

Supporting Information: Synthesis, Characterization and Copper(2+) Coordination Chemistry of a Polytopic Paramagnetic Ligand

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¹H

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PROCNO 1

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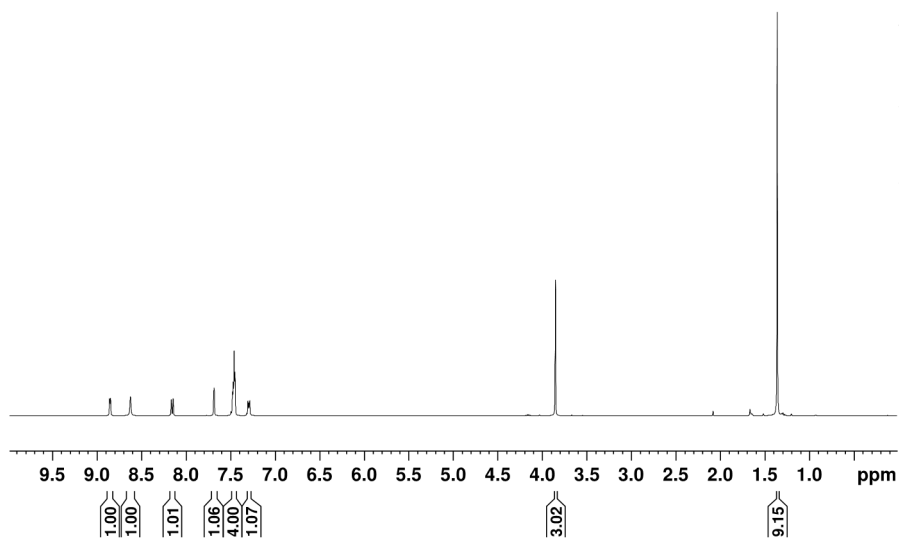
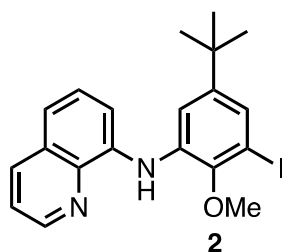
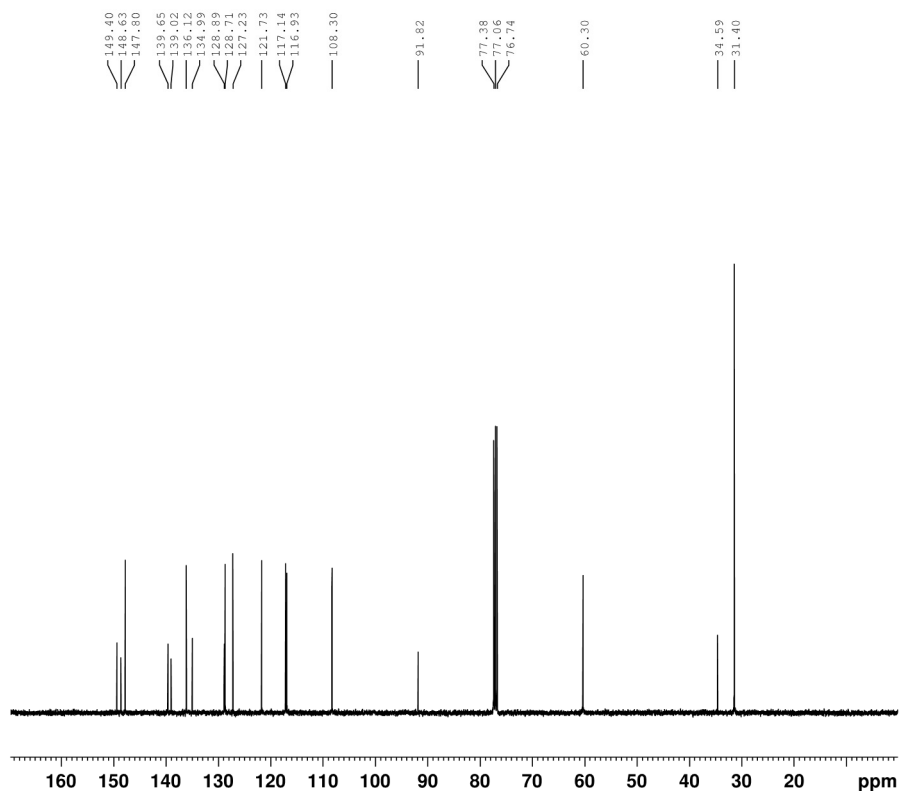


Figure S1. ¹H NMR spectrum of **2** (CDCl₃).



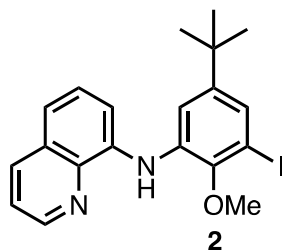
¹³C with ¹H decoupling

BRUKER

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 AQ 0.7077888 sec
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 DW 21.600 usec
 DE 6.50 usec
 TE 298.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1
 SFO1 100.630068 MHz
 NUC1 ¹³C
 P1 12.00 usec
 PLW1 54.00000000 W
 SFO2 400.2516010 MHz
 NUC2 ¹H
 CPDPRG2 waltz65
 PCPD2 80.00 usec
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 PLW12 0.35200000 W
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F2 - Processing parameters
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Figure S2. ¹³C NMR spectrum of **2** (CDCl₃).

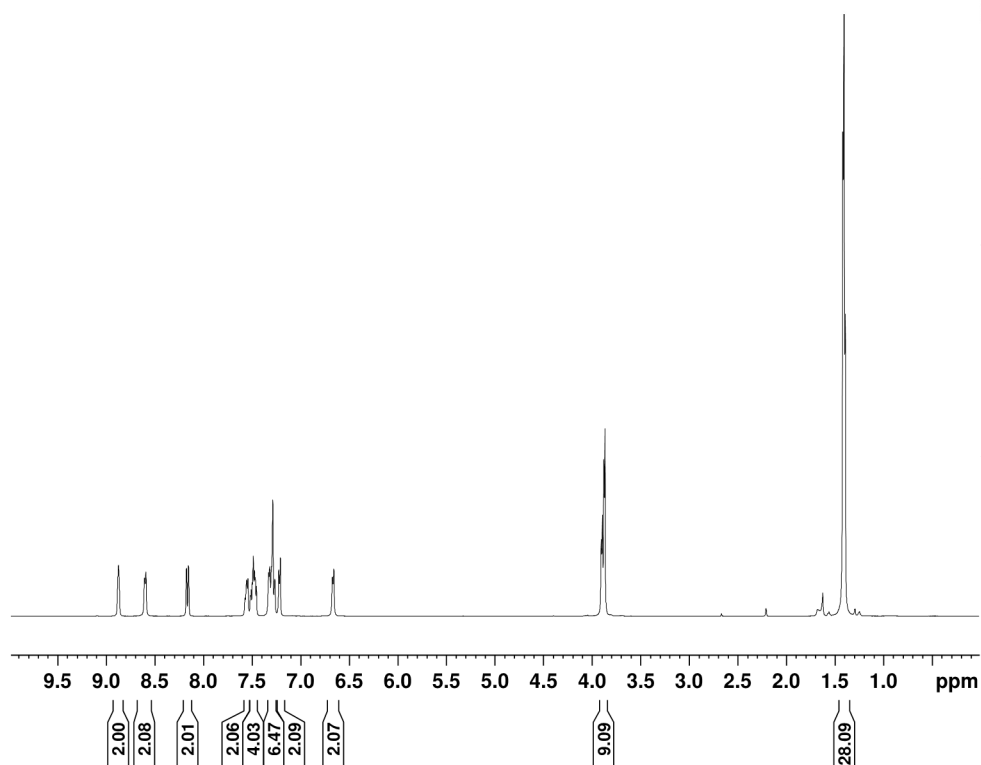


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FIDRES              0.244532 Hz
AQ                  2.0444723 sec
RG                   71.76
DW                  62.400 usec
DE                   6.50 usec
TE                  298.1 K
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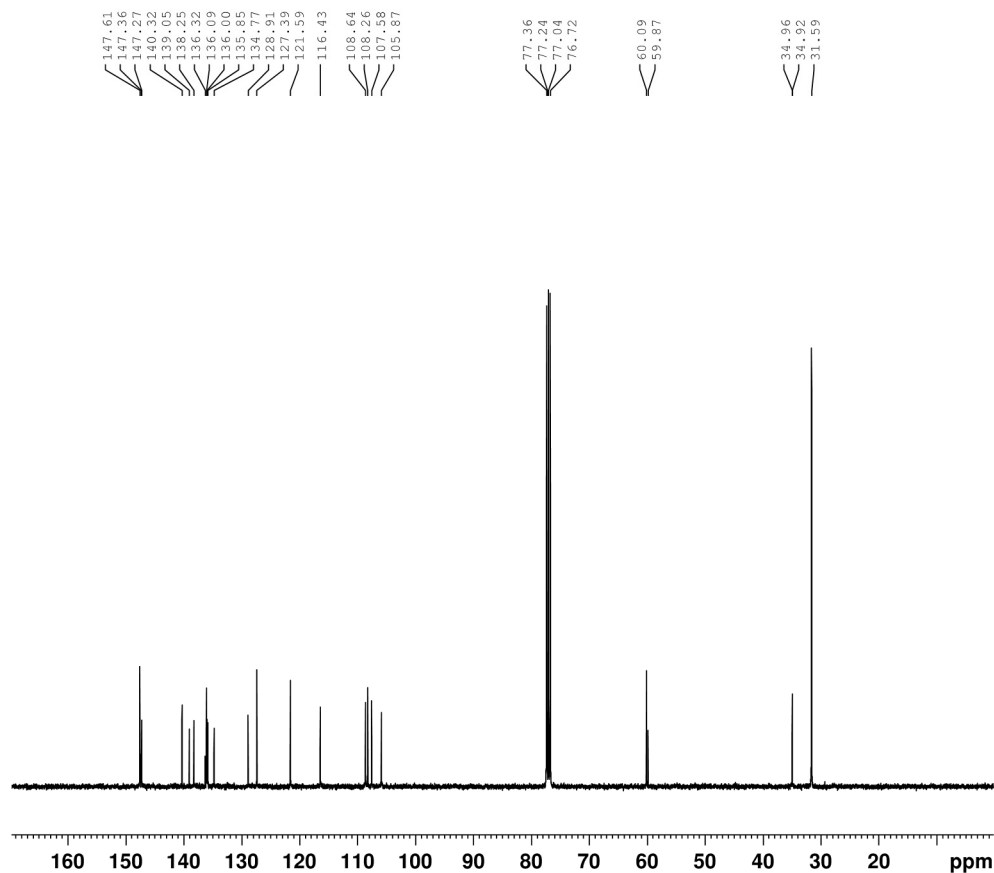
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3

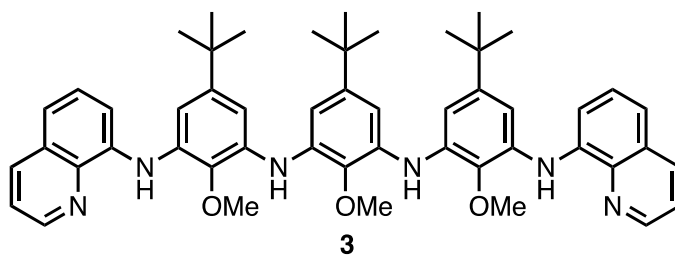
13C with 1H decoupling



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FIDRES 0.250007 Hz
AQ 1.9999440 sec
RG 210.82
DW 21.600 usec
DE 6.50 usec
TE 298.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO
SFO1 100.6530068 MHz
NUC1 13C
P1 10.00 usec
PLW1 54.00000000 W
SFO2 400.2516010 MHz
NUC2 1H
CPDPRG2 waltz165
PCPD2 80.00 usec
PLW2 10.71500015 W
PLW12 0.35200000 W
PLW13 0.22528000 W

F2 - Processing parameters
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S4. 13C NMR spectrum of 3 (CDCl₃).

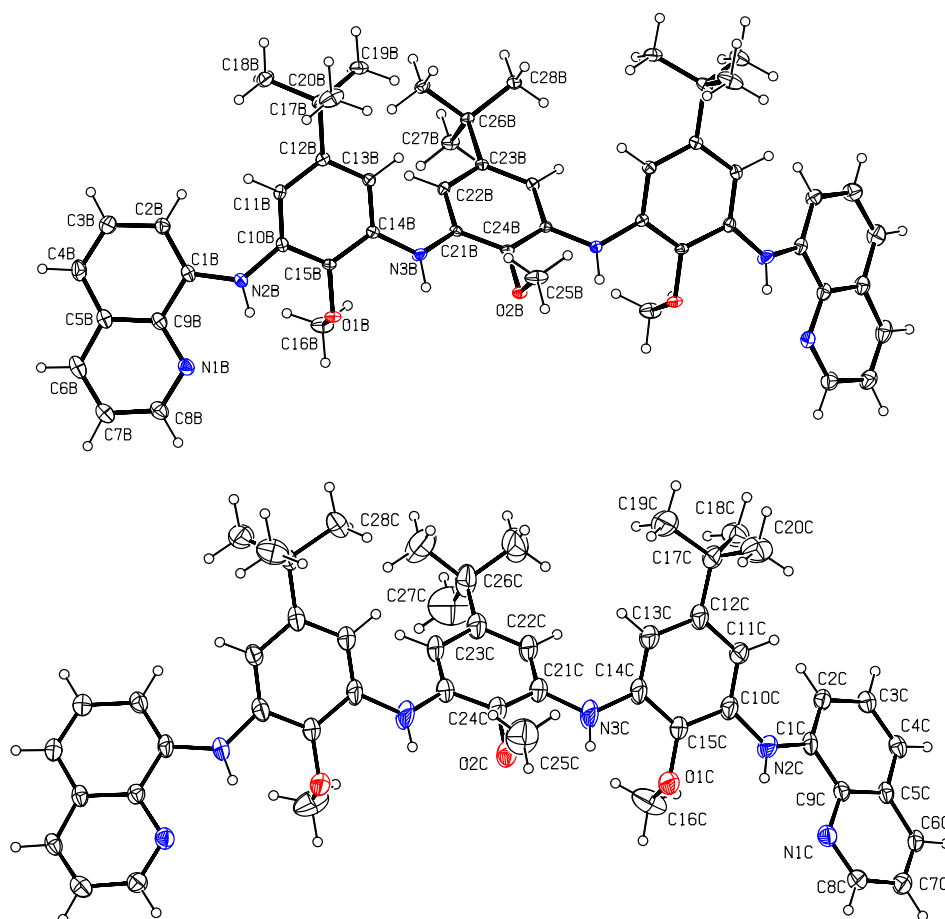


Figure S5. Displacement ellipsoid plots of two independent molecules of **3** in the asymmetric unit.

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File Name: MLH0506

Ion Source Type(Polarity): ESI+
Solvent: DCM/MeOH

Sample has to be very diluted to show

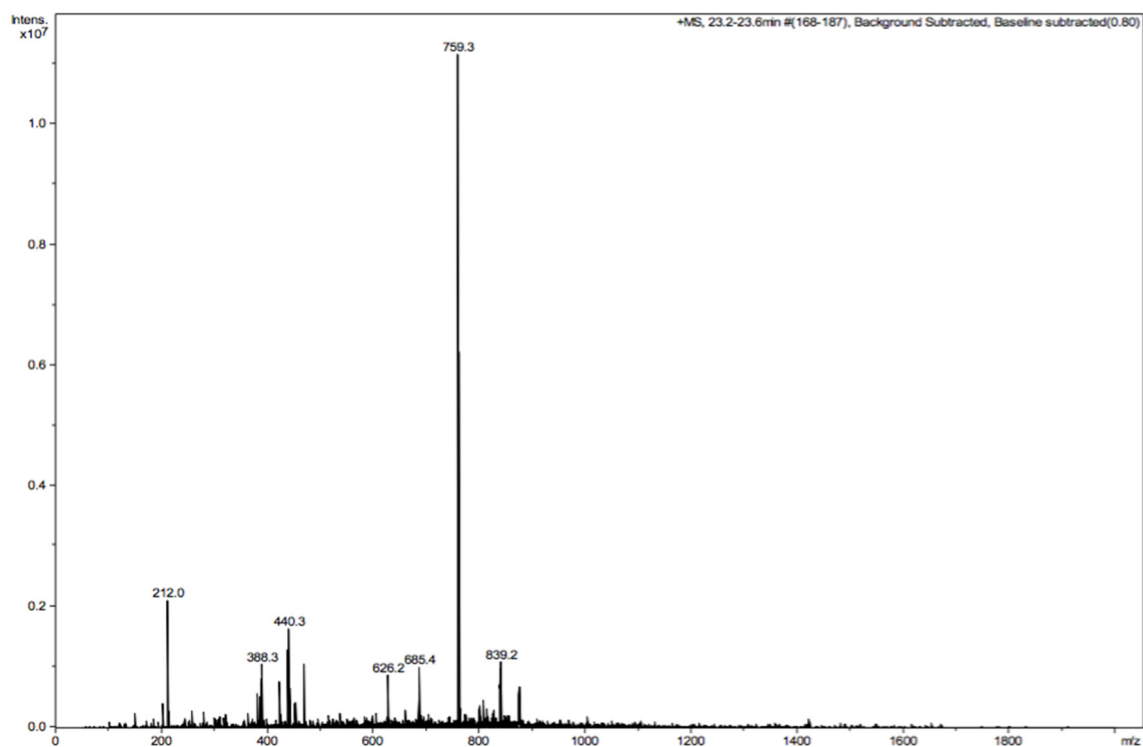


Figure S6. ESI mass spectrum of 4 (positive ion mode).

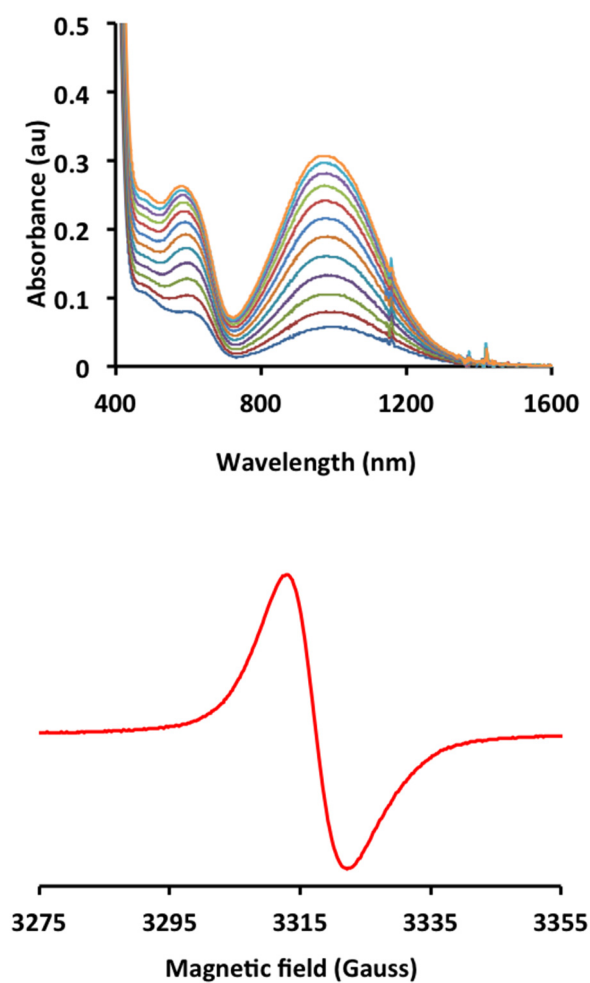


Figure S7. Left: UV-visible spectrum (CH_2Cl_2) of 4 over time changing to oxidized 4 (most intense absorptions belong to oxidized 4). Right: EPR spectrum of 4 in solid state at 298 K.

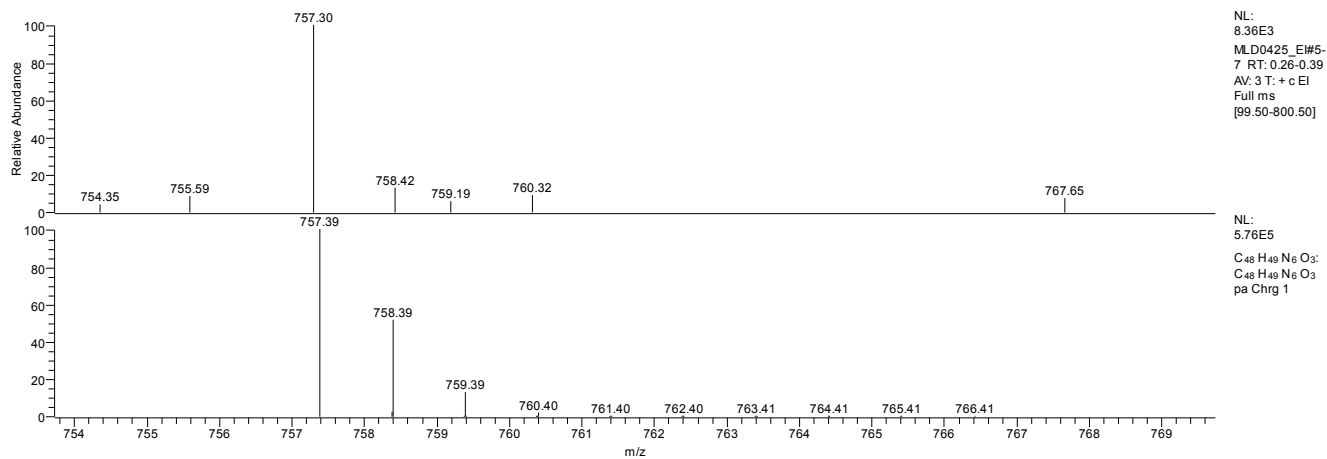


Figure S8. HR-FAB mass spectrum of oxidized 4.

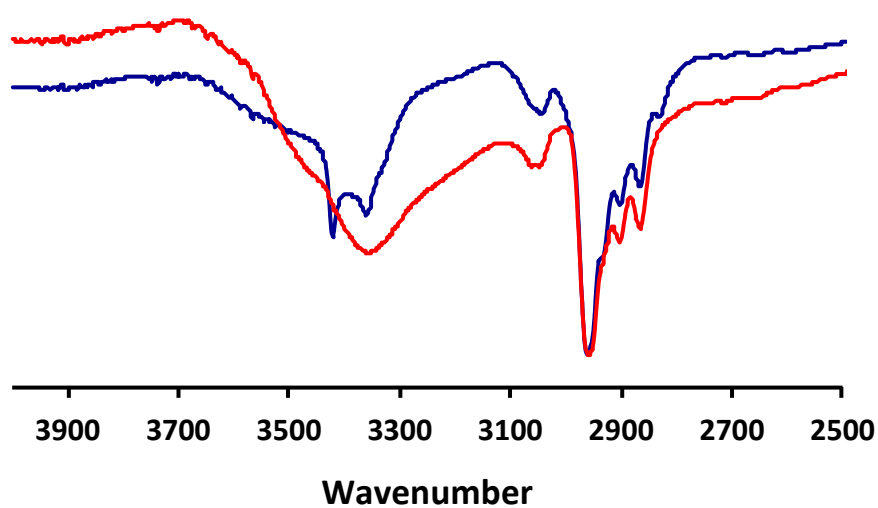


Figure S9. Comparison of the FT-IR spectra of 3 (blue trace) and oxidized 4 (red trace) (KBr).

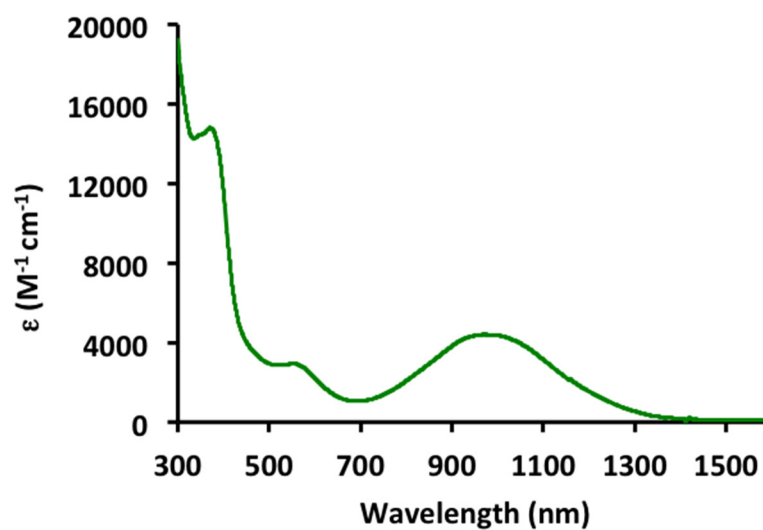


Figure S10. UV-visible spectrum of oxidized 4 in CH₂Cl₂ (298 K).

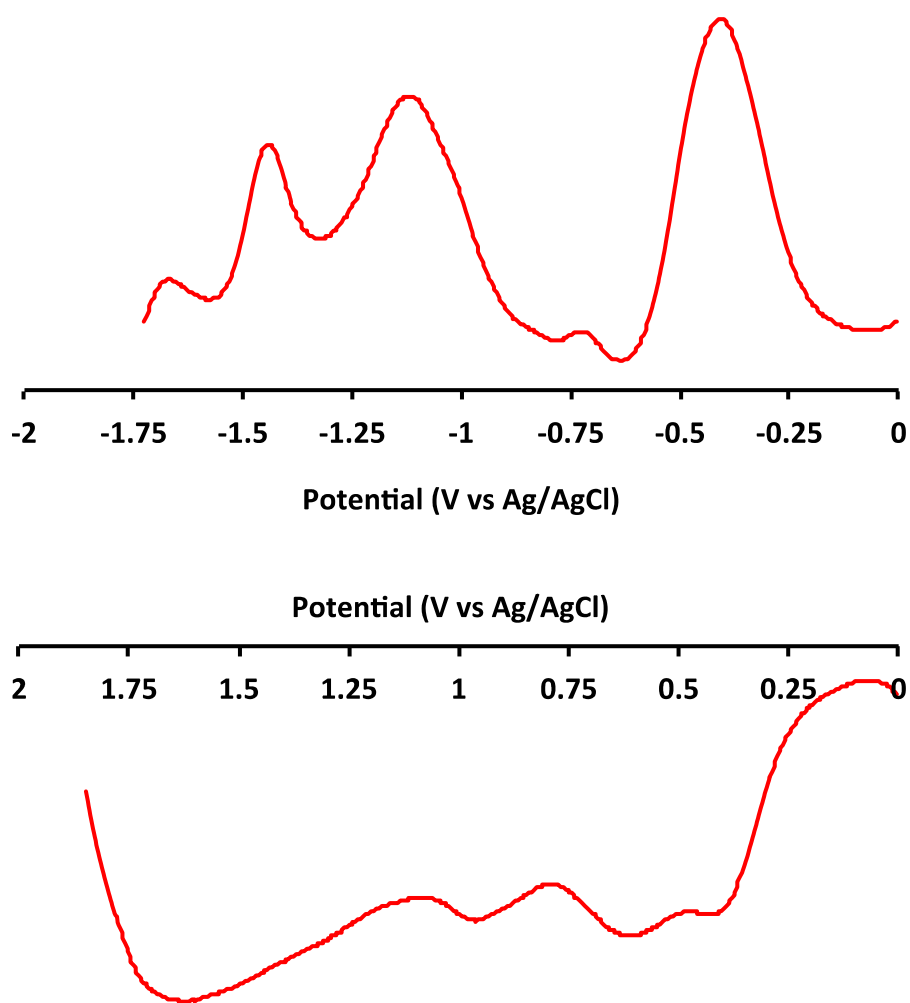


Figure S11. Cathodic (top) and Anodic (bottom) DPVs of oxidized 4 in CH₂Cl₂ (containing 0.5 M Bu₄NPF₆).

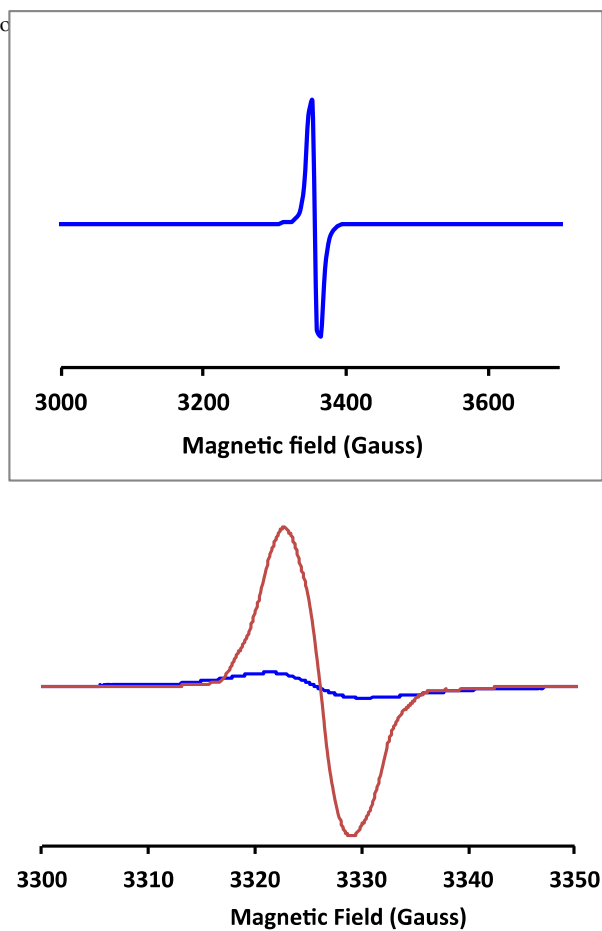


Figure S12. Left: EPR spectrum of oxidized 4 (powder, 100 K). Right: EPR spectrum of oxidized 4 in CH₂Cl₂ (red trace = 298 K and blue trace = 100 K).

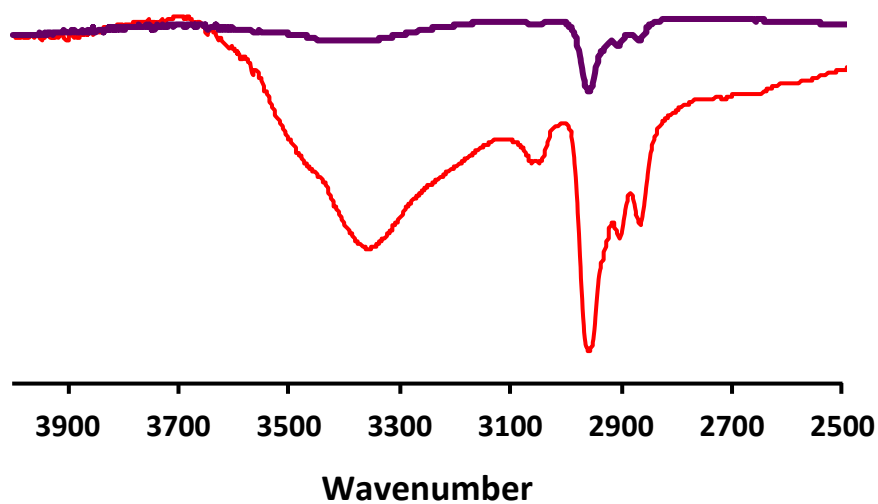
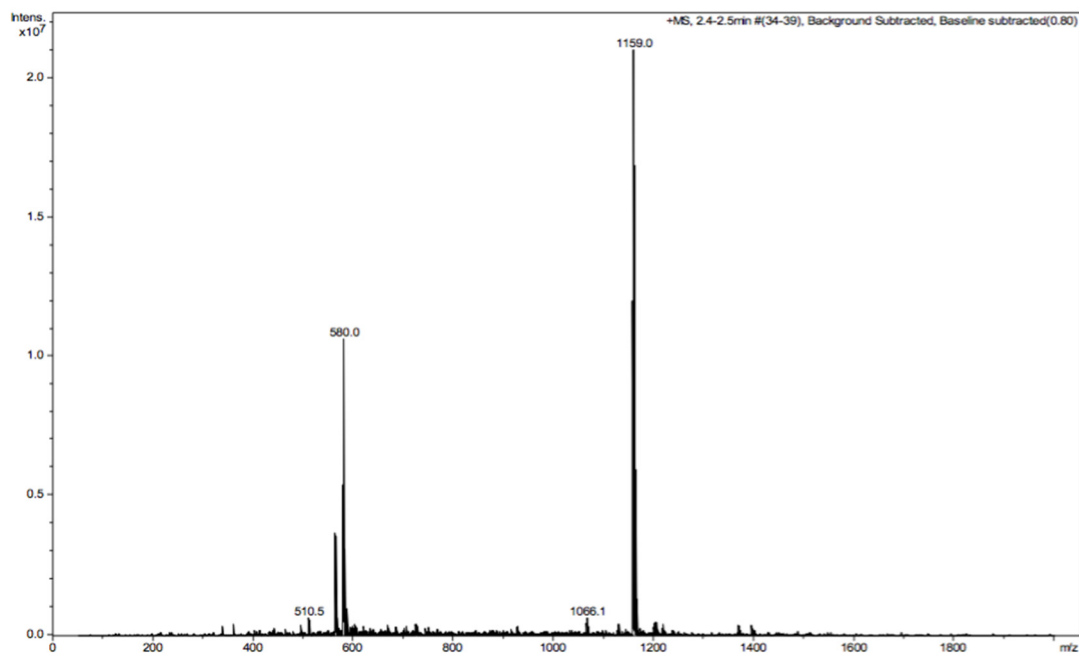


Figure S13. Comparison of the FT-IR spectra of oxidized 4 (red trace) and 5 (purple trace) (KBr).

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File Name: MLH0511

Ion Source Type(Polarity): ESI+
Solvent: MeOH (0.1% FA)



Sample Name: NB-05-14-2
File Name: MLH0511

Ion Source Type(Polarity): ESI+
Solvent: MeOH (0.1% FA)

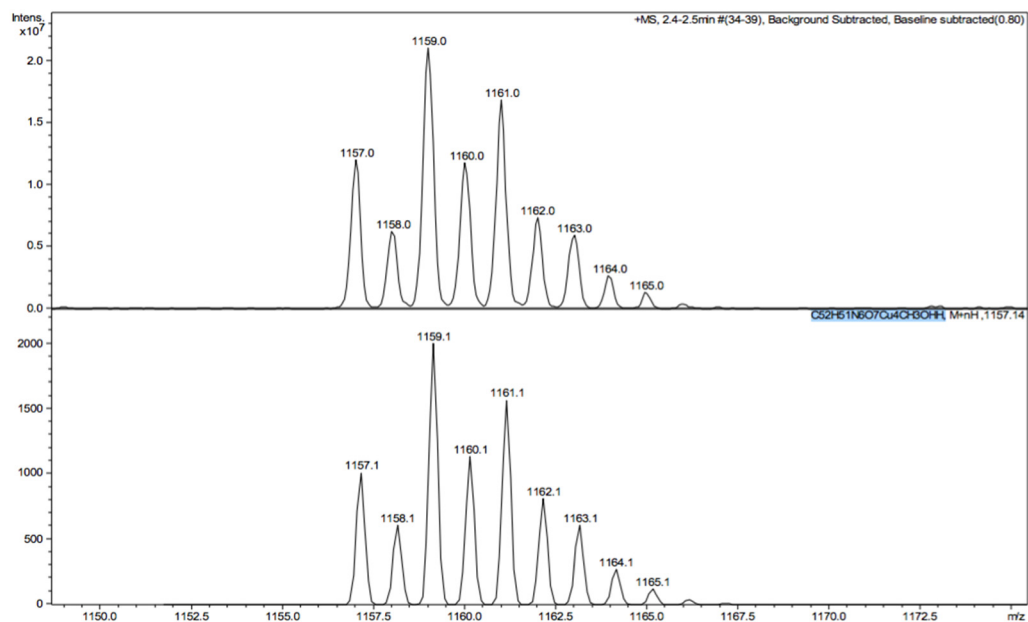


Figure S14. Top: ESI mass spec of 5 (positive ion mode, CH₃OH containing 0.1% formic acid). Bottom: Isotope distribution for m/z 1159 with theoretical distribution below.

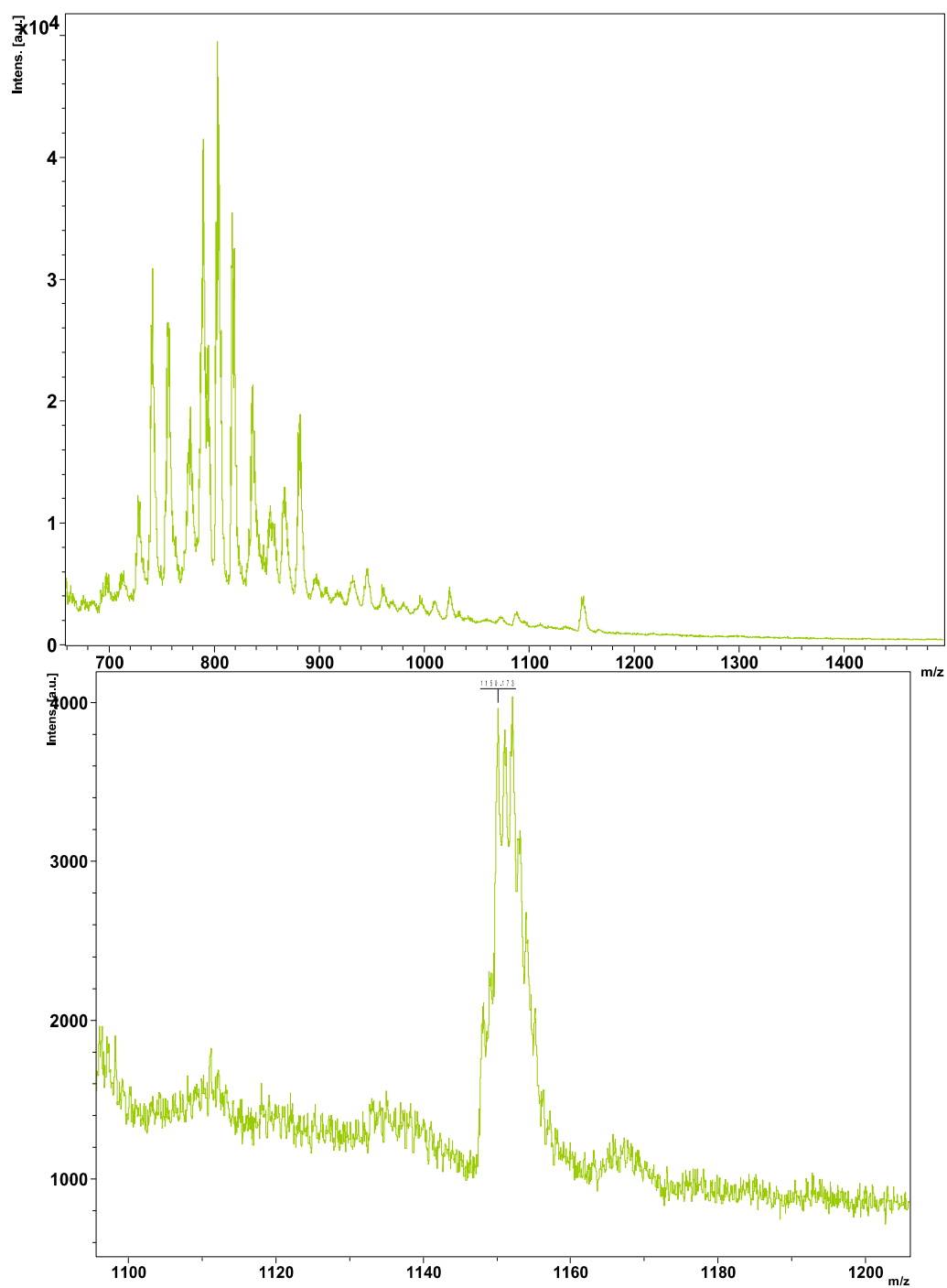


Figure S15. MALDI mass spectrum of 5 (positive ion mode).

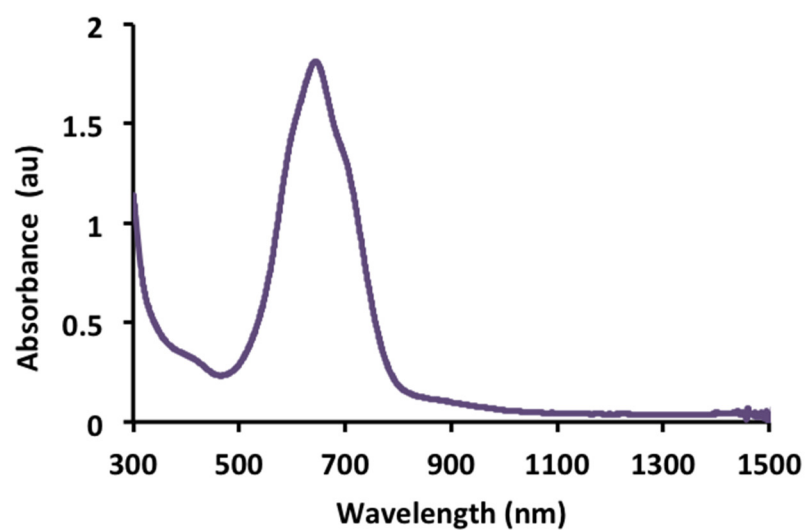


Figure S16. UV-visible spectrum of 5 in methanol (298 K).

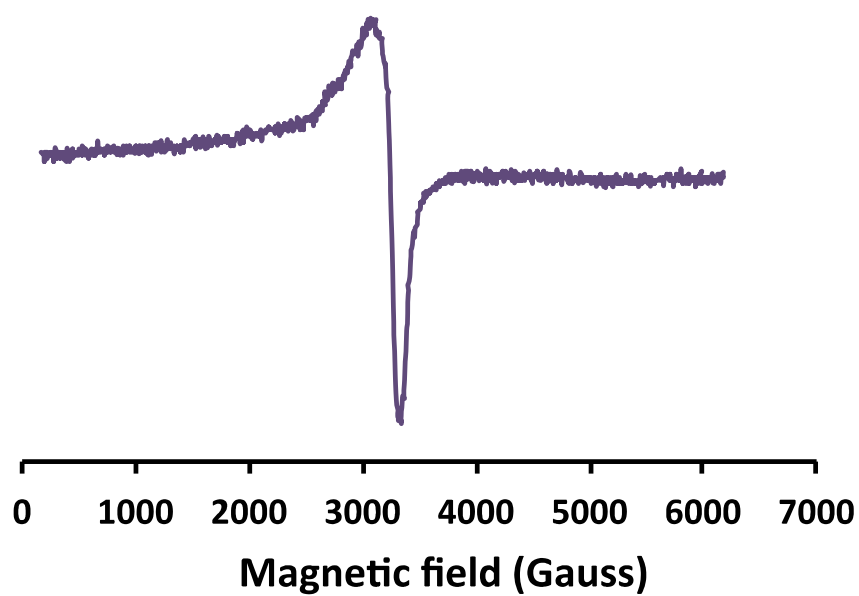


Figure S17. EPR spectrum of 5 (powder, 100 K).

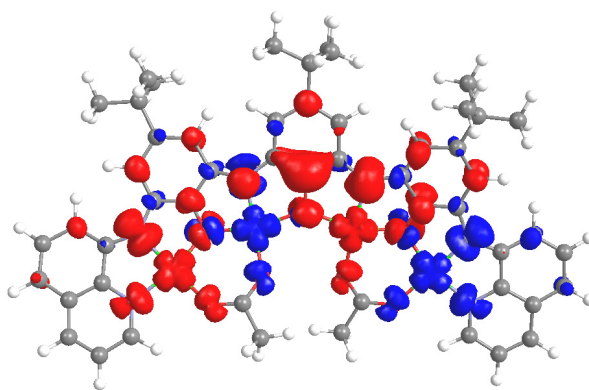


Figure S18. Spin-density distribution in the BS doublet state of 5. B3LYP/def2-SVP level of theory. Isovalue 0.004.

Table S1. Crystal data for 3.

Empirical formula	C ₁₅₇ H ₁₈₂ N ₁₈ O ₁₀		
Formula weight	2481.20		
Temperature	147(2) K		
Wavelength	1.54178 Å		
Crystal system	Orthorhombic		
Space group	Pmc2 ₁		
Unit cell dimensions	a = 40.5622(15) Å	α = 90°.	
	b = 16.6179(6) Å	β = 90°.	
	c = 11.4245(4) Å	γ = 90°.	
Volume	7700.8(5) Å ³		
Z	2		
Density (calculated)	1.070 Mg/m ³		
Absorption coefficient	0.529 mm ⁻¹		
F(000)	2660		
Crystal size	0.410 x 0.150 x 0.020 mm ³		
Theta range for data collection	2.178 to 67.304°.		
Index ranges	-48<=h<=48, -19<=k<=19, -13<=l<=13		
Reflections collected	147458		
Independent reflections	13873 [R(int) = 0.0814]		
Completeness to theta = 67.304°	99.3 %		
Absorption correction	Semi-empirical from equivalents		
Refinement method	Full-matrix least-squares on F ²		
Data / restraints / parameters	13873 / 6 / 883		
Goodness-of-fit on F ²	1.022		
Final R indices [I>2sigma(I)]	R1 = 0.0584, wR2 = 0.1628		
R indices (all data)	R1 = 0.0673, wR2 = 0.1712		
Absolute structure parameter	-0.07(9)		
Extinction coefficient	n/a		
Largest diff. peak and hole	0.408 and -0.337 e.Å ⁻³		

Table S2. Bond distances (Å) and angles (°) for **3**.

O(1A)-C(15A)	1.386(4)
O(1A)-C(16A)	1.439(5)
O(2A)-C(24A)	1.396(5)
O(2A)-C(25A)	1.436(6)
N(1A)-C(8A)	1.323(5)
N(1A)-C(9A)	1.366(5)
N(2A)-C(1A)	1.388(5)
N(2A)-C(10A)	1.399(5)
N(2A)-H(2A)	0.8800
N(3A)-C(14A)	1.393(4)
N(3A)-C(21A)	1.399(4)
N(3A)-H(3A)	0.8800
C(1A)-C(2A)	1.390(5)
C(1A)-C(9A)	1.426(5)
C(2A)-C(3A)	1.403(6)
C(2A)-H(2AA)	0.9500
C(3A)-C(4A)	1.362(6)
C(3A)-H(3AA)	0.9500
C(4A)-C(5A)	1.417(6)
C(4A)-H(4AA)	0.9500
C(5A)-C(6A)	1.403(6)
C(5A)-C(9A)	1.411(5)
C(6A)-C(7A)	1.355(7)
C(6A)-H(6AA)	0.9500
C(7A)-C(8A)	1.417(6)
C(7A)-H(7AA)	0.9500
C(8A)-H(8AA)	0.9500
C(10A)-C(15A)	1.393(5)
C(10A)-C(11A)	1.399(5)
C(11A)-C(12A)	1.398(5)
C(11A)-H(11A)	0.9500
C(12A)-C(13A)	1.392(5)
C(12A)-C(17A)	1.520(4)
C(13A)-C(14A)	1.407(5)
C(13A)-H(13A)	0.9500
C(14A)-C(15A)	1.394(5)
C(16A)-H(16A)	0.9800
C(16A)-H(16B)	0.9800
C(16A)-H(16C)	0.9800
C(17A)-C(19A)	1.528(5)
C(17A)-C(20A)	1.531(5)
C(17A)-C(18A)	1.533(5)
C(18A)-H(18A)	0.9800
C(18A)-H(18B)	0.9800
C(18A)-H(18C)	0.9800
C(19A)-H(19A)	0.9800
C(19A)-H(19B)	0.9800
C(19A)-H(19C)	0.9800
C(20A)-H(20A)	0.9800
C(20A)-H(20B)	0.9800
C(20A)-H(20C)	0.9800
C(21A)-C(24A)	1.387(4)
C(21A)-C(22A)	1.403(4)

C(22A)-C(23A)	1.386(4)
C(22A)-H(22A)	0.9500
C(23A)-C(22A)#1	1.386(4)
C(23A)-C(26A)	1.536(6)
C(24A)-C(21A)#1	1.387(4)
C(25A)-H(25A)	0.9800
C(25A)-H(25B)	0.9800
C(25A)-H(25C)	0.9800
C(26A)-C(28A)	1.533(4)
C(26A)-C(28A)#1	1.533(4)
C(26A)-C(27A)	1.541(6)
C(27A)-H(27A)	0.9800
C(27A)-H(27B)	0.9800
C(27A)-H(27C)	0.9800
C(28A)-H(28A)	0.9800
C(28A)-H(28B)	0.9800
C(28A)-H(28C)	0.9800
O(1B)-C(15B)	1.386(4)
O(1B)-C(16B)	1.454(4)
O(2B)-C(24B)	1.386(5)
O(2B)-C(25B)	1.435(6)
N(1B)-C(8B)	1.318(5)
N(1B)-C(9B)	1.358(5)
N(2B)-C(1B)	1.382(5)
N(2B)-C(10B)	1.399(5)
N(2B)-H(2B)	0.8800
N(3B)-C(21B)	1.384(4)
N(3B)-C(14B)	1.402(4)
N(3B)-H(3B)	0.8800
C(1B)-C(2B)	1.379(5)
C(1B)-C(9B)	1.439(5)
C(2B)-C(3B)	1.413(6)
C(2B)-H(2BA)	0.9500
C(3B)-C(4B)	1.379(6)
C(3B)-H(3BA)	0.9500
C(4B)-C(5B)	1.404(6)
C(4B)-H(4BA)	0.9500
C(5B)-C(9B)	1.415(6)
C(5B)-C(6B)	1.418(6)
C(6B)-C(7B)	1.374(7)
C(6B)-H(6BA)	0.9500
C(7B)-C(8B)	1.401(6)
C(7B)-H(7BA)	0.9500
C(8B)-H(8BA)	0.9500
C(10B)-C(11B)	1.389(5)
C(10B)-C(15B)	1.398(5)
C(11B)-C(12B)	1.397(5)
C(11B)-H(11B)	0.9500
C(12B)-C(13B)	1.388(5)
C(12B)-C(17B)	1.538(5)
C(13B)-C(14B)	1.384(5)
C(13B)-H(13B)	0.9500
C(14B)-C(15B)	1.393(5)
C(16B)-H(16D)	0.9800

C(16B)-H(16E)	0.9800
C(16B)-H(16F)	0.9800
C(17B)-C(19B)	1.524(6)
C(17B)-C(20B)	1.524(5)
C(17B)-C(18B)	1.531(5)
C(18B)-H(18D)	0.9800
C(18B)-H(18E)	0.9800
C(18B)-H(18F)	0.9800
C(19B)-H(19D)	0.9800
C(19B)-H(19E)	0.9800
C(19B)-H(19F)	0.9800
C(20B)-H(20D)	0.9800
C(20B)-H(20E)	0.9800
C(20B)-H(20F)	0.9800
C(21B)-C(24B)	1.394(4)
C(21B)-C(22B)	1.400(5)
C(22B)-C(23B)	1.392(4)
C(22B)-H(22B)	0.9500
C(23B)-C(22B)#1	1.392(4)
C(23B)-C(26B)	1.544(6)
C(24B)-C(21B)#1	1.394(4)
C(25B)-H(25D)	0.9800
C(25B)-H(25E)	0.9800
C(25B)-H(25F)	0.9800
C(26B)-C(28B)	1.533(4)
C(26B)-C(28B)#1	1.533(4)
C(26B)-C(27B)	1.539(7)
C(27B)-H(27D)	0.9800
C(27B)-H(27E)	0.9800
C(27B)-H(27F)	0.9800
C(28B)-H(28D)	0.9800
C(28B)-H(28E)	0.9800
C(28B)-H(28F)	0.9800
O(1C)-C(15C)	1.387(7)
O(1C)-C(16C)	1.432(10)
O(2C)-C(24C)	1.406(11)
O(2C)-C(25C)	1.511(17)
N(1C)-C(8C)	1.325(6)
N(1C)-C(9C)	1.391(6)
N(2C)-C(1C)	1.397(6)
N(2C)-C(10C)	1.401(6)
N(2C)-H(2C)	0.8800
N(3C)-C(14C)	1.406(7)
N(3C)-C(21C)	1.409(7)
N(3C)-H(3C)	0.8800
C(1C)-C(2C)	1.373(7)
C(1C)-C(9C)	1.426(7)
C(2C)-C(3C)	1.412(7)
C(2C)-H(2CA)	0.9500
C(3C)-C(4C)	1.355(7)
C(3C)-H(3CA)	0.9500
C(4C)-C(5C)	1.415(6)
C(4C)-H(4CA)	0.9500
C(5C)-C(6C)	1.408(6)

C(5C)-C(9C)	1.409(6)
C(6C)-C(7C)	1.343(7)
C(6C)-H(6CA)	0.9500
C(7C)-C(8C)	1.406(7)
C(7C)-H(7CA)	0.9500
C(8C)-H(8CA)	0.9500
C(10C)-C(11C)	1.384(7)
C(10C)-C(15C)	1.391(7)
C(11C)-C(12C)	1.398(7)
C(11C)-H(11C)	0.9500
C(12C)-C(13C)	1.382(7)
C(12C)-C(17C)	1.528(7)
C(13C)-C(14C)	1.370(8)
C(13C)-H(13C)	0.9500
C(14C)-C(15C)	1.418(7)
C(16C)-H(16G)	0.9800
C(16C)-H(16H)	0.9800
C(16C)-H(16I)	0.9800
C(17C)-C(19C)	1.512(8)
C(17C)-C(18C)	1.535(8)
C(17C)-C(20C)	1.555(9)
C(18C)-H(18G)	0.9800
C(18C)-H(18H)	0.9800
C(18C)-H(18I)	0.9800
C(19C)-H(19G)	0.9800
C(19C)-H(19H)	0.9800
C(19C)-H(19I)	0.9800
C(20C)-H(20G)	0.9800
C(20C)-H(20H)	0.9800
C(20C)-H(20I)	0.9800
C(21C)-C(24C)	1.383(7)
C(21C)-C(22C)	1.384(9)
C(22C)-C(23C)	1.403(7)
C(22C)-H(22C)	0.9500
C(23C)-C(22C)#2	1.403(7)
C(23C)-C(26C)	1.502(12)
C(24C)-C(21C)#2	1.382(7)
C(25C)-H(25G)	0.9800
C(25C)-H(25H)	0.9800
C(25C)-H(25I)	0.9800
C(26C)-C(28C)	1.512(11)
C(26C)-C(28C)#2	1.512(11)
C(26C)-C(27C)	1.528(18)
C(27C)-H(27G)	0.9800
C(27C)-H(27H)	0.9800
C(27C)-H(27I)	0.9800
C(28C)-H(28G)	0.9800
C(28C)-H(28H)	0.9800
C(28C)-H(28I)	0.9800
O(1S)-C(4S)	1.362(12)
O(1S)-C(1S)	1.425(13)
C(1S)-C(2S)	1.446(13)
C(1S)-H(1SA)	0.9900
C(1S)-H(1SB)	0.9900

C(2S)-C(3S)	1.467(13)
C(2S)-H(2SA)	0.9900
C(2S)-H(2SB)	0.9900
C(3S)-C(4S)	1.448(13)
C(3S)-H(3SA)	0.9900
C(3S)-H(3SB)	0.9900
C(4S)-H(4SA)	0.9900
C(4S)-H(4SB)	0.9900
C(15A)-O(1A)-C(16A)	111.4(3)
C(24A)-O(2A)-C(25A)	113.0(3)
C(8A)-N(1A)-C(9A)	117.9(4)
C(1A)-N(2A)-C(10A)	129.6(3)
C(1A)-N(2A)-H(2A)	115.2
C(10A)-N(2A)-H(2A)	115.2
C(14A)-N(3A)-C(21A)	126.4(3)
C(14A)-N(3A)-H(3A)	116.8
C(21A)-N(3A)-H(3A)	116.8
N(2A)-C(1A)-C(2A)	124.9(3)
N(2A)-C(1A)-C(9A)	116.2(3)
C(2A)-C(1A)-C(9A)	118.8(3)
C(1A)-C(2A)-C(3A)	119.8(4)
C(1A)-C(2A)-H(2AA)	120.1
C(3A)-C(2A)-H(2AA)	120.1
C(4A)-C(3A)-C(2A)	122.5(4)
C(4A)-C(3A)-H(3AA)	118.8
C(2A)-C(3A)-H(3AA)	118.8
C(3A)-C(4A)-C(5A)	119.1(4)
C(3A)-C(4A)-H(4AA)	120.4
C(5A)-C(4A)-H(4AA)	120.4
C(6A)-C(5A)-C(9A)	116.7(4)
C(6A)-C(5A)-C(4A)	123.8(4)
C(9A)-C(5A)-C(4A)	119.5(4)
C(7A)-C(6A)-C(5A)	120.7(4)
C(7A)-C(6A)-H(6AA)	119.7
C(5A)-C(6A)-H(6AA)	119.7
C(6A)-C(7A)-C(8A)	118.9(4)
C(6A)-C(7A)-H(7AA)	120.6
C(8A)-C(7A)-H(7AA)	120.6
N(1A)-C(8A)-C(7A)	122.7(4)
N(1A)-C(8A)-H(8AA)	118.6
C(7A)-C(8A)-H(8AA)	118.6
N(1A)-C(9A)-C(5A)	123.1(3)
N(1A)-C(9A)-C(1A)	116.7(3)
C(5A)-C(9A)-C(1A)	120.2(3)
C(15A)-C(10A)-C(11A)	119.1(3)
C(15A)-C(10A)-N(2A)	118.0(3)
C(11A)-C(10A)-N(2A)	122.9(3)
C(12A)-C(11A)-C(10A)	121.3(3)
C(12A)-C(11A)-H(11A)	119.3
C(10A)-C(11A)-H(11A)	119.3
C(13A)-C(12A)-C(11A)	118.4(3)
C(13A)-C(12A)-C(17A)	122.2(3)
C(11A)-C(12A)-C(17A)	119.3(3)

C(12A)-C(13A)-C(14A)	121.5(3)
C(12A)-C(13A)-H(13A)	119.3
C(14A)-C(13A)-H(13A)	119.3
N(3A)-C(14A)-C(15A)	118.5(3)
N(3A)-C(14A)-C(13A)	122.8(3)
C(15A)-C(14A)-C(13A)	118.7(3)
O(1A)-C(15A)-C(10A)	119.7(3)
O(1A)-C(15A)-C(14A)	119.3(3)
C(10A)-C(15A)-C(14A)	121.0(3)
O(1A)-C(16A)-H(16A)	109.5
O(1A)-C(16A)-H(16B)	109.5
H(16A)-C(16A)-H(16B)	109.5
O(1A)-C(16A)-H(16C)	109.5
H(16A)-C(16A)-H(16C)	109.5
H(16B)-C(16A)-H(16C)	109.5
C(12A)-C(17A)-C(19A)	111.7(3)
C(12A)-C(17A)-C(20A)	109.1(3)
C(19A)-C(17A)-C(20A)	108.6(3)
C(12A)-C(17A)-C(18A)	110.4(3)
C(19A)-C(17A)-C(18A)	107.1(3)
C(20A)-C(17A)-C(18A)	109.8(3)
C(17A)-C(18A)-H(18A)	109.5
C(17A)-C(18A)-H(18B)	109.5
H(18A)-C(18A)-H(18B)	109.5
C(17A)-C(18A)-H(18C)	109.5
H(18A)-C(18A)-H(18C)	109.5
H(18B)-C(18A)-H(18C)	109.5
C(17A)-C(19A)-H(19A)	109.5
C(17A)-C(19A)-H(19B)	109.5
H(19A)-C(19A)-H(19B)	109.5
C(17A)-C(19A)-H(19C)	109.5
H(19A)-C(19A)-H(19C)	109.5
H(19B)-C(19A)-H(19C)	109.5
C(17A)-C(20A)-H(20A)	109.5
C(17A)-C(20A)-H(20B)	109.5
H(20A)-C(20A)-H(20B)	109.5
C(17A)-C(20A)-H(20C)	109.5
H(20A)-C(20A)-H(20C)	109.5
H(20B)-C(20A)-H(20C)	109.5
C(24A)-C(21A)-N(3A)	119.6(3)
C(24A)-C(21A)-C(22A)	119.0(3)
N(3A)-C(21A)-C(22A)	121.4(3)
C(23A)-C(22A)-C(21A)	121.0(3)
C(23A)-C(22A)-H(22A)	119.5
C(21A)-C(22A)-H(22A)	119.5
C(22A)#1-C(23A)-C(22A)	119.0(4)
C(22A)#1-C(23A)-C(26A)	120.4(2)
C(22A)-C(23A)-C(26A)	120.4(2)
C(21A)-C(24A)-C(21A)#1	120.9(4)
C(21A)-C(24A)-O(2A)	119.5(2)
C(21A)#1-C(24A)-O(2A)	119.5(2)
O(2A)-C(25A)-H(25A)	109.5
O(2A)-C(25A)-H(25B)	109.5
H(25A)-C(25A)-H(25B)	109.5

O(2A)-C(25A)-H(25C)	109.5
H(25A)-C(25A)-H(25C)	109.5
H(25B)-C(25A)-H(25C)	109.5
C(28A)-C(26A)-C(28A)#1	107.6(4)
C(28A)-C(26A)-C(23A)	111.7(2)
C(28A)#1-C(26A)-C(23A)	111.7(2)
C(28A)-C(26A)-C(27A)	108.8(3)
C(28A)#1-C(26A)-C(27A)	108.8(3)
C(23A)-C(26A)-C(27A)	108.3(4)
C(26A)-C(27A)-H(27A)	109.5
C(26A)-C(27A)-H(27B)	109.5
H(27A)-C(27A)-H(27B)	109.5
C(26A)-C(27A)-H(27C)	109.5
H(27A)-C(27A)-H(27C)	109.5
H(27B)-C(27A)-H(27C)	109.5
C(26A)-C(28A)-H(28A)	109.5
C(26A)-C(28A)-H(28B)	109.5
H(28A)-C(28A)-H(28B)	109.5
C(26A)-C(28A)-H(28C)	109.5
H(28A)-C(28A)-H(28C)	109.5
H(28B)-C(28A)-H(28C)	109.5
C(15B)-O(1B)-C(16B)	111.7(3)
C(24B)-O(2B)-C(25B)	112.6(4)
C(8B)-N(1B)-C(9B)	117.1(4)
C(1B)-N(2B)-C(10B)	130.0(3)
C(1B)-N(2B)-H(2B)	115.0
C(10B)-N(2B)-H(2B)	115.0
C(21B)-N(3B)-C(14B)	125.9(3)
C(21B)-N(3B)-H(3B)	117.0
C(14B)-N(3B)-H(3B)	117.0
C(2B)-C(1B)-N(2B)	126.7(3)
C(2B)-C(1B)-C(9B)	119.0(3)
N(2B)-C(1B)-C(9B)	114.3(3)
C(1B)-C(2B)-C(3B)	120.5(4)
C(1B)-C(2B)-H(2BA)	119.8
C(3B)-C(2B)-H(2BA)	119.8
C(4B)-C(3B)-C(2B)	121.4(4)
C(4B)-C(3B)-H(3BA)	119.3
C(2B)-C(3B)-H(3BA)	119.3
C(3B)-C(4B)-C(5B)	119.3(4)
C(3B)-C(4B)-H(4BA)	120.3
C(5B)-C(4B)-H(4BA)	120.3
C(4B)-C(5B)-C(9B)	120.4(4)
C(4B)-C(5B)-C(6B)	122.5(4)
C(9B)-C(5B)-C(6B)	117.1(4)
C(7B)-C(6B)-C(5B)	119.6(4)
C(7B)-C(6B)-H(6BA)	120.2
C(5B)-C(6B)-H(6BA)	120.2
C(6B)-C(7B)-C(8B)	118.1(4)
C(6B)-C(7B)-H(7BA)	121.0
C(8B)-C(7B)-H(7BA)	121.0
N(1B)-C(8B)-C(7B)	125.0(4)
N(1B)-C(8B)-H(8BA)	117.5
C(7B)-C(8B)-H(8BA)	117.5

N(1B)-C(9B)-C(5B)	123.2(4)
N(1B)-C(9B)-C(1B)	117.5(3)
C(5B)-C(9B)-C(1B)	119.3(4)
C(11B)-C(10B)-C(15B)	119.1(3)
C(11B)-C(10B)-N(2B)	125.9(3)
C(15B)-C(10B)-N(2B)	115.0(3)
C(10B)-C(11B)-C(12B)	121.2(3)
C(10B)-C(11B)-H(11B)	119.4
C(12B)-C(11B)-H(11B)	119.4
C(13B)-C(12B)-C(11B)	118.5(3)
C(13B)-C(12B)-C(17B)	121.0(3)
C(11B)-C(12B)-C(17B)	120.5(3)
C(14B)-C(13B)-C(12B)	121.3(3)
C(14B)-C(13B)-H(13B)	119.3
C(12B)-C(13B)-H(13B)	119.3
C(13B)-C(14B)-C(15B)	119.6(3)
C(13B)-C(14B)-N(3B)	122.8(3)
C(15B)-C(14B)-N(3B)	117.6(3)
O(1B)-C(15B)-C(14B)	119.7(3)
O(1B)-C(15B)-C(10B)	120.0(3)
C(14B)-C(15B)-C(10B)	120.2(3)
O(1B)-C(16B)-H(16D)	109.5
O(1B)-C(16B)-H(16E)	109.5
H(16D)-C(16B)-H(16E)	109.5
O(1B)-C(16B)-H(16F)	109.5
H(16D)-C(16B)-H(16F)	109.5
H(16E)-C(16B)-H(16F)	109.5
C(19B)-C(17B)-C(20B)	108.6(4)
C(19B)-C(17B)-C(18B)	107.2(3)
C(20B)-C(17B)-C(18B)	109.4(3)
C(19B)-C(17B)-C(12B)	111.4(3)
C(20B)-C(17B)-C(12B)	109.1(3)
C(18B)-C(17B)-C(12B)	111.1(3)
C(17B)-C(18B)-H(18D)	109.5
C(17B)-C(18B)-H(18E)	109.5
H(18D)-C(18B)-H(18E)	109.5
C(17B)-C(18B)-H(18F)	109.5
H(18D)-C(18B)-H(18F)	109.5
H(18E)-C(18B)-H(18F)	109.5
C(17B)-C(19B)-H(19D)	109.5
C(17B)-C(19B)-H(19E)	109.5
H(19D)-C(19B)-H(19E)	109.5
C(17B)-C(19B)-H(19F)	109.5
H(19D)-C(19B)-H(19F)	109.5
H(19E)-C(19B)-H(19F)	109.5
C(17B)-C(20B)-H(20D)	109.5
C(17B)-C(20B)-H(20E)	109.5
H(20D)-C(20B)-H(20E)	109.5
C(17B)-C(20B)-H(20F)	109.5
H(20D)-C(20B)-H(20F)	109.5
H(20E)-C(20B)-H(20F)	109.5
N(3B)-C(21B)-C(24B)	118.4(3)
N(3B)-C(21B)-C(22B)	122.4(3)
C(24B)-C(21B)-C(22B)	119.2(3)

C(23B)-C(22B)-C(21B)	121.2(3)
C(23B)-C(22B)-H(22B)	119.4
C(21B)-C(22B)-H(22B)	119.4
C(22B)-C(23B)-C(22B)#1	118.7(4)
C(22B)-C(23B)-C(26B)	120.6(2)
C(22B)#1-C(23B)-C(26B)	120.6(2)
O(2B)-C(24B)-C(21B)	119.7(2)
O(2B)-C(24B)-C(21B)#1	119.7(2)
C(21B)-C(24B)-C(21B)#1	120.5(4)
O(2B)-C(25B)-H(25D)	109.5
O(2B)-C(25B)-H(25E)	109.5
H(25D)-C(25B)-H(25E)	109.5
O(2B)-C(25B)-H(25F)	109.5
H(25D)-C(25B)-H(25F)	109.5
H(25E)-C(25B)-H(25F)	109.5
C(28B)-C(26B)-C(28B)#1	108.3(4)
C(28B)-C(26B)-C(27B)	109.0(3)
C(28B)#1-C(26B)-C(27B)	109.0(3)
C(28B)-C(26B)-C(23B)	111.2(2)
C(28B)#1-C(26B)-C(23B)	111.2(2)
C(27B)-C(26B)-C(23B)	108.1(4)
C(26B)-C(27B)-H(27D)	109.5
C(26B)-C(27B)-H(27E)	109.5
H(27D)-C(27B)-H(27E)	109.5
C(26B)-C(27B)-H(27F)	109.5
H(27D)-C(27B)-H(27F)	109.5
H(27E)-C(27B)-H(27F)	109.5
C(26B)-C(28B)-H(28D)	109.5
C(26B)-C(28B)-H(28E)	109.5
H(28D)-C(28B)-H(28E)	109.5
C(26B)-C(28B)-H(28F)	109.5
H(28D)-C(28B)-H(28F)	109.5
H(28E)-C(28B)-H(28F)	109.5
C(15C)-O(1C)-C(16C)	112.9(5)
C(24C)-O(2C)-C(25C)	112.3(9)
C(8C)-N(1C)-C(9C)	118.0(4)
C(1C)-N(2C)-C(10C)	129.3(5)
C(1C)-N(2C)-H(2C)	115.3
C(10C)-N(2C)-H(2C)	115.3
C(14C)-N(3C)-C(21C)	124.8(5)
C(14C)-N(3C)-H(3C)	117.6
C(21C)-N(3C)-H(3C)	117.6
C(2C)-C(1C)-N(2C)	125.8(4)
C(2C)-C(1C)-C(9C)	118.8(4)
N(2C)-C(1C)-C(9C)	115.4(4)
C(1C)-C(2C)-C(3C)	120.0(4)
C(1C)-C(2C)-H(2CA)	120.0
C(3C)-C(2C)-H(2CA)	120.0
C(4C)-C(3C)-C(2C)	122.1(5)
C(4C)-C(3C)-H(3CA)	118.9
C(2C)-C(3C)-H(3CA)	118.9
C(3C)-C(4C)-C(5C)	119.6(4)
C(3C)-C(4C)-H(4CA)	120.2
C(5C)-C(4C)-H(4CA)	120.2

C(6C)-C(5C)-C(9C)	117.2(4)
C(6C)-C(5C)-C(4C)	123.9(4)
C(9C)-C(5C)-C(4C)	118.9(4)
C(7C)-C(6C)-C(5C)	120.9(4)
C(7C)-C(6C)-H(6CA)	119.5
C(5C)-C(6C)-H(6CA)	119.5
C(6C)-C(7C)-C(8C)	119.2(5)
C(6C)-C(7C)-H(7CA)	120.4
C(8C)-C(7C)-H(7CA)	120.4
N(1C)-C(8C)-C(7C)	123.0(5)
N(1C)-C(8C)-H(8CA)	118.5
C(7C)-C(8C)-H(8CA)	118.5
N(1C)-C(9C)-C(5C)	121.6(4)
N(1C)-C(9C)-C(1C)	117.8(4)
C(5C)-C(9C)-C(1C)	120.6(4)
C(11C)-C(10C)-C(15C)	119.4(4)
C(11C)-C(10C)-N(2C)	125.1(5)
C(15C)-C(10C)-N(2C)	115.3(5)
C(10C)-C(11C)-C(12C)	121.9(5)
C(10C)-C(11C)-H(11C)	119.1
C(12C)-C(11C)-H(11C)	119.1
C(13C)-C(12C)-C(11C)	118.2(5)
C(13C)-C(12C)-C(17C)	121.4(5)
C(11C)-C(12C)-C(17C)	120.3(4)
C(14C)-C(13C)-C(12C)	121.3(5)
C(14C)-C(13C)-H(13C)	119.4
C(12C)-C(13C)-H(13C)	119.4
C(13C)-C(14C)-N(3C)	123.5(5)
C(13C)-C(14C)-C(15C)	120.4(5)
N(3C)-C(14C)-C(15C)	116.0(6)
O(1C)-C(15C)-C(10C)	120.6(5)
O(1C)-C(15C)-C(14C)	120.6(5)
C(10C)-C(15C)-C(14C)	118.8(5)
O(1C)-C(16C)-H(16G)	109.5
O(1C)-C(16C)-H(16H)	109.5
H(16G)-C(16C)-H(16H)	109.5
O(1C)-C(16C)-H(16I)	109.5
H(16G)-C(16C)-H(16I)	109.5
H(16H)-C(16C)-H(16I)	109.5
C(19C)-C(17C)-C(12C)	113.5(5)
C(19C)-C(17C)-C(18C)	109.2(6)
C(12C)-C(17C)-C(18C)	110.1(4)
C(19C)-C(17C)-C(20C)	106.9(6)
C(12C)-C(17C)-C(20C)	109.7(5)
C(18C)-C(17C)-C(20C)	107.2(5)
C(17C)-C(18C)-H(18G)	109.5
C(17C)-C(18C)-H(18H)	109.5
H(18G)-C(18C)-H(18H)	109.5
C(17C)-C(18C)-H(18I)	109.5
H(18G)-C(18C)-H(18I)	109.5
H(18H)-C(18C)-H(18I)	109.5
C(17C)-C(19C)-H(19G)	109.5
C(17C)-C(19C)-H(19H)	109.5
H(19G)-C(19C)-H(19H)	109.5

C(17C)-C(19C)-H(19I)	109.5
H(19G)-C(19C)-H(19I)	109.5
H(19H)-C(19C)-H(19I)	109.5
C(17C)-C(20C)-H(20G)	109.5
C(17C)-C(20C)-H(20H)	109.5
H(20G)-C(20C)-H(20H)	109.5
C(17C)-C(20C)-H(20I)	109.5
H(20G)-C(20C)-H(20I)	109.5
H(20H)-C(20C)-H(20I)	109.5
C(24C)-C(21C)-C(22C)	119.4(5)
C(24C)-C(21C)-N(3C)	116.6(6)
C(22C)-C(21C)-N(3C)	124.0(5)
C(21C)-C(22C)-C(23C)	121.8(5)
C(21C)-C(22C)-H(22C)	119.1
C(23C)-C(22C)-H(22C)	119.1
C(22C)#2-C(23C)-C(22C)	116.8(8)
C(22C)#2-C(23C)-C(26C)	121.6(4)
C(22C)-C(23C)-C(26C)	121.6(4)
C(21C)#2-C(24C)-C(21C)	120.5(8)
C(21C)#2-C(24C)-O(2C)	119.5(4)
C(21C)-C(24C)-O(2C)	119.5(4)
O(2C)-C(25C)-H(25G)	109.5
O(2C)-C(25C)-H(25H)	109.5
H(25G)-C(25C)-H(25H)	109.5
O(2C)-C(25C)-H(25I)	109.5
H(25G)-C(25C)-H(25I)	109.5
H(25H)-C(25C)-H(25I)	109.5
C(23C)-C(26C)-C(28C)	110.6(6)
C(23C)-C(26C)-C(28C)#2	110.6(6)
C(28C)-C(26C)-C(28C)#2	107.3(11)
C(23C)-C(26C)-C(27C)	107.1(11)
C(28C)-C(26C)-C(27C)	110.7(8)
C(28C)#2-C(26C)-C(27C)	110.7(8)
C(26C)-C(27C)-H(27G)	109.5
C(26C)-C(27C)-H(27H)	109.5
H(27G)-C(27C)-H(27H)	109.5
C(26C)-C(27C)-H(27I)	109.5
H(27G)-C(27C)-H(27I)	109.5
H(27H)-C(27C)-H(27I)	109.5
C(26C)-C(28C)-H(28G)	109.5
C(26C)-C(28C)-H(28H)	109.5
H(28G)-C(28C)-H(28H)	109.5
C(26C)-C(28C)-H(28I)	109.5
H(28G)-C(28C)-H(28I)	109.5
H(28H)-C(28C)-H(28I)	109.5
C(4S)-O(1S)-C(1S)	111.2(14)
O(1S)-C(1S)-C(2S)	108.9(14)
O(1S)-C(1S)-H(1SA)	109.9
C(2S)-C(1S)-H(1SA)	109.9
O(1S)-C(1S)-H(1SB)	109.9
C(2S)-C(1S)-H(1SB)	109.9
H(1SA)-C(1S)-H(1SB)	108.3
C(1S)-C(2S)-C(3S)	97.6(15)
C(1S)-C(2S)-H(2SA)	112.2

C(3S)-C(2S)-H(2SA)	112.2
C(1S)-C(2S)-H(2SB)	112.2
C(3S)-C(2S)-H(2SB)	112.2
H(2SA)-C(2S)-H(2SB)	109.8
C(4S)-C(3S)-C(2S)	114.6(15)
C(4S)-C(3S)-H(3SA)	108.6
C(2S)-C(3S)-H(3SA)	108.6
C(4S)-C(3S)-H(3SB)	108.6
C(2S)-C(3S)-H(3SB)	108.6
H(3SA)-C(3S)-H(3SB)	107.6
O(1S)-C(4S)-C(3S)	101.7(14)
O(1S)-C(4S)-H(4SA)	111.4
C(3S)-C(4S)-H(4SA)	111.4
O(1S)-C(4S)-H(4SB)	111.4
C(3S)-C(4S)-H(4SB)	111.4
H(4SA)-C(4S)-H(4SB)	109.3

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,z #2 -x+2,y,z