Inorganic Chemistry
including bioinorganic chemistry
Inorg. Chem., 1998, 37(13), 3361-3370, DOI:10.1021/ic971550+

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Experimental details for $[C_1][Ni(dmit)_2]$ (phase1)

Crystal data

Chemical formula	$C_{28}H_{26}N_4Ni_2S_{20}$
Chemical formula weight	1177.16
Crystal system	Monoclinic
Space group	$P2_1/c$
a, (Å)	17.450 (2)
b, (Å)	10.646 (1)
c, (Å)	23.891 (2)
β, deg	97.42 (1)
V, (Å^3)	4401.1
Z	4
F(000)	2403.1
ρ(calcd), (g.cm^{-3})	1.776
μ (MoKα), (cm^{-1})	18.04
Crystal form	Elongated plate
Crystal color	black
Crystal size, (mm)	0.75 x 0.1 x 0.05
T, K	160

Data Collection

diffractometer	IPdS Stoe
monochromator	graphite
radiation	MoKα (λ = 0.71069 Å)
scan mode	ϕ
detector distance, mm	80
collimator size, mm	0.5
scan range ϕ, deg	$0 < \phi < 200$
ϕ increment, deg	1
exposure time, min	5

[C1][Ni(dmit)2] (phase 1)

NI(1)	- S(1)	2.163(1)
NI(1)	- S(2)	2.162(1)
NI(1)	- S(6)	2.165(1)
NI(1)	- S(7)	2.169(1)
S(1)	- C(1)	1.713(5)
S(2)	- C(2)	1.695(5)
S(3)	- C(1)	1.746(4)
S(3)	- C(3)	1.726(5)
S(4)	- C(2)	1.755(5)
S(4)	- C(3)	1.730(5)
S(5)	- C(3)	1.658(5)
S(6)	- C(4)	1.720(5)
S(7)	- C(5)	1.728(5)
S(8)	- C(4)	1.743(5)
S(8)	- C(6)	1.710(6)
S(9)	- C(5)	1.737(5)
S(9)	- C(6)	1.742(6)
S(10)	- C(6)	1.658(5)
C(1)	- C(2)	1.373(7)
C(4)	- C(5)	1.357(7)
N(3)	- C(23)	1.318(7)
N(3)	- C(24)	1.438(7)
N(3)	- C(25)	1.486(7)
N(4)	- C(21)	1.373(7)
N(4)	- C(27)	1.348(7)
N(4)	- C(28)	1.454(8)
C(21)	- C(22)	1.346(8)
C(21)	- H(211)	1.059(6)
C(22)	- C(23)	1.425(7)
C(22)	- H(221)	1.066(6)
C(23)	- C(26)	1.417(8)
C(24)	- H(241)	1.054(6)
C(24)	- H(242)	1.052(6)
C(24)	- H(243)	1.064(6)
C(25)	- H(251)	1.062(6)
C(25)	- H(252)	1.047(6)
C(25)	- H(253)	1.057(6)
C(26)	- C(27)	1.355(8)
C(26)	- H(261)	1.065(5)
C(27)	- H(271)	1.077(6)
C(28)	- H(281)	1.056(7)
C(28)	- H(282)	1.054(6)
C(28)	- H(283)	1.052(7)
NI(2)	- S(11)	2.163(1)
NI(2)	- S(12)	2.166(1)
NI(2)	- S(16)	2.164(1)
NI(2)	- S(17)	2.164(1)
S(11)	- C(7)	1.730(5)
S(12)	- C(8)	1.715(5)
S(13)	- C(7)	1.736(5)
S(13)	- C(9)	1.731(5)
S(14)	- C(8)	1.753(5)
S(14)	- C(9)	1.728(5)
S(15)	- C(9)	1.653(5)
S(16)	- C(10)	1.727(5)
S(17)	- C(11)	1.719(4)
S(18)	- C(10)	1.734(5)
S(18)	- C(12)	1.736(6)
S(19)	- C(11)	1.755(5)
S(19)	- C(12)	1.750(6)
S(20)	- C(12)	1.630(5)
C(7)	- C(8)	1.353(6)
C(10)	- C(11)	1.354(7)
N(1)	- C(15)	1.324(7)

2θ range, deg	$2.9 < 2\theta < 48.4$
Absorption Correction	None
No of measured reflections	28505
No. of independent reflections (R_m)	6928 (0.081)
No of observed reflections	4836
Criterion for observed reflections	$I > 0.5\ \sigma(I)$
Range of *h, k, l*	$-15 \leq h < 15$
	$0 \leq k \leq 12$
	$0 \leq l \leq 27$
Intensity decay (%)	Not significant

Refinement

Refinement on	F
R	0.0480
R_w	0.0408
S	1.09
No. of reflections used in refinement	4836
No. of parameters used	488
H-atoms treatment	calculated
Weighting scheme	Chebychev
coeff. Ar	1.676 1.687 1.829 0.680 0.507
$(\Delta / \sigma)_{max}$	0.04
$\Delta\rho_{max}$, e Å^{-3}	0.61
$\Delta\rho_{min}$, e Å^{-3}	-0.81
Source of atomic scattering factors	*International Tables for X-ray Crystallography (1974, vol IV)*

N(1)	- C(16)	1.483(8)
N(1)	- C(17)	1.468(8)
N(2)	- C(13)	1.367(8)
N(2)	- C(19)	1.323(8)
N(2)	- C(20)	1.467(8)
C(13)	- C(14)	1.367(9)
C(13)	- H(131)	1.078(6)
C(14)	- C(15)	1.392(8)
C(14)	- H(141)	1.066(5)
C(15)	- C(18)	1.451(8)
C(16)	- H(161)	1.047(7)
C(16)	- H(162)	1.058(9)
C(16)	- H(163)	1.071(9)
C(17)	- H(171)	1.056(7)
C(17)	- H(172)	1.073(9)
C(17)	- H(173)	1.041(8)
C(18)	- C(19)	1.349(9)
C(18)	- H(181)	1.061(6)
C(19)	- H(191)	1.069(7)
C(20)	- H(201)	1.05(1)
C(20)	- H(202)	1.058(9)
C(20)	- H(203)	1.07(1)

S(1)	- NI(1)	- S(2)	92.76(5)
S(1)	- NI(1)	- S(6)	179.12(6)
S(2)	- NI(1)	- S(6)	86.45(5)
S(1)	- NI(1)	- S(7)	87.62(5)
S(2)	- NI(1)	- S(7)	179.48(6)
S(6)	- NI(1)	- S(7)	93.18(5)
NI(1)	- S(1)	- C(1)	102.6(2)
NI(1)	- S(2)	- C(2)	102.5(2)
C(1)	- S(3)	- C(3)	97.1(2)
C(2)	- S(4)	- C(3)	97.4(2)
NI(1)	- S(6)	- C(4)	102.3(2)
NI(1)	- S(7)	- C(5)	101.9(2)
C(4)	- S(8)	- C(6)	97.6(3)
C(5)	- S(9)	- C(6)	97.1(3)
S(1)	- C(1)	- S(3)	123.0(3)
S(1)	- C(1)	- C(2)	120.4(3)
S(3)	- C(1)	- C(2)	116.7(4)
S(2)	- C(2)	- S(4)	123.3(3)
S(2)	- C(2)	- C(1)	121.7(4)
S(4)	- C(2)	- C(1)	115.0(3)
S(3)	- C(3)	- S(4)	113.9(3)
S(3)	- C(3)	- S(5)	123.0(3)
S(4)	- C(3)	- S(5)	123.1(3)
S(6)	- C(4)	- S(8)	122.7(3)
S(6)	- C(4)	- C(5)	121.3(4)
S(8)	- C(4)	- C(5)	116.0(4)
S(7)	- C(5)	- S(9)	122.7(3)
S(7)	- C(5)	- C(4)	121.3(4)
S(9)	- C(5)	- C(4)	115.9(4)
S(8)	- C(6)	- S(9)	113.2(3)
S(8)	- C(6)	- S(10)	124.3(4)
S(9)	- C(6)	- S(10)	122.5(4)
C(23)	- N(3)	- C(24)	123.1(5)
C(23)	- N(3)	- C(25)	121.3(5)
C(24)	- N(3)	- C(25)	115.2(5)
C(21)	- N(4)	- C(27)	118.3(5)
C(21)	- N(4)	- C(28)	120.4(5)
C(27)	- N(4)	- C(28)	121.3(5)
N(4)	- C(21)	- C(22)	122.0(5)
N(4)	- C(21)	- H(211)	118.8(6)
C(22)	- C(21)	- H(211)	119.3(5)

C(21) - C(22) - C(23)	121.4(5)
C(21) - C(22) - H(221)	118.5(5)
C(23) - C(22) - H(221)	120.1(6)
N(3) - C(23) - C(22)	121.8(5)
N(3) - C(23) - C(26)	123.6(5)
C(22) - C(23) - C(26)	114.6(5)
N(3) - C(24) - H(241)	110.6(5)
N(3) - C(24) - H(242)	110.8(5)
H(241)- C(24) - H(242)	109.0(6)
N(3) - C(24) - H(243)	110.0(5)
H(241)- C(24) - H(243)	108.1(6)
H(242)- C(24) - H(243)	108.2(5)
N(3) - C(25) - H(251)	109.9(5)
N(3) - C(25) - H(252)	110.9(5)
H(251)- C(25) - H(252)	108.7(6)
N(3) - C(25) - H(253)	110.2(5)
H(251)- C(25) - H(253)	108.0(5)
H(252)- C(25) - H(253)	109.1(5)
C(23) - C(26) - C(27)	121.7(5)
C(23) - C(26) - H(261)	118.6(5)
C(27) - C(26) - H(261)	119.7(5)
N(4) - C(27) - C(26)	122.1(5)
N(4) - C(27) - H(271)	119.6(6)
C(26) - C(27) - H(271)	118.4(5)
N(4) - C(28) - H(281)	109.6(6)
N(4) - C(28) - H(282)	110.2(5)
H(281)- C(28) - H(282)	108.7(6)
N(4) - C(28) - H(283)	110.5(5)
H(281)- C(28) - H(283)	108.8(5)
H(282)- C(28) - H(283)	109.0(6)
S(11) - NI(2) - S(12)	93.03(5)
S(11) - NI(2) - S(16)	178.64(6)
S(12) - NI(2) - S(16)	87.64(5)
S(11) - NI(2) - S(17)	86.33(5)
S(12) - NI(2) - S(17)	178.49(6)
S(16) - NI(2) - S(17)	92.97(5)
NI(2) - S(11) - C(7)	102.3(2)
NI(2) - S(12) - C(8)	102.1(2)
C(7) - S(13) - C(9)	97.2(2)
C(8) - S(14) - C(9)	97.5(2)
NI(2) - S(16) - C(10)	102.4(2)
NI(2) - S(17) - C(11)	102.1(2)
C(10) - S(18) - C(12)	98.2(2)
C(11) - S(19) - C(12)	97.5(2)
S(11) - C(7) - S(13)	122.6(3)
S(11) - C(7) - C(8)	120.5(4)
S(13) - C(7) - C(8)	116.9(4)
S(12) - C(8) - S(14)	122.7(3)
S(12) - C(8) - C(7)	122.0(4)
S(14) - C(8) - C(7)	115.3(4)
S(13) - C(9) - S(14)	113.1(3)
S(13) - C(9) - S(15)	123.0(3)
S(14) - C(9) - S(15)	123.9(3)
S(16) - C(10) - S(18)	123.1(3)
S(16) - C(10) - C(11)	120.5(4)
S(18) - C(10) - C(11)	116.4(4)
S(17) - C(11) - S(19)	122.2(3)
S(17) - C(11) - C(10)	121.9(4)
S(19) - C(11) - C(10)	115.9(3)
S(18) - C(12) - S(19)	112.0(3)
S(18) - C(12) - S(20)	124.8(3)
S(19) - C(12) - S(20)	123.1(4)
C(15) - N(1) - C(16)	121.3(5)
C(15) - N(1) - C(17)	122.4(5)
C(16) - N(1) - C(17)	116.1(5)
C(13) - N(2) - C(19)	118.2(5)
C(13) - N(2) - C(20)	119.5(6)

C(19) - N(2) - C(20)	122.2(6)
N(2) - C(13) - C(14)	121.1(6)
N(2) - C(13) - H(131)	120.9(6)
C(14) - C(13) - H(131)	117.9(6)
C(13) - C(14) - C(15)	121.6(6)
C(13) - C(14) - H(141)	119.6(5)
C(15) - C(14) - H(141)	118.8(5)
N(1) - C(15) - C(14)	123.5(5)
N(1) - C(15) - C(18)	120.8(5)
C(14) - C(15) - C(18)	115.7(5)
N(1) - C(16) - H(161)	111.3(6)
N(1) - C(16) - H(162)	110.9(6)
H(161)- C(16) - H(162)	109.1(7)
N(1) - C(16) - H(163)	109.9(6)
H(161)- C(16) - H(163)	108.2(7)
H(162)- C(16) - H(163)	107.3(7)
N(1) - C(17) - H(171)	110.4(6)
N(1) - C(17) - H(172)	109.4(6)
H(171)- C(17) - H(172)	107.3(7)
N(1) - C(17) - H(173)	111.6(6)
H(171)- C(17) - H(173)	109.7(6)
H(172)- C(17) - H(173)	108.4(7)
C(15) - C(18) - C(19)	118.6(6)
C(15) - C(18) - H(181)	120.3(5)
C(19) - C(18) - H(181)	121.1(6)
N(2) - C(19) - C(18)	124.8(6)
N(2) - C(19) - H(191)	117.5(6)
C(18) - C(19) - H(191)	117.8(7)
N(2) - C(20) - H(201)	111.3(8)
N(2) - C(20) - H(202)	110.6(7)
H(201)- C(20) - H(202)	109.2(8)
N(2) - C(20) - H(203)	109.5(7)
H(201)- C(20) - H(203)	108.5(7)
H(202)- C(20) - H(203)	107.7(8)

Atom	x/a	y/b	z/c	U(iso)	Occ
NI(1)	0.65675(3)	0.07312(6)	0.12554(2)	0.0194	
S(1)	0.58174(7)	0.0894(1)	0.19050(5)	0.0262	
S(2)	0.56078(7)	0.0741(1)	0.05854(5)	0.0247	
S(3)	0.40726(7)	0.1147(1)	0.18326(5)	0.0255	
S(4)	0.38819(7)	0.1039(1)	0.06111(5)	0.0262	
S(5)	0.24949(7)	0.1389(1)	0.12027(6)	0.0334	
S(6)	0.73039(7)	0.0555(1)	0.05966(5)	0.0293	
S(7)	0.75352(7)	0.0707(1)	0.19238(5)	0.0273	
S(8)	0.90521(8)	0.0447(1)	0.06529(6)	0.0347	
S(9)	0.92628(7)	0.0502(1)	0.18693(6)	0.0348	
S(10)	1.06434(8)	0.0204(2)	0.12650(9)	0.0546	
C(1)	0.4918(3)	0.0965(5)	0.1522(2)	0.0220	
C(2)	0.4836(3)	0.0909(5)	0.0943(2)	0.0203	
C(3)	0.3440(3)	0.1206(4)	0.1215(2)	0.0246	
C(4)	0.8213(3)	0.0556(5)	0.0974(2)	0.0264	
C(5)	0.8314(3)	0.0604(5)	0.1546(2)	0.0233	
C(6)	0.9697(3)	0.0377(5)	0.1255(3)	0.0370	
N(3)	0.2735(3)	0.7916(4)	0.1229(2)	0.0364	
N(4)	0.5094(3)	0.7583(4)	0.1225(2)	0.0365	
C(21)	0.4596(4)	0.7572(5)	0.0730(2)	0.0371	
C(22)	0.3828(4)	0.7704(6)	0.0723(2)	0.0370	
C(23)	0.3488(3)	0.7823(5)	0.1231(2)	0.0321	
C(24)	0.2202(3)	0.8029(6)	0.0720(2)	0.0417	
C(25)	0.2388(4)	0.8058(6)	0.1762(2)	0.0428	
C(26)	0.4024(3)	0.7823(5)	0.1730(2)	0.0325	
C(27)	0.4794(4)	0.7703(5)	0.1714(2)	0.0392	
C(28)	0.5922(4)	0.7470(6)	0.1216(3)	0.0493	
H(211)	0.4826	0.7457	0.0344	0.0351	

H(221)	0.3472	0.7710	0.0325	0.0431
H(241)	0.1630	0.8082	0.0814	0.0501
H(242)	0.2323	0.8835	0.0491	0.0501
H(243)	0.2246	0.7230	0.0458	0.0501
H(251)	0.1777	0.8110	0.1672	0.0509
H(252)	0.2590	0.8875	0.1977	0.0509
H(253)	0.2527	0.7272	0.2027	0.0509
H(261)	0.3809	0.7887	0.2127	0.0338
H(271)	0.5175	0.7731	0.2107	0.0437
H(281)	0.6210	0.7496	0.1633	0.0535
H(282)	0.6125	0.8219	0.0986	0.0535
H(283)	0.6054	0.6616	0.1027	0.0535
NI(2)	0.42859(3)	-0.07507(6)	0.37384(2)	0.0188
S(11)	0.50140(7)	-0.0600(1)	0.30743(5)	0.0234
S(12)	0.52610(7)	-0.0731(1)	0.43988(5)	0.0233
S(13)	0.67566(7)	-0.0343(1)	0.31251(5)	0.0267
S(14)	0.69837(7)	-0.0430(1)	0.43428(5)	0.0256
S(15)	0.83531(7)	-0.0118(1)	0.37255(6)	0.0343
S(16)	0.35442(7)	-0.0860(1)	0.43961(5)	0.0265
S(17)	0.33192(7)	-0.0721(1)	0.30728(5)	0.0267
S(18)	0.17961(7)	-0.1082(1)	0.43285(6)	0.0302
S(19)	0.15916(7)	-0.0998(1)	0.31092(5)	0.0289
S(20)	0.02070(8)	-0.1292(1)	0.37035(7)	0.0393
C(7)	0.5929(3)	-0.0507(5)	0.3450(2)	0.0218
C(8)	0.6026(3)	-0.0565(4)	0.4021(2)	0.0207
C(9)	0.7413(3)	-0.0289(5)	0.3733(2)	0.0252
C(10)	0.2634(3)	-0.0931(5)	0.4015(2)	0.0225
C(11)	0.2545(3)	-0.0884(5)	0.3444(2)	0.0231
C(12)	0.1139(3)	-0.1137(5)	0.3718(2)	0.0293
N(1)	0.9320(3)	0.7095(5)	0.0466(2)	0.0381
N(2)	0.8584(3)	0.7336(5)	0.2036(2)	0.0403
C(13)	0.9349(4)	0.7159(6)	0.1989(3)	0.0518
C(14)	0.9602(3)	0.7060(6)	0.1473(2)	0.0361
C(15)	0.9096(3)	0.7158(5)	0.0974(2)	0.0375
C(16)	1.0143(4)	0.6909(8)	0.0392(3)	0.0666
C(17)	0.8786(4)	0.7305(8)	-0.0053(3)	0.0641
C(18)	0.8289(3)	0.7334(5)	0.1041(2)	0.0348
C(19)	0.8092(4)	0.7421(6)	0.1567(3)	0.0539
C(20)	0.8334(6)	0.7422(8)	0.2598(3)	0.0860
H(131)	0.9772	0.7095	0.2359	0.0600
H(141)	1.0201	0.6916	0.1448	0.0439
H(161)	1.0218	0.6879	-0.0035	0.0808
H(162)	1.0361	0.6069	0.0590	0.0808
H(163)	1.0484	0.7667	0.0586	0.0808
H(171)	0.9080	0.7218	-0.0410	0.0666
H(172)	0.8563	0.8245	-0.0052	0.0666
H(173)	0.8322	0.6682	-0.0085	0.0666
H(181)	0.7865	0.7394	0.0681	0.0396
H(191)	0.7496	0.7562	0.1610	0.0675
H(201)	0.7736	0.7555	0.2571	0.0945
H(202)	0.8488	0.6600	0.2834	0.0945
H(203)	0.8615	0.8196	0.2822	0.0945

Atom	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
NI(1)	0.0156(3)	0.0247(3)	0.0189(3)	0.0012(3)	0.0058(2)	-0.0005(3)
S(1)	0.0198(6)	0.0417(8)	0.0177(6)	-0.0008(6)	0.0048(5)	0.0028(6)
S(2)	0.0197(6)	0.0366(7)	0.0189(6)	0.0022(6)	0.0067(5)	0.0015(6)
S(3)	0.0201(6)	0.0332(7)	0.0249(6)	-0.0011(5)	0.0097(5)	0.0045(5)
S(4)	0.0197(6)	0.0340(8)	0.0253(6)	0.0003(5)	0.0034(5)	0.0020(5)
S(5)	0.0162(6)	0.0366(8)	0.0485(8)	0.0015(7)	0.0085(6)	0.0017(6)
S(6)	0.0222(6)	0.0450(8)	0.0221(6)	0.0031(6)	0.0084(5)	-0.0004(6)
S(7)	0.0175(6)	0.0421(8)	0.0229(6)	-0.0033(6)	0.0047(5)	-0.0009(6)
S(8)	0.0228(7)	0.0401(8)	0.0451(8)	-0.0017(7)	0.0187(6)	-0.0017(6)
S(9)	0.0177(6)	0.0391(8)	0.0468(8)	-0.0016(7)	0.0011(6)	-0.0003(6)

S(10)	0.0167(7)	0.053(1)	0.096(1)	-0.0066(9)	0.0162(8)	0.0006(7)
C(1)	0.015(2)	0.024(3)	0.028(3)	0.002(2)	0.010(2)	0.005(2)
C(2)	0.016(2)	0.027(3)	0.018(2)	0.003(2)	0.003(2)	0.001(2)
C(3)	0.026(3)	0.018(2)	0.032(3)	0.002(2)	0.011(2)	-0.003(2)
C(4)	0.017(2)	0.027(3)	0.038(3)	0.001(2)	0.014(2)	0.002(2)
C(5)	0.016(2)	0.024(3)	0.031(3)	-0.004(2)	0.005(2)	-0.000(2)
C(6)	0.021(3)	0.030(3)	0.063(4)	-0.000(3)	0.017(3)	-0.007(2)
N(3)	0.047(3)	0.034(3)	0.028(2)	0.002(2)	0.003(2)	-0.003(2)
N(4)	0.050(3)	0.019(2)	0.042(3)	-0.002(2)	0.011(2)	-0.006(2)
C(21)	0.062(4)	0.019(3)	0.031(3)	0.001(2)	0.008(3)	0.002(3)
C(22)	0.054(4)	0.038(3)	0.021(3)	-0.003(2)	0.009(3)	0.005(3)
C(23)	0.047(3)	0.017(3)	0.033(3)	0.004(2)	0.007(3)	-0.003(2)
C(24)	0.040(3)	0.051(4)	0.034(3)	0.003(3)	0.008(3)	0.002(3)
C(25)	0.053(4)	0.050(4)	0.028(3)	-0.002(3)	0.014(3)	0.000(3)
C(26)	0.050(4)	0.022(3)	0.026(3)	-0.004(2)	0.005(2)	0.003(3)
C(27)	0.057(4)	0.026(3)	0.034(3)	-0.003(2)	0.004(3)	0.001(3)
C(28)	0.045(4)	0.025(3)	0.078(5)	0.008(3)	0.008(3)	-0.000(3)
NI(2)	0.0173(3)	0.0222(3)	0.0181(3)	-0.0014(3)	0.0075(2)	-0.0015(3)
S(11)	0.0179(6)	0.0349(7)	0.0184(6)	-0.0038(5)	0.0056(5)	-0.0005(5)
S(12)	0.0193(6)	0.0344(7)	0.0176(6)	0.0006(5)	0.0076(5)	0.0009(5)
S(13)	0.0185(6)	0.0402(8)	0.0232(6)	-0.0005(6)	0.0104(5)	0.0015(5)
S(14)	0.0179(6)	0.0381(8)	0.0209(6)	-0.0004(5)	0.0035(5)	0.0022(5)
S(15)	0.0174(6)	0.0451(9)	0.0415(8)	0.0007(7)	0.0078(6)	0.0023(6)
S(16)	0.0196(6)	0.0398(8)	0.0211(6)	0.0037(6)	0.0068(5)	-0.0013(6)
S(17)	0.0197(6)	0.0419(8)	0.0197(6)	-0.0032(6)	0.0072(5)	-0.0060(6)
S(18)	0.0228(7)	0.0381(8)	0.0325(7)	0.0050(6)	0.0139(6)	-0.0005(6)
S(19)	0.0190(6)	0.0375(8)	0.0304(7)	-0.0005(6)	0.0038(5)	-0.0019(5)
S(20)	0.0198(7)	0.0415(9)	0.059(1)	0.0014(7)	0.0146(7)	-0.0019(6)
C(7)	0.021(3)	0.021(3)	0.025(3)	-0.000(2)	0.012(2)	0.003(2)
C(8)	0.024(3)	0.019(3)	0.022(2)	-0.000(2)	0.011(2)	0.001(2)
C(9)	0.023(3)	0.025(3)	0.030(3)	-0.001(2)	0.013(2)	-0.001(2)
C(10)	0.020(2)	0.024(3)	0.026(3)	0.002(2)	0.011(2)	0.004(2)
C(11)	0.016(2)	0.023(3)	0.033(3)	-0.001(2)	0.013(2)	-0.005(2)
C(12)	0.021(2)	0.023(3)	0.046(3)	0.005(3)	0.015(2)	0.002(2)
N(1)	0.036(3)	0.047(3)	0.032(3)	-0.003(2)	0.006(2)	-0.005(2)
N(2)	0.051(3)	0.032(3)	0.039(3)	0.006(2)	0.010(2)	0.006(2)
C(13)	0.063(5)	0.046(4)	0.042(4)	0.002(3)	-0.005(3)	0.001(3)
C(14)	0.031(3)	0.036(3)	0.039(3)	0.009(3)	-0.001(3)	0.008(3)
C(15)	0.046(4)	0.028(3)	0.040(3)	0.002(3)	0.008(3)	-0.004(3)
C(16)	0.051(4)	0.088(6)	0.066(5)	-0.000(4)	0.029(4)	0.005(4)
C(17)	0.069(5)	0.089(6)	0.033(4)	-0.006(4)	0.002(3)	-0.016(4)
C(18)	0.031(3)	0.034(3)	0.040(3)	-0.006(3)	0.005(2)	0.001(2)
C(19)	0.061(4)	0.044(4)	0.059(5)	-0.002(3)	0.015(4)	0.002(3)
C(20)	0.144(9)	0.073(6)	0.051(5)	0.006(4)	0.051(5)	0.022(6)