Table 1. Crystal data and structure refinement for a:zh1.

complex 1

cm010688u

Identification code	zh1
Empirical formula	$C_{40}H_{30}FeN_{12}S_2$
Formula weight	798.73
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 9.120(3) Å alpha = 76.256(15)° b = 9.2563(18) Å beta = 76.405(18)° c = 11.576(2) Å gamma = 84.983(19)°
Volume, Z	922.1(4) $Å^3$, 1
Density (calculated)	1.438 Mg/m^3
Absorption coefficient	0.571 mm^{-1}
F(000)	412
Crystal size	0.30 x 0.21 x 0.18 mm
θ range for data collection	1.86 to 25.00°
Limiting indices	$-1 \le h \le 10$, $-10 \le k \le 10$, $-13 \le l \le 13$
Reflections collected	3902
Independent reflections	3226 (R_{int} = 0.1048)
Completeness to θ = 25.00°	99.6 %
Absorption correction	Empirical
Max. and min. transmission	0.3632 and 0.3276
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3226 / 0 / 247
Goodness-of-fit on F^2	1.029
Final R indices [I>2σ(I)]	R1 = 0.0541, wR2 = 0.1372
R indices (all data)	R1 = 0.0741, wR2 = 0.1513
Largest diff. peak and hole	0.575 and -0.796 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for a:zh1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe(1)	0	0	0	34(1)
S(1)	550(1)	3941(1)	-3484(1)	65(1)
N(1)	188(3)	752(3)	1636(3)	38(1)
N(2)	2291(3)	-658(3)	253(2)	34(1)
N(3)	3412(3)	-1555(3)	-262(2)	34(1)
N(4)	3678(3)	-1536(3)	1585(2)	31(1)
N(5)	6095(3)	-3823(3)	1290(3)	45(1)
N(6)	639(4)	2037(4)	-1241(3)	51(1)
C(1)	-841(4)	1593(4)	2229(4)	49(1)
C(2)	-714(5)	1959(5)	3278(4)	58(1)
C(3)	522(5)	1441(5)	3759(4)	52(1)
C(4)	1597(4)	540(4)	3171(3)	43(1)
C(5)	1396(3)	228(4)	2117(3)	34(1)
C(6)	2456(3)	-649(3)	1342(3)	32(1)
C(7)	4239(3)	-2078(3)	552(3)	31(1)
C(8)	5562(3)	-3094(3)	332(3)	32(1)
C(9)	6160(4)	-3252(4)	-848(3)	46(1)
C(10)	7378(4)	-4232(5)	-1042(4)	54(1)
C(11)	7951(4)	-4986(4)	-78(4)	49(1)
C(12)	7302(4)	-4751(4)	1063(4)	52(1)
C(13)	4193(3)	-1903(3)	2722(3)	31(1)
C(14)	3471(3)	-2990(4)	3662(3)	35(1)
C(15)	3945(4)	-3347(4)	4751(3)	38(1)
C(16)	5117(4)	-2592(4)	4906(3)	40(1)
C(17)	5812(4)	-1501(4)	3935(3)	47(1)
C(18)	5361(4)	-1149(4)	2839(3)	39(1)
C(19)	5622(3)	-2969(3)	6095(3)	65(1)
C(20)	610(3)	2835(3)	-2177(3)	43(1)

Table 3. Bond lengths [Å] and angles [°] for a:zh1.

Fe(1)-N(6)	2.114(3)	Fe(1)-N(6)#1	2.114(3)
Fe(1)-N(2)	2.192(2)	Fe(1)-N(2)#1	2.192(2)
Fe(1)-N(1)	2.213(3)	Fe(1)-N(1)#1	2.213(3)
S(1)-C(20)	1.622(3)	N(1)-C(1)	1.335(4)
N(1)-C(5)	1.351(4)	N(2)-C(6)	1.306(4)
N(2)-N(3)	1.374(4)	N(3)-C(7)	1.321(4)
N(4)-C(6)	1.368(4)	N(4)-C(7)	1.376(4)
N(4)-C(13)	1.456(4)	N(5)-C(8)	1.328(4)
N(5)-C(12)	1.350(5)	N(6)-C(20)	1.162(4)
C(1)-C(2)	1.368(6)	C(2)-C(3)	1.373(6)
C(3)-C(4)	1.390(5)	C(4)-C(5)	1.374(5)
C(5)-C(6)	1.483(4)	C(7)-C(8)	1.476(4)
C(8)-C(9)	1.384(5)	C(9)-C(10)	1.382(5)
C(10)-C(11)	1.358(6)	C(11)-C(12)	1.374(6)
C(13)-C(18)	1.372(5)	C(13)-C(14)	1.375(5)
C(14)-C(15)	1.384(5)	C(15)-C(16)	1.395(5)
C(16)-C(17)	1.387(5)	C(16)-C(19)	1.506(4)
C(17)-C(18)	1.382(5)		

N(6)-Fe(1)-N(6)#1	180.0(2)	N(6)-Fe(1)-N(2)	94.52(11)
N(6)#1-Fe(1)-N(2)	85.48(11)	N(6)-Fe(1)-N(2)#1	85.48(11)
N(6)#1-Fe(1)-N(2)#1	94.52(11)	N(2)-Fe(1)-N(2)#1	180.00(13)
N(6)-Fe(1)-N(1)	95.30(12)	N(6)#1-Fe(1)-N(1)	84.70(12)
N(2)-Fe(1)-N(1)	74.17(10)	N(2)#1-Fe(1)-N(1)	105.83(10)
N(6)-Fe(1)-N(1)#1	84.70(12)	N(6)#1-Fe(1)-N(1)#1	95.30(12)
N(2)-Fe(1)-N(1)#1	105.83(10)	N(2)#1-Fe(1)-N(1)#1	74.17(10)
N(1)-Fe(1)-N(1)#1	180.00(12)	C(1)-N(1)-C(5)	117.6(3)
C(1)-N(1)-Fe(1)	125.4(2)	C(5)-N(1)-Fe(1)	116.9(2)
C(6)-N(2)-N(3)	109.0(2)	C(6)-N(2)-Fe(1)	113.0(2)
N(3)-N(2)-Fe(1)	133.3(2)	C(7)-N(3)-N(2)	106.5(2)
C(6)-N(4)-C(7)	104.8(2)	C(6)-N(4)-C(13)	127.1(3)
C(7)-N(4)-C(13)	128.0(2)	C(8)-N(5)-C(12)	116.3(3)
C(20)-N(6)-Fe(1)	148.3(3)	N(1)-C(1)-C(2)	123.2(3)
C(1)-C(2)-C(3)	119.1(3)	C(2)-C(3)-C(4)	118.8(3)
C(5)-C(4)-C(3)	118.7(3)	N(1)-C(5)-C(4)	122.6(3)
N(1)-C(5)-C(6)	111.3(3)	C(4)-C(5)-C(6)	126.1(3)
N(2)-C(6)-N(4)	109.6(3)	N(2)-C(6)-C(5)	120.9(3)
N(4)-C(6)-C(5)	129.5(3)	N(3)-C(7)-N(4)	110.1(3)
N(3)-C(7)-C(8)	122.7(3)	N(4)-C(7)-C(8)	127.2(3)
N(5)-C(8)-C(9)	123.8(3)	N(5)-C(8)-C(7)	117.5(3)
C(9)-C(8)-C(7)	118.6(3)	C(10)-C(9)-C(8)	118.2(3)
C(11)-C(10)-C(9)	119.2(4)	C(10)-C(11)-C(12)	118.9(3)
N(5)-C(12)-C(11)	123.5(3)	C(18)-C(13)-C(14)	121.7(3)
C(18)-C(13)-N(4)	119.7(3)	C(14)-C(13)-N(4)	118.6(3)
C(13)-C(14)-C(15)	119.2(3)	C(14)-C(15)-C(16)	120.6(3)
C(17)-C(16)-C(15)	118.2(3)	C(17)-C(16)-C(19)	121.1(3)
C(15)-C(16)-C(19)	120.6(3)	C(18)-C(17)-C(16)	121.6(3)
C(13)-C(18)-C(17)	118.6(3)	N(6)-C(20)-S(1)	179.3(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for a:zh1.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Fe(1)	28(1)	36(1)	36(1)	-6(1)	-12(1)	8(1)
S(1)	57(1)	71(1)	57(1)	11(1)	-16(1)	-5(1)
N(1)	32(1)	40(2)	42(2)	-12(1)	-10(1)	10(1)
N(2)	29(1)	41(2)	35(2)	-11(1)	-12(1)	12(1)
N(3)	29(1)	40(2)	31(1)	-8(1)	-7(1)	8(1)
N(4)	25(1)	38(1)	32(1)	-8(1)	-11(1)	7(1)
N(5)	43(2)	50(2)	43(2)	-16(1)	-16(1)	18(1)
N(6)	48(2)	45(2)	55(2)	-1(2)	-14(2)	-2(1)
C(1)	41(2)	50(2)	52(2)	-15(2)	-9(2)	18(2)
C(2)	50(2)	63(3)	60(3)	-28(2)	-7(2)	24(2)
C(3)	60(3)	58(2)	44(2)	-24(2)	-10(2)	5(2)
C(4)	44(2)	47(2)	43(2)	-16(2)	-13(2)	8(2)
C(5)	29(2)	34(2)	36(2)	-8(1)	-7(1)	5(1)
C(6)	25(2)	36(2)	35(2)	-7(1)	-11(1)	4(1)
C(7)	27(2)	36(2)	29(2)	-7(1)	-7(1)	3(1)
C(8)	25(2)	34(2)	38(2)	-9(1)	-11(1)	2(1)
C(9)	39(2)	58(2)	38(2)	-14(2)	-7(2)	11(2)
C(10)	44(2)	66(3)	51(2)	-25(2)	4(2)	8(2)
C(11)	31(2)	46(2)	72(3)	-22(2)	-11(2)	14(2)
C(12)	49(2)	50(2)	63(3)	-17(2)	-29(2)	21(2)
C(13)	25(2)	38(2)	30(2)	-10(1)	-9(1)	8(1)
C(14)	27(2)	40(2)	39(2)	-12(1)	-8(1)	3(1)
C(15)	41(2)	37(2)	32(2)	-5(1)	-4(1)	5(1)
C(16)	44(2)	47(2)	33(2)	-13(2)	-15(2)	6(2)
C(17)	45(2)	55(2)	46(2)	-11(2)	-21(2)	-8(2)
C(18)	39(2)	43(2)	34(2)	-2(1)	-9(1)	-8(2)
C(19)	94(3)	62(3)	45(2)	-3(2)	-37(2)	-6(2)
C(20)	32(2)	42(2)	52(2)	-9(2)	-7(2)	0(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for a:zh1.

	x	y	z	U(eq)
H(1A)	-1685	1947	1913	59
H(2A)	-1456	2552	3661	69
H(3A)	638	1687	4465	63
H(4A)	2436	156	3485	52
H(9A)	5754	-2712	-1493	55
H(10A)	7800	-4373	-1822	65
H(11A)	8770	-5651	-188	59
H(12A)	7717	-5257	1713	62
H(14A)	2673	-3480	3568	42
H(15A)	3477	-4098	5384	46
H(17A)	6601	-993	4023	56
H(18A)	5839	-417	2195	47
H(19A)	5013	-3742	6657	97
H(19B)	5512	-2101	6429	97
H(19C)	6661	-3305	5956	97

Table 1. Crystal data and structure refinement for zd2. complex 2

Identification code	zd2
Empirical formula	$C_{40}H_{30}FeN_{12}S_2$
Formula weight	798.73
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 21.851(3) Å alpha = 90° b = 13.4113(15) Å beta = 128.153(9)° c = 16.859(3) Å gamma = 90°
Volume, Z	3885.0(9) Å^3, 4
Density (calculated)	1.366 Mg/m^3
Absorption coefficient	0.542 mm^{-1}
F(000)	1648
Crystal size	0.60 x 0.56 x 0.40 mm
θ range for data collection	1.95 to 25.01°
Limiting indices	$-1 \le h \le 25$, $-1 \le k \le 15$, $-20 \le l \le 16$
Reflections collected	4052
Independent reflections	3412 (R_{int} = 0.0367)
Completeness to θ = 25.01°	99.6 %
Absorption correction	Empirical
Max. and min. transmission	0.7113 and 0.6634
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3412 / 12 / 250
Goodness-of-fit on F^2	1.015
Final R indices [I>2σ(I)]	R1 = 0.0697, wR2 = 0.1789
R indices (all data)	R1 = 0.1320, wR2 = 0.2265
Extinction coefficient	0.0116(7)
Largest diff. peak and hole	0.315 and -0.318 eÅ^{-3}

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for zd2. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe(1)	0	2098(1)	2500	78(1)
S(1)	1364(1)	356(1)	1577(1)	163(1)
N(1)	1020(1)	2339(2)	4098(2)	78(1)
N(2)	648(1)	3421(2)	2536(2)	86(1)
N(3)	422(1)	4161(2)	1840(2)	92(1)
N(4)	1257(1)	4782(2)	3377(2)	81(1)
N(5)	522(1)	1137(2)	2136(2)	103(1)
N(6)	671(2)	6768(3)	2321(2)	115(1)
C(1)	1254(2)	1699(3)	4841(2)	89(1)
C(2)	1888(2)	1869(3)	5843(2)	99(1)
C(3)	2305(2)	2734(3)	6074(2)	98(1)
C(4)	2090(2)	3387(3)	5317(2)	95(1)
C(5)	1442(2)	3183(2)	4340(2)	77(1)
C(6)	1140(2)	3795(2)	3442(2)	79(1)
C(7)	791(2)	4977(3)	2350(2)	84(1)
C(8)	668(2)	5939(3)	1869(2)	88(1)
C(9)	496(2)	5946(3)	955(2)	110(1)
C(10)	278(2)	6835(4)	430(3)	138(2)
C(11)	276(2)	7670(3)	853(3)	122(2)
C(12)	471(2)	7622(3)	1786(3)	125(2)
C(13)	1553(2)	5753(3)	4786(2)	102(1)
C(14)	2073(2)	6307(4)	5640(3)	135(2)
C(15)	2769(3)	6530(4)	5898(4)	175(3)
C(16)	2990(2)	6226(4)	5335(4)	159(2)
C(17)	2475(2)	5663(3)	4458(3)	115(2)
C(18)	1771(2)	5441(2)	4220(2)	84(1)
C(19)	875(2)	794(2)	1904(2)	88(1)
C(20)	1882(4)	6644(7)	6273(6)	187(3)
C(20A)	3827(7)	6237(12)	5864(10)	115(5)

Table 3. Bond lengths [Å] and angles [°] for zd2.

Fe(1)-N(5)#1	2.051(3)	Fe(1)-N(5)	2.051(3)
Fe(1)-N(1)#1	2.2166(19)	Fe(1)-N(1)	2.2166(19)
Fe(1)-N(2)	2.248(3)	Fe(1)-N(2)#1	2.248(3)
S(1)-C(19)	1.586(4)	N(1)-C(1)	1.332(4)
N(1)-C(5)	1.354(4)	N(2)-C(6)	1.308(3)
N(2)-N(3)	1.375(4)	N(3)-C(7)	1.315(4)
N(4)-C(6)	1.365(4)	N(4)-C(7)	1.387(3)
N(4)-C(18)	1.446(3)	N(5)-C(19)	1.154(5)
N(6)-C(8)	1.346(5)	N(6)-C(12)	1.351(5)
C(1)-C(2)	1.390(4)	C(2)-C(3)	1.374(5)
C(3)-C(4)	1.370(5)	C(4)-C(5)	1.382(3)
C(5)-C(6)	1.472(4)	C(7)-C(8)	1.458(5)
C(8)-C(9)	1.343(5)	C(9)-C(10)	1.381(5)
C(10)-C(11)	1.329(6)	C(11)-C(12)	1.354(6)
C(13)-C(18)	1.368(6)	C(13)-C(14)	1.377(5)
C(14)-C(15)	1.332(7)	C(14)-C(20)	1.439(10)
C(15)-C(16)	1.366(9)	C(16)-C(17)	1.403(6)
C(16)-C(20A)	1.457(13)	C(17)-C(18)	1.362(5)

N(5)#1-Fe(1)-N(5)	102.13(18)	N(5)#1-Fe(1)-N(1)#1	97.34(9)
N(5)-Fe(1)-N(1)#1	93.17(9)	N(5)#1-Fe(1)-N(1)	93.17(9)
N(5)-Fe(1)-N(1)	97.34(9)	N(1)#1-Fe(1)-N(1)	163.24(13)
N(5)#1-Fe(1)-N(2)	161.05(11)	N(5)-Fe(1)-N(2)	92.66(12)
N(1)#1-Fe(1)-N(2)	93.54(8)	N(1)-Fe(1)-N(2)	73.03(9)
N(5)#1-Fe(1)-N(2)#1	92.66(12)	N(5)-Fe(1)-N(2)#1	161.05(11)
N(1)#1-Fe(1)-N(2)#1	73.03(9)	N(1)-Fe(1)-N(2)#1	93.54(8)
N(2)-Fe(1)-N(2)#1	75.72(15)	C(1)-N(1)-C(5)	117.5(2)
C(1)-N(1)-Fe(1)	124.21(19)	C(5)-N(1)-Fe(1)	118.32(18)
C(6)-N(2)-N(3)	108.8(3)	C(6)-N(2)-Fe(1)	112.6(2)
N(3)-N(2)-Fe(1)	131.17(16)	C(7)-N(3)-N(2)	106.9(2)
C(6)-N(4)-C(7)	104.7(2)	C(6)-N(4)-C(18)	125.7(2)
C(7)-N(4)-C(18)	129.6(3)	C(19)-N(5)-Fe(1)	164.5(3)
C(8)-N(6)-C(12)	115.9(3)	N(1)-C(1)-C(2)	123.5(3)
C(3)-C(2)-C(1)	118.2(3)	C(4)-C(3)-C(2)	119.3(3)
C(3)-C(4)-C(5)	119.5(3)	N(1)-C(5)-C(4)	122.0(3)
N(1)-C(5)-C(6)	111.5(2)	C(4)-C(5)-C(6)	126.4(3)
N(2)-C(6)-N(4)	109.7(3)	N(2)-C(6)-C(5)	120.7(3)
N(4)-C(6)-C(5)	129.5(2)	N(3)-C(7)-N(4)	109.9(3)
N(3)-C(7)-C(8)	123.0(2)	N(4)-C(7)-C(8)	127.0(3)
C(9)-C(8)-N(6)	122.9(3)	C(9)-C(8)-C(7)	118.0(3)
N(6)-C(8)-C(7)	118.9(3)	C(8)-C(9)-C(10)	118.8(4)
C(11)-C(10)-C(9)	119.8(4)	C(10)-C(11)-C(12)	118.7(4)
N(6)-C(12)-C(11)	123.7(4)	C(18)-C(13)-C(14)	118.5(4)
C(15)-C(14)-C(13)	120.0(5)	C(15)-C(14)-C(20)	119.0(5)
C(13)-C(14)-C(20)	121.0(5)	C(14)-C(15)-C(16)	122.0(5)
C(15)-C(16)-C(17)	119.7(5)	C(15)-C(16)-C(20A)	114.8(8)
C(17)-C(16)-C(20A)	122.5(8)	C(18)-C(17)-C(16)	116.9(5)
C(17)-C(18)-C(13)	122.9(3)	C(17)-C(18)-N(4)	118.2(4)
C(13)-C(18)-N(4)	118.7(3)	N(5)-C(19)-S(1)	178.2(4)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for zd2.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Fe(1)	83(1)	67(1)	91(1)	0	58(1)	0
S(1)	194(1)	150(1)	224(1)	-17(1)	169(1)	21(1)
N(1)	83(1)	69(1)	93(1)	3(1)	60(1)	2(1)
N(2)	99(1)	85(2)	76(1)	-9(1)	54(1)	-14(1)
N(3)	114(1)	86(2)	82(1)	-8(1)	63(1)	-25(1)
N(4)	88(1)	76(2)	78(1)	-9(1)	51(1)	-15(1)
N(5)	100(1)	95(2)	119(2)	-16(1)	70(1)	-4(1)
N(6)	146(2)	98(2)	96(1)	1(1)	72(1)	-13(2)
C(1)	92(1)	79(2)	97(2)	6(2)	58(1)	5(2)
C(2)	98(2)	90(2)	95(2)	14(2)	53(1)	10(2)
C(3)	97(2)	97(3)	85(2)	2(2)	49(1)	1(2)
C(4)	94(2)	90(2)	90(2)	-3(2)	51(1)	-7(2)
C(5)	79(1)	76(2)	76(1)	-4(1)	48(1)	-2(1)
C(6)	90(1)	76(2)	84(1)	-8(1)	60(1)	-12(1)
C(7)	97(1)	84(2)	78(1)	-9(1)	57(1)	-21(2)
C(8)	103(1)	89(2)	78(1)	-14(1)	59(1)	-31(2)
C(9)	158(2)	95(2)	100(2)	-19(2)	91(1)	-44(2)
C(10)	187(3)	135(3)	90(2)	-12(2)	85(2)	-62(3)
C(11)	134(2)	119(3)	96(2)	11(2)	63(2)	-33(2)
C(12)	162(2)	102(3)	115(2)	5(2)	88(2)	-1(2)
C(13)	109(2)	102(2)	78(2)	-17(2)	50(1)	-4(2)
C(14)	148(3)	132(3)	97(2)	-30(2)	61(2)	18(3)
C(15)	134(3)	152(4)	177(4)	-76(3)	65(3)	-29(3)
C(16)	96(2)	147(4)	190(4)	-53(3)	67(2)	-42(3)
C(17)	98(2)	96(3)	133(2)	-15(2)	63(2)	-19(2)
C(18)	83(1)	76(2)	75(1)	-9(1)	40(1)	-11(2)
C(19)	90(1)	75(2)	98(2)	-10(2)	58(1)	4(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for zd2.

	x	y	z	U(eq)
H(1A)	977	1108	4681	107
H(2A)	2026	1410	6342	119
H(3A)	2728	2874	6738	118
H(4A)	2378	3964	5459	114
H(9A)	524	5363	679	132
H(10A)	132	6849	-218	165
H(11A)	144	8275	515	146
H(12A)	466	8209	2076	150
H(13A)	1065	5595	4598	122
H(14A)	1939	6526	6038	162
H(15A)	3115	6903	6478	209
H(16A)	3480	6393	5531	191
H(17A)	2609	5450	4057	138
H(20A)	2310	7016	6830	280
H(20B)	1777	6079	6523	280
H(20C)	1429	7063	5888	280
H(20D)	4074	6666	6442	172
H(20E)	3929	6478	5420	172
H(20F)	4029	5573	6080	172

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pascal constant = -.000432

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271.9	.0107111	4.826882	93.36106
258.9	1.116046E-02	4.807863	89.60203
247.8	1.139322E-02	4.752464	87.77151
237.9	1.122933E-02	4.62295	89.05249
228	4.062735E-03	2.72221	246.1396
220	1.916559E-03	1.836612	521.7684
211.8	1.426212E-03	1.554533	701.1579
203.8	1.020272E-03	1.289749	980.1307
195.9	8.576147E-04	1.159333	1166.025
188	8.817449E-04	1.151583	1134.115
180	7.213484E-04	1.019187	1386.293
173	7.722231E-04	1.033807	1294.963
166	6.663465E-04	.9406955	1500.721
159	7.947237E-04	1.00543	1258.299
152	6.898378E-04	.9158836	1449.616
145	6.629875E-04	.8769638	1508.324
138	7.897731E-04	.9337609	1266.187
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126.1	7.11319E-04	.8471001	1405.839
120	7.865334E-04	.8689488	1271.402
114	7.85742E-04	.8465203	1272.682
109.4	8.60947E-04	.8680443	1161.512
104.2	8.856333E-04	.8592229	1129.135
100.5	6.586803E-04	.7277218	1518.187
96.3	9.103522E-04	.8374577	1098.476
92.5	6.837375E-04	.7113127	1462.55
88.3	7.089635E-04	.7076806	1410.51
85.2	7.846243E-04	.7313001	1274.495
82.3	7.596016E-04	.7071928	1316.48
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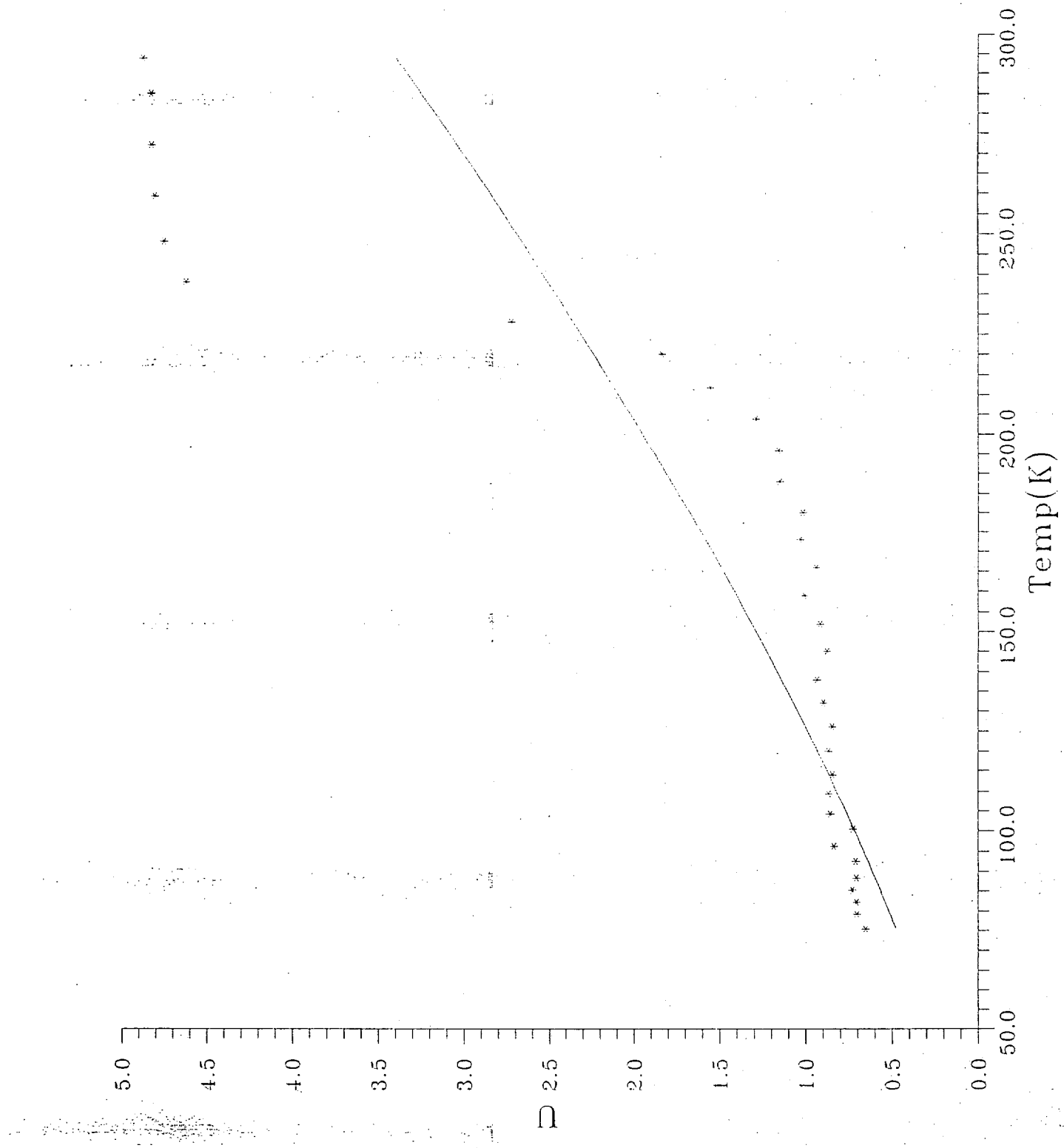
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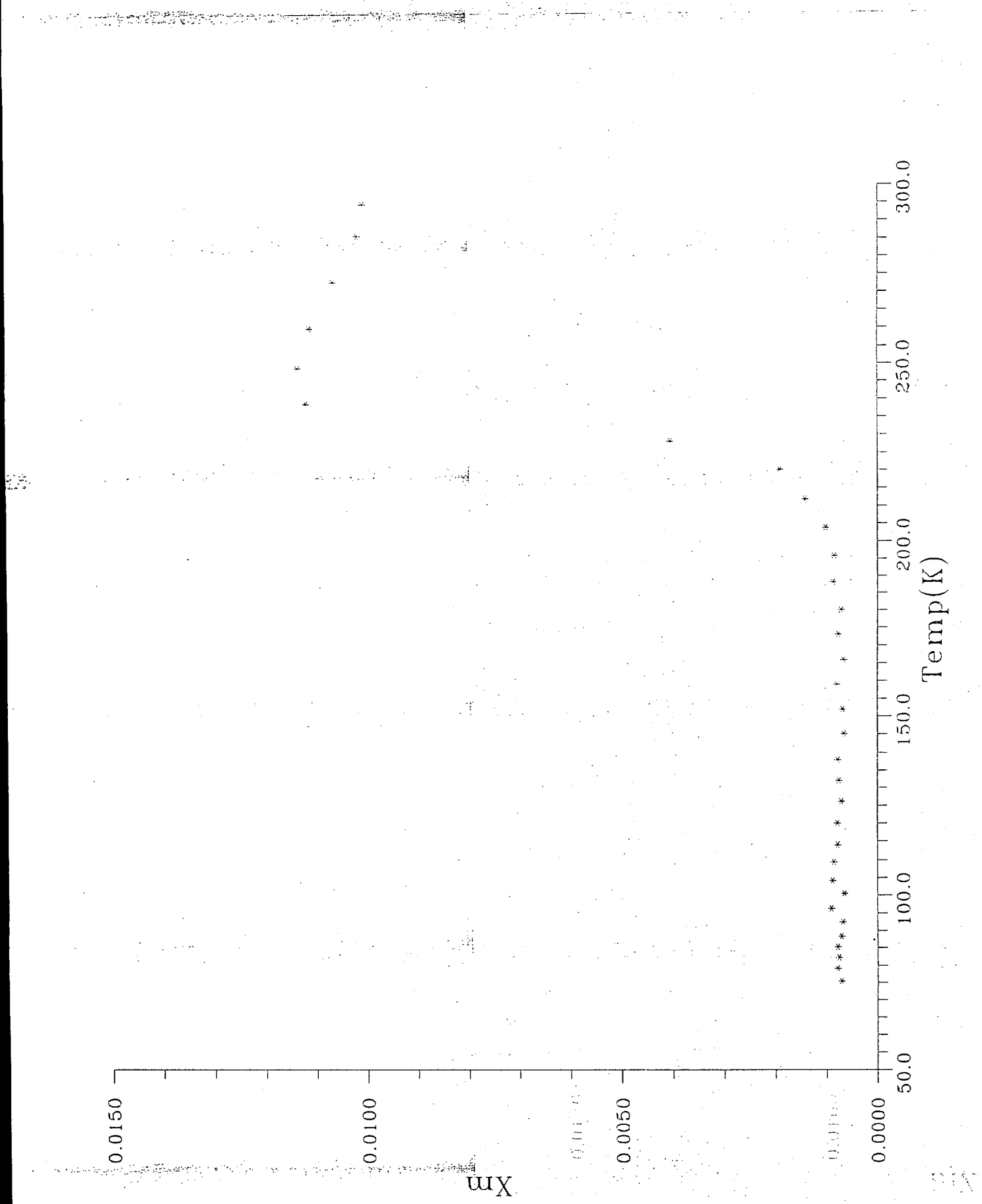
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88.4	3.163333E-02	4.729809	31.61223
92.4	3.048469E-02	4.747028	32.80336
96.2	2.963519E-02	4.775693	33.74367
100.3	2.871953E-02	4.800474	34.81952
104.5	2.816049E-02	4.852027	35.51075
109.3	2.727555E-02	4.883619	36.66288
114.3	2.584805E-02	4.861631	38.68764
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126.4	2.399217E-02	4.925534	41.68026
132.4	.0228695	4.921724	43.72636
138.4	2.198624E-02	4.933879	45.483
145.3	2.087874E-02	4.926403	47.89561
152.3	2.016517E-02	4.956737	49.59046
159.4	1.896469E-02	4.9177	52.72958
166.4	1.851348E-02	4.964388	54.01469
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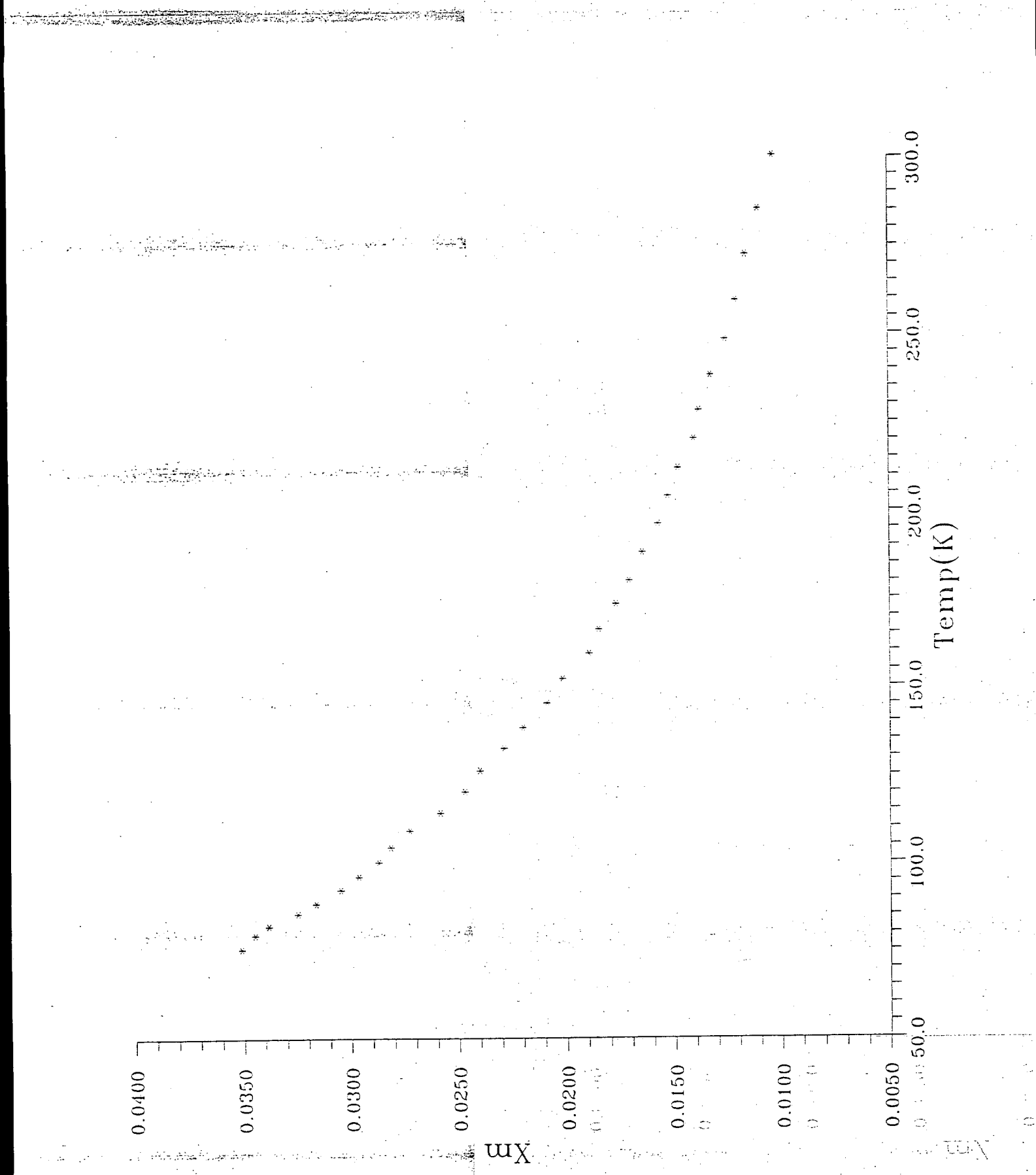
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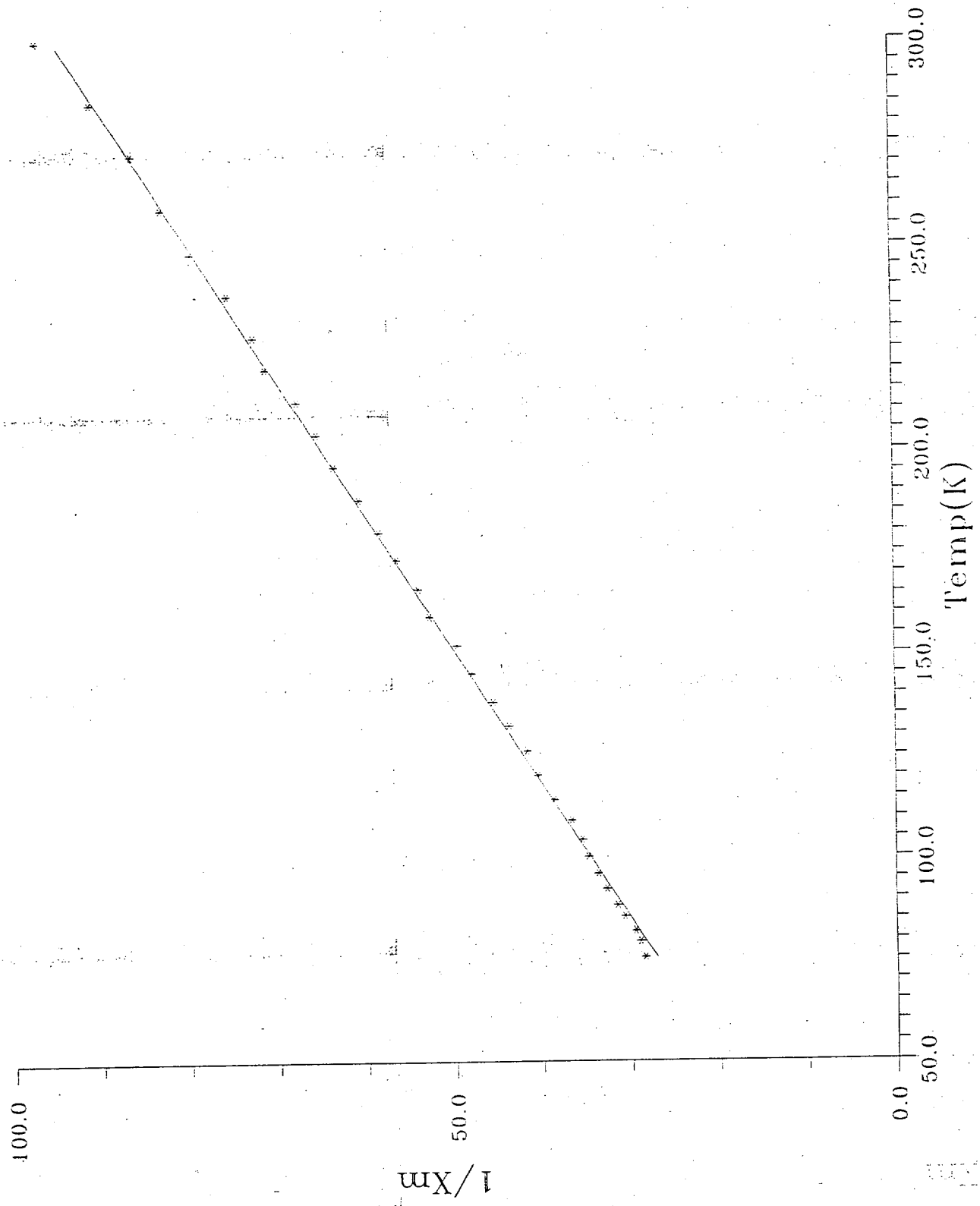
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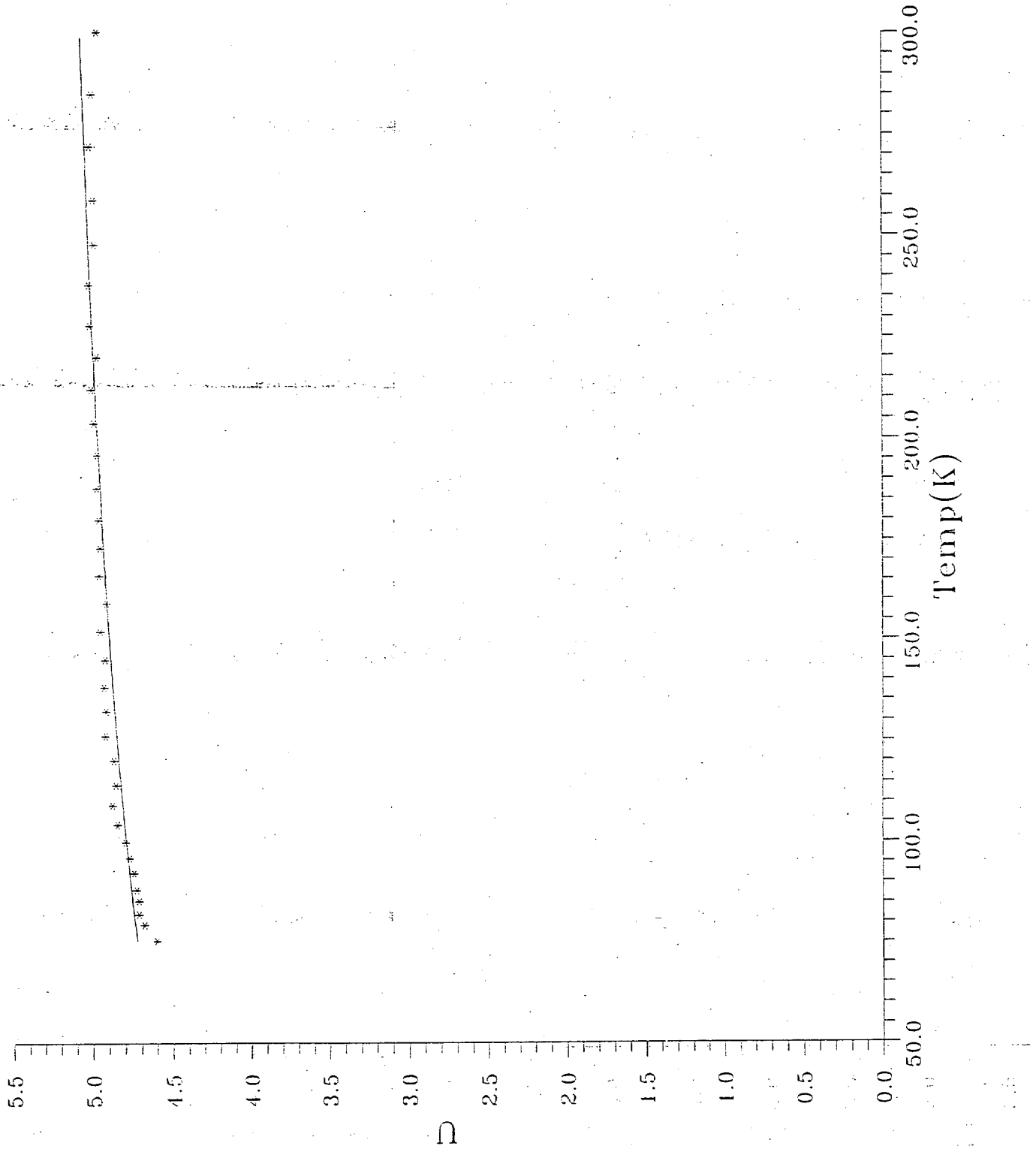
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C4 C 0.1597(4) 0.0540(4) 0.3171(3) 0.0434(8) Uani 1 1 d . . .
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C5 C 0.1396(3) 0.0228(4) 0.2117(3) 0.0337(7) Uani 1 1 d . . .
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C18 C 0.5361(4) -0.1149(4) 0.2839(3) 0.0393(8) Uani 1 1 d . . .
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C19 C 0.5622(3) -0.2969(3) 0.6095(3) 0.0648(12) Uani 1 1 d . . .
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C20 C 0.0610(3) 0.2835(3) -0.2177(3) 0.0427(8) Uani 1 1 d R . .

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S1 0.0574(7) 0.0708(7) 0.0572(7) 0.0111(5) -0.0162(5) -0.0052(5)
N1 0.0322(14) 0.0396(15) 0.0424(16) -0.0115(12) -0.0099(12) 0.0100(12)
N2 0.0289(14) 0.0405(15) 0.0352(15) -0.0106(12) -0.0120(11) 0.0115(12)
N3 0.0294(14) 0.0398(15) 0.0307(14) -0.0084(11) -0.0074(11) 0.0075(11)
N4 0.0248(13) 0.0380(14) 0.0316(14) -0.0080(11) -0.0109(11) 0.0068(11)
N5 0.0428(17) 0.0503(18) 0.0429(17) -0.0156(14) -0.0162(13) 0.0178(14)
N6 0.0475(18) 0.0453(18) 0.055(2) -0.0013(16) -0.0137(15) -0.0020(14)
C1 0.041(2) 0.050(2) 0.052(2) -0.0147(18) -0.0085(17) 0.0183(16)
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C2 0.050(2) 0.063(3) 0.060(3) -0.028(2) -0.0067(19) 0.024(2)
C3 0.060(3) 0.058(2) 0.044(2) -0.0236(19) -0.0097(18) 0.0052(19)
C4 0.044(2) 0.047(2) 0.043(2) -0.0157(16) -0.0130(16) 0.0083(16)
C5 0.0292(16) 0.0342(16) 0.0364(17) -0.0077(13) -0.0074(13) 0.0046(13)
C6 0.0248(15) 0.0357(17) 0.0352(17) -0.0069(13) -0.0106(13) 0.0036(13)
C7 0.0267(15) 0.0360(16) 0.0292(16) -0.0068(13) -0.0066(13) 0.0028(13)
C8 0.0253(15) 0.0337(17) 0.0383(18) -0.0094(14) -0.0106(13) 0.0024(13)
C9 0.0393(19) 0.058(2) 0.0377(19) -0.0140(17) -0.0069(15) 0.0109(17)
C10 0.044(2) 0.066(3) 0.051(2) -0.025(2) 0.0036(18) 0.0076(19)
C11 0.0306(18) 0.046(2) 0.072(3) -0.0222(19) -0.0109(18) 0.0140(16)
C12 0.049(2) 0.050(2) 0.063(3) -0.0174(19) -0.0285(19) 0.0211(18)
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C15 0.0408(19) 0.0370(18) 0.0320(17) -0.0052(14) -0.0036(14) 0.0049(14)
C16 0.0436(19) 0.047(2) 0.0329(18) -0.0127(15) -0.0147(15) 0.0055(16)
C17 0.045(2) 0.055(2) 0.046(2) -0.0112(17) -0.0206(17) -0.0078(17)
C18 0.0388(19) 0.0432(19) 0.0339(18) -0.0017(14) -0.0088(14) -0.0078(15)
C19 0.094(3) 0.062(3) 0.045(2) -0.003(2) -0.037(2) -0.006(2)
C20 0.0319(18) 0.0418(19) 0.052(2) -0.0087(17) -0.0074(16) -0.0003(15)

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All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
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S1 C20 1.622(3) . ?
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N6 Fe1 N1 95.30(12) . . ?
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N2 Fe1 N1 74.17(10) . . ?
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N6 Fe1 N1 84.70(12) . 2 ?
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N1 Fe1 N1 180.00(12) . 2 ?
C1 N1 C5 117.6(3) . . ?
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C6 N2 N3 109.0(2) . . ?
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C7 N3 N2 106.5(2) . . ?
C6 N4 C7 104.8(2) . . ?
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C14 C15 C16 120.6(3) . . ?
C17 C16 C15 118.2(3) . . ?
C17 C16 C19 121.1(3) . . ?
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'H'  'H'   0.0000   0.0000
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'x, -y, z-1/2'
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_cell_angle_beta                128.153(9)
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Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
goodness of fit S are based on F^2^, conventional R-factors R are based
on F, with F set to zero for negative F^2^. The threshold expression of
F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement.  R-factors based
on F^2^ are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
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_refine_ls_weighting_details
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S1 S 0.13642(6) 0.03561(12) 0.15769(9) 0.1629(5) Uani 1 1 d . . .
N1 N 0.10203(11) 0.23388(18) 0.40983(16) 0.0776(7) Uani 1 1 d . . .
N2 N 0.06482(13) 0.3421(2) 0.25363(16) 0.0863(8) Uani 1 1 d . . .
N3 N 0.04217(13) 0.4161(2) 0.18399(17) 0.0922(9) Uani 1 1 d . . .
N4 N 0.12574(12) 0.47818(19) 0.33767(16) 0.0805(8) Uani 1 1 d . A .
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N5 N 0.05223(14) 0.1137(2) 0.21357(19) 0.1032(10) Uani 1 1 d . . .
N6 N 0.06713(17) 0.6768(3) 0.23209(19) 0.1152(12) Uani 1 1 d . . .
C1 C 0.12535(16) 0.1699(3) 0.4841(2) 0.0893(11) Uani 1 1 d . . .
H1A H 0.0977 0.1108 0.4681 0.107 Uiso 1 1 calc R . .
C2 C 0.18878(17) 0.1869(3) 0.5843(2) 0.0989(13) Uani 1 1 d . . .
H2A H 0.2026 0.1410 0.6342 0.119 Uiso 1 1 calc R . .
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C5 C 0.14423(15) 0.3183(2) 0.43403(19) 0.0773(9) Uani 1 1 d . . .
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C7 C 0.07905(15) 0.4977(3) 0.23499(19) 0.0844(10) Uani 1 1 d . . .
C8 C 0.06682(16) 0.5939(3) 0.1869(2) 0.0883(10) Uani 1 1 d . . .
C9 C 0.04962(18) 0.5946(3) 0.0955(2) 0.1104(12) Uani 1 1 d . . .
H9A H 0.0524 0.5363 0.0679 0.132 Uiso 1 1 calc R . .
C10 C 0.0278(2) 0.6835(4) 0.0430(3) 0.1375(17) Uani 1 1 d . . .
H10A H 0.0132 0.6849 -0.0218 0.165 Uiso 1 1 calc R . .
C11 C 0.0276(2) 0.7670(3) 0.0853(3) 0.1215(15) Uani 1 1 d . . .
H11A H 0.0144 0.8275 0.0515 0.146 Uiso 1 1 calc R . .
C12 C 0.0471(2) 0.7622(3) 0.1786(3) 0.1248(16) Uani 1 1 d . . .
H12A H 0.0466 0.8209 0.2076 0.150 Uiso 1 1 calc R . .
C13 C 0.15534(19) 0.5753(3) 0.4786(2) 0.1015(13) Uani 1 1 d . A .
H13A H 0.1065 0.5595 0.4598 0.122 Uiso 1 1 calc R . .
C14 C 0.2073(2) 0.6307(4) 0.5640(3) 0.1353(18) Uani 1 1 d . . .
H14A H 0.1939 0.6526 0.6038 0.162 Uiso 0.274(6) 1 calc PR A 2
C15 C 0.2769(3) 0.6530(4) 0.5898(4) 0.175(3) Uani 1 1 d U A .
H15A H 0.3115 0.6903 0.6478 0.209 Uiso 1 1 calc R . .
C16 C 0.2990(2) 0.6226(4) 0.5335(4) 0.159(2) Uani 1 1 d U . .
H16A H 0.3480 0.6393 0.5531 0.191 Uiso 0.726(6) 1 calc PR A 1
C17 C 0.24752(19) 0.5663(3) 0.4458(3) 0.1152(15) Uani 1 1 d . A .
H17A H 0.2609 0.5450 0.4057 0.138 Uiso 1 1 calc R . .
C18 C 0.17707(16) 0.5441(2) 0.4220(2) 0.0837(11) Uani 1 1 d . . .
C19 C 0.08752(17) 0.0794(2) 0.1904(2) 0.0879(11) Uani 1 1 d . . .
C20 C 0.1882(4) 0.6644(7) 0.6273(6) 0.187(3) Uiso 0.726(6) 1 d P A 1
H20A H 0.2310 0.7016 0.6830 0.280 Uiso 0.726(6) 1 calc PR A 1
H20B H 0.1777 0.6079 0.6523 0.280 Uiso 0.726(6) 1 calc PR A 1
H20C H 0.1429 0.7063 0.5888 0.280 Uiso 0.726(6) 1 calc PR A 1
C20A C 0.3827(7) 0.6237(12) 0.5864(10) 0.115(5) Uiso 0.274(6) 1 d P A 2
H20D H 0.4074 0.6666 0.6442 0.172 Uiso 0.274(6) 1 calc PR A 2
H20E H 0.3929 0.6478 0.5420 0.172 Uiso 0.274(6) 1 calc PR A 2
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S1 0.1940(5) 0.1498(11) 0.2243(7) -0.0167(7) 0.1689(4) 0.0208(7)
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N2 0.0985(11) 0.0846(16) 0.0757(10) -0.0089(12) 0.0538(9) -0.0137(13)
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N4 0.0876(10) 0.0763(15) 0.0775(10) -0.0089(11) 0.0510(8) -0.0150(11)
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N6 0.1461(18) 0.098(2) 0.0957(14) 0.0010(14) 0.0717(13) -0.0129(17)
C1 0.0920(14) 0.0786(19) 0.0967(15) 0.0056(15) 0.0579(11) 0.0053(15)
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C3 0.0967(16) 0.097(3) 0.0848(16) 0.0020(17) 0.0485(13) 0.0009(18)
C4 0.0935(15) 0.090(2) 0.0897(16) -0.0031(17) 0.0512(13) -0.0065(17)

C5 0.0793(12) 0.0755(18) 0.0763(13) -0.0036(13) 0.0476(10) -0.0024(14)
C6 0.0900(12) 0.0762(19) 0.0837(12) -0.0076(13) 0.0599(9) -0.0116(14)
C7 0.0973(13) 0.084(2) 0.0780(12) -0.0086(14) 0.0572(10) -0.0208(15)
C8 0.1029(14) 0.089(2) 0.0783(13) -0.0140(14) 0.0585(10) -0.0308(15)
C9 0.1583(18) 0.095(2) 0.1001(15) -0.0194(16) 0.0912(13) -0.0443(19)
C10 0.187(3) 0.135(3) 0.0899(17) -0.0115(19) 0.0852(16) -0.062(3)
C11 0.134(2) 0.119(3) 0.0955(18) 0.011(2) 0.0630(16) -0.033(2)
C12 0.162(2) 0.102(3) 0.115(2) 0.005(2) 0.0877(17) -0.001(2)
C13 0.1092(18) 0.102(2) 0.0784(15) -0.0165(16) 0.0504(13) -0.0040(19)
C14 0.148(3) 0.132(3) 0.0966(19) -0.030(2) 0.0609(18) 0.018(3)
C15 0.134(3) 0.152(4) 0.177(4) -0.076(3) 0.065(3) -0.029(3)
C16 0.096(2) 0.147(4) 0.190(4) -0.053(3) 0.067(2) -0.042(3)
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C18 0.0828(14) 0.0759(19) 0.0745(14) -0.0087(14) 0.0396(11) -0.0105(15)
C19 0.0897(14) 0.075(2) 0.0984(16) -0.0099(15) 0.0577(12) 0.0035(15)

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;
All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
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Fe1 N5 2.051(3) . ?
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