)-C(191)	-171.1(9)	O(181)-As(3)-O(191)-C(191)	-83.2(9)

O(201)-As(3)-O(192)-C(196)	173.9(9)	O(202)-As(3)-O(192)-C(196)	-97.3(9)
O(191)-As(3)-O(192)-C(196)	-6.4(9)	O(182)-As(3)-O(192)-C(196)	33(5)
O(181)-As(3)-O(192)-C(196)	86.0(9)	O(202)-As(3)-O(201)-C(201)	-11.0(8)
O(192)-As(3)-O(201)-C(201)	84.2(9)	O(191)-As(3)-O(201)-C(201)	79(7)
O(182)-As(3)-O(201)-C(201)	-99.1(8)	O(181)-As(3)-O(201)-C(201)	173.2(9)
O(201)-As(3)-O(202)-C(206)	12.4(8)	O(192)-As(3)-O(202)-C(206)	-75.5(8)
O(191)-As(3)-O(202)-C(206)	-164.0(8)	O(182)-As(3)-O(202)-C(206)	108.6(8)
O(181)-As(3)-O(202)-C(206)	65(5)	As(3)-O(181)-C(181)-C(182)	169.4(13)
As(3)-O(181)-C(181)-C(186)	-6.7(15)	C(186)-C(181)-C(182)-C(183)	-5(2)
O(181)-C(181)-C(182)-C(183)	179.2(14)	C(181)-C(182)-C(183)-C(184)	3(3)
C(182)-C(183)-C(184)-C(185)	0(3)	C(183)-C(184)-C(185)-C(186)	-1(2)
C(182)-C(181)-C(186)-C(185)	4(2)	O(181)-C(181)-C(186)-C(185)	179.6(12)
C(182)-C(181)-C(186)-O(182)	-178.1(14)	O(181)-C(181)-C(186)-O(182)	-2.1(18)
C(184)-C(185)-C(186)-C(181)	0(2)	C(184)-C(185)-C(186)-O(182)	-178.4(13)
As(3)-O(182)-C(186)-C(181)	9.9(15)	As(3)-O(182)-C(186)-C(185)	-171.9(11)
As(3)-O(191)-C(191)-C(192)	168.1(11)	As(3)-O(191)-C(191)-C(196)	-3.3(14)
O(191)-C(191)-C(192)-C(193)	-179.5(13)	C(196)-C(191)-C(192)-C(193)	-9(2)
C(191)-C(192)-C(193)-C(194)	5(2)	C(192)-C(193)-C(194)-C(195)	-1(2)
C(193)-C(194)-C(195)-C(196)	1(2)	C(194)-C(195)-C(196)-O(192)	178.3(13)
C(194)-C(195)-C(196)-C(191)	-4(2)	As(3)-O(192)-C(196)-C(195)	-176.4(12)
As(3)-O(192)-C(196)-C(191)	6.1(14)	O(191)-C(191)-C(196)-C(195)	-179.4(12)
C(192)-C(191)-C(196)-C(195)	9(2)	O(191)-C(191)-C(196)-O(192)	-1.9(17)
C(192)-C(191)-C(196)-O(192)	-173.8(12)	As(3)-O(201)-C(201)-C(206)	7.4(14)
As(3)-O(201)-C(201)-C(202)	-169.3(11)	O(201)-C(201)-C(202)-C(203)	-179.6(13)
C(206)-C(201)-C(202)-C(203)	4(2)	C(201)-C(202)-C(203)-C(204)	-1(2)
C(202)-C(203)-C(204)-C(205)	-2(2)	C(203)-C(204)-C(205)-C(206)	2(2)
C(204)-C(205)-C(206)-O(202)	177.4(12)	C(204)-C(205)-C(206)-C(201)	0(2)
As(3)-O(202)-C(206)-C(205)	171.9(11)	As(3)-O(202)-C(206)-C(201)	-10.8(13)
O(201)-C(201)-C(206)-C(205)	179.7(12)	C(202)-C(201)-C(206)-C(205)	-3(2)
O(201)-C(201)-C(206)-O(202)	2.3(17)	C(202)-C(201)-C(206)-O(202)	179.2(12)
O(232)-As(4)-O(211)-C(211)	94.1(10)	O(222)-As(4)-O(211)-C(211)	-177.1(10)
O(221)-As(4)-O(211)-C(211)	-88.4(10)	O(212)-As(4)-O(211)-C(211)	-0.8(10)
O(231)-As(4)-O(211)-C(211)	42(5)	O(211)-As(4)-O(212)-C(216)	1.2(10)
O(232)-As(4)-O(212)-C(216)	-86.2(10)	O(222)-As(4)-O(212)-C(216)	66(6)
O(221)-As(4)-O(212)-C(216)	94.8(10)	O(231)-As(4)-O(212)-C(216)	-174.8(10)
O(211)-As(4)-O(221)-C(221)	-87.5(9)	O(232)-As(4)-O(221)-C(221)	25(10)
O(222)-As(4)-O(221)-C(221)	2.7(9)	O(212)-As(4)-O(221)-C(221)	-175.3(9)
O(231)-As(4)-O(221)-C(221)	96.9(9)	O(211)-As(4)-O(222)-C(226)	89.5(9)
O(232)-As(4)-O(222)-C(226)	177.0(9)	O(221)-As(4)-O(222)-C(226)	-4.0(9)
O(212)-As(4)-O(222)-C(226)	25(6)	O(231)-As(4)-O(222)-C(226)	-94.2(9)
O(211)-As(4)-O(231)-C(231)	59(5)	O(232)-As(4)-O(231)-C(231)	7.2(9)
O(222)-As(4)-O(231)-C(231)	-81.6(9)	O(221)-As(4)-O(231)-C(231)	-170.3(9)
O(212)-As(4)-O(231)-C(231)	102.0(9)	O(211)-As(4)-O(232)-C(236)	177.5(9)
O(222)-As(4)-O(232)-C(236)	87.2(9)	O(221)-As(4)-O(232)-C(236)	65(9)
O(212)-As(4)-O(232)-C(236)	-94.7(9)	O(231)-As(4)-O(232)-C(236)	-7.1(9)
As(4)-O(211)-C(211)-C(212)	-176.2(13)	As(4)-O(211)-C(211)-C(216)	0.2(16)

O(211)-C(211)-C(212)-C(213)	-177.7(16)	C(216)-C(211)-C(212)-C(213)	6(2)
C(211)-C(212)-C(213)-C(214)	-5(3)	C(212)-C(213)-C(214)-C(215)	1(3)
C(213)-C(214)-C(215)-C(216)	2(3)	C(214)-C(215)-C(216)-O(212)	178.3(15)
C(214)-C(215)-C(216)-C(211)	-1(2)	As(4)-O(212)-C(216)-C(215)	179.2(14)
As(4)-O(212)-C(216)-C(211)	-1.4(16)	C(212)-C(211)-C(216)-C(215)	-3(2)
O(211)-C(211)-C(216)-C(215)	-179.8(14)	C(212)-C(211)-C(216)-O(212)	177.4(14)
O(211)-C(211)-C(216)-O(212)	1(2)	As(4)-O(221)-C(221)-C(222)	175.5(12)
As(4)-O(221)-C(221)-C(226)	-0.7(14)	O(221)-C(221)-C(222)-C(223)	-177.8(14)
C(226)-C(221)-C(222)-C(223)	-2(2)	C(221)-C(222)-C(223)-C(224)	1(2)
C(222)-C(223)-C(224)-C(225)	-1(2)	C(223)-C(224)-C(225)-C(226)	2(2)
C(224)-C(225)-C(226)-O(222)	179.3(12)	C(224)-C(225)-C(226)-C(221)	-2(2)
As(4)-O(222)-C(226)-C(225)	-177.0(11)	As(4)-O(222)-C(226)-C(221)	4.5(14)
O(221)-C(221)-C(226)-C(225)	179.0(12)	C(222)-C(221)-C(226)-C(225)	2(2)
O(221)-C(221)-C(226)-O(222)	-2.5(17)	C(222)-C(221)-C(226)-O(222)	-179.2(12)
As(4)-O(231)-C(231)-C(232)	177.5(11)	As(4)-O(231)-C(231)-C(236)	-5.8(15)
O(231)-C(231)-C(232)-C(233)	-179.2(14)	C(236)-C(231)-C(232)-C(233)	4(2)
C(231)-C(232)-C(233)-C(234)	-3(3)	C(232)-C(233)-C(234)-C(235)	4(3)
C(233)-C(234)-C(235)-C(236)	-5(3)	As(4)-O(232)-C(236)-C(235)	-171.3(12)
As(4)-O(232)-C(236)-C(231)	5.4(15)	C(234)-C(235)-C(236)-O(232)	-177.2(14)
C(234)-C(235)-C(236)-C(231)	6(2)	C(232)-C(231)-C(236)-O(232)	177.2(12)
O(231)-C(231)-C(236)-O(232)	0.4(18)	C(232)-C(231)-C(236)-C(235)	-6(2)
O(231)-C(231)-C(236)-C(235)	177.1(13)		

Symmetry transformations used to generate equivalent atoms:

Lemus, Lappin Compound 2 (nd1014z_x)

Table 1. Crystal data and structure refinement for nd1014z_x.

Identification code	nd1014z	
Empirical formula	C98 H78 As2 Cu2 N10 O12	
Formula weight	1864.62	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 17.1177(6) Å	α = 90°
	b = 17.4161(6) Å	β = 90.228(2)°
	c = 28.7700(9) Å	γ = 90°
Volume	8576.9(5) $Å^3$	
Z	4	
Density (calculated)	1.444 $g.cm^{-3}$	
Absorption coefficient (μ)	1.332 mm^{-1}	
F(000)	3824	
Crystal color, habit	orange/red, blade	
Crystal size	0.285 × 0.097 × 0.087 mm^3	
θ range for data collection	0.708 to 23.358°	
Index ranges	$-18 \le h \le 19$, $-19 \le k \le 19$, $-31 \le l \le 31$	
Reflections collected	86434	
Independent reflections	24173 [R_{int} = 0.0736]	
Completeness to θ = 25.242°	80.3 %	
Absorption correction	Numerical	
Max. and min. transmission	0.8929 and 0.7027	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	24173 / 1509 / 2185	
Goodness-of-fit on F^2	1.019	
Final R indices [I>2σ(I)]	R_1 = 0.0791, wR_2 = 0.2007	
R indices (all data)	R_1 = 0.1267, wR_2 = 0.2312	
Absolute structure parameter	0.037(5)	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.374 and -0.608 $e^-.Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for nd1014z_x. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cu(1)	0.30946(12)	0.73475(11)	0.43677(7)	0.030(1)
Cu(2)	0.41882(12)	0.55472(11)	0.62172(7)	0.033(1)
N(1)	0.2299(9)	0.8155(8)	0.4187(5)	0.040(3)
N(2)	0.2134(8)	0.6669(8)	0.4441(5)	0.035(3)
N(3)	0.3236(8)	0.6120(8)	0.6470(4)	0.030(2)
N(4)	0.3774(8)	0.4691(8)	0.6622(4)	0.032(2)
N(5)	0.3875(8)	0.6909(7)	0.3903(4)	0.028(2)
N(6)	0.4072(8)	0.7560(7)	0.4736(4)	0.025(2)
N(7)	0.4601(8)	0.5339(7)	0.5563(4)	0.029(2)
N(8)	0.5262(8)	0.6044(8)	0.6299(5)	0.033(2)
C(1)	0.3213(12)	0.9194(10)	0.4116(7)	0.052(5)
C(2)	0.2395(11)	0.8879(10)	0.4093(6)	0.045(3)
C(3)	0.1729(12)	0.9361(11)	0.3963(7)	0.050(3)
C(4)	0.1026(12)	0.9044(11)	0.3942(7)	0.052(3)
C(5)	0.0901(12)	0.8256(11)	0.4043(7)	0.050(3)
C(6)	0.1565(11)	0.7844(10)	0.4179(6)	0.042(3)
C(7)	0.0177(12)	0.7888(12)	0.4012(7)	0.058(3)
C(8)	0.0094(12)	0.7130(12)	0.4124(7)	0.057(3)
C(9)	0.0741(11)	0.6702(11)	0.4277(7)	0.050(3)
C(10)	0.1475(11)	0.7040(10)	0.4301(6)	0.040(3)
C(11)	0.0676(12)	0.5901(11)	0.4390(7)	0.049(3)
C(12)	0.1352(10)	0.5551(10)	0.4528(6)	0.043(3)
C(13)	0.2087(10)	0.5940(10)	0.4548(6)	0.038(3)
C(14)	0.2802(10)	0.5510(9)	0.4683(6)	0.039(3)
C(15)	0.2821(10)	0.5257(9)	0.5196(6)	0.038(3)
C(16)	0.3438(10)	0.4647(9)	0.5298(6)	0.034(3)
C(17)	0.4255(10)	0.4967(9)	0.5211(6)	0.032(2)
C(18)	0.4636(10)	0.4867(9)	0.4782(6)	0.032(3)
C(19)	0.5389(10)	0.5135(9)	0.4728(6)	0.031(3)
C(20)	0.5772(10)	0.5516(9)	0.5102(5)	0.030(2)
C(21)	0.5324(10)	0.5608(9)	0.5502(5)	0.030(2)
C(22)	0.6535(10)	0.5785(9)	0.5080(6)	0.034(3)
C(23)	0.6880(10)	0.6152(9)	0.5445(6)	0.032(3)
C(24)	0.6458(10)	0.6283(9)	0.5866(6)	0.033(2)
C(25)	0.5699(10)	0.5982(9)	0.5904(6)	0.031(2)
C(26)	0.6769(11)	0.6666(10)	0.6247(6)	0.037(3)
C(27)	0.6321(10)	0.6726(10)	0.6645(6)	0.038(3)
C(28)	0.5573(10)	0.6393(10)	0.6660(6)	0.038(3)
C(29)	0.5081(11)	0.6419(11)	0.7104(6)	0.046(4)
C(30)	0.2925(10)	0.6533(10)	0.3331(6)	0.035(4)
C(31)	0.3754(10)	0.6547(9)	0.3498(5)	0.033(3)

C(32)	0.4364(10)	0.6216(9)	0.3259(6)	0.034(3)
C(33)	0.5122(10)	0.6253(9)	0.3419(5)	0.033(3)
C(34)	0.5267(10)	0.6664(9)	0.3832(5)	0.031(2)
C(35)	0.4620(10)	0.6936(9)	0.4066(5)	0.028(2)
C(36)	0.6033(10)	0.6785(9)	0.4019(5)	0.033(3)
C(37)	0.6132(10)	0.7142(9)	0.4420(5)	0.034(3)
C(38)	0.5490(10)	0.7406(9)	0.4691(5)	0.033(2)
C(39)	0.4734(9)	0.7306(9)	0.4511(5)	0.027(2)
C(40)	0.5552(10)	0.7757(9)	0.5130(5)	0.033(3)
C(41)	0.4896(10)	0.8002(9)	0.5351(5)	0.030(3)
C(42)	0.4162(9)	0.7905(9)	0.5149(5)	0.028(2)
C(43)	0.3432(9)	0.8208(9)	0.5380(5)	0.029(3)
C(44)	0.2994(9)	0.7601(9)	0.5659(5)	0.028(3)
C(45)	0.3463(9)	0.7346(10)	0.6091(5)	0.030(3)
C(46)	0.3000(10)	0.6827(10)	0.6406(5)	0.032(2)
C(47)	0.2350(10)	0.7130(11)	0.6627(6)	0.037(3)
C(48)	0.1908(10)	0.6681(11)	0.6909(6)	0.039(3)
C(49)	0.2128(10)	0.5903(11)	0.6979(6)	0.037(2)
C(50)	0.2800(10)	0.5645(10)	0.6754(6)	0.033(2)
C(51)	0.1710(10)	0.5373(10)	0.7285(6)	0.035(3)
C(52)	0.1994(10)	0.4676(10)	0.7348(6)	0.035(3)
C(53)	0.2691(10)	0.4405(10)	0.7149(6)	0.035(2)
C(54)	0.3113(10)	0.4891(10)	0.6834(5)	0.032(2)
C(55)	0.3031(11)	0.3678(10)	0.7208(6)	0.038(3)
C(56)	0.3724(11)	0.3469(10)	0.7001(6)	0.039(3)
C(57)	0.4063(10)	0.3967(10)	0.6685(6)	0.036(3)
C(58)	0.4747(11)	0.3753(10)	0.6416(6)	0.044(4)
Cu(3)	0.41242(14)	0.45485(12)	0.12092(7)	0.038(1)
Cu(4)	0.31998(12)	0.64092(12)	-0.07263(8)	0.038(1)
N(9)	0.3644(9)	0.3731(8)	0.1620(4)	0.044(3)
N(10)	0.3194(9)	0.5175(8)	0.1425(5)	0.041(3)
N(11)	0.4149(7)	0.6587(7)	-0.0313(4)	0.028(2)
N(12)	0.4008(8)	0.5988(7)	-0.1174(4)	0.032(2)
N(13)	0.5215(9)	0.4983(8)	0.1325(5)	0.038(3)
N(14)	0.4568(8)	0.4333(7)	0.0573(4)	0.029(2)
N(15)	0.2199(9)	0.5790(11)	-0.0605(7)	0.063(3)
N(16)	0.2430(11)	0.7214(11)	-0.0893(8)	0.079(4)
C(1A)	0.4579(13)	0.2736(12)	0.1449(7)	0.059(5)
C(2A)	0.3862(13)	0.3007(11)	0.1696(6)	0.049(3)
C(3A)	0.3424(13)	0.2529(12)	0.2006(6)	0.053(3)
C(4A)	0.2811(13)	0.2791(12)	0.2227(6)	0.052(3)
C(5A)	0.2568(12)	0.3519(12)	0.2141(6)	0.049(3)
C(6A)	0.2971(12)	0.3977(11)	0.1830(6)	0.045(3)
C(7A)	0.1858(12)	0.3854(13)	0.2344(6)	0.053(3)
C(8A)	0.1631(13)	0.4546(12)	0.2237(6)	0.053(3)
C(9A)	0.2086(12)	0.5049(12)	0.1954(6)	0.048(3)

C(10A)	0.2742(11)	0.4751(11)	0.1735(6)	0.044(3)
C(11A)	0.1906(12)	0.5811(12)	0.1849(6)	0.050(3)
C(12A)	0.2351(11)	0.6228(12)	0.1567(6)	0.047(3)
C(13A)	0.2988(11)	0.5891(11)	0.1344(6)	0.042(3)
C(14A)	0.3482(11)	0.6340(10)	0.0995(6)	0.042(3)
C(15A)	0.3010(10)	0.6642(10)	0.0579(6)	0.039(3)
C(16A)	0.3468(10)	0.7236(9)	0.0296(6)	0.035(3)
C(17A)	0.4203(9)	0.6914(9)	0.0096(5)	0.030(2)
C(18A)	0.4934(9)	0.6979(9)	0.0329(5)	0.029(3)
C(19A)	0.5580(9)	0.6709(9)	0.0131(5)	0.027(3)
C(20A)	0.5542(9)	0.6366(9)	-0.0307(5)	0.027(2)
C(21A)	0.4822(9)	0.6307(9)	-0.0514(5)	0.027(2)
C(22A)	0.6219(10)	0.6059(9)	-0.0566(5)	0.031(3)
C(23A)	0.6145(10)	0.5729(9)	-0.0973(5)	0.030(3)
C(24A)	0.5392(10)	0.5663(9)	-0.1190(5)	0.029(2)
C(25A)	0.4740(10)	0.5960(9)	-0.0968(5)	0.029(2)
C(26A)	0.5275(10)	0.5316(9)	-0.1632(5)	0.032(3)
C(27A)	0.4538(10)	0.5340(9)	-0.1838(6)	0.035(3)
C(28A)	0.3932(10)	0.5696(9)	-0.1605(6)	0.034(3)
C(29A)	0.3147(11)	0.5804(11)	-0.1812(6)	0.050(4)
C(30A)	0.5053(12)	0.5264(11)	0.2145(6)	0.050(4)
C(31A)	0.5532(12)	0.5248(10)	0.1723(6)	0.045(3)
C(32A)	0.6282(11)	0.5511(11)	0.1729(6)	0.049(3)
C(33A)	0.6757(12)	0.5512(11)	0.1335(6)	0.047(3)
C(34A)	0.6438(11)	0.5192(10)	0.0927(6)	0.039(3)
C(35A)	0.5676(10)	0.4935(10)	0.0947(5)	0.033(2)
C(36A)	0.6898(11)	0.5078(10)	0.0506(6)	0.040(3)
C(37A)	0.6571(10)	0.4751(10)	0.0137(6)	0.038(3)
C(38A)	0.5802(10)	0.4492(10)	0.0137(5)	0.033(2)
C(39A)	0.5324(10)	0.4582(9)	0.0533(5)	0.031(2)
C(40A)	0.5415(10)	0.4152(10)	-0.0255(6)	0.033(3)
C(41A)	0.4652(10)	0.3907(10)	-0.0221(5)	0.033(3)
C(42A)	0.4252(10)	0.3995(9)	0.0199(6)	0.033(2)
C(43A)	0.3436(10)	0.3716(10)	0.0251(6)	0.039(3)
C(44A)	0.2825(11)	0.4336(11)	0.0144(6)	0.046(3)
C(45A)	0.2828(11)	0.4609(12)	-0.0349(7)	0.051(3)
C(46A)	0.2123(11)	0.5042(14)	-0.0479(8)	0.061(3)
C(47A)	0.1381(12)	0.4650(15)	-0.0453(9)	0.073(4)
C(48A)	0.0742(14)	0.5092(16)	-0.0573(9)	0.083(4)
C(49A)	0.0838(14)	0.5878(17)	-0.0656(10)	0.086(3)
C(50A)	0.1563(13)	0.6211(15)	-0.0693(9)	0.076(3)
C(51A)	0.0171(15)	0.6350(17)	-0.0730(10)	0.095(4)
C(52A)	0.0285(15)	0.7076(17)	-0.0836(10)	0.096(4)
C(53A)	0.1008(15)	0.7469(17)	-0.0889(11)	0.093(4)
C(54A)	0.1693(14)	0.6980(15)	-0.0827(10)	0.082(3)
C(55A)	0.1199(15)	0.8246(17)	-0.1012(10)	0.094(4)

C(56A)	0.1931(14)	0.8488(16)	-0.1072(10)	0.090(4)
C(57A)	0.2550(14)	0.7934(15)	-0.1009(10)	0.085(4)
C(58A)	0.3356(14)	0.8170(14)	-0.1081(10)	0.088(6)
As(1)	0.25381(13)	-0.00792(11)	0.65199(7)	0.046(1)
O(1)	0.2759(9)	-0.0727(8)	0.7017(5)	0.060(3)
O(2)	0.3521(8)	-0.0311(7)	0.6286(4)	0.045(3)
O(3)	0.3002(8)	0.0760(7)	0.6806(4)	0.054(3)
O(4)	0.1633(10)	0.0189(9)	0.6819(5)	0.078(4)
O(5)	0.2041(7)	-0.0875(7)	0.6232(5)	0.051(3)
O(6)	0.2348(7)	0.0505(6)	0.6005(4)	0.040(3)
C(61)	0.3514(14)	-0.0969(12)	0.7008(7)	0.058(3)
C(62)	0.3851(14)	-0.1401(12)	0.7358(7)	0.065(3)
C(63)	0.4594(15)	-0.1604(13)	0.7313(8)	0.068(4)
C(64)	0.5043(15)	-0.1392(12)	0.6927(7)	0.065(4)
C(65)	0.4685(13)	-0.0929(11)	0.6574(7)	0.058(3)
C(66)	0.3935(13)	-0.0730(11)	0.6616(7)	0.052(3)
C(67)	0.2528(15)	0.1052(12)	0.7132(8)	0.067(3)
C(68)	0.2768(16)	0.1623(13)	0.7431(8)	0.075(4)
C(69)	0.2241(17)	0.1850(14)	0.7782(9)	0.082(4)
C(70)	0.1556(17)	0.1562(15)	0.7809(9)	0.087(4)
C(71)	0.1305(16)	0.0980(14)	0.7517(8)	0.084(4)
C(72)	0.1799(16)	0.0759(14)	0.7156(9)	0.077(3)
C(73)	0.1680(11)	-0.0608(10)	0.5843(7)	0.049(3)
C(74)	0.1147(11)	-0.1042(11)	0.5580(7)	0.052(3)
C(75)	0.0751(12)	-0.0687(11)	0.5187(7)	0.051(3)
C(76)	0.0955(11)	0.0036(10)	0.5073(7)	0.047(3)
C(77)	0.1501(10)	0.0464(10)	0.5334(7)	0.045(3)
C(78)	0.1837(11)	0.0134(10)	0.5721(7)	0.044(3)
As(2)	0.14541(11)	0.29221(9)	0.46274(6)	0.035(1)
O(7)	0.2473(7)	0.3070(6)	0.4458(4)	0.041(3)
O(8)	0.1168(8)	0.3552(7)	0.4151(4)	0.050(3)
O(9)	0.1405(7)	0.3758(6)	0.5016(4)	0.037(3)
O(10)	0.1809(7)	0.2345(6)	0.5123(4)	0.037(2)
O(11)	0.0420(7)	0.2728(6)	0.4753(4)	0.038(3)
O(12)	0.1456(7)	0.2061(6)	0.4255(4)	0.036(2)
C(79)	0.2482(12)	0.3580(10)	0.4088(6)	0.045(3)
C(80)	0.3183(13)	0.3819(11)	0.3885(6)	0.052(3)
C(81)	0.3152(14)	0.4338(11)	0.3523(7)	0.058(3)
C(82)	0.2457(13)	0.4587(12)	0.3362(7)	0.057(3)
C(83)	0.1793(13)	0.4347(11)	0.3560(7)	0.054(3)
C(84)	0.1812(12)	0.3841(11)	0.3926(6)	0.048(3)
C(85)	0.1550(10)	0.3540(10)	0.5460(6)	0.038(2)
C(86)	0.1472(10)	0.4025(10)	0.5842(6)	0.039(3)
C(87)	0.1624(10)	0.3714(10)	0.6282(6)	0.041(3)
C(88)	0.1839(10)	0.2967(10)	0.6336(6)	0.042(3)
C(89)	0.1925(10)	0.2480(10)	0.5955(6)	0.038(3)

C(90)	0.1779(10)	0.2776(10)	0.5527(6)	0.037(2)
C(91)	0.0160(10)	0.2134(9)	0.4490(6)	0.037(2)
C(92)	-0.0619(10)	0.1904(9)	0.4485(6)	0.038(3)
C(93)	-0.0783(11)	0.1299(9)	0.4182(6)	0.039(3)
C(94)	-0.0237(10)	0.0933(10)	0.3895(6)	0.038(3)
C(95)	0.0498(10)	0.1186(9)	0.3905(6)	0.037(3)
C(96)	0.0731(10)	0.1777(9)	0.4206(6)	0.036(2)
As(3)	0.84701(11)	0.69825(10)	0.04496(7)	0.039(1)
O(13)	0.8478(7)	0.6147(7)	0.0834(4)	0.045(3)
O(14)	0.9502(7)	0.6811(7)	0.0333(5)	0.048(3)
O(15)	0.7439(6)	0.7114(6)	0.0602(4)	0.034(2)
O(16)	0.8718(7)	0.7666(7)	0.0917(4)	0.043(3)
O(17)	0.8139(6)	0.6389(6)	-0.0042(4)	0.035(2)
O(18)	0.8498(7)	0.7808(7)	0.0045(4)	0.042(3)
C(97)	0.9211(12)	0.5841(11)	0.0875(7)	0.051(3)
C(98)	0.9420(12)	0.5253(11)	0.1188(8)	0.058(3)
C(99)	1.0178(12)	0.5003(12)	0.1172(8)	0.061(3)
C(100)	1.0735(13)	0.5319(11)	0.0874(8)	0.060(3)
C(101)	1.0539(12)	0.5938(11)	0.0574(8)	0.057(3)
C(102)	0.9751(12)	0.6204(11)	0.0597(8)	0.052(3)
C(103)	0.7363(11)	0.7661(10)	0.0938(6)	0.037(3)
C(104)	0.6663(11)	0.7915(10)	0.1115(6)	0.039(3)
C(105)	0.6655(12)	0.8527(10)	0.1432(6)	0.042(3)
C(106)	0.7351(11)	0.8845(11)	0.1568(6)	0.044(3)
C(107)	0.8063(12)	0.8591(10)	0.1424(6)	0.043(3)
C(108)	0.8062(11)	0.7978(10)	0.1106(6)	0.041(3)
C(109)	0.8212(10)	0.6784(10)	-0.0450(6)	0.039(3)
C(110)	0.8089(10)	0.6476(11)	-0.0886(6)	0.045(3)
C(111)	0.8181(11)	0.6939(12)	-0.1280(7)	0.052(3)
C(112)	0.8368(11)	0.7692(12)	-0.1210(7)	0.054(3)
C(113)	0.8476(11)	0.8039(12)	-0.0754(7)	0.050(3)
C(114)	0.8387(10)	0.7554(11)	-0.0386(7)	0.043(3)
As(4)	0.24123(11)	0.88951(10)	0.14428(6)	0.038(1)
O(19)	0.1479(8)	0.9097(7)	0.1717(4)	0.051(3)
O(20)	0.2840(8)	0.9700(7)	0.1776(4)	0.048(3)
O(21)	0.2629(7)	0.8194(7)	0.1907(4)	0.042(3)
O(22)	0.3403(7)	0.8705(7)	0.1228(4)	0.035(2)
O(23)	0.1941(6)	0.8130(6)	0.1120(4)	0.034(2)
O(24)	0.2248(6)	0.9529(6)	0.0948(4)	0.036(3)
C(115)	0.1568(13)	0.9696(12)	0.2038(7)	0.054(3)
C(116)	0.0956(14)	0.9914(12)	0.2325(7)	0.060(3)
C(117)	0.1103(14)	1.0522(12)	0.2645(7)	0.063(3)
C(118)	0.1833(13)	1.0834(12)	0.2675(7)	0.060(3)
C(119)	0.2439(13)	1.0583(12)	0.2376(6)	0.056(3)
C(120)	0.2309(13)	1.0015(11)	0.2067(7)	0.051(3)
C(121)	0.3402(12)	0.7982(10)	0.1904(6)	0.043(3)

C(122)	0.3744(12)	0.7523(11)	0.2229(6)	0.047(3)
C(123)	0.4502(12)	0.7357(11)	0.2174(6)	0.048(3)
C(124)	0.4948(12)	0.7636(11)	0.1819(6)	0.046(3)
C(125)	0.4605(11)	0.8118(10)	0.1493(6)	0.043(3)
C(126)	0.3814(11)	0.8270(10)	0.1539(6)	0.039(3)
C(127)	0.1542(10)	0.8423(10)	0.0742(6)	0.039(3)
C(128)	0.0992(11)	0.8034(11)	0.0505(7)	0.045(3)
C(129)	0.0637(11)	0.8398(11)	0.0140(7)	0.052(3)
C(130)	0.0835(11)	0.9179(11)	0.0026(7)	0.051(3)
C(131)	0.1372(10)	0.9563(10)	0.0274(7)	0.043(3)
C(132)	0.1726(10)	0.9189(10)	0.0651(6)	0.039(3)
N(1S)	-0.0455(12)	0.8421(12)	0.2233(7)	0.090(6)
C(1S)	-0.0130(14)	0.8022(13)	0.1977(8)	0.077(6)
C(2S)	0.0208(13)	0.7512(13)	0.1630(7)	0.067(6)
N(2S)	0.5662(14)	0.4491(15)	0.7343(9)	0.116(8)
C(3S)	0.6276(15)	0.4344(19)	0.7179(11)	0.119(8)
C(4S)	0.6977(14)	0.3911(17)	0.7046(9)	0.100(8)
N(3S)	-0.0276(18)	0.318(2)	0.3394(11)	0.151(10)
C(5S)	0.016(2)	0.282(3)	0.3177(14)	0.173(12)
C(6S)	0.092(2)	0.248(3)	0.3091(14)	0.181(14)
N(4S)	0.9125(18)	0.1428(18)	0.7104(11)	0.143(9)
C(7S)	0.898(2)	0.2074(19)	0.7163(15)	0.153(10)
C(8S)	0.864(2)	0.2839(19)	0.7183(14)	0.160(12)
H(1A)	0.3585	0.8792	0.4027	0.078
H(1B)	0.3327	0.9365	0.4433	0.078
H(1C)	0.3260	0.9629	0.3902	0.078
H(3A)	0.1800	0.9891	0.3894	0.060
H(4A)	0.0592	0.9355	0.3857	0.062
H(7A)	-0.0267	0.8171	0.3912	0.070
H(8A)	-0.0404	0.6891	0.4098	0.068
H(11A)	0.0194	0.5633	0.4371	0.059
H(12A)	0.1333	0.5025	0.4615	0.051
H(14A)	0.3264	0.5837	0.4622	0.047
H(14B)	0.2845	0.5049	0.4483	0.047
H(15A)	0.2924	0.5711	0.5394	0.045
H(15B)	0.2301	0.5052	0.5281	0.045
H(16A)	0.3348	0.4195	0.5096	0.041
H(16B)	0.3396	0.4480	0.5626	0.041
H(18A)	0.4377	0.4618	0.4532	0.039
H(19A)	0.5652	0.5064	0.4441	0.038
H(22A)	0.6824	0.5709	0.4803	0.041
H(23A)	0.7406	0.6322	0.5419	0.038
H(26A)	0.7279	0.6881	0.6236	0.044
H(27A)	0.6519	0.6993	0.6908	0.045
H(29A)	0.4910	0.5898	0.7183	0.069
H(29B)	0.4622	0.6745	0.7052	0.069

H(29C)	0.5395	0.6629	0.7359	0.069
H(30A)	0.2745	0.7060	0.3275	0.052
H(30B)	0.2595	0.6292	0.3567	0.052
H(30C)	0.2892	0.6239	0.3041	0.052
H(32A)	0.4258	0.5954	0.2975	0.041
H(33A)	0.5535	0.6010	0.3256	0.040
H(36A)	0.6475	0.6606	0.3853	0.039
H(37A)	0.6648	0.7226	0.4532	0.041
H(40A)	0.6050	0.7823	0.5271	0.039
H(41A)	0.4939	0.8243	0.5646	0.036
H(43A)	0.3078	0.8415	0.5137	0.034
H(43B)	0.3577	0.8636	0.5589	0.034
H(44A)	0.2891	0.7150	0.5459	0.033
H(44B)	0.2485	0.7812	0.5759	0.033
H(45A)	0.3940	0.7074	0.5988	0.036
H(45B)	0.3629	0.7807	0.6267	0.036
H(47A)	0.2214	0.7653	0.6581	0.044
H(48A)	0.1459	0.6884	0.7058	0.047
H(51A)	0.1243	0.5528	0.7435	0.042
H(52A)	0.1709	0.4334	0.7540	0.042
H(55A)	0.2773	0.3314	0.7400	0.046
H(56A)	0.3964	0.2991	0.7073	0.046
H(58A)	0.5086	0.4202	0.6378	0.067
H(58B)	0.4581	0.3567	0.6109	0.067
H(58C)	0.5033	0.3347	0.6579	0.067
H(1AA)	0.4947	0.3164	0.1416	0.088
H(1AB)	0.4434	0.2544	0.1140	0.088
H(1AC)	0.4826	0.2323	0.1628	0.088
H(3AA)	0.3582	0.2012	0.2053	0.064
H(4AA)	0.2541	0.2476	0.2443	0.063
H(7AA)	0.1558	0.3559	0.2556	0.064
H(8AA)	0.1144	0.4724	0.2352	0.063
H(11B)	0.1455	0.6038	0.1982	0.060
H(12B)	0.2235	0.6755	0.1517	0.056
H(14C)	0.3905	0.6003	0.0879	0.051
H(14D)	0.3730	0.6780	0.1156	0.051
H(15C)	0.2867	0.6206	0.0374	0.047
H(15D)	0.2521	0.6878	0.0692	0.047
H(16C)	0.3133	0.7429	0.0041	0.042
H(16D)	0.3600	0.7677	0.0499	0.042
H(18B)	0.4962	0.7216	0.0626	0.034
H(19B)	0.6067	0.6750	0.0289	0.032
H(22B)	0.6725	0.6103	-0.0432	0.037
H(23B)	0.6593	0.5532	-0.1126	0.036
H(26B)	0.5697	0.5069	-0.1786	0.038
H(27B)	0.4451	0.5115	-0.2134	0.042

H(29D)	0.3007	0.6350	-0.1801	0.075
H(29E)	0.2763	0.5506	-0.1636	0.075
H(29F)	0.3151	0.5630	-0.2136	0.075
H(30D)	0.5383	0.5389	0.2413	0.075
H(30E)	0.4811	0.4760	0.2191	0.075
H(30F)	0.4645	0.5655	0.2111	0.075
H(32B)	0.6491	0.5703	0.2012	0.058
H(33B)	0.7270	0.5718	0.1342	0.056
H(36B)	0.7428	0.5238	0.0497	0.048
H(37B)	0.6873	0.4691	-0.0137	0.045
H(40B)	0.5686	0.4095	-0.0540	0.040
H(41B)	0.4399	0.3681	-0.0481	0.039
H(43C)	0.3361	0.3531	0.0573	0.047
H(43D)	0.3353	0.3275	0.0039	0.047
H(44C)	0.2300	0.4130	0.0216	0.055
H(44D)	0.2919	0.4781	0.0351	0.055
H(45C)	0.3291	0.4940	-0.0397	0.062
H(45D)	0.2878	0.4160	-0.0557	0.062
H(47B)	0.1337	0.4128	-0.0361	0.087
H(48B)	0.0240	0.4863	-0.0599	0.100
H(51B)	-0.0342	0.6147	-0.0704	0.114
H(52B)	-0.0172	0.7376	-0.0884	0.115
H(55B)	0.0785	0.8603	-0.1053	0.113
H(56B)	0.2041	0.9005	-0.1153	0.109
H(58D)	0.3652	0.7741	-0.1213	0.132
H(58E)	0.3590	0.8320	-0.0784	0.132
H(58F)	0.3370	0.8606	-0.1296	0.132
H(62A)	0.3559	-0.1549	0.7623	0.077
H(63A)	0.4830	-0.1905	0.7551	0.081
H(64A)	0.5572	-0.1552	0.6901	0.078
H(65A)	0.4978	-0.0765	0.6313	0.070
H(68A)	0.3268	0.1856	0.7402	0.090
H(69A)	0.2399	0.2224	0.8003	0.099
H(70A)	0.1207	0.1755	0.8037	0.104
H(71A)	0.0813	0.0739	0.7561	0.101
H(74A)	0.1046	-0.1563	0.5658	0.062
H(75A)	0.0361	-0.0956	0.5017	0.061
H(76A)	0.0724	0.0265	0.4806	0.057
H(77A)	0.1635	0.0972	0.5244	0.054
H(80A)	0.3670	0.3627	0.3994	0.062
H(81A)	0.3622	0.4521	0.3388	0.070
H(82A)	0.2437	0.4934	0.3107	0.069
H(83A)	0.1305	0.4528	0.3446	0.065
H(86A)	0.1321	0.4546	0.5806	0.047
H(87A)	0.1577	0.4032	0.6548	0.049
H(88A)	0.1932	0.2773	0.6640	0.051

H(89A)	0.2080	0.1961	0.5994	0.046
H(92A)	-0.1007	0.2140	0.4672	0.045
H(93A)	-0.1307	0.1119	0.4169	0.047
H(94A)	-0.0386	0.0518	0.3700	0.045
H(95A)	0.0872	0.0961	0.3704	0.044
H(98A)	0.9054	0.5042	0.1400	0.069
H(99A)	1.0333	0.4596	0.1372	0.073
H(10A)	1.1250	0.5117	0.0872	0.072
H(10B)	1.0911	0.6162	0.0371	0.068
H(10D)	0.6188	0.7677	0.1022	0.047
H(10E)	0.6175	0.8717	0.1551	0.051
H(10F)	0.7337	0.9269	0.1776	0.053
H(10G)	0.8535	0.8817	0.1532	0.052
H(11C)	0.7944	0.5953	-0.0919	0.054
H(11D)	0.8115	0.6737	-0.1584	0.062
H(11E)	0.8431	0.8009	-0.1476	0.065
H(11F)	0.8600	0.8567	-0.0716	0.060
H(11G)	0.0461	0.9668	0.2309	0.072
H(11I)	0.0695	1.0709	0.2838	0.075
H(11J)	0.1936	1.1223	0.2898	0.073
H(11K)	0.2940	1.0817	0.2393	0.067
H(12C)	0.3457	0.7329	0.2485	0.057
H(12D)	0.4743	0.7025	0.2394	0.058
H(12E)	0.5485	0.7503	0.1797	0.055
H(12F)	0.4900	0.8336	0.1247	0.051
H(12G)	0.0855	0.7524	0.0589	0.054
H(12H)	0.0256	0.8133	-0.0040	0.063
H(13A)	0.0583	0.9425	-0.0228	0.061
H(13B)	0.1509	1.0076	0.0197	0.052
H(2SA)	0.0724	0.7705	0.1540	0.101
H(2SB)	-0.0133	0.7493	0.1356	0.101
H(2SC)	0.0262	0.6995	0.1761	0.101
H(4SA)	0.7382	0.4268	0.6940	0.150
H(4SB)	0.6847	0.3553	0.6795	0.150
H(4SC)	0.7172	0.3623	0.7315	0.150
H(6SA)	0.1074	0.2581	0.2769	0.271
H(6SB)	0.0890	0.1923	0.3141	0.271
H(6SC)	0.1306	0.2701	0.3303	0.271
H(8SA)	0.8998	0.3184	0.7350	0.240
H(8SB)	0.8141	0.2816	0.7345	0.240
H(8SC)	0.8559	0.3032	0.6866	0.240

Table 3. Anisotropic displacement parameters ($Å^2$) for nd1014z_x.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cu(1)	0.0383(13)	0.0135(10)	0.0384(12)	0.0026(9)	-0.0041(10)	-0.0010(9)
Cu(2)	0.0434(13)	0.0228(12)	0.0322(12)	0.0041(9)	0.0029(10)	0.0005(10)
N(1)	0.051(6)	0.018(5)	0.051(6)	0.000(5)	0.002(5)	0.006(5)
N(2)	0.043(5)	0.015(5)	0.048(5)	0.001(5)	0.007(5)	0.000(5)
N(3)	0.036(5)	0.025(5)	0.029(5)	0.003(4)	-0.001(4)	-0.006(5)
N(4)	0.046(6)	0.026(5)	0.025(5)	0.001(4)	-0.007(5)	-0.003(5)
N(5)	0.045(5)	0.014(5)	0.025(5)	0.012(4)	0.002(5)	-0.002(5)
N(6)	0.043(5)	0.011(5)	0.020(5)	0.004(4)	0.001(4)	0.003(4)
N(7)	0.044(5)	0.013(5)	0.031(5)	0.005(4)	-0.003(5)	0.006(4)
N(8)	0.042(5)	0.027(5)	0.031(5)	0.005(5)	-0.001(5)	0.002(5)
C(1)	0.073(11)	0.019(8)	0.064(10)	0.001(8)	-0.019(9)	-0.002(8)
C(2)	0.059(6)	0.020(5)	0.055(6)	0.000(5)	0.001(6)	0.010(5)
C(3)	0.064(7)	0.025(6)	0.060(6)	0.005(6)	0.002(6)	0.012(6)
C(4)	0.061(6)	0.030(6)	0.065(6)	0.004(6)	0.004(6)	0.016(6)
C(5)	0.054(5)	0.031(5)	0.066(6)	0.007(5)	0.007(5)	0.010(5)
C(6)	0.048(5)	0.024(5)	0.054(5)	0.001(5)	0.006(5)	0.006(5)
C(7)	0.053(6)	0.042(6)	0.079(7)	0.010(6)	0.009(6)	0.013(6)
C(8)	0.051(6)	0.041(6)	0.078(7)	0.011(6)	0.011(6)	0.006(6)
C(9)	0.049(5)	0.033(5)	0.067(6)	0.006(5)	0.010(5)	0.004(5)
C(10)	0.045(5)	0.023(5)	0.053(5)	0.001(5)	0.008(5)	0.004(4)
C(11)	0.050(6)	0.031(6)	0.066(6)	0.007(6)	0.011(6)	0.001(5)
C(12)	0.049(6)	0.021(6)	0.059(6)	0.007(5)	0.006(6)	0.000(5)
C(13)	0.046(5)	0.015(5)	0.054(5)	-0.001(5)	0.008(5)	0.000(5)
C(14)	0.052(6)	0.012(5)	0.053(6)	-0.001(5)	0.003(5)	-0.006(5)
C(15)	0.051(6)	0.013(5)	0.049(6)	-0.005(5)	0.002(6)	-0.003(5)
C(16)	0.048(6)	0.009(5)	0.044(6)	-0.005(5)	-0.001(5)	-0.002(5)
C(17)	0.047(5)	0.011(5)	0.037(5)	0.000(4)	-0.004(5)	0.002(4)
C(18)	0.048(6)	0.014(5)	0.035(5)	0.001(5)	-0.003(5)	0.004(5)
C(19)	0.048(6)	0.014(5)	0.032(5)	0.005(5)	0.004(5)	0.006(5)
C(20)	0.042(5)	0.015(5)	0.034(5)	0.010(4)	0.003(4)	0.006(4)
C(21)	0.044(5)	0.016(5)	0.031(5)	0.008(4)	0.000(4)	0.006(4)
C(22)	0.044(6)	0.020(5)	0.040(6)	0.008(5)	0.004(5)	0.006(5)
C(23)	0.039(6)	0.019(5)	0.037(6)	0.012(5)	0.001(5)	0.005(5)
C(24)	0.041(5)	0.021(5)	0.037(5)	0.011(4)	-0.001(4)	0.008(4)
C(25)	0.041(5)	0.021(5)	0.031(5)	0.009(4)	0.002(4)	0.005(4)
C(26)	0.045(6)	0.025(6)	0.040(6)	0.009(5)	-0.002(5)	0.005(5)
C(27)	0.048(6)	0.028(6)	0.037(6)	0.008(5)	-0.005(5)	-0.002(5)
C(28)	0.047(6)	0.032(6)	0.034(5)	0.007(5)	-0.002(5)	0.000(5)
C(29)	0.056(10)	0.045(10)	0.037(9)	0.001(8)	-0.004(8)	-0.006(9)
C(30)	0.049(9)	0.025(8)	0.030(8)	0.002(7)	-0.001(7)	-0.005(7)

C(31)	0.049(6)	0.020(5)	0.029(5)	0.007(5)	-0.002(5)	0.001(5)
C(32)	0.052(6)	0.023(5)	0.028(6)	0.005(5)	-0.002(5)	0.002(5)
C(33)	0.051(6)	0.021(5)	0.029(5)	0.009(5)	-0.001(5)	0.001(5)
C(34)	0.047(5)	0.018(5)	0.029(5)	0.006(4)	0.001(4)	0.000(5)
C(35)	0.045(5)	0.012(4)	0.029(5)	0.005(4)	0.003(4)	0.000(4)
C(36)	0.048(6)	0.022(5)	0.028(5)	0.006(5)	0.006(5)	0.000(5)
C(37)	0.047(6)	0.025(6)	0.031(5)	0.006(5)	0.004(5)	-0.002(5)
C(38)	0.048(5)	0.020(5)	0.030(5)	0.006(4)	0.000(4)	-0.003(5)
C(39)	0.043(5)	0.012(4)	0.028(5)	0.008(4)	0.002(4)	0.000(4)
C(40)	0.048(6)	0.020(5)	0.029(5)	0.005(5)	-0.006(5)	-0.007(5)
C(41)	0.048(6)	0.018(5)	0.025(5)	0.007(5)	-0.007(5)	-0.004(5)
C(42)	0.045(5)	0.013(5)	0.026(5)	0.006(4)	-0.001(4)	0.004(4)
C(43)	0.042(6)	0.016(5)	0.027(5)	0.003(5)	0.001(5)	0.006(5)
C(44)	0.039(6)	0.018(5)	0.027(5)	0.002(5)	0.000(5)	0.002(5)
C(45)	0.036(6)	0.023(5)	0.030(5)	0.004(5)	-0.001(5)	0.002(5)
C(46)	0.037(5)	0.028(5)	0.031(5)	0.005(4)	-0.001(4)	0.001(5)
C(47)	0.037(6)	0.037(6)	0.036(6)	0.007(5)	0.002(5)	0.002(5)
C(48)	0.038(6)	0.042(6)	0.036(6)	0.006(5)	-0.003(5)	-0.001(5)
C(49)	0.039(5)	0.039(5)	0.032(5)	0.006(5)	-0.006(4)	-0.008(5)
C(50)	0.039(5)	0.031(5)	0.029(5)	0.003(4)	-0.004(4)	-0.009(4)
C(51)	0.037(6)	0.037(6)	0.032(5)	0.009(5)	-0.009(5)	-0.012(5)
C(52)	0.040(6)	0.036(6)	0.029(5)	0.006(5)	-0.011(5)	-0.014(5)
C(53)	0.046(5)	0.031(5)	0.030(5)	0.002(5)	-0.011(4)	-0.013(5)
C(54)	0.042(5)	0.029(5)	0.025(5)	0.001(4)	-0.008(4)	-0.009(5)
C(55)	0.054(6)	0.027(6)	0.033(6)	0.006(5)	-0.012(5)	-0.012(5)
C(56)	0.054(6)	0.025(6)	0.036(6)	0.006(5)	-0.011(5)	-0.004(5)
C(57)	0.054(6)	0.022(5)	0.031(5)	0.005(5)	-0.010(5)	0.000(5)
C(58)	0.077(11)	0.016(8)	0.040(9)	0.011(7)	0.004(8)	0.022(8)
Cu(3)	0.0589(15)	0.0223(12)	0.0333(12)	-0.0053(9)	0.0107(11)	-0.0059(11)
Cu(4)	0.0315(12)	0.0284(13)	0.0535(14)	-0.0144(11)	-0.0138(10)	0.0055(10)
N(9)	0.078(7)	0.031(5)	0.023(5)	-0.004(5)	-0.010(5)	-0.019(5)
N(10)	0.059(6)	0.031(5)	0.033(5)	-0.009(5)	0.007(5)	-0.009(5)
N(11)	0.033(5)	0.016(5)	0.035(5)	-0.006(4)	-0.003(4)	-0.005(4)
N(12)	0.046(5)	0.021(5)	0.028(5)	0.000(4)	-0.014(5)	0.003(5)
N(13)	0.056(6)	0.026(5)	0.031(5)	-0.005(5)	-0.010(5)	-0.001(5)
N(14)	0.039(5)	0.021(5)	0.028(5)	-0.005(4)	-0.002(4)	-0.006(5)
N(15)	0.032(5)	0.057(6)	0.100(7)	-0.029(6)	-0.011(6)	0.006(5)
N(16)	0.053(6)	0.058(7)	0.125(8)	-0.024(7)	-0.030(7)	0.027(6)
C(1A)	0.100(12)	0.037(10)	0.039(9)	0.001(8)	-0.015(9)	-0.009(9)
C(2A)	0.086(7)	0.032(6)	0.028(5)	0.000(5)	-0.011(5)	-0.018(6)
C(3A)	0.086(7)	0.040(6)	0.033(6)	0.007(5)	-0.015(6)	-0.020(6)
C(4A)	0.080(7)	0.045(6)	0.032(6)	0.005(6)	-0.015(6)	-0.022(6)
C(5A)	0.074(6)	0.047(5)	0.027(5)	0.000(5)	-0.010(5)	-0.023(5)
C(6A)	0.070(6)	0.039(5)	0.025(5)	-0.005(5)	-0.005(5)	-0.021(5)
C(7A)	0.072(7)	0.056(6)	0.032(6)	-0.004(6)	-0.006(6)	-0.022(6)
C(8A)	0.068(7)	0.057(6)	0.034(6)	-0.010(6)	0.002(6)	-0.017(6)

C(9A)	0.061(6)	0.049(5)	0.034(5)	-0.011(5)	0.005(5)	-0.012(5)
C(10A)	0.063(6)	0.040(5)	0.028(5)	-0.009(5)	0.002(5)	-0.013(5)
C(11A)	0.059(6)	0.050(6)	0.041(6)	-0.013(6)	0.012(5)	-0.005(6)
C(12A)	0.057(6)	0.039(6)	0.045(6)	-0.010(5)	0.011(5)	-0.006(6)
C(13A)	0.056(6)	0.030(5)	0.040(5)	-0.012(5)	0.009(5)	-0.006(5)
C(14A)	0.056(6)	0.028(6)	0.043(6)	-0.011(5)	0.008(5)	-0.002(5)
C(15A)	0.050(6)	0.025(6)	0.044(6)	-0.009(5)	0.007(5)	0.002(5)
C(16A)	0.045(6)	0.021(6)	0.039(6)	-0.008(5)	0.008(5)	0.000(5)
C(17A)	0.038(5)	0.017(5)	0.033(5)	-0.006(4)	0.000(4)	-0.006(4)
C(18A)	0.039(6)	0.017(5)	0.029(5)	-0.003(5)	-0.002(5)	-0.007(5)
C(19A)	0.035(5)	0.018(5)	0.027(5)	0.000(5)	-0.006(5)	-0.007(5)
C(20A)	0.034(5)	0.018(5)	0.029(5)	0.001(4)	-0.005(4)	-0.001(4)
C(21A)	0.034(5)	0.017(5)	0.030(5)	-0.001(4)	-0.005(4)	0.002(4)
C(22A)	0.035(5)	0.023(5)	0.034(5)	0.002(5)	-0.004(5)	-0.003(5)
C(23A)	0.036(6)	0.020(5)	0.033(5)	0.004(5)	-0.002(5)	0.002(5)
C(24A)	0.041(5)	0.018(5)	0.029(5)	0.002(4)	-0.005(4)	0.002(4)
C(25A)	0.039(5)	0.018(5)	0.029(5)	-0.002(4)	-0.008(4)	0.002(4)
C(26A)	0.047(6)	0.022(5)	0.027(5)	-0.002(5)	-0.006(5)	-0.001(5)
C(27A)	0.051(6)	0.026(6)	0.029(6)	-0.004(5)	-0.013(5)	0.001(5)
C(28A)	0.050(6)	0.020(5)	0.031(5)	-0.004(5)	-0.017(5)	0.002(5)
C(29A)	0.071(10)	0.030(9)	0.048(9)	-0.013(8)	-0.032(8)	0.007(8)
C(30A)	0.083(11)	0.035(9)	0.031(8)	-0.004(8)	-0.001(8)	-0.002(9)
C(31A)	0.063(6)	0.033(6)	0.037(5)	-0.007(5)	-0.011(5)	0.001(5)
C(32A)	0.064(7)	0.039(6)	0.043(6)	-0.011(6)	-0.018(6)	0.000(6)
C(33A)	0.060(6)	0.037(6)	0.043(6)	-0.009(6)	-0.019(5)	-0.004(6)
C(34A)	0.051(5)	0.030(5)	0.037(5)	-0.008(5)	-0.015(5)	-0.003(5)
C(35A)	0.048(5)	0.023(5)	0.028(5)	-0.005(4)	-0.011(4)	-0.003(5)
C(36A)	0.048(6)	0.031(6)	0.041(6)	-0.006(5)	-0.012(5)	-0.002(5)
C(37A)	0.046(6)	0.030(6)	0.038(6)	-0.002(5)	-0.007(5)	0.000(5)
C(38A)	0.042(5)	0.028(5)	0.030(5)	-0.004(4)	-0.005(4)	0.001(5)
C(39A)	0.043(5)	0.024(5)	0.027(4)	-0.005(4)	-0.007(4)	-0.002(4)
C(40A)	0.043(6)	0.031(6)	0.026(5)	-0.008(5)	0.000(5)	0.003(5)
C(41A)	0.042(6)	0.028(6)	0.028(5)	-0.008(5)	0.000(5)	-0.003(5)
C(42A)	0.040(5)	0.026(5)	0.033(5)	-0.007(4)	-0.004(4)	-0.007(5)
C(43A)	0.042(6)	0.035(6)	0.041(6)	-0.012(5)	-0.002(5)	-0.013(5)
C(44A)	0.044(6)	0.040(6)	0.053(6)	-0.019(6)	0.004(6)	-0.011(5)
C(45A)	0.041(6)	0.047(6)	0.067(6)	-0.023(6)	0.006(6)	-0.005(6)
C(46A)	0.037(5)	0.057(6)	0.088(6)	-0.024(6)	-0.002(5)	-0.002(5)
C(47A)	0.041(6)	0.072(7)	0.105(7)	-0.022(7)	-0.005(6)	-0.002(6)
C(48A)	0.049(6)	0.080(7)	0.120(8)	-0.021(7)	-0.008(7)	0.001(7)
C(49A)	0.051(6)	0.081(7)	0.127(7)	-0.022(7)	-0.011(6)	0.012(6)
C(50A)	0.043(5)	0.067(6)	0.118(7)	-0.025(6)	-0.017(6)	0.013(5)
C(51A)	0.061(7)	0.088(8)	0.135(8)	-0.023(8)	-0.011(7)	0.018(7)
C(52A)	0.065(7)	0.086(8)	0.136(8)	-0.024(8)	-0.016(7)	0.022(7)
C(53A)	0.066(6)	0.080(7)	0.132(7)	-0.025(7)	-0.021(6)	0.025(6)
C(54A)	0.054(6)	0.068(6)	0.125(7)	-0.025(6)	-0.023(6)	0.023(6)

C(55A)	0.072(7)	0.076(7)	0.133(8)	-0.022(8)	-0.027(7)	0.031(7)
C(56A)	0.069(7)	0.070(7)	0.132(9)	-0.021(8)	-0.034(8)	0.029(7)
C(57A)	0.061(7)	0.061(7)	0.132(8)	-0.021(7)	-0.035(7)	0.027(7)
C(58A)	0.079(12)	0.043(11)	0.141(14)	-0.008(11)	-0.049(12)	0.009(10)
As(1)	0.0631(14)	0.0227(11)	0.0525(12)	0.0109(9)	0.0217(10)	0.0029(10)
O(1)	0.099(8)	0.036(6)	0.045(6)	0.017(5)	0.015(6)	0.009(6)
O(2)	0.064(7)	0.034(6)	0.038(6)	0.005(5)	0.005(5)	0.008(5)
O(3)	0.092(8)	0.026(6)	0.044(6)	0.005(5)	0.027(6)	0.011(6)
O(4)	0.097(8)	0.059(8)	0.079(8)	0.020(6)	0.043(7)	0.005(7)
O(5)	0.052(6)	0.023(6)	0.079(7)	0.010(5)	0.007(6)	-0.010(5)
O(6)	0.045(6)	0.012(5)	0.062(6)	0.012(5)	0.010(5)	-0.001(5)
C(61)	0.093(7)	0.037(6)	0.046(5)	0.009(5)	0.008(6)	0.013(5)
C(62)	0.099(8)	0.041(7)	0.054(6)	0.008(6)	0.002(7)	0.013(6)
C(63)	0.101(8)	0.044(7)	0.058(7)	0.005(6)	-0.005(7)	0.011(7)
C(64)	0.095(8)	0.045(7)	0.057(7)	-0.001(6)	-0.002(7)	0.013(7)
C(65)	0.086(8)	0.039(7)	0.050(6)	-0.003(6)	0.001(6)	0.015(6)
C(66)	0.079(6)	0.035(6)	0.043(5)	0.002(5)	0.005(5)	0.013(5)
C(67)	0.104(7)	0.036(6)	0.062(6)	0.010(5)	0.035(6)	0.012(6)
C(68)	0.116(8)	0.040(7)	0.069(7)	0.007(6)	0.036(7)	0.016(7)
C(69)	0.122(9)	0.046(7)	0.079(8)	0.005(7)	0.040(8)	0.016(7)
C(70)	0.119(9)	0.056(8)	0.085(8)	0.003(7)	0.045(8)	0.019(8)
C(71)	0.113(9)	0.058(7)	0.082(8)	0.007(6)	0.045(7)	0.014(7)
C(72)	0.105(8)	0.050(6)	0.076(7)	0.012(5)	0.043(6)	0.013(6)
C(73)	0.052(6)	0.021(5)	0.075(6)	0.006(5)	0.012(5)	-0.010(5)
C(74)	0.057(7)	0.023(6)	0.076(7)	-0.001(6)	0.016(6)	-0.013(5)
C(75)	0.054(7)	0.025(6)	0.075(7)	-0.009(6)	0.016(6)	-0.013(6)
C(76)	0.050(7)	0.023(6)	0.069(7)	-0.011(6)	0.018(6)	-0.012(5)
C(77)	0.047(6)	0.021(6)	0.069(7)	-0.006(5)	0.017(6)	-0.008(5)
C(78)	0.045(6)	0.017(5)	0.069(6)	0.003(5)	0.015(5)	-0.007(5)
As(2)	0.0518(12)	0.0127(9)	0.0399(11)	0.0002(8)	-0.0058(9)	0.0000(8)
O(7)	0.063(6)	0.024(6)	0.036(6)	0.006(5)	-0.003(5)	-0.008(5)
O(8)	0.077(7)	0.029(6)	0.043(6)	0.006(5)	-0.015(6)	-0.003(6)
O(9)	0.057(6)	0.014(5)	0.040(5)	-0.010(5)	-0.002(5)	-0.004(5)
O(10)	0.048(6)	0.020(5)	0.041(5)	0.000(5)	-0.005(5)	0.005(5)
O(11)	0.042(6)	0.013(5)	0.059(6)	0.001(5)	-0.009(5)	0.008(5)
O(12)	0.042(6)	0.016(5)	0.050(6)	-0.003(5)	-0.003(5)	-0.001(5)
C(79)	0.069(6)	0.027(5)	0.039(5)	0.004(5)	-0.009(5)	-0.011(5)
C(80)	0.078(7)	0.031(6)	0.046(6)	0.003(5)	-0.013(6)	-0.018(6)
C(81)	0.085(8)	0.036(6)	0.053(7)	0.002(6)	-0.016(6)	-0.019(6)
C(82)	0.086(8)	0.033(6)	0.054(7)	0.005(6)	-0.020(6)	-0.014(6)
C(83)	0.082(7)	0.031(6)	0.049(6)	0.004(5)	-0.020(6)	-0.009(6)
C(84)	0.075(6)	0.026(5)	0.042(5)	0.004(5)	-0.015(5)	-0.007(5)
C(85)	0.046(5)	0.024(5)	0.044(5)	-0.008(5)	-0.002(5)	-0.004(5)
C(86)	0.041(6)	0.030(6)	0.046(6)	-0.010(5)	-0.004(5)	-0.007(5)
C(87)	0.042(6)	0.035(6)	0.046(6)	-0.011(5)	-0.010(6)	-0.001(5)
C(88)	0.042(6)	0.037(6)	0.048(6)	-0.010(5)	-0.010(6)	0.002(6)

C(89)	0.040(6)	0.031(6)	0.044(6)	-0.006(5)	-0.007(5)	0.003(5)
C(90)	0.043(5)	0.026(5)	0.041(5)	-0.005(4)	-0.003(5)	0.001(5)
C(91)	0.042(5)	0.013(5)	0.056(6)	0.007(4)	-0.010(5)	0.002(4)
C(92)	0.042(6)	0.014(5)	0.058(6)	0.010(5)	-0.013(5)	0.001(5)
C(93)	0.044(6)	0.016(6)	0.058(7)	0.010(5)	-0.015(6)	-0.002(5)
C(94)	0.043(6)	0.016(6)	0.054(6)	0.008(5)	-0.012(6)	-0.004(5)
C(95)	0.044(6)	0.014(5)	0.053(6)	0.007(5)	-0.009(5)	0.001(5)
C(96)	0.044(5)	0.012(5)	0.053(5)	0.006(4)	-0.006(5)	0.003(4)
As(3)	0.0380(11)	0.0220(10)	0.0561(12)	0.0020(9)	-0.0197(9)	-0.0082(8)
O(13)	0.048(6)	0.024(6)	0.063(6)	0.003(5)	-0.033(5)	-0.008(5)
O(14)	0.045(6)	0.020(5)	0.080(7)	0.005(5)	-0.021(6)	-0.008(5)
O(15)	0.043(6)	0.028(5)	0.031(5)	-0.001(4)	-0.011(5)	-0.002(5)
O(16)	0.052(6)	0.025(6)	0.052(6)	-0.001(5)	-0.023(5)	-0.012(5)
O(17)	0.037(5)	0.019(5)	0.049(6)	-0.002(5)	-0.019(5)	-0.003(5)
O(18)	0.040(6)	0.034(6)	0.052(6)	0.013(5)	-0.013(5)	-0.005(5)
C(97)	0.053(6)	0.024(5)	0.074(6)	-0.003(5)	-0.036(5)	-0.005(5)
C(98)	0.060(7)	0.028(6)	0.085(7)	-0.005(6)	-0.041(6)	-0.004(6)
C(99)	0.062(7)	0.031(6)	0.090(8)	-0.004(6)	-0.044(6)	-0.002(6)
C(100)	0.057(7)	0.032(6)	0.091(8)	-0.002(6)	-0.041(6)	-0.003(6)
C(101)	0.053(6)	0.029(6)	0.088(7)	-0.001(6)	-0.035(6)	-0.001(6)
C(102)	0.050(6)	0.025(5)	0.081(6)	-0.001(5)	-0.031(5)	-0.005(5)
C(103)	0.051(5)	0.025(5)	0.034(5)	0.001(4)	-0.012(5)	-0.004(5)
C(104)	0.057(6)	0.027(6)	0.034(6)	0.000(5)	-0.008(5)	-0.005(6)
C(105)	0.064(7)	0.028(6)	0.034(6)	0.000(5)	-0.009(6)	-0.006(6)
C(106)	0.067(7)	0.029(6)	0.037(6)	0.002(5)	-0.012(6)	-0.005(6)
C(107)	0.063(6)	0.028(6)	0.038(6)	0.004(5)	-0.017(6)	-0.008(6)
C(108)	0.056(6)	0.025(5)	0.042(5)	0.003(5)	-0.017(5)	-0.005(5)
C(109)	0.035(5)	0.031(5)	0.050(5)	0.006(5)	-0.016(5)	-0.002(5)
C(110)	0.041(6)	0.039(6)	0.055(6)	0.006(6)	-0.016(6)	0.000(6)
C(111)	0.047(6)	0.050(6)	0.058(7)	0.011(6)	-0.018(6)	0.001(6)
C(112)	0.050(6)	0.052(7)	0.061(7)	0.015(6)	-0.019(6)	-0.001(6)
C(113)	0.045(6)	0.045(6)	0.060(6)	0.009(6)	-0.017(6)	-0.006(6)
C(114)	0.039(5)	0.037(5)	0.054(5)	0.010(5)	-0.017(5)	-0.004(5)
As(4)	0.0506(12)	0.0236(10)	0.0401(10)	-0.0055(8)	0.0126(9)	-0.0103(9)
O(19)	0.067(7)	0.037(6)	0.049(6)	-0.018(5)	0.018(6)	-0.010(6)
O(20)	0.069(7)	0.036(6)	0.039(6)	-0.011(5)	0.008(5)	-0.006(5)
O(21)	0.062(6)	0.028(6)	0.037(5)	0.000(5)	0.001(5)	-0.015(5)
O(22)	0.047(6)	0.032(6)	0.026(5)	0.001(5)	0.006(5)	-0.003(5)
O(23)	0.043(6)	0.012(5)	0.046(6)	-0.004(4)	0.001(5)	-0.004(4)
O(24)	0.040(6)	0.024(5)	0.046(6)	0.000(5)	0.005(5)	-0.009(5)
C(115)	0.075(6)	0.041(6)	0.048(6)	-0.015(5)	0.013(5)	-0.008(5)
C(116)	0.084(7)	0.047(7)	0.049(6)	-0.014(6)	0.012(6)	-0.007(6)
C(117)	0.090(8)	0.048(7)	0.051(7)	-0.008(6)	0.011(7)	-0.005(7)
C(118)	0.088(8)	0.044(7)	0.050(7)	-0.003(6)	0.010(6)	-0.007(7)
C(119)	0.084(7)	0.039(6)	0.045(6)	-0.003(6)	0.010(6)	-0.014(6)
C(120)	0.075(6)	0.036(6)	0.043(5)	-0.008(5)	0.010(5)	-0.010(5)

C(121)	0.061(6)	0.031(5)	0.037(5)	0.000(5)	0.000(5)	-0.008(5)
C(122)	0.067(7)	0.034(6)	0.041(6)	0.004(5)	0.002(6)	-0.008(6)
C(123)	0.066(7)	0.037(6)	0.041(6)	0.007(6)	0.002(6)	-0.004(6)
C(124)	0.059(7)	0.039(6)	0.039(6)	0.006(5)	0.001(6)	-0.002(6)
C(125)	0.058(6)	0.036(6)	0.033(6)	0.003(5)	0.001(6)	-0.001(6)
C(126)	0.054(5)	0.032(5)	0.031(5)	0.002(4)	0.001(5)	-0.005(5)
C(127)	0.040(5)	0.023(5)	0.054(5)	-0.005(5)	0.000(5)	-0.002(5)
C(128)	0.045(6)	0.028(6)	0.063(7)	-0.006(5)	-0.007(6)	-0.003(5)
C(129)	0.051(6)	0.034(6)	0.071(7)	-0.004(6)	-0.016(6)	-0.005(6)
C(130)	0.050(6)	0.031(6)	0.071(7)	0.001(6)	-0.018(6)	-0.004(6)
C(131)	0.040(6)	0.026(6)	0.064(7)	0.005(5)	-0.009(5)	-0.010(5)
C(132)	0.038(5)	0.025(5)	0.054(6)	-0.001(5)	-0.001(5)	-0.006(5)

Table 4. Bond lengths [Å] for nd1014z_x.

atom-atom	distance	atom-atom	distance
Cu(1)-N(6)	2.011(13)	Cu(1)-N(1)	2.024(14)
Cu(1)-N(2)	2.036(14)	Cu(1)-N(5)	2.042(13)
Cu(2)-N(4)	2.021(13)	Cu(2)-N(8)	2.044(14)
Cu(2)-N(7)	2.045(13)	Cu(2)-N(3)	2.046(14)
N(1)-C(2)	1.30(2)	N(1)-C(6)	1.37(2)
N(2)-C(13)	1.31(2)	N(2)-C(10)	1.36(2)
N(3)-C(46)	1.31(2)	N(3)-C(50)	1.38(2)
N(4)-C(54)	1.33(2)	N(4)-C(57)	1.37(2)
N(5)-C(31)	1.34(2)	N(5)-C(35)	1.36(2)
N(6)-C(42)	1.341(19)	N(6)-C(39)	1.380(19)
N(7)-C(21)	1.33(2)	N(7)-C(17)	1.34(2)
N(8)-C(28)	1.31(2)	N(8)-C(25)	1.37(2)
C(1)-C(2)	1.50(3)	C(2)-C(3)	1.46(3)
C(3)-C(4)	1.33(3)	C(4)-C(5)	1.42(3)
C(5)-C(7)	1.40(3)	C(5)-C(6)	1.40(3)
C(6)-C(10)	1.45(2)	C(7)-C(8)	1.37(3)
C(8)-C(9)	1.40(3)	C(9)-C(10)	1.39(3)
C(9)-C(11)	1.44(3)	C(11)-C(12)	1.37(3)
C(12)-C(13)	1.43(2)	C(13)-C(14)	1.48(2)
C(14)-C(15)	1.54(2)	C(15)-C(16)	1.53(2)
C(16)-C(17)	1.53(2)	C(17)-C(18)	1.41(2)
C(18)-C(19)	1.38(2)	C(19)-C(20)	1.42(2)
C(20)-C(22)	1.39(2)	C(20)-C(21)	1.39(2)
C(21)-C(25)	1.47(2)	C(22)-C(23)	1.36(2)
C(23)-C(24)	1.43(2)	C(24)-C(26)	1.39(2)
C(24)-C(25)	1.41(2)	C(26)-C(27)	1.38(2)
C(27)-C(28)	1.41(2)	C(28)-C(29)	1.53(2)
C(30)-C(31)	1.50(2)	C(31)-C(32)	1.38(2)
C(32)-C(33)	1.38(2)	C(33)-C(34)	1.41(2)
C(34)-C(35)	1.38(2)	C(34)-C(36)	1.43(2)
C(35)-C(39)	1.45(2)	C(36)-C(37)	1.32(2)
C(37)-C(38)	1.43(2)	C(38)-C(39)	1.40(2)
C(38)-C(40)	1.41(2)	C(40)-C(41)	1.36(2)
C(41)-C(42)	1.39(2)	C(42)-C(43)	1.51(2)
C(43)-C(44)	1.53(2)	C(44)-C(45)	1.54(2)
C(45)-C(46)	1.51(2)	C(46)-C(47)	1.39(2)
C(47)-C(48)	1.36(2)	C(48)-C(49)	1.42(3)
C(49)-C(50)	1.40(2)	C(49)-C(51)	1.46(2)
C(50)-C(54)	1.44(2)	C(51)-C(52)	1.32(2)
C(52)-C(53)	1.41(2)	C(53)-C(55)	1.40(2)
C(53)-C(54)	1.44(2)	C(55)-C(56)	1.38(2)
C(56)-C(57)	1.39(2)	C(57)-C(58)	1.45(2)

Cu(3)-N(14)	2.018(13)	Cu(3)-N(9)	2.027(14)
Cu(3)-N(10)	2.029(15)	Cu(3)-N(13)	2.041(15)
Cu(4)-N(16)	1.981(17)	Cu(4)-N(12)	2.032(14)
Cu(4)-N(11)	2.032(13)	Cu(4)-N(15)	2.055(17)
N(9)-C(2A)	1.33(2)	N(9)-C(6A)	1.37(2)
N(10)-C(13A)	1.32(2)	N(10)-C(10A)	1.39(2)
N(11)-C(17A)	1.312(19)	N(11)-C(21A)	1.381(19)
N(12)-C(28A)	1.34(2)	N(12)-C(25A)	1.39(2)
N(13)-C(31A)	1.35(2)	N(13)-C(35A)	1.35(2)
N(14)-C(42A)	1.339(19)	N(14)-C(39A)	1.37(2)
N(15)-C(50A)	1.34(3)	N(15)-C(46A)	1.36(3)
N(16)-C(57A)	1.31(3)	N(16)-C(54A)	1.34(3)
C(1A)-C(2A)	1.50(3)	C(2A)-C(3A)	1.43(3)
C(3A)-C(4A)	1.31(3)	C(4A)-C(5A)	1.36(3)
C(5A)-C(6A)	1.38(3)	C(5A)-C(7A)	1.47(3)
C(6A)-C(10A)	1.43(3)	C(7A)-C(8A)	1.30(3)
C(8A)-C(9A)	1.43(3)	C(9A)-C(10A)	1.39(3)
C(9A)-C(11A)	1.39(3)	C(11A)-C(12A)	1.33(3)
C(12A)-C(13A)	1.40(2)	C(13A)-C(14A)	1.53(2)
C(14A)-C(15A)	1.53(2)	C(15A)-C(16A)	1.53(2)
C(16A)-C(17A)	1.50(2)	C(17A)-C(18A)	1.42(2)
C(18A)-C(19A)	1.33(2)	C(19A)-C(20A)	1.40(2)
C(20A)-C(21A)	1.37(2)	C(20A)-C(22A)	1.48(2)
C(21A)-C(25A)	1.44(2)	C(22A)-C(23A)	1.31(2)
C(23A)-C(24A)	1.43(2)	C(24A)-C(25A)	1.39(2)
C(24A)-C(26A)	1.42(2)	C(26A)-C(27A)	1.39(2)
C(27A)-C(28A)	1.38(2)	C(28A)-C(29A)	1.48(2)
C(30A)-C(31A)	1.47(2)	C(31A)-C(32A)	1.36(3)
C(32A)-C(33A)	1.40(3)	C(33A)-C(34A)	1.41(2)
C(34A)-C(35A)	1.38(2)	C(34A)-C(36A)	1.46(2)
C(35A)-C(39A)	1.47(2)	C(36A)-C(37A)	1.33(2)
C(37A)-C(38A)	1.39(2)	C(38A)-C(39A)	1.41(2)
C(38A)-C(40A)	1.43(2)	C(40A)-C(41A)	1.38(2)
C(41A)-C(42A)	1.40(2)	C(42A)-C(43A)	1.49(2)
C(43A)-C(44A)	1.53(2)	C(44A)-C(45A)	1.49(3)
C(45A)-C(46A)	1.47(3)	C(46A)-C(47A)	1.44(3)
C(47A)-C(48A)	1.38(3)	C(48A)-C(49A)	1.40(4)
C(49A)-C(50A)	1.37(3)	C(49A)-C(51A)	1.42(3)
C(50A)-C(54A)	1.41(4)	C(51A)-C(52A)	1.32(4)
C(52A)-C(53A)	1.42(4)	C(53A)-C(55A)	1.44(4)
C(53A)-C(54A)	1.46(3)	C(55A)-C(56A)	1.33(3)
C(56A)-C(57A)	1.44(3)	C(57A)-C(58A)	1.46(3)
As(1)-O(5)	1.823(13)	As(1)-O(6)	1.825(11)
As(1)-O(4)	1.836(15)	As(1)-O(3)	1.854(14)
As(1)-O(1)	1.859(13)	As(1)-O(2)	1.860(12)
O(1)-C(61)	1.36(2)	O(2)-C(66)	1.39(2)

O(3)-C(67)	1.34(2)	O(4)-C(72)	1.42(3)
O(5)-C(73)	1.36(2)	O(6)-C(78)	1.36(2)
C(61)-C(62)	1.38(3)	C(61)-C(66)	1.40(3)
C(62)-C(63)	1.33(3)	C(63)-C(64)	1.40(3)
C(64)-C(65)	1.43(3)	C(65)-C(66)	1.34(3)
C(67)-C(72)	1.35(3)	C(67)-C(68)	1.38(3)
C(68)-C(69)	1.41(3)	C(69)-C(70)	1.28(3)
C(70)-C(71)	1.38(4)	C(71)-C(72)	1.40(3)
C(73)-C(78)	1.37(2)	C(73)-C(74)	1.40(3)
C(74)-C(75)	1.45(3)	C(75)-C(76)	1.35(2)
C(76)-C(77)	1.41(3)	C(77)-C(78)	1.38(3)
As(2)-O(8)	1.822(12)	As(2)-O(7)	1.831(12)
As(2)-O(9)	1.838(10)	As(2)-O(11)	1.839(12)
As(2)-O(12)	1.843(11)	As(2)-O(10)	1.845(11)
O(7)-C(79)	1.39(2)	O(8)-C(84)	1.37(2)
O(9)-C(85)	1.35(2)	O(10)-C(90)	1.39(2)
O(11)-C(91)	1.35(2)	O(12)-C(96)	1.34(2)
C(79)-C(84)	1.32(3)	C(79)-C(80)	1.40(3)
C(80)-C(81)	1.38(3)	C(81)-C(82)	1.35(3)
C(82)-C(83)	1.34(3)	C(83)-C(84)	1.37(3)
C(85)-C(86)	1.39(2)	C(85)-C(90)	1.40(2)
C(86)-C(87)	1.40(2)	C(87)-C(88)	1.36(2)
C(88)-C(89)	1.39(2)	C(89)-C(90)	1.36(2)
C(91)-C(92)	1.39(2)	C(91)-C(96)	1.42(2)
C(92)-C(93)	1.40(2)	C(93)-C(94)	1.40(2)
C(94)-C(95)	1.33(2)	C(95)-C(96)	1.40(2)
As(3)-O(14)	1.823(12)	As(3)-O(13)	1.828(12)
As(3)-O(15)	1.835(11)	As(3)-O(17)	1.840(11)
As(3)-O(16)	1.845(11)	As(3)-O(18)	1.850(11)
O(13)-C(97)	1.37(2)	O(14)-C(102)	1.37(2)
O(15)-C(103)	1.364(19)	O(16)-C(108)	1.36(2)
O(17)-C(109)	1.37(2)	O(18)-C(114)	1.33(2)
C(97)-C(102)	1.38(3)	C(97)-C(98)	1.41(3)
C(98)-C(99)	1.37(3)	C(99)-C(100)	1.40(3)
C(100)-C(101)	1.42(3)	C(101)-C(102)	1.43(3)
C(103)-C(104)	1.38(2)	C(103)-C(108)	1.40(2)
C(104)-C(105)	1.40(2)	C(105)-C(106)	1.37(2)
C(106)-C(107)	1.36(3)	C(107)-C(108)	1.41(2)
C(109)-C(110)	1.38(3)	C(109)-C(114)	1.39(3)
C(110)-C(111)	1.40(3)	C(111)-C(112)	1.36(3)
C(112)-C(113)	1.46(3)	C(113)-C(114)	1.37(3)
As(4)-O(23)	1.811(11)	As(4)-O(19)	1.818(12)
As(4)-O(24)	1.821(11)	As(4)-O(22)	1.837(11)
As(4)-O(21)	1.846(12)	As(4)-O(20)	1.848(12)
O(19)-C(115)	1.40(2)	O(20)-C(120)	1.35(2)
O(21)-C(121)	1.37(2)	O(22)-C(126)	1.37(2)

O(23)-C(127)	1.38(2)	O(24)-C(132)	1.37(2)
C(115)-C(120)	1.39(3)	C(115)-C(116)	1.39(3)
C(116)-C(117)	1.43(3)	C(117)-C(118)	1.36(3)
C(118)-C(119)	1.42(3)	C(119)-C(120)	1.35(3)
C(121)-C(122)	1.36(2)	C(121)-C(126)	1.36(2)
C(122)-C(123)	1.34(3)	C(123)-C(124)	1.37(2)
C(124)-C(125)	1.39(2)	C(125)-C(126)	1.39(2)
C(127)-C(128)	1.34(2)	C(127)-C(132)	1.39(2)
C(128)-C(129)	1.37(3)	C(129)-C(130)	1.44(3)
C(130)-C(131)	1.34(2)	C(131)-C(132)	1.40(2)
N(1S)-C(1S)	1.157(12)	C(1S)-C(2S)	1.458(13)
N(2S)-C(3S)	1.182(13)	C(3S)-C(4S)	1.469(13)
N(3S)-C(5S)	1.168(14)	C(5S)-C(6S)	1.443(14)
N(4S)-C(7S)	1.165(13)	C(7S)-C(8S)	1.455(13)

Symmetry transformations used to generate equivalent atoms:

Table 5. Bond angles [°] for nd1014z_x.

atom-atom-atom	angle	atom-atom-atom	angle
N(6)-Cu(1)-N(1)	124.4(5)	N(6)-Cu(1)-N(2)	136.3(5)
N(1)-Cu(1)-N(2)	83.5(6)	N(6)-Cu(1)-N(5)	82.4(5)
N(1)-Cu(1)-N(5)	122.2(5)	N(2)-Cu(1)-N(5)	112.4(5)
N(4)-Cu(2)-N(8)	124.3(5)	N(4)-Cu(2)-N(7)	121.5(5)
N(8)-Cu(2)-N(7)	82.4(5)	N(4)-Cu(2)-N(3)	82.7(5)
N(8)-Cu(2)-N(3)	118.0(5)	N(7)-Cu(2)-N(3)	133.7(5)
C(2)-N(1)-C(6)	119.8(16)	C(2)-N(1)-Cu(1)	130.0(14)
C(6)-N(1)-Cu(1)	110.2(11)	C(13)-N(2)-C(10)	118.7(16)
C(13)-N(2)-Cu(1)	129.6(12)	C(10)-N(2)-Cu(1)	111.2(11)
C(46)-N(3)-C(50)	118.5(14)	C(46)-N(3)-Cu(2)	130.9(11)
C(50)-N(3)-Cu(2)	110.5(11)	C(54)-N(4)-C(57)	119.1(14)
C(54)-N(4)-Cu(2)	111.8(11)	C(57)-N(4)-Cu(2)	129.0(12)
C(31)-N(5)-C(35)	117.3(14)	C(31)-N(5)-Cu(1)	130.2(12)
C(35)-N(5)-Cu(1)	112.1(10)	C(42)-N(6)-C(39)	117.9(14)
C(42)-N(6)-Cu(1)	129.9(11)	C(39)-N(6)-Cu(1)	112.2(10)
C(21)-N(7)-C(17)	118.5(14)	C(21)-N(7)-Cu(2)	112.5(10)
C(17)-N(7)-Cu(2)	129.0(11)	C(28)-N(8)-C(25)	118.1(15)
C(28)-N(8)-Cu(2)	130.4(12)	C(25)-N(8)-Cu(2)	111.5(11)
N(1)-C(2)-C(3)	120.8(18)	N(1)-C(2)-C(1)	117.5(16)
C(3)-C(2)-C(1)	121.7(16)	C(4)-C(3)-C(2)	118.6(18)
C(3)-C(4)-C(5)	122.1(19)	C(7)-C(5)-C(6)	120.1(18)
C(7)-C(5)-C(4)	124.4(19)	C(6)-C(5)-C(4)	115.5(19)
N(1)-C(6)-C(5)	123.1(17)	N(1)-C(6)-C(10)	118.5(16)
C(5)-C(6)-C(10)	118.4(17)	C(8)-C(7)-C(5)	121(2)
C(7)-C(8)-C(9)	120(2)	C(10)-C(9)-C(8)	120.2(18)
C(10)-C(9)-C(11)	118.1(18)	C(8)-C(9)-C(11)	121.6(19)
N(2)-C(10)-C(9)	124.2(16)	N(2)-C(10)-C(6)	116.2(16)
C(9)-C(10)-C(6)	119.6(17)	C(12)-C(11)-C(9)	115.6(18)
C(11)-C(12)-C(13)	123.0(17)	N(2)-C(13)-C(12)	120.3(17)
N(2)-C(13)-C(14)	120.0(16)	C(12)-C(13)-C(14)	119.7(15)
C(13)-C(14)-C(15)	114.1(15)	C(16)-C(15)-C(14)	113.3(14)
C(15)-C(16)-C(17)	110.4(13)	N(7)-C(17)-C(18)	121.2(15)
N(7)-C(17)-C(16)	117.0(14)	C(18)-C(17)-C(16)	121.8(15)
C(19)-C(18)-C(17)	119.6(16)	C(18)-C(19)-C(20)	120.0(15)
C(22)-C(20)-C(21)	121.4(16)	C(22)-C(20)-C(19)	123.5(15)
C(21)-C(20)-C(19)	115.1(15)	N(7)-C(21)-C(20)	125.6(15)
N(7)-C(21)-C(25)	117.0(14)	C(20)-C(21)-C(25)	117.3(15)
C(23)-C(22)-C(20)	121.8(16)	C(22)-C(23)-C(24)	120.5(16)
C(26)-C(24)-C(25)	118.0(15)	C(26)-C(24)-C(23)	123.5(16)
C(25)-C(24)-C(23)	118.4(16)	N(8)-C(25)-C(24)	122.9(15)
N(8)-C(25)-C(21)	116.6(15)	C(24)-C(25)-C(21)	120.4(15)
C(27)-C(26)-C(24)	118.5(17)	C(26)-C(27)-C(28)	120.1(17)

N(8)-C(28)-C(27)	122.2(16)	N(8)-C(28)-C(29)	116.6(16)
C(27)-C(28)-C(29)	121.1(16)	N(5)-C(31)-C(32)	121.1(16)
N(5)-C(31)-C(30)	115.5(15)	C(32)-C(31)-C(30)	123.4(15)
C(33)-C(32)-C(31)	121.8(16)	C(32)-C(33)-C(34)	118.0(16)
C(35)-C(34)-C(33)	116.5(16)	C(35)-C(34)-C(36)	120.1(15)
C(33)-C(34)-C(36)	123.4(16)	N(5)-C(35)-C(34)	125.0(15)
N(5)-C(35)-C(39)	116.4(14)	C(34)-C(35)-C(39)	118.5(15)
C(37)-C(36)-C(34)	120.8(16)	C(36)-C(37)-C(38)	122.2(17)
C(39)-C(38)-C(40)	116.9(15)	C(39)-C(38)-C(37)	118.1(15)
C(40)-C(38)-C(37)	125.0(16)	N(6)-C(39)-C(38)	123.1(14)
N(6)-C(39)-C(35)	116.7(14)	C(38)-C(39)-C(35)	120.2(15)
C(41)-C(40)-C(38)	119.7(16)	C(40)-C(41)-C(42)	120.8(15)
N(6)-C(42)-C(41)	121.7(15)	N(6)-C(42)-C(43)	116.9(14)
C(41)-C(42)-C(43)	121.4(14)	C(42)-C(43)-C(44)	113.4(13)
C(43)-C(44)-C(45)	111.7(13)	C(46)-C(45)-C(44)	112.6(13)
N(3)-C(46)-C(47)	122.9(15)	N(3)-C(46)-C(45)	119.0(15)
C(47)-C(46)-C(45)	118.1(15)	C(48)-C(47)-C(46)	120.2(17)
C(47)-C(48)-C(49)	119.1(17)	C(50)-C(49)-C(48)	117.4(16)
C(50)-C(49)-C(51)	118.8(16)	C(48)-C(49)-C(51)	123.8(17)
N(3)-C(50)-C(49)	122.0(16)	N(3)-C(50)-C(54)	116.1(15)
C(49)-C(50)-C(54)	121.8(15)	C(52)-C(51)-C(49)	118.8(17)
C(51)-C(52)-C(53)	124.5(17)	C(55)-C(53)-C(52)	127.3(16)
C(55)-C(53)-C(54)	113.5(16)	C(52)-C(53)-C(54)	119.2(16)
N(4)-C(54)-C(50)	118.8(15)	N(4)-C(54)-C(53)	124.4(16)
C(50)-C(54)-C(53)	116.9(16)	C(56)-C(55)-C(53)	122.9(16)
C(55)-C(56)-C(57)	118.8(17)	N(4)-C(57)-C(56)	120.9(17)
N(4)-C(57)-C(58)	117.2(15)	C(56)-C(57)-C(58)	121.9(16)
N(14)-Cu(3)-N(9)	123.6(6)	N(14)-Cu(3)-N(10)	132.5(6)
N(9)-Cu(3)-N(10)	83.0(6)	N(14)-Cu(3)-N(13)	82.5(5)
N(9)-Cu(3)-N(13)	122.5(6)	N(10)-Cu(3)-N(13)	118.0(6)
N(16)-Cu(4)-N(12)	123.7(8)	N(16)-Cu(4)-N(11)	124.3(7)
N(12)-Cu(4)-N(11)	83.2(5)	N(16)-Cu(4)-N(15)	81.8(8)
N(12)-Cu(4)-N(15)	119.3(6)	N(11)-Cu(4)-N(15)	130.2(7)
C(2A)-N(9)-C(6A)	117.3(16)	C(2A)-N(9)-Cu(3)	130.3(14)
C(6A)-N(9)-Cu(3)	112.3(12)	C(13A)-N(10)-C(10A)	117.7(16)
C(13A)-N(10)-Cu(3)	131.7(13)	C(10A)-N(10)-Cu(3)	110.5(12)
C(17A)-N(11)-C(21A)	118.2(13)	C(17A)-N(11)-Cu(4)	130.2(11)
C(21A)-N(11)-Cu(4)	111.6(10)	C(28A)-N(12)-C(25A)	117.7(14)
C(28A)-N(12)-Cu(4)	131.1(12)	C(25A)-N(12)-Cu(4)	111.0(10)
C(31A)-N(13)-C(35A)	118.2(15)	C(31A)-N(13)-Cu(3)	129.1(13)
C(35A)-N(13)-Cu(3)	112.5(10)	C(42A)-N(14)-C(39A)	116.7(13)
C(42A)-N(14)-Cu(3)	131.1(11)	C(39A)-N(14)-Cu(3)	112.2(10)
C(50A)-N(15)-C(46A)	119.9(19)	C(50A)-N(15)-Cu(4)	111.1(17)
C(46A)-N(15)-Cu(4)	128.9(14)	C(57A)-N(16)-C(54A)	118(2)
C(57A)-N(16)-Cu(4)	129.3(17)	C(54A)-N(16)-Cu(4)	112.1(17)
N(9)-C(2A)-C(3A)	120(2)	N(9)-C(2A)-C(1A)	116.7(17)

C(3A)-C(2A)-C(1A)	123.0(18)	C(4A)-C(3A)-C(2A)	121(2)
C(3A)-C(4A)-C(5A)	119(2)	C(4A)-C(5A)-C(6A)	120(2)
C(4A)-C(5A)-C(7A)	123.4(19)	C(6A)-C(5A)-C(7A)	116.3(19)
N(9)-C(6A)-C(5A)	121.7(19)	N(9)-C(6A)-C(10A)	116.1(16)
C(5A)-C(6A)-C(10A)	122.0(19)	C(8A)-C(7A)-C(5A)	121.2(19)
C(7A)-C(8A)-C(9A)	123(2)	C(10A)-C(9A)-C(11A)	115.7(18)
C(10A)-C(9A)-C(8A)	118(2)	C(11A)-C(9A)-C(8A)	126(2)
C(9A)-C(10A)-N(10)	123.0(18)	C(9A)-C(10A)-C(6A)	119.0(18)
N(10)-C(10A)-C(6A)	118.0(17)	C(12A)-C(11A)-C(9A)	121.7(19)
C(11A)-C(12A)-C(13A)	120.0(19)	N(10)-C(13A)-C(12A)	121.8(17)
N(10)-C(13A)-C(14A)	116.8(16)	C(12A)-C(13A)-C(14A)	121.4(17)
C(13A)-C(14A)-C(15A)	113.3(15)	C(16A)-C(15A)-C(14A)	112.1(15)
C(17A)-C(16A)-C(15A)	112.6(14)	N(11)-C(17A)-C(18A)	121.1(15)
N(11)-C(17A)-C(16A)	116.8(14)	C(18A)-C(17A)-C(16A)	122.0(14)
C(19A)-C(18A)-C(17A)	120.1(15)	C(18A)-C(19A)-C(20A)	120.1(15)
C(21A)-C(20A)-C(19A)	117.5(14)	C(21A)-C(20A)-C(22A)	117.3(14)
C(19A)-C(20A)-C(22A)	125.2(14)	C(20A)-C(21A)-N(11)	122.8(14)
C(20A)-C(21A)-C(25A)	120.5(14)	N(11)-C(21A)-C(25A)	116.6(14)
C(23A)-C(22A)-C(20A)	122.4(16)	C(22A)-C(23A)-C(24A)	120.5(16)
C(25A)-C(24A)-C(26A)	117.4(15)	C(25A)-C(24A)-C(23A)	119.5(14)
C(26A)-C(24A)-C(23A)	123.1(15)	N(12)-C(25A)-C(24A)	122.9(14)
N(12)-C(25A)-C(21A)	117.2(14)	C(24A)-C(25A)-C(21A)	119.8(14)
C(27A)-C(26A)-C(24A)	119.3(16)	C(28A)-C(27A)-C(26A)	119.2(15)
N(12)-C(28A)-C(27A)	123.1(15)	N(12)-C(28A)-C(29A)	114.0(15)
C(27A)-C(28A)-C(29A)	122.9(15)	N(13)-C(31A)-C(32A)	120.1(17)
N(13)-C(31A)-C(30A)	119.0(17)	C(32A)-C(31A)-C(30A)	120.9(17)
C(31A)-C(32A)-C(33A)	122.8(17)	C(32A)-C(33A)-C(34A)	116.8(18)
C(35A)-C(34A)-C(33A)	117.2(17)	C(35A)-C(34A)-C(36A)	120.2(15)
C(33A)-C(34A)-C(36A)	122.4(17)	N(13)-C(35A)-C(34A)	124.7(15)
N(13)-C(35A)-C(39A)	116.1(15)	C(34A)-C(35A)-C(39A)	119.1(15)
C(37A)-C(36A)-C(34A)	119.7(17)	C(36A)-C(37A)-C(38A)	122.3(17)
C(37A)-C(38A)-C(39A)	121.0(15)	C(37A)-C(38A)-C(40A)	124.6(15)
C(39A)-C(38A)-C(40A)	114.3(15)	N(14)-C(39A)-C(38A)	125.6(14)
N(14)-C(39A)-C(35A)	116.7(14)	C(38A)-C(39A)-C(35A)	117.6(15)
C(41A)-C(40A)-C(38A)	120.5(15)	C(40A)-C(41A)-C(42A)	119.7(15)
N(14)-C(42A)-C(41A)	123.0(15)	N(14)-C(42A)-C(43A)	116.1(14)
C(41A)-C(42A)-C(43A)	120.9(15)	C(42A)-C(43A)-C(44A)	113.0(15)
C(45A)-C(44A)-C(43A)	114.2(15)	C(46A)-C(45A)-C(44A)	113.5(17)
N(15)-C(46A)-C(47A)	123(2)	N(15)-C(46A)-C(45A)	118.7(18)
C(47A)-C(46A)-C(45A)	118(2)	C(48A)-C(47A)-C(46A)	115(2)
C(47A)-C(48A)-C(49A)	120(2)	C(50A)-C(49A)-C(48A)	122(2)
C(50A)-C(49A)-C(51A)	118(3)	C(48A)-C(49A)-C(51A)	120(2)
N(15)-C(50A)-C(49A)	119(2)	N(15)-C(50A)-C(54A)	116(2)
C(49A)-C(50A)-C(54A)	124(2)	C(52A)-C(51A)-C(49A)	118(3)
C(51A)-C(52A)-C(53A)	128(3)	C(52A)-C(53A)-C(55A)	133(3)
C(52A)-C(53A)-C(54A)	114(3)	C(55A)-C(53A)-C(54A)	113(3)

N(16)-C(54A)-C(50A)	118(2)	N(16)-C(54A)-C(53A)	124(3)
C(50A)-C(54A)-C(53A)	117(2)	C(56A)-C(55A)-C(53A)	123(3)
C(55A)-C(56A)-C(57A)	118(3)	N(16)-C(57A)-C(56A)	124(2)
N(16)-C(57A)-C(58A)	117(2)	C(56A)-C(57A)-C(58A)	119(3)
O(5)-As(1)-O(6)	88.5(6)	O(5)-As(1)-O(4)	90.8(7)
O(6)-As(1)-O(4)	95.2(6)	O(5)-As(1)-O(3)	177.2(6)
O(6)-As(1)-O(3)	89.7(5)	O(4)-As(1)-O(3)	87.3(7)
O(5)-As(1)-O(1)	88.9(6)	O(6)-As(1)-O(1)	176.0(6)
O(4)-As(1)-O(1)	87.9(7)	O(3)-As(1)-O(1)	93.0(6)
O(5)-As(1)-O(2)	95.2(6)	O(6)-As(1)-O(2)	89.2(5)
O(4)-As(1)-O(2)	172.7(7)	O(3)-As(1)-O(2)	86.9(6)
O(1)-As(1)-O(2)	88.0(6)	C(61)-O(1)-As(1)	111.3(12)
C(66)-O(2)-As(1)	109.0(11)	C(67)-O(3)-As(1)	110.5(14)
C(72)-O(4)-As(1)	109.4(15)	C(73)-O(5)-As(1)	108.9(11)
C(78)-O(6)-As(1)	109.5(10)	O(1)-C(61)-C(62)	123.3(19)
O(1)-C(61)-C(66)	114.5(18)	C(62)-C(61)-C(66)	122(2)
C(63)-C(62)-C(61)	118(2)	C(62)-C(63)-C(64)	122(2)
C(63)-C(64)-C(65)	118(2)	C(66)-C(65)-C(64)	119(2)
C(65)-C(66)-O(2)	124.2(18)	C(65)-C(66)-C(61)	119(2)
O(2)-C(66)-C(61)	116.4(19)	O(3)-C(67)-C(72)	117(2)
O(3)-C(67)-C(68)	122(2)	C(72)-C(67)-C(68)	121(2)
C(67)-C(68)-C(69)	117(3)	C(70)-C(69)-C(68)	122(3)
C(69)-C(70)-C(71)	122(2)	C(70)-C(71)-C(72)	118(3)
C(67)-C(72)-C(71)	120(3)	C(67)-C(72)-O(4)	114(2)
C(71)-C(72)-O(4)	126(2)	O(5)-C(73)-C(78)	116.5(18)
O(5)-C(73)-C(74)	123.6(16)	C(78)-C(73)-C(74)	120(2)
C(73)-C(74)-C(75)	119.4(17)	C(76)-C(75)-C(74)	117.8(19)
C(75)-C(76)-C(77)	122(2)	C(78)-C(77)-C(76)	119.0(17)
O(6)-C(78)-C(73)	115.0(18)	O(6)-C(78)-C(77)	123.6(15)
C(73)-C(78)-C(77)	121.3(19)	O(8)-As(2)-O(7)	88.1(6)
O(8)-As(2)-O(9)	88.2(5)	O(7)-As(2)-O(9)	95.6(5)
O(8)-As(2)-O(11)	90.2(6)	O(7)-As(2)-O(11)	175.3(5)
O(9)-As(2)-O(11)	88.8(5)	O(8)-As(2)-O(12)	93.1(5)
O(7)-As(2)-O(12)	87.5(5)	O(9)-As(2)-O(12)	176.8(5)
O(11)-As(2)-O(12)	88.2(5)	O(8)-As(2)-O(10)	175.1(6)
O(7)-As(2)-O(10)	88.4(5)	O(9)-As(2)-O(10)	88.7(5)
O(11)-As(2)-O(10)	93.6(5)	O(12)-As(2)-O(10)	90.3(5)
C(79)-O(7)-As(2)	108.0(11)	C(84)-O(8)-As(2)	111.1(11)
C(85)-O(9)-As(2)	110.1(10)	C(90)-O(10)-As(2)	109.9(10)
C(91)-O(11)-As(2)	110.2(11)	C(96)-O(12)-As(2)	110.9(10)
C(84)-C(79)-O(7)	118.6(18)	C(84)-C(79)-C(80)	119.9(18)
O(7)-C(79)-C(80)	121.6(18)	C(81)-C(80)-C(79)	119(2)
C(82)-C(81)-C(80)	120(2)	C(83)-C(82)-C(81)	120(2)
C(82)-C(83)-C(84)	121(2)	C(79)-C(84)-C(83)	121(2)
C(79)-C(84)-O(8)	114.1(17)	C(83)-C(84)-O(8)	125.4(19)
O(9)-C(85)-C(86)	123.9(16)	O(9)-C(85)-C(90)	116.6(15)

C(86)-C(85)-C(90)	119.5(17)	C(85)-C(86)-C(87)	117.5(17)
C(88)-C(87)-C(86)	121.5(17)	C(87)-C(88)-C(89)	121.3(18)
C(90)-C(89)-C(88)	117.6(17)	C(89)-C(90)-O(10)	123.3(16)
C(89)-C(90)-C(85)	122.5(17)	O(10)-C(90)-C(85)	114.1(15)
O(11)-C(91)-C(92)	122.6(16)	O(11)-C(91)-C(96)	115.5(15)
C(92)-C(91)-C(96)	121.9(16)	C(91)-C(92)-C(93)	114.6(17)
C(92)-C(93)-C(94)	125.2(17)	C(95)-C(94)-C(93)	118.0(17)
C(94)-C(95)-C(96)	121.5(18)	O(12)-C(96)-C(95)	126.6(16)
O(12)-C(96)-C(91)	114.6(15)	C(95)-C(96)-C(91)	118.9(16)
O(14)-As(3)-O(13)	88.7(6)	O(14)-As(3)-O(15)	176.2(5)
O(13)-As(3)-O(15)	87.7(5)	O(14)-As(3)-O(17)	93.6(5)
O(13)-As(3)-O(17)	91.2(5)	O(15)-As(3)-O(17)	87.7(5)
O(14)-As(3)-O(16)	91.2(6)	O(13)-As(3)-O(16)	94.1(5)
O(15)-As(3)-O(16)	87.9(5)	O(17)-As(3)-O(16)	173.0(5)
O(14)-As(3)-O(18)	89.1(5)	O(13)-As(3)-O(18)	177.5(6)
O(15)-As(3)-O(18)	94.6(5)	O(17)-As(3)-O(18)	87.8(5)
O(16)-As(3)-O(18)	87.2(5)	C(97)-O(13)-As(3)	111.6(12)
C(102)-O(14)-As(3)	108.9(12)	C(103)-O(15)-As(3)	110.5(10)
C(108)-O(16)-As(3)	111.2(10)	C(109)-O(17)-As(3)	110.4(10)
C(114)-O(18)-As(3)	108.9(11)	O(13)-C(97)-C(102)	112.8(17)
O(13)-C(97)-C(98)	125(2)	C(102)-C(97)-C(98)	122.4(19)
C(99)-C(98)-C(97)	117(2)	C(98)-C(99)-C(100)	123(2)
C(99)-C(100)-C(101)	121(2)	C(100)-C(101)-C(102)	116(2)
O(14)-C(102)-C(97)	117.9(17)	O(14)-C(102)-C(101)	121.2(19)
C(97)-C(102)-C(101)	120.9(18)	O(15)-C(103)-C(104)	124.9(16)
O(15)-C(103)-C(108)	115.9(16)	C(104)-C(103)-C(108)	119.3(17)
C(103)-C(104)-C(105)	119.8(17)	C(106)-C(105)-C(104)	118.8(19)
C(107)-C(106)-C(105)	124.0(18)	C(106)-C(107)-C(108)	116.6(18)
O(16)-C(108)-C(103)	114.1(15)	O(16)-C(108)-C(107)	124.3(16)
C(103)-C(108)-C(107)	121.5(18)	O(17)-C(109)-C(110)	124.9(16)
O(17)-C(109)-C(114)	113.1(16)	C(110)-C(109)-C(114)	121.9(18)
C(109)-C(110)-C(111)	119.7(19)	C(112)-C(111)-C(110)	118(2)
C(111)-C(112)-C(113)	124(2)	C(114)-C(113)-C(112)	115.4(19)
O(18)-C(114)-C(113)	120.1(17)	O(18)-C(114)-C(109)	118.5(16)
C(113)-C(114)-C(109)	121.3(19)	O(23)-As(4)-O(19)	88.5(5)
O(23)-As(4)-O(24)	88.8(5)	O(19)-As(4)-O(24)	95.1(6)
O(23)-As(4)-O(22)	96.0(5)	O(19)-As(4)-O(22)	173.9(5)
O(24)-As(4)-O(22)	89.2(5)	O(23)-As(4)-O(21)	88.4(5)
O(19)-As(4)-O(21)	89.4(6)	O(24)-As(4)-O(21)	174.7(5)
O(22)-As(4)-O(21)	86.6(5)	O(23)-As(4)-O(20)	176.9(6)
O(19)-As(4)-O(20)	88.6(6)	O(24)-As(4)-O(20)	90.3(5)
O(22)-As(4)-O(20)	87.0(5)	O(21)-As(4)-O(20)	92.7(5)
C(115)-O(19)-As(4)	109.6(12)	C(120)-O(20)-As(4)	111.3(12)
C(121)-O(21)-As(4)	111.4(10)	C(126)-O(22)-As(4)	110.7(10)
C(127)-O(23)-As(4)	110.5(10)	C(132)-O(24)-As(4)	108.9(10)
C(120)-C(115)-C(116)	123.1(19)	C(120)-C(115)-O(19)	115.8(17)

C(116)-C(115)-O(19)	121.0(18)	C(115)-C(116)-C(117)	117(2)
C(118)-C(117)-C(116)	120(2)	C(117)-C(118)-C(119)	121(2)
C(120)-C(119)-C(118)	120(2)	C(119)-C(120)-O(20)	127(2)
C(119)-C(120)-C(115)	118.9(19)	O(20)-C(120)-C(115)	114.5(17)
C(122)-C(121)-C(126)	121.5(19)	C(122)-C(121)-O(21)	124.5(17)
C(126)-C(121)-O(21)	114.0(16)	C(123)-C(122)-C(121)	117.4(18)
C(122)-C(123)-C(124)	123.8(19)	C(123)-C(124)-C(125)	118.9(19)
C(126)-C(125)-C(124)	117.5(17)	C(121)-C(126)-O(22)	116.2(17)
C(121)-C(126)-C(125)	120.8(17)	O(22)-C(126)-C(125)	123.0(15)
C(128)-C(127)-O(23)	123.8(16)	C(128)-C(127)-C(132)	123.2(18)
O(23)-C(127)-C(132)	112.9(15)	C(127)-C(128)-C(129)	117.6(18)
C(128)-C(129)-C(130)	120.5(18)	C(131)-C(130)-C(129)	120.8(19)
C(130)-C(131)-C(132)	118.2(17)	O(24)-C(132)-C(127)	116.4(16)
O(24)-C(132)-C(131)	124.1(15)	C(127)-C(132)-C(131)	119.5(17)
N(1S)-C(1S)-C(2S)	175(3)	N(2S)-C(3S)-C(4S)	161(3)
N(3S)-C(5S)-C(6S)	154(4)	N(4S)-C(7S)-C(8S)	167(5)

Symmetry transformations used to generate equivalent atoms:

Table 6. Torsion angles [°] for nd1014z_x.

atom-atom-atom-atom	angle	atom-atom-atom-atom	angle
C(6)-N(1)-C(2)-C(3)	-2(3)	Cu(1)-N(1)-C(2)-C(3)	179.2(13)
C(6)-N(1)-C(2)-C(1)	178.9(16)	Cu(1)-N(1)-C(2)-C(1)	0(3)
N(1)-C(2)-C(3)-C(4)	0(3)	C(1)-C(2)-C(3)-C(4)	178.9(18)
C(2)-C(3)-C(4)-C(5)	0(3)	C(3)-C(4)-C(5)-C(7)	-178(2)
C(3)-C(4)-C(5)-C(6)	2(3)	C(2)-N(1)-C(6)-C(5)	4(3)
Cu(1)-N(1)-C(6)-C(5)	-176.7(15)	C(2)-N(1)-C(6)-C(10)	-178.0(17)
Cu(1)-N(1)-C(6)-C(10)	1(2)	C(7)-C(5)-C(6)-N(1)	175.7(18)
C(4)-C(5)-C(6)-N(1)	-4(3)	C(7)-C(5)-C(6)-C(10)	-2(3)
C(4)-C(5)-C(6)-C(10)	178.2(18)	C(6)-C(5)-C(7)-C(8)	2(3)
C(4)-C(5)-C(7)-C(8)	-179(2)	C(5)-C(7)-C(8)-C(9)	1(3)
C(7)-C(8)-C(9)-C(10)	-2(3)	C(7)-C(8)-C(9)-C(11)	-179(2)
C(13)-N(2)-C(10)-C(9)	2(3)	Cu(1)-N(2)-C(10)-C(9)	174.8(15)
C(13)-N(2)-C(10)-C(6)	-178.9(16)	Cu(1)-N(2)-C(10)-C(6)	-6(2)
C(8)-C(9)-C(10)-N(2)	-179.5(18)	C(11)-C(9)-C(10)-N(2)	-2(3)
C(8)-C(9)-C(10)-C(6)	2(3)	C(11)-C(9)-C(10)-C(6)	178.7(18)
N(1)-C(6)-C(10)-N(2)	4(3)	C(5)-C(6)-C(10)-N(2)	-178.5(17)
N(1)-C(6)-C(10)-C(9)	-177.4(17)	C(5)-C(6)-C(10)-C(9)	0(3)
C(10)-C(9)-C(11)-C(12)	2(3)	C(8)-C(9)-C(11)-C(12)	179.1(19)
C(9)-C(11)-C(12)-C(13)	-2(3)	C(10)-N(2)-C(13)-C(12)	-2(3)
Cu(1)-N(2)-C(13)-C(12)	-172.6(13)	C(10)-N(2)-C(13)-C(14)	177.3(16)
Cu(1)-N(2)-C(13)-C(14)	6(3)	C(11)-C(12)-C(13)-N(2)	1(3)
C(11)-C(12)-C(13)-C(14)	-177.4(17)	N(2)-C(13)-C(14)-C(15)	112.1(18)
C(12)-C(13)-C(14)-C(15)	-69(2)	C(13)-C(14)-C(15)-C(16)	164.8(14)
C(14)-C(15)-C(16)-C(17)	63.5(18)	C(21)-N(7)-C(17)-C(18)	-1(2)
Cu(2)-N(7)-C(17)-C(18)	-179.0(11)	C(21)-N(7)-C(17)-C(16)	178.2(13)
Cu(2)-N(7)-C(17)-C(16)	0(2)	C(15)-C(16)-C(17)-N(7)	86.8(18)
C(15)-C(16)-C(17)-C(18)	-94.0(18)	N(7)-C(17)-C(18)-C(19)	2(2)
C(16)-C(17)-C(18)-C(19)	-176.9(14)	C(17)-C(18)-C(19)-C(20)	-1(2)
C(18)-C(19)-C(20)-C(22)	178.3(15)	C(18)-C(19)-C(20)-C(21)	-2(2)
C(17)-N(7)-C(21)-C(20)	-2(2)	Cu(2)-N(7)-C(21)-C(20)	176.4(13)
C(17)-N(7)-C(21)-C(25)	-177.2(13)	Cu(2)-N(7)-C(21)-C(25)	1.1(17)
C(22)-C(20)-C(21)-N(7)	-176.8(15)	C(19)-C(20)-C(21)-N(7)	3(2)
C(22)-C(20)-C(21)-C(25)	-2(2)	C(19)-C(20)-C(21)-C(25)	178.6(13)
C(21)-C(20)-C(22)-C(23)	0(2)	C(19)-C(20)-C(22)-C(23)	179.6(15)
C(20)-C(22)-C(23)-C(24)	-1(2)	C(22)-C(23)-C(24)-C(26)	-178.8(15)
C(22)-C(23)-C(24)-C(25)	4(2)	C(28)-N(8)-C(25)-C(24)	-1(2)
Cu(2)-N(8)-C(25)-C(24)	179.4(12)	C(28)-N(8)-C(25)-C(21)	-178.3(14)
Cu(2)-N(8)-C(25)-C(21)	1.9(17)	C(26)-C(24)-C(25)-N(8)	-1(2)
C(23)-C(24)-C(25)-N(8)	176.8(14)	C(26)-C(24)-C(25)-C(21)	176.7(14)
C(23)-C(24)-C(25)-C(21)	-6(2)	N(7)-C(21)-C(25)-N(8)	-2(2)
C(20)-C(21)-C(25)-N(8)	-177.8(14)	N(7)-C(21)-C(25)-C(24)	-179.7(14)
C(20)-C(21)-C(25)-C(24)	5(2)	C(25)-C(24)-C(26)-C(27)	1(2)

C(23)-C(24)-C(26)-C(27)	-176.8(15)	C(24)-C(26)-C(27)-C(28)	1(2)
C(25)-N(8)-C(28)-C(27)	2(2)	Cu(2)-N(8)-C(28)-C(27)	-177.8(12)
C(25)-N(8)-C(28)-C(29)	-177.2(15)	Cu(2)-N(8)-C(28)-C(29)	3(2)
C(26)-C(27)-C(28)-N(8)	-3(3)	C(26)-C(27)-C(28)-C(29)	177.0(16)
C(35)-N(5)-C(31)-C(32)	0(2)	Cu(1)-N(5)-C(31)-C(32)	-172.5(11)
C(35)-N(5)-C(31)-C(30)	-179.9(13)	Cu(1)-N(5)-C(31)-C(30)	8(2)
N(5)-C(31)-C(32)-C(33)	-1(2)	C(30)-C(31)-C(32)-C(33)	178.7(15)
C(31)-C(32)-C(33)-C(34)	-2(2)	C(32)-C(33)-C(34)-C(35)	6(2)
C(32)-C(33)-C(34)-C(36)	-176.1(15)	C(31)-N(5)-C(35)-C(34)	5(2)
Cu(1)-N(5)-C(35)-C(34)	178.4(12)	C(31)-N(5)-C(35)-C(39)	-178.0(13)
Cu(1)-N(5)-C(35)-C(39)	-4.1(16)	C(33)-C(34)-C(35)-N(5)	-8(2)
C(36)-C(34)-C(35)-N(5)	174.4(14)	C(33)-C(34)-C(35)-C(39)	175.0(14)
C(36)-C(34)-C(35)-C(39)	-3(2)	C(35)-C(34)-C(36)-C(37)	1(2)
C(33)-C(34)-C(36)-C(37)	-176.6(15)	C(34)-C(36)-C(37)-C(38)	2(2)
C(36)-C(37)-C(38)-C(39)	-3(2)	C(36)-C(37)-C(38)-C(40)	176.9(16)
C(42)-N(6)-C(39)-C(38)	-1(2)	Cu(1)-N(6)-C(39)-C(38)	178.3(12)
C(42)-N(6)-C(39)-C(35)	179.9(13)	Cu(1)-N(6)-C(39)-C(35)	-0.6(16)
C(40)-C(38)-C(39)-N(6)	2(2)	C(37)-C(38)-C(39)-N(6)	-178.0(14)
C(40)-C(38)-C(39)-C(35)	-178.7(14)	C(37)-C(38)-C(39)-C(35)	1(2)
N(5)-C(35)-C(39)-N(6)	3(2)	C(34)-C(35)-C(39)-N(6)	-179.1(13)
N(5)-C(35)-C(39)-C(38)	-175.7(14)	C(34)-C(35)-C(39)-C(38)	2(2)
C(39)-C(38)-C(40)-C(41)	-2(2)	C(37)-C(38)-C(40)-C(41)	178.5(15)
C(38)-C(40)-C(41)-C(42)	0(2)	C(39)-N(6)-C(42)-C(41)	0(2)
Cu(1)-N(6)-C(42)-C(41)	-179.9(11)	C(39)-N(6)-C(42)-C(43)	177.5(12)
Cu(1)-N(6)-C(42)-C(43)	-1.9(19)	C(40)-C(41)-C(42)-N(6)	1(2)
C(40)-C(41)-C(42)-C(43)	-177.0(14)	N(6)-C(42)-C(43)-C(44)	84.6(17)
C(41)-C(42)-C(43)-C(44)	-97.5(17)	C(42)-C(43)-C(44)-C(45)	67.7(17)
C(43)-C(44)-C(45)-C(46)	172.4(13)	C(50)-N(3)-C(46)-C(47)	3(2)
Cu(2)-N(3)-C(46)-C(47)	-176.8(12)	C(50)-N(3)-C(46)-C(45)	-179.0(14)
Cu(2)-N(3)-C(46)-C(45)	1(2)	C(44)-C(45)-C(46)-N(3)	116.2(17)
C(44)-C(45)-C(46)-C(47)	-65.5(19)	N(3)-C(46)-C(47)-C(48)	-3(3)
C(45)-C(46)-C(47)-C(48)	179.0(15)	C(46)-C(47)-C(48)-C(49)	1(3)
C(47)-C(48)-C(49)-C(50)	1(2)	C(47)-C(48)-C(49)-C(51)	178.3(16)
C(46)-N(3)-C(50)-C(49)	-1(2)	Cu(2)-N(3)-C(50)-C(49)	178.5(13)
C(46)-N(3)-C(50)-C(54)	-176.3(14)	Cu(2)-N(3)-C(50)-C(54)	3.3(17)
C(48)-C(49)-C(50)-N(3)	-1(2)	C(51)-C(49)-C(50)-N(3)	-178.3(15)
C(48)-C(49)-C(50)-C(54)	174.3(15)	C(51)-C(49)-C(50)-C(54)	-3(2)
C(50)-C(49)-C(51)-C(52)	2(2)	C(48)-C(49)-C(51)-C(52)	-175.7(16)
C(49)-C(51)-C(52)-C(53)	2(3)	C(51)-C(52)-C(53)-C(55)	178.7(17)
C(51)-C(52)-C(53)-C(54)	-4(3)	C(57)-N(4)-C(54)-C(50)	-178.1(14)
Cu(2)-N(4)-C(54)-C(50)	-0.2(18)	C(57)-N(4)-C(54)-C(53)	3(2)
Cu(2)-N(4)-C(54)-C(53)	-179.0(12)	N(3)-C(50)-C(54)-N(4)	-2(2)
C(49)-C(50)-C(54)-N(4)	-177.3(15)	N(3)-C(50)-C(54)-C(53)	176.6(14)
C(49)-C(50)-C(54)-C(53)	1(2)	C(55)-C(53)-C(54)-N(4)	-1(2)
C(52)-C(53)-C(54)-N(4)	-179.3(15)	C(55)-C(53)-C(54)-C(50)	179.9(14)
C(52)-C(53)-C(54)-C(50)	2(2)	C(52)-C(53)-C(55)-C(56)	-179.3(16)

C(54)-C(53)-C(55)-C(56)	3(2)	C(53)-C(55)-C(56)-C(57)	-6(2)
C(54)-N(4)-C(57)-C(56)	-7(2)	Cu(2)-N(4)-C(57)-C(56)	176.0(12)
C(54)-N(4)-C(57)-C(58)	174.8(15)	Cu(2)-N(4)-C(57)-C(58)	-3(2)
C(55)-C(56)-C(57)-N(4)	8(2)	C(55)-C(56)-C(57)-C(58)	-173.4(16)
C(6A)-N(9)-C(2A)-C(3A)	-3(2)	Cu(3)-N(9)-C(2A)-C(3A)	-180.0(12)
C(6A)-N(9)-C(2A)-C(1A)	177.5(15)	Cu(3)-N(9)-C(2A)-C(1A)	1(2)
N(9)-C(2A)-C(3A)-C(4A)	-1(3)	C(1A)-C(2A)-C(3A)-C(4A)	178.2(18)
C(2A)-C(3A)-C(4A)-C(5A)	3(3)	C(3A)-C(4A)-C(5A)-C(6A)	-1(3)
C(3A)-C(4A)-C(5A)-C(7A)	175.7(17)	C(2A)-N(9)-C(6A)-C(5A)	5(2)
Cu(3)-N(9)-C(6A)-C(5A)	-177.2(13)	C(2A)-N(9)-C(6A)-C(10A)	-178.7(15)
Cu(3)-N(9)-C(6A)-C(10A)	-1.3(18)	C(4A)-C(5A)-C(6A)-N(9)	-3(3)
C(7A)-C(5A)-C(6A)-N(9)	179.7(15)	C(4A)-C(5A)-C(6A)-C(10A)	-179.1(17)
C(7A)-C(5A)-C(6A)-C(10A)	4(3)	C(4A)-C(5A)-C(7A)-C(8A)	-177.3(18)
C(6A)-C(5A)-C(7A)-C(8A)	-1(3)	C(5A)-C(7A)-C(8A)-C(9A)	-6(3)
C(7A)-C(8A)-C(9A)-C(10A)	9(3)	C(7A)-C(8A)-C(9A)-C(11A)	-175.8(19)
C(11A)-C(9A)-C(10A)-N(10)	-1(3)	C(8A)-C(9A)-C(10A)-N(10)	175.2(16)
C(11A)-C(9A)-C(10A)-C(6A)	179.0(16)	C(8A)-C(9A)-C(10A)-C(6A)	-5(3)
C(13A)-N(10)-C(10A)-C(9A)	1(3)	Cu(3)-N(10)-C(10A)-C(9A)	177.1(14)
C(13A)-N(10)-C(10A)-C(6A)	-178.8(16)	Cu(3)-N(10)-C(10A)-C(6A)	-2.6(19)
N(9)-C(6A)-C(10A)-C(9A)	-177.0(16)	C(5A)-C(6A)-C(10A)-C(9A)	-1(3)
N(9)-C(6A)-C(10A)-N(10)	3(2)	C(5A)-C(6A)-C(10A)-N(10)	178.6(16)
C(10A)-C(9A)-C(11A)-C(12A)	-2(3)	C(8A)-C(9A)-C(11A)-C(12A)	-177.4(19)
C(9A)-C(11A)-C(12A)-C(13A)	4(3)	C(10A)-N(10)-C(13A)-C(12A)	1(3)
Cu(3)-N(10)-C(13A)-C(12A)	-173.8(13)	C(10A)-N(10)-C(13A)-C(14A)	-178.8(15)
Cu(3)-N(10)-C(13A)-C(14A)	6(3)	C(11A)-C(12A)-C(13A)-N(10)	-4(3)
C(11A)-C(12A)-C(13A)-C(14A)	176.2(18)	N(10)-C(13A)-C(14A)-C(15A)	121.1(18)
C(12A)-C(13A)-C(14A)-C(15A)	-59(2)	C(13A)-C(14A)-C(15A)-C(16A)	166.9(14)
C(14A)-C(15A)-C(16A)-C(17A)	61.1(18)	C(21A)-N(11)-C(17A)-C(18A)	0(2)
Cu(4)-N(11)-C(17A)-C(18A)	179.9(11)	C(21A)-N(11)-C(17A)-C(16A)	177.9(14)
Cu(4)-N(11)-C(17A)-C(16A)	-2(2)	C(15A)-C(16A)-C(17A)-N(11)	88.2(18)
C(15A)-C(16A)-C(17A)-C(18A)	-93.8(18)	N(11)-C(17A)-C(18A)-C(19A)	0(2)
C(16A)-C(17A)-C(18A)-C(19A)	-177.6(15)	C(17A)-C(18A)-C(19A)-C(20A)	0(2)
C(18A)-C(19A)-C(20A)-C(21A)	-1(2)	C(18A)-C(19A)-C(20A)-C(22A)	178.7(15)
C(19A)-C(20A)-C(21A)-N(11)	2(2)	C(22A)-C(20A)-C(21A)-N(11)	-178.4(14)
C(19A)-C(20A)-C(21A)-C(25A)	179.8(14)	C(22A)-C(20A)-C(21A)-C(25A)	0(2)
C(17A)-N(11)-C(21A)-C(20A)	-1(2)	Cu(4)-N(11)-C(21A)-C(20A)	179.1(12)
C(17A)-N(11)-C(21A)-C(25A)	-179.1(14)	Cu(4)-N(11)-C(21A)-C(25A)	1.0(17)
C(21A)-C(20A)-C(22A)-C(23A)	-1(2)	C(19A)-C(20A)-C(22A)-C(23A)	178.7(16)
C(20A)-C(22A)-C(23A)-C(24A)	1(2)	C(22A)-C(23A)-C(24A)-C(25A)	1(2)
C(22A)-C(23A)-C(24A)-C(26A)	179.6(15)	C(28A)-N(12)-C(25A)-C(24A)	1(2)
Cu(4)-N(12)-C(25A)-C(24A)	177.0(12)	C(28A)-N(12)-C(25A)-C(21A)	177.3(14)
Cu(4)-N(12)-C(25A)-C(21A)	-7.2(17)	C(26A)-C(24A)-C(25A)-N(12)	-5(2)
C(23A)-C(24A)-C(25A)-N(12)	173.4(14)	C(26A)-C(24A)-C(25A)-C(21A)	178.8(14)
C(23A)-C(24A)-C(25A)-C(21A)	-2(2)	C(20A)-C(21A)-C(25A)-N(12)	-173.9(14)
N(11)-C(21A)-C(25A)-N(12)	4(2)	C(20A)-C(21A)-C(25A)-C(24A)	2(2)
N(11)-C(21A)-C(25A)-C(24A)	-179.7(14)	C(25A)-C(24A)-C(26A)-C(27A)	5(2)

C(23A)-C(24A)-C(26A)-C(27A)	-173.9(15)	C(24A)-C(26A)-C(27A)-C(28A)	-1(2)
C(25A)-N(12)-C(28A)-C(27A)	3(2)	Cu(4)-N(12)-C(28A)-C(27A)	-171.2(12)
C(25A)-N(12)-C(28A)-C(29A)	-175.4(15)	Cu(4)-N(12)-C(28A)-C(29A)	10(2)
C(26A)-C(27A)-C(28A)-N(12)	-4(3)	C(26A)-C(27A)-C(28A)-C(29A)	174.9(17)
C(35A)-N(13)-C(31A)-C(32A)	5(3)	Cu(3)-N(13)-C(31A)-C(32A)	179.5(14)
C(35A)-N(13)-C(31A)-C(30A)	-176.7(16)	Cu(3)-N(13)-C(31A)-C(30A)	-2(2)
N(13)-C(31A)-C(32A)-C(33A)	-1(3)	C(30A)-C(31A)-C(32A)-C(33A)	-179.5(18)
C(31A)-C(32A)-C(33A)-C(34A)	-3(3)	C(32A)-C(33A)-C(34A)-C(35A)	3(3)
C(32A)-C(33A)-C(34A)-C(36A)	-173.1(17)	C(31A)-N(13)-C(35A)-C(34A)	-5(3)
Cu(3)-N(13)-C(35A)-C(34A)	179.4(14)	C(31A)-N(13)-C(35A)-C(39A)	174.9(15)
Cu(3)-N(13)-C(35A)-C(39A)	-0.7(19)	C(33A)-C(34A)-C(35A)-N(13)	1(3)
C(36A)-C(34A)-C(35A)-N(13)	177.0(16)	C(33A)-C(34A)-C(35A)-C(39A)	-178.7(16)
C(36A)-C(34A)-C(35A)-C(39A)	-3(3)	C(35A)-C(34A)-C(36A)-C(37A)	2(3)
C(33A)-C(34A)-C(36A)-C(37A)	177.8(18)	C(34A)-C(36A)-C(37A)-C(38A)	-1(3)
C(36A)-C(37A)-C(38A)-C(39A)	1(3)	C(36A)-C(37A)-C(38A)-C(40A)	178.5(17)
C(42A)-N(14)-C(39A)-C(38A)	-2(2)	Cu(3)-N(14)-C(39A)-C(38A)	177.8(14)
C(42A)-N(14)-C(39A)-C(35A)	-178.5(14)	Cu(3)-N(14)-C(39A)-C(35A)	1.2(18)
C(37A)-C(38A)-C(39A)-N(14)	-178.4(16)	C(40A)-C(38A)-C(39A)-N(14)	4(2)
C(37A)-C(38A)-C(39A)-C(35A)	-2(2)	C(40A)-C(38A)-C(39A)-C(35A)	-179.3(15)
N(13)-C(35A)-C(39A)-N(14)	0(2)	C(34A)-C(35A)-C(39A)-N(14)	179.6(15)
N(13)-C(35A)-C(39A)-C(38A)	-177.2(15)	C(34A)-C(35A)-C(39A)-C(38A)	3(2)
C(37A)-C(38A)-C(40A)-C(41A)	179.5(17)	C(39A)-C(38A)-C(40A)-C(41A)	-3(2)
C(38A)-C(40A)-C(41A)-C(42A)	0(3)	C(39A)-N(14)-C(42A)-C(41A)	-2(2)
Cu(3)-N(14)-C(42A)-C(41A)	178.8(12)	C(39A)-N(14)-C(42A)-C(43A)	179.0(14)
Cu(3)-N(14)-C(42A)-C(43A)	-1(2)	C(40A)-C(41A)-C(42A)-N(14)	2(3)
C(40A)-C(41A)-C(42A)-C(43A)	-178.2(16)	N(14)-C(42A)-C(43A)-C(44A)	86.7(19)
C(41A)-C(42A)-C(43A)-C(44A)	-92.8(19)	C(42A)-C(43A)-C(44A)-C(45A)	64(2)
C(43A)-C(44A)-C(45A)-C(46A)	164.8(16)	C(50A)-N(15)-C(46A)-C(47A)	3(4)
Cu(4)-N(15)-C(46A)-C(47A)	-173.0(16)	C(50A)-N(15)-C(46A)-C(45A)	-175(2)
Cu(4)-N(15)-C(46A)-C(45A)	9(3)	C(44A)-C(45A)-C(46A)-N(15)	117(2)
C(44A)-C(45A)-C(46A)-C(47A)	-61(3)	N(15)-C(46A)-C(47A)-C(48A)	1(4)
C(45A)-C(46A)-C(47A)-C(48A)	179(2)	C(46A)-C(47A)-C(48A)-C(49A)	-7(4)
C(47A)-C(48A)-C(49A)-C(50A)	10(5)	C(47A)-C(48A)-C(49A)-C(51A)	-173(3)
C(46A)-N(15)-C(50A)-C(49A)	0(4)	Cu(4)-N(15)-C(50A)-C(49A)	176(2)
C(46A)-N(15)-C(50A)-C(54A)	-179(2)	Cu(4)-N(15)-C(50A)-C(54A)	-3(3)
C(48A)-C(49A)-C(50A)-N(15)	-6(4)	C(51A)-C(49A)-C(50A)-N(15)	177(2)
C(48A)-C(49A)-C(50A)-C(54A)	173(3)	C(51A)-C(49A)-C(50A)-C(54A)	-4(4)
C(50A)-C(49A)-C(51A)-C(52A)	1(4)	C(48A)-C(49A)-C(51A)-C(52A)	-176(3)
C(49A)-C(51A)-C(52A)-C(53A)	0(5)	C(51A)-C(52A)-C(53A)-C(55A)	178(3)
C(51A)-C(52A)-C(53A)-C(54A)	2(5)	C(57A)-N(16)-C(54A)-C(50A)	-179(3)
Cu(4)-N(16)-C(54A)-C(50A)	-5(3)	C(57A)-N(16)-C(54A)-C(53A)	2(4)
Cu(4)-N(16)-C(54A)-C(53A)	175(2)	N(15)-C(50A)-C(54A)-N(16)	5(4)
C(49A)-C(50A)-C(54A)-N(16)	-174(3)	N(15)-C(50A)-C(54A)-C(53A)	-175(2)
C(49A)-C(50A)-C(54A)-C(53A)	6(4)	C(52A)-C(53A)-C(54A)-N(16)	175(3)
C(55A)-C(53A)-C(54A)-N(16)	-2(4)	C(52A)-C(53A)-C(54A)-C(50A)	-5(4)
C(55A)-C(53A)-C(54A)-C(50A)	178(3)	C(52A)-C(53A)-C(55A)-C(56A)	-175(3)

C(54A)-C(53A)-C(55A)-C(56A)	1(4)	C(53A)-C(55A)-C(56A)-C(57A)	0(4)
C(54A)-N(16)-C(57A)-C(56A)	0(4)	Cu(4)-N(16)-C(57A)-C(56A)	-172.6(19)
C(54A)-N(16)-C(57A)-C(58A)	-180(2)	Cu(4)-N(16)-C(57A)-C(58A)	8(4)
C(55A)-C(56A)-C(57A)-N(16)	-1(4)	C(55A)-C(56A)-C(57A)-C(58A)	179(3)
O(5)-As(1)-O(1)-C(61)	102.7(14)	O(4)-As(1)-O(1)-C(61)	-166.5(14)
O(3)-As(1)-O(1)-C(61)	-79.3(14)	O(2)-As(1)-O(1)-C(61)	7.4(14)
O(5)-As(1)-O(2)-C(66)	-97.2(12)	O(6)-As(1)-O(2)-C(66)	174.4(12)
O(3)-As(1)-O(2)-C(66)	84.6(12)	O(1)-As(1)-O(2)-C(66)	-8.5(12)
O(6)-As(1)-O(3)-C(67)	105.5(13)	O(4)-As(1)-O(3)-C(67)	10.3(13)
O(1)-As(1)-O(3)-C(67)	-77.4(13)	O(2)-As(1)-O(3)-C(67)	-165.3(13)
O(5)-As(1)-O(4)-C(72)	171.0(13)	O(6)-As(1)-O(4)-C(72)	-100.4(13)
O(3)-As(1)-O(4)-C(72)	-10.9(13)	O(1)-As(1)-O(4)-C(72)	82.2(14)
O(6)-As(1)-O(5)-C(73)	-10.5(12)	O(4)-As(1)-O(5)-C(73)	84.6(12)
O(1)-As(1)-O(5)-C(73)	172.5(12)	O(2)-As(1)-O(5)-C(73)	-99.6(12)
O(5)-As(1)-O(6)-C(78)	11.1(11)	O(4)-As(1)-O(6)-C(78)	-79.5(12)
O(3)-As(1)-O(6)-C(78)	-166.8(11)	O(2)-As(1)-O(6)-C(78)	106.4(11)
As(1)-O(1)-C(61)-C(62)	174.2(17)	As(1)-O(1)-C(61)-C(66)	-4(2)
O(1)-C(61)-C(62)-C(63)	-180(2)	C(66)-C(61)-C(62)-C(63)	-1(3)
C(61)-C(62)-C(63)-C(64)	0(3)	C(62)-C(63)-C(64)-C(65)	1(3)
C(63)-C(64)-C(65)-C(66)	-2(3)	C(64)-C(65)-C(66)-O(2)	-177.1(18)
C(64)-C(65)-C(66)-C(61)	1(3)	As(1)-O(2)-C(66)-C(65)	-173.8(17)
As(1)-O(2)-C(66)-C(61)	8(2)	O(1)-C(61)-C(66)-C(65)	179.4(18)
C(62)-C(61)-C(66)-C(65)	1(3)	O(1)-C(61)-C(66)-O(2)	-3(3)
C(62)-C(61)-C(66)-O(2)	178.7(19)	As(1)-O(3)-C(67)-C(72)	-7(2)
As(1)-O(3)-C(67)-C(68)	172.6(17)	O(3)-C(67)-C(68)-C(69)	-175.5(19)
C(72)-C(67)-C(68)-C(69)	4(3)	C(67)-C(68)-C(69)-C(70)	-3(4)
C(68)-C(69)-C(70)-C(71)	4(4)	C(69)-C(70)-C(71)-C(72)	-6(4)
O(3)-C(67)-C(72)-C(71)	173(2)	C(68)-C(67)-C(72)-C(71)	-7(4)
O(3)-C(67)-C(72)-O(4)	-2(3)	C(68)-C(67)-C(72)-O(4)	179(2)
C(70)-C(71)-C(72)-C(67)	7(4)	C(70)-C(71)-C(72)-O(4)	-178(2)
As(1)-O(4)-C(72)-C(67)	10(2)	As(1)-O(4)-C(72)-C(71)	-165(2)
As(1)-O(5)-C(73)-C(78)	8(2)	As(1)-O(5)-C(73)-C(74)	-169.8(15)
O(5)-C(73)-C(74)-C(75)	175.9(17)	C(78)-C(73)-C(74)-C(75)	-2(3)
C(73)-C(74)-C(75)-C(76)	4(3)	C(74)-C(75)-C(76)-C(77)	-4(3)
C(75)-C(76)-C(77)-C(78)	0(3)	As(1)-O(6)-C(78)-C(73)	-9.3(19)
As(1)-O(6)-C(78)-C(77)	171.6(15)	O(5)-C(73)-C(78)-O(6)	1(2)
C(74)-C(73)-C(78)-O(6)	178.7(16)	O(5)-C(73)-C(78)-C(77)	-179.9(17)
C(74)-C(73)-C(78)-C(77)	-2(3)	C(76)-C(77)-C(78)-O(6)	-177.7(16)
C(76)-C(77)-C(78)-C(73)	3(3)	O(8)-As(2)-O(7)-C(79)	2.2(11)
O(9)-As(2)-O(7)-C(79)	-85.8(11)	O(12)-As(2)-O(7)-C(79)	95.4(11)
O(10)-As(2)-O(7)-C(79)	-174.3(11)	O(7)-As(2)-O(8)-C(84)	-2.8(11)
O(9)-As(2)-O(8)-C(84)	92.8(11)	O(11)-As(2)-O(8)-C(84)	-178.4(11)
O(12)-As(2)-O(8)-C(84)	-90.2(11)	O(8)-As(2)-O(9)-C(85)	176.8(11)
O(7)-As(2)-O(9)-C(85)	-95.3(11)	O(11)-As(2)-O(9)-C(85)	86.6(11)
O(10)-As(2)-O(9)-C(85)	-7.0(11)	O(7)-As(2)-O(10)-C(90)	102.0(11)
O(9)-As(2)-O(10)-C(90)	6.4(11)	O(11)-As(2)-O(10)-C(90)	-82.3(11)

O(12)-As(2)-O(10)-C(90)	-170.5(11)	O(8)-As(2)-O(11)-C(91)	87.0(10)
O(9)-As(2)-O(11)-C(91)	175.2(10)	O(12)-As(2)-O(11)-C(91)	-6.0(10)
O(10)-As(2)-O(11)-C(91)	-96.2(10)	O(8)-As(2)-O(12)-C(96)	-82.5(11)
O(7)-As(2)-O(12)-C(96)	-170.5(11)	O(11)-As(2)-O(12)-C(96)	7.6(11)
O(10)-As(2)-O(12)-C(96)	101.1(11)	As(2)-O(7)-C(79)-C(84)	-1(2)
As(2)-O(7)-C(79)-C(80)	178.9(14)	C(84)-C(79)-C(80)-C(81)	1(3)
O(7)-C(79)-C(80)-C(81)	-178.9(16)	C(79)-C(80)-C(81)-C(82)	-2(3)
C(80)-C(81)-C(82)-C(83)	2(3)	C(81)-C(82)-C(83)-C(84)	0(3)
O(7)-C(79)-C(84)-C(83)	-179.9(16)	C(80)-C(79)-C(84)-C(83)	0(3)
O(7)-C(79)-C(84)-O(8)	-1(2)	C(80)-C(79)-C(84)-O(8)	178.9(16)
C(82)-C(83)-C(84)-C(79)	0(3)	C(82)-C(83)-C(84)-O(8)	-179.2(18)
As(2)-O(8)-C(84)-C(79)	3(2)	As(2)-O(8)-C(84)-C(83)	-178.3(16)
As(2)-O(9)-C(85)-C(86)	-172.7(14)	As(2)-O(9)-C(85)-C(90)	6.2(19)
O(9)-C(85)-C(86)-C(87)	178.4(16)	C(90)-C(85)-C(86)-C(87)	0(3)
C(85)-C(86)-C(87)-C(88)	0(3)	C(86)-C(87)-C(88)-C(89)	1(3)
C(87)-C(88)-C(89)-C(90)	-1(3)	C(88)-C(89)-C(90)-O(10)	-177.1(15)
C(88)-C(89)-C(90)-C(85)	0(3)	As(2)-O(10)-C(90)-C(89)	172.8(14)
As(2)-O(10)-C(90)-C(85)	-4.5(18)	O(9)-C(85)-C(90)-C(89)	-178.5(16)
C(86)-C(85)-C(90)-C(89)	0(3)	O(9)-C(85)-C(90)-O(10)	-1(2)
C(86)-C(85)-C(90)-O(10)	177.8(15)	As(2)-O(11)-C(91)-C(92)	-174.4(13)
As(2)-O(11)-C(91)-C(96)	3.4(17)	O(11)-C(91)-C(92)-C(93)	178.0(14)
C(96)-C(91)-C(92)-C(93)	0(2)	C(91)-C(92)-C(93)-C(94)	-1(2)
C(92)-C(93)-C(94)-C(95)	-1(3)	C(93)-C(94)-C(95)-C(96)	3(2)
As(2)-O(12)-C(96)-C(95)	171.8(14)	As(2)-O(12)-C(96)-C(91)	-7.4(17)
C(94)-C(95)-C(96)-O(12)	178.0(16)	C(94)-C(95)-C(96)-C(91)	-3(2)
O(11)-C(91)-C(96)-O(12)	3(2)	C(92)-C(91)-C(96)-O(12)	-179.5(15)
O(11)-C(91)-C(96)-C(95)	-176.5(14)	C(92)-C(91)-C(96)-C(95)	1(2)
O(14)-As(3)-O(13)-C(97)	3.8(12)	O(15)-As(3)-O(13)-C(97)	-175.0(12)
O(17)-As(3)-O(13)-C(97)	97.3(12)	O(16)-As(3)-O(13)-C(97)	-87.2(12)
O(13)-As(3)-O(14)-C(102)	-2.9(11)	O(17)-As(3)-O(14)-C(102)	-94.0(11)
O(16)-As(3)-O(14)-C(102)	91.1(11)	O(18)-As(3)-O(14)-C(102)	178.2(11)
O(13)-As(3)-O(15)-C(103)	98.6(10)	O(17)-As(3)-O(15)-C(103)	-170.2(10)
O(16)-As(3)-O(15)-C(103)	4.4(10)	O(18)-As(3)-O(15)-C(103)	-82.6(10)
O(14)-As(3)-O(16)-C(108)	177.9(11)	O(13)-As(3)-O(16)-C(108)	-93.4(11)
O(15)-As(3)-O(16)-C(108)	-5.8(11)	O(18)-As(3)-O(16)-C(108)	88.9(11)
O(14)-As(3)-O(17)-C(109)	-78.3(11)	O(13)-As(3)-O(17)-C(109)	-167.0(11)
O(15)-As(3)-O(17)-C(109)	105.3(11)	O(18)-As(3)-O(17)-C(109)	10.7(11)
O(14)-As(3)-O(18)-C(114)	84.7(11)	O(15)-As(3)-O(18)-C(114)	-96.4(11)
O(17)-As(3)-O(18)-C(114)	-8.9(11)	O(16)-As(3)-O(18)-C(114)	175.9(11)
As(3)-O(13)-C(97)-C(102)	-3.7(19)	As(3)-O(13)-C(97)-C(98)	172.2(15)
O(13)-C(97)-C(98)-C(99)	178.3(17)	C(102)-C(97)-C(98)-C(99)	-6(3)
C(97)-C(98)-C(99)-C(100)	2(3)	C(98)-C(99)-C(100)-C(101)	1(3)
C(99)-C(100)-C(101)-C(102)	0(3)	As(3)-O(14)-C(102)-C(97)	2(2)
As(3)-O(14)-C(102)-C(101)	179.8(15)	O(13)-C(97)-C(102)-O(14)	1(2)
C(98)-C(97)-C(102)-O(14)	-174.6(17)	O(13)-C(97)-C(102)-C(101)	-176.8(17)
C(98)-C(97)-C(102)-C(101)	7(3)	C(100)-C(101)-C(102)-O(14)	178.2(17)

C(100)-C(101)-C(102)-C(97)	-4(3)	As(3)-O(15)-C(103)-C(104)	177.3(14)
As(3)-O(15)-C(103)-C(108)	-2.2(17)	O(15)-C(103)-C(104)-C(105)	-174.5(15)
C(108)-C(103)-C(104)-C(105)	5(2)	C(103)-C(104)-C(105)-C(106)	-2(2)
C(104)-C(105)-C(106)-C(107)	-2(3)	C(105)-C(106)-C(107)-C(108)	2(3)
As(3)-O(16)-C(108)-C(103)	5.9(18)	As(3)-O(16)-C(108)-C(107)	-171.0(14)
O(15)-C(103)-C(108)-O(16)	-2(2)	C(104)-C(103)-C(108)-O(16)	178.0(15)
O(15)-C(103)-C(108)-C(107)	174.5(15)	C(104)-C(103)-C(108)-C(107)	-5(3)
C(106)-C(107)-C(108)-O(16)	178.3(16)	C(106)-C(107)-C(108)-C(103)	2(3)
As(3)-O(17)-C(109)-C(110)	173.2(14)	As(3)-O(17)-C(109)-C(114)	-10.1(18)
O(17)-C(109)-C(110)-C(111)	179.8(16)	C(114)-C(109)-C(110)-C(111)	3(3)
C(109)-C(110)-C(111)-C(112)	-2(3)	C(110)-C(111)-C(112)-C(113)	0(3)
C(111)-C(112)-C(113)-C(114)	1(3)	As(3)-O(18)-C(114)-C(113)	-172.0(15)
As(3)-O(18)-C(114)-C(109)	5(2)	C(112)-C(113)-C(114)-O(18)	177.9(16)
C(112)-C(113)-C(114)-C(109)	1(3)	O(17)-C(109)-C(114)-O(18)	3(2)
C(110)-C(109)-C(114)-O(18)	180.0(16)	O(17)-C(109)-C(114)-C(113)	-179.5(16)
C(110)-C(109)-C(114)-C(113)	-3(3)	O(23)-As(4)-O(19)-C(115)	178.3(12)
O(24)-As(4)-O(19)-C(115)	-93.1(12)	O(21)-As(4)-O(19)-C(115)	89.8(12)
O(20)-As(4)-O(19)-C(115)	-2.9(12)	O(19)-As(4)-O(20)-C(120)	3.2(13)
O(24)-As(4)-O(20)-C(120)	98.3(13)	O(22)-As(4)-O(20)-C(120)	-172.6(13)
O(21)-As(4)-O(20)-C(120)	-86.1(13)	O(23)-As(4)-O(21)-C(121)	104.6(11)
O(19)-As(4)-O(21)-C(121)	-166.8(11)	O(22)-As(4)-O(21)-C(121)	8.5(11)
O(20)-As(4)-O(21)-C(121)	-78.3(11)	O(23)-As(4)-O(22)-C(126)	-97.3(11)
O(24)-As(4)-O(22)-C(126)	174.0(11)	O(21)-As(4)-O(22)-C(126)	-9.2(11)
O(20)-As(4)-O(22)-C(126)	83.7(11)	O(19)-As(4)-O(23)-C(127)	80.6(11)
O(24)-As(4)-O(23)-C(127)	-14.5(11)	O(22)-As(4)-O(23)-C(127)	-103.6(10)
O(21)-As(4)-O(23)-C(127)	170.0(11)	O(23)-As(4)-O(24)-C(132)	13.6(11)
O(19)-As(4)-O(24)-C(132)	-74.8(11)	O(22)-As(4)-O(24)-C(132)	109.6(11)
O(20)-As(4)-O(24)-C(132)	-163.4(11)	As(4)-O(19)-C(115)-C(120)	2(2)
As(4)-O(19)-C(115)-C(116)	-174.1(17)	C(120)-C(115)-C(116)-C(117)	3(3)
O(19)-C(115)-C(116)-C(117)	179.2(18)	C(115)-C(116)-C(117)-C(118)	-3(3)
C(116)-C(117)-C(118)-C(119)	3(3)	C(117)-C(118)-C(119)-C(120)	-2(3)
C(118)-C(119)-C(120)-O(20)	-177.1(19)	C(118)-C(119)-C(120)-C(115)	2(3)
As(4)-O(20)-C(120)-C(119)	176.3(18)	As(4)-O(20)-C(120)-C(115)	-3(2)
C(116)-C(115)-C(120)-C(119)	-3(3)	O(19)-C(115)-C(120)-C(119)	-178.7(18)
C(116)-C(115)-C(120)-O(20)	176.5(19)	O(19)-C(115)-C(120)-O(20)	0(3)
As(4)-O(21)-C(121)-C(122)	174.3(15)	As(4)-O(21)-C(121)-C(126)	-6.0(19)
C(126)-C(121)-C(122)-C(123)	-1(3)	O(21)-C(121)-C(122)-C(123)	178.9(17)
C(121)-C(122)-C(123)-C(124)	2(3)	C(122)-C(123)-C(124)-C(125)	0(3)
C(123)-C(124)-C(125)-C(126)	-2(3)	C(122)-C(121)-C(126)-O(22)	178.2(16)
O(21)-C(121)-C(126)-O(22)	-2(2)	C(122)-C(121)-C(126)-C(125)	-2(3)
O(21)-C(121)-C(126)-C(125)	178.7(15)	As(4)-O(22)-C(126)-C(121)	8.3(19)
As(4)-O(22)-C(126)-C(125)	-172.0(14)	C(124)-C(125)-C(126)-C(121)	3(3)
C(124)-C(125)-C(126)-O(22)	-176.8(16)	As(4)-O(23)-C(127)-C(128)	-163.4(15)
As(4)-O(23)-C(127)-C(132)	12.0(18)	O(23)-C(127)-C(128)-C(129)	179.3(17)
C(132)-C(127)-C(128)-C(129)	4(3)	C(127)-C(128)-C(129)-C(130)	-2(3)
C(128)-C(129)-C(130)-C(131)	0(3)	C(129)-C(130)-C(131)-C(132)	-1(3)

As(4)-O(24)-C(132)-C(127)	-10.0(18)	As(4)-O(24)-C(132)-C(131)	169.3(15)
C(128)-C(127)-C(132)-O(24)	174.2(16)	O(23)-C(127)-C(132)-O(24)	-1(2)
C(128)-C(127)-C(132)-C(131)	-5(3)	O(23)-C(127)-C(132)-C(131)	179.4(15)
C(130)-C(131)-C(132)-O(24)	-176.1(17)	C(130)-C(131)-C(132)-C(127)	3(3)

Symmetry transformations used to generate equivalent atoms:

Lemus, Lappin Compound 3 (nd029a)

Table 1. Crystal data and structure refinement for nd029a.

Identification code	nd029a	
Empirical formula	C87 H72 Cl3 Cu3 N12 O12	
Formula weight	1774.54	
Temperature	150(2) K	
Wavelength	0.77490 Å	
Crystal system	Trigonal	
Space group	P-31c	
Unit cell dimensions	a = 16.9700(5) Å	α = 90°
	b = 16.9700(5) Å	β = 90°
	c = 17.6573(6) Å	γ = 120°
Volume	4403.7(2) $Å^3$	
Z	2	
Density (calculated)	1.338 $g.cm^{-3}$	
Absorption coefficient (μ)	1.102 mm^{-1}	
F(000)	1824	
Crystal color, habit	orange, rod	
Crystal size	0.07 × 0.07 × 0.06 mm^3	
θ range for data collection	1.97 to 29.01°	
Index ranges	$-21 \le h \le 21$, $-21 \le k \le 21$, $-22 \le l \le 22$	
Reflections collected	64420	
Independent reflections	3028 [R_{int} = 0.0655]	
Completeness to θ = 29.01°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9368 and 0.9268	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3028 / 21 / 190	
Goodness-of-fit on F^2	1.064	
Final R indices [I>2σ(I)]	R_1 = 0.0646, wR_2 = 0.2195	
R indices (all data)	R_1 = 0.0716, wR_2 = 0.2302	
Largest diff. peak and hole	1.237 and -0.569 $e^-.Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for nd029a. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cu(1)	0.52585(2)	0.47415(2)	0.2500	0.034(1)
N(1)	0.5893(2)	0.5849(2)	0.31874(16)	0.037(1)
N(2)	0.52001(19)	0.4084(2)	0.35251(16)	0.033(1)
C(1)	0.6051(4)	0.6930(3)	0.2231(2)	0.056(1)
C(2)	0.6244(3)	0.6725(3)	0.3004(2)	0.044(1)
C(3)	0.6783(3)	0.7434(3)	0.3515(2)	0.053(1)
C(4)	0.6919(3)	0.7222(3)	0.4238(2)	0.049(1)
C(5)	0.6536(3)	0.6307(3)	0.44500(19)	0.040(1)
C(6)	0.6039(2)	0.5640(2)	0.39017(19)	0.034(1)
C(7)	0.6624(3)	0.6027(3)	0.5202(2)	0.043(1)
C(8)	0.6239(3)	0.5136(3)	0.5376(2)	0.044(1)
C(9)	0.5742(3)	0.4448(3)	0.48270(19)	0.038(1)
C(10)	0.5649(2)	0.4691(2)	0.40861(19)	0.033(1)
C(11)	0.5313(3)	0.3507(3)	0.4991(2)	0.045(1)
C(12)	0.4833(3)	0.2899(3)	0.4435(2)	0.045(1)
C(13)	0.4784(2)	0.3199(3)	0.3702(2)	0.037(1)
C(14)	0.4253(3)	0.2517(3)	0.3096(2)	0.040(1)
C(15)	0.4853(3)	0.24263(17)	0.2500	0.037(1)
Cl(1)	0.6667	0.3333	0.7793(3)	0.082(1)
O(1)	0.5884(11)	0.3254(12)	0.6918(7)	0.219(6)
Cl(2)	0.9610(4)	0.8310(3)	0.3774(4)	0.096(2)
O(2)	0.9017(9)	0.7607(10)	0.4189(8)	0.101(4)
O(3)	1.0429(11)	0.8501(13)	0.4031(11)	0.157(8)
O(4)	0.9580(16)	0.8153(15)	0.3054(10)	0.208(12)
O(5)	0.9483(14)	0.9006(12)	0.3896(12)	0.170(9)
H(1A)	0.5822	0.6385	0.1914	0.085
H(1B)	0.6612	0.7422	0.2009	0.085
H(1C)	0.5593	0.7120	0.2260	0.085
H(3A)	0.7048	0.8051	0.3360	0.064
H(4A)	0.7270	0.7692	0.4591	0.059
H(7A)	0.6956	0.6473	0.5577	0.051
H(8A)	0.6300	0.4964	0.5875	0.053
H(11A)	0.5358	0.3303	0.5481	0.055
H(12A)	0.4529	0.2266	0.4542	0.053
H(14A)	0.3847	0.2698	0.2844	0.048
H(14B)	0.3865	0.1916	0.3336	0.048
H(15A)	0.5246	0.2223	0.2742	0.044

Table 3. Anisotropic displacement parameters ($Å^2$) for nd029a.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cu(1)	0.0444(4)	0.0444(4)	0.0215(4)	-0.0058(2)	-0.0058(2)	0.0282(3)
N(1)	0.0523(17)	0.0445(16)	0.0254(13)	-0.0066(12)	-0.0071(12)	0.0334(15)
N(2)	0.0401(15)	0.0441(16)	0.0243(14)	-0.0028(11)	0.0003(10)	0.0275(13)
C(1)	0.095(3)	0.049(2)	0.037(2)	-0.0066(17)	-0.017(2)	0.045(2)
C(2)	0.062(2)	0.0435(19)	0.0349(19)	-0.0047(15)	-0.0077(17)	0.0333(19)
C(3)	0.078(3)	0.046(2)	0.042(2)	-0.0084(18)	-0.011(2)	0.035(2)
C(4)	0.063(3)	0.049(2)	0.039(2)	-0.0157(16)	-0.0137(18)	0.031(2)
C(5)	0.051(2)	0.053(2)	0.0273(16)	-0.0092(14)	-0.0055(14)	0.0346(18)
C(6)	0.0438(18)	0.0444(18)	0.0244(15)	-0.0049(13)	-0.0027(13)	0.0299(16)
C(7)	0.054(2)	0.059(2)	0.0246(16)	-0.0127(15)	-0.0073(15)	0.0351(19)
C(8)	0.058(2)	0.068(3)	0.0206(16)	-0.0052(16)	-0.0026(15)	0.042(2)
C(9)	0.047(2)	0.054(2)	0.0246(17)	-0.0015(14)	0.0015(14)	0.0352(17)
C(10)	0.0392(17)	0.0458(19)	0.0242(16)	-0.0033(13)	0.0000(13)	0.0285(15)
C(11)	0.061(2)	0.062(2)	0.0278(18)	0.0053(16)	0.0031(15)	0.041(2)
C(12)	0.061(2)	0.049(2)	0.034(2)	0.0040(15)	0.0057(16)	0.0354(19)
C(13)	0.047(2)	0.0449(19)	0.0285(17)	-0.0007(14)	0.0029(13)	0.0290(16)
C(14)	0.0459(19)	0.0434(19)	0.0340(18)	-0.0031(15)	0.0011(14)	0.0242(16)
C(15)	0.044(3)	0.0373(17)	0.031(2)	-0.0046(16)	0.000	0.0221(13)
Cl(1)	0.0782(17)	0.0782(17)	0.089(3)	0.000	0.000	0.0391(8)
Cl(2)	0.095(3)	0.072(3)	0.121(4)	0.004(3)	0.018(3)	0.043(3)

Table 4. Bond lengths [Å] for nd029a.

atom-atom	distance	atom-atom	distance
Cu(1)-N(1)#1	2.035(3)	Cu(1)-N(1)	2.035(3)
Cu(1)-N(2)	2.103(3)	Cu(1)-N(2)#1	2.103(3)
N(1)-C(2)	1.335(5)	N(1)-C(6)	1.366(4)
N(2)-C(13)	1.338(5)	N(2)-C(10)	1.356(4)
C(1)-C(2)	1.486(5)	C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800	C(1)-H(1C)	0.9800
C(2)-C(3)	1.413(6)	C(3)-C(4)	1.378(6)
C(3)-H(3A)	0.9500	C(4)-C(5)	1.402(6)
C(4)-H(4A)	0.9500	C(5)-C(6)	1.405(5)
C(5)-C(7)	1.443(5)	C(6)-C(10)	1.439(5)
C(7)-C(8)	1.349(6)	C(7)-H(7A)	0.9500
C(8)-C(9)	1.424(5)	C(8)-H(8A)	0.9500
C(9)-C(10)	1.404(5)	C(9)-C(11)	1.415(6)
C(11)-C(12)	1.360(6)	C(11)-H(11A)	0.9500
C(12)-C(13)	1.408(5)	C(12)-H(12A)	0.9500
C(13)-C(14)	1.501(5)	C(14)-C(15)	1.525(4)
C(14)-H(14A)	0.9900	C(14)-H(14B)	0.9900
C(15)-C(14)#2	1.525(4)	C(15)-H(15A)	0.9886
Cl(1)-Cl(1)#3	1.034(11)	Cl(1)-O(1)#4	1.366(15)
Cl(1)-O(1)#5	1.366(16)	Cl(1)-O(1)#3	1.366(15)
Cl(1)-O(1)	1.998(14)	Cl(1)-O(1)#6	1.998(14)
Cl(1)-O(1)#7	1.998(15)	O(1)-Cl(1)#3	1.366(15)
Cl(2)-O(4)	1.295(16)	Cl(2)-O(5)	1.320(15)
Cl(2)-O(2)	1.331(13)	Cl(2)-O(3)	1.340(16)

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

Table 5. Bond angles [°] for nd029a.

atom-atom-atom	angle	atom-atom-atom	angle
N(1)#1-Cu(1)-N(1)	140.06(16)	N(1)#1-Cu(1)-N(2)	116.52(12)
N(1)-Cu(1)-N(2)	80.77(11)	N(1)#1-Cu(1)-N(2)#1	80.77(11)
N(1)-Cu(1)-N(2)#1	116.52(12)	N(2)-Cu(1)-N(2)#1	130.47(15)
C(2)-N(1)-C(6)	118.4(3)	C(2)-N(1)-Cu(1)	128.2(2)
C(6)-N(1)-Cu(1)	113.1(2)	C(13)-N(2)-C(10)	117.6(3)
C(13)-N(2)-Cu(1)	130.9(2)	C(10)-N(2)-Cu(1)	111.5(2)
C(2)-C(1)-H(1A)	109.5	C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5	C(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5	H(1B)-C(1)-H(1C)	109.5
N(1)-C(2)-C(3)	122.2(3)	N(1)-C(2)-C(1)	117.1(3)
C(3)-C(2)-C(1)	120.7(4)	C(4)-C(3)-C(2)	119.4(4)
C(4)-C(3)-H(3A)	120.3	C(2)-C(3)-H(3A)	120.3
C(3)-C(4)-C(5)	119.4(4)	C(3)-C(4)-H(4A)	120.3
C(5)-C(4)-H(4A)	120.3	C(4)-C(5)-C(6)	117.8(3)
C(4)-C(5)-C(7)	122.9(3)	C(6)-C(5)-C(7)	119.2(4)
N(1)-C(6)-C(5)	122.8(3)	N(1)-C(6)-C(10)	117.3(3)
C(5)-C(6)-C(10)	120.0(3)	C(8)-C(7)-C(5)	120.5(3)
C(8)-C(7)-H(7A)	119.8	C(5)-C(7)-H(7A)	119.8
C(7)-C(8)-C(9)	121.3(3)	C(7)-C(8)-H(8A)	119.3
C(9)-C(8)-H(8A)	119.3	C(10)-C(9)-C(11)	116.9(3)
C(10)-C(9)-C(8)	120.1(4)	C(11)-C(9)-C(8)	123.1(3)
N(2)-C(10)-C(9)	124.1(3)	N(2)-C(10)-C(6)	117.0(3)
C(9)-C(10)-C(6)	118.9(3)	C(12)-C(11)-C(9)	119.0(3)
C(12)-C(11)-H(11A)	120.5	C(9)-C(11)-H(11A)	120.5
C(11)-C(12)-C(13)	120.6(4)	C(11)-C(12)-H(12A)	119.7
C(13)-C(12)-H(12A)	119.7	N(2)-C(13)-C(12)	121.8(3)
N(2)-C(13)-C(14)	118.4(3)	C(12)-C(13)-C(14)	119.8(3)
C(13)-C(14)-C(15)	113.4(3)	C(13)-C(14)-H(14A)	108.9
C(15)-C(14)-H(14A)	108.9	C(13)-C(14)-H(14B)	108.9
C(15)-C(14)-H(14B)	108.9	H(14A)-C(14)-H(14B)	107.7
C(14)#2-C(15)-C(14)	109.4(4)	C(14)#2-C(15)-H(15A)	109.7
C(14)-C(15)-H(15A)	109.8	Cl(1)#3-Cl(1)-O(1)#4	112.0(6)
Cl(1)#3-Cl(1)-O(1)#5	112.0(7)	O(1)#4-Cl(1)-O(1)#5	106.9(7)
Cl(1)#3-Cl(1)-O(1)#3	112.0(6)	O(1)#4-Cl(1)-O(1)#3	106.9(7)
O(1)#5-Cl(1)-O(1)#3	106.9(7)	Cl(1)#3-Cl(1)-O(1)	39.3(4)
O(1)#4-Cl(1)-O(1)	150.1(6)	O(1)#5-Cl(1)-O(1)	84.7(10)
O(1)#3-Cl(1)-O(1)	95.4(11)	Cl(1)#3-Cl(1)-O(1)#6	39.3(4)
O(1)#4-Cl(1)-O(1)#6	84.7(10)	O(1)#5-Cl(1)-O(1)#6	95.4(11)
O(1)#3-Cl(1)-O(1)#6	150.1(6)	O(1)-Cl(1)-O(1)#6	66.6(7)
Cl(1)#3-Cl(1)-O(1)#7	39.3(4)	O(1)#4-Cl(1)-O(1)#7	95.4(11)
O(1)#5-Cl(1)-O(1)#7	150.1(6)	O(1)#3-Cl(1)-O(1)#7	84.7(10)
O(1)-Cl(1)-O(1)#7	66.6(7)	O(1)#6-Cl(1)-O(1)#7	66.6(7)

Cl(1)#3-O(1)-Cl(1)	28.7(5)	O(4)-Cl(2)-O(5)	109.8(11)
O(4)-Cl(2)-O(2)	115.0(11)	O(5)-Cl(2)-O(2)	108.8(9)
O(4)-Cl(2)-O(3)	108.1(10)	O(5)-Cl(2)-O(3)	110.0(10)
O(2)-Cl(2)-O(3)	104.9(9)		

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

Table 6. Torsion angles [°] for nd029a.

atom-atom-atom-atom	angle	atom-atom-atom-atom	angle
N(1)#1-Cu(1)-N(1)-C(2)	-60.3(3)	N(2)-Cu(1)-N(1)-C(2)	179.0(3)
N(2)#1-Cu(1)-N(1)-C(2)	48.2(4)	N(1)#1-Cu(1)-N(1)-C(6)	126.6(3)
N(2)-Cu(1)-N(1)-C(6)	5.9(2)	N(2)#1-Cu(1)-N(1)-C(6)	-124.9(2)
N(1)#1-Cu(1)-N(2)-C(13)	31.4(3)	N(1)-Cu(1)-N(2)-C(13)	173.3(3)
N(2)#1-Cu(1)-N(2)-C(13)	-69.5(3)	N(1)#1-Cu(1)-N(2)-C(10)	-146.4(2)
N(1)-Cu(1)-N(2)-C(10)	-4.5(2)	N(2)#1-Cu(1)-N(2)-C(10)	112.6(2)
C(6)-N(1)-C(2)-C(3)	2.2(6)	Cu(1)-N(1)-C(2)-C(3)	-170.6(3)
C(6)-N(1)-C(2)-C(1)	-178.2(4)	Cu(1)-N(1)-C(2)-C(1)	9.0(6)
N(1)-C(2)-C(3)-C(4)	-3.0(7)	C(1)-C(2)-C(3)-C(4)	177.4(4)
C(2)-C(3)-C(4)-C(5)	1.2(7)	C(3)-C(4)-C(5)-C(6)	1.2(6)
C(3)-C(4)-C(5)-C(7)	-178.1(4)	C(2)-N(1)-C(6)-C(5)	0.4(5)
Cu(1)-N(1)-C(6)-C(5)	174.3(3)	C(2)-N(1)-C(6)-C(10)	179.7(3)
Cu(1)-N(1)-C(6)-C(10)	-6.4(4)	C(4)-C(5)-C(6)-N(1)	-2.1(6)
C(7)-C(5)-C(6)-N(1)	177.2(3)	C(4)-C(5)-C(6)-C(10)	178.6(3)
C(7)-C(5)-C(6)-C(10)	-2.0(5)	C(4)-C(5)-C(7)-C(8)	179.7(4)
C(6)-C(5)-C(7)-C(8)	0.4(6)	C(5)-C(7)-C(8)-C(9)	0.4(6)
C(7)-C(8)-C(9)-C(10)	0.3(6)	C(7)-C(8)-C(9)-C(11)	-178.7(4)
C(13)-N(2)-C(10)-C(9)	3.4(5)	Cu(1)-N(2)-C(10)-C(9)	-178.4(3)
C(13)-N(2)-C(10)-C(6)	-175.7(3)	Cu(1)-N(2)-C(10)-C(6)	2.5(4)
C(11)-C(9)-C(10)-N(2)	-1.9(5)	C(8)-C(9)-C(10)-N(2)	179.1(3)
C(11)-C(9)-C(10)-C(6)	177.2(3)	C(8)-C(9)-C(10)-C(6)	-1.9(5)
N(1)-C(6)-C(10)-N(2)	2.6(5)	C(5)-C(6)-C(10)-N(2)	-178.1(3)
N(1)-C(6)-C(10)-C(9)	-176.6(3)	C(5)-C(6)-C(10)-C(9)	2.7(5)
C(10)-C(9)-C(11)-C(12)	-0.7(5)	C(8)-C(9)-C(11)-C(12)	178.3(4)
C(9)-C(11)-C(12)-C(13)	1.6(6)	C(10)-N(2)-C(13)-C(12)	-2.4(5)
Cu(1)-N(2)-C(13)-C(12)	179.9(3)	C(10)-N(2)-C(13)-C(14)	177.7(3)
Cu(1)-N(2)-C(13)-C(14)	-0.1(5)	C(11)-C(12)-C(13)-N(2)	-0.1(6)
C(11)-C(12)-C(13)-C(14)	179.9(3)	N(2)-C(13)-C(14)-C(15)	72.6(4)
C(12)-C(13)-C(14)-C(15)	-107.3(4)	C(13)-C(14)-C(15)-C(14)#2	-178.8(4)
O(1)#4-Cl(1)-O(1)-Cl(1)#3	-20(3)	O(1)#5-Cl(1)-O(1)-Cl(1)#3	-134.9(14)
O(1)#3-Cl(1)-O(1)-Cl(1)#3	118.6(12)	O(1)#6-Cl(1)-O(1)-Cl(1)#3	-36.75(16)
O(1)#7-Cl(1)-O(1)-Cl(1)#3	36.74(16)		

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

Lemus, Lappin Compound 4 (nd1024_x)

Table 1. Crystal data and structure refinement for nd1024_x.

Identification code	nd1024	
Empirical formula	$C_{141}H_{114}As_3Cu_3N_{12}O_{21}$	
Formula weight	2727.81	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 20.9348(6) Å	α = 90°
	b = 17.0379(5) Å	β = 98.473(2)°
	c = 58.1561(17) Å	γ = 90°
Volume	20517.0(10) Å^3	
Z	6	
Density (calculated)	1.325 g.cm^{-3}	
Absorption coefficient (μ)	1.252 mm^{-1}	
F(000)	8388	
Crystal color, habit	dark red, rod	
Crystal size	0.29 × 0.17 × 0.09 mm^3	
θ range for data collection	0.983 to 20.926°	
Index ranges	$-20 \le h \le 20$, $-17 \le k \le 17$, $-56 \le l \le 58$	
Reflections collected	137432	
Independent reflections	42913 [R_{int} = 0.1126]	
Completeness to θ = 25.242°	58.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7446 and 0.5909	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	42913 / 40 / 1496	
Goodness-of-fit on F^2	1.014	
Final R indices [I>2σ(I)]	R_1 = 0.1193, wR_2 = 0.2793	
R indices (all data)	R_1 = 0.1589, wR_2 = 0.3022	
Absolute structure parameter	0.14(2)	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.278 and -0.895 e$^-$.Å^{-3}	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for nd1024_x. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cu11	0.39973(16)	0.9382(2)	0.83820(6)	0.035(1)
Cu21	0.13865(16)	0.9563(2)	0.73400(6)	0.035(1)
Cu31	0.48660(18)	0.9526(2)	0.71974(7)	0.041(1)
N11	0.4721(8)	0.8607(9)	0.8437(3)	0.044(7)
C21	0.5353(9)	0.8729(9)	0.8543(3)	0.043(9)
C31	0.5803(7)	0.8126(11)	0.8551(3)	0.051(9)
C41	0.5622(8)	0.7401(10)	0.8453(4)	0.049(9)
C51	0.4990(9)	0.7279(9)	0.8347(3)	0.040(8)
C61	0.4540(7)	0.7882(11)	0.8339(3)	0.048(9)
N21	0.3560(8)	0.8436(8)	0.8203(3)	0.039(6)
C101	0.3969(6)	0.7790(10)	0.8212(3)	0.043(8)
C91	0.3761(7)	0.7106(9)	0.8094(3)	0.024(7)
C111	0.3145(8)	0.7067(8)	0.7967(3)	0.038(8)
C121	0.2737(6)	0.7713(10)	0.7958(3)	0.038(8)
C131	0.2944(7)	0.8397(9)	0.8076(3)	0.039(8)
N31	0.1752(7)	1.0610(7)	0.7448(3)	0.017(5)
C171	0.2021(8)	1.0860(8)	0.7668(2)	0.023(7)
C181	0.2245(8)	1.1626(9)	0.7702(2)	0.034(8)
C191	0.2199(9)	1.2141(7)	0.7515(3)	0.044(9)
C201	0.1930(9)	1.1891(8)	0.7294(3)	0.022(7)
C211	0.1707(8)	1.1126(9)	0.7261(2)	0.039(8)
N41	0.1194(8)	1.0120(9)	0.7034(3)	0.033(6)
C251	0.1420(8)	1.0888(10)	0.7050(3)	0.024(7)
C241	0.1326(10)	1.1375(8)	0.6856(3)	0.045(9)
C261	0.1006(10)	1.1094(11)	0.6646(3)	0.061(10)
C271	0.0780(10)	1.0326(12)	0.6630(2)	0.057(10)
C281	0.0874(9)	0.9839(9)	0.6823(3)	0.047(8)
N51	0.0859(7)	0.8981(8)	0.7545(3)	0.030(6)
C311	0.0398(9)	0.9287(8)	0.7669(3)	0.050(9)
C321	0.0145(8)	0.8823(11)	0.7831(3)	0.063(11)
C331	0.0354(9)	0.8053(10)	0.7868(3)	0.049(9)
C341	0.0816(9)	0.7747(7)	0.7744(3)	0.054(9)
C351	0.1068(7)	0.8211(9)	0.7583(3)	0.014(6)
N61	0.1811(9)	0.8470(8)	0.7327(3)	0.042(7)
C391	0.1516(8)	0.7944(11)	0.7461(3)	0.036(8)
C381	0.1699(10)	0.7159(10)	0.7470(3)	0.056(10)
C401	0.2177(10)	0.6900(9)	0.7346(4)	0.085(13)
C411	0.2472(9)	0.7426(12)	0.7212(4)	0.065(11)
C421	0.2289(9)	0.8211(11)	0.7203(3)	0.056(10)
N71	0.4361(7)	1.0504(8)	0.7224(3)	0.025(6)
C461	0.3708(7)	1.0624(10)	0.7148(3)	0.027(7)

C471	0.3430(7)	1.1351(12)	0.7179(4)	0.095(14)
C481	0.3807(10)	1.1958(9)	0.7286(4)	0.068(11)
C491	0.4461(9)	1.1838(10)	0.7362(4)	0.071(11)
C501	0.4738(6)	1.1111(11)	0.7331(3)	0.049(9)
N81	0.5572(11)	1.0189(12)	0.7348(4)	0.067(9)
C541	0.5361(8)	1.0947(14)	0.7384(4)	0.059(10)
C531	0.5795(12)	1.1507(11)	0.7486(5)	0.120(18)
C551	0.6441(10)	1.1311(15)	0.7551(5)	0.088(14)
C561	0.6652(9)	1.0554(17)	0.7515(5)	0.110(16)
C571	0.6217(12)	0.9993(12)	0.7413(5)	0.106(16)
N91	0.4643(10)	0.8916(13)	0.6894(3)	0.065(9)
C601	0.4602(11)	0.9211(11)	0.6670(4)	0.101(15)
C611	0.4303(11)	0.8774(13)	0.6483(3)	0.060(10)
C621	0.4045(10)	0.8041(13)	0.6520(3)	0.054(10)
C631	0.4086(11)	0.7746(10)	0.6744(4)	0.054(9)
C641	0.4384(11)	0.8183(13)	0.6932(3)	0.069(11)
N101	0.4651(8)	0.8465(9)	0.7337(3)	0.033(6)
C681	0.4400(10)	0.7933(12)	0.7166(2)	0.050(9)
C671	0.4193(11)	0.7198(11)	0.7228(3)	0.067(11)
C691	0.4239(10)	0.6995(9)	0.7461(4)	0.053(9)
C701	0.4491(11)	0.7526(12)	0.7632(3)	0.067(11)
C711	0.4697(9)	0.8261(11)	0.7570(3)	0.048(9)
N111	0.4019(8)	1.0416(8)	0.8219(3)	0.027(6)
C751	0.4336(7)	1.0609(9)	0.8033(3)	0.027(7)
C761	0.4235(9)	1.1338(10)	0.7927(3)	0.038(8)
C771	0.3819(9)	1.1875(8)	0.8007(3)	0.050(9)
C781	0.3503(9)	1.1682(9)	0.8193(3)	0.041(8)
C791	0.3603(8)	1.0952(10)	0.8300(3)	0.043(8)
N121	0.3411(7)	0.9979(9)	0.8569(3)	0.035(6)
C831	0.3318(8)	1.0743(10)	0.8486(3)	0.021(7)
C821	0.2890(8)	1.1237(8)	0.8577(3)	0.045(9)
C841	0.2554(7)	1.0967(9)	0.8751(3)	0.024(7)
C851	0.2647(8)	1.0203(10)	0.8833(3)	0.041(8)
C861	0.3075(9)	0.9710(8)	0.8742(3)	0.050(9)
C11	0.5506(13)	0.9560(16)	0.8628(5)	0.033(7)
C71	0.4823(16)	0.655(2)	0.8245(6)	0.052(9)
C81	0.4157(16)	0.643(2)	0.8118(6)	0.056(10)
C141	0.2505(15)	0.9055(18)	0.8060(6)	0.049(9)
C151	0.2566(13)	0.9658(17)	0.7850(5)	0.040(8)
C161	0.2047(14)	1.0291(17)	0.7859(5)	0.037(8)
C221	0.1792(12)	1.2436(17)	0.7093(5)	0.028(7)
C231	0.1558(15)	1.218(2)	0.6900(6)	0.054(10)
C291	0.0598(17)	0.905(2)	0.6830(6)	0.064(10)
C301	0.0170(17)	1.012(2)	0.7599(6)	0.064(11)
C371	0.1417(13)	0.6662(9)	0.7616(5)	0.059(10)
C361	0.0997(14)	0.6961(9)	0.7758(5)	0.076(12)

C431	0.2571(15)	0.8853(18)	0.7058(5)	0.048(9)
C441	0.3015(19)	0.946(3)	0.7192(7)	0.085(13)
C451	0.3310(15)	0.9990(19)	0.7033(5)	0.050(9)
C511	0.4885(9)	1.2388(14)	0.7477(7)	0.101(15)
C521	0.5544(9)	1.2248(12)	0.7516(8)	0.13(2)
C581	0.6429(19)	0.915(2)	0.7378(7)	0.083(13)
C591	0.4899(18)	1.002(2)	0.6640(6)	0.073(12)
C651	0.3827(16)	0.694(2)	0.6823(6)	0.057(10)
C661	0.3918(14)	0.6701(19)	0.7040(5)	0.042(8)
C721	0.4987(15)	0.8805(18)	0.7752(5)	0.044(9)
C731	0.4509(13)	0.9452(18)	0.7793(5)	0.041(8)
C741	0.4805(14)	1.0001(17)	0.7970(5)	0.041(8)
C801	0.2976(16)	1.222(2)	0.8299(6)	0.055(10)
C811	0.2729(15)	1.1987(19)	0.8483(6)	0.048(9)
C871	0.3148(15)	0.8905(17)	0.8823(5)	0.045(9)
Cu42	0.16153(15)	0.9836(2)	0.36466(6)	0.035(1)
Cu52	0.38234(16)	0.9853(2)	0.47791(6)	0.035(1)
Cu62	0.52298(16)	0.9814(2)	0.36877(6)	0.033(1)
N1A2	0.1577(9)	1.0418(10)	0.3339(3)	0.033(6)
C2A2	0.1434(9)	1.0126(8)	0.3114(3)	0.054(10)
C3A2	0.1483(10)	1.0610(11)	0.2926(2)	0.036(8)
C4A2	0.1677(10)	1.1387(11)	0.2961(3)	0.050(9)
C5A2	0.1820(10)	1.1679(8)	0.3186(4)	0.053(9)
C6A2	0.1771(10)	1.1195(11)	0.3375(3)	0.057(10)
N2A2	0.1931(8)	1.0906(8)	0.3777(3)	0.030(6)
C10A2	0.1961(9)	1.1445(11)	0.3599(2)	0.051(9)
C9A2	0.2172(11)	1.2206(10)	0.3652(3)	0.043(9)
C11A2	0.2353(10)	1.2428(8)	0.3883(4)	0.081(13)
C12A2	0.2322(10)	1.1889(11)	0.4060(3)	0.040(8)
C13A2	0.2111(9)	1.1128(10)	0.4007(3)	0.039(8)
N3A2	0.3466(7)	0.8852(7)	0.4611(3)	0.024(5)
C17A2	0.2857(6)	0.8711(8)	0.4488(3)	0.026(7)
C18A2	0.2693(6)	0.7963(10)	0.4404(3)	0.041(8)
C19A2	0.3140(8)	0.7356(7)	0.4443(3)	0.061(10)
C20A2	0.3749(7)	0.7497(8)	0.4567(3)	0.035(8)
C21A2	0.3912(5)	0.8245(9)	0.4651(3)	0.024(7)
N4A2	0.4595(6)	0.9155(8)	0.4865(3)	0.033(6)
C25A2	0.4472(6)	0.8397(10)	0.4781(3)	0.037(8)
C24A2	0.4960(8)	0.7837(8)	0.4810(3)	0.057(10)
C26A2	0.5572(7)	0.8035(9)	0.4922(3)	0.045(9)
C27A2	0.5695(6)	0.8793(10)	0.5006(3)	0.046(9)
C28A2	0.5207(8)	0.9353(7)	0.4977(3)	0.028(7)
N5A2	0.3145(8)	1.0396(10)	0.4931(3)	0.037(6)
C31A2	0.2761(10)	1.0075(9)	0.5083(3)	0.040(8)
C32A2	0.2314(10)	1.0542(14)	0.5174(4)	0.081(13)
C33A2	0.2252(10)	1.1330(13)	0.5113(4)	0.104(16)

C34A2	0.2636(11)	1.1651(9)	0.4961(4)	0.047(9)
C35A2	0.3083(9)	1.1184(10)	0.4870(3)	0.044(9)
N6A2	0.3900(7)	1.0958(7)	0.4642(3)	0.030(6)
C39A2	0.3430(7)	1.1441(10)	0.4712(3)	0.017(6)
C38A2	0.3350(8)	1.2202(9)	0.4627(3)	0.058(10)
C40A2	0.3740(9)	1.2480(8)	0.4471(3)	0.046(9)
C41A2	0.4210(8)	1.1997(10)	0.4400(3)	0.034(8)
C42A2	0.4290(7)	1.1236(9)	0.4486(3)	0.035(8)
N7A2	0.4970(8)	0.8847(7)	0.3862(3)	0.034(6)
C46A2	0.4939(9)	0.8745(9)	0.4097(2)	0.028(7)
C47A2	0.4733(10)	0.8032(11)	0.4177(2)	0.059(10)
C48A2	0.4559(9)	0.7423(8)	0.4022(3)	0.047(9)
C49A2	0.4590(9)	0.7526(8)	0.3787(3)	0.029(7)
C50A2	0.4795(8)	0.8238(9)	0.3707(2)	0.017(6)
N8A2	0.5142(7)	0.9053(8)	0.3429(2)	0.027(6)
C54A2	0.4875(8)	0.8350(9)	0.3490(2)	0.025(7)
C53A2	0.4726(8)	0.7764(7)	0.3325(3)	0.025(7)
C55A2	0.4845(8)	0.7882(8)	0.3098(2)	0.025(7)
C56A2	0.5112(9)	0.8585(10)	0.3037(2)	0.044(9)
C57A2	0.5260(8)	0.9171(8)	0.3203(3)	0.028(7)
N9A2	0.5893(8)	1.0544(9)	0.3853(3)	0.039(7)
C60A2	0.6531(8)	1.0393(9)	0.3948(3)	0.045(9)
C61A2	0.6895(6)	1.0969(12)	0.4076(3)	0.056(10)
C62A2	0.6621(9)	1.1696(10)	0.4110(3)	0.049(9)
C63A2	0.5984(9)	1.1846(8)	0.4015(4)	0.066(11)
C64A2	0.5620(6)	1.1270(10)	0.3887(3)	0.023(7)
N10A2	0.4645(7)	1.0796(7)	0.3683(3)	0.024(6)
C68A2	0.4997(6)	1.1394(9)	0.3805(3)	0.028(7)
C67A2	0.4707(8)	1.2113(8)	0.3835(3)	0.029(7)
C69A2	0.4063(8)	1.2234(8)	0.3742(3)	0.056(10)
C70A2	0.3711(6)	1.1637(10)	0.3620(3)	0.033(8)
C71A2	0.4002(7)	1.0917(8)	0.3591(3)	0.026(7)
N11A2	0.2081(7)	0.8761(7)	0.3698(3)	0.023(5)
C75A2	0.2635(7)	0.8487(9)	0.3618(3)	0.047(9)
C76A2	0.2845(7)	0.7724(10)	0.3668(3)	0.034(8)
C77A2	0.2503(9)	0.7234(8)	0.3797(3)	0.040(8)
C78A2	0.1949(9)	0.7508(9)	0.3876(3)	0.077(12)
C79A2	0.1739(7)	0.8272(10)	0.3827(3)	0.020(6)
N12A2	0.0979(7)	0.9265(9)	0.3822(3)	0.026(5)
C83A2	0.1172(7)	0.8520(9)	0.3901(3)	0.039(8)
C82A2	0.0830(8)	0.8124(8)	0.4052(3)	0.023(7)
C84A2	0.0294(8)	0.8474(10)	0.4125(3)	0.035(8)
C85A2	0.0101(7)	0.9220(10)	0.4046(3)	0.042(8)
C86A2	0.0443(8)	0.9615(8)	0.3895(3)	0.055(10)
C1A2	0.1196(15)	0.927(2)	0.3082(6)	0.059(10)
C7A2	0.2080(15)	1.246(2)	0.3247(6)	0.055(10)

C8A2	0.2171(15)	1.272(2)	0.3443(6)	0.052(9)
C14A2	0.2035(14)	1.0613(17)	0.4184(5)	0.038(8)
C15A2	0.2546(13)	0.9925(18)	0.4243(5)	0.040(8)
C16A2	0.2426(13)	0.9437(18)	0.4431(5)	0.038(8)
C22A2	0.4210(7)	0.6907(8)	0.4610(4)	0.034(8)
C23A2	0.4828(8)	0.7085(9)	0.4721(5)	0.047(9)
C29A2	0.5336(13)	1.0204(16)	0.5061(5)	0.031(7)
C30A2	0.2785(16)	0.929(2)	0.5133(6)	0.061(10)
C36A2	0.2536(14)	1.2441(18)	0.4868(5)	0.041(8)
C37A2	0.2867(15)	1.274(2)	0.4708(6)	0.056(10)
C43A2	0.4839(14)	1.0657(17)	0.4435(5)	0.037(8)
C44A2	0.4550(14)	0.9946(18)	0.4273(5)	0.041(8)
C45A2	0.5090(15)	0.944(2)	0.4239(6)	0.053(9)
C51A2	0.4390(12)	0.6913(16)	0.3609(5)	0.025(7)
C52A2	0.4481(13)	0.7020(17)	0.3400(5)	0.033(8)
C58A2	0.5527(15)	0.9964(18)	0.3151(5)	0.050(9)
C59A2	0.6767(14)	0.9596(18)	0.3910(5)	0.048(9)
C65A2	0.5700(13)	1.2592(17)	0.4047(5)	0.032(7)
C66A2	0.5095(15)	1.273(2)	0.3963(5)	0.048(9)
C72A2	0.3661(14)	1.0270(17)	0.3483(5)	0.039(8)
C73A2	0.3317(11)	0.9709(14)	0.3632(4)	0.020(6)
C74A2	0.2939(15)	0.9013(19)	0.3477(6)	0.052(9)
C80A2	0.1564(16)	0.705(2)	0.4006(6)	0.057(10)
C81A2	0.1095(17)	0.730(2)	0.4114(7)	0.067(11)
C87A2	0.0222(14)	1.0418(17)	0.3812(5)	0.042(8)
Cu73	0.36529(16)	0.9321(2)	0.12858(6)	0.038(1)
Cu83	0.38663(17)	0.9401(2)	0.00303(7)	0.040(1)
Cu93	0.05459(19)	0.9244(3)	0.04350(8)	0.058(1)
N1B3	0.3133(7)	0.9909(9)	0.1511(3)	0.035(6)
C2B3	0.2890(8)	0.9669(8)	0.1710(3)	0.040(8)
C3B3	0.2525(9)	1.0184(11)	0.1823(3)	0.037(8)
C4B3	0.2403(10)	1.0939(10)	0.1737(3)	0.093(14)
C5B3	0.2647(10)	1.1180(8)	0.1538(3)	0.054(10)
C6B3	0.3011(8)	1.0665(10)	0.1426(2)	0.023(7)
N2B3	0.3606(8)	1.0383(8)	0.1117(3)	0.044(7)
C10B3	0.3229(8)	1.0906(10)	0.1223(2)	0.021(7)
C9B3	0.3101(8)	1.1650(9)	0.1129(3)	0.032(7)
C11B3	0.3351(9)	1.1872(9)	0.0930(3)	0.046(9)
C12B3	0.3727(10)	1.1349(12)	0.0825(3)	0.068(11)
C13B3	0.3855(9)	1.0605(11)	0.0918(3)	0.072(12)
N3B3	0.3886(7)	0.8406(7)	0.0224(3)	0.023(5)
C17B3	0.4157(8)	0.8227(10)	0.0451(3)	0.038(8)
C18B3	0.4105(10)	0.7471(11)	0.0536(2)	0.072(11)
C19B3	0.3782(10)	0.6895(8)	0.0395(3)	0.054(10)
C20B3	0.3511(9)	0.7074(8)	0.0169(3)	0.042(8)
C21B3	0.3563(8)	0.7829(9)	0.0083(2)	0.018(6)

N4B3	0.3419(8)	0.8709(10)	-0.0223(3)	0.057(8)
C25B3	0.3316(8)	0.7953(11)	-0.0146(3)	0.027(7)
C24B3	0.2892(9)	0.7454(9)	-0.0282(3)	0.050(9)
C26B3	0.2570(9)	0.7711(11)	-0.0495(3)	0.052(9)
C27B3	0.2674(9)	0.8467(12)	-0.0572(3)	0.044(8)
C28B3	0.3098(9)	0.8966(9)	-0.0436(3)	0.051(9)
N5B3	0.4645(6)	1.0091(9)	0.0098(3)	0.038(7)
C31B3	0.5285(7)	0.9853(8)	0.0112(3)	0.024(6)
C32B3	0.5780(5)	1.0354(10)	0.0206(3)	0.040(8)
C33B3	0.5634(7)	1.1093(10)	0.0285(4)	0.058(10)
C34B3	0.4995(8)	1.1330(8)	0.0271(4)	0.061(10)
C35B3	0.4500(6)	1.0829(10)	0.0177(3)	0.032(7)
N6B3	0.3399(9)	1.0446(8)	0.0075(3)	0.053(8)
C39B3	0.3864(6)	1.0988(10)	0.0168(3)	0.020(6)
C38B3	0.3683(8)	1.1750(9)	0.0214(3)	0.033(8)
C40B3	0.3038(9)	1.1972(9)	0.0167(4)	0.110(17)
C41B3	0.2573(6)	1.1430(13)	0.0074(4)	0.084(13)
C42B3	0.2754(8)	1.0668(11)	0.0028(4)	0.045(9)
N7B3	0.1129(8)	0.8323(9)	0.0367(3)	0.040(7)
C46B3	0.1575(8)	0.8282(9)	0.0212(3)	0.024(7)
C47B3	0.1933(8)	0.7601(12)	0.0198(3)	0.063(10)
C48B3	0.1844(10)	0.6961(10)	0.0339(4)	0.059(10)
C49B3	0.1398(11)	0.7003(10)	0.0493(4)	0.074(12)
C50B3	0.1040(9)	0.7684(12)	0.0507(3)	0.041(8)
N8B3	0.0319(10)	0.8441(11)	0.0666(3)	0.044(7)
C54B3	0.0638(10)	0.7728(13)	0.0659(3)	0.069(11)
C53B3	0.0584(11)	0.7159(10)	0.0826(4)	0.041(8)
C55B3	0.0211(13)	0.7302(14)	0.1000(4)	0.18(2)
C56B3	-0.0108(13)	0.8016(17)	0.1007(4)	0.092(14)
C57B3	-0.0054(10)	0.8585(12)	0.0840(4)	0.080(13)
N9B3	0.0164(11)	0.9892(12)	0.0158(4)	0.064(8)
C60B3	-0.0253(12)	0.9641(12)	-0.0036(5)	0.092(13)
C61B3	-0.0369(13)	1.0118(16)	-0.0232(4)	0.17(2)
C62B3	-0.0070(12)	1.0846(14)	-0.0233(3)	0.073(11)
C63B3	0.0347(11)	1.1097(11)	-0.0038(4)	0.061(10)
C64B3	0.0463(10)	1.0620(13)	0.0157(3)	0.058(10)
N10B3	0.1021(9)	1.0274(10)	0.0523(3)	0.047(7)
C68B3	0.0897(10)	1.0814(13)	0.0342(3)	0.071(11)
C67B3	0.1231(11)	1.1522(12)	0.0354(3)	0.072(12)
C69B3	0.1688(11)	1.1690(11)	0.0546(4)	0.077(12)
C70B3	0.1812(10)	1.1150(13)	0.0727(3)	0.086(13)
C71B3	0.1478(10)	1.0443(11)	0.0715(3)	0.043(8)
N11B3	0.3235(7)	0.8258(7)	0.1169(3)	0.029(6)
C75B3	0.2595(6)	0.8077(9)	0.1086(3)	0.046(9)
C76B3	0.2432(5)	0.7326(10)	0.1004(3)	0.041(8)
C77B3	0.2908(8)	0.6757(8)	0.1005(3)	0.062(10)

C78B3	0.3547(7)	0.6938(8)	0.1088(3)	0.024(7)
C79B3	0.3711(5)	0.7689(9)	0.1170(3)	0.031(7)
N12B3	0.4475(7)	0.8665(8)	0.1317(3)	0.025(6)
C83B3	0.4333(6)	0.7893(9)	0.1251(3)	0.040(8)
C82B3	0.4826(8)	0.7342(7)	0.1262(3)	0.035(8)
C84B3	0.5461(7)	0.7562(9)	0.1339(3)	0.048(9)
C85B3	0.5603(6)	0.8334(10)	0.1405(3)	0.041(8)
C86B3	0.5110(8)	0.8886(7)	0.1394(3)	0.041(8)
C1B3	0.3054(18)	0.873(2)	0.1768(7)	0.073(12)
C7B3	0.2498(14)	1.1918(11)	0.1444(4)	0.064(11)
C8B3	0.2724(18)	1.2151(12)	0.1241(5)	0.097(15)
C14B3	0.4307(11)	1.0050(14)	0.0834(4)	0.020(6)
C15B3	0.3938(11)	0.9415(16)	0.0682(4)	0.026(7)
C16B3	0.4462(12)	0.8877(15)	0.0571(5)	0.026(7)
C22B3	0.3137(16)	0.648(2)	0.0033(6)	0.057(10)
C23B3	0.2867(17)	0.664(2)	-0.0190(7)	0.067(11)
C29B3	0.3311(14)	0.9738(19)	-0.0525(5)	0.050(9)
C30B3	0.535(2)	0.912(3)	-0.0026(8)	0.103(15)
C36B3	0.4804(8)	1.2071(10)	0.0335(6)	0.070(11)
C37B3	0.4156(7)	1.2286(10)	0.0303(6)	0.071(11)
C43B3	0.2288(14)	1.0068(17)	-0.0056(5)	0.041(8)
C44B3	0.2187(13)	0.9477(17)	0.0127(5)	0.035(7)
C45B3	0.1657(14)	0.8954(17)	0.0061(5)	0.038(8)
C51B3	0.1353(13)	0.6362(17)	0.0637(5)	0.033(8)
C52B3	0.0962(18)	0.648(2)	0.0805(7)	0.072(11)
C58B3	-0.0360(19)	0.937(3)	0.0829(7)	0.092(13)
C59B3	-0.059(3)	0.886(3)	-0.0008(10)	0.15(2)
C65B3	0.0675(16)	1.1807(14)	-0.0031(4)	0.092(14)
C66B3	0.110(2)	1.2028(15)	0.0166(5)	0.13(2)
C72B3	0.1524(15)	0.984(2)	0.0911(6)	0.056(9)
C73B3	0.2053(13)	0.9279(18)	0.0889(5)	0.040(8)
C74B3	0.2116(16)	0.8693(19)	0.1100(6)	0.055(10)
C80B3	0.4044(6)	0.6393(9)	0.1092(5)	0.040(8)
C81B3	0.4676(7)	0.6586(9)	0.1181(5)	0.045(9)
C87B3	0.5236(13)	0.9685(16)	0.1472(5)	0.033(7)
As14	0.34157(17)	0.41108(19)	0.91145(6)	0.047(1)
O14	0.2669(9)	0.3584(11)	0.9137(3)	0.039(5)
O24	0.3103(8)	0.4298(12)	0.8810(3)	0.039(5)
O34	0.3814(10)	0.3206(13)	0.9022(4)	0.052(6)
O44	0.3739(11)	0.3858(14)	0.9417(4)	0.070(7)
O54	0.3087(8)	0.5057(11)	0.9218(3)	0.034(5)
O64	0.4120(10)	0.4660(13)	0.9075(4)	0.055(6)
C14	0.2291(9)	0.3488(13)	0.8931(3)	0.052(9)
C24	0.1730(10)	0.3050(12)	0.8876(3)	0.052(9)
C34	0.1411(8)	0.3037(11)	0.8649(3)	0.062(10)
C44	0.1653(8)	0.3462(12)	0.8477(3)	0.035(8)

C54	0.2215(9)	0.3900(11)	0.8532(3)	0.042(8)
C64	0.2534(8)	0.3913(11)	0.8759(3)	0.040(8)
C74	0.3933(11)	0.2716(12)	0.9205(3)	0.068(11)
C84	0.4090(10)	0.1925(12)	0.9197(3)	0.042(8)
C94	0.4222(10)	0.1494(9)	0.9401(4)	0.053(9)
C104	0.4196(11)	0.1855(12)	0.9614(3)	0.068(11)
C114	0.4039(11)	0.2646(13)	0.9622(3)	0.061(10)
C124	0.3908(10)	0.3077(10)	0.9418(4)	0.046(9)
C134	0.3412(11)	0.5654(13)	0.9166(4)	0.095(15)
C144	0.3228(10)	0.6434(15)	0.9183(4)	0.066(11)
C154	0.3624(13)	0.7031(11)	0.9123(4)	0.084(13)
C164	0.4204(12)	0.6849(14)	0.9045(5)	0.082(13)
C174	0.4388(10)	0.6070(16)	0.9029(4)	0.116(17)
C184	0.3992(12)	0.5473(12)	0.9089(4)	0.044(9)
As25	0.83198(16)	0.7859(2)	0.78133(7)	0.053(1)
O1A5	0.7917(10)	0.7054(13)	0.7639(4)	0.056(6)
O2A5	0.7600(9)	0.8044(11)	0.7944(3)	0.039(5)
O3A5	0.8032(12)	0.8631(15)	0.7599(4)	0.078(8)
O4A5	0.8983(10)	0.7685(13)	0.7644(4)	0.051(6)
O5A5	0.8638(9)	0.7108(11)	0.8031(3)	0.035(5)
O6A5	0.8721(11)	0.8592(14)	0.8000(4)	0.063(7)
C1A5	0.7324(9)	0.6959(14)	0.7707(4)	0.048(9)
C2A5	0.6905(13)	0.6344(13)	0.7635(4)	0.066(11)
C3A5	0.6331(12)	0.6265(14)	0.7727(5)	0.19(3)
C4A5	0.6176(10)	0.6800(17)	0.7890(5)	0.079(12)
C5A5	0.6595(12)	0.7415(14)	0.7962(4)	0.081(13)
C6A5	0.7169(10)	0.7494(12)	0.7871(4)	0.048(9)
C7A5	0.8420(12)	0.8604(16)	0.7447(4)	0.053(9)
C8A5	0.8285(12)	0.9088(15)	0.7254(5)	0.096(14)
C9A5	0.8674(16)	0.9066(18)	0.7080(4)	0.13(2)
C10A5	0.9199(14)	0.856(2)	0.7099(5)	0.107(16)
C11A5	0.9335(12)	0.8073(17)	0.7293(6)	0.131(19)
C12A5	0.8945(13)	0.8096(15)	0.7466(4)	0.082(13)
C13A5	0.9017(10)	0.7409(13)	0.8203(4)	0.040(8)
C14A5	0.9287(12)	0.7015(10)	0.8404(4)	0.070(11)
C15A5	0.9636(12)	0.7429(15)	0.8587(3)	0.106(16)
C16A5	0.9714(11)	0.8236(14)	0.8569(4)	0.069(11)
C17A5	0.9444(11)	0.8629(10)	0.8369(4)	0.055(10)
C18A5	0.9096(11)	0.8216(13)	0.8186(3)	0.088(13)
As36	0.15099(16)	0.2677(2)	0.60890(6)	0.048(1)
O1B6	0.1255(10)	0.3238(13)	0.5812(4)	0.051(6)
O2B6	0.1454(9)	0.1794(12)	0.5913(4)	0.046(6)
O3B6	0.0694(8)	0.2448(10)	0.6157(3)	0.028(5)
O4B6	0.1461(10)	0.3603(13)	0.6254(4)	0.055(6)
O5B6	0.2344(10)	0.2852(13)	0.6046(4)	0.052(6)
O6B6	0.1879(9)	0.2071(12)	0.6352(3)	0.044(5)

C1B6	0.1091(11)	0.2734(11)	0.5639(4)	0.069(11)
C2B6	0.0850(11)	0.2937(11)	0.5411(4)	0.072(11)
C3B6	0.0725(11)	0.2357(15)	0.5242(3)	0.065(11)
C4B6	0.0843(12)	0.1575(13)	0.5301(4)	0.080(12)
C5B6	0.1085(11)	0.1371(10)	0.5529(4)	0.072(12)
C6B6	0.1209(10)	0.1951(13)	0.5698(3)	0.033(8)
C7B6	0.0576(11)	0.2920(13)	0.6340(4)	0.057(10)
C8B6	0.0079(10)	0.2795(12)	0.6470(4)	0.065(11)
C9B6	0.0000(11)	0.3299(16)	0.6652(4)	0.097(15)
C10B6	0.0418(13)	0.3930(14)	0.6703(4)	0.078(12)
C11B6	0.0915(11)	0.4055(12)	0.6573(4)	0.081(12)
C12B6	0.0994(10)	0.3550(14)	0.6392(4)	0.062(10)
C13B6	0.2757(9)	0.2443(12)	0.6203(3)	0.083(13)
C14B6	0.3422(9)	0.2422(11)	0.6205(3)	0.031(7)
C15B6	0.3813(7)	0.2030(13)	0.6382(4)	0.058(10)
C16B6	0.3540(9)	0.1660(13)	0.6557(3)	0.073(12)
C17B6	0.2875(9)	0.1681(12)	0.6555(3)	0.050(9)
C18B6	0.2484(7)	0.2073(12)	0.6377(4)	0.029(7)
As47	0.14502(16)	0.8107(2)	0.56028(7)	0.049(1)
O1C7	0.0558(10)	0.7980(13)	0.5550(4)	0.062(7)
O2C7	0.1386(10)	0.8703(12)	0.5329(4)	0.050(6)
O3C7	0.1606(9)	0.7200(12)	0.5432(4)	0.047(6)
O4C7	0.1406(9)	0.7485(12)	0.5851(3)	0.046(6)
O5C7	0.1381(11)	0.8933(14)	0.5797(4)	0.066(7)
O6C7	0.2339(9)	0.8256(11)	0.5646(3)	0.039(5)
C1C7	0.0338(11)	0.8514(13)	0.5370(4)	0.076(12)
C2C7	-0.0318(10)	0.8657(13)	0.5305(4)	0.064(11)
C3C7	-0.0524(7)	0.9165(13)	0.5123(4)	0.043(8)
C4C7	-0.0075(9)	0.9531(12)	0.5005(3)	0.057(10)
C5C7	0.0580(8)	0.9389(13)	0.5070(4)	0.059(10)
C6C7	0.0787(7)	0.8880(14)	0.5253(4)	0.055(10)
C7C7	0.1504(10)	0.6577(11)	0.5559(3)	0.034(8)
C8C7	0.1517(11)	0.5807(13)	0.5481(3)	0.080(13)
C9C7	0.1470(11)	0.5189(9)	0.5633(4)	0.051(9)
C10C7	0.1409(11)	0.5341(11)	0.5864(4)	0.062(10)
C11C7	0.1395(12)	0.6111(14)	0.5942(3)	0.083(13)
C12C7	0.1442(10)	0.6729(10)	0.5789(4)	0.045(9)
C13C7	0.1942(9)	0.9303(16)	0.5823(5)	0.069(11)
C14C7	0.2024(12)	1.0000(16)	0.5948(5)	0.101(15)
C15C7	0.2638(15)	1.0312(14)	0.6010(5)	0.119(18)
C16C7	0.3172(11)	0.9927(16)	0.5947(5)	0.121(17)
C17C7	0.3090(9)	0.9230(15)	0.5822(4)	0.060(10)
C18C7	0.2475(11)	0.8918(12)	0.5760(4)	0.058(10)
As58	0.36107(15)	0.48016(18)	0.40433(6)	0.040(1)
O1D8	0.3165(9)	0.5472(11)	0.3836(3)	0.038(5)
O2D8	0.3784(9)	0.4212(12)	0.3803(3)	0.050(6)

O3D8	0.2920(8)	0.4193(11)	0.4058(3)	0.036(5)
O4D8	0.3367(10)	0.5414(12)	0.4282(4)	0.051(6)
O5D8	0.4127(9)	0.4117(12)	0.4234(3)	0.049(6)
O6D8	0.4338(9)	0.5449(11)	0.4047(3)	0.041(5)
C1D8	0.3149(10)	0.5167(11)	0.3625(3)	0.028(7)
C2D8	0.2795(10)	0.5512(11)	0.3430(4)	0.073(12)
C3D8	0.2770(12)	0.5158(15)	0.3214(3)	0.098(15)
C4D8	0.3099(12)	0.4459(15)	0.3192(3)	0.084(12)
C5D8	0.3452(10)	0.4115(11)	0.3387(4)	0.058(10)
C6D8	0.3477(9)	0.4469(12)	0.3604(3)	0.042(8)
C7D8	0.2594(10)	0.4433(13)	0.4226(3)	0.036(7)
C8D8	0.2035(11)	0.4089(14)	0.4282(5)	0.111(16)
C9D8	0.1772(11)	0.4353(18)	0.4474(5)	0.109(16)
C10D8	0.2067(14)	0.4962(19)	0.4609(4)	0.117(17)
C11D8	0.2625(13)	0.5306(14)	0.4553(4)	0.116(17)
C12D8	0.2889(9)	0.5041(12)	0.4361(4)	0.037(8)
C13D8	0.4673(8)	0.4389(12)	0.4315(4)	0.031(7)
C14D8	0.5122(12)	0.4065(12)	0.4488(4)	0.103(15)
C15D8	0.5688(10)	0.4468(16)	0.4569(4)	0.094(14)
C16D8	0.5805(9)	0.5196(15)	0.4475(4)	0.079(12)
C17D8	0.5356(11)	0.5520(11)	0.4301(4)	0.083(13)
C18D8	0.4790(10)	0.5117(12)	0.4221(3)	0.050(9)
As69	0.19946(16)	0.84383(19)	0.24020(6)	0.043(1)
O1E9	0.2262(9)	0.8912(11)	0.2685(3)	0.037(5)
O2E9	0.2848(8)	0.8434(10)	0.2347(3)	0.030(5)
O3E9	0.1861(9)	0.9407(12)	0.2256(3)	0.041(5)
O4E9	0.1157(10)	0.8454(13)	0.2452(4)	0.053(6)
O5E9	0.1735(9)	0.7962(12)	0.2125(3)	0.045(6)
O6E9	0.2089(9)	0.7464(12)	0.2557(4)	0.047(6)
C1E9	0.2863(7)	0.9203(13)	0.2687(4)	0.054(9)
C2E9	0.3181(9)	0.9672(13)	0.2863(3)	0.047(9)
C3E9	0.3810(9)	0.9918(12)	0.2854(3)	0.070(11)
C4E9	0.4121(7)	0.9694(13)	0.2669(4)	0.053(9)
C5E9	0.3802(9)	0.9225(12)	0.2493(3)	0.046(9)
C6E9	0.3173(9)	0.8979(12)	0.2502(3)	0.053(9)
C7E9	0.1328(8)	0.9707(12)	0.2308(4)	0.040(8)
C8E9	0.1126(9)	1.0467(11)	0.2249(4)	0.051(9)
C9E9	0.0531(10)	1.0731(10)	0.2296(4)	0.076(12)
C10E9	0.0138(8)	1.0235(13)	0.2404(4)	0.061(10)
C11E9	0.0341(9)	0.9476(12)	0.2464(4)	0.060(10)
C12E9	0.0935(10)	0.9212(10)	0.2416(4)	0.051(9)
C13E9	0.1659(12)	0.7173(10)	0.2166(4)	0.060(10)
C14E9	0.1456(12)	0.6626(14)	0.1994(3)	0.099(15)
C15E9	0.1390(11)	0.5842(12)	0.2052(3)	0.050(9)
C16E9	0.1525(10)	0.5606(9)	0.2283(4)	0.051(9)
C17E9	0.1728(10)	0.6154(12)	0.2455(3)	0.041(8)

C18E9	0.1795(10)	0.6937(10)	0.2397(3)	0.045(9)
As710	0.32515(16)	0.45081(18)	0.75132(7)	0.049(1)
O1F10	0.3992(9)	0.5028(12)	0.7537(3)	0.045(6)
O2F10	0.3680(9)	0.3793(11)	0.7726(3)	0.041(5)
O3F10	0.3432(10)	0.3916(12)	0.7274(4)	0.047(6)
O4F10	0.2925(9)	0.5212(12)	0.7286(3)	0.046(6)
O5F10	0.2466(10)	0.4013(12)	0.7508(4)	0.052(6)
O6F10	0.3039(9)	0.5172(12)	0.7742(3)	0.047(6)
C1F10	0.4444(8)	0.4752(10)	0.7703(3)	0.034(7)
C2F10	0.5035(9)	0.5084(9)	0.7793(3)	0.047(9)
C3F10	0.5432(7)	0.4715(12)	0.7974(3)	0.050(9)
C4F10	0.5239(9)	0.4014(12)	0.8064(3)	0.085(13)
C5F10	0.4648(9)	0.3682(9)	0.7975(3)	0.046(9)
C6F10	0.4250(7)	0.4051(10)	0.7794(3)	0.027(7)
C7F10	0.3129(10)	0.4139(12)	0.7057(3)	0.058(10)
C8F10	0.3061(10)	0.3740(9)	0.6846(4)	0.062(11)
C9F10	0.2750(10)	0.4098(12)	0.6645(3)	0.044(8)
C10F10	0.2508(9)	0.4855(12)	0.6655(3)	0.050(9)
C11F10	0.2577(10)	0.5254(10)	0.6866(4)	0.058(10)
C12F10	0.2887(10)	0.4896(12)	0.7067(3)	0.042(8)
C13F10	0.2167(11)	0.4270(14)	0.7673(4)	0.071(11)
C14F10	0.1575(12)	0.3996(13)	0.7721(4)	0.081(12)
C15F10	0.1282(9)	0.4346(16)	0.7894(5)	0.127(18)
C16F10	0.1582(11)	0.4972(15)	0.8020(4)	0.069(11)
C17F10	0.2175(11)	0.5246(12)	0.7973(4)	0.065(11)
C18F10	0.2467(8)	0.4895(13)	0.7800(4)	0.041(8)
As811	0.90257(16)	0.4938(2)	0.08064(6)	0.054(1)
O1G11	0.8881(8)	0.5421(10)	0.1061(3)	0.030(5)
O2G11	0.9846(10)	0.4728(14)	0.0940(4)	0.062(6)
O3G11	0.9320(10)	0.5838(13)	0.0669(4)	0.058(6)
O4G11	0.8182(10)	0.5195(13)	0.0689(4)	0.054(6)
O5G11	0.8696(10)	0.4025(12)	0.0925(4)	0.051(6)
O6G11	0.9219(12)	0.4391(17)	0.0555(4)	0.086(8)
C1G11	0.9436(8)	0.5583(13)	0.1207(4)	0.038(8)
C2G11	0.9504(10)	0.6078(13)	0.1399(4)	0.057(10)
C3G11	1.0110(13)	0.6198(15)	0.1528(4)	0.115(17)
C4G11	1.0648(9)	0.5823(17)	0.1465(4)	0.113(17)
C5G11	1.0579(9)	0.5328(15)	0.1273(4)	0.061(10)
C6G11	0.9973(11)	0.5208(13)	0.1144(4)	0.069(11)
C7G11	0.8801(9)	0.6328(14)	0.0607(4)	0.063(11)
C8G11	0.8848(9)	0.7097(14)	0.0532(4)	0.098(15)
C9G11	0.8296(11)	0.7554(11)	0.0481(4)	0.063(10)
C10G11	0.7696(9)	0.7242(12)	0.0505(4)	0.061(10)
C11G11	0.7648(8)	0.6473(13)	0.0581(4)	0.054(9)
C12G11	0.8201(11)	0.6016(10)	0.0632(4)	0.053(9)
C13G11	0.8866(15)	0.3399(19)	0.0806(6)	0.096(14)

C14G11	0.8861(16)	0.264(2)	0.0891(5)	0.104(15)
C15G11	0.912(2)	0.2029(17)	0.0776(8)	0.31(5)
C16G11	0.939(2)	0.218(2)	0.0576(8)	0.16(2)
C17G11	0.9397(17)	0.295(3)	0.0491(5)	0.20(3)
C18G11	0.9134(17)	0.355(2)	0.0606(6)	0.100(15)
As912	0.27720(17)	0.4320(2)	0.04871(10)	0.083(2)
O1H12	0.3366(12)	0.3556(15)	0.0618(4)	0.078(8)
O2H12	0.3456(8)	0.4935(10)	0.0496(3)	0.026(4)
O3H12	0.2246(10)	0.5072(12)	0.0327(4)	0.050(6)
O4H12	0.2884(12)	0.3939(15)	0.0180(4)	0.074(8)
O5H12	0.2110(13)	0.3584(17)	0.0450(5)	0.090(9)
O6H12	0.2665(13)	0.4582(17)	0.0726(5)	0.091(9)
C1H12	0.3933(8)	0.3883(13)	0.0684(4)	0.048(9)
C2H12	0.4449(11)	0.3483(10)	0.0810(4)	0.114(17)
C3H12	0.5039(9)	0.3860(12)	0.0871(4)	0.050(9)
C4H12	0.5111(8)	0.4637(12)	0.0807(4)	0.055(10)
C5H12	0.4595(10)	0.5038(10)	0.0682(4)	0.062(10)
C6H12	0.4006(8)	0.4661(13)	0.0621(4)	0.058(10)
C7H12	0.2136(12)	0.4852(16)	0.0098(3)	0.104(15)
C8H12	0.1722(11)	0.5326(13)	-0.0051(4)	0.064(11)
C9H12	0.1685(11)	0.5239(13)	-0.0290(4)	0.057(10)
C10H12	0.2061(13)	0.4677(16)	-0.0380(3)	0.103(15)
C11H12	0.2475(11)	0.4203(13)	-0.0231(5)	0.088(13)
C12H12	0.2512(11)	0.4290(14)	0.0008(4)	0.056(9)
C13H12	0.1947(18)	0.376(2)	0.0664(6)	0.097(15)
C14H12	0.1378(18)	0.336(2)	0.0683(6)	0.15(2)
C15H12	0.1125(15)	0.337(2)	0.0891(8)	0.14(2)
C16H12	0.144(2)	0.379(2)	0.1080(6)	0.126(19)
C17H12	0.201(2)	0.419(2)	0.1061(6)	0.30(5)
C18H12	0.2262(15)	0.418(2)	0.0853(8)	0.119(17)
O(1W)	0.0292(7)	0.2251(9)	0.7451(3)	0.013(4)
O(2W)	0.0713(7)	0.2564(9)	0.4076(3)	0.014(4)
O(3W)	0.0608(7)	0.2033(9)	0.7933(3)	0.019(4)
O(4W)	0.0999(7)	0.9353(10)	0.1483(3)	0.022(4)
O(5W)	0.3854(7)	0.7299(8)	0.5299(2)	0.008(4)
O(6W)	0.4443(7)	0.1858(10)	0.3108(3)	0.021(4)
O(7W)	0.0200(8)	0.8435(10)	0.1751(3)	0.027(4)
O(8W)	-0.0357(9)	0.2551(11)	0.3696(3)	0.038(5)
O(9W)	0.1318(8)	0.8160(11)	0.4693(3)	0.034(5)
H3A1	0.6235	0.8209	0.8624	0.061
H4A1	0.5929	0.6989	0.8458	0.059
H11A1	0.3003	0.6599	0.7886	0.046
H12A1	0.2316	0.7686	0.7871	0.045
H18A1	0.2428	1.1797	0.7853	0.041
H19A1	0.2352	1.2665	0.7538	0.053
H26A1	0.0942	1.1426	0.6513	0.074

H27A1	0.0561	1.0134	0.6486	0.068
H32A1	-0.0170	0.9032	0.7915	0.076
H33A1	0.0181	0.7736	0.7978	0.058
H40A1	0.2301	0.6363	0.7353	0.102
H41A1	0.2799	0.7249	0.7127	0.078
H47A1	0.2984	1.1433	0.7127	0.114
H48A1	0.3618	1.2455	0.7307	0.082
H55A1	0.6738	1.1694	0.7621	0.106
H56A1	0.7093	1.0419	0.7560	0.132
H61A1	0.4276	0.8976	0.6329	0.072
H62A1	0.3841	0.7742	0.6392	0.065
H69A1	0.4098	0.6492	0.7504	0.064
H70A1	0.4522	0.7387	0.7792	0.080
H76A1	0.4451	1.1470	0.7800	0.046
H77A1	0.3751	1.2373	0.7934	0.059
H84A1	0.2262	1.1305	0.8813	0.028
H85A1	0.2417	1.0019	0.8952	0.049
H1A1	0.5111	0.9877	0.8604	0.049
H1B1	0.5826	0.9791	0.8541	0.049
H1C1	0.5681	0.9550	0.8794	0.049
H7A1	0.5131	0.6139	0.8256	0.063
H8A1	0.4010	0.5931	0.8057	0.067
H14A1	0.2581	0.9348	0.8209	0.059
H14B1	0.2058	0.8851	0.8042	0.059
H15A1	0.3001	0.9899	0.7870	0.048
H15B1	0.2494	0.9380	0.7699	0.048
H16A1	0.1620	1.0034	0.7851	0.045
H16B1	0.2136	1.0573	0.8009	0.045
H22A1	0.1882	1.2981	0.7113	0.034
H23A1	0.1528	1.2530	0.6772	0.065
H29A1	0.0396	0.8902	0.6674	0.096
H29B1	0.0271	0.9053	0.6935	0.096
H29C1	0.0940	0.8679	0.6887	0.096
H30A1	-0.0161	1.0281	0.7692	0.096
H30B1	-0.0012	1.0123	0.7433	0.096
H30C1	0.0537	1.0479	0.7626	0.096
H37A1	0.1513	0.6116	0.7619	0.071
H36A1	0.0833	0.6626	0.7866	0.091
H43A1	0.2813	0.8590	0.6945	0.057
H43B1	0.2206	0.9137	0.6966	0.057
H44A1	0.2766	0.9770	0.7291	0.102
H44B1	0.3363	0.9179	0.7295	0.102
H45A1	0.3581	0.9672	0.6942	0.060
H45B1	0.2959	1.0225	0.6922	0.060
H51A1	0.4720	1.2865	0.7529	0.121
H52A1	0.5830	1.2668	0.7565	0.157

H58A1	0.6896	0.9099	0.7427	0.124
H58B1	0.6325	0.9006	0.7213	0.124
H58C1	0.6203	0.8790	0.7471	0.124
H59A1	0.4831	1.0169	0.6475	0.110
H59B1	0.5363	1.0008	0.6697	0.110
H59C1	0.4692	1.0414	0.6729	0.110
H65A1	0.3596	0.6604	0.6708	0.068
H66A1	0.3797	0.6181	0.7074	0.051
H72A1	0.5379	0.9044	0.7705	0.053
H72B1	0.5117	0.8511	0.7898	0.053
H73A1	0.4371	0.9738	0.7646	0.049
H73B1	0.4122	0.9214	0.7844	0.049
H74A1	0.5170	1.0270	0.7913	0.049
H74B1	0.4981	0.9704	0.8112	0.049
H80A1	0.2844	1.2703	0.8227	0.067
H81A1	0.2445	1.2320	0.8551	0.058
H87A1	0.2867	0.8811	0.8941	0.068
H87B1	0.3599	0.8812	0.8891	0.068
H87C1	0.3029	0.8547	0.8692	0.068
H3AA2	0.1385	1.0411	0.2772	0.043
H4AA2	0.1710	1.1718	0.2832	0.060
H11B2	0.2497	1.2948	0.3919	0.097
H12B2	0.2446	1.2040	0.4218	0.048
H18B2	0.2277	0.7866	0.4319	0.049
H19B2	0.3028	0.6844	0.4386	0.074
H26B2	0.5905	0.7652	0.4942	0.054
H27B2	0.6113	0.8928	0.5082	0.055
H32B2	0.2052	1.0323	0.5277	0.098
H33B2	0.1946	1.1649	0.5175	0.125
H40B2	0.3685	1.3000	0.4412	0.055
H41B2	0.4477	1.2187	0.4293	0.041
H47B2	0.4712	0.7962	0.4338	0.071
H48B2	0.4418	0.6936	0.4076	0.056
H55B2	0.4743	0.7481	0.2985	0.030
H56B2	0.5193	0.8665	0.2883	0.053
H61B2	0.7330	1.0866	0.4141	0.068
H62B2	0.6870	1.2090	0.4198	0.059
H69B2	0.3865	1.2726	0.3763	0.067
H70B2	0.3271	1.1719	0.3557	0.040
H76B2	0.3224	0.7536	0.3613	0.041
H77B2	0.2647	0.6712	0.3831	0.048
H84B2	0.0060	0.8204	0.4229	0.042
H85B2	-0.0265	0.9459	0.4096	0.050
H1AA2	0.1110	0.9148	0.2915	0.088
H1AB2	0.0799	0.9207	0.3150	0.088
H1AC2	0.1528	0.8916	0.3159	0.088

H7AA2	0.2186	1.2782	0.3125	0.065
H8AA2	0.2243	1.3267	0.3464	0.062
H14C2	0.1603	1.0371	0.4147	0.046
H14D2	0.2034	1.0926	0.4328	0.046
H15C2	0.2544	0.9596	0.4103	0.048
H15D2	0.2982	1.0158	0.4281	0.048
H16C2	0.1973	0.9256	0.4398	0.046
H16D2	0.2464	0.9767	0.4572	0.046
H22B2	0.4103	0.6383	0.4564	0.040
H23B2	0.5158	0.6697	0.4736	0.056
H29D2	0.5786	1.0255	0.5134	0.047
H29E2	0.5049	1.0336	0.5174	0.047
H29F2	0.5253	1.0562	0.4928	0.047
H30D2	0.3112	0.9037	0.5053	0.091
H30E2	0.2362	0.9052	0.5079	0.091
H30F2	0.2896	0.9214	0.5301	0.091
H36B2	0.2220	1.2761	0.4924	0.049
H37B2	0.2799	1.3261	0.4650	0.067
H43C2	0.5067	1.0448	0.4583	0.045
H43D2	0.5157	1.0947	0.4357	0.045
H44C2	0.4230	0.9651	0.4349	0.049
H44D2	0.4333	1.0145	0.4122	0.049
H45C2	0.5306	0.9267	0.4394	0.063
H45D2	0.5406	0.9755	0.4168	0.063
H51B2	0.4194	0.6442	0.3651	0.029
H52B2	0.4387	0.6607	0.3291	0.040
H58D2	0.5580	0.9990	0.2987	0.075
H58E2	0.5947	1.0041	0.3248	0.075
H58F2	0.5228	1.0375	0.3186	0.075
H59D2	0.7213	0.9543	0.3988	0.071
H59E2	0.6751	0.9502	0.3743	0.071
H59F2	0.6493	0.9211	0.3975	0.071
H65B2	0.5951	1.2994	0.4130	0.038
H66B2	0.4909	1.3223	0.3985	0.058
H72C2	0.3969	0.9955	0.3408	0.047
H72D2	0.3332	1.0476	0.3358	0.047
H73C2	0.3004	1.0009	0.3709	0.024
H73D2	0.3639	0.9475	0.3754	0.024
H74C2	0.2609	0.9245	0.3357	0.062
H74D2	0.3249	0.8718	0.3397	0.062
H80B2	0.1654	0.6504	0.4015	0.068
H81B2	0.0928	0.6989	0.4226	0.081
H87D2	-0.0154	1.0569	0.3884	0.063
H87E2	0.0105	1.0414	0.3643	0.063
H87F2	0.0572	1.0796	0.3856	0.063
H3BA3	0.2359	1.0020	0.1958	0.044

H4BA3	0.2154	1.1291	0.1814	0.112
H11C3	0.3264	1.2380	0.0866	0.056
H12C3	0.3898	1.1501	0.0689	0.081
H18C3	0.4290	0.7349	0.0691	0.087
H19C3	0.3746	0.6378	0.0454	0.065
H26C3	0.2280	0.7370	-0.0589	0.062
H27C3	0.2454	0.8643	-0.0718	0.052
H32C3	0.6217	1.0192	0.0215	0.048
H33C3	0.5972	1.1435	0.0350	0.070
H40C3	0.2914	1.2493	0.0198	0.132
H41C3	0.2132	1.1582	0.0042	0.101
H47C3	0.2238	0.7572	0.0093	0.076
H48C3	0.2089	0.6496	0.0329	0.071
H55B3	0.0174	0.6913	0.1114	0.214
H56B3	-0.0363	0.8114	0.1127	0.111
H61B3	-0.0654	0.9947	-0.0365	0.201
H62B3	-0.0149	1.1172	-0.0367	0.088
H69C3	0.1916	1.2174	0.0555	0.093
H70C3	0.2124	1.1265	0.0858	0.103
H76C3	0.1994	0.7203	0.0947	0.050
H77C3	0.2796	0.6244	0.0949	0.075
H84C3	0.5798	0.7185	0.1346	0.058
H85C3	0.6037	0.8485	0.1457	0.049
H1BA3	0.3310	0.8524	0.1654	0.109
H1BB3	0.2649	0.8440	0.1759	0.109
H1BC3	0.3298	0.8688	0.1924	0.109
H7BA3	0.2239	1.2267	0.1518	0.077
H8BA3	0.2620	1.2659	0.1179	0.117
H14E3	0.4578	0.9802	0.0968	0.024
H14F3	0.4595	1.0337	0.0742	0.024
H15E3	0.3633	0.9660	0.0556	0.031
H15F3	0.3688	0.9085	0.0777	0.031
H16E3	0.4676	0.9198	0.0463	0.031
H16F3	0.4797	0.8689	0.0697	0.031
H22C3	0.3078	0.5985	0.0100	0.069
H23C3	0.2665	0.6229	-0.0285	0.080
H29G3	0.3056	0.9854	-0.0676	0.074
H29H3	0.3770	0.9709	-0.0542	0.074
H29I3	0.3248	1.0155	-0.0414	0.074
H30G3	0.4927	0.8875	-0.0068	0.155
H30H3	0.5643	0.8753	0.0067	0.155
H30I3	0.5529	0.9254	-0.0168	0.155
H36C3	0.5121	1.2436	0.0403	0.084
H37C3	0.4037	1.2801	0.0342	0.085
H43E3	0.2436	0.9792	-0.0189	0.050
H43F3	0.1870	1.0322	-0.0114	0.050

H44E3	0.2587	0.9163	0.0166	0.042
H44F3	0.2115	0.9761	0.0270	0.042
H45E3	0.1695	0.8746	-0.0095	0.046
H45F3	0.1255	0.9268	0.0046	0.046
H51D3	0.1573	0.5881	0.0620	0.039
H52C3	0.0946	0.6074	0.0916	0.086
H58G3	-0.0630	0.9417	0.0952	0.137
H58H3	-0.0628	0.9438	0.0677	0.137
H58I3	-0.0024	0.9775	0.0849	0.137
H59G3	-0.0869	0.8731	-0.0152	0.218
H59H3	-0.0846	0.8905	0.0119	0.218
H59I3	-0.0262	0.8450	0.0029	0.218
H65C3	0.0612	1.2146	-0.0162	0.111
H66C3	0.1292	1.2532	0.0172	0.161
H72E3	0.1609	1.0107	0.1063	0.067
H72F3	0.1110	0.9551	0.0902	0.067
H73E3	0.2463	0.9566	0.0889	0.048
H73F3	0.1957	0.8985	0.0741	0.048
H74E3	0.2237	0.8991	0.1246	0.066
H74F3	0.1691	0.8446	0.1106	0.066
H80C3	0.3948	0.5880	0.1032	0.048
H81E3	0.5007	0.6201	0.1187	0.054
H87G3	0.5701	0.9754	0.1522	0.050
H87H3	0.5004	0.9793	0.1604	0.050
H87I3	0.5089	1.0048	0.1345	0.050
H2A4	0.1564	0.2759	0.8993	0.062
H3B4	0.1027	0.2737	0.8611	0.075
H4B4	0.1435	0.3453	0.8322	0.042
H5A4	0.2381	0.4191	0.8415	0.050
H8B4	0.4108	0.1679	0.9051	0.050
H9A4	0.4329	0.0954	0.9395	0.063
H10A4	0.4286	0.1560	0.9754	0.081
H11D4	0.4021	0.2892	0.9768	0.073
H14G4	0.2832	0.6558	0.9236	0.079
H15G4	0.3498	0.7564	0.9134	0.101
H16G4	0.4474	0.7258	0.9004	0.099
H17A4	0.4784	0.5946	0.8976	0.139
H2AA5	0.7011	0.5979	0.7523	0.080
H3AB5	0.6045	0.5845	0.7677	0.223
H4AB5	0.5784	0.6746	0.7953	0.095
H5AA5	0.6489	0.7781	0.8074	0.097
H8AB5	0.7926	0.9435	0.7241	0.115
H9AA5	0.8582	0.9397	0.6948	0.160
H10B5	0.9466	0.8543	0.6980	0.128
H11E5	0.9694	0.7727	0.7306	0.157
H14H5	0.9233	0.6464	0.8415	0.085

H15H5	0.9820	0.7160	0.8723	0.127
H16H5	0.9952	0.8519	0.8694	0.083
H17B5	0.9498	0.9181	0.8357	0.066
H2BA6	0.0769	0.3472	0.5371	0.087
H3BB6	0.0560	0.2496	0.5087	0.077
H4BB6	0.0758	0.1178	0.5186	0.096
H5BA6	0.1165	0.0836	0.5569	0.087
H8BB6	-0.0207	0.2364	0.6435	0.077
H9BA6	-0.0340	0.3214	0.6741	0.116
H10C6	0.0364	0.4275	0.6827	0.093
H11F6	0.1201	0.4486	0.6608	0.097
H14I6	0.3608	0.2675	0.6085	0.037
H15I6	0.4267	0.2016	0.6384	0.069
H16I6	0.3808	0.1392	0.6678	0.088
H17C6	0.2689	0.1428	0.6674	0.060
H2CA7	-0.0625	0.8406	0.5386	0.077
H3CA7	-0.0972	0.9263	0.5078	0.052
H4CA7	-0.0217	0.9879	0.4880	0.069
H5CA7	0.0887	0.9639	0.4989	0.070
H8CA7	0.1559	0.5703	0.5323	0.096
H9CA7	0.1479	0.4663	0.5580	0.062
H10D7	0.1376	0.4918	0.5968	0.074
H11G7	0.1353	0.6215	0.6099	0.100
H14J7	0.1659	1.0262	0.5992	0.121
H15J7	0.2694	1.0788	0.6096	0.142
H16J7	0.3592	1.0140	0.5989	0.145
H17D7	0.3455	0.8967	0.5779	0.072
H2DA8	0.2570	0.5990	0.3445	0.088
H3DA8	0.2528	0.5394	0.3080	0.118
H4DA8	0.3082	0.4218	0.3044	0.101
H5DA8	0.3677	0.3637	0.3372	0.069
H8DA8	0.1834	0.3673	0.4190	0.133
H9DA8	0.1390	0.4118	0.4513	0.131
H10E8	0.1887	0.5142	0.4741	0.141
H11H8	0.2827	0.5722	0.4645	0.139
H14K8	0.5042	0.3567	0.4552	0.123
H15K8	0.5996	0.4246	0.4688	0.113
H16K8	0.6192	0.5472	0.4530	0.095
H17E8	0.5436	0.6018	0.4238	0.100
H2EA9	0.2969	0.9825	0.2990	0.056
H3EA9	0.4028	1.0238	0.2975	0.084
H4EA9	0.4551	0.9861	0.2663	0.064
H5EA9	0.4014	0.9072	0.2367	0.056
H8EA9	0.1395	1.0806	0.2175	0.061
H9EA9	0.0393	1.1250	0.2256	0.091
H10F9	-0.0268	1.0416	0.2437	0.073

H11I9	0.0072	0.9137	0.2537	0.073
H14L9	0.1364	0.6787	0.1836	0.119
H15L9	0.1251	0.5467	0.1934	0.060
H16L9	0.1480	0.5070	0.2323	0.061
H17F9	0.1821	0.5992	0.2613	0.049
H2FA10	0.5167	0.5563	0.7731	0.057
H3FA10	0.5836	0.4942	0.8035	0.060
H4FA10	0.5511	0.3762	0.8188	0.102
H5FA10	0.4516	0.3203	0.8037	0.055
H8FA10	0.3226	0.3223	0.6839	0.075
H9FA10	0.2704	0.3825	0.6501	0.053
H10G10	0.2296	0.5100	0.6518	0.060
H11J10	0.2411	0.5771	0.6873	0.070
H14M10	0.1370	0.3568	0.7634	0.097
H15M10	0.0877	0.4159	0.7926	0.153
H16M10	0.1382	0.5211	0.8139	0.083
H17G10	0.2380	0.5673	0.8060	0.078
H2GA11	0.9137	0.6335	0.1442	0.069
H3GA11	1.0157	0.6537	0.1659	0.138
H4GA11	1.1062	0.5905	0.1553	0.136
H5GA11	1.0947	0.5071	0.1230	0.073
H8GA11	0.9258	0.7310	0.0515	0.118
H9GA11	0.8328	0.8080	0.0430	0.075
H10H11	0.7318	0.7555	0.0471	0.074
H11K11	0.7238	0.6260	0.0597	0.064
H14N11	0.8678	0.2532	0.1028	0.125
H15N11	0.9121	0.1508	0.0834	0.367
H16N11	0.9571	0.1768	0.0497	0.196
H17H11	0.9580	0.3051	0.0354	0.239
H2HA12	0.4400	0.2951	0.0853	0.137
H3HA12	0.5391	0.3586	0.0956	0.060
H4HA12	0.5514	0.4895	0.0849	0.066
H5HA12	0.4645	0.5569	0.0638	0.074
H8HA12	0.1465	0.5709	0.0011	0.076
H9HA12	0.1402	0.5563	-0.0392	0.069
H10I12	0.2036	0.4618	-0.0544	0.123
H11L12	0.2732	0.3819	-0.0293	0.106
H14O12	0.1163	0.3075	0.0554	0.186
H15O12	0.0736	0.3101	0.0903	0.170
H16O12	0.1266	0.3801	0.1222	0.151
H17I12	0.2223	0.4475	0.1190	0.356

Table 3. Anisotropic displacement parameters ($Å^2$) for nd1024_x.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cu11	0.042(2)	0.021(2)	0.044(2)	-0.0093(19)	0.0131(18)	-0.0034(18)
Cu21	0.041(2)	0.018(2)	0.048(2)	-0.0027(18)	0.0090(18)	0.0028(16)
Cu31	0.055(2)	0.018(2)	0.051(3)	0.0018(19)	0.0157(19)	0.0091(18)
Cu42	0.030(2)	0.0128(19)	0.062(3)	-0.0048(19)	0.0083(18)	-0.0015(17)
Cu52	0.042(2)	0.021(2)	0.043(2)	0.0024(19)	0.0129(18)	-0.0059(18)
Cu62	0.040(2)	0.0128(19)	0.048(2)	-0.0026(18)	0.0174(17)	-0.0021(17)
Cu73	0.043(2)	0.022(2)	0.050(2)	-0.0023(19)	0.0145(18)	0.0019(18)
Cu83	0.045(2)	0.020(2)	0.057(3)	0.004(2)	0.0162(19)	0.0052(18)
Cu93	0.046(2)	0.052(3)	0.073(3)	0.006(2)	0.001(2)	0.034(2)
As14	0.056(2)	0.024(2)	0.065(3)	-0.0029(18)	0.0184(19)	0.0051(16)
As25	0.047(2)	0.025(2)	0.090(3)	-0.0117(19)	0.025(2)	-0.0121(17)
As36	0.045(2)	0.042(2)	0.059(2)	0.0157(19)	0.0163(18)	0.0133(17)
As47	0.044(2)	0.041(2)	0.065(3)	0.0036(19)	0.0164(18)	0.0049(17)
As58	0.057(2)	0.0054(16)	0.057(2)	-0.0060(16)	0.0079(17)	-0.0023(16)
As69	0.048(2)	0.0246(19)	0.058(2)	0.0057(17)	0.0110(18)	-0.0052(16)
As710	0.057(2)	0.0106(18)	0.084(3)	0.0000(18)	0.0212(19)	0.0039(16)
As811	0.048(2)	0.055(3)	0.061(2)	0.011(2)	0.0089(18)	0.0080(19)
As912	0.041(2)	0.015(2)	0.199(5)	0.018(3)	0.035(3)	0.0071(17)

Table 4. Bond lengths [Å] for nd1024_x.

atom-atom	distance	atom-atom	distance
Cu11-N11	2.000(13)	Cu11-N111	2.003(13)
Cu11-N121	2.029(12)	Cu11-N21	2.058(13)
Cu21-N31	2.006(12)	Cu21-N51	2.003(13)
Cu21-N41	2.007(13)	Cu21-N61	2.069(15)
Cu31-N81	1.961(19)	Cu31-N71	1.992(13)
Cu31-N91	2.040(17)	Cu31-N101	2.057(15)
N11-C21	1.3900	N11-C61	1.3900
C21-C31	1.3900	C21-C11	1.52(3)
C31-C41	1.3900	C41-C51	1.3900
C51-C61	1.3900	C51-C71	1.40(4)
C61-C101	1.319(17)	N21-C101	1.3900
N21-C131	1.3900	C101-C91	1.3900
C91-C111	1.3900	C91-C81	1.42(4)
C111-C121	1.3900	C121-C131	1.3900
C131-C141	1.44(3)	N31-C171	1.3900
N31-C211	1.3900	C171-C181	1.3900
C171-C161	1.47(3)	C181-C191	1.3900
C191-C201	1.3900	C201-C211	1.3900
C201-C221	1.49(3)	C211-C251	1.345(17)
N41-C251	1.3900	N41-C281	1.3900
C251-C241	1.3900	C241-C261	1.3900
C241-C231	1.47(4)	C261-C271	1.3900
C271-C281	1.3900	C281-C291	1.46(4)
N51-C311	1.3900	N51-C351	1.3900
C311-C321	1.3900	C311-C301	1.53(4)
C321-C331	1.3900	C331-C341	1.3900
C341-C351	1.3900	C341-C361	1.391(7)
C351-C391	1.335(16)	N61-C391	1.3900
N61-C421	1.3900	C391-C381	1.3900
C381-C401	1.3900	C381-C371	1.391(7)
C401-C411	1.3900	C411-C421	1.3900
C421-C431	1.55(3)	N71-C461	1.3900
N71-C501	1.3900	C461-C471	1.3900
C461-C451	1.46(3)	C471-C481	1.3900
C481-C491	1.3900	C491-C501	1.3900
C491-C511	1.391(7)	C501-C541	1.325(19)
N81-C541	1.3900	N81-C571	1.3900
C541-C531	1.3900	C531-C521	1.388(7)
C531-C551	1.3900	C551-C561	1.3900
C561-C571	1.3900	C571-C581	1.53(4)
N91-C601	1.3900	N91-C641	1.3900
C601-C611	1.3900	C601-C591	1.54(4)

C611-C621	1.3900	C621-C631	1.3900
C631-C641	1.3900	C631-C651	1.57(4)
C641-C681	1.42(2)	N101-C681	1.3900
N101-C711	1.3900	C681-C671	1.3900
C671-C691	1.3900	C671-C661	1.43(3)
C691-C701	1.3900	C701-C711	1.3900
C711-C721	1.47(3)	N111-C751	1.3900
N111-C791	1.3900	C751-C761	1.3900
C751-C741	1.51(3)	C761-C771	1.3900
C771-C781	1.3900	C781-C791	1.3900
C781-C801	1.62(4)	C791-C831	1.361(17)
N121-C831	1.3900	N121-C861	1.3900
C831-C821	1.3900	C821-C841	1.3900
C821-C811	1.41(3)	C841-C851	1.3900
C851-C861	1.3900	C861-C871	1.45(3)
C71-C81	1.49(4)	C141-C151	1.62(4)
C151-C161	1.54(4)	C221-C231	1.24(4)
C371-C361	1.389(7)	C431-C441	1.52(5)
C441-C451	1.49(5)	C511-C521	1.386(7)
C651-C661	1.31(4)	C721-C731	1.53(4)
C731-C741	1.46(4)	C801-C811	1.31(4)
Cu42-N12A2	2.038(12)	Cu42-N1A2	2.036(14)
Cu42-N2A2	2.046(14)	Cu42-N11A2	2.075(12)
Cu52-N5A2	2.006(14)	Cu52-N4A2	2.010(12)
Cu52-N3A2	2.050(12)	Cu52-N6A2	2.061(13)
Cu62-N8A2	1.972(12)	Cu62-N9A2	2.002(14)
Cu62-N7A2	2.050(13)	Cu62-N10A2	2.071(12)
N1A2-C2A2	1.3900	N1A2-C6A2	1.3900
C2A2-C3A2	1.3900	C2A2-C1A2	1.54(4)
C3A2-C4A2	1.3900	C4A2-C5A2	1.3900
C5A2-C6A2	1.3900	C5A2-C7A2	1.46(4)
C6A2-C10A2	1.373(19)	N2A2-C10A2	1.3900
N2A2-C13A2	1.3900	C10A2-C9A2	1.3900
C9A2-C11A2	1.3900	C9A2-C8A2	1.50(4)
C11A2-C12A2	1.3900	C12A2-C13A2	1.3900
C13A2-C14A2	1.38(3)	N3A2-C17A2	1.3900
N3A2-C21A2	1.3900	C17A2-C18A2	1.3900
C17A2-C16A2	1.54(3)	C18A2-C19A2	1.3900
C19A2-C20A2	1.3900	C20A2-C22A2	1.390(7)
C20A2-C21A2	1.3900	C21A2-C25A2	1.324(15)
N4A2-C25A2	1.3900	N4A2-C28A2	1.3900
C25A2-C24A2	1.3900	C24A2-C26A2	1.3900
C24A2-C23A2	1.394(7)	C26A2-C27A2	1.3900
C27A2-C28A2	1.3900	C28A2-C29A2	1.54(3)
N5A2-C31A2	1.3900	N5A2-C35A2	1.3900
C31A2-C30A2	1.37(4)	C31A2-C32A2	1.3900

C32A2-C33A2	1.3900	C33A2-C34A2	1.3900
C34A2-C35A2	1.3900	C34A2-C36A2	1.45(3)
C35A2-C39A2	1.328(19)	N6A2-C39A2	1.3900
N6A2-C42A2	1.3900	C39A2-C38A2	1.3900
C38A2-C40A2	1.3900	C38A2-C37A2	1.49(3)
C40A2-C41A2	1.3900	C41A2-C42A2	1.3900
C42A2-C43A2	1.58(3)	N7A2-C46A2	1.3900
N7A2-C50A2	1.3900	C46A2-C47A2	1.3900
C46A2-C45A2	1.45(3)	C47A2-C48A2	1.3900
C48A2-C49A2	1.3900	C49A2-C50A2	1.3900
C49A2-C51A2	1.49(3)	C50A2-C54A2	1.308(16)
N8A2-C54A2	1.3900	N8A2-C57A2	1.3900
C54A2-C53A2	1.3900	C53A2-C55A2	1.3900
C53A2-C52A2	1.46(3)	C55A2-C56A2	1.3900
C56A2-C57A2	1.3900	C57A2-C58A2	1.51(3)
N9A2-C60A2	1.3900	N9A2-C64A2	1.3900
C60A2-C61A2	1.3900	C60A2-C59A2	1.47(3)
C61A2-C62A2	1.3900	C62A2-C63A2	1.3900
C63A2-C64A2	1.3900	C63A2-C65A2	1.43(3)
C64A2-C68A2	1.336(17)	N10A2-C68A2	1.3900
N10A2-C71A2	1.3900	C68A2-C67A2	1.3900
C67A2-C69A2	1.3900	C67A2-C66A2	1.46(3)
C69A2-C70A2	1.3900	C70A2-C71A2	1.3900
C71A2-C72A2	1.41(3)	N11A2-C75A2	1.3900
N11A2-C79A2	1.3900	C75A2-C76A2	1.3900
C75A2-C74A2	1.43(3)	C76A2-C77A2	1.3900
C77A2-C78A2	1.3900	C78A2-C79A2	1.3900
C78A2-C80A2	1.41(4)	C79A2-C83A2	1.385(16)
N12A2-C83A2	1.3900	N12A2-C86A2	1.3900
C83A2-C82A2	1.3900	C82A2-C84A2	1.3900
C82A2-C81A2	1.53(4)	C84A2-C85A2	1.3900
C85A2-C86A2	1.3900	C86A2-C87A2	1.50(3)
C7A2-C8A2	1.21(4)	C14A2-C15A2	1.59(4)
C15A2-C16A2	1.43(4)	C22A2-C23A2	1.391(7)
C36A2-C37A2	1.34(4)	C43A2-C44A2	1.60(4)
C44A2-C45A2	1.46(4)	C51A2-C52A2	1.27(3)
C65A2-C66A2	1.31(4)	C72A2-C73A2	1.54(4)
C73A2-C74A2	1.62(4)	C80A2-C81A2	1.32(4)
Cu73-N12B3	2.038(12)	Cu73-N2B3	2.054(14)
Cu73-N11B3	2.081(13)	Cu73-N1B3	2.080(13)
Cu83-N5B3	2.001(13)	Cu83-N4B3	2.008(14)
Cu83-N3B3	2.034(13)	Cu83-N6B3	2.067(15)
Cu93-N8B3	2.021(17)	Cu93-N9B3	2.018(18)
Cu93-N10B3	2.045(16)	Cu93-N7B3	2.061(14)
N1B3-C2B3	1.3900	N1B3-C6B3	1.3900
C2B3-C3B3	1.3900	C2B3-C1B3	1.65(4)

C3B3-C4B3	1.3900	C4B3-C5B3	1.3900
C5B3-C7B3	1.390(7)	C5B3-C6B3	1.3900
C6B3-C10B3	1.388(16)	N2B3-C10B3	1.3900
N2B3-C13B3	1.3900	C10B3-C9B3	1.3900
C9B3-C11B3	1.3900	C9B3-C8B3	1.390(7)
C11B3-C12B3	1.3900	C12B3-C13B3	1.3900
C13B3-C14B3	1.47(3)	N3B3-C17B3	1.3900
N3B3-C21B3	1.3900	C17B3-C18B3	1.3900
C17B3-C16B3	1.41(3)	C18B3-C19B3	1.3900
C19B3-C20B3	1.3900	C20B3-C21B3	1.3900
C20B3-C22B3	1.43(4)	C21B3-C25B3	1.373(18)
N4B3-C25B3	1.3900	N4B3-C28B3	1.3900
C25B3-C24B3	1.3900	C24B3-C26B3	1.3900
C24B3-C23B3	1.50(4)	C26B3-C27B3	1.3900
C27B3-C28B3	1.3900	C28B3-C29B3	1.51(3)
N5B3-C31B3	1.3900	N5B3-C35B3	1.3900
C31B3-C32B3	1.3900	C31B3-C30B3	1.50(4)
C32B3-C33B3	1.3900	C33B3-C34B3	1.3900
C34B3-C35B3	1.3900	C34B3-C36B3	1.392(7)
C35B3-C39B3	1.353(16)	N6B3-C39B3	1.3900
N6B3-C42B3	1.3900	C39B3-C38B3	1.3900
C38B3-C37B3	1.390(7)	C38B3-C40B3	1.3900
C40B3-C41B3	1.3900	C41B3-C42B3	1.3900
C42B3-C43B3	1.45(3)	N7B3-C46B3	1.3900
N7B3-C50B3	1.3900	C46B3-C47B3	1.3900
C46B3-C45B3	1.47(3)	C47B3-C48B3	1.3900
C48B3-C49B3	1.3900	C49B3-C50B3	1.3900
C49B3-C51B3	1.39(3)	C50B3-C54B3	1.31(2)
N8B3-C54B3	1.3900	N8B3-C57B3	1.3900
C54B3-C53B3	1.3900	C53B3-C55B3	1.3900
C53B3-C52B3	1.42(4)	C55B3-C56B3	1.3900
C56B3-C57B3	1.3900	C57B3-C58B3	1.48(4)
N9B3-C60B3	1.3900	N9B3-C64B3	1.3900
C60B3-C61B3	1.3900	C60B3-C59B3	1.52(6)
C61B3-C62B3	1.3900	C62B3-C63B3	1.3900
C63B3-C65B3	1.390(7)	C63B3-C64B3	1.3900
C64B3-C68B3	1.34(2)	N10B3-C68B3	1.3900
N10B3-C71B3	1.3900	C68B3-C67B3	1.3900
C67B3-C69B3	1.3900	C67B3-C66B3	1.390(7)
C69B3-C70B3	1.3900	C70B3-C71B3	1.3900
C71B3-C72B3	1.53(3)	N11B3-C75B3	1.3900
N11B3-C79B3	1.3900	C75B3-C76B3	1.3900
C75B3-C74B3	1.46(3)	C76B3-C77B3	1.3900
C77B3-C78B3	1.3900	C78B3-C79B3	1.3900
C78B3-C80B3	1.392(7)	C79B3-C83B3	1.363(15)
N12B3-C83B3	1.3900	N12B3-C86B3	1.3900

C83B3-C82B3	1.3900	C82B3-C84B3	1.3900
C82B3-C81B3	1.391(7)	C84B3-C85B3	1.3900
C85B3-C86B3	1.3900	C86B3-C87B3	1.45(3)
C7B3-C8B3	1.389(7)	C14B3-C15B3	1.53(3)
C15B3-C16B3	1.63(3)	C22B3-C23B3	1.36(4)
C36B3-C37B3	1.389(7)	C43B3-C44B3	1.50(4)
C44B3-C45B3	1.43(4)	C51B3-C52B3	1.38(4)
C65B3-C66B3	1.388(7)	C72B3-C73B3	1.48(4)
C73B3-C74B3	1.57(4)	C80B3-C81B3	1.389(7)
As14-O64	1.79(2)	As14-O14	1.825(19)
As14-O24	1.825(18)	As14-O44	1.84(2)
As14-O34	1.87(2)	As14-O54	1.886(18)
O14-C14	1.35(2)	O24-C64	1.35(2)
O34-C74	1.35(2)	O44-C124	1.38(3)
O54-C134	1.28(2)	O64-C184	1.42(3)
C14-C24	1.3900	C14-C64	1.3900
C24-C34	1.3900	C34-C44	1.3900
C44-C54	1.3900	C54-C64	1.3900
C74-C84	1.3900	C74-C124	1.3900
C84-C94	1.3900	C94-C104	1.3900
C104-C114	1.3900	C114-C124	1.3900
C134-C144	1.3900	C134-C184	1.3900
C144-C154	1.3900	C154-C164	1.3900
C164-C174	1.3900	C174-C184	1.3900
As25-O6A5	1.78(2)	As25-O2A5	1.813(19)
As25-O4A5	1.84(2)	As25-O1A5	1.84(2)
As25-O5A5	1.852(19)	As25-O3A5	1.85(3)
O1A5-C1A5	1.37(3)	O2A5-C6A5	1.33(2)
O3A5-C7A5	1.29(3)	O4A5-C12A5	1.24(3)
O5A5-C13A5	1.29(2)	O6A5-C18A5	1.39(3)
C1A5-C2A5	1.3900	C1A5-C6A5	1.3900
C2A5-C3A5	1.3900	C3A5-C4A5	1.3900
C4A5-C5A5	1.3900	C5A5-C6A5	1.3900
C7A5-C8A5	1.3900	C7A5-C12A5	1.3900
C8A5-C9A5	1.3900	C9A5-C10A5	1.3900
C10A5-C11A5	1.3900	C11A5-C12A5	1.3900
C13A5-C14A5	1.3900	C13A5-C18A5	1.3900
C14A5-C15A5	1.3900	C15A5-C16A5	1.3900
C16A5-C17A5	1.3900	C17A5-C18A5	1.3900
As36-O2B6	1.81(2)	As36-O5B6	1.83(2)
As36-O4B6	1.86(2)	As36-O3B6	1.850(17)
As36-O1B6	1.88(2)	As36-O6B6	1.91(2)
O1B6-C1B6	1.33(3)	O2B6-C6B6	1.31(2)
O3B6-C7B6	1.39(2)	O4B6-C12B6	1.35(3)
O5B6-C13B6	1.35(2)	O6B6-C18B6	1.25(2)
C1B6-C2B6	1.3900	C1B6-C6B6	1.3900

C2B6-C3B6	1.3900	C3B6-C4B6	1.3900
C4B6-C5B6	1.3900	C5B6-C6B6	1.3900
C7B6-C8B6	1.3900	C7B6-C12B6	1.3900
C8B6-C9B6	1.3900	C9B6-C10B6	1.3900
C10B6-C11B6	1.3900	C11B6-C12B6	1.3900
C13B6-C14B6	1.3900	C13B6-C18B6	1.3900
C14B6-C15B6	1.3900	C15B6-C16B6	1.3900
C16B6-C17B6	1.3900	C17B6-C18B6	1.3900
As47-O6C7	1.859(19)	As47-O4C7	1.80(2)
As47-O5C7	1.83(2)	As47-O1C7	1.86(2)
As47-O2C7	1.88(2)	As47-O3C7	1.89(2)
O1C7-C1C7	1.41(3)	O2C7-C6C7	1.30(2)
O3C7-C7C7	1.33(2)	O4C7-C12C7	1.34(2)
O5C7-C13C7	1.32(3)	O6C7-C18C7	1.32(3)
C1C7-C2C7	1.3900	C1C7-C6C7	1.3900
C2C7-C3C7	1.3900	C3C7-C4C7	1.3900
C4C7-C5C7	1.3900	C5C7-C6C7	1.3900
C7C7-C8C7	1.3900	C7C7-C12C7	1.3900
C8C7-C9C7	1.3900	C9C7-C10C7	1.3900
C10C7-C11C7	1.3900	C11C7-C12C7	1.3900
C13C7-C14C7	1.3900	C13C7-C18C7	1.3900
C14C7-C15C7	1.3900	C15C7-C16C7	1.3900
C16C7-C17C7	1.3900	C17C7-C18C7	1.3900
As58-O2D8	1.80(2)	As58-O3D8	1.792(18)
As58-O1D8	1.814(19)	As58-O5D8	1.85(2)
As58-O4D8	1.87(2)	As58-O6D8	1.877(19)
O1D8-C1D8	1.33(2)	O2D8-C6D8	1.31(2)
O3D8-C7D8	1.33(2)	O4D8-C12D8	1.33(3)
O5D8-C13D8	1.26(2)	O6D8-C18D8	1.40(2)
C1D8-C2D8	1.3900	C1D8-C6D8	1.3900
C2D8-C3D8	1.3900	C3D8-C4D8	1.3900
C4D8-C5D8	1.3900	C5D8-C6D8	1.3900
C7D8-C8D8	1.3900	C7D8-C12D8	1.3900
C8D8-C9D8	1.3900	C9D8-C10D8	1.3900
C10D8-C11D8	1.3900	C11D8-C12D8	1.3900
C13D8-C14D8	1.3900	C13D8-C18D8	1.3900
C14D8-C15D8	1.3900	C15D8-C16D8	1.3900
C16D8-C17D8	1.3900	C17D8-C18D8	1.3900
As69-O5E9	1.81(2)	As69-O3E9	1.86(2)
As69-O4E9	1.82(2)	As69-O1E9	1.843(19)
As69-O6E9	1.88(2)	As69-O2E9	1.862(17)
O1E9-C1E9	1.35(2)	O2E9-C6E9	1.40(2)
O3E9-C7E9	1.30(2)	O4E9-C12E9	1.38(3)
O5E9-C13E9	1.38(2)	O6E9-C18E9	1.37(2)
C1E9-C2E9	1.3900	C1E9-C6E9	1.3900
C2E9-C3E9	1.3900	C3E9-C4E9	1.3900

C4E9-C5E9	1.3900	C5E9-C6E9	1.3900
C7E9-C8E9	1.3900	C7E9-C12E9	1.3900
C8E9-C9E9	1.3900	C9E9-C10E9	1.3900
C10E9-C11E9	1.3900	C11E9-C12E9	1.3900
C13E9-C14E9	1.3900	C13E9-C18E9	1.3900
C14E9-C15E9	1.3900	C15E9-C16E9	1.3900
C16E9-C17E9	1.3900	C17E9-C18E9	1.3900
As710-O1F10	1.77(2)	As710-O3F10	1.81(2)
As710-O5F10	1.84(2)	As710-O4F10	1.84(2)
As710-O6F10	1.85(2)	As710-O2F10	1.870(19)
O1F10-C1F10	1.33(2)	O2F10-C6F10	1.28(2)
O3F10-C7F10	1.38(2)	O4F10-C12F10	1.38(2)
O5F10-C13F10	1.30(3)	O6F10-C18F10	1.37(2)
C1F10-C2F10	1.3900	C1F10-C6F10	1.3900
C2F10-C3F10	1.3900	C3F10-C4F10	1.3900
C4F10-C5F10	1.3900	C5F10-C6F10	1.3900
C7F10-C8F10	1.3900	C7F10-C12F10	1.3900
C8F10-C9F10	1.3900	C9F10-C10F10	1.3900
C10F10-C11F10	1.3900	C11F10-C12F10	1.3900
C13F10-C14F10	1.3900	C13F10-C18F10	1.3900
C14F10-C15F10	1.3900	C15F10-C16F10	1.3900
C16F10-C17F10	1.3900	C17F10-C18F10	1.3900
As811-O1G11	1.760(18)	As811-O2G11	1.81(2)
As811-O6G11	1.83(3)	As811-O3G11	1.87(2)
As811-O4G11	1.85(2)	As811-O5G11	1.87(2)
As811-C13G11	2.64(3)	O1G11-C1G11	1.36(2)
O2G11-C6G11	1.43(3)	O3G11-C7G11	1.38(3)
O4G11-C12G11	1.44(3)	O5G11-C13G11	1.35(3)
O5G11-C14G11	2.40(4)	O6G11-C18G11	1.47(4)
C1G11-C2G11	1.3900	C1G11-C6G11	1.3900
C2G11-C3G11	1.3900	C3G11-C4G11	1.3900
C4G11-C5G11	1.3900	C5G11-C6G11	1.3900
C7G11-C8G11	1.3900	C7G11-C12G11	1.3900
C8G11-C9G11	1.3900	C9G11-C10G11	1.3900
C10G11-C11G11	1.3900	C11G11-C12G11	1.3900
C13G11-C14G11	1.3900	C13G11-C18G11	1.3900
C14G11-C15G11	1.3900	C15G11-C16G11	1.3900
C16G11-C17G11	1.3900	C17G11-C18G11	1.3900
As912-O6H12	1.51(3)	As912-O2H12	1.770(17)
As912-O3H12	1.85(2)	As912-O1H12	1.88(3)
As912-O5H12	1.86(3)	As912-O4H12	1.95(3)
As912-C13H12	2.34(3)	O1H12-C1H12	1.32(3)
O2H12-C6H12	1.35(2)	O3H12-C7H12	1.37(3)
O4H12-C12H12	1.32(3)	O5H12-C13H12	1.37(4)
O6H12-C18H12	1.39(4)	C1H12-C2H12	1.3900
C1H12-C6H12	1.3900	C2H12-C3H12	1.3900

C3H12-C4H12	1.3900	C4H12-C5H12	1.3900
C5H12-C6H12	1.3900	C7H12-C8H12	1.3900
C7H12-C12H12	1.3900	C8H12-C9H12	1.3900
C9H12-C10H12	1.3900	C10H12-C11H12	1.3900
C11H12-C12H12	1.3900	C13H12-C14H12	1.3900
C13H12-C18H12	1.3900	C14H12-C15H12	1.3900
C15H12-C16H12	1.3900	C16H12-C17H12	1.3900
C17H12-C18H12	1.3900		

Symmetry transformations used to generate equivalent atoms:

Table 5. Bond angles [°] for nd1024_x.

atom-atom-atom	angle	atom-atom-atom	angle
N11-Cu11-N111	125.9(7)	N11-Cu11-N121	138.5(7)
N111-Cu11-N121	82.5(7)	N11-Cu11-N21	80.5(7)
N111-Cu11-N21	119.3(7)	N121-Cu11-N21	113.8(7)
N31-Cu21-N51	118.2(7)	N31-Cu21-N41	82.7(6)
N51-Cu21-N41	135.0(7)	N31-Cu21-N61	131.8(7)
N51-Cu21-N61	81.6(7)	N41-Cu21-N61	115.1(7)
N81-Cu31-N71	81.7(9)	N81-Cu31-N91	137.8(10)
N71-Cu31-N91	115.9(8)	N81-Cu31-N101	121.7(9)
N71-Cu31-N101	123.7(7)	N91-Cu31-N101	81.8(9)
C21-N11-C61	120.0	C21-N11-Cu11	128.4(10)
C61-N11-Cu11	111.4(10)	C31-C21-N11	120.0
C31-C21-C11	124.7(16)	N11-C21-C11	115.2(15)
C21-C31-C41	120.0	C51-C41-C31	120.0
C41-C51-C61	120.0	C41-C51-C71	118.9(19)
C61-C51-C71	121.1(19)	C101-C61-C51	119.0(15)
C101-C61-N11	120.4(15)	C51-C61-N11	120.0
C101-N21-C131	120.0	C101-N21-Cu11	112.1(9)
C131-N21-Cu11	127.9(9)	C61-C101-C91	124.6(14)
C61-C101-N21	115.4(14)	C91-C101-N21	120.0
C101-C91-C111	120.0	C101-C91-C81	120.0(18)
C111-C91-C81	119.8(19)	C91-C111-C121	120.0
C131-C121-C111	120.0	C121-C131-N21	120.0
C121-C131-C141	118.1(18)	N21-C131-C141	121.9(18)
C171-N31-C211	120.0	C171-N31-Cu21	130.2(8)
C211-N31-Cu21	109.8(8)	N31-C171-C181	120.0
N31-C171-C161	117.3(16)	C181-C171-C161	122.7(15)
C191-C181-C171	120.0	C201-C191-C181	120.0
C191-C201-C211	120.0	C191-C201-C221	122.6(16)
C211-C201-C221	116.9(15)	C251-C211-C201	120.5(13)
C251-C211-N31	119.5(13)	C201-C211-N31	120.0
C251-N41-C281	120.0	C251-N41-Cu21	111.3(9)
C281-N41-Cu21	128.7(9)	C211-C251-C241	123.4(14)
C211-C251-N41	116.6(13)	C241-C251-N41	120.0
C251-C241-C261	120.0	C251-C241-C231	114.4(19)
C261-C241-C231	125.5(19)	C271-C261-C241	120.0
C261-C271-C281	120.0	C271-C281-N41	120.0
C271-C281-C291	124.0(19)	N41-C281-C291	115.7(19)
C311-N51-C351	120.0	C311-N51-Cu21	127.6(9)
C351-N51-Cu21	111.8(9)	N51-C311-C321	120.0
N51-C311-C301	114.9(18)	C321-C311-C301	124.9(18)
C331-C321-C311	120.0	C321-C331-C341	120.0
C351-C341-C331	120.0	C351-C341-C361	117.4(11)

C331-C341-C361	122.4(11)	C391-C351-C341	122.1(14)
C391-C351-N51	117.9(14)	C341-C351-N51	120.0
C391-N61-C421	120.0	C391-N61-Cu21	109.3(10)
C421-N61-Cu21	130.6(10)	C351-C391-N61	118.9(15)
C351-C391-C381	121.1(15)	N61-C391-C381	120.0
C401-C381-C391	120.0	C401-C381-C371	121.7(13)
C391-C381-C371	118.2(13)	C381-C401-C411	120.0
C401-C411-C421	120.0	C411-C421-N61	120.0
C411-C421-C431	125.2(18)	N61-C421-C431	114.8(18)
C461-N71-C501	120.0	C461-N71-Cu31	127.3(9)
C501-N71-Cu31	112.6(9)	C471-C461-N71	120.0
C471-C461-C451	119.8(18)	N71-C461-C451	120.2(17)
C461-C471-C481	120.0	C491-C481-C471	120.0
C501-C491-C481	120.0	C501-C491-C511	114.4(14)
C481-C491-C511	125.6(13)	C541-C501-C491	125.0(17)
C541-C501-N71	114.9(17)	C491-C501-N71	120.0
C541-N81-C571	120.0	C541-N81-Cu31	111.6(14)
C571-N81-Cu31	128.4(14)	C501-C541-C531	121(2)
C501-C541-N81	119(2)	C531-C541-N81	120.0
C521-C531-C541	116.3(16)	C521-C531-C551	123.7(16)
C541-C531-C551	120.0	C561-C551-C531	120.0
C551-C561-C571	120.0	C561-C571-N81	120.0
C561-C571-C581	121(2)	N81-C571-C581	119(2)
C601-N91-C641	120.0	C601-N91-Cu31	127.0(13)
C641-N91-Cu31	111.6(13)	C611-C601-N91	120.0
C611-C601-C591	123(2)	N91-C601-C591	117(2)
C621-C611-C601	120.0	C611-C621-C631	120.0
C641-C631-C621	120.0	C641-C631-C651	112(2)
C621-C631-C651	128(2)	C631-C641-N91	120.0
C631-C641-C681	122.2(17)	N91-C641-C681	117.6(17)
C681-N101-C711	120.0	C681-N101-Cu31	111.9(10)
C711-N101-Cu31	128.0(10)	N101-C681-C671	120.0
N101-C681-C641	116.2(16)	C671-C681-C641	123.7(16)
C691-C671-C681	120.0	C691-C671-C661	124(2)
C681-C671-C661	116.1(19)	C671-C691-C701	120.0
C711-C701-C691	120.0	C701-C711-N101	120.0
C701-C711-C721	119.4(18)	N101-C711-C721	120.5(18)
C751-N111-C791	120.0	C751-N111-Cu11	128.5(9)
C791-N111-Cu11	111.2(9)	C761-C751-N111	120.0
C761-C751-C741	124.5(16)	N111-C751-C741	115.4(16)
C751-C761-C771	120.0	C781-C771-C761	120.0
C771-C781-C791	120.0	C771-C781-C801	126.2(17)
C791-C781-C801	113.7(17)	C831-C791-C781	122.3(13)
C831-C791-N111	117.7(13)	C781-C791-N111	120.0
C831-N121-C861	120.0	C831-N121-Cu11	110.5(9)
C861-N121-Cu11	129.3(9)	C791-C831-C821	121.9(13)

C791-C831-N121	117.7(13)	C821-C831-N121	120.0
C831-C821-C841	120.0	C831-C821-C811	121.9(18)
C841-C821-C811	117.7(18)	C851-C841-C821	120.0
C861-C851-C841	120.0	C851-C861-N121	120.0
C851-C861-C871	119.5(17)	N121-C861-C871	120.5(17)
C51-C71-C81	120(3)	C91-C81-C71	115(3)
C131-C141-C151	115(2)	C161-C151-C141	107(2)
C171-C161-C151	113(2)	C231-C221-C201	120(3)
C221-C231-C241	124(3)	C361-C371-C381	120.1(11)
C371-C361-C341	120.6(11)	C441-C431-C421	117(3)
C451-C441-C431	112(3)	C461-C451-C441	115(3)
C521-C511-C491	120.9(12)	C511-C521-C531	121.5(12)
C661-C651-C631	123(3)	C651-C661-C671	123(3)
C711-C721-C731	111(2)	C741-C731-C721	111(2)
C731-C741-C751	113(2)	C811-C801-C781	121(3)
C801-C811-C821	119(3)	N12A2-Cu42-N1A2	136.7(7)
N12A2-Cu42-N2A2	116.1(7)	N1A2-Cu42-N2A2	81.9(7)
N12A2-Cu42-N11A2	80.5(6)	N1A2-Cu42-N11A2	120.9(7)
N2A2-Cu42-N11A2	127.9(7)	N5A2-Cu52-N4A2	139.4(7)
N5A2-Cu52-N3A2	111.2(7)	N4A2-Cu52-N3A2	81.3(6)
N5A2-Cu52-N6A2	81.4(7)	N4A2-Cu52-N6A2	122.1(7)
N3A2-Cu52-N6A2	128.3(6)	N8A2-Cu62-N9A2	139.1(7)
N8A2-Cu62-N7A2	81.2(6)	N9A2-Cu62-N7A2	118.4(7)
N8A2-Cu62-N10A2	122.2(6)	N9A2-Cu62-N10A2	82.6(6)
N7A2-Cu62-N10A2	117.1(6)	C2A2-N1A2-C6A2	120.0
C2A2-N1A2-Cu42	128.8(10)	C6A2-N1A2-Cu42	111.1(10)
N1A2-C2A2-C3A2	120.0	N1A2-C2A2-C1A2	118.4(17)
C3A2-C2A2-C1A2	121.5(17)	C4A2-C3A2-C2A2	120.0
C3A2-C4A2-C5A2	120.0	C6A2-C5A2-C4A2	120.0
C6A2-C5A2-C7A2	115(2)	C4A2-C5A2-C7A2	125(2)
C10A2-C6A2-C5A2	121.4(15)	C10A2-C6A2-N1A2	118.4(15)
C5A2-C6A2-N1A2	120.0	C10A2-N2A2-C13A2	120.0
C10A2-N2A2-Cu42	111.2(10)	C13A2-N2A2-Cu42	128.8(10)
C6A2-C10A2-N2A2	117.4(15)	C6A2-C10A2-C9A2	122.6(15)
N2A2-C10A2-C9A2	120.0	C11A2-C9A2-C10A2	120.0
C11A2-C9A2-C8A2	126.3(19)	C10A2-C9A2-C8A2	113.7(19)
C12A2-C11A2-C9A2	120.0	C11A2-C12A2-C13A2	120.0
C14A2-C13A2-C12A2	119.6(18)	C14A2-C13A2-N2A2	120.2(18)
C12A2-C13A2-N2A2	120.0	C17A2-N3A2-C21A2	120.0
C17A2-N3A2-Cu52	129.2(8)	C21A2-N3A2-Cu52	110.6(8)
N3A2-C17A2-C18A2	120.0	N3A2-C17A2-C16A2	115.9(15)
C18A2-C17A2-C16A2	123.8(15)	C19A2-C18A2-C17A2	120.0
C20A2-C19A2-C18A2	120.0	C22A2-C20A2-C19A2	121.9(11)
C22A2-C20A2-C21A2	118.1(11)	C19A2-C20A2-C21A2	120.0
C25A2-C21A2-C20A2	122.1(13)	C25A2-C21A2-N3A2	117.8(13)
C20A2-C21A2-N3A2	120.0	C25A2-N4A2-C28A2	120.0

C25A2-N4A2-Cu52	111.2(9)	C28A2-N4A2-Cu52	128.6(9)
C21A2-C25A2-C24A2	120.5(13)	C21A2-C25A2-N4A2	119.0(13)
C24A2-C25A2-N4A2	120.0	C25A2-C24A2-C26A2	120.0
C25A2-C24A2-C23A2	118.9(11)	C26A2-C24A2-C23A2	121.0(11)
C24A2-C26A2-C27A2	120.0	C28A2-C27A2-C26A2	120.0
C27A2-C28A2-N4A2	120.0	C27A2-C28A2-C29A2	121.1(14)
N4A2-C28A2-C29A2	118.9(14)	C31A2-N5A2-C35A2	120.0
C31A2-N5A2-Cu52	127.7(11)	C35A2-N5A2-Cu52	112.3(11)
C30A2-C31A2-N5A2	121(2)	C30A2-C31A2-C32A2	119(2)
N5A2-C31A2-C32A2	120.0	C31A2-C32A2-C33A2	120.0
C34A2-C33A2-C32A2	120.0	C35A2-C34A2-C33A2	120.0
C35A2-C34A2-C36A2	117.2(19)	C33A2-C34A2-C36A2	122.3(19)
C39A2-C35A2-C34A2	122.8(15)	C39A2-C35A2-N5A2	117.0(15)
C34A2-C35A2-N5A2	120.0	C39A2-N6A2-C42A2	120.0
C39A2-N6A2-Cu52	109.1(8)	C42A2-N6A2-Cu52	130.7(9)
C35A2-C39A2-C38A2	120.3(14)	C35A2-C39A2-N6A2	119.6(14)
C38A2-C39A2-N6A2	120.0	C40A2-C38A2-C39A2	120.0
C40A2-C38A2-C37A2	119.2(18)	C39A2-C38A2-C37A2	120.8(18)
C38A2-C40A2-C41A2	120.0	C40A2-C41A2-C42A2	120.0
C41A2-C42A2-N6A2	120.0	C41A2-C42A2-C43A2	124.7(15)
N6A2-C42A2-C43A2	115.1(15)	C46A2-N7A2-C50A2	120.0
C46A2-N7A2-Cu62	130.0(9)	C50A2-N7A2-Cu62	110.0(9)
N7A2-C46A2-C47A2	120.0	N7A2-C46A2-C45A2	114.9(18)
C47A2-C46A2-C45A2	125.0(17)	C46A2-C47A2-C48A2	120.0
C47A2-C48A2-C49A2	120.0	C50A2-C49A2-C48A2	120.0
C50A2-C49A2-C51A2	116.8(15)	C48A2-C49A2-C51A2	123.2(15)
C54A2-C50A2-C49A2	122.6(13)	C54A2-C50A2-N7A2	117.3(13)
C49A2-C50A2-N7A2	120.0	C54A2-N8A2-C57A2	120.0
C54A2-N8A2-Cu62	111.7(8)	C57A2-N8A2-Cu62	128.1(8)
C50A2-C54A2-N8A2	118.9(12)	C50A2-C54A2-C53A2	121.0(12)
N8A2-C54A2-C53A2	120.0	C55A2-C53A2-C54A2	120.0
C55A2-C53A2-C52A2	122.0(16)	C54A2-C53A2-C52A2	117.9(16)
C56A2-C55A2-C53A2	120.0	C55A2-C56A2-C57A2	120.0
C56A2-C57A2-N8A2	120.0	C56A2-C57A2-C58A2	123.8(16)
N8A2-C57A2-C58A2	116.2(16)	C60A2-N9A2-C64A2	120.0
C60A2-N9A2-Cu62	129.3(10)	C64A2-N9A2-Cu62	110.5(10)
C61A2-C60A2-N9A2	120.0	C61A2-C60A2-C59A2	124.2(17)
N9A2-C60A2-C59A2	115.8(17)	C62A2-C61A2-C60A2	120.0
C61A2-C62A2-C63A2	120.0	C62A2-C63A2-C64A2	120.0
C62A2-C63A2-C65A2	120.5(17)	C64A2-C63A2-C65A2	119.5(17)
C68A2-C64A2-C63A2	120.5(14)	C68A2-C64A2-N9A2	119.4(14)
C63A2-C64A2-N9A2	120.0	C68A2-N10A2-C71A2	120.0
C68A2-N10A2-Cu62	108.5(8)	C71A2-N10A2-Cu62	131.4(8)
C64A2-C68A2-C67A2	121.1(13)	C64A2-C68A2-N10A2	118.9(13)
C67A2-C68A2-N10A2	120.0	C68A2-C67A2-C69A2	120.0
C68A2-C67A2-C66A2	118.2(17)	C69A2-C67A2-C66A2	121.8(17)

C70A2-C69A2-C67A2	120.0	C71A2-C70A2-C69A2	120.0
C70A2-C71A2-N10A2	120.0	C70A2-C71A2-C72A2	122.9(16)
N10A2-C71A2-C72A2	117.0(16)	C75A2-N11A2-C79A2	120.0
C75A2-N11A2-Cu42	130.2(9)	C79A2-N11A2-Cu42	109.7(9)
C76A2-C75A2-N11A2	120.0	C76A2-C75A2-C74A2	123.4(17)
N11A2-C75A2-C74A2	116.5(17)	C77A2-C76A2-C75A2	120.0
C76A2-C77A2-C78A2	120.0	C77A2-C78A2-C79A2	120.0
C77A2-C78A2-C80A2	124.1(19)	C79A2-C78A2-C80A2	115.9(19)
C78A2-C79A2-N11A2	120.0	C78A2-C79A2-C83A2	118.8(13)
N11A2-C79A2-C83A2	121.2(13)	C83A2-N12A2-C86A2	120.0
C83A2-N12A2-Cu42	114.9(9)	C86A2-N12A2-Cu42	124.3(9)
N12A2-C83A2-C82A2	120.0	N12A2-C83A2-C79A2	113.4(13)
C82A2-C83A2-C79A2	126.4(13)	C83A2-C82A2-C84A2	120.0
C83A2-C82A2-C81A2	112.9(18)	C84A2-C82A2-C81A2	127.0(18)
C85A2-C84A2-C82A2	120.0	C84A2-C85A2-C86A2	120.0
C85A2-C86A2-N12A2	120.0	C85A2-C86A2-C87A2	118.7(16)
N12A2-C86A2-C87A2	121.3(16)	C8A2-C7A2-C5A2	124(3)
C7A2-C8A2-C9A2	122(3)	C13A2-C14A2-C15A2	119(2)
C16A2-C15A2-C14A2	114(2)	C15A2-C16A2-C17A2	118(2)
C20A2-C22A2-C23A2	120.0(10)	C22A2-C23A2-C24A2	119.5(10)
C37A2-C36A2-C34A2	123(3)	C36A2-C37A2-C38A2	115(3)
C42A2-C43A2-C44A2	111(2)	C45A2-C44A2-C43A2	107(2)
C44A2-C45A2-C46A2	117(2)	C52A2-C51A2-C49A2	120(3)
C51A2-C52A2-C53A2	121(3)	C66A2-C65A2-C63A2	120(3)
C65A2-C66A2-C67A2	120(3)	C71A2-C72A2-C73A2	119(2)
C72A2-C73A2-C74A2	112(2)	C75A2-C74A2-C73A2	111(2)
C81A2-C80A2-C78A2	127(3)	C80A2-C81A2-C82A2	117(3)
N12B3-Cu73-N2B3	120.4(7)	N12B3-Cu73-N11B3	82.0(6)
N2B3-Cu73-N11B3	128.6(7)	N12B3-Cu73-N1B3	136.2(7)
N2B3-Cu73-N1B3	83.3(7)	N11B3-Cu73-N1B3	113.0(7)
N5B3-Cu83-N4B3	140.1(7)	N5B3-Cu83-N3B3	115.6(7)
N4B3-Cu83-N3B3	83.4(7)	N5B3-Cu83-N6B3	81.8(7)
N4B3-Cu83-N6B3	114.9(7)	N3B3-Cu83-N6B3	128.3(7)
N8B3-Cu93-N9B3	142.7(9)	N8B3-Cu93-N10B3	124.6(8)
N9B3-Cu93-N10B3	81.4(9)	N8B3-Cu93-N7B3	79.4(8)
N9B3-Cu93-N7B3	116.1(8)	N10B3-Cu93-N7B3	114.9(7)
C2B3-N1B3-C6B3	120.0	C2B3-N1B3-Cu73	132.1(9)
C6B3-N1B3-Cu73	107.8(9)	N1B3-C2B3-C3B3	120.0
N1B3-C2B3-C1B3	111.3(17)	C3B3-C2B3-C1B3	128.5(17)
C4B3-C3B3-C2B3	120.0	C3B3-C4B3-C5B3	120.0
C7B3-C5B3-C4B3	120.6(12)	C7B3-C5B3-C6B3	119.3(12)
C4B3-C5B3-C6B3	120.0	C10B3-C6B3-C5B3	119.1(14)
C10B3-C6B3-N1B3	120.8(14)	C5B3-C6B3-N1B3	120.0
C10B3-N2B3-C13B3	120.0	C10B3-N2B3-Cu73	110.2(10)
C13B3-N2B3-Cu73	129.7(10)	C6B3-C10B3-C9B3	122.3(14)
C6B3-C10B3-N2B3	117.6(14)	C9B3-C10B3-N2B3	120.0

C11B3-C9B3-C10B3	120.0	C11B3-C9B3-C8B3	122.2(11)
C10B3-C9B3-C8B3	117.8(11)	C9B3-C11B3-C12B3	120.0
C13B3-C12B3-C11B3	120.0	C12B3-C13B3-N2B3	120.0
C12B3-C13B3-C14B3	123.4(16)	N2B3-C13B3-C14B3	116.2(16)
C17B3-N3B3-C21B3	120.0	C17B3-N3B3-Cu83	132.9(9)
C21B3-N3B3-Cu83	107.1(9)	C18B3-C17B3-N3B3	120.0
C18B3-C17B3-C16B3	127.1(16)	N3B3-C17B3-C16B3	112.9(16)
C19B3-C18B3-C17B3	120.0	C18B3-C19B3-C20B3	120.0
C21B3-C20B3-C19B3	120.0	C21B3-C20B3-C22B3	121.1(19)
C19B3-C20B3-C22B3	118.7(19)	C25B3-C21B3-C20B3	116.9(13)
C25B3-C21B3-N3B3	123.0(13)	C20B3-C21B3-N3B3	120.0
C25B3-N4B3-C28B3	120.0	C25B3-N4B3-Cu83	112.7(10)
C28B3-N4B3-Cu83	125.5(10)	C21B3-C25B3-N4B3	113.6(14)
C21B3-C25B3-C24B3	125.2(14)	N4B3-C25B3-C24B3	120.0
C26B3-C24B3-C25B3	120.0	C26B3-C24B3-C23B3	125.2(19)
C25B3-C24B3-C23B3	114.6(19)	C27B3-C26B3-C24B3	120.0
C26B3-C27B3-C28B3	120.0	C27B3-C28B3-N4B3	120.0
C27B3-C28B3-C29B3	122.4(17)	N4B3-C28B3-C29B3	116.9(17)
C31B3-N5B3-C35B3	120.0	C31B3-N5B3-Cu83	126.2(9)
C35B3-N5B3-Cu83	112.6(9)	N5B3-C31B3-C32B3	120.0
N5B3-C31B3-C30B3	112(2)	C32B3-C31B3-C30B3	127(2)
C33B3-C32B3-C31B3	120.0	C32B3-C33B3-C34B3	120.0
C35B3-C34B3-C33B3	120.0	C35B3-C34B3-C36B3	115.8(12)
C33B3-C34B3-C36B3	124.1(12)	C39B3-C35B3-C34B3	124.4(14)
C39B3-C35B3-N5B3	115.5(14)	C34B3-C35B3-N5B3	120.0
C39B3-N6B3-C42B3	120.0	C39B3-N6B3-Cu83	107.7(10)
C42B3-N6B3-Cu83	132.3(10)	C35B3-C39B3-C38B3	118.2(14)
C35B3-C39B3-N6B3	120.8(14)	C38B3-C39B3-N6B3	120.0
C39B3-C38B3-C37B3	119.1(12)	C39B3-C38B3-C40B3	120.0
C37B3-C38B3-C40B3	120.9(12)	C41B3-C40B3-C38B3	120.0
C42B3-C41B3-C40B3	120.0	C41B3-C42B3-N6B3	120.0
C41B3-C42B3-C43B3	122.4(18)	N6B3-C42B3-C43B3	117.5(18)
C46B3-N7B3-C50B3	120.0	C46B3-N7B3-Cu93	129.6(10)
C50B3-N7B3-Cu93	110.4(10)	N7B3-C46B3-C47B3	120.0
N7B3-C46B3-C45B3	119.7(17)	C47B3-C46B3-C45B3	120.3(17)
C46B3-C47B3-C48B3	120.0	C49B3-C48B3-C47B3	120.0
C50B3-C49B3-C48B3	120.0	C50B3-C49B3-C51B3	122.6(19)
C48B3-C49B3-C51B3	117.4(19)	C54B3-C50B3-C49B3	119.6(17)
C54B3-C50B3-N7B3	120.4(17)	C49B3-C50B3-N7B3	120.0
C54B3-N8B3-C57B3	120.0	C54B3-N8B3-Cu93	114.2(12)
C57B3-N8B3-Cu93	125.3(13)	C50B3-C54B3-N8B3	115.5(18)
C50B3-C54B3-C53B3	124.0(18)	N8B3-C54B3-C53B3	120.0
C54B3-C53B3-C55B3	120.0	C54B3-C53B3-C52B3	114(2)
C55B3-C53B3-C52B3	126(2)	C56B3-C55B3-C53B3	120.0
C57B3-C56B3-C55B3	120.0	C56B3-C57B3-N8B3	120.0
C56B3-C57B3-C58B3	126(2)	N8B3-C57B3-C58B3	114(2)

C60B3-N9B3-C64B3	120.0	C60B3-N9B3-Cu93	127.5(13)
C64B3-N9B3-Cu93	111.4(13)	N9B3-C60B3-C61B3	120.0
N9B3-C60B3-C59B3	115(3)	C61B3-C60B3-C59B3	125(3)
C62B3-C61B3-C60B3	120.0	C61B3-C62B3-C63B3	120.0
C65B3-C63B3-C64B3	117.2(15)	C65B3-C63B3-C62B3	122.8(15)
C64B3-C63B3-C62B3	120.0	C68B3-C64B3-C63B3	121.9(19)
C68B3-C64B3-N9B3	118.0(19)	C63B3-C64B3-N9B3	120.0
C68B3-N10B3-C71B3	120.0	C68B3-N10B3-Cu93	110.5(11)
C71B3-N10B3-Cu93	129.0(11)	C64B3-C68B3-C67B3	121.9(18)
C64B3-C68B3-N10B3	118.0(18)	C67B3-C68B3-N10B3	120.0
C69B3-C67B3-C68B3	120.0	C69B3-C67B3-C66B3	122.8(14)
C68B3-C67B3-C66B3	117.2(14)	C67B3-C69B3-C70B3	120.0
C71B3-C70B3-C69B3	120.0	C70B3-C71B3-N10B3	120.0
C70B3-C71B3-C72B3	124.9(19)	N10B3-C71B3-C72B3	114.9(19)
C75B3-N11B3-C79B3	120.0	C75B3-N11B3-Cu73	130.1(8)
C79B3-N11B3-Cu73	109.8(8)	C76B3-C75B3-N11B3	120.0
C76B3-C75B3-C74B3	122.9(17)	N11B3-C75B3-C74B3	117.1(17)
C75B3-C76B3-C77B3	120.0	C78B3-C77B3-C76B3	120.0
C79B3-C78B3-C77B3	120.0	C79B3-C78B3-C80B3	117.6(11)
C77B3-C78B3-C80B3	122.4(11)	C83B3-C79B3-C78B3	121.9(13)
C83B3-C79B3-N11B3	118.1(13)	C78B3-C79B3-N11B3	120.0
C83B3-N12B3-C86B3	120.0	C83B3-N12B3-Cu73	110.6(9)
C86B3-N12B3-Cu73	129.4(8)	C79B3-C83B3-C82B3	120.6(13)
C79B3-C83B3-N12B3	119.4(13)	C82B3-C83B3-N12B3	120.0
C83B3-C82B3-C84B3	120.0	C83B3-C82B3-C81B3	118.8(11)
C84B3-C82B3-C81B3	121.1(11)	C85B3-C84B3-C82B3	120.0
C84B3-C85B3-C86B3	120.0	C85B3-C86B3-N12B3	120.0
C85B3-C86B3-C87B3	121.4(15)	N12B3-C86B3-C87B3	118.5(15)
C8B3-C7B3-C5B3	120.8(11)	C7B3-C8B3-C9B3	120.7(11)
C13B3-C14B3-C15B3	110.6(19)	C14B3-C15B3-C16B3	108.3(19)
C17B3-C16B3-C15B3	111(2)	C23B3-C22B3-C20B3	120(3)
C22B3-C23B3-C24B3	119(3)	C37B3-C36B3-C34B3	121.0(11)
C36B3-C37B3-C38B3	120.4(11)	C42B3-C43B3-C44B3	113(2)
C45B3-C44B3-C43B3	114(2)	C44B3-C45B3-C46B3	119(2)
C52B3-C51B3-C49B3	114(3)	C51B3-C52B3-C53B3	125(3)
C66B3-C65B3-C63B3	120.9(11)	C65B3-C66B3-C67B3	120.8(12)
C73B3-C72B3-C71B3	110(2)	C72B3-C73B3-C74B3	109(2)
C75B3-C74B3-C73B3	113(2)	C81B3-C80B3-C78B3	121.0(10)
C80B3-C81B3-C82B3	120.1(10)	O64-As14-O14	176.2(9)
O64-As14-O24	88.3(9)	O14-As14-O24	88.1(8)
O64-As14-O44	92.9(10)	O14-As14-O44	90.8(10)
O24-As14-O44	176.4(10)	O64-As14-O34	89.0(9)
O14-As14-O34	92.2(9)	O24-As14-O34	88.6(9)
O44-As14-O34	88.0(10)	O64-As14-O54	86.6(9)
O14-As14-O54	92.3(8)	O24-As14-O54	93.7(8)
O44-As14-O54	89.8(9)	O34-As14-O54	175.0(9)

C14-O14-As14	113.1(15)	C64-O24-As14	107.7(14)
C74-O34-As14	108.7(16)	C124-O44-As14	106.8(17)
C134-O54-As14	111.9(16)	C184-O64-As14	109.7(16)
O14-C14-C24	129.6(16)	O14-C14-C64	110.4(16)
C24-C14-C64	120.0	C34-C24-C14	120.0
C24-C34-C44	120.0	C54-C44-C34	120.0
C44-C54-C64	120.0	O24-C64-C54	119.8(15)
O24-C64-C14	120.0(15)	C54-C64-C14	120.0
O34-C74-C84	126.1(18)	O34-C74-C124	113.8(18)
C84-C74-C124	120.0	C74-C84-C94	120.0
C104-C94-C84	120.0	C114-C104-C94	120.0
C104-C114-C124	120.0	O44-C124-C114	122.2(18)
O44-C124-C74	117.8(18)	C114-C124-C74	120.0
O54-C134-C144	125(2)	O54-C134-C184	115(2)
C144-C134-C184	120.0	C134-C144-C154	120.0
C164-C154-C144	120.0	C154-C164-C174	120.00(5)
C184-C174-C164	120.0	C174-C184-C134	120.0
C174-C184-O64	125.2(19)	C134-C184-O64	114.7(19)
O6A5-As25-O2A5	88.3(10)	O6A5-As25-O4A5	96.5(10)
O2A5-As25-O4A5	172.5(9)	O6A5-As25-O1A5	175.9(10)
O2A5-As25-O1A5	91.1(9)	O4A5-As25-O1A5	84.6(10)
O6A5-As25-O5A5	88.7(10)	O2A5-As25-O5A5	94.2(8)
O4A5-As25-O5A5	91.7(9)	O1A5-As25-O5A5	87.2(9)
O6A5-As25-O3A5	89.4(11)	O2A5-As25-O3A5	87.1(10)
O4A5-As25-O3A5	87.2(11)	O1A5-As25-O3A5	94.7(10)
O5A5-As25-O3A5	177.7(10)	C1A5-O1A5-As25	106.9(16)
C6A5-O2A5-As25	108.2(15)	C7A5-O3A5-As25	105(2)
C12A5-O4A5-As25	113.2(19)	C13A5-O5A5-As25	112.0(16)
C18A5-O6A5-As25	108.1(18)	O1A5-C1A5-C2A5	124.1(19)
O1A5-C1A5-C6A5	115.8(19)	C2A5-C1A5-C6A5	120.0
C1A5-C2A5-C3A5	120.0	C2A5-C3A5-C4A5	120.0
C5A5-C4A5-C3A5	120.0	C6A5-C5A5-C4A5	120.0
O2A5-C6A5-C5A5	122.1(18)	O2A5-C6A5-C1A5	117.8(18)
C5A5-C6A5-C1A5	120.0	O3A5-C7A5-C8A5	117(2)
O3A5-C7A5-C12A5	123(2)	C8A5-C7A5-C12A5	120.0
C7A5-C8A5-C9A5	120.0	C10A5-C9A5-C8A5	120.0
C11A5-C10A5-C9A5	120.0	C10A5-C11A5-C12A5	120.0
O4A5-C12A5-C11A5	128(2)	O4A5-C12A5-C7A5	112(2)
C11A5-C12A5-C7A5	120.0	O5A5-C13A5-C14A5	126.0(19)
O5A5-C13A5-C18A5	113.7(19)	C14A5-C13A5-C18A5	120.0
C13A5-C14A5-C15A5	120.0	C16A5-C15A5-C14A5	120.0
C15A5-C16A5-C17A5	120.0	C18A5-C17A5-C16A5	120.0
O6A5-C18A5-C17A5	122.1(19)	O6A5-C18A5-C13A5	116.9(19)
C17A5-C18A5-C13A5	120.0	O2B6-As36-O5B6	92.4(9)
O2B6-As36-O4B6	172.9(9)	O5B6-As36-O4B6	93.4(10)
O2B6-As36-O3B6	87.7(8)	O5B6-As36-O3B6	174.7(9)

O4B6-As36-O3B6	86.8(9)	O2B6-As36-O1B6	87.3(9)
O5B6-As36-O1B6	87.5(9)	O4B6-As36-O1B6	88.9(10)
O3B6-As36-O1B6	97.8(8)	O2B6-As36-O6B6	89.3(9)
O5B6-As36-O6B6	85.1(9)	O4B6-As36-O6B6	95.2(9)
O3B6-As36-O6B6	89.5(8)	O1B6-As36-O6B6	171.7(9)
C1B6-O1B6-As36	109.2(17)	C6B6-O2B6-As36	110.7(16)
C7B6-O3B6-As36	108.6(14)	C12B6-O4B6-As36	110.4(17)
C13B6-O5B6-As36	110.7(15)	C18B6-O6B6-As36	112.0(16)
O1B6-C1B6-C2B6	125.3(19)	O1B6-C1B6-C6B6	114.6(19)
C2B6-C1B6-C6B6	120.0	C1B6-C2B6-C3B6	120.0
C4B6-C3B6-C2B6	120.0	C3B6-C4B6-C5B6	120.0
C6B6-C5B6-C4B6	120.0	O2B6-C6B6-C5B6	122.4(18)
O2B6-C6B6-C1B6	117.5(18)	C5B6-C6B6-C1B6	120.0
C8B6-C7B6-C12B6	120.0	C8B6-C7B6-O3B6	124.2(18)
C12B6-C7B6-O3B6	115.8(18)	C9B6-C8B6-C7B6	120.0
C8B6-C9B6-C10B6	120.0	C11B6-C10B6-C9B6	120.0
C10B6-C11B6-C12B6	120.0	O4B6-C12B6-C11B6	125.7(19)
O4B6-C12B6-C7B6	114.3(19)	C11B6-C12B6-C7B6	120.0
C14B6-C13B6-C18B6	120.0	C14B6-C13B6-O5B6	124.0(16)
C18B6-C13B6-O5B6	115.8(16)	C15B6-C14B6-C13B6	120.0
C14B6-C15B6-C16B6	120.0	C17B6-C16B6-C15B6	120.0
C18B6-C17B6-C16B6	120.0	O6B6-C18B6-C17B6	124.2(17)
O6B6-C18B6-C13B6	115.6(17)	C17B6-C18B6-C13B6	120.0
O6C7-As47-O4C7	98.1(9)	O6C7-As47-O5C7	88.8(10)
O4C7-As47-O5C7	86.5(10)	O6C7-As47-O1C7	177.9(10)
O4C7-As47-O1C7	84.0(9)	O5C7-As47-O1C7	91.3(10)
O6C7-As47-O2C7	89.2(9)	O4C7-As47-O2C7	172.3(9)
O5C7-As47-O2C7	96.1(10)	O1C7-As47-O2C7	88.7(10)
O6C7-As47-O3C7	86.3(9)	O4C7-As47-O3C7	88.4(9)
O5C7-As47-O3C7	172.4(10)	O1C7-As47-O3C7	93.8(9)
O2C7-As47-O3C7	89.7(9)	C1C7-O1C7-As47	105.1(16)
C6C7-O2C7-As47	111.1(17)	C7C7-O3C7-As47	108.0(16)
C12C7-O4C7-As47	109.8(16)	C13C7-O5C7-As47	106.7(19)
C18C7-O6C7-As47	108.9(16)	C2C7-C1C7-C6C7	120.0
C2C7-C1C7-O1C7	121.1(18)	C6C7-C1C7-O1C7	118.8(18)
C3C7-C2C7-C1C7	120.0	C2C7-C3C7-C4C7	120.0
C5C7-C4C7-C3C7	120.0	C6C7-C5C7-C4C7	120.0
O2C7-C6C7-C5C7	125.5(18)	O2C7-C6C7-C1C7	114.5(18)
C5C7-C6C7-C1C7	120.0	O3C7-C7C7-C8C7	124.2(17)
O3C7-C7C7-C12C7	115.5(18)	C8C7-C7C7-C12C7	120.0
C7C7-C8C7-C9C7	120.0	C10C7-C9C7-C8C7	120.0
C11C7-C10C7-C9C7	120.0	C12C7-C11C7-C10C7	120.0
O4C7-C12C7-C11C7	123.0(17)	O4C7-C12C7-C7C7	117.0(17)
C11C7-C12C7-C7C7	120.0	O5C7-C13C7-C14C7	120(2)
O5C7-C13C7-C18C7	119(2)	C14C7-C13C7-C18C7	120.0
C15C7-C14C7-C13C7	120.0	C14C7-C15C7-C16C7	120.0

C17C7-C16C7-C15C7	120.0	C16C7-C17C7-C18C7	120.0
O6C7-C18C7-C17C7	125.5(19)	O6C7-C18C7-C13C7	114.4(19)
C17C7-C18C7-C13C7	120.0	O2D8-As58-O3D8	88.4(9)
O2D8-As58-O1D8	88.7(9)	O3D8-As58-O1D8	93.3(8)
O2D8-As58-O5D8	87.0(9)	O3D8-As58-O5D8	90.6(9)
O1D8-As58-O5D8	174.1(9)	O2D8-As58-O4D8	175.7(9)
O3D8-As58-O4D8	88.7(9)	O1D8-As58-O4D8	88.3(9)
O5D8-As58-O4D8	96.2(9)	O2D8-As58-O6D8	94.6(9)
O3D8-As58-O6D8	176.5(8)	O1D8-As58-O6D8	88.5(8)
O5D8-As58-O6D8	87.8(9)	O4D8-As58-O6D8	88.4(9)
C1D8-O1D8-As58	107.9(15)	C6D8-O2D8-As58	111.8(16)
C7D8-O3D8-As58	111.2(15)	C12D8-O4D8-As58	107.1(16)
C13D8-O5D8-As58	114.2(17)	C18D8-O6D8-As58	103.4(15)
O1D8-C1D8-C2D8	121.8(17)	O1D8-C1D8-C6D8	118.1(17)
C2D8-C1D8-C6D8	120.0	C3D8-C2D8-C1D8	120.0
C2D8-C3D8-C4D8	120.0	C5D8-C4D8-C3D8	120.0
C6D8-C5D8-C4D8	120.0	O2D8-C6D8-C5D8	127.0(17)
O2D8-C6D8-C1D8	112.9(17)	C5D8-C6D8-C1D8	120.0
O3D8-C7D8-C8D8	125.6(18)	O3D8-C7D8-C12D8	114.2(18)
C8D8-C7D8-C12D8	120.0	C7D8-C8D8-C9D8	120.0
C10D8-C9D8-C8D8	120.0	C9D8-C10D8-C11D8	120.0
C12D8-C11D8-C10D8	120.0	O4D8-C12D8-C11D8	122.3(19)
O4D8-C12D8-C7D8	117.1(19)	C11D8-C12D8-C7D8	120.0
O5D8-C13D8-C14D8	127.2(19)	O5D8-C13D8-C18D8	112.7(19)
C14D8-C13D8-C18D8	120.0	C15D8-C14D8-C13D8	120.0
C14D8-C15D8-C16D8	120.0	C17D8-C16D8-C15D8	120.0
C16D8-C17D8-C18D8	120.0	C17D8-C18D8-C13D8	120.0
C17D8-C18D8-O6D8	119.7(17)	C13D8-C18D8-O6D8	120.3(17)
O5E9-As69-O3E9	89.2(9)	O5E9-As69-O4E9	88.8(9)
O3E9-As69-O4E9	88.6(9)	O5E9-As69-O1E9	179.3(9)
O3E9-As69-O1E9	91.4(8)	O4E9-As69-O1E9	91.5(9)
O5E9-As69-O6E9	91.6(9)	O3E9-As69-O6E9	176.9(9)
O4E9-As69-O6E9	88.4(9)	O1E9-As69-O6E9	87.8(9)
O5E9-As69-O2E9	90.8(8)	O3E9-As69-O2E9	90.5(8)
O4E9-As69-O2E9	179.0(10)	O1E9-As69-O2E9	89.0(8)
O6E9-As69-O2E9	92.5(8)	C1E9-O1E9-As69	109.4(14)
C6E9-O2E9-As69	105.8(13)	C7E9-O3E9-As69	108.5(15)
C12E9-O4E9-As69	107.6(15)	C13E9-O5E9-As69	108.0(16)
C18E9-O6E9-As69	104.3(15)	O1E9-C1E9-C2E9	124.4(16)
O1E9-C1E9-C6E9	115.5(16)	C2E9-C1E9-C6E9	120.0
C1E9-C2E9-C3E9	120.0	C4E9-C3E9-C2E9	120.0
C5E9-C4E9-C3E9	120.0	C4E9-C5E9-C6E9	120.0
C5E9-C6E9-C1E9	120.0	C5E9-C6E9-O2E9	123.2(15)
C1E9-C6E9-O2E9	116.4(15)	O3E9-C7E9-C8E9	123.1(17)
O3E9-C7E9-C12E9	116.8(17)	C8E9-C7E9-C12E9	120.0
C7E9-C8E9-C9E9	120.0	C10E9-C9E9-C8E9	120.0

C9E9-C10E9-C11E9	120.0	C12E9-C11E9-C10E9	120.0
O4E9-C12E9-C11E9	124.5(16)	O4E9-C12E9-C7E9	115.3(16)
C11E9-C12E9-C7E9	120.0	O5E9-C13E9-C14E9	124.1(18)
O5E9-C13E9-C18E9	115.9(18)	C14E9-C13E9-C18E9	120.0
C13E9-C14E9-C15E9	120.0	C14E9-C15E9-C16E9	120.0
C15E9-C16E9-C17E9	120.0	C18E9-C17E9-C16E9	120.0
C17E9-C18E9-C13E9	120.0	C17E9-C18E9-O6E9	120.9(17)
C13E9-C18E9-O6E9	118.3(17)	O1F10-As710-O3F10	93.4(9)
O1F10-As710-O5F10	175.5(9)	O3F10-As710-O5F10	91.1(9)
O1F10-As710-O4F10	87.6(9)	O3F10-As710-O4F10	84.8(9)
O5F10-As710-O4F10	92.8(9)	O1F10-As710-O6F10	86.5(9)
O3F10-As710-O6F10	175.6(9)	O5F10-As710-O6F10	89.1(9)
O4F10-As710-O6F10	90.8(9)	O1F10-As710-O2F10	86.9(9)
O3F10-As710-O2F10	90.7(9)	O5F10-As710-O2F10	93.0(9)
O4F10-As710-O2F10	172.7(9)	O6F10-As710-O2F10	93.7(9)
C1F10-O1F10-As710	113.5(15)	C6F10-O2F10-As710	108.4(15)
C7F10-O3F10-As710	115.5(16)	C12F10-O4F10-As710	112.0(15)
C13F10-O5F10-As710	111.0(17)	C18F10-O6F10-As710	106.1(15)
O1F10-C1F10-C2F10	128.7(15)	O1F10-C1F10-C6F10	111.3(15)
C2F10-C1F10-C6F10	120.0	C1F10-C2F10-C3F10	120.0
C4F10-C3F10-C2F10	120.0	C5F10-C4F10-C3F10	120.0
C4F10-C5F10-C6F10	120.0	O2F10-C6F10-C5F10	120.4(16)
O2F10-C6F10-C1F10	119.2(16)	C5F10-C6F10-C1F10	120.0
C8F10-C7F10-C12F10	120.0	C8F10-C7F10-O3F10	130.2(17)
C12F10-C7F10-O3F10	109.8(17)	C7F10-C8F10-C9F10	120.0
C10F10-C9F10-C8F10	120.0	C11F10-C10F10-C9F10	120.0
C12F10-C11F10-C10F10	120.0	O4F10-C12F10-C11F10	124.2(17)
O4F10-C12F10-C7F10	115.5(17)	C11F10-C12F10-C7F10	120.0
O5F10-C13F10-C14F10	125(2)	O5F10-C13F10-C18F10	115(2)
C14F10-C13F10-C18F10	120.0	C13F10-C14F10-C15F10	120.0
C16F10-C15F10-C14F10	120.0	C15F10-C16F10-C17F10	120.0
C18F10-C17F10-C16F10	120.0	O6F10-C18F10-C17F10	121.5(18)
O6F10-C18F10-C13F10	118.4(18)	C17F10-C18F10-C13F10	120.0
O1G11-As811-O2G11	90.1(9)	O1G11-As811-O6G11	175.8(10)
O2G11-As811-O6G11	86.2(11)	O1G11-As811-O3G11	94.8(9)
O2G11-As811-O3G11	89.7(10)	O6G11-As811-O3G11	87.3(11)
O1G11-As811-O4G11	85.7(9)	O2G11-As811-O4G11	175.8(10)
O6G11-As811-O4G11	98.0(10)	O3G11-As811-O4G11	90.3(10)
O1G11-As811-O5G11	87.7(9)	O2G11-As811-O5G11	93.1(10)
O6G11-As811-O5G11	90.4(11)	O3G11-As811-O5G11	176.3(10)
O4G11-As811-O5G11	87.1(9)	O1G11-As811-C13G11	115.2(9)
O2G11-As811-C13G11	85.1(10)	O6G11-As811-C13G11	62.4(12)
O3G11-As811-C13G11	149.5(10)	O4G11-As811-C13G11	97.0(10)
O5G11-As811-C13G11	28.8(9)	C1G11-O1G11-As811	112.5(14)
C6G11-O2G11-As811	106.9(16)	C7G11-O3G11-As811	108.2(17)
C12G11-O4G11-As811	105.0(15)	C13G11-O5G11-As811	109(2)

C13G11-O5G11-C14G11	29.1(16)	As811-O5G11-C14G11	136.2(12)
C18G11-O6G11-As811	107(2)	O1G11-C1G11-C2G11	127.0(17)
O1G11-C1G11-C6G11	113.0(17)	C2G11-C1G11-C6G11	120.0
C1G11-C2G11-C3G11	120.0	C4G11-C3G11-C2G11	120.0
C3G11-C4G11-C5G11	120.0	C6G11-C5G11-C4G11	120.0
C5G11-C6G11-C1G11	120.0	C5G11-C6G11-O2G11	125.0(17)
C1G11-C6G11-O2G11	115.0(17)	O3G11-C7G11-C8G11	124.4(19)
O3G11-C7G11-C12G11	115.6(19)	C8G11-C7G11-C12G11	120.0
C7G11-C8G11-C9G11	120.0	C8G11-C9G11-C10G11	120.0
C9G11-C10G11-C11G11	120.0	C10G11-C11G11-C12G11	120.0
C11G11-C12G11-C7G11	120.0	C11G11-C12G11-O4G11	122.9(17)
C7G11-C12G11-O4G11	116.8(17)	O5G11-C13G11-C14G11	123(3)
O5G11-C13G11-C18G11	117(3)	C14G11-C13G11-C18G11	120.0
O5G11-C13G11-As811	42.1(14)	C14G11-C13G11-As811	159.1(19)
C18G11-C13G11-As811	75.3(19)	C15G11-C14G11-C13G11	120.0
C15G11-C14G11-O5G11	147.6(15)	C13G11-C14G11-O5G11	28.2(15)
C14G11-C15G11-C16G11	120.0	C17G11-C16G11-C15G11	120.0
C18G11-C17G11-C16G11	120.0	C17G11-C18G11-C13G11	120.0
C17G11-C18G11-O6G11	124(3)	C13G11-C18G11-O6G11	115(3)
O6H12-As912-O2H12	91.6(12)	O6H12-As912-O3H12	95.7(13)
O2H12-As912-O3H12	91.3(8)	O6H12-As912-O1H12	90.6(13)
O2H12-As912-O1H12	85.1(10)	O3H12-As912-O1H12	172.9(10)
O6H12-As912-O5H12	95.6(14)	O2H12-As912-O5H12	171.9(11)
O3H12-As912-O5H12	91.8(11)	O1H12-As912-O5H12	91.0(12)
O6H12-As912-O4H12	177.3(13)	O2H12-As912-O4H12	91.0(9)
O3H12-As912-O4H12	85.0(10)	O1H12-As912-O4H12	88.9(11)
O5H12-As912-O4H12	81.8(12)	O6H12-As912-C13H12	59.7(15)
O2H12-As912-C13H12	151.1(11)	O3H12-As912-C13H12	94.6(11)
O1H12-As912-C13H12	91.5(12)	O5H12-As912-C13H12	35.8(12)
O4H12-As912-C13H12	117.7(12)	C1H12-O1H12-As912	110(2)
C6H12-O2H12-As912	115.6(15)	C7H12-O3H12-As912	107.5(17)
C12H12-O4H12-As912	114(2)	C13H12-O5H12-As912	92(2)
As912-O6H12-C18H12	122(3)	O1H12-C1H12-C2H12	123(2)
O1H12-C1H12-C6H12	117(2)	C2H12-C1H12-C6H12	120.0
C1H12-C2H12-C3H12	120.0	C4H12-C3H12-C2H12	120.0
C5H12-C4H12-C3H12	120.0	C6H12-C5H12-C4H12	120.0
O2H12-C6H12-C5H12	129.2(17)	O2H12-C6H12-C1H12	110.8(17)
C5H12-C6H12-C1H12	120.0	C8H12-C7H12-C12H12	120.0
C8H12-C7H12-O3H12	116(2)	C12H12-C7H12-O3H12	122(2)
C9H12-C8H12-C7H12	120.0	C8H12-C9H12-C10H12	120.0
C11H12-C10H12-C9H12	120.0	C10H12-C11H12-C12H12	120.0
O4H12-C12H12-C11H12	131(2)	O4H12-C12H12-C7H12	109(2)
C11H12-C12H12-C7H12	120.0	O5H12-C13H12-C14H12	107(3)
O5H12-C13H12-C18H12	133(3)	C14H12-C13H12-C18H12	120.0
O5H12-C13H12-As912	52.5(16)	C14H12-C13H12-As912	159(2)
C18H12-C13H12-As912	81(2)	C15H12-C14H12-C13H12	120.0

C14H12-C15H12-C16H12	120.0	C17H12-C16H12-C15H12	120.0
C16H12-C17H12-C18H12	120.0	C17H12-C18H12-C13H12	120.0
C17H12-C18H12-O6H12	143(3)	C13H12-C18H12-O6H12	95(3)

Symmetry transformations used to generate equivalent atoms:

Table 6. Torsion angles [°] for nd1024_x.

atom-atom-atom-atom	angle	atom-atom-atom-atom	angle
C61-N11-C21-C31	0.0	Cu11-N11-C21-C31	-175.4(14)
C61-N11-C21-C11	175.6(19)	Cu11-N11-C21-C11	0.2(19)
N11-C21-C31-C41	0.0	C11-C21-C31-C41	-175(2)
C21-C31-C41-C51	0.0	C31-C41-C51-C61	0.0
C31-C41-C51-C71	178(2)	C41-C51-C61-C101	171(2)
C71-C51-C61-C101	-7(2)	C41-C51-C61-N11	0.0
C71-C51-C61-N11	-178(2)	C21-N11-C61-C101	-171(2)
Cu11-N11-C61-C101	5.0(17)	C21-N11-C61-C51	0.0
Cu11-N11-C61-C51	176.1(12)	C51-C61-C101-C91	4(2)
N11-C61-C101-C91	175.4(11)	C51-C61-C101-N21	-176.6(10)
N11-C61-C101-N21	-5(2)	C131-N21-C101-C61	-179.3(18)
Cu11-N21-C101-C61	2.9(16)	C131-N21-C101-C91	0.0
Cu11-N21-C101-C91	-177.8(11)	C61-C101-C91-C111	179(2)
N21-C101-C91-C111	0.0	C61-C101-C91-C81	4(2)
N21-C101-C91-C81	-175(2)	C101-C91-C111-C121	0.0
C81-C91-C111-C121	175(2)	C91-C111-C121-C131	0.0
C111-C121-C131-N21	0.0	C111-C121-C131-C141	180(2)
C101-N21-C131-C121	0.0	Cu11-N21-C131-C121	177.4(13)
C101-N21-C131-C141	-179(2)	Cu11-N21-C131-C141	-2(2)
C211-N31-C171-C181	0.0	Cu21-N31-C171-C181	-179.9(12)
C211-N31-C171-C161	179.2(18)	Cu21-N31-C171-C161	-0.6(19)
N31-C171-C181-C191	0.0	C161-C171-C181-C191	-179.2(19)
C171-C181-C191-C201	0.0	C181-C191-C201-C211	0.0
C181-C191-C201-C221	172.0(19)	C191-C201-C211-C251	177.1(17)
C221-C201-C211-C251	4.6(19)	C191-C201-C211-N31	0.0
C221-C201-C211-N31	-172.5(18)	C171-N31-C211-C251	-177.1(17)
Cu21-N31-C211-C251	2.8(15)	C171-N31-C211-C201	0.0
Cu21-N31-C211-C201	179.9(10)	C201-C211-C251-C241	-0.3(19)
N31-C211-C251-C241	176.8(10)	C201-C211-C251-N41	-178.1(10)
N31-C211-C251-N41	-1.0(19)	C281-N41-C251-C211	177.9(17)
Cu21-N41-C251-C211	-1.3(16)	C281-N41-C251-C241	0.0
Cu21-N41-C251-C241	-179.2(11)	C211-C251-C241-C261	-177.8(19)
N41-C251-C241-C261	0.0	C211-C251-C241-C231	-1(2)
N41-C251-C241-C231	177(2)	C251-C241-C261-C271	0.0
C231-C241-C261-C271	-177(2)	C241-C261-C271-C281	0.0
C261-C271-C281-N41	0.0	C261-C271-C281-C291	173(2)
C251-N41-C281-C271	0.0	Cu21-N41-C281-C271	179.1(13)
C251-N41-C281-C291	-174(2)	Cu21-N41-C281-C291	5(2)
C351-N51-C311-C321	0.0	Cu21-N51-C311-C321	-170.4(13)
C351-N51-C311-C301	-175(2)	Cu21-N51-C311-C301	14(2)
N51-C311-C321-C331	0.0	C301-C311-C321-C331	175(2)
C311-C321-C331-C341	0.0	C321-C331-C341-C351	0.0

C321-C331-C341-C361	-174(3)	C331-C341-C351-C391	179.5(18)
C361-C341-C351-C391	-6(2)	C331-C341-C351-N51	0.0
C361-C341-C351-N51	174(2)	C311-N51-C351-C391	-179.5(18)
Cu21-N51-C351-C391	-7.7(16)	C311-N51-C351-C341	0.0
Cu21-N51-C351-C341	171.8(11)	C341-C351-C391-N61	-171.1(11)
N51-C351-C391-N61	8(2)	C341-C351-C391-C381	7(2)
N51-C351-C391-C381	-173.1(11)	C421-N61-C391-C351	178.5(19)
Cu21-N61-C391-C351	-4.5(17)	C421-N61-C391-C381	0.0
Cu21-N61-C391-C381	177.0(12)	C351-C391-C381-C401	-178.5(19)
N61-C391-C381-C401	0.0	C351-C391-C381-C371	-2(2)
N61-C391-C381-C371	176(2)	C391-C381-C401-C411	0.0
C371-C381-C401-C411	-176(3)	C381-C401-C411-C421	0.0
C401-C411-C421-N61	0.0	C401-C411-C421-C431	-179(2)
C391-N61-C421-C411	0.0	Cu21-N61-C421-C411	-176.2(15)
C391-N61-C421-C431	179(2)	Cu21-N61-C421-C431	3(2)
C501-N71-C461-C471	0.0	Cu31-N71-C461-C471	-179.3(14)
C501-N71-C461-C451	179(2)	Cu31-N71-C461-C451	0(2)
N71-C461-C471-C481	0.0	C451-C461-C471-C481	-179(2)
C461-C471-C481-C491	0.0	C471-C481-C491-C501	0.0
C471-C481-C491-C511	-178(3)	C481-C491-C501-C541	176(2)
C511-C491-C501-C541	-6(3)	C481-C491-C501-N71	0.0
C511-C491-C501-N71	178(3)	C461-N71-C501-C541	-176(2)
Cu31-N71-C501-C541	3.3(19)	C461-N71-C501-C491	0.0
Cu31-N71-C501-C491	179.4(12)	C491-C501-C541-C531	2(2)
N71-C501-C541-C531	178.2(13)	C491-C501-C541-N81	179.0(14)
N71-C501-C541-N81	-5(3)	C571-N81-C541-C501	-177(2)
Cu31-N81-C541-C501	4(2)	C571-N81-C541-C531	0.0
Cu31-N81-C541-C531	-179.0(15)	C501-C541-C531-C521	-3(3)
N81-C541-C531-C521	-180(3)	C501-C541-C531-C551	177(2)
N81-C541-C531-C551	0.0	C521-C531-C551-C561	180(4)
C541-C531-C551-C561	0.0	C531-C551-C561-C571	0.0
C551-C561-C571-N81	0.0	C551-C561-C571-C581	-178(3)
C541-N81-C571-C561	0.0	Cu31-N81-C571-C561	178.8(18)
C541-N81-C571-C581	178(3)	Cu31-N81-C571-C581	-3(3)
C641-N91-C601-C611	0.0	Cu31-N91-C601-C611	-165.2(16)
C641-N91-C601-C591	-180(2)	Cu31-N91-C601-C591	15(2)
N91-C601-C611-C621	0.0	C591-C601-C611-C621	180(3)
C601-C611-C621-C631	0.0	C611-C621-C631-C641	0.0
C611-C621-C631-C651	-180(3)	C621-C631-C641-N91	0.0
C651-C631-C641-N91	180(2)	C621-C631-C641-C681	176(2)
C651-C631-C641-C681	-5(2)	C601-N91-C641-C631	0.0
Cu31-N91-C641-C631	167.3(14)	C601-N91-C641-C681	-176(2)
Cu31-N91-C641-C681	-8.5(18)	C711-N101-C681-C671	0.0
Cu31-N101-C681-C671	-176.5(12)	C711-N101-C681-C641	-178.6(19)
Cu31-N101-C681-C641	4.9(18)	C631-C641-C681-N101	-173.2(12)
N91-C641-C681-N101	2(2)	C631-C641-C681-C671	8(2)

N91-C641-C681-C671	-176.1(12)	N101-C681-C671-C691	0.0
C641-C681-C671-C691	179(2)	N101-C681-C671-C661	178(2)
C641-C681-C671-C661	-4(2)	C681-C671-C691-C701	0.0
C661-C671-C691-C701	-177(2)	C671-C691-C701-C711	0.0
C691-C701-C711-N101	0.0	C691-C701-C711-C721	-177(2)
C681-N101-C711-C701	0.0	Cu31-N101-C711-C701	175.9(14)
C681-N101-C711-C721	177(2)	Cu31-N101-C711-C721	-7(2)
C791-N111-C751-C761	0.0	Cu11-N111-C751-C761	172.8(13)
C791-N111-C751-C741	176.5(18)	Cu11-N111-C751-C741	-10.7(19)
N111-C751-C761-C771	0.0	C741-C751-C761-C771	-176(2)
C751-C761-C771-C781	0.0	C761-C771-C781-C791	0.0
C761-C771-C781-C801	-176(2)	C771-C781-C791-C831	178.3(19)
C801-C781-C791-C831	-5(2)	C771-C781-C791-N111	0.0
C801-C781-C791-N111	177(2)	C751-N111-C791-C831	-178.4(18)
Cu11-N111-C791-C831	7.6(16)	C751-N111-C791-C781	0.0
Cu11-N111-C791-C781	-174.0(11)	C781-C791-C831-C821	2.3(19)
N111-C791-C831-C821	-179.3(10)	C781-C791-C831-N121	175.2(10)
N111-C791-C831-N121	-6.5(19)	C861-N121-C831-C791	-173.0(17)
Cu11-N121-C831-C791	1.8(16)	C861-N121-C831-C821	0.0
Cu11-N121-C831-C821	174.8(11)	C791-C831-C821-C841	172.7(18)
N121-C831-C821-C841	0.0	C791-C831-C821-C811	0(2)
N121-C831-C821-C811	-173(2)	C831-C821-C841-C851	0.0
C811-C821-C841-C851	173(2)	C821-C841-C851-C861	0.0
C841-C851-C861-N121	0.0	C841-C851-C861-C871	-178(2)
C831-N121-C861-C851	0.0	Cu11-N121-C861-C851	-173.7(13)
C831-N121-C861-C871	178(2)	Cu11-N121-C861-C871	4(2)
C41-C51-C71-C81	-176(2)	C61-C51-C71-C81	2(4)
C101-C91-C81-C71	-9(3)	C111-C91-C81-C71	176(2)
C51-C71-C81-C91	6(4)	C121-C131-C141-C151	-91(3)
N21-C131-C141-C151	88(3)	C131-C141-C151-C161	178(2)
N31-C171-C161-C151	74(3)	C181-C171-C161-C151	-107(2)
C141-C151-C161-C171	-177(2)	C191-C201-C221-C231	179(2)
C211-C201-C221-C231	-9(3)	C201-C221-C231-C241	8(5)
C251-C241-C231-C221	-3(4)	C261-C241-C231-C221	173(2)
C401-C381-C371-C361	172(3)	C391-C381-C371-C361	-4(4)
C381-C371-C361-C341	5(5)	C351-C341-C361-C371	0(4)
C331-C341-C361-C371	174(3)	C411-C421-C431-C441	-108(3)
N61-C421-C431-C441	73(3)	C421-C431-C441-C451	174(3)
C471-C461-C451-C441	-93(3)	N71-C461-C451-C441	88(3)
C431-C441-C451-C461	176(3)	C501-C491-C511-C521	11(5)
C481-C491-C511-C521	-171(3)	C491-C511-C521-C531	-13(7)
C541-C531-C521-C511	8(6)	C551-C531-C521-C511	-171(3)
C641-C631-C651-C661	-3(4)	C621-C631-C651-C661	177(2)
C631-C651-C661-C671	7(5)	C691-C671-C661-C651	174(2)
C681-C671-C661-C651	-4(4)	C701-C711-C721-C731	-104(2)
N101-C711-C721-C731	78(3)	C711-C721-C731-C741	-179(2)

C721-C731-C741-C751	-175(2)	C761-C751-C741-C731	-91(3)
N111-C751-C741-C731	92(2)	C771-C781-C801-C811	-177(2)
C791-C781-C801-C811	6(4)	C781-C801-C811-C821	-5(5)
C831-C821-C811-C801	2(4)	C841-C821-C811-C801	-171(2)
C6A2-N1A2-C2A2-C3A2	0.0	Cu42-N1A2-C2A2-C3A2	-174.9(14)
C6A2-N1A2-C2A2-C1A2	-178(2)	Cu42-N1A2-C2A2-C1A2	7(2)
N1A2-C2A2-C3A2-C4A2	0.0	C1A2-C2A2-C3A2-C4A2	178(2)
C2A2-C3A2-C4A2-C5A2	0.0	C3A2-C4A2-C5A2-C6A2	0.0
C3A2-C4A2-C5A2-C7A2	174(2)	C4A2-C5A2-C6A2-C10A2	174(2)
C7A2-C5A2-C6A2-C10A2	-1(2)	C4A2-C5A2-C6A2-N1A2	0.0
C7A2-C5A2-C6A2-N1A2	-175(2)	C2A2-N1A2-C6A2-C10A2	-174.5(19)
Cu42-N1A2-C6A2-C10A2	1.2(17)	C2A2-N1A2-C6A2-C5A2	0.0
Cu42-N1A2-C6A2-C5A2	175.7(11)	C5A2-C6A2-C10A2-N2A2	-176.2(11)
N1A2-C6A2-C10A2-N2A2	-2(2)	C5A2-C6A2-C10A2-C9A2	4(2)
N1A2-C6A2-C10A2-C9A2	178.9(11)	C13A2-N2A2-C10A2-C6A2	-179.3(19)
Cu42-N2A2-C10A2-C6A2	1.4(17)	C13A2-N2A2-C10A2-C9A2	0.0
Cu42-N2A2-C10A2-C9A2	-179.3(12)	C6A2-C10A2-C9A2-C11A2	179.3(19)
N2A2-C10A2-C9A2-C11A2	0.0	C6A2-C10A2-C9A2-C8A2	0(2)
N2A2-C10A2-C9A2-C8A2	-179(2)	C10A2-C9A2-C11A2-C12A2	0.0
C8A2-C9A2-C11A2-C12A2	179(2)	C9A2-C11A2-C12A2-C13A2	0.0
C11A2-C12A2-C13A2-C14A2	-175(2)	C11A2-C12A2-C13A2-N2A2	0.0
C10A2-N2A2-C13A2-C14A2	175(2)	Cu42-N2A2-C13A2-C14A2	-6(2)
C10A2-N2A2-C13A2-C12A2	0.0	Cu42-N2A2-C13A2-C12A2	179.2(14)
C21A2-N3A2-C17A2-C18A2	0.0	Cu52-N3A2-C17A2-C18A2	-174.4(13)
C21A2-N3A2-C17A2-C16A2	-173.6(18)	Cu52-N3A2-C17A2-C16A2	12.0(18)
N3A2-C17A2-C18A2-C19A2	0.0	C16A2-C17A2-C18A2-C19A2	173.1(19)
C17A2-C18A2-C19A2-C20A2	0.0	C18A2-C19A2-C20A2-C22A2	-180(2)
C18A2-C19A2-C20A2-C21A2	0.0	C22A2-C20A2-C21A2-C25A2	-4(2)
C19A2-C20A2-C21A2-C25A2	175.9(18)	C22A2-C20A2-C21A2-N3A2	180(2)
C19A2-C20A2-C21A2-N3A2	0.0	C17A2-N3A2-C21A2-C25A2	-176.0(17)
Cu52-N3A2-C21A2-C25A2	-0.7(15)	C17A2-N3A2-C21A2-C20A2	0.0
Cu52-N3A2-C21A2-C20A2	175.4(11)	C20A2-C21A2-C25A2-C24A2	9.9(19)
N3A2-C21A2-C25A2-C24A2	-174.2(10)	C20A2-C21A2-C25A2-N4A2	-178.2(10)
N3A2-C21A2-C25A2-N4A2	-2(2)	C28A2-N4A2-C25A2-C21A2	-171.9(18)
Cu52-N4A2-C25A2-C21A2	4.1(16)	C28A2-N4A2-C25A2-C24A2	0.0
Cu52-N4A2-C25A2-C24A2	176.0(11)	C21A2-C25A2-C24A2-C26A2	171.8(19)
N4A2-C25A2-C24A2-C26A2	0.0	C21A2-C25A2-C24A2-C23A2	-7(2)
N4A2-C25A2-C24A2-C23A2	-179(2)	C25A2-C24A2-C26A2-C27A2	0.0
C23A2-C24A2-C26A2-C27A2	179(2)	C24A2-C26A2-C27A2-C28A2	0.0
C26A2-C27A2-C28A2-N4A2	0.0	C26A2-C27A2-C28A2-C29A2	-178.1(19)
C25A2-N4A2-C28A2-C27A2	0.0	Cu52-N4A2-C28A2-C27A2	-175.2(13)
C25A2-N4A2-C28A2-C29A2	178.1(19)	Cu52-N4A2-C28A2-C29A2	2.9(19)
C35A2-N5A2-C31A2-C30A2	176(3)	Cu52-N5A2-C31A2-C30A2	-5(3)
C35A2-N5A2-C31A2-C32A2	0.0	Cu52-N5A2-C31A2-C32A2	179.7(15)
C30A2-C31A2-C32A2-C33A2	-176(2)	N5A2-C31A2-C32A2-C33A2	0.0
C31A2-C32A2-C33A2-C34A2	0.0	C32A2-C33A2-C34A2-C35A2	0.0

C32A2-C33A2-C34A2-C36A2	172(2)	C33A2-C34A2-C35A2-C39A2	175(2)
C36A2-C34A2-C35A2-C39A2	3(2)	C33A2-C34A2-C35A2-N5A2	0.0
C36A2-C34A2-C35A2-N5A2	-172(2)	C31A2-N5A2-C35A2-C39A2	-175.3(19)
Cu52-N5A2-C35A2-C39A2	4.9(17)	C31A2-N5A2-C35A2-C34A2	0.0
Cu52-N5A2-C35A2-C34A2	-179.7(13)	C34A2-C35A2-C39A2-C38A2	-1(2)
N5A2-C35A2-C39A2-C38A2	174.1(11)	C34A2-C35A2-C39A2-N6A2	175.5(11)
N5A2-C35A2-C39A2-N6A2	-9(2)	C42A2-N6A2-C39A2-C35A2	-176.6(18)
Cu52-N6A2-C39A2-C35A2	8.5(17)	C42A2-N6A2-C39A2-C38A2	0.0
Cu52-N6A2-C39A2-C38A2	-174.9(11)	C35A2-C39A2-C38A2-C40A2	176.5(18)
N6A2-C39A2-C38A2-C40A2	0.0	C35A2-C39A2-C38A2-C37A2	-1(2)
N6A2-C39A2-C38A2-C37A2	-177(2)	C39A2-C38A2-C40A2-C41A2	0.0
C37A2-C38A2-C40A2-C41A2	177(2)	C38A2-C40A2-C41A2-C42A2	0.0
C40A2-C41A2-C42A2-N6A2	0.0	C40A2-C41A2-C42A2-C43A2	-175(2)
C39A2-N6A2-C42A2-C41A2	0.0	Cu52-N6A2-C42A2-C41A2	173.7(13)
C39A2-N6A2-C42A2-C43A2	175.4(18)	Cu52-N6A2-C42A2-C43A2	-10.9(18)
C50A2-N7A2-C46A2-C47A2	0.0	Cu62-N7A2-C46A2-C47A2	178.6(13)
C50A2-N7A2-C46A2-C45A2	-175.9(19)	Cu62-N7A2-C46A2-C45A2	3(2)
N7A2-C46A2-C47A2-C48A2	0.0	C45A2-C46A2-C47A2-C48A2	175(2)
C46A2-C47A2-C48A2-C49A2	0.0	C47A2-C48A2-C49A2-C50A2	0.0
C47A2-C48A2-C49A2-C51A2	-177.8(19)	C48A2-C49A2-C50A2-C54A2	175.3(18)
C51A2-C49A2-C50A2-C54A2	-6.7(19)	C48A2-C49A2-C50A2-N7A2	0.0
C51A2-C49A2-C50A2-N7A2	177.9(17)	C46A2-N7A2-C50A2-C54A2	-175.6(17)
Cu62-N7A2-C50A2-C54A2	5.6(14)	C46A2-N7A2-C50A2-C49A2	0.0
Cu62-N7A2-C50A2-C49A2	-178.8(11)	C49A2-C50A2-C54A2-N8A2	-173.8(10)
N7A2-C50A2-C54A2-N8A2	1.7(18)	C49A2-C50A2-C54A2-C53A2	3.0(18)
N7A2-C50A2-C54A2-C53A2	178.5(9)	C57A2-N8A2-C54A2-C50A2	176.8(17)
Cu62-N8A2-C54A2-C50A2	-8.4(15)	C57A2-N8A2-C54A2-C53A2	0.0
Cu62-N8A2-C54A2-C53A2	174.8(10)	C50A2-C54A2-C53A2-C55A2	-176.8(17)
N8A2-C54A2-C53A2-C55A2	0.0	C50A2-C54A2-C53A2-C52A2	-0.1(19)
N8A2-C54A2-C53A2-C52A2	176.6(18)	C54A2-C53A2-C55A2-C56A2	0.0
C52A2-C53A2-C55A2-C56A2	-176.5(19)	C53A2-C55A2-C56A2-C57A2	0.0
C55A2-C56A2-C57A2-N8A2	0.0	C55A2-C56A2-C57A2-C58A2	-178(2)
C54A2-N8A2-C57A2-C56A2	0.0	Cu62-N8A2-C57A2-C56A2	-173.8(12)
C54A2-N8A2-C57A2-C58A2	177.8(19)	Cu62-N8A2-C57A2-C58A2	4.0(19)
C64A2-N9A2-C60A2-C61A2	0.0	Cu62-N9A2-C60A2-C61A2	-173.9(14)
C64A2-N9A2-C60A2-C59A2	178(2)	Cu62-N9A2-C60A2-C59A2	4(2)
N9A2-C60A2-C61A2-C62A2	0.0	C59A2-C60A2-C61A2-C62A2	-177(2)
C60A2-C61A2-C62A2-C63A2	0.0	C61A2-C62A2-C63A2-C64A2	0.0
C61A2-C62A2-C63A2-C65A2	-179(2)	C62A2-C63A2-C64A2-C68A2	176.6(19)
C65A2-C63A2-C64A2-C68A2	-4(2)	C62A2-C63A2-C64A2-N9A2	0.0
C65A2-C63A2-C64A2-N9A2	179(2)	C60A2-N9A2-C64A2-C68A2	-176.7(18)
Cu62-N9A2-C64A2-C68A2	-1.7(17)	C60A2-N9A2-C64A2-C63A2	0.0
Cu62-N9A2-C64A2-C63A2	174.9(12)	C63A2-C64A2-C68A2-C67A2	3.6(19)
N9A2-C64A2-C68A2-C67A2	-179.8(11)	C63A2-C64A2-C68A2-N10A2	-178.3(10)
N9A2-C64A2-C68A2-N10A2	-2(2)	C71A2-N10A2-C68A2-C64A2	-178.2(17)
Cu62-N10A2-C68A2-C64A2	4.0(15)	C71A2-N10A2-C68A2-C67A2	0.0

Cu62-N10A2-C68A2-C67A2	-177.9(10)	C64A2-C68A2-C67A2-C69A2	178.1(18)
N10A2-C68A2-C67A2-C69A2	0.0	C64A2-C68A2-C67A2-C66A2	-1(2)
N10A2-C68A2-C67A2-C66A2	-180(2)	C68A2-C67A2-C69A2-C70A2	0.0
C66A2-C67A2-C69A2-C70A2	180(2)	C67A2-C69A2-C70A2-C71A2	0.0
C69A2-C70A2-C71A2-N10A2	0.0	C69A2-C70A2-C71A2-C72A2	175(2)
C68A2-N10A2-C71A2-C70A2	0.0	Cu62-N10A2-C71A2-C70A2	177.3(13)
C68A2-N10A2-C71A2-C72A2	-175.7(19)	Cu62-N10A2-C71A2-C72A2	2(2)
C79A2-N11A2-C75A2-C76A2	0.0	Cu42-N11A2-C75A2-C76A2	-177.4(13)
C79A2-N11A2-C75A2-C74A2	177(2)	Cu42-N11A2-C75A2-C74A2	-1(2)
N11A2-C75A2-C76A2-C77A2	0.0	C74A2-C75A2-C76A2-C77A2	-177(2)
C75A2-C76A2-C77A2-C78A2	0.0	C76A2-C77A2-C78A2-C79A2	0.0
C76A2-C77A2-C78A2-C80A2	179(2)	C77A2-C78A2-C79A2-N11A2	0.0
C80A2-C78A2-C79A2-N11A2	-179(2)	C77A2-C78A2-C79A2-C83A2	177.5(17)
C80A2-C78A2-C79A2-C83A2	-2(2)	C75A2-N11A2-C79A2-C78A2	0.0
Cu42-N11A2-C79A2-C78A2	177.9(10)	C75A2-N11A2-C79A2-C83A2	-177.5(18)
Cu42-N11A2-C79A2-C83A2	0.4(17)	C86A2-N12A2-C83A2-C82A2	0.0
Cu42-N12A2-C83A2-C82A2	170.0(11)	C86A2-N12A2-C83A2-C79A2	-175.6(17)
Cu42-N12A2-C83A2-C79A2	-5.5(15)	C78A2-C79A2-C83A2-N12A2	-174.1(10)
N11A2-C79A2-C83A2-N12A2	3.3(19)	C78A2-C79A2-C83A2-C82A2	10.6(19)
N11A2-C79A2-C83A2-C82A2	-171.9(11)	N12A2-C83A2-C82A2-C84A2	0.0
C79A2-C83A2-C82A2-C84A2	175.0(19)	N12A2-C83A2-C82A2-C81A2	178(2)
C79A2-C83A2-C82A2-C81A2	-7(2)	C83A2-C82A2-C84A2-C85A2	0.0
C81A2-C82A2-C84A2-C85A2	-178(2)	C82A2-C84A2-C85A2-C86A2	0.0
C84A2-C85A2-C86A2-N12A2	0.0	C84A2-C85A2-C86A2-C87A2	180(2)
C83A2-N12A2-C86A2-C85A2	0.0	Cu42-N12A2-C86A2-C85A2	-169.0(12)
C83A2-N12A2-C86A2-C87A2	-180(2)	Cu42-N12A2-C86A2-C87A2	11(2)
C6A2-C5A2-C7A2-C8A2	-9(4)	C4A2-C5A2-C7A2-C8A2	176(3)
C5A2-C7A2-C8A2-C9A2	15(5)	C11A2-C9A2-C8A2-C7A2	171(3)
C10A2-C9A2-C8A2-C7A2	-10(4)	C12A2-C13A2-C14A2-C15A2	-107(2)
N2A2-C13A2-C14A2-C15A2	78(3)	C13A2-C14A2-C15A2-C16A2	179(3)
C14A2-C15A2-C16A2-C17A2	175(2)	N3A2-C17A2-C16A2-C15A2	78(3)
C18A2-C17A2-C16A2-C15A2	-95(3)	C19A2-C20A2-C22A2-C23A2	176(2)
C21A2-C20A2-C22A2-C23A2	-4(3)	C20A2-C22A2-C23A2-C24A2	7(4)
C25A2-C24A2-C23A2-C22A2	-1(3)	C26A2-C24A2-C23A2-C22A2	180(2)
C35A2-C34A2-C36A2-C37A2	-2(4)	C33A2-C34A2-C36A2-C37A2	-175(2)
C34A2-C36A2-C37A2-C38A2	1(4)	C40A2-C38A2-C37A2-C36A2	-176(2)
C39A2-C38A2-C37A2-C36A2	1(3)	C41A2-C42A2-C43A2-C44A2	-111(2)
N6A2-C42A2-C43A2-C44A2	74(2)	C42A2-C43A2-C44A2-C45A2	-179(2)
C43A2-C44A2-C45A2-C46A2	180(2)	N7A2-C46A2-C45A2-C44A2	91(3)
C47A2-C46A2-C45A2-C44A2	-84(3)	C50A2-C49A2-C51A2-C52A2	8(3)
C48A2-C49A2-C51A2-C52A2	-174(2)	C49A2-C51A2-C52A2-C53A2	-6(4)
C55A2-C53A2-C52A2-C51A2	178(2)	C54A2-C53A2-C52A2-C51A2	2(3)
C62A2-C63A2-C65A2-C66A2	-178(2)	C64A2-C63A2-C65A2-C66A2	2(3)
C63A2-C65A2-C66A2-C67A2	0(4)	C68A2-C67A2-C66A2-C65A2	0(3)
C69A2-C67A2-C66A2-C65A2	-180(2)	C70A2-C71A2-C72A2-C73A2	-87(3)
N10A2-C71A2-C72A2-C73A2	88(3)	C71A2-C72A2-C73A2-C74A2	179(2)

C76A2-C75A2-C74A2-C73A2	-109(2)	N11A2-C75A2-C74A2-C73A2	74(2)
C72A2-C73A2-C74A2-C75A2	179(2)	C77A2-C78A2-C80A2-C81A2	169(3)
C79A2-C78A2-C80A2-C81A2	-12(4)	C78A2-C80A2-C81A2-C82A2	15(5)
C83A2-C82A2-C81A2-C80A2	-5(4)	C84A2-C82A2-C81A2-C80A2	172(2)
C6B3-N1B3-C2B3-C3B3	0.0	Cu73-N1B3-C2B3-C3B3	-176.7(14)
C6B3-N1B3-C2B3-C1B3	176.1(19)	Cu73-N1B3-C2B3-C1B3	-1(2)
N1B3-C2B3-C3B3-C4B3	0.0	C1B3-C2B3-C3B3-C4B3	-175(2)
C2B3-C3B3-C4B3-C5B3	0.0	C3B3-C4B3-C5B3-C7B3	176(2)
C3B3-C4B3-C5B3-C6B3	0.0	C7B3-C5B3-C6B3-C10B3	1(2)
C4B3-C5B3-C6B3-C10B3	177.5(17)	C7B3-C5B3-C6B3-N1B3	-176(2)
C4B3-C5B3-C6B3-N1B3	0.0	C2B3-N1B3-C6B3-C10B3	-177.5(17)
Cu73-N1B3-C6B3-C10B3	-0.1(16)	C2B3-N1B3-C6B3-C5B3	0.0
Cu73-N1B3-C6B3-C5B3	177.4(11)	C5B3-C6B3-C10B3-C9B3	0.8(18)
N1B3-C6B3-C10B3-C9B3	178.3(11)	C5B3-C6B3-C10B3-N2B3	178.5(11)
N1B3-C6B3-C10B3-N2B3	-4(2)	C13B3-N2B3-C10B3-C6B3	-177.7(17)
Cu73-N2B3-C10B3-C6B3	5.8(16)	C13B3-N2B3-C10B3-C9B3	0.0
Cu73-N2B3-C10B3-C9B3	-176.5(11)	C6B3-C10B3-C9B3-C11B3	177.6(18)
N2B3-C10B3-C9B3-C11B3	0.0	C6B3-C10B3-C9B3-C8B3	-2(3)
N2B3-C10B3-C9B3-C8B3	-180(3)	C10B3-C9B3-C11B3-C12B3	0.0
C8B3-C9B3-C11B3-C12B3	180(3)	C9B3-C11B3-C12B3-C13B3	0.0
C11B3-C12B3-C13B3-N2B3	0.0	C11B3-C12B3-C13B3-C14B3	-173(2)
C10B3-N2B3-C13B3-C12B3	0.0	Cu73-N2B3-C13B3-C12B3	175.7(14)
C10B3-N2B3-C13B3-C14B3	173(2)	Cu73-N2B3-C13B3-C14B3	-11.0(19)
C21B3-N3B3-C17B3-C18B3	0.0	Cu83-N3B3-C17B3-C18B3	-178.3(13)
C21B3-N3B3-C17B3-C16B3	-179.5(18)	Cu83-N3B3-C17B3-C16B3	2.2(19)
N3B3-C17B3-C18B3-C19B3	0.0	C16B3-C17B3-C18B3-C19B3	179(2)
C17B3-C18B3-C19B3-C20B3	0.0	C18B3-C19B3-C20B3-C21B3	0.0
C18B3-C19B3-C20B3-C22B3	-175(2)	C19B3-C20B3-C21B3-C25B3	176.4(17)
C22B3-C20B3-C21B3-C25B3	-9(2)	C19B3-C20B3-C21B3-N3B3	0.0
C22B3-C20B3-C21B3-N3B3	175(2)	C17B3-N3B3-C21B3-C25B3	-176.2(18)
Cu83-N3B3-C21B3-C25B3	2.5(16)	C17B3-N3B3-C21B3-C20B3	0.0
Cu83-N3B3-C21B3-C20B3	178.7(10)	C20B3-C21B3-C25B3-N4B3	-176.4(10)
N3B3-C21B3-C25B3-N4B3	-0.1(19)	C20B3-C21B3-C25B3-C24B3	16.2(19)
N3B3-C21B3-C25B3-C24B3	-167.5(11)	C28B3-N4B3-C25B3-C21B3	-168.1(17)
Cu83-N4B3-C25B3-C21B3	-2.4(15)	C28B3-N4B3-C25B3-C24B3	0.0
Cu83-N4B3-C25B3-C24B3	165.7(12)	C21B3-C25B3-C24B3-C26B3	166.6(19)
N4B3-C25B3-C24B3-C26B3	0.0	C21B3-C25B3-C24B3-C23B3	-18(2)
N4B3-C25B3-C24B3-C23B3	175(2)	C25B3-C24B3-C26B3-C27B3	0.0
C23B3-C24B3-C26B3-C27B3	-174(2)	C24B3-C26B3-C27B3-C28B3	0.0
C26B3-C27B3-C28B3-N4B3	0.0	C26B3-C27B3-C28B3-C29B3	170(2)
C25B3-N4B3-C28B3-C27B3	0.0	Cu83-N4B3-C28B3-C27B3	-163.7(14)
C25B3-N4B3-C28B3-C29B3	-171(2)	Cu83-N4B3-C28B3-C29B3	25.7(19)
C35B3-N5B3-C31B3-C32B3	0.0	Cu83-N5B3-C31B3-C32B3	-166.8(13)
C35B3-N5B3-C31B3-C30B3	-168(2)	Cu83-N5B3-C31B3-C30B3	25(2)
N5B3-C31B3-C32B3-C33B3	0.0	C30B3-C31B3-C32B3-C33B3	166(3)
C31B3-C32B3-C33B3-C34B3	0.0	C32B3-C33B3-C34B3-C35B3	0.0

C32B3-C33B3-C34B3-C36B3	-177(3)	C33B3-C34B3-C35B3-C39B3	176.1(19)
C36B3-C34B3-C35B3-C39B3	-7(2)	C33B3-C34B3-C35B3-N5B3	0.0
C36B3-C34B3-C35B3-N5B3	177(2)	C31B3-N5B3-C35B3-C39B3	-176.5(18)
Cu83-N5B3-C35B3-C39B3	-7.9(16)	C31B3-N5B3-C35B3-C34B3	0.0
Cu83-N5B3-C35B3-C34B3	168.5(11)	C34B3-C35B3-C39B3-C38B3	13(2)
N5B3-C35B3-C39B3-C38B3	-171.1(11)	C34B3-C35B3-C39B3-N6B3	-178.7(11)
N5B3-C35B3-C39B3-N6B3	-2(2)	C42B3-N6B3-C39B3-C35B3	-168.5(19)
Cu83-N6B3-C39B3-C35B3	10.8(16)	C42B3-N6B3-C39B3-C38B3	0.0
Cu83-N6B3-C39B3-C38B3	179.3(13)	C35B3-C39B3-C38B3-C37B3	-10(3)
N6B3-C39B3-C38B3-C37B3	-179(2)	C35B3-C39B3-C38B3-C40B3	168.8(18)
N6B3-C39B3-C38B3-C40B3	0.0	C39B3-C38B3-C40B3-C41B3	0.0
C37B3-C38B3-C40B3-C41B3	179(2)	C38B3-C40B3-C41B3-C42B3	0.0
C40B3-C41B3-C42B3-N6B3	0.0	C40B3-C41B3-C42B3-C43B3	177(2)
C39B3-N6B3-C42B3-C41B3	0.0	Cu83-N6B3-C42B3-C41B3	-179.1(17)
C39B3-N6B3-C42B3-C43B3	-177(2)	Cu83-N6B3-C42B3-C43B3	4(2)
C50B3-N7B3-C46B3-C47B3	0.0	Cu93-N7B3-C46B3-C47B3	178.3(14)
C50B3-N7B3-C46B3-C45B3	179(2)	Cu93-N7B3-C46B3-C45B3	-3(2)
N7B3-C46B3-C47B3-C48B3	0.0	C45B3-C46B3-C47B3-C48B3	-179(2)
C46B3-C47B3-C48B3-C49B3	0.0	C47B3-C48B3-C49B3-C50B3	0.0
C47B3-C48B3-C49B3-C51B3	-177(2)	C48B3-C49B3-C50B3-C54B3	-178(2)
C51B3-C49B3-C50B3-C54B3	-1(2)	C48B3-C49B3-C50B3-N7B3	0.0
C51B3-C49B3-C50B3-N7B3	177(2)	C46B3-N7B3-C50B3-C54B3	178(2)
Cu93-N7B3-C50B3-C54B3	-1.1(19)	C46B3-N7B3-C50B3-C49B3	0.0
Cu93-N7B3-C50B3-C49B3	-178.6(12)	C49B3-C50B3-C54B3-N8B3	177.8(12)
N7B3-C50B3-C54B3-N8B3	0(2)	C49B3-C50B3-C54B3-C53B3	6(2)
N7B3-C50B3-C54B3-C53B3	-171.1(13)	C57B3-N8B3-C54B3-C50B3	-172(2)
Cu93-N8B3-C54B3-C50B3	0.8(19)	C57B3-N8B3-C54B3-C53B3	0.0
Cu93-N8B3-C54B3-C53B3	172.5(14)	C50B3-C54B3-C53B3-C55B3	171(2)
N8B3-C54B3-C53B3-C55B3	0.0	C50B3-C54B3-C53B3-C52B3	-6(3)
N8B3-C54B3-C53B3-C52B3	-177(2)	C54B3-C53B3-C55B3-C56B3	0.0
C52B3-C53B3-C55B3-C56B3	176(3)	C53B3-C55B3-C56B3-C57B3	0.0
C55B3-C56B3-C57B3-N8B3	0.0	C55B3-C56B3-C57B3-C58B3	-179(3)
C54B3-N8B3-C57B3-C56B3	0.0	Cu93-N8B3-C57B3-C56B3	-171.6(16)
C54B3-N8B3-C57B3-C58B3	179(3)	Cu93-N8B3-C57B3-C58B3	8(3)
C64B3-N9B3-C60B3-C61B3	0.0	Cu93-N9B3-C60B3-C61B3	-167.0(16)
C64B3-N9B3-C60B3-C59B3	-176(3)	Cu93-N9B3-C60B3-C59B3	17(3)
N9B3-C60B3-C61B3-C62B3	0.0	C59B3-C60B3-C61B3-C62B3	175(4)
C60B3-C61B3-C62B3-C63B3	0.0	C61B3-C62B3-C63B3-C65B3	178(3)
C61B3-C62B3-C63B3-C64B3	0.0	C65B3-C63B3-C64B3-C68B3	-3(3)
C62B3-C63B3-C64B3-C68B3	175(3)	C65B3-C63B3-C64B3-N9B3	-178(3)
C62B3-C63B3-C64B3-N9B3	0.0	C60B3-N9B3-C64B3-C68B3	-175(2)
Cu93-N9B3-C64B3-C68B3	-6(2)	C60B3-N9B3-C64B3-C63B3	0.0
Cu93-N9B3-C64B3-C63B3	169.0(14)	C63B3-C64B3-C68B3-C67B3	3(3)
N9B3-C64B3-C68B3-C67B3	178.6(13)	C63B3-C64B3-C68B3-N10B3	-174.9(13)
N9B3-C64B3-C68B3-N10B3	0(3)	C71B3-N10B3-C68B3-C64B3	178(2)
Cu93-N10B3-C68B3-C64B3	6(2)	C71B3-N10B3-C68B3-C67B3	0.0

Cu93-N10B3-C68B3-C67B3	-172.5(13)	C64B3-C68B3-C67B3-C69B3	-178(2)
N10B3-C68B3-C67B3-C69B3	0.0	C64B3-C68B3-C67B3-C66B3	0(3)
N10B3-C68B3-C67B3-C66B3	179(3)	C68B3-C67B3-C69B3-C70B3	0.0
C66B3-C67B3-C69B3-C70B3	-178(3)	C67B3-C69B3-C70B3-C71B3	0.0
C69B3-C70B3-C71B3-N10B3	0.0	C69B3-C70B3-C71B3-C72B3	-174(2)
C68B3-N10B3-C71B3-C70B3	0.0	Cu93-N10B3-C71B3-C70B3	171.0(16)
C68B3-N10B3-C71B3-C72B3	175(2)	Cu93-N10B3-C71B3-C72B3	-14(2)
C79B3-N11B3-C75B3-C76B3	0.0	Cu73-N11B3-C75B3-C76B3	176.1(13)
C79B3-N11B3-C75B3-C74B3	177(2)	Cu73-N11B3-C75B3-C74B3	-7(2)
N11B3-C75B3-C76B3-C77B3	0.0	C74B3-C75B3-C76B3-C77B3	-177(2)
C75B3-C76B3-C77B3-C78B3	0.0	C76B3-C77B3-C78B3-C79B3	0.0
C76B3-C77B3-C78B3-C80B3	-180(2)	C77B3-C78B3-C79B3-C83B3	-179.2(18)
C80B3-C78B3-C79B3-C83B3	0(2)	C77B3-C78B3-C79B3-N11B3	0.0
C80B3-C78B3-C79B3-N11B3	180(2)	C75B3-N11B3-C79B3-C83B3	179.2(17)
Cu73-N11B3-C79B3-C83B3	2.4(15)	C75B3-N11B3-C79B3-C78B3	0.0
Cu73-N11B3-C79B3-C78B3	-176.8(11)	C78B3-C79B3-C83B3-C82B3	-2.6(19)
N11B3-C79B3-C83B3-C82B3	178.2(10)	C78B3-C79B3-C83B3-N12B3	175.9(11)
N11B3-C79B3-C83B3-N12B3	-3.3(19)	C86B3-N12B3-C83B3-C79B3	-178.5(18)
Cu73-N12B3-C83B3-C79B3	2.3(16)	C86B3-N12B3-C83B3-C82B3	0.0
Cu73-N12B3-C83B3-C82B3	-179.2(11)	C79B3-C83B3-C82B3-C84B3	178.4(18)
N12B3-C83B3-C82B3-C84B3	0.0	C79B3-C83B3-C82B3-C81B3	2(2)
N12B3-C83B3-C82B3-C81B3	-176(2)	C83B3-C82B3-C84B3-C85B3	0.0
C81B3-C82B3-C84B3-C85B3	176(2)	C82B3-C84B3-C85B3-C86B3	0.0
C84B3-C85B3-C86B3-N12B3	0.0	C84B3-C85B3-C86B3-C87B3	177(2)
C83B3-N12B3-C86B3-C85B3	0.0	Cu73-N12B3-C86B3-C85B3	179.0(13)
C83B3-N12B3-C86B3-C87B3	-177(2)	Cu73-N12B3-C86B3-C87B3	2(2)
C4B3-C5B3-C7B3-C8B3	-178(3)	C6B3-C5B3-C7B3-C8B3	-2(4)
C5B3-C7B3-C8B3-C9B3	0(6)	C11B3-C9B3-C8B3-C7B3	-178(3)
C10B3-C9B3-C8B3-C7B3	2(5)	C12B3-C13B3-C14B3-C15B3	-103(2)
N2B3-C13B3-C14B3-C15B3	84(2)	C13B3-C14B3-C15B3-C16B3	174(2)
C18B3-C17B3-C16B3-C15B3	-96(2)	N3B3-C17B3-C16B3-C15B3	84(2)
C14B3-C15B3-C16B3-C17B3	173(2)	C21B3-C20B3-C22B3-C23B3	5(4)
C19B3-C20B3-C22B3-C23B3	-180(3)	C20B3-C22B3-C23B3-C24B3	-8(5)
C26B3-C24B3-C23B3-C22B3	-172(2)	C25B3-C24B3-C23B3-C22B3	14(4)
C35B3-C34B3-C36B3-C37B3	-1(4)	C33B3-C34B3-C36B3-C37B3	176(3)
C34B3-C36B3-C37B3-C38B3	3(5)	C39B3-C38B3-C37B3-C36B3	3(4)
C40B3-C38B3-C37B3-C36B3	-176(3)	C41B3-C42B3-C43B3-C44B3	-106(2)
N6B3-C42B3-C43B3-C44B3	71(3)	C42B3-C43B3-C44B3-C45B3	170(2)
C43B3-C44B3-C45B3-C46B3	171(2)	N7B3-C46B3-C45B3-C44B3	100(3)
C47B3-C46B3-C45B3-C44B3	-82(3)	C50B3-C49B3-C51B3-C52B3	-5(3)
C48B3-C49B3-C51B3-C52B3	172(2)	C49B3-C51B3-C52B3-C53B3	5(5)
C54B3-C53B3-C52B3-C51B3	-1(4)	C55B3-C53B3-C52B3-C51B3	-177(3)
C64B3-C63B3-C65B3-C66B3	-1(5)	C62B3-C63B3-C65B3-C66B3	-179(4)
C63B3-C65B3-C66B3-C67B3	4(7)	C69B3-C67B3-C66B3-C65B3	174(3)
C68B3-C67B3-C66B3-C65B3	-4(6)	C70B3-C71B3-C72B3-C73B3	-90(3)
N10B3-C71B3-C72B3-C73B3	96(3)	C71B3-C72B3-C73B3-C74B3	177(2)

C76B3-C75B3-C74B3-C73B3	-98(3)	N11B3-C75B3-C74B3-C73B3	84(3)
C72B3-C73B3-C74B3-C75B3	176(3)	C79B3-C78B3-C80B3-C81B3	2(3)
C77B3-C78B3-C80B3-C81B3	-179(2)	C78B3-C80B3-C81B3-C82B3	-2(4)
C83B3-C82B3-C81B3-C80B3	0(3)	C84B3-C82B3-C81B3-C80B3	-176(2)
O24-As14-O14-C14	7.6(17)	O44-As14-O14-C14	-169.0(17)
O34-As14-O14-C14	-81.0(17)	O54-As14-O14-C14	101.2(16)
O64-As14-O24-C64	176.7(16)	O14-As14-O24-C64	-4.6(15)
O34-As14-O24-C64	87.7(15)	O54-As14-O24-C64	-96.8(15)
O64-As14-O34-C74	113.0(17)	O14-As14-O34-C74	-70.6(17)
O24-As14-O34-C74	-158.7(16)	O44-As14-O34-C74	20.1(17)
O64-As14-O44-C124	-106.7(18)	O14-As14-O44-C124	74.4(17)
O34-As14-O44-C124	-17.8(17)	O54-As14-O44-C124	166.7(17)
O64-As14-O54-C134	14.4(18)	O14-As14-O54-C134	-161.9(18)
O24-As14-O54-C134	-73.6(18)	O44-As14-O54-C134	107.4(18)
O24-As14-O64-C184	80.9(17)	O44-As14-O64-C184	-102.5(18)
O34-As14-O64-C184	169.6(17)	O54-As14-O64-C184	-12.9(17)
As14-O14-C14-C24	172.2(12)	As14-O14-C14-C64	-8.2(18)
O14-C14-C24-C34	180(2)	C64-C14-C24-C34	0.0
C14-C24-C34-C44	0.0	C24-C34-C44-C54	0.0
C34-C44-C54-C64	0.0	As14-O24-C64-C54	-174.5(10)
As14-O24-C64-C14	1.1(19)	C44-C54-C64-O24	176(2)
C44-C54-C64-C14	0.0	O14-C14-C64-O24	5(2)
C24-C14-C64-O24	-176(2)	O14-C14-C64-C54	-179.7(19)
C24-C14-C64-C54	0.0	As14-O34-C74-C84	164.9(12)
As14-O34-C74-C124	-17.1(19)	O34-C74-C84-C94	178(2)
C124-C74-C84-C94	0.0	C74-C84-C94-C104	0.0
C84-C94-C104-C114	0.0	C94-C104-C114-C124	0.0
As14-O44-C124-C114	-166.0(12)	As14-O44-C124-C74	13(2)
C104-C114-C124-O44	179(2)	C104-C114-C124-C74	0.0
O34-C74-C124-O44	3(2)	C84-C74-C124-O44	-179(2)
O34-C74-C124-C114	-178(2)	C84-C74-C124-C114	0.0
As14-O54-C134-C144	168.4(13)	As14-O54-C134-C184	-12(2)
O54-C134-C144-C154	180(3)	C184-C134-C144-C154	0.0
C134-C144-C154-C164	0.0	C144-C154-C164-C174	0.0
C154-C164-C174-C184	0.0	C164-C174-C184-C134	0.0
C164-C174-C184-O64	179(2)	O54-C134-C184-C174	-180(2)
C144-C134-C184-C174	0.0	O54-C134-C184-O64	1(2)
C144-C134-C184-O64	-179(2)	As14-O64-C184-C174	-168.6(14)
As14-O64-C184-C134	10(2)	O2A5-As25-O1A5-C1A5	-5.1(17)
O4A5-As25-O1A5-C1A5	-179.0(18)	O5A5-As25-O1A5-C1A5	89.1(17)
O3A5-As25-O1A5-C1A5	-92.2(18)	O6A5-As25-O2A5-C6A5	-170.6(17)
O1A5-As25-O2A5-C6A5	5.3(17)	O5A5-As25-O2A5-C6A5	-82.0(16)
O3A5-As25-O2A5-C6A5	100.0(17)	O6A5-As25-O3A5-C7A5	99(2)
O2A5-As25-O3A5-C7A5	-172(2)	O4A5-As25-O3A5-C7A5	3(2)
O1A5-As25-O3A5-C7A5	-81(2)	O6A5-As25-O4A5-C12A5	-92(2)
O1A5-As25-O4A5-C12A5	92(2)	O5A5-As25-O4A5-C12A5	179(2)

O3A5-As25-O4A5-C12A5	-3(2)	O6A5-As25-O5A5-C13A5	-3.8(17)
O2A5-As25-O5A5-C13A5	-92.0(17)	O4A5-As25-O5A5-C13A5	92.7(17)
O1A5-As25-O5A5-C13A5	177.1(17)	O2A5-As25-O6A5-C18A5	100.5(18)
O4A5-As25-O6A5-C18A5	-85.3(18)	O5A5-As25-O6A5-C18A5	6.3(17)
O3A5-As25-O6A5-C18A5	-172.4(18)	As25-O1A5-C1A5-C2A5	-171.9(13)
As25-O1A5-C1A5-C6A5	4(2)	O1A5-C1A5-C2A5-C3A5	176(2)
C6A5-C1A5-C2A5-C3A5	0.0	C1A5-C2A5-C3A5-C4A5	0.0
C2A5-C3A5-C4A5-C5A5	0.0	C3A5-C4A5-C5A5-C6A5	0.0
As25-O2A5-C6A5-C5A5	171.8(12)	As25-O2A5-C6A5-C1A5	-4(2)
C4A5-C5A5-C6A5-O2A5	-176(2)	C4A5-C5A5-C6A5-C1A5	0.0
O1A5-C1A5-C6A5-O2A5	0(2)	C2A5-C1A5-C6A5-O2A5	176(2)
O1A5-C1A5-C6A5-C5A5	-176(2)	C2A5-C1A5-C6A5-C5A5	0.0
As25-O3A5-C7A5-C8A5	175.2(14)	As25-O3A5-C7A5-C12A5	-3(3)
O3A5-C7A5-C8A5-C9A5	-178(3)	C12A5-C7A5-C8A5-C9A5	0.0
C7A5-C8A5-C9A5-C10A5	0.0	C8A5-C9A5-C10A5-C11A5	0.0
C9A5-C10A5-C11A5-C12A5	0.0	As25-O4A5-C12A5-C11A5	-174.9(15)
As25-O4A5-C12A5-C7A5	2(2)	C10A5-C11A5-C12A5-O4A5	177(3)
C10A5-C11A5-C12A5-C7A5	0.0	O3A5-C7A5-C12A5-O4A5	0(3)
C8A5-C7A5-C12A5-O4A5	-177(3)	O3A5-C7A5-C12A5-C11A5	178(3)
C8A5-C7A5-C12A5-C11A5	0.0	As25-O5A5-C13A5-C14A5	173.9(13)
As25-O5A5-C13A5-C18A5	0.0(19)	O5A5-C13A5-C14A5-C15A5	-174(2)
C18A5-C13A5-C14A5-C15A5	0.0	C13A5-C14A5-C15A5-C16A5	0.0
C14A5-C15A5-C16A5-C17A5	0.0	C15A5-C16A5-C17A5-C18A5	0.0
As25-O6A5-C18A5-C17A5	-176.7(12)	As25-O6A5-C18A5-C13A5	-8(2)
C16A5-C17A5-C18A5-O6A5	168(2)	C16A5-C17A5-C18A5-C13A5	0.0
O5A5-C13A5-C18A5-O6A5	5(2)	C14A5-C13A5-C18A5-O6A5	-169(2)
O5A5-C13A5-C18A5-C17A5	174(2)	C14A5-C13A5-C18A5-C17A5	0.0
O2B6-As36-O1B6-C1B6	7.3(17)	O5B6-As36-O1B6-C1B6	99.8(17)
O4B6-As36-O1B6-C1B6	-166.7(17)	O3B6-As36-O1B6-C1B6	-80.1(17)
O5B6-As36-O2B6-C6B6	-94.2(17)	O3B6-As36-O2B6-C6B6	91.1(16)
O1B6-As36-O2B6-C6B6	-6.8(16)	O6B6-As36-O2B6-C6B6	-179.3(16)
O2B6-As36-O3B6-C7B6	167.0(16)	O4B6-As36-O3B6-C7B6	-17.6(15)
O1B6-As36-O3B6-C7B6	-106.1(15)	O6B6-As36-O3B6-C7B6	77.7(15)
O5B6-As36-O4B6-C12B6	-156.8(18)	O3B6-As36-O4B6-C12B6	17.9(17)
O1B6-As36-O4B6-C12B6	115.8(18)	O6B6-As36-O4B6-C12B6	-71.4(18)
O2B6-As36-O5B6-C13B6	-85.0(17)	O4B6-As36-O5B6-C13B6	99.1(17)
O1B6-As36-O5B6-C13B6	-172.2(18)	O6B6-As36-O5B6-C13B6	4.1(17)
As36-O1B6-C1B6-C2B6	176.8(11)	As36-O1B6-C1B6-C6B6	-6(2)
O1B6-C1B6-C2B6-C3B6	177(2)	C6B6-C1B6-C2B6-C3B6	0.0
C1B6-C2B6-C3B6-C4B6	0.0	C2B6-C3B6-C4B6-C5B6	0.0
C3B6-C4B6-C5B6-C6B6	0.0	As36-O2B6-C6B6-C5B6	-176.8(12)
As36-O2B6-C6B6-C1B6	5(2)	C4B6-C5B6-C6B6-O2B6	-178(2)
C4B6-C5B6-C6B6-C1B6	0.0	O1B6-C1B6-C6B6-O2B6	1(2)
C2B6-C1B6-C6B6-O2B6	178(2)	O1B6-C1B6-C6B6-C5B6	-177(2)
C2B6-C1B6-C6B6-C5B6	0.0	As36-O3B6-C7B6-C8B6	-165.3(13)
As36-O3B6-C7B6-C12B6	14.4(18)	C12B6-C7B6-C8B6-C9B6	0.0

O3B6-C7B6-C8B6-C9B6	180(2)	C7B6-C8B6-C9B6-C10B6	0.0
C8B6-C9B6-C10B6-C11B6	0.0	C9B6-C10B6-C11B6-C12B6	0.0
As36-O4B6-C12B6-C11B6	165.4(13)	As36-O4B6-C12B6-C7B6	-14(2)
C10B6-C11B6-C12B6-O4B6	-179(3)	C10B6-C11B6-C12B6-C7B6	0.0
C8B6-C7B6-C12B6-O4B6	179(2)	O3B6-C7B6-C12B6-O4B6	0(2)
C8B6-C7B6-C12B6-C11B6	0.0	O3B6-C7B6-C12B6-C11B6	-180(2)
As36-O5B6-C13B6-C14B6	176.2(12)	As36-O5B6-C13B6-C18B6	-8(2)
C18B6-C13B6-C14B6-C15B6	0.0	O5B6-C13B6-C14B6-C15B6	175(2)
C13B6-C14B6-C15B6-C16B6	0.0	C14B6-C15B6-C16B6-C17B6	0.0
C15B6-C16B6-C17B6-C18B6	0.0	As36-O6B6-C18B6-C17B6	179.9(12)
As36-O6B6-C18B6-C13B6	-6(2)	C16B6-C17B6-C18B6-O6B6	174(2)
C16B6-C17B6-C18B6-C13B6	0.0	C14B6-C13B6-C18B6-O6B6	-175(2)
O5B6-C13B6-C18B6-O6B6	9(2)	C14B6-C13B6-C18B6-C17B6	0.0
O5B6-C13B6-C18B6-C17B6	-176(2)	O4C7-As47-O1C7-C1C7	170.9(17)
O5C7-As47-O1C7-C1C7	84.6(17)	O2C7-As47-O1C7-C1C7	-11.5(17)
O3C7-As47-O1C7-C1C7	-101.1(17)	O6C7-As47-O2C7-C6C7	-168.5(18)
O5C7-As47-O2C7-C6C7	-79.8(19)	O1C7-As47-O2C7-C6C7	11.4(18)
O3C7-As47-O2C7-C6C7	105.1(18)	O6C7-As47-O3C7-C7C7	108.1(16)
O4C7-As47-O3C7-C7C7	9.9(16)	O1C7-As47-O3C7-C7C7	-73.9(16)
O2C7-As47-O3C7-C7C7	-162.7(16)	O6C7-As47-O4C7-C12C7	-91.5(16)
O5C7-As47-O4C7-C12C7	-179.8(17)	O1C7-As47-O4C7-C12C7	88.5(17)
O3C7-As47-O4C7-C12C7	-5.4(16)	O6C7-As47-O5C7-C13C7	13.7(19)
O4C7-As47-O5C7-C13C7	111.9(19)	O1C7-As47-O5C7-C13C7	-164.2(19)
O2C7-As47-O5C7-C13C7	-75.4(19)	O4C7-As47-O6C7-C18C7	-95.4(17)
O5C7-As47-O6C7-C18C7	-9.1(17)	O2C7-As47-O6C7-C18C7	87.0(17)
O3C7-As47-O6C7-C18C7	176.7(17)	As47-O1C7-C1C7-C2C7	-171.4(12)
As47-O1C7-C1C7-C6C7	11(2)	C6C7-C1C7-C2C7-C3C7	0.0
O1C7-C1C7-C2C7-C3C7	-178(2)	C1C7-C2C7-C3C7-C4C7	0.0
C2C7-C3C7-C4C7-C5C7	0.0	C3C7-C4C7-C5C7-C6C7	0.0
As47-O2C7-C6C7-C5C7	172.2(13)	As47-O2C7-C6C7-C1C7	-8(2)
C4C7-C5C7-C6C7-O2C7	-180(2)	C4C7-C5C7-C6C7-C1C7	0.0
C2C7-C1C7-C6C7-O2C7	180(2)	O1C7-C1C7-C6C7-O2C7	-2(2)
C2C7-C1C7-C6C7-C5C7	0.0	O1C7-C1C7-C6C7-C5C7	178(2)
As47-O3C7-C7C7-C8C7	174.2(11)	As47-O3C7-C7C7-C12C7	-12.2(19)
O3C7-C7C7-C8C7-C9C7	173(2)	C12C7-C7C7-C8C7-C9C7	0.0
C7C7-C8C7-C9C7-C10C7	0.0	C8C7-C9C7-C10C7-C11C7	0.0
C9C7-C10C7-C11C7-C12C7	0.0	As47-O4C7-C12C7-C11C7	-177.3(11)
As47-O4C7-C12C7-C7C7	0(2)	C10C7-C11C7-C12C7-O4C7	177(2)
C10C7-C11C7-C12C7-C7C7	0.0	O3C7-C7C7-C12C7-O4C7	9(2)
C8C7-C7C7-C12C7-O4C7	-177(2)	O3C7-C7C7-C12C7-C11C7	-174(2)
C8C7-C7C7-C12C7-C11C7	0.0	As47-O5C7-C13C7-C14C7	174.9(13)
As47-O5C7-C13C7-C18C7	-16(2)	O5C7-C13C7-C14C7-C15C7	169(3)
C18C7-C13C7-C14C7-C15C7	0.0	C13C7-C14C7-C15C7-C16C7	0.0
C14C7-C15C7-C16C7-C17C7	0.0	C15C7-C16C7-C17C7-C18C7	0.0
As47-O6C7-C18C7-C17C7	-179.2(14)	As47-O6C7-C18C7-C13C7	2(2)
C16C7-C17C7-C18C7-O6C7	-179(3)	C16C7-C17C7-C18C7-C13C7	0.0

O5C7-C13C7-C18C7-O6C7	10(2)	C14C7-C13C7-C18C7-O6C7	179(2)
O5C7-C13C7-C18C7-C17C7	-169(3)	C14C7-C13C7-C18C7-C17C7	0.0
O2D8-As58-O1D8-C1D8	5.0(15)	O3D8-As58-O1D8-C1D8	-83.3(15)
O4D8-As58-O1D8-C1D8	-171.9(15)	O6D8-As58-O1D8-C1D8	99.6(15)
O3D8-As58-O2D8-C6D8	87.1(17)	O1D8-As58-O2D8-C6D8	-6.2(17)
O5D8-As58-O2D8-C6D8	177.8(17)	O6D8-As58-O2D8-C6D8	-94.7(17)
O2D8-As58-O3D8-C7D8	-178.8(16)	O1D8-As58-O3D8-C7D8	-90.1(16)
O5D8-As58-O3D8-C7D8	94.3(16)	O4D8-As58-O3D8-C7D8	-1.9(16)
O3D8-As58-O4D8-C12D8	8.8(16)	O1D8-As58-O4D8-C12D8	102.1(16)
O5D8-As58-O4D8-C12D8	-81.6(17)	O6D8-As58-O4D8-C12D8	-169.3(16)
O2D8-As58-O5D8-C13D8	105.4(18)	O3D8-As58-O5D8-C13D8	-166.3(18)
O4D8-As58-O5D8-C13D8	-77.5(18)	O6D8-As58-O5D8-C13D8	10.7(18)
O2D8-As58-O6D8-C18D8	-97.5(15)	O1D8-As58-O6D8-C18D8	173.8(15)
O5D8-As58-O6D8-C18D8	-10.8(15)	O4D8-As58-O6D8-C18D8	85.5(15)
As58-O1D8-C1D8-C2D8	174.6(11)	As58-O1D8-C1D8-C6D8	-3.0(19)
O1D8-C1D8-C2D8-C3D8	-178(2)	C6D8-C1D8-C2D8-C3D8	0.0
C1D8-C2D8-C3D8-C4D8	0.0	C2D8-C3D8-C4D8-C5D8	0.0
C3D8-C4D8-C5D8-C6D8	0.0	As58-O2D8-C6D8-C5D8	-173.6(12)
As58-O2D8-C6D8-C1D8	6(2)	C4D8-C5D8-C6D8-O2D8	179(2)
C4D8-C5D8-C6D8-C1D8	0.0	O1D8-C1D8-C6D8-O2D8	-2(2)
C2D8-C1D8-C6D8-O2D8	-179(2)	O1D8-C1D8-C6D8-C5D8	177.6(19)
C2D8-C1D8-C6D8-C5D8	0.0	As58-O3D8-C7D8-C8D8	179.9(12)
As58-O3D8-C7D8-C12D8	-5(2)	O3D8-C7D8-C8D8-C9D8	174(2)
C12D8-C7D8-C8D8-C9D8	0.0	C7D8-C8D8-C9D8-C10D8	0.0
C8D8-C9D8-C10D8-C11D8	0.0	C9D8-C10D8-C11D8-C12D8	0.0
As58-O4D8-C12D8-C11D8	174.8(12)	As58-O4D8-C12D8-C7D8	-14(2)
C10D8-C11D8-C12D8-O4D8	171(2)	C10D8-C11D8-C12D8-C7D8	0.0
O3D8-C7D8-C12D8-O4D8	14(2)	C8D8-C7D8-C12D8-O4D8	-171(2)
O3D8-C7D8-C12D8-C11D8	-175(2)	C8D8-C7D8-C12D8-C11D8	0.0
As58-O5D8-C13D8-C14D8	169.4(13)	As58-O5D8-C13D8-C18D8	-7(2)
O5D8-C13D8-C14D8-C15D8	-176(2)	C18D8-C13D8-C14D8-C15D8	0.0
C13D8-C14D8-C15D8-C16D8	0.0	C14D8-C15D8-C16D8-C17D8	0.0
C15D8-C16D8-C17D8-C18D8	0.0	C16D8-C17D8-C18D8-C13D8	0.0
C16D8-C17D8-C18D8-O6D8	180(2)	O5D8-C13D8-C18D8-C17D8	176(2)
C14D8-C13D8-C18D8-C17D8	0.0	O5D8-C13D8-C18D8-O6D8	-3(2)
C14D8-C13D8-C18D8-O6D8	-180(2)	As58-O6D8-C18D8-C17D8	-169.0(11)
As58-O6D8-C18D8-C13D8	11(2)	O3E9-As69-O1E9-C1E9	-74.5(16)
O4E9-As69-O1E9-C1E9	-163.1(16)	O6E9-As69-O1E9-C1E9	108.5(16)
O2E9-As69-O1E9-C1E9	15.9(16)	O5E9-As69-O2E9-C6E9	162.9(15)
O3E9-As69-O2E9-C6E9	73.7(14)	O1E9-As69-O2E9-C6E9	-17.7(14)
O6E9-As69-O2E9-C6E9	-105.5(15)	O5E9-As69-O3E9-C7E9	104.3(16)
O4E9-As69-O3E9-C7E9	15.6(16)	O1E9-As69-O3E9-C7E9	-75.9(16)
O2E9-As69-O3E9-C7E9	-164.8(15)	O5E9-As69-O4E9-C12E9	-104.7(16)
O3E9-As69-O4E9-C12E9	-15.5(16)	O1E9-As69-O4E9-C12E9	75.9(16)
O6E9-As69-O4E9-C12E9	163.7(16)	O3E9-As69-O5E9-C13E9	-169.8(16)
O4E9-As69-O5E9-C13E9	-81.2(17)	O6E9-As69-O5E9-C13E9	7.2(16)

O2E9-As69-O5E9-C13E9	99.8(16)	O5E9-As69-O6E9-C18E9	-12.0(15)
O4E9-As69-O6E9-C18E9	76.7(15)	O1E9-As69-O6E9-C18E9	168.2(15)
O2E9-As69-O6E9-C18E9	-102.9(15)	As69-O1E9-C1E9-C2E9	172.5(12)
As69-O1E9-C1E9-C6E9	-10.0(18)	O1E9-C1E9-C2E9-C3E9	177(2)
C6E9-C1E9-C2E9-C3E9	0.0	C1E9-C2E9-C3E9-C4E9	0.0
C2E9-C3E9-C4E9-C5E9	0.0	C3E9-C4E9-C5E9-C6E9	0.0
C4E9-C5E9-C6E9-C1E9	0.0	C4E9-C5E9-C6E9-O2E9	-172(2)
O1E9-C1E9-C6E9-C5E9	-178(2)	C2E9-C1E9-C6E9-C5E9	0.0
O1E9-C1E9-C6E9-O2E9	-4.8(19)	C2E9-C1E9-C6E9-O2E9	173(2)
As69-O2E9-C6E9-C5E9	-170.9(12)	As69-O2E9-C6E9-C1E9	16.6(17)
As69-O3E9-C7E9-C8E9	172.6(11)	As69-O3E9-C7E9-C12E9	-11.7(18)
O3E9-C7E9-C8E9-C9E9	176(2)	C12E9-C7E9-C8E9-C9E9	0.0
C7E9-C8E9-C9E9-C10E9	0.0	C8E9-C9E9-C10E9-C11E9	0.0
C9E9-C10E9-C11E9-C12E9	0.0	As69-O4E9-C12E9-C11E9	-172.2(11)
As69-O4E9-C12E9-C7E9	12.9(19)	C10E9-C11E9-C12E9-O4E9	-175(2)
C10E9-C11E9-C12E9-C7E9	0.0	O3E9-C7E9-C12E9-O4E9	-1(2)
C8E9-C7E9-C12E9-O4E9	175(2)	O3E9-C7E9-C12E9-C11E9	-176(2)
C8E9-C7E9-C12E9-C11E9	0.0	As69-O5E9-C13E9-C14E9	179.2(11)
As69-O5E9-C13E9-C18E9	0(2)	O5E9-C13E9-C14E9-C15E9	-180(2)
C18E9-C13E9-C14E9-C15E9	0.0	C13E9-C14E9-C15E9-C16E9	0.0
C14E9-C15E9-C16E9-C17E9	0.0	C15E9-C16E9-C17E9-C18E9	0.0
C16E9-C17E9-C18E9-C13E9	0.0	C16E9-C17E9-C18E9-O6E9	-170(2)
O5E9-C13E9-C18E9-C17E9	180(2)	C14E9-C13E9-C18E9-C17E9	0.0
O5E9-C13E9-C18E9-O6E9	-10(2)	C14E9-C13E9-C18E9-O6E9	170(2)
As69-O6E9-C18E9-C17E9	-175.4(11)	As69-O6E9-C18E9-C13E9	14.8(18)
O3F10-As710-O1F10-C1F10	-98.3(17)	O4F10-As710-O1F10-C1F10	177.1(17)
O6F10-As710-O1F10-C1F10	86.1(17)	O2F10-As710-O1F10-C1F10	-7.8(16)
O1F10-As710-O2F10-C6F10	4.8(16)	O3F10-As710-O2F10-C6F10	98.2(16)
O5F10-As710-O2F10-C6F10	-170.7(15)	O6F10-As710-O2F10-C6F10	-81.4(16)
O1F10-As710-O3F10-C7F10	-102.0(17)	O5F10-As710-O3F10-C7F10	78.0(17)
O4F10-As710-O3F10-C7F10	-14.7(17)	O2F10-As710-O3F10-C7F10	171.1(17)
O1F10-As710-O4F10-C12F10	103.3(16)	O3F10-As710-O4F10-C12F10	9.7(16)
O5F10-As710-O4F10-C12F10	-81.1(16)	O6F10-As710-O4F10-C12F10	-170.2(16)
O3F10-As710-O5F10-C13F10	177.4(18)	O4F10-As710-O5F10-C13F10	-97.8(18)
O6F10-As710-O5F10-C13F10	-7.1(18)	O2F10-As710-O5F10-C13F10	86.6(18)
O1F10-As710-O6F10-C18F10	-173.4(16)	O5F10-As710-O6F10-C18F10	6.2(16)
O4F10-As710-O6F10-C18F10	99.0(16)	O2F10-As710-O6F10-C18F10	-86.8(16)
As710-O1F10-C1F10-C2F10	-169.1(11)	As710-O1F10-C1F10-C6F10	8.8(19)
O1F10-C1F10-C2F10-C3F10	178(2)	C6F10-C1F10-C2F10-C3F10	0.0
C1F10-C2F10-C3F10-C4F10	0.0	C2F10-C3F10-C4F10-C5F10	0.0
C3F10-C4F10-C5F10-C6F10	0.0	As710-O2F10-C6F10-C5F10	172.1(11)
As710-O2F10-C6F10-C1F10	-1.1(19)	C4F10-C5F10-C6F10-O2F10	-173(2)
C4F10-C5F10-C6F10-C1F10	0.0	O1F10-C1F10-C6F10-O2F10	-5(2)
C2F10-C1F10-C6F10-O2F10	173(2)	O1F10-C1F10-C6F10-C5F10	-178.1(19)
C2F10-C1F10-C6F10-C5F10	0.0	As710-O3F10-C7F10-C8F10	-166.2(12)
As710-O3F10-C7F10-C12F10	15.9(19)	C12F10-C7F10-C8F10-C9F10	0.0

O3F10-C7F10-C8F10-C9F10	-178(2)	C7F10-C8F10-C9F10-C10F10	0.0
C8F10-C9F10-C10F10-C11F10	0.0	C9F10-C10F10-C11F10-C12F10	0.0
As710-O4F10-C12F10-C11F10	170.5(11)	As710-O4F10-C12F10-C7F10	-3.3(19)
C10F10-C11F10-C12F10-O4F10	-174(2)	C10F10-C11F10-C12F10-C7F10	0.0
C8F10-C7F10-C12F10-O4F10	174.2(19)	O3F10-C7F10-C12F10-O4F10	-7.7(18)
C8F10-C7F10-C12F10-C11F10	0.0	O3F10-C7F10-C12F10-C11F10	178.1(19)
As710-O5F10-C13F10-C14F10	-177.7(13)	As710-O5F10-C13F10-C18F10	6(2)
O5F10-C13F10-C14F10-C15F10	-176(3)	C18F10-C13F10-C14F10-C15F10	0.0
C13F10-C14F10-C15F10-C16F10	0.0	C14F10-C15F10-C16F10-C17F10	0.0
C15F10-C16F10-C17F10-C18F10	0.0	As710-O6F10-C18F10-C17F10	178.1(12)
As710-O6F10-C18F10-C13F10	-5(2)	C16F10-C17F10-C18F10-O6F10	177(2)
C16F10-C17F10-C18F10-C13F10	0.0	O5F10-C13F10-C18F10-O6F10	-1(2)
C14F10-C13F10-C18F10-O6F10	-177(2)	O5F10-C13F10-C18F10-C17F10	177(2)
C14F10-C13F10-C18F10-C17F10	0.0	O2G11-As811-O1G11-C1G11	14.6(17)
O3G11-As811-O1G11-C1G11	-75.1(16)	O4G11-As811-O1G11-C1G11	-165.0(16)
O5G11-As811-O1G11-C1G11	107.7(16)	C13G11-As811-O1G11-C1G11	99.3(16)
O1G11-As811-O2G11-C6G11	-13.6(17)	O6G11-As811-O2G11-C6G11	168.5(18)
O3G11-As811-O2G11-C6G11	81.2(17)	O5G11-As811-O2G11-C6G11	-101.3(17)
C13G11-As811-O2G11-C6G11	-128.9(17)	O1G11-As811-O3G11-C7G11	-70.5(17)
O2G11-As811-O3G11-C7G11	-160.6(18)	O6G11-As811-O3G11-C7G11	113.2(18)
O4G11-As811-O3G11-C7G11	15.2(18)	C13G11-As811-O3G11-C7G11	120(2)
O1G11-As811-O4G11-C12G11	76.6(16)	O6G11-As811-O4G11-C12G11	-105.5(17)
O3G11-As811-O4G11-C12G11	-18.2(16)	O5G11-As811-O4G11-C12G11	164.5(16)
C13G11-As811-O4G11-C12G11	-168.5(16)	O1G11-As811-O5G11-C13G11	-163.9(19)
O2G11-As811-O5G11-C13G11	-74(2)	O6G11-As811-O5G11-C13G11	12(2)
O4G11-As811-O5G11-C13G11	110(2)	O1G11-As811-O5G11-C14G11	-150.7(19)
O2G11-As811-O5G11-C14G11	-61(2)	O6G11-As811-O5G11-C14G11	26(2)
O4G11-As811-O5G11-C14G11	123.5(19)	C13G11-As811-O5G11-C14G11	13.3(13)
O2G11-As811-O6G11-C18G11	83(2)	O3G11-As811-O6G11-C18G11	172(2)
O4G11-As811-O6G11-C18G11	-98(2)	O5G11-As811-O6G11-C18G11	-11(2)
C13G11-As811-O6G11-C18G11	-4.0(15)	As811-O1G11-C1G11-C2G11	167.2(14)
As811-O1G11-C1G11-C6G11	-11.3(19)	O1G11-C1G11-C2G11-C3G11	-178(2)
C6G11-C1G11-C2G11-C3G11	0.0	C1G11-C2G11-C3G11-C4G11	0.0
C2G11-C3G11-C4G11-C5G11	0.0	C3G11-C4G11-C5G11-C6G11	0.0
C4G11-C5G11-C6G11-C1G11	0.0	C4G11-C5G11-C6G11-O2G11	178(2)
O1G11-C1G11-C6G11-C5G11	179(2)	C2G11-C1G11-C6G11-C5G11	0.0
O1G11-C1G11-C6G11-O2G11	0(2)	C2G11-C1G11-C6G11-O2G11	-179(2)
As811-O2G11-C6G11-C5G11	-168.0(13)	As811-O2G11-C6G11-C1G11	10(2)
As811-O3G11-C7G11-C8G11	170.2(12)	As811-O3G11-C7G11-C12G11	-8(2)
O3G11-C7G11-C8G11-C9G11	-178(2)	C12G11-C7G11-C8G11-C9G11	0.0
C7G11-C8G11-C9G11-C10G11	0.0	C8G11-C9G11-C10G11-C11G11	0.0
C9G11-C10G11-C11G11-C12G11	0.0	C10G11-C11G11-C12G11-C7G11	0.0
C10G11-C11G11-C12G11-O4G11	-174(2)	O3G11-C7G11-C12G11-C11G11	178(2)
C8G11-C7G11-C12G11-C11G11	0.0	O3G11-C7G11-C12G11-O4G11	-8(2)
C8G11-C7G11-C12G11-O4G11	174(2)	As811-O4G11-C12G11-C11G11	-167.1(12)
As811-O4G11-C12G11-C7G11	18.6(19)	As811-O5G11-C13G11-C14G11	161.0(19)

As811-O5G11-C13G11-C18G11 -11(2)
C14G11-O5G11-C13G11-As811 -161.0(19)
C18G11-C13G11-C14G11-C15G11 0.0
C18G11-C13G11-C14G11-O5G11 171(3)
C13G11-C14G11-C15G11-C16G11 0.0
C14G11-C15G11-C16G11-C17G11 0.0
C16G11-C17G11-C18G11-C13G11 0.0
O5G11-C13G11-C18G11-C17G11 172(3)
As811-C13G11-C18G11-C17G11 164.5(19)
C14G11-C13G11-C18G11-O6G11 -170(3)
As811-O6G11-C18G11-C17G11 -161.7(19)
O6H12-As912-O1H12-C1H12 -81(2)
O5H12-As912-O1H12-C1H12 -177(2)
C13H12-As912-O1H12-C1H12 -141(2)
O3H12-As912-O2H12-C6H12 174.7(16)
O4H12-As912-O2H12-C6H12 -100.3(17)
O6H12-As912-O3H12-C7H12 -166.0(19)
O5H12-As912-O3H12-C7H12 -70.2(19)
C13H12-As912-O3H12-C7H12 -106.0(19)
O3H12-As912-O5H12-C13H12 -95(2)
O4H12-As912-O5H12-C13H12 180(2)
O3H12-As912-O6H12-C18H12 104(3)
O5H12-As912-O6H12-C18H12 11(3)
As912-O1H12-C1H12-C2H12 173.0(11)
O1H12-C1H12-C2H12-C3H12 179(2)
C1H12-C2H12-C3H12-C4H12 0.0
C3H12-C4H12-C5H12-C6H12 0.0
As912-O2H12-C6H12-C1H12 9.8(18)
C4H12-C5H12-C6H12-C1H12 0.0
C2H12-C1H12-C6H12-O2H12 178.5(19)
C2H12-C1H12-C6H12-C5H12 0.0
As912-O3H12-C7H12-C12H12 -16(2)
O3H12-C7H12-C8H12-C9H12 167(2)
C8H12-C9H12-C10H12-C11H12 0.0
As912-O4H12-C12H12-C11H12 177.0(15)
C10H12-C11H12-C12H12-O4H12 -176(3)
C8H12-C7H12-C12H12-O4H12 177(2)
C8H12-C7H12-C12H12-C11H12 0.0
As912-O5H12-C13H12-C14H12 172.2(16)
O5H12-C13H12-C14H12-C15H12 175(3)
As912-C13H12-C14H12-C15H12 -168(5)
C14H12-C15H12-C16H12-C17H12 0.0
C16H12-C17H12-C18H12-C13H12 0.0
O5H12-C13H12-C18H12-C17H12 -173(4)
As912-C13H12-C18H12-C17H12 175.7(18)
C14H12-C13H12-C18H12-O6H12 -166(3)
C14G11-O5G11-C13G11-C18G11 -171(3)
O5G11-C13G11-C14G11-C15G11 -171(3)
As811-C13G11-C14G11-C15G11 -134(5)
As811-C13G11-C14G11-O5G11 38(4)
O5G11-C14G11-C15G11-C16G11 -8(3)
C15G11-C16G11-C17G11-C18G11 0.0
C16G11-C17G11-C18G11-O6G11 169(3)
C14G11-C13G11-C18G11-C17G11 0.0
O5G11-C13G11-C18G11-O6G11 2(3)
As811-C13G11-C18G11-O6G11 -5.1(18)
As811-O6G11-C18G11-C13G11 7(3)
O2H12-As912-O1H12-C1H12 10.5(19)
O4H12-As912-O1H12-C1H12 102(2)
O6H12-As912-O2H12-C6H12 78.9(18)
O1H12-As912-O2H12-C6H12 -11.5(17)
C13H12-As912-O2H12-C6H12 73(3)
O2H12-As912-O3H12-C7H12 102.3(17)
O4H12-As912-O3H12-C7H12 11.4(18)
O6H12-As912-O5H12-C13H12 0(2)
O1H12-As912-O5H12-C13H12 91(2)
O2H12-As912-O6H12-C18H12 -165(3)
O1H12-As912-O6H12-C18H12 -80(3)
C13H12-As912-O6H12-C18H12 12(2)
As912-O1H12-C1H12-C6H12 -8(2)
C6H12-C1H12-C2H12-C3H12 0.0
C2H12-C3H12-C4H12-C5H12 0.0
As912-O2H12-C6H12-C5H12 -171.9(12)
C4H12-C5H12-C6H12-O2H12 -178(2)
O1H12-C1H12-C6H12-O2H12 -1(2)
O1H12-C1H12-C6H12-C5H12 -179(2)
As912-O3H12-C7H12-C8H12 177.1(11)
C12H12-C7H12-C8H12-C9H12 0.0
C7H12-C8H12-C9H12-C10H12 0.0
C9H12-C10H12-C11H12-C12H12 0.0
As912-O4H12-C12H12-C7H12 0(2)
C10H12-C11H12-C12H12-C7H12 0.0
O3H12-C7H12-C12H12-O4H12 11(2)
O3H12-C7H12-C12H12-C11H12 -166(3)
As912-O5H12-C13H12-C18H12 -14(3)
C18H12-C13H12-C14H12-C15H12 0.0
C13H12-C14H12-C15H12-C16H12 0.0
C15H12-C16H12-C17H12-C18H12 0.0
C16H12-C17H12-C18H12-O6H12 157(5)
C14H12-C13H12-C18H12-C17H12 0.0
O5H12-C13H12-C18H12-O6H12 21(4)
As912-C13H12-C18H12-O6H12 9.3(17)

As912-O6H12-C18H12-C17H12 -177(3) As912-O6H12-C18H12-C13H12 -17(3)

Symmetry transformations used to generate equivalent atoms: