Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for Zn IDS Hydrate.

Atom	x	y	z	U(eq)
Zn(1)	249(1)	6323(1)	2237(1)	23(1)
Zn(2)	1074(1)	1234(1)	1963(1)	22(1)
O(1)	-1118(2)	-2204(2)	2085(1)	28(1)
O(2)	596(2)	-741(2)	2260(2)	33(1)
O(3)	-1795(2)	-823(2)	-607(1)	29(1)
O(4)	-4058(2)	-1265(2)	-1074(2)	37(1)
O(5)	-1005(2)	4784(2)	1778(1)	28(1)
O(6)	594(2)	3179(2)	2299(1)	30(1)
O(7)	-2119(2)	3724(2)	-1822(1)	28(1)
O(8)	-345(2)	3197(2)	-416(2)	35(1)
OW	-3945(7)	-3856(6)	497(6)	113(3)
N(1)	-1073(2)	1221(2)	1147(2)	19(1)
C(1)	-662(2)	-1032(2)	1999(2)	22(1)
C(2)	-1726(2)	89(2)	1598(2)	19(1)
C(3)	-3064(2)	-413(2)	778(2)	23(1)
C(4)	-2952(2)	-871(2)	-396(2)	22(1)
C(5)	-598(2)	3575(2)	1791(2)	22(1)
C(6)	-1708(2)	2555(2)	1185(2)	21(1)
C(7)	-2525(2)	3073(2)	0(2)	26(1)
C(8)	-1606(2)	3341(2)	-771(2)	24(1)

(U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor)

Bond lengths [Å] and angles [°] for Zinc IDS Hydrate:

Zn(1)-O(5)	1.9604(16)
Zn(1)-O(4)#1	1.9677(18)
Zn(1)-O(1)#2	1.9794(15)
Zn(1)-O(7)#3	2.0751(18)
Zn(1)-O(8)#3	2.2731(17)
Zn(1)-C(8)#3	2.530(2)
Zn(2)-O(3)#4	2.0006(16)
Zn(2)-O(7)#1	2.0066(16)
Zn(2)-O(6)	2.0506(17)
Zn(2)-O(2)	2.0667(17)
Zn(2)-N(1)	2.1213(18)
O(1)-C(1)	1.262(3)
O(1)-Zn(1)#5	1.9794(15)
O(2)-C(1)	1.254(3)
O(3)-C(4)	1.259(3)
O(3)-Zn(2)#4	2.0006(16)
O(4)-C(4)	1.253(3)
O(4)-Zn(1)#6	1.9677(18)
O(5)-C(5)	1.263(3)
O(6)-C(5)	1.254(3)
O(7)-C(8)	1.289(3)
O(7)-Zn(2)#6	2.0066(16)
O(7)-Zn(1)#3	2.0751(17)
O(8)-C(8)	1.234(3)
O(8)-Zn(1)#3	2.2731(17)
OW-HW1	0.817(15)
OW-HW2	0.800(15)
N(1)-C(6)	1.472(3)
N(1)-C(2)	1.475(3)
N(1)-H(1N1)	0.84(3)
C(1)-C(2)	1.527(3)
C(2)-C(3)	1.523(3)
C(2)-H(2)	0.9800
C(3)-C(4)	1.519(3)

C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(5)-C(6)	1.537(3)
C(6)-C(7)	1.533(3)
C(6)-H(6)	0.9800
C(7)-C(8)	1.501(3)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(8)-Zn(1)#3	2.530(2)

O(5)-Zn(1)-O(4)#1	106.93(8)
O(5)-Zn(1)-O(1)#2	99.60(7)
O(4)#1-Zn(1)-O(1)#2	99.31(7)
O(5)-Zn(1)-O(7)#3	118.16(7)
O(4)#1-Zn(1)-O(7)#3	98.99(7)
O(1)#2-Zn(1)-O(7)#3	130.40(6)
O(5)-Zn(1)-O(8)#3	94.68(7)
O(4)#1-Zn(1)-O(8)#3	155.48(7)
O(1)#2-Zn(1)-O(8)#3	88.06(7)
O(7)#3-Zn(1)-O(8)#3	59.64(6)
O(5)-Zn(1)-C(8)#3	109.48(7)
O(4)#1-Zn(1)-C(8)#3	128.20(8)
O(1)#2-Zn(1)-C(8)#3	109.36(7)
O(7)#3-Zn(1)-C(8)#3	30.53(7)
O(8)#3-Zn(1)-C(8)#3	29.16(6)
O(3)#4-Zn(2)-O(7)#1	98.23(7)
O(3)#4-Zn(2)-O(6)	120.57(7)
O(7)#1-Zn(2)-O(6)	93.01(6)
O(3)#4-Zn(2)-O(2)	95.86(7)
O(7)#1-Zn(2)-O(2)	95.80(6)
O(6)-Zn(2)-O(2)	140.77(7)
O(3)#4-Zn(2)-N(1)	99.74(7)
O(7)#1-Zn(2)-N(1)	161.80(7)
O(6)-Zn(2)-N(1)	80.31(6)
O(2)-Zn(2)-N(1)	79.55(6)
C(1)-O(1)-Zn(1)#5	115.16(14)

C(1)-O(2)-Zn(2)	116.11(14)
C(4)-O(3)-Zn(2)#4	135.76(15)
C(4)-O(4)-Zn(1)#6	133.59(16)
C(5)-O(5)-Zn(1)	123.35(15)
C(5)-O(6)-Zn(2)	116.29(14)
C(8)-O(7)-Zn(2)#6	140.17(16)
C(8)-O(7)-Zn(1)#3	94.62(14)
Zn(2)#6-O(7)-Zn(1)#3	121.90(8)
C(8)-O(8)-Zn(1)#3	87.03(13)
HW1-OW-HW2	107(2)
C(6)-N(1)-C(2)	115.39(17)
C(6)-N(1)-Zn(2)	112.18(13)
C(2)-N(1)-Zn(2)	109.51(12)
C(6)-N(1)-H(1N1)	108.6(16)
C(2)-N(1)-H(1N1)	109.5(16)
Zn(2)-N(1)-H(1N1)	100.6(17)
O(2)-C(1)-O(1)	123.7(2)
O(2)-C(1)-C(2)	119.24(19)
O(1)-C(1)-C(2)	116.97(19)
N(1)-C(2)-C(3)	114.39(17)
N(1)-C(2)-C(1)	108.89(16)
C(3)-C(2)-C(1)	113.06(17)
N(1)-C(2)-H(2)	106.7
C(3)-C(2)-H(2)	106.7
C(1)-C(2)-H(2)	106.7
C(4)-C(3)-C(2)	115.31(18)
C(4)-C(3)-H(3A)	108.4
C(2)-C(3)-H(3A)	108.4
C(4)-C(3)-H(3B)	108.4
C(2)-C(3)-H(3B)	108.4
H(3A)-C(3)-H(3B)	107.5
O(4)-C(4)-O(3)	126.1(2)
O(4)-C(4)-C(3)	115.1(2)
O(3)-C(4)-C(3)	118.76(19)
O(6)-C(5)-O(5)	124.5(2)
O(6)-C(5)-C(6)	120.29(19)

O(5)-C(5)-C(6)	115.08(19)
N(1)-C(6)-C(7)	113.53(17)
N(1)-C(6)-C(5)	109.68(17)
C(7)-C(6)-C(5)	111.27(18)
N(1)-C(6)-H(6)	107.4
C(7)-C(6)-H(6)	107.4
C(5)-C(6)-H(6)	107.4
C(8)-C(7)-C(6)	111.75(18)
C(8)-C(7)-H(7A)	109.3
C(6)-C(7)-H(7A)	109.3
C(8)-C(7)-H(7B)	109.3
C(6)-C(7)-H(7B)	109.3
H(7A)-C(7)-H(7B)	107.9
O(8)-C(8)-O(7)	118.5(2)
O(8)-C(8)-C(7)	120.9(2)
O(7)-C(8)-C(7)	120.6(2)
O(8)-C(8)-Zn(1)#3	63.81(13)
O(7)-C(8)-Zn(1)#3	54.85(11)
C(7)-C(8)-Zn(1)#3	174.03(16)

Symmetry transformations used to generate equivalent atoms:

#1 x+1/2,-y+1/2,z+1/2 #2 x,y+1,z #3 -x,-y+1,-z

#4 -x,-y,-z #5 x,y-1,z #6 x-1/2,-y+1/2,z-1/2

Anisotropic displacement parameters ($Å^2$ x 10^3) for Zinc IDS Hydrate:

(The anisotropic displacement factor exponent takes the form: $-2p^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$)

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn(1)	20(1)	23(1)	25(1)	2(1)	5(1)	1(1)
Zn(2)	19(1)	24(1)	23(1)	-5(1)	5(1)	0(1)
O(1)	28(1)	21(1)	35(1)	5(1)	11(1)	2(1)
O(2)	23(1)	27(1)	45(1)	5(1)	1(1)	0(1)
O(3)	22(1)	42(1)	24(1)	-9(1)	8(1)	-1(1)
O(4)	26(1)	59(1)	26(1)	-8(1)	3(1)	-12(1)
O(5)	31(1)	19(1)	36(1)	-2(1)	11(1)	0(1)
O(6)	27(1)	25(1)	32(1)	-6(1)	-1(1)	0(1)
O(7)	24(1)	37(1)	21(1)	8(1)	1(1)	-1(1)
O(8)	24(1)	52(1)	28(1)	8(1)	9(1)	7(1)
OW	99(5)	57(4)	151(7)	14(4)	-20(4)	5(3)
N(1)	22(1)	19(1)	17(1)	-2(1)	8(1)	0(1)
C(1)	26(1)	22(1)	18(1)	-1(1)	7(1)	2(1)
C(2)	21(1)	21(1)	17(1)	-1(1)	7(1)	1(1)
C(3)	20(1)	26(1)	24(1)	-1(1)	8(1)	0(1)
C(4)	22(1)	21(1)	23(1)	1(1)	4(1)	1(1)
C(5)	29(1)	21(1)	19(1)	-1(1)	10(1)	-2(1)
C(6)	22(1)	19(1)	24(1)	1(1)	11(1)	3(1)
C(7)	22(1)	30(1)	27(1)	3(1)	7(1)	3(1)
C(8)	29(1)	21(1)	23(1)	0(1)	7(1)	-1(1)

Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for Zinc IDS Hydrate:

	x	y	z	U(eq)
HW1	-3380(70)	-3720(110)	140(70)	135
HW2	-4630(50)	-4110(100)	40(60)	135
H(1N1)	-1070(20)	1060(20)	460(20)	18(6)
H(2)	-1961	425	2286	23
H(3A)	-3407	-1161	1141	27
H(3B)	-3741	307	667	27
H(6)	-2357	2463	1658	25
H(7A)	-3214	2408	-360	31
H(7B)	-3000	3900	95	31

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for Tetraaquanickel(II) DDPD.

Atom	x	y	z	U(eq)
Ni(1)	0	0	5000	29(1)
O(1)	12350(5)	8198(4)	219(2)	33(1)
O(2)	10426(5)	9005(4)	1745(2)	38(1)
O(3)	1938(5)	4726(4)	3574(2)	38(1)
O(4)	2681(4)	1274(4)	3655(2)	32(1)
O(5)	2326(4)	946(4)	6106(2)	34(1)
O(6)	-2198(5)	2779(4)	4847(2)	35(1)
C(1)	14516(6)	7517(5)	-1471(3)	29(1)
C(2)	12628(6)	6977(5)	-575(3)	27(1)
C(3)	10455(7)	7815(5)	1121(3)	30(1)
C(4)	8673(6)	6016(5)	1253(3)	29(1)
C(5)	9016(6)	4758(5)	461(3)	27(1)
C(6)	6729(7)	5530(5)	2138(3)	31(1)
C(7)	5163(6)	3758(5)	2259(3)	28(1)
C(8)	3097(6)	3218(5)	3248(3)	30(1)

(U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor)

Bond lengths [Å] and angles [°] for Tetraaquanickel(II) DDPD:

Ni(1)-O(6)#1	2.062(2)
Ni(1)-O(6)	2.062(2)
Ni(1)-O(5)#1	2.076(2)
Ni(1)-O(5)	2.076(2)
Ni(1)-O(4)#1	2.077(2)
Ni(1)-O(4)	2.077(2)
O(2)-C(3)	1.208(4)
O(5)-H(5A)	0.7917
O(5)-H(5B)	0.7850
O(6)-H(6A)	0.7729
O(6)-H(6B)	0.7789
O(3)-C(8)	1.248(4)
O(4)-C(8)	1.272(4)
O(1)-C(3)	1.380(4)
O(1)-C(2)	1.389(4)
C(5)-C(2)#2	1.402(4)
C(5)-C(4)	1.406(4)
C(5)-C(5)#2	1.424(6)
C(1)-C(2)	1.379(4)
C(1)-C(7)#2	1.410(4)
C(1)-H(1)	0.9300
C(6)-C(4)	1.385(5)
C(6)-C(7)	1.397(5)
C(6)-H(6)	0.9300
C(8)-C(7)	1.514(4)
C(3)-C(4)	1.475(5)
C(2)-C(5)#2	1.402(4)
C(7)-C(1)#2	1.410(4)
O(6)#1-Ni(1)-O(6)	180.000(1)
O(6)#1-Ni(1)-O(5)#1	89.66(10)
O(6)-Ni(1)-O(5)#1	90.34(10)
O(6)#1-Ni(1)-O(5)	90.34(10)
O(6)-Ni(1)-O(5)	89.66(10)

O(5)#1-Ni(1)-O(5)	180.0
O(6)#1-Ni(1)-O(4)#1	92.38(9)
O(6)-Ni(1)-O(4)#1	87.62(9)
O(5)#1-Ni(1)-O(4)#1	91.10(10)
O(5)-Ni(1)-O(4)#1	88.90(10)
O(6)#1-Ni(1)-O(4)	87.62(9)
O(6)-Ni(1)-O(4)	92.38(9)
O(5)#1-Ni(1)-O(4)	88.90(10)
O(5)-Ni(1)-O(4)	91.10(10)
O(4)#1-Ni(1)-O(4)	180.0
Ni(1)-O(5)-H(5A)	113.0
Ni(1)-O(5)-H(5B)	107.6
H(5A)-O(5)-H(5B)	106.7
Ni(1)-O(6)-H(6A)	104.5
Ni(1)-O(6)-H(6B)	119.5
H(6A)-O(6)-H(6B)	108.0
C(8)-O(4)-Ni(1)	126.73(19)
C(3)-O(1)-C(2)	122.8(2)
C(2)#2-C(5)-C(4)	119.4(3)
C(2)#2-C(5)-C(5)#2	119.7(3)
C(4)-C(5)-C(5)#2	120.8(4)
C(2)-C(1)-C(7)#2	118.7(3)
C(2)-C(1)-H(1)	120.6
C(7)#2-C(1)-H(1)	120.6
C(4)-C(6)-C(7)	120.0(3)
C(4)-C(6)-H(6)	120.0
C(7)-C(6)-H(6)	120.0
O(3)-C(8)-O(4)	126.4(3)
O(3)-C(8)-C(7)	116.7(3)
O(4)-C(8)-C(7)	116.9(3)
O(2)-C(3)-O(1)	115.9(3)
O(2)-C(3)-C(4)	125.6(3)
O(1)-C(3)-C(4)	118.5(3)
C(6)-C(4)-C(5)	119.9(3)
C(6)-C(4)-C(3)	121.9(3)
C(5)-C(4)-C(3)	118.2(3)

C(1)-C(2)-O(1)	118.9(3)
C(1)-C(2)-C(5)#2	121.3(3)
O(1)-C(2)-C(5)#2	119.8(3)
C(6)-C(7)-C(1)#2	120.7(3)
C(6)-C(7)-C(8)	119.3(3)
C(1)#2-C(7)-C(8)	120.1(3)

Symmetry transformations used to generate equivalent atoms:

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

Anisotropic displacement parameters ($Å^2$ x 10^3) for Tetraaquanickel(II) DDPD:
(The anisotropic displacement factor exponent takes the form: $-2p^2$ [$h^2 a^{*2} U^{11}$ + ... + 2 h k a* b* U^{12}])

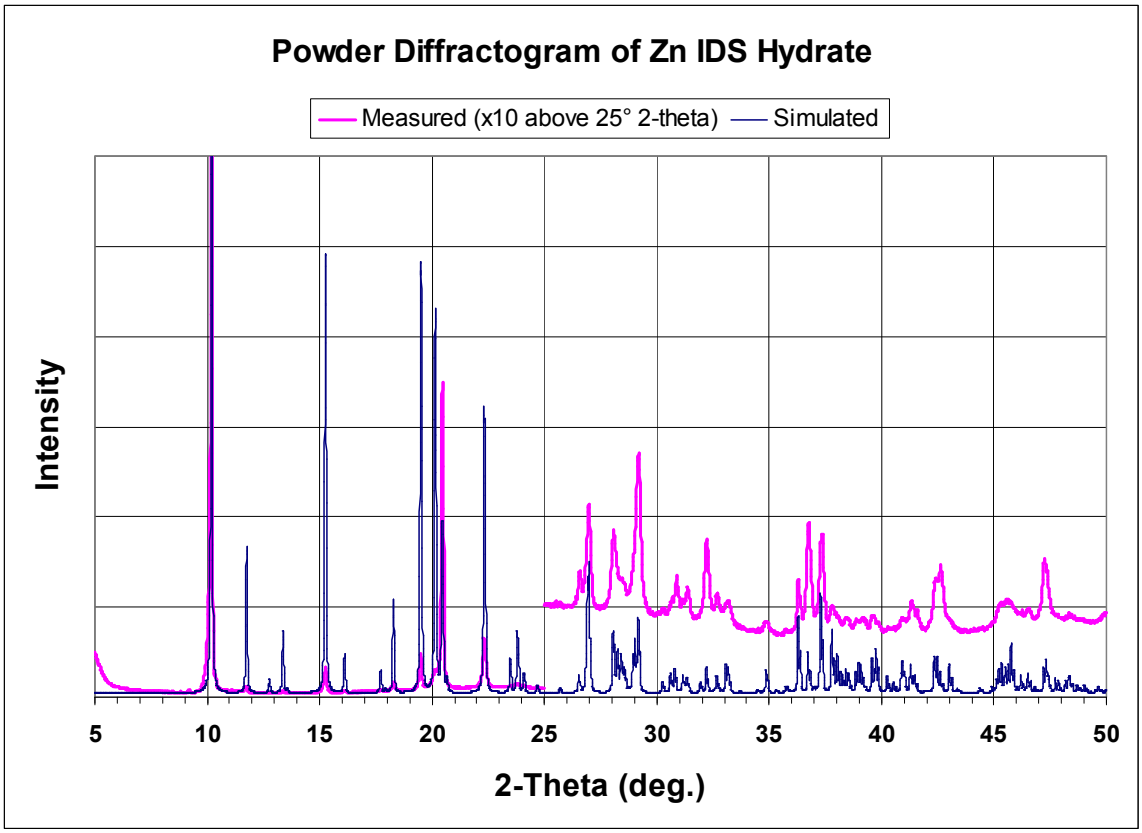
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni(1)	22(1)	35(1)	30(1)	-11(1)	7(1)	-9(1)
O(1)	30(1)	40(1)	30(1)	-13(1)	9(1)	-15(1)
O(2)	42(1)	41(1)	35(1)	-17(1)	11(1)	-18(1)
O(3)	32(1)	39(1)	43(2)	-13(1)	15(1)	-7(1)
O(4)	28(1)	35(1)	32(1)	-9(1)	9(1)	-9(1)
O(5)	25(1)	47(1)	30(1)	-13(1)	5(1)	-5(1)
O(6)	28(1)	37(1)	39(1)	-12(1)	10(1)	-8(1)
C(1)	25(2)	30(2)	31(2)	-5(1)	4(1)	-9(1)
C(2)	25(2)	30(2)	27(2)	-8(1)	3(1)	-7(1)
C(3)	28(2)	32(2)	28(2)	-7(1)	6(1)	-8(1)
C(4)	24(2)	33(2)	29(2)	-8(1)	3(1)	-7(1)
C(5)	21(2)	30(2)	27(2)	-5(1)	3(1)	-6(1)
C(6)	29(2)	34(2)	30(2)	-11(1)	6(1)	-6(1)
C(7)	20(2)	35(2)	28(2)	-6(1)	3(1)	-5(1)
C(8)	20(2)	39(2)	31(2)	-10(1)	3(1)	-7(1)

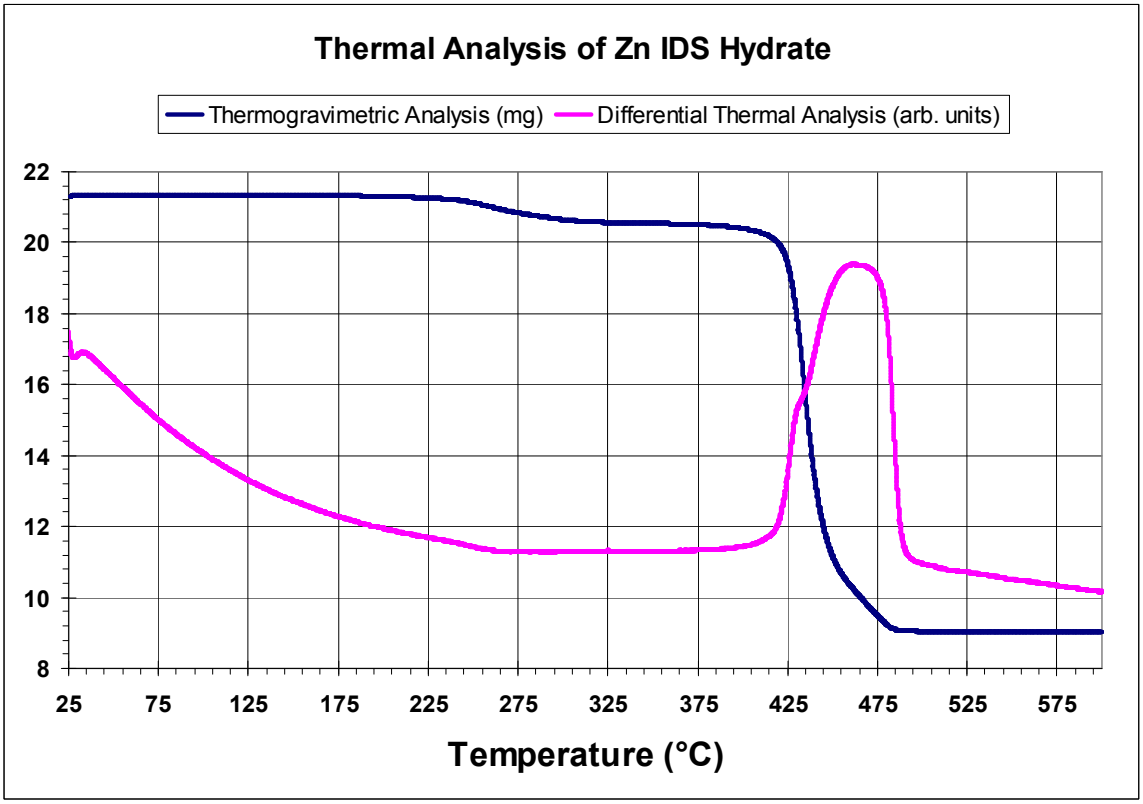
Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for Tetraaquanickel(II) DDPD:

	x	y	z	U(eq)
H(5A)	3610	215	6241	40
H(5B)	1448	862	6675	40
H(6A)	-1403	3567	4379	41
H(6B)	-2461	3287	5363	41
H(1)	15556	8698	-1553	35
H(6)	6466	6383	2651	37

Hydrogen bonds in the structure of Tetraaquanickel(II) DDPD:

D-H	d(D-H)	d(H...A)	Angle DHA	d(D...A)	A
O5-H(5A)	0.792	2.061	169.0	2.842	O4 [-x+1, -y, -z+1]
O5-H(5B)	0.785	2.103	170.1	2.880	O2 [-x+1, -y+1, -z+1]
O6-H(6A)	0.773	1.957	152.5	2.667	O3
O6-H(6B)	0.779	2.079	158.5	2.818	O3 [-x, -y+1, -z+1]


Powder Diffractogram of Zn IDS Hydrate
Measured (x10 above 25° 2-theta)
Simulated
Intensity
5
10
15
20
25
30
35
40
45
50
2-Theta (deg.)


Thermal Analysis of Zn IDS Hydrate
Thermogravimetric Analysis (mg)
Differential Thermal Analysis (arb. units)
22
20
18
16
14
12
10
8
25
75
125
175
225
275
325
375
425
475
525
575
Temperature (°C)