

**Eisen(III)-Oximat 2b mit der Struktur [Fe<sub>3</sub><sup>III</sup>O(H<sub>2</sub>O)<sub>3</sub>L<sub>6</sub>][HCO<sub>3</sub>]**

Empirical formula	C <sub>25</sub> H <sub>45</sub> Fe <sub>3</sub> N <sub>6</sub> O <sub>26</sub>	
Color	orange	
Formula weight	1013.22 g · mol <sup>-1</sup>	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	TRICLINIC	
Space group	P <sup>-</sup> 1, (no. 2)	
Unit cell dimensions	a = 10.336(3) Å	α = 83.297(5)°.
	b = 13.928(4) Å	β = 77.990(4)°.
	c = 16.287(4) Å	β = 86.457(4)°.
Volume	2276.0(10) Å <sup>3</sup>	
Z	2	
Density (calculated)	1.478 Mg · m <sup>-3</sup>	
Absorption coefficient	1.032 mm <sup>-1</sup>	
F(000)	1046 e	
Crystal size	0.12 x 0.12 x 0.01 mm <sup>3</sup>	
θ range for data collection	1.473 to 26.354°.	
Index ranges -	12 ≤ h ≤ 12, -17 ≤ k ≤ 17, -20 ≤ l ≤ 20	
Reflections collected	42748	
Independent reflections	9247 [Rint = 0.0959]	
Reflections with I > 2σ (I)	5992	
Completeness to θ = 27.500°	88.4 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.99 and 0.91	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	9247 / 0 / 550	
Goodness-of-fit on F <sup>2</sup>	0.973	
Final R indices [I > 2σ (I)]	R <sub>1</sub> = 0.0558   wR <sup>2</sup> = 0.1406	
R indices (all data)	R <sub>1</sub> = 0.0952   wR <sup>2</sup> = 0.1551	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.7 and -0.8 e · Å <sup>-3</sup>	

Atomic parameters						
Atom	Wyck	Site	S.O.F.	x/a	y/b	z/c
Fe1	2i	1		0.33278(6)	0.81841(5)	0.28969(4)
Fe2	2i	1		0.46903(5)	0.60333(5)	0.33907(4)
Fe3	2i	1		0.64848(5)	0.76835(5)	0.21121(4)
O1	2i	1		0.4830(3)	0.7303(2)	0.28184(17)
O2	2i	1		0.2223(3)	0.7185(2)	0.2611(2)
O3	2i	1		0.3272(3)	0.5749(2)	0.2771(2)
O4	2i	1		0.2648(3)	0.7869(2)	0.41574(19)
O5	2i	1		0.3390(3)	0.6352(2)	0.44310(19)
O6	2i	1		0.5988(3)	0.5323(2)	0.25633(19)
O7	2i	1		0.6798(3)	0.6464(2)	0.15268(19)
O8	2i	1		0.6162(3)	0.6206(2)	0.40244(18)
O9	2i	1		0.7510(3)	0.7051(2)	0.2964(2)
O10	2i	1		0.6451(3)	0.8924(2)	0.2644(2)
O11	2i	1		0.4305(3)	0.9249(2)	0.3188(2)
O12	2i	1		0.5722(3)	0.8284(2)	0.11366(19)
O13	2i	1		0.3621(3)	0.8697(2)	0.16672(19)
O14	2i	1		0.1699(3)	0.9109(2)	0.29989(19)
O15	2i	1		0.4456(3)	0.4641(2)	0.40042(19)
O16	2i	1		0.8249(3)	0.8088(2)	0.1400(2)
O17	2i	1		0.0765(4)	0.4676(3)	0.1554(3)
O18	2i	1		0.0511(3)	0.7702(3)	0.6513(2)
O19	2i	1		0.7886(4)	0.3338(3)	0.1101(3)
O20A	2i	1	0.5	0.8872(7)	0.6495(6)	0.5423(5)
O20B	2i	1	0.5	0.9215(7)	0.6085(6)	0.5254(5)
O21	2i	1		0.5431(4)	1.1451(3)	0.4235(3)
O22	2i	1		0.5068(3)	0.9023(3)	-0.1186(2)
O95	2i	1		0.1824(3)	1.1917(3)	0.0198(2)
O97	2i	1		-0.0030(3)	0.9221(3)	0.1952(2)
O98	2i	1		0.0689(3)	1.0666(3)	0.1603(2)
O99	2i	1		-0.0775(4)	1.0167(3)	0.1009(3)
N1	2i	1		0.1613(4)	0.4995(4)	0.2022(3)
N2	2i	1		0.1172(4)	0.7768(3)	0.5684(2)
N3	2i	1		0.7172(4)	0.3981(3)	0.1637(3)
N4A	2i	1	0.5	0.7926(8)	0.6328(7)	0.4972(5)
N4B	2i	1	0.5	0.8148(9)	0.6009(7)	0.4850(6)
N5	2i	1		0.4981(4)	1.0693(3)	0.3892(3)
N6	2i	1		0.5351(4)	0.8771(3)	-0.0393(2)
C1	2i	1		0.2435(4)	0.6318(4)	0.2487(3)
C2	2i	1		0.1573(5)	0.5926(4)	0.1978(3)
C3	2i	1		0.0730(6)	0.6593(5)	0.1516(5)
H3A	2i	1		0.08700	0.64430	0.09300
H3B	2i	1		0.09660	0.72620	0.15260
H3C	2i	1		-0.02020	0.65140	0.17880
C4	2i	1		0.0919(7)	0.3632(5)	0.1577(4)
H4A	2i	1		0.18030	0.34550	0.12670
H4B	2i	1		0.02480	0.33890	0.13160
H4C	2i	1		0.08090	0.33440	0.21650
C5	2i	1		0.2742(4)	0.7113(3)	0.4636(3)
C6	2i	1		0.2013(4)	0.7062(3)	0.5536(3)
C7	2i	1		0.2282(6)	0.6256(5)	0.6156(4)
H7A	2i	1		0.20740	0.56450	0.59800
H7B	2i	1		0.17320	0.63490	0.67110
H7C	2i	1		0.32180	0.62400	0.61910
C8	2i	1		-0.0527(5)	0.8433(4)	0.6615(4)
H8A	2i	1		-0.12150	0.82880	0.63200
H8B	2i	1		-0.01680	0.90640	0.63780
H8C	2i	1		-0.09100	0.84480	0.72170
C9	2i	1		0.6657(4)	0.5608(3)	0.1840(3)
C10	2i	1		0.7360(4)	0.4857(4)	0.1305(3)

C11	2i	1		0.8188(5)	0.5165(4)	0.0472(3)
H11A	2i	1		0.78690	0.48810	0.00320
H11B	2i	1		0.91090	0.49460	0.04670
H11C	2i	1		0.81360	0.58720	0.03650
C12	2i	1		0.7755(8)	0.2374(4)	0.1540(5)
H12A	2i	1		0.82520	0.19080	0.11750
H12B	2i	1		0.68190	0.22160	0.16860
H12C	2i	1		0.81070	0.23460	0.20570
C13	2i	1		0.7204(4)	0.6641(4)	0.3699(3)
C14A	2i	1	0.5	0.8172(10)	0.6827(8)	0.4241(6)
C14B	2i	1	0.5	0.8297(11)	0.6528(9)	0.4186(7)
C15A	2i	1	0.7	0.9257(8)	0.7492(6)	0.3943(5)
H15A	2i	1	0.7	1.00840	0.71210	0.37600
H15B	2i	1	0.7	0.93490	0.78630	0.44020
H15C	2i	1	0.7	0.90650	0.79360	0.34670
C15B	2i	1	0.3	0.9623(18)	0.6910(15)	0.3748(13)
H15D	2i	1	0.3	0.95300	0.73160	0.32280
H15E	2i	1	0.3	1.02490	0.63670	0.36090
H15F	2i	1	0.3	0.99530	0.72960	0.41210
C16A	2i	1	0.5	0.8606(12)	0.5947(9)	0.6247(8)
H16A	2i	1	0.5	0.85330	0.52620	0.61830
H16B	2i	1	0.5	0.77740	0.61900	0.65800
H16C	2i	1	0.5	0.93300	0.60160	0.65380
C16B	2i	1	0.5	0.9008(14)	0.5480(11)	0.6007(9)
H16D	2i	1	0.5	0.90560	0.48050	0.58840
H16E	2i	1	0.5	0.81330	0.56310	0.63430
H16F	2i	1	0.5	0.96900	0.55780	0.63240
C17	2i	1		0.5532(4)	0.9397(3)	0.3073(3)
C18	2i	1		0.5945(5)	1.0213(4)	0.3463(3)
C19	2i	1		0.7370(5)	1.0391(5)	0.3355(5)
H19A	2i	1		0.76060	1.03580	0.39110
H19B	2i	1		0.75540	1.10340	0.30530
H19C	2i	1		0.78940	0.99000	0.30310
C20	2i	1		0.4308(7)	1.1931(5)	0.4701(4)
H20A	2i	1		0.36240	1.20510	0.43620
H20B	2i	1		0.45680	1.25480	0.48400
H20C	2i	1		0.39590	1.15240	0.52240
C21	2i	1		0.4579(4)	0.8607(3)	0.1070(3)
C22	2i	1		0.4316(4)	0.8907(3)	0.0201(3)
C23	2i	1		0.2990(4)	0.9293(4)	0.0092(3)
H23A	2i	1		0.23990	0.87560	0.01420
H23B	2i	1		0.30600	0.96580	-0.04660
H23C	2i	1		0.26300	0.97210	0.05290
C24	2i	1		0.6241(5)	0.8821(4)	-0.1801(3)
H24A	2i	1		0.60460	0.89410	-0.23690
H24B	2i	1		0.65320	0.81430	-0.16970
H24C	2i	1		0.69430	0.92420	-0.17560
C96	2i	1		-0.0047(4)	1.0029(3)	0.1512(3)

#### Anisotropic displacement parameters, in Å<sup>2</sup>

Atom	U <sub>11</sub>	U <sub>22</sub>	U <sub>33</sub>	U <sub>12</sub>	U <sub>13</sub>	U <sub>23</sub>
Fe1	0.0153(3)	0.0256(4)	0.0232(4)	0.0010(2)	-0.0035(2)	-0.0041(3)
Fe2	0.0147(3)	0.0238(4)	0.0225(3)	0.0004(2)	-0.0050(2)	-0.0040(3)
Fe3	0.0154(3)	0.0266(4)	0.0220(3)	-0.0002(2)	-0.0045(2)	-0.0029(3)
O1	0.0153(14)	0.0292(17)	0.0184(16)	-0.0013(12)	-0.0042(11)	-0.0028(13)
O2	0.0218(16)	0.031(2)	0.054(2)	0.0049(14)	-0.0151(15)	-0.0164(17)
O3	0.0237(16)	0.0284(18)	0.0361(19)	-0.0020(13)	-0.0151(14)	-0.0056(15)
O4	0.0317(17)	0.0282(18)	0.0221(17)	0.0005(14)	-0.0013(13)	-0.0017(14)

O5	0.0252(16)	0.0281(18)	0.0287(18)	0.0051(13)	-0.0002(13)	-0.0018(14)
O6	0.0258(16)	0.0265(18)	0.0265(18)	0.0016(13)	-0.0035(13)	-0.0050(14)
O7	0.0245(16)	0.0279(19)	0.0261(17)	0.0022(13)	-0.0033(13)	-0.0050(14)
O8	0.0172(15)	0.0303(18)	0.0256(17)	-0.0021(13)	-0.0055(12)	-0.0032(14)
O9	0.0199(15)	0.044(2)	0.0251(18)	-0.0030(14)	-0.0065(13)	0.0028(15)
O10	0.0240(16)	0.0332(19)	0.040(2)	-0.0078(14)	0.0007(14)	-0.0135(16)
O11	0.0243(16)	0.0283(18)	0.0371(19)	-0.0007(13)	-0.0073(14)	-0.0047(15)
O12	0.0215(15)	0.0355(19)	0.0270(18)	0.0023(13)	-0.0064(13)	0.0024(14)
O13	0.0208(16)	0.042(2)	0.0251(18)	0.0081(14)	-0.0043(13)	-0.0020(15)
O14	0.0247(16)	0.0307(18)	0.0277(18)	0.0069(13)	-0.0031(13)	-0.0057(14)
O15	0.0216(15)	0.0272(18)	0.0311(18)	-0.0022(13)	-0.0061(13)	0.0002(14)
O16	0.0178(15)	0.0348(19)	0.0315(18)	-0.0007(13)	-0.0056(13)	-0.0017(15)
O17	0.059(2)	0.052(3)	0.052(3)	-0.012(2)	-0.025(2)	-0.012(2)
O18	0.0386(19)	0.041(2)	0.0252(19)	0.0033(16)	-0.0010(14)	-0.0105(16)
O19	0.075(3)	0.037(2)	0.050(2)	0.009(2)	-0.010(2)	-0.0211(19)
O21	0.053(2)	0.050(3)	0.073(3)	0.0050(19)	-0.027(2)	-0.037(2)
O22	0.0344(18)	0.046(2)	0.0276(19)	0.0037(15)	-0.0116(14)	-0.0025(16)
O95	0.0354(18)	0.040(2)	0.0279(19)	0.0003(15)	-0.0040(14)	-0.0055(16)
O97	0.0273(18)	0.039(2)	0.063(3)	-0.0053(16)	-0.0116(17)	0.005(2)
O98	0.0350(19)	0.040(2)	0.038(2)	-0.0056(16)	-0.0085(15)	-0.0015(17)
O99	0.060(3)	0.058(3)	0.078(3)	0.006(2)	-0.049(2)	-0.009(2)
N1	0.045(3)	0.050(3)	0.035(3)	-0.015(2)	-0.015(2)	-0.015(2)
N2	0.027(2)	0.038(2)	0.026(2)	-0.0021(17)	-0.0002(16)	-0.0122(18)
N3	0.049(3)	0.037(3)	0.039(3)	0.011(2)	-0.014(2)	-0.022(2)
N5	0.059(3)	0.031(2)	0.037(3)	0.001(2)	-0.022(2)	-0.014(2)
N6	0.039(2)	0.032(2)	0.025(2)	-0.0025(18)	-0.0119(18)	0.0005(18)
C1	0.021(2)	0.036(3)	0.030(3)	0.000(2)	-0.0081(19)	-0.005(2)
C2	0.032(3)	0.037(3)	0.039(3)	0.006(2)	-0.021(2)	-0.013(2)
C3	0.066(4)	0.051(4)	0.092(5)	0.015(3)	-0.057(4)	-0.026(4)
C4	0.095(5)	0.047(4)	0.050(4)	-0.022(4)	-0.022(4)	-0.012(3)
C5	0.017(2)	0.031(3)	0.023(2)	-0.0045(18)	-0.0066(17)	-0.005(2)
C6	0.018(2)	0.034(3)	0.027(3)	-0.0030(19)	-0.0044(18)	-0.004(2)
C7	0.057(4)	0.057(4)	0.038(3)	0.022(3)	0.005(3)	0.011(3)
C8	0.047(3)	0.053(4)	0.043(3)	0.018(3)	0.002(3)	-0.018(3)
C9	0.017(2)	0.032(3)	0.026(3)	0.0021(18)	-0.0076(18)	-0.003(2)
C10	0.026(2)	0.033(3)	0.026(3)	0.006(2)	-0.0063(19)	-0.010(2)
C11	0.040(3)	0.052(4)	0.039(3)	0.007(3)	-0.004(2)	-0.017(3)
C12	0.104(6)	0.032(3)	0.074(5)	0.007(3)	-0.029(4)	-0.020(3)
C13	0.016(2)	0.034(3)	0.029(3)	0.0002(19)	-0.0065(18)	-0.005(2)
C17	0.026(2)	0.026(3)	0.029(3)	-0.0013(19)	-0.0072(19)	-0.001(2)
C18	0.031(3)	0.026(3)	0.045(3)	-0.002(2)	-0.014(2)	-0.011(2)
C19	0.034(3)	0.048(4)	0.116(6)	-0.007(3)	-0.019(3)	-0.035(4)
C20	0.073(4)	0.051(4)	0.067(5)	0.003(3)	-0.010(3)	-0.032(4)
C21	0.018(2)	0.021(2)	0.026(2)	-0.0004(17)	-0.0086(18)	-0.0012(19)
C22	0.024(2)	0.024(2)	0.027(3)	0.0018(18)	-0.0104(19)	-0.006(2)
C23	0.027(2)	0.041(3)	0.041(3)	0.003(2)	-0.013(2)	-0.005(2)
C24	0.034(3)	0.052(3)	0.025(3)	0.004(2)	-0.001(2)	-0.010(2)
C96	0.0106(19)	0.020(2)	0.030(3)	-0.0023(16)	-0.0080(17)	-0.0090(19)

## Bond length [Å] und angles [°]

Fe(1)-O(1)	1.909(3)	Fe(1)-O(11)	1.998(3)	Fe(1)-O(2)	2.005(3)
Fe(1)-O(13)	2.014(3)	Fe(1)-O(4)	2.031(3)	Fe(1)-O(14)	2.039(3)
Fe(2)-O(1)	1.901(3)	Fe(2)-O(6)	1.998(3)	Fe(2)-O(5)	2.003(3)
Fe(2)-O(3)	2.025(3)	Fe(2)-O(8)	2.048(3)	Fe(2)-O(15)	2.068(3)
Fe(3)-O(1)	1.918(3)	Fe(3)-O(12)	1.995(3)	Fe(3)-O(9)	2.007(3)
Fe(3)-O(16)	2.011(3)	Fe(3)-O(10)	2.012(3)	Fe(3)-O(7)	2.019(3)

Na(1)-O(98)	2.799(5)	Na(1)-O(12)	2.996(5)	O(2)-C(1)	1.246(6)
O(3)-C(1)	1.263(5)	O(4)-C(5)	1.247(5)	O(5)-C(5)	1.259(5)
O(6)-C(9)	1.262(6)	O(7)-C(9)	1.246(6)	O(8)-C(13)	1.258(5)
O(9)-C(13)	1.252(6)	O(10)-C(17)	1.257(6)	O(11)-C(17)	1.268(5)
O(12)-C(21)	1.258(5)	O(13)-C(21)	1.251(5)	O(17)-N(1)	1.400(6)
O(17)-C(4)	1.450(8)	O(18)-N(2)	1.377(5)	O(18)-C(8)	1.439(6)
O(19)-N(3)	1.388(6)	O(19)-C(12)	1.434(8)	O(20A)-N(4A)	1.385(11)
O(20A)-C(16A)	1.468(15)	O(20B)-N(4B)	1.406(12)	O(20B)-C(16B)	1.408(16)
O(21)-N(5)	1.395(6)	O(21)-C(20)	1.430(7)	O(22)-N(6)	1.381(5)
O(22)-C(24)	1.446(6)	O(97)-C(96)	1.256(6)	O(98)-C(96)	1.246(5)
O(99)-C(96)	1.216(6)	N(1)-C(2)	1.285(7)	N(2)-C(6)	1.282(6)
N(3)-C(10)	1.280(7)	N(4A)-C(14A)	1.291(13)	N(4B)-C(14B)	1.202(15)
N(5)-C(18)	1.283(7)	N(6)-C(22)	1.300(6)	C(1)-C(2)	1.498(7)
C(2)-C(3)	1.482(7)	C(5)-C(6)	1.507(6)	C(6)-C(7)	1.469(7)
C(9)-C(10)	1.506(6)	C(10)-C(11)	1.475(7)	C(13)-C(14B)	1.506(13)
C(13)-C(14A)	1.513(11)	C(14A)-C(15A)	1.470(13)	C(14B)-C(15B)	1.51(2)
C(17)-C(18)	1.495(7)	C(18)-C(19)	1.488(7)	C(21)-C(22)	1.507(6)
C(22)-C(23)	1.477(6)				
O(1)-Fe(1)-O(11)	93.06(13)	O(1)-Fe(1)-O(2)	91.36(13)		
O(11)-Fe(1)-O(2)	175.58(13)	O(1)-Fe(1)-O(13)	97.28(13)		
O(11)-Fe(1)-O(13)	93.09(14)	O(2)-Fe(1)-O(13)	86.41(15)		
O(1)-Fe(1)-O(4)	96.09(13)	O(11)-Fe(1)-O(4)	86.89(14)		
O(2)-Fe(1)-O(4)	92.58(15)	O(13)-Fe(1)-O(4)	166.61(13)		
O(1)-Fe(1)-O(14)	179.06(14)	O(11)-Fe(1)-O(14)	87.58(14)		
O(2)-Fe(1)-O(14)	88.00(14)	O(13)-Fe(1)-O(14)	83.37(13)		
O(4)-Fe(1)-O(14)	83.25(13)	O(1)-Fe(2)-O(6)	99.70(13)		
O(1)-Fe(2)-O(5)	97.78(13)	O(6)-Fe(2)-O(5)	162.39(14)		
O(1)-Fe(2)-O(3)	90.80(13)	O(6)-Fe(2)-O(3)	87.86(13)		
O(5)-Fe(2)-O(3)	94.00(14)	O(1)-Fe(2)-O(8)	93.33(13)		
O(6)-Fe(2)-O(8)	89.47(13)	O(5)-Fe(2)-O(8)	87.43(13)		
O(3)-Fe(2)-O(8)	175.41(13)	O(1)-Fe(2)-O(15)	177.32(12)		
O(6)-Fe(2)-O(15)	81.43(13)	O(5)-Fe(2)-O(15)	81.19(13)		
O(3)-Fe(2)-O(15)	86.82(13)	O(8)-Fe(2)-O(15)	89.10(13)		
O(1)-Fe(3)-O(12)	96.05(13)	O(1)-Fe(3)-O(9)	92.08(13)		
O(12)-Fe(3)-O(9)	171.07(13)	O(1)-Fe(3)-O(16)	178.07(14)		
O(12)-Fe(3)-O(16)	85.46(13)	O(9)-Fe(3)-O(16)	86.50(13)		
O(1)-Fe(3)-O(10)	92.59(13)	O(12)-Fe(3)-O(10)	95.17(15)		
O(9)-Fe(3)-O(10)	88.12(15)	O(16)-Fe(3)-O(10)	86.06(14)		
O(1)-Fe(3)-O(7)	94.92(13)	O(12)-Fe(3)-O(7)	87.01(14)		
O(9)-Fe(3)-O(7)	88.63(14)	O(16)-Fe(3)-O(7)	86.36(13)		
O(10)-Fe(3)-O(7)	171.92(13)	O(98)-Na(1)-O(12)	131.79(16)		
Fe(2)-O(1)-Fe(1)	120.91(15)	Fe(2)-O(1)-Fe(3)	119.28(15)		
Fe(1)-O(1)-Fe(3)	119.74(16)	C(1)-O(2)-Fe(1)	133.4(3)		
C(1)-O(3)-Fe(2)	129.3(3)	C(5)-O(4)-Fe(1)	131.1(3)		

C(5)-O(5)-Fe(2)	133.1(3)	C(9)-O(6)-Fe(2)	130.8(3)
C(9)-O(7)-Fe(3)	128.7(3)	C(13)-O(8)-Fe(2)	123.7(3)
C(13)-O(9)-Fe(3)	134.6(3)	C(17)-O(10)-Fe(3)	132.3(3)
C(17)-O(11)-Fe(1)	131.7(3)	C(21)-O(12)-Fe(3)	132.7(3)
C(21)-O(12)-Na(1)	130.1(3)	Fe(3)-O(12)-Na(1)	97.06(13)
C(21)-O(13)-Fe(1)	131.6(3)	N(1)-O(17)-C(4)	108.9(4)
N(2)-O(18)-C(8)	109.8(4)	N(3)-O(19)-C(12)	108.1(5)
N(4A)-O(20A)-C(16A)	110.3(8)	N(4B)-O(20B)-C(16B)	108.6(9)
N(5)-O(21)-C(20)	107.9(4)	N(6)-O(22)-C(24)	108.0(3)
C(96)-O(98)-Na(1)	119.6(3)	C(2)-N(1)-O(17)	111.3(4)
C(6)-N(2)-O(18)	111.8(4)	C(10)-N(3)-O(19)	110.4(4)
C(14A)-N(4A)-O(20A)	109.3(8)	C(14B)-N(4B)-O(20B)	110.6(10)
C(18)-N(5)-O(21)	112.0(4)	C(22)-N(6)-O(22)	111.3(4)
O(2)-C(1)-O(3)	125.7(4)	O(2)-C(1)-C(2)	116.2(4)
O(3)-C(1)-C(2)	118.1(5)	N(1)-C(2)-C(3)	125.6(5)
N(1)-C(2)-C(1)	114.0(4)	C(3)-C(2)-C(1)	120.3(5)
O(4)-C(5)-O(5)	126.0(4)	O(4)-C(5)-C(6)	119.1(4)
O(5)-C(5)-C(6)	114.9(4)	N(2)-C(6)-C(7)	126.3(5)
N(2)-C(6)-C(5)	113.0(4)	C(7)-C(6)-C(5)	120.7(4)
O(7)-C(9)-O(6)	126.6(4)	O(7)-C(9)-C(10)	115.6(4)
O(6)-C(9)-C(10)	117.8(4)	N(3)-C(10)-C(11)	126.5(5)
N(3)-C(10)-C(9)	114.5(4)	C(11)-C(10)-C(9)	119.0(5)
O(9)-C(13)-O(8)	127.2(4)	O(9)-C(13)-C(14B)	115.6(6)
O(8)-C(13)-C(14B)	116.4(6)	O(9)-C(13)-C(14A)	112.3(5)
O(8)-C(13)-C(14A)	120.1(5)	C(14B)-C(13)-C(14A)	17.1(6)
N(4A)-C(14A)-C(15A)	125.5(9)	N(4A)-C(14A)-C(13)	111.9(8)
C(15A)-C(14A)-C(13)	122.6(8)	N(4B)-C(14B)-C(13)	119.8(10)
N(4B)-C(14B)-C(15B)	122.2(13)	C(13)-C(14B)-C(15B)	117.3(11)
O(10)-C(17)-O(11)	126.2(5)	O(10)-C(17)-C(18)	116.1(4)
O(11)-C(17)-C(18)	117.8(4)	N(5)-C(18)-C(19)	125.8(5)
N(5)-C(18)-C(17)	114.9(4)	C(19)-C(18)-C(17)	119.3(5)
O(13)-C(21)-O(12)	126.0(4)	O(13)-C(21)-C(22)	115.7(4)
O(12)-C(21)-C(22)	118.2(4)	N(6)-C(22)-C(23)	127.0(4)
N(6)-C(22)-C(21)	112.5(4)	C(23)-C(22)-C(21)	120.5(4)
O(99)-C(96)-O(98)	121.5(5)	O(99)-C(96)-O(97)	119.5(4)
O(98)-C(96)-O(97)	119.0(4)		

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