Electronic supplementary information (ESI)

Figs. 1-2

IR Spectra of $(GunH)_2(Hpzdc).H_2O$ **(2)** and $(AgunH)_2(Hpzdc).H_2O$ **(4)**

Figs. 3-4

IR Spectra of $(DagunH)(H_2pzdc).H_2O$ **(6)** and $(TagunH)(H_2pzdc)(H_3pzdc)$ **(9)**

Fig. 5-9

PXRD Patterns of compounds **3, 5, 6,** 7 & **8**

Fig. 10-11

Simultaneous TG/DTA of free acid (H_3pzdc) and $(AgunH)(H_2pzdc).H_2O$ **(3)**

Fig. 12-13

Simultaneous TG/DTA of $(AgunH)(H_2pdc)(H_3pzdc)$ **(5)** and $(DagunH)(H_2pzdc).H_2O$ **(6)**

Fig. 14-15

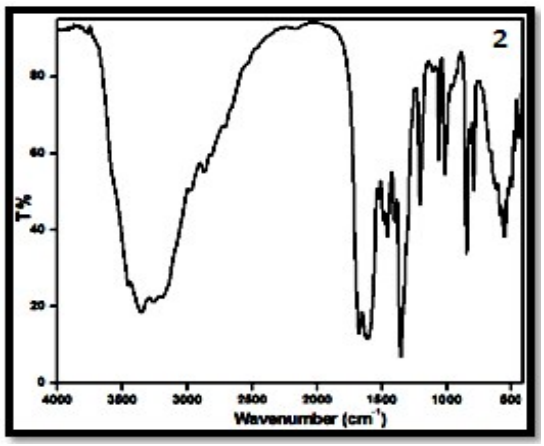
Simultaneous TG/DTA of $(DagunH)_2(Hpzdc).H_2O$ **(7)** and $(DagunH)(H_2pzdc)(H_3pzdc)$ **(8)**

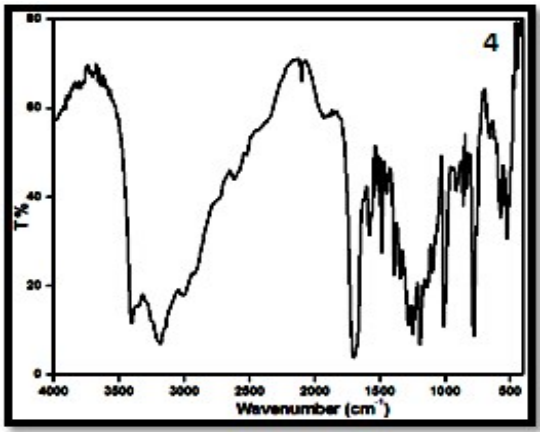
Table 1

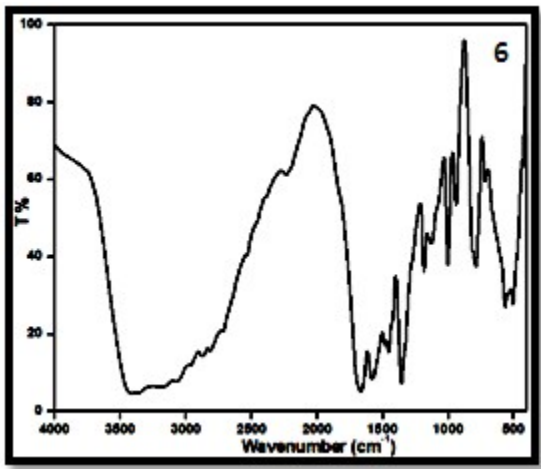
Selected bond lengths (Å) for the compounds **1, 2, 4** & **9**

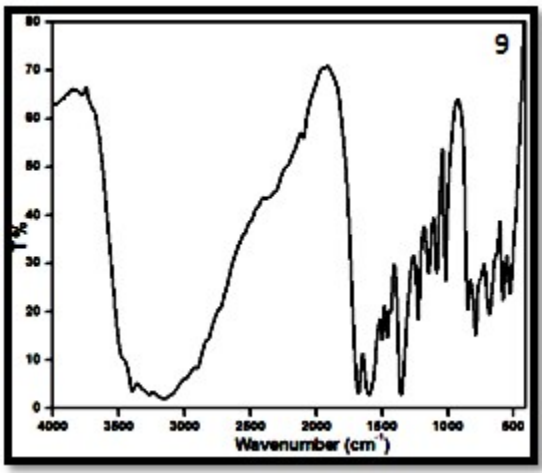
Table 2

Selected bond angles (°) for the compounds **1, 2, 4** & **9**

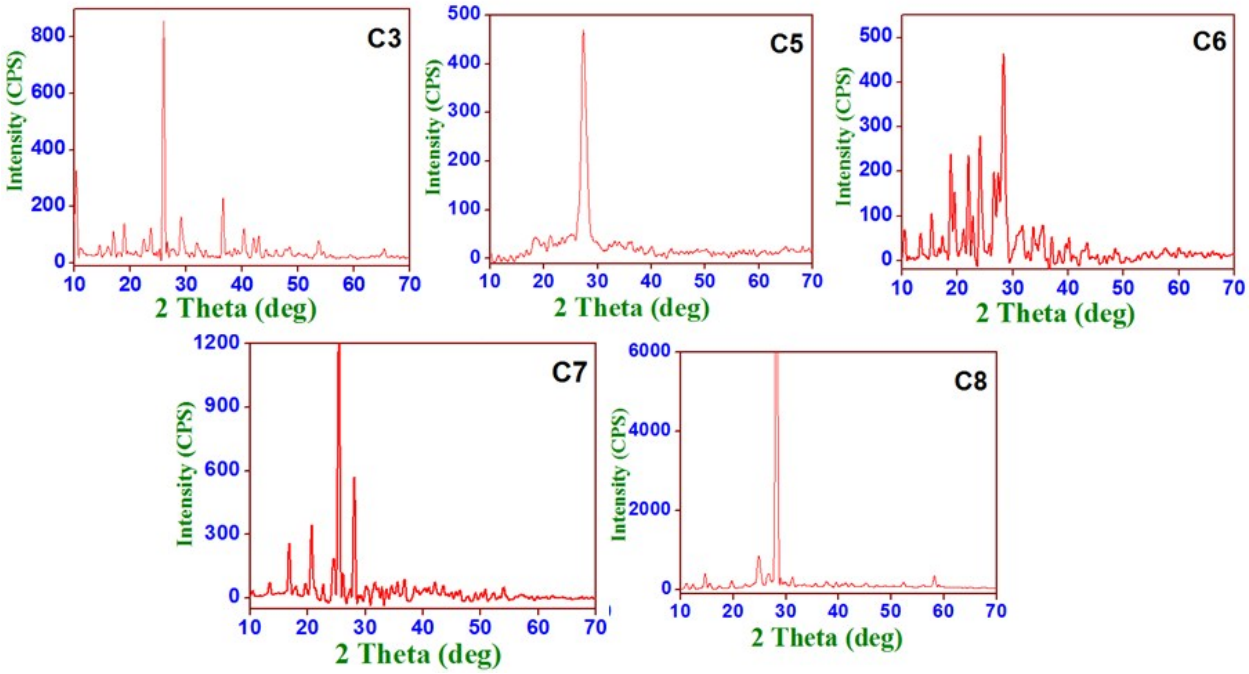

2
T%
Wavenumber (cm-1)


4
T%
Wavenumber (cm-1)

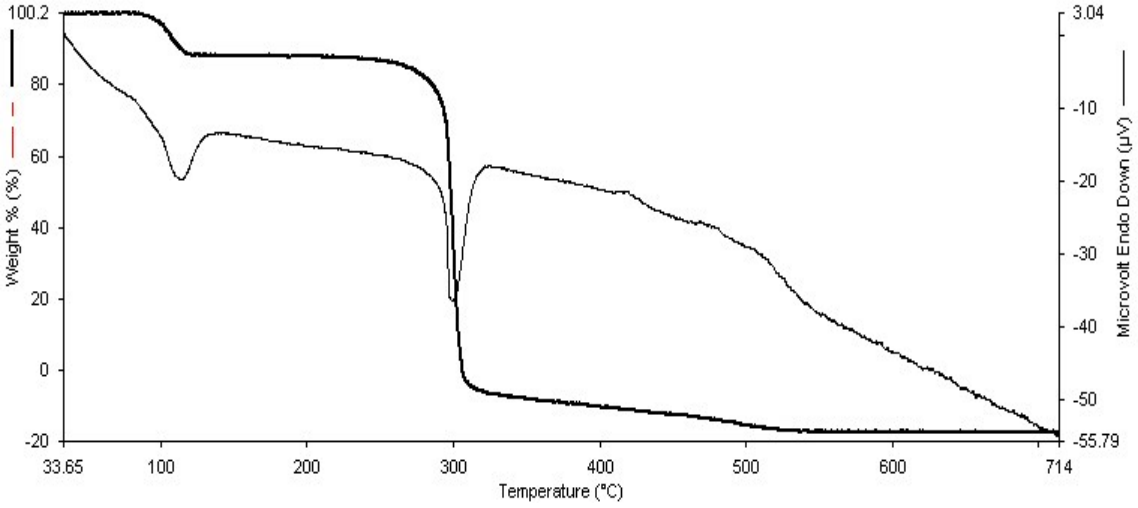

6
T%
Wavenumber (cm-1)

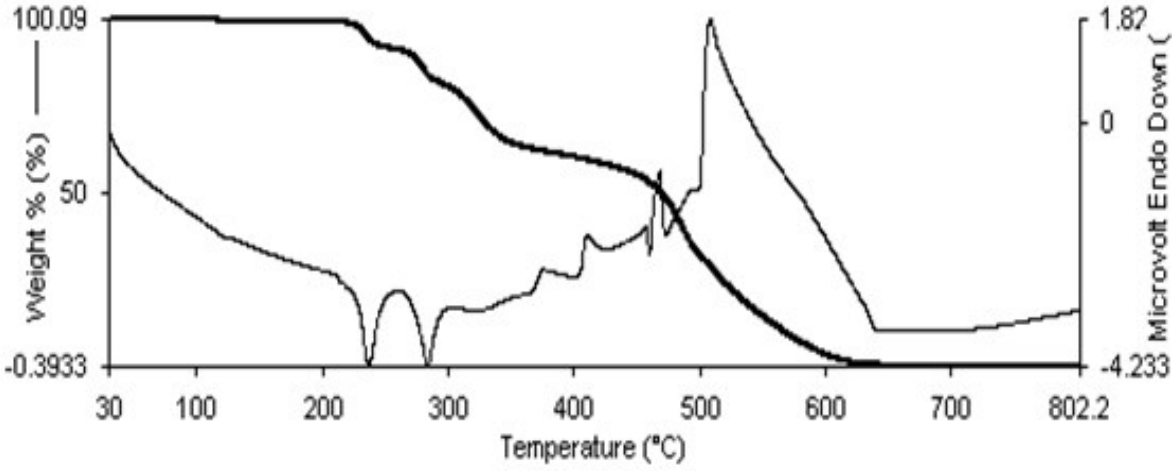

9
T%
Wavenumber (cm-1)

Figs. 1-4

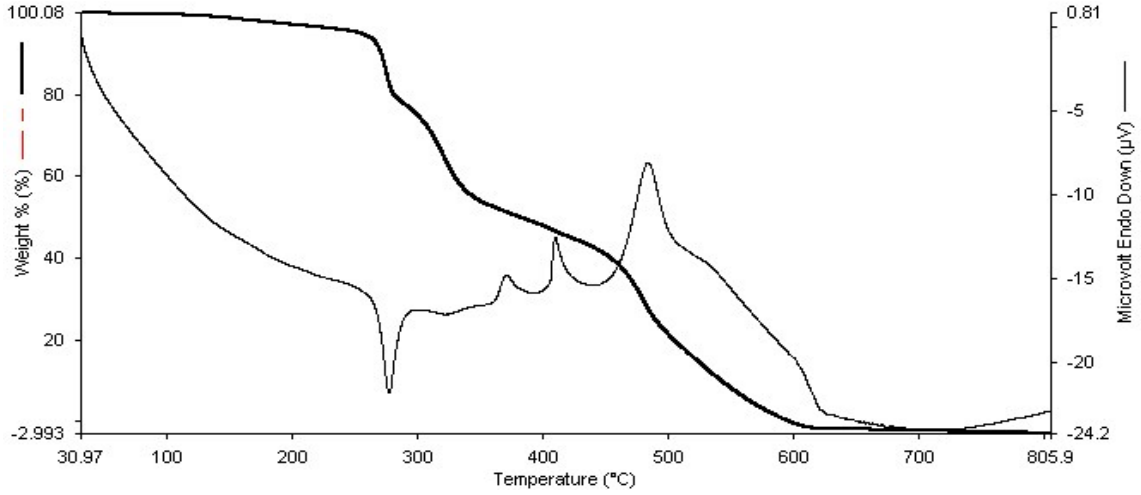


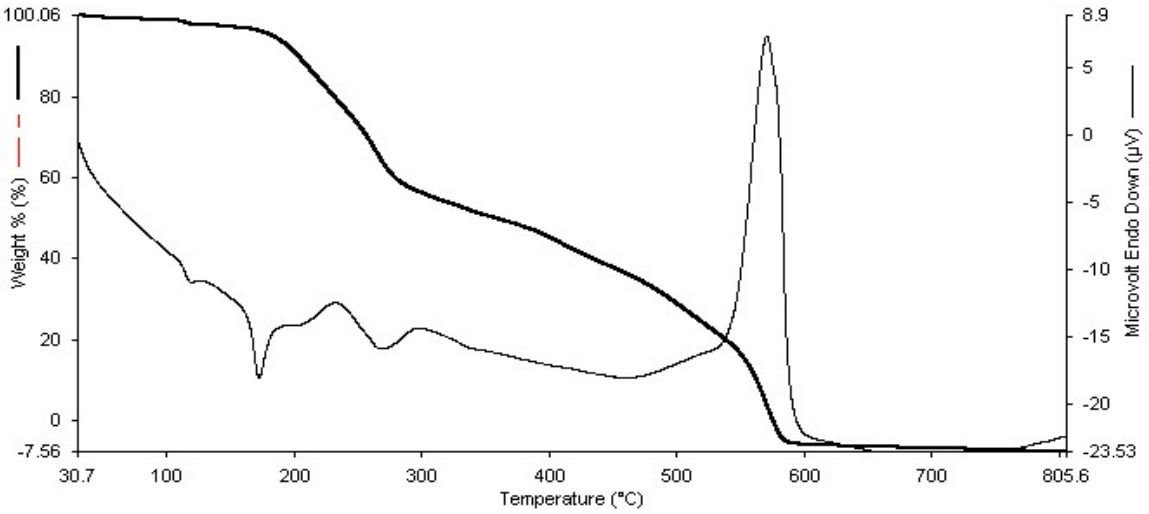
Figs. 5-9


100.2
80
60
40
20
0
-20
Weight % (%)
3.04
-10
-20
-30
-40
-50
-55.79
Microvolt Endo Down (µV)
33.65
100
200
300
400
500
600
714
Temperature (°C)

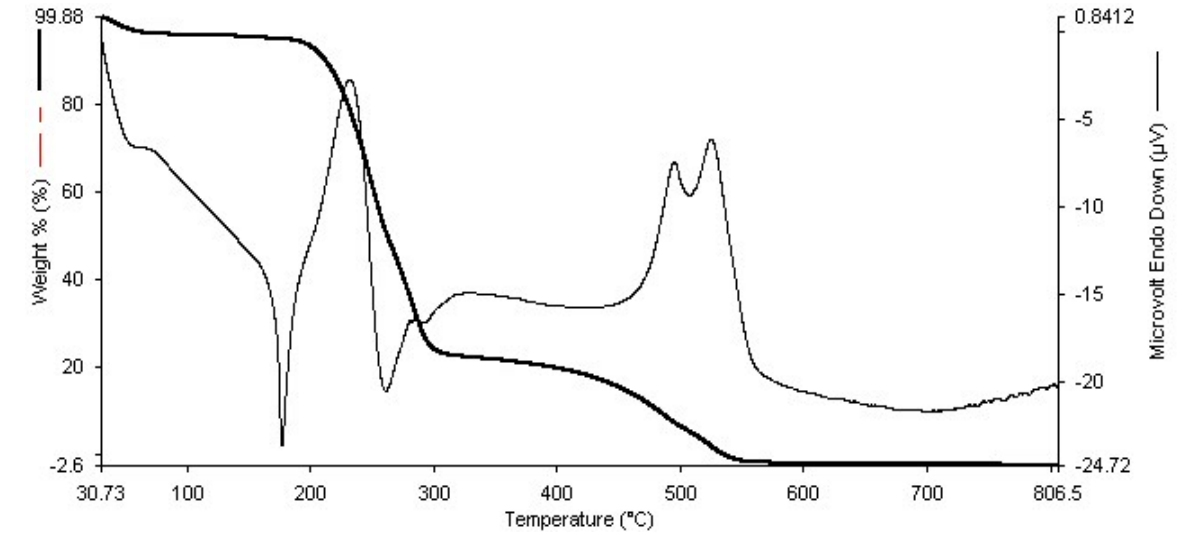

100.09
50
-0.3933
Weight % (%)
1.82
0
-4.233
Microvolt Endo Down (
30
100
200
300
400
500
600
700
802.2
Temperature (°C)

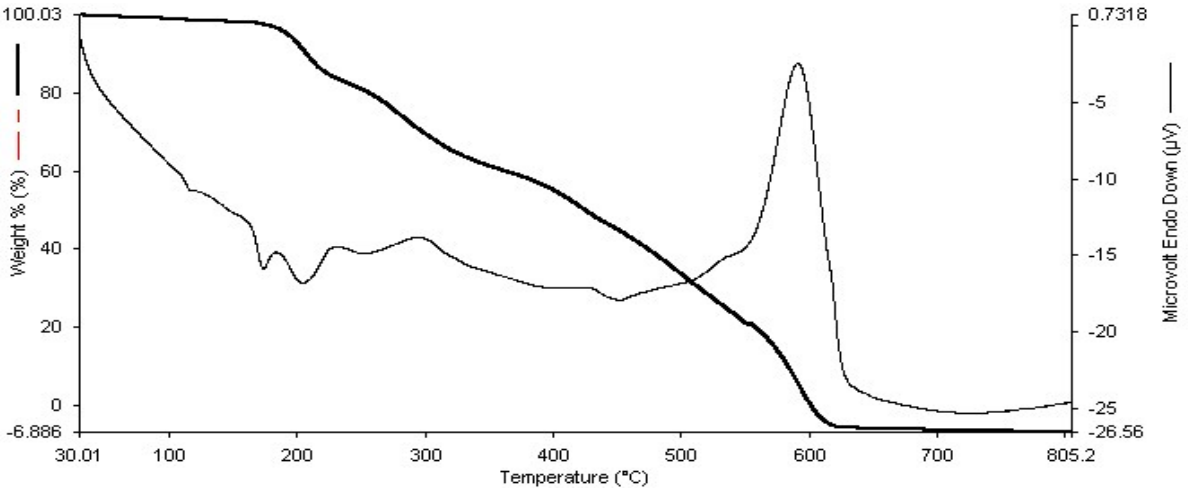
Figs. 10-11


100.08
80
60
40
20
-2.993
Weight % (%)
0.81
-5
-10
-15
-20
-24.2
Microvolt Endo Down (µV)
30.97
100
200
300
400
500
600
700
805.9
Temperature (°C)


100.06
80
60
40
20
0
-7.56
Weight % (%)
8.9
5
0
-5
-10
-15
-20
-23.53
Microvolt Endo Down (µV)
30.7
100
200
300
400
500
600
700
805.6
Temperature (°C)

Figs. 12-13


99.88
80
60
40
20
-2.6
Weight % (%)
0.8412
-5
-10
-15
-20
-24.72
Microvolt Endo Down (µV)
30.73
100
200
300
400
500
600
700
806.5
Temperature (°C)


100.03
80
60
40
20
0
-6.886
Weight % (%)
0.7318
-5
-10
-15
-20
-25
-26.56
Microvolt Endo Down (µV)
30.01
100
200
300
400
500
600
700
805.2
Temperature (°C)

Figs. 14-15

Table 1 Selected bond lengths (Å) for the compounds 1, 2, 4 & 9

O1	C1	1.2984(14)	N5	C6	1.3220(15)		C2	N2	1.3382(14)	N1	N2	1.3346(12)
O2	C5	1.2663(14)	N3	C6	1.3154(15)	**1**	C3	C4	1.3763(15)	C6	N4	1.3279(15)
O3	C1	1.2150(14)	C1	C2	1.4819(14)		C4	C5	1.4856(14)			
O4	C5	1.2481(13)	C2	C3	1.3967(14)		C4	N1	1.3497(13)			
C1	C2	1.497(7)	C3	C4	1.397(7)		C7	N3	1.324(7)	C8	N8	1.334(7)
C1	O1	1.256(6)	C4	C5	1.491(7)		C7	N4	1.316(6)	N1	N2	1.334(6)
C1	O3	1.261(5)	C4	N1	1.338(6)	**2**	C7	N5	1.319(7)			
C2	C3	1.369(6)	C5	O2	1.244(6)		C8	N6	1.325(7)			
C2	N2	1.330(6)	C5	O4	1.270(6)		C8	N7	1.319(7)			
O1	C1	1.2558(13)	N2	C4	1.3546(13)		C4	C5	1.4809(14)	N21	C21	1.3215(14)
N1	N2	1.3427(12)	C2	C3	1.4026(14)		N11	C11	1.3270(14)	C21	N22	1.3362(14)
N1	C2	1.3452(13)	O3	C5	1.2646(13)	**4**	C11	N12	1.3377(15)	C21	N23	1.3299(14)
C1	O2	1.2569(13)	C3	C4	1.3811(14)		C11	N13	1.3235(14)	N23	N24	1.4074(13)
C1	C2	1.4961(14)	O4	C5	1.2555(13)		N13	N14	1.4158(14)			
O2	C1	1.2429(16)	N9	N10	1.4141(18)		C2	N1	1.3555(17)	C10	C9	1.4757(17)
O3	C5	1.2412(18)	O8	C10	1.2912(16)		N6	N5	1.3988(19)	C9	C8	1.3738(18)
O4	C5	1.2835(16)	O5	C6	1.2842(17)		N6	C11	1.326(2)	C9	N4	1.3503(17)
O1	C1	1.2672(16)	O6	C6	1.2394(18)	**9**	C3	C4	1.3952(18)	C8	C7	1.3965(18)
N8	N7	1.4124(19)	O7	C10	1.2234(16)		C4	C5	1.4679(18)	C7	C6	1.4644(18)
N7	C11	1.326(2)	C1	C2	1.4807(17)		C4	N2	1.3347(18)	C7	N3	1.3352(17)
N9	C11	1.3264(19)	C2	C3	1.3759(18)		N2	N1	1.3301(15)	N3	N4	1.3265(15)

Table 2 Selected bond angles (°) for the compounds 1, 2, 4 & 9

O1	C1	C2	113.03(9)	C4	C3	C2	104.86(9)		O4	C5	C4	116.84(10)
O3	C1	O1	125.01(10)	C3	C4	C5	133.09(10)		N2	N1	C4	113.01(9)
O3	C1	C2	121.95(10)	N1	C4	C3	106.27(9)		N1	N2	C2	104.50(8)
C3	C2	C1	127.56(10)	N1	C4	C5	120.58(9)	**1**	N5	C6	N4	120.81(11)
N2	C2	C1	121.07(9)	O2	C5	C4	117.15(9)		N3	C6	N5	120.72(11)
N2	C2	C3	111.35(9)	O4	C5	O2	126.00(10)		N3	C6	N4	118.47(11)
O1	C1	C2	117.7(4)	C3	C4	C5	127.9(4)		N4	C7	N3	119.9(5)
O1	C1	O3	125.3(4)	N1	C4	C3	110.6(4)		N4	C7	N5	120.7(5)
O3	C1	C2	117.0(4)	N1	C4	C5	121.5(4)		N7	C8	N6	119.4(5)
C3	C2	C1	131.7(4)	O2	C5	C4	117.1(4)	**2**	N7	C8	N8	120.3(5)
N2	C2	C1	121.5(4)	O4	C5	C4	118.0(4)		N8	C8	N6	120.3(5)
N2	C2	C3	106.7(4)	O4	C5	O2	124.9(4)		N2	N1	C4	104.6(4)
C2	C3	C4	105.0(4)	N3	C7	N5	119.4(5)		N1	N2	C2	113.1(4)
N2	N1	C2	104.56(8)	C4	C3	C2	104.77(9)		N13	C11	N11	121.24(11)
O1	C1	O2	124.89(10)	N2	C4	C3	106.58(9)		N13	C11	N12	119.49(10)
O1	C1	C2	116.91(9)	N2	C4	C5	121.64(9)		C11	N13	N14	117.61(9)
O2	C1	C2	118.19(9)	C3	C4	C5	131.75(10)	**4**	N21	C21	N22	120.18(10)
N1	N2	C4	112.74(9)	O3	C5	C4	117.08(9)		N21	C21	N23	121.86(10)
N1	C2	C1	121.02(9)	O4	C5	O3	124.86(10)		N23	C21	N22	117.95(10)
N1	C2	C3	111.35(9)	O4	C5	C4	118.03(9)		C21	N23	N24	119.98(9)
C3	C2	C1	127.63(9)	N11	C11	N12	119.27(11)					
C11	N7	N8	118.39(14)	N2	C4	C5	120.18(12)		C8	C9	C10	132.72(12)
C11	N9	N10	119.51(13)	O3	C5	O4	124.63(13)		N4	C9	C10	120.61(11)
O2	C1	O1	125.45(12)	O3	C5	C4	119.24(12)		N4	C9	C8	106.67(11)
O2	C1	C2	118.75(12)	O4	C5	C4	116.13(12)		C9	C8	C7	104.17(11)
O1	C1	C2	115.80(11)	N1	N2	C4	104.41(11)		C8	C7	C6	127.92(13)
C3	C2	C1	132.14(12)	N2	N1	C2	112.92(11)	**9**	N3	C7	C8	111.81(11)
N1	C2	C1	121.54(11)	N7	C11	N9	120.05(14)		N3	C7	C6	120.25(12)
N1	C2	C3	106.31(11)	N6	C11	N7	119.60(13)		O5	C6	C7	116.21(13)
C11	N6	N5	124.11(12)	N6	C11	N9	120.32(13)		O6	C6	O5	124.32(13)
C2	C3	C4	104.47(11)	O8	C10	C9	114.11(11)		O6	C6	C7	119.47(13)
C3	C4	C5	127.94(12)	O7	C10	O8	124.79(12)		N4	N3	C7	104.45(11)
N2	C4	C3	111.89(11)	O7	C10	C9	121.10(12)		N3	N4	C9	112.90(11)