

**Table 39A-4-001.** [N(CH<sub>3</sub>)<sub>4</sub>]<sub>2</sub>MnCl<sub>4</sub>. Crystal structure of phase I [89Mas]. Fractional coordinates [ $\cdot 10^{-4}$ ] and equivalent isotropic temperature parameters  $B_{\text{eq}}$  [ $\cdot 10^{-2} \text{ \AA}^2$ ].  $T = 293 \text{ K}$ .  $B_{\text{eq}} = (4/3)\Sigma b_{ij}\mathbf{a}_i \cdot \mathbf{a}_j$ , where  $b_{ij}$  is defined by Eq. (b) in Introduction. Fixed parameters are denoted by (\*).

Atom	$x$	$y$	$z$	$B_{\text{eq}}$
Mn	2500(*)	4074(1)	2456(1)	375(3)
Cl(1)	2682(7)	4064(3)	566(2)	695(10)
Cl(2)	2854(5)	5454(2)	3167(3)	716(15)
Cl(3)	270(4)	3537(3)	3060(4)	712(12)
Cl(4)	4491(5)	3227(3)	3085(4)	684(11)
N(1)	2500(*)	964(5)	1494(6)	459(20)
N(2)	7500(*)	3259(5)	84(6)	438(21)
C(1)	2135(36)	995(13)	2641(10)	1321(90)
C(2)	2028(27)	71(10)	1121(14)	1064(96)
C(3)	1557(25)	1630(12)	949(19)	1212(74)
C(4)	4033(21)	1138(20)	1200(21)	1460(104)
C(5)	7702(32)	2389(9)	566(15)	1243(57)
C(6)	6868(25)	3845(13)	916(15)	1196(87)
C(7)	6649(24)	3244(15)	−903(16)	1294(73)
C(8)	9002(16)	3566(10)	−171(17)	810(57)

**Table 39A-4-002.** [N(CH<sub>3</sub>)<sub>4</sub>]<sub>2</sub>MnCl<sub>4</sub>. Crystal structure of phase III [89Mas]. Fractional coordinates [ $\cdot 10^{-4}$ ] and equivalent isotropic temperature parameters  $B_{\text{eq}}$  [ $\cdot 10^{-2} \text{ \AA}^2$ ].  $T = 273 \text{ K}$ .  $B_{\text{eq}} = (4/3)\Sigma b_{ij}a_i \cdot a_j$ , where  $b_{ij}$  is defined by Eq. (b) in Introduction.

Atom	$x$	$y$	$z$	$B_{\text{eq}}$
Mn( <i>a</i> )	2543(1)	4075(1)	1222(1)	370(3)
Mn( <i>b</i> )	2705(1)	933(1)	3730(1)	359(3)
Cl(1 <i>a</i> )	2659(4)	4078(3)	279(1)	663(9)
Cl(2 <i>a</i> )	2894(4)	5450(2)	1593(1)	727(10)
Cl(3 <i>a</i> )	228(3)	3545(3)	1510(1)	699(10)
Cl(4 <i>a</i> )	4450(4)	3209(2)	1566(1)	721(10)
Cl(1 <i>b</i> )	2679(4)	939(3)	2780(1)	742(10)
Cl(2 <i>b</i> )	3034(4)	−451(2)	4085(2)	705(10)
Cl(3 <i>b</i> )	447(4)	1474(3)	4053(2)	779(10)
Cl(4 <i>b</i> )	4684(4)	1799(2)	4019(2)	716(9)
N(1 <i>a</i> )	2655(9)	936(6)	737(3)	484(22)
N(1 <i>b</i> )	2553(8)	4033(6)	3250(3)	417(20)
N(2 <i>a</i> )	7555(9)	3287(5)	54(3)	346(19)
N(2 <i>b</i> )	7618(9)	1771(6)	2528(4)	512(24)
C(1 <i>a</i> )	2425(22)	894(12)	1364(5)	1122(61)
C(2 <i>a</i> )	2228(19)	107(9)	484(7)	981(53)
C(3 <i>a</i> )	1691(21)	1604(10)	472(7)	1051(60)
C(4 <i>a</i> )	4210(16)	1134(14)	614(7)	1162(67)
C(1 <i>b</i> )	2373(20)	3925(10)	3826(4)	890(50)
C(2 <i>b</i> )	2106(19)	4909(8)	3071(5)	847(47)
C(3 <i>b</i> )	1622(20)	3362(10)	2983(7)	1053(56)
C(4 <i>b</i> )	4120(16)	3879(13)	3081(7)	1103(63)
C(5 <i>a</i> )	7757(18)	2398(9)	286(7)	1040(53)
C(6 <i>a</i> )	6686(18)	3766(12)	391(8)	1416(61)
C(7 <i>a</i> )	6785(21)	3185(12)	−464(6)	1436(59)
C(8 <i>a</i> )	9000(15)	3632(9)	−57(7)	936(52)
C(5 <i>b</i> )	7566(20)	2665(9)	2715(7)	1136(58)
C(6 <i>b</i> )	7441(28)	1100(11)	2980(6)	1386(84)
C(7 <i>b</i> )	6410(21)	1578(13)	2190(8)	1611(69)
C(8 <i>b</i> )	9070(19)	1568(11)	2303(8)	1298(66)

**Table 39A-4-003.** [N(CH<sub>3</sub>)<sub>4</sub>]<sub>2</sub>MnCl<sub>4</sub>. Crystal structure of phase IV [89Mas]. Fractional coordinates [ $\cdot 10^{-4}$ ] and equivalent isotropic temperature parameters  $B_{\text{eq}}$  [ $\cdot 10^{-2} \text{ \AA}^2$ ].  $T = 261 \text{ K}$ .  $B_{\text{eq}} = (4/3)\Sigma b_{ij}a_i \cdot a_j$ , where  $b_{ij}$  is defined by Eq. (b) in Introduction.

Atom	$x$	$y$	$z$	$B_{\text{eq}}$
Mn( <i>a</i> )	2526(2)	4088(1)	816(1)	324(4)
Mn( <i>b</i> )	2794(2)	4092(1)	4157(1)	328(4)
Mn( <i>c</i> )	2256(2)	4021(1)	7489(1)	338(4)
Cl(1 <i>a</i> )	2739(4)	4061(3)	184(1)	609(12)
Cl(2 <i>a</i> )	2847(5)	5477(3)	1054(1)	632(12)
Cl(3 <i>a</i> )	181(4)	3555(3)	995(1)	651(13)
Cl(4 <i>a</i> )	4401(4)	3230(3)	1065(1)	619(11)
Cl(1 <i>b</i> )	2604(5)	4110(3)	3523(1)	629(12)
Cl(2 <i>b</i> )	3194(5)	5482(3)	4384(1)	603(12)
Cl(3 <i>b</i> )	569(4)	3567(3)	4406(1)	643(12)
Cl(4 <i>b</i> )	4810(4)	3197(3)	4323(1)	613(11)
Cl(1 <i>c</i> )	2152(5)	4070(3)	6855(1)	649(12)
Cl(2 <i>c</i> )	1890(5)	5380(3)	7761(1)	633(12)
Cl(3 <i>c</i> )	371(5)	3120(3)	7695(1)	670(12)
Cl(4 <i>c</i> )	4578(4)	3491(3)	7666(1)	644(12)
N(1 <i>a</i> )	2749(10)	954(8)	496(3)	426(30)
N(1 <i>b</i> )	2564(10)	989(6)	3828(2)	273(23)
N(1 <i>c</i> )	2316(12)	882(9)	7161(3)	548(35)
N(2 <i>a</i> )	7572(10)	3241(7)	35(3)	370(28)
N(2 <i>b</i> )	7631(11)	3263(7)	3343(3)	408(29)
N(2 <i>c</i> )	7258(11)	3264(7)	6693(3)	420(29)
C(1 <i>a</i> )	2372(23)	907(21)	896(5)	1167(93)
C(2 <i>a</i> )	2331(20)	88(12)	357(5)	799(56)
C(3 <i>a</i> )	1789(22)	1608(12)	303(6)	908(65)
C(4 <i>a</i> )	4370(18)	1042(15)	429(7)	941(73)
C(1 <i>b</i> )	2487(27)	1037(14)	4228(5)	951(74)
C(2 <i>b</i> )	2013(21)	130(12)	3711(5)	810(57)
C(3 <i>b</i> )	1541(27)	1559(19)	3670(7)	1411(94)
C(4 <i>b</i> )	4062(18)	1165(15)	3711(5)	858(65)
C(1 <i>c</i> )	2552(25)	996(13)	7565(4)	965(66)
C(2 <i>c</i> )	2766(23)	33(11)	7005(6)	798(63)
C(3 <i>c</i> )	756(18)	1129(20)	7082(6)	1218(89)
C(4 <i>c</i> )	3216(21)	1627(11)	6989(4)	683(53)
C(5 <i>a</i> )	7868(25)	2400(14)	186(7)	1046(77)
C(6 <i>a</i> )	6854(20)	3862(14)	323(4)	882(58)
C(7 <i>a</i> )	6478(21)	3166(14)	-260(5)	1004(60)
C(8 <i>a</i> )	9022(18)	3650(13)	-65(6)	838(65)
C(5 <i>b</i> )	7490(21)	2366(10)	3439(6)	853(61)
C(6 <i>b</i> )	8622(32)	3661(21)	3564(8)	2183(148)
C(7 <i>b</i> )	6200(21)	3616(17)	3307(9)	1476(117)
C(8 <i>b</i> )	8135(36)	3245(17)	2967(6)	1762(103)
C(5 <i>c</i> )	7282(23)	2294(10)	6826(6)	960(61)
C(6 <i>c</i> )	7885(27)	3824(13)	6954(6)	1048(114)
C(7 <i>c</i> )	5775(17)	3508(10)	6585(5)	711(63)
C(8 <i>c</i> )	8291(23)	3438(15)	6400(6)	1343(77)

**Table 39A-4-004.** [N(CH<sub>3</sub>)<sub>4</sub>]<sub>2</sub>MnCl<sub>4</sub>. Crystal structure of phase V [89Mas]. Fractional coordinates [ $\cdot 10^{-4}$ ] and equivalent isotropic temperature parameters  $B_{\text{eq}}$  [ $\cdot 10^{-2} \text{ \AA}^2$ ].  $T = 168 \text{ K}$ .  $B_{\text{eq}} = (4/3) \sum b_{ij} \mathbf{a}_i \cdot \mathbf{a}_j$ , where  $b_{ij}$  is defined by Eq. (b) in Introduction.

Atom	$x$	$y$	$z$	$B_{\text{eq}}$
Mn	2252(1)	4054(1)	2469(1)	157(1)
Cl(1)	2732(2)	4073(1)	573(1)	236(3)
Cl(2)	1875(2)	5462(1)	3187(1)	298(4)
Cl(3)	91(2)	3217(1)	2844(1)	264(4)
Cl(4)	4360(2)	3435(1)	3316(1)	329(3)
N(1)	2641(6)	972(3)	1496(3)	205(10)
N(2)	7520(5)	3295(3)	36(4)	186(10)
C(1)	2208(9)	1030(4)	2682(4)	350(16)
C(2)	2462(12)	46(4)	1115(6)	466(23)
C(3)	1635(9)	1557(5)	815(6)	393(18)
C(4)	4205(9)	1250(7)	1344(7)	599(27)
C(5)	7673(9)	2345(4)	336(6)	337(16)
C(6)	6806(8)	3783(5)	964(6)	358(17)
C(7)	6537(9)	3380(5)	−959(5)	383(16)
C(8)	9018(7)	3650(4)	−203(6)	292(17)

**Table 39A-4-005.** [N(CH<sub>3</sub>)<sub>4</sub>]<sub>2</sub>MnCl<sub>4</sub>. Crystal structure [89Mas]. Bond distances [ $\text{\AA}$ ] and angles [ $^\circ$ ] in phase I.  $T = 293 \text{ K}$ .

Mn–Cl(1)	2.338(4)	N(1)–C(1)	1.453(17)	N(2)–C(5)	1.497(19)
Mn–Cl(2)	2.354(13)	N(1)–C(2)	1.534(20)	N(2)–C(6)	1.491(24)
Mn–Cl(3)	2.309(13)	N(1)–C(3)	1.507(24)	N(2)–C(7)	1.442(23)
Mn–Cl(4)	2.369(16)	N(1)–C(4)	1.460(21)	N(2)–C(8)	1.475(17)
Cl(1)–Mn–Cl(2)	111.6(7)	Cl(1)–Mn–Cl(3)	112.4(7)		
Cl(1)–Mn–Cl(4)	105.6(7)	Cl(2)–Mn–Cl(3)	109.5(6)		
Cl(2)–Mn–Cl(4)	106.8(5)	Cl(3)–Mn–Cl(4)	110.7(4)		
C(1)–N(1)–C(2)	105.0(11)	C(1)–N(1)–C(3)	106.4(13)		
C(1)–N(1)–C(4)	116.9(14)	C(2)–N(1)–C(3)	109.9(11)		
C(2)–N(1)–C(4)	111.1(11)	C(3)–N(1)–C(4)	107.3(9)		
C(5)–N(2)–C(6)	109.5(8)	C(5)–N(2)–C(7)	112.7(9)		
C(5)–N(2)–C(8)	105.6(13)	C(6)–N(2)–C(7)	112.8(11)		
C(6)–N(2)–C(8)	107.4(9)	C(7)–N(2)–C(8)	108.4(10)		

**Table 39A-4-006.** [N(CH<sub>3</sub>)<sub>4</sub>]<sub>2</sub>MnCl<sub>4</sub>. Crystal structure [89Mas]. Bond distances [Å] and angles [°] in phase III. *T* = 273 K.

Mn( <i>a</i> )–Cl(1 <i>a</i> )	2.329(3)	Mn( <i>b</i> )–Cl(1 <i>b</i> )	2.344(3)
Mn( <i>a</i> )–Cl(2 <i>a</i> )	2.356(25)	Mn( <i>b</i> )–Cl(2 <i>b</i> )	2.352(24)
Mn( <i>a</i> )–Cl(3 <i>a</i> )	2.360(8)	Mn( <i>b</i> )–Cl(3 <i>b</i> )	2.349(9)
Mn( <i>a</i> )–Cl(4 <i>a</i> )	2.349(15)	Mn( <i>b</i> )–Cl(4 <i>b</i> )	2.354(13)
N(1 <i>a</i> )–C(1 <i>a</i> )	1.562(16)	N(1 <i>b</i> )–C(1 <i>b</i> )	1.439(14)
N(1 <i>a</i> )–C(2 <i>a</i> )	1.490(24)	N(1 <i>b</i> )–C(2 <i>b</i> )	1.494(20)
N(1 <i>a</i> )–C(3 <i>a</i> )	1.508(24)	N(1 <i>b</i> )–C(3 <i>b</i> )	1.497(23)
N(1 <i>a</i> )–C(4 <i>a</i> )	1.472(18)	N(1 <i>b</i> )–C(4 <i>b</i> )	1.496(17)
N(2 <i>a</i> )–C(5 <i>a</i> )	1.514(23)	N(2 <i>b</i> )–C(5 <i>b</i> )	1.472(22)
N(2 <i>a</i> )–C(6 <i>a</i> )	1.367(24)	N(2 <i>b</i> )–C(6 <i>b</i> )	1.538(29)
N(2 <i>a</i> )–C(7 <i>a</i> )	1.466(18)	N(2 <i>b</i> )–C(7 <i>b</i> )	1.407(22)
N(2 <i>a</i> )–C(8 <i>a</i> )	1.439(16)	N(2 <i>b</i> )–C(8 <i>b</i> )	1.460(20)
Cl(1 <i>a</i> )–Mn( <i>a</i> )–Cl(2 <i>a</i> )	112.3(14)	Cl(1 <i>b</i> )–Mn( <i>b</i> )–Cl(2 <i>b</i> )	112.1(15)
Cl(1 <i>a</i> )–Mn( <i>a</i> )–Cl(3 <i>a</i> )	109.9(6)	Cl(1 <i>b</i> )–Mn( <i>b</i> )–Cl(3 <i>b</i> )	109.2(6)
Cl(1 <i>a</i> )–Mn( <i>a</i> )–Cl(4 <i>a</i> )	109.1(9)	Cl(1 <i>b</i> )–Mn( <i>b</i> )–Cl(4 <i>b</i> )	107.9(10)
Cl(2 <i>a</i> )–Mn( <i>a</i> )–Cl(3 <i>a</i> )	108.8(4)	Cl(2 <i>b</i> )–Mn( <i>b</i> )–Cl(3 <i>b</i> )	108.4(5)
Cl(2 <i>a</i> )–Mn( <i>a</i> )–Cl(4 <i>a</i> )	106.7(3)	Cl(2 <i>b</i> )–Mn( <i>b</i> )–Cl(4 <i>b</i> )	108.7(2)
Cl(3 <i>a</i> )–Mn( <i>a</i> )–Cl(4 <i>a</i> )	109.9(7)	Cl(3 <i>b</i> )–Mn( <i>b</i> )–Cl(4 <i>b</i> )	110.5(8)
C(1 <i>a</i> )–N(1 <i>a</i> )–C(2 <i>a</i> )	110.1(14)	C(1 <i>b</i> )–N(1 <i>b</i> )–C(2 <i>b</i> )	111.5(15)
C(1 <i>a</i> )–N(1 <i>a</i> )–C(3 <i>a</i> )	112.4(13)	C(1 <i>b</i> )–N(1 <i>b</i> )–C(3 <i>b</i> )	106.8(12)
C(1 <i>a</i> )–N(1 <i>a</i> )–C(4 <i>a</i> )	109.9(8)	C(1 <i>b</i> )–N(1 <i>b</i> )–C(4 <i>b</i> )	111.3(8)
C(2 <i>a</i> )–N(1 <i>a</i> )–C(3 <i>a</i> )	105.7(7)	C(2 <i>b</i> )–N(1 <i>b</i> )–C(3 <i>b</i> )	111.1(8)
C(2 <i>a</i> )–N(1 <i>a</i> )–C(4 <i>a</i> )	110.1(8)	C(2 <i>b</i> )–N(1 <i>b</i> )–C(4 <i>b</i> )	108.7(8)
C(3 <i>a</i> )–N(1 <i>a</i> )–C(4 <i>a</i> )	108.5(8)	C(3 <i>b</i> )–N(1 <i>b</i> )–C(4 <i>b</i> )	107.3(9)
C(5 <i>a</i> )–N(2 <i>a</i> )–C(6 <i>a</i> )	110.0(8)	C(5 <i>b</i> )–N(2 <i>b</i> )–C(6 <i>b</i> )	114.6(8)
C(5 <i>a</i> )–N(2 <i>a</i> )–C(7 <i>a</i> )	106.7(13)	C(5 <i>b</i> )–N(2 <i>b</i> )–C(7 <i>b</i> )	111.4(12)
C(5 <i>a</i> )–N(2 <i>a</i> )–C(8 <i>a</i> )	107.8(9)	C(5 <i>b</i> )–N(2 <i>b</i> )–C(8 <i>b</i> )	110.8(10)
C(6 <i>a</i> )–N(2 <i>a</i> )–C(7 <i>a</i> )	108.6(12)	C(6 <i>b</i> )–N(2 <i>b</i> )–C(7 <i>b</i> )	101.6(10)
C(6 <i>a</i> )–N(2 <i>a</i> )–C(8 <i>a</i> )	115.7(7)	C(6 <i>b</i> )–N(2 <i>b</i> )–C(8 <i>b</i> )	102.8(9)
C(7 <i>a</i> )–N(2 <i>a</i> )–C(8 <i>a</i> )	107.7(8)	C(7 <i>b</i> )–N(2 <i>b</i> )–C(8 <i>b</i> )	115.2(7)

**Table 39A-4-007.** [N(CH<sub>3</sub>)<sub>4</sub>]<sub>2</sub>MnCl<sub>4</sub>. Crystal structure [89Mas]. Bond distances [Å] and angles [°] in phase IV. *T* = 261 K.

	Type <i>a</i>	Type <i>b</i>	Type <i>c</i>
Mn–Cl(1)	2.345(4)	2.349(4)	2.345(4)
Mn–Cl(2)	2.356(9)	2.350(11)	2.370(10)
Mn–Cl(3)	2.368(23)	2.356(22)	2.332(32)
Mn–Cl(4)	2.351(30)	2.381(3)	2.352(23)
N(1)–C(1)	1.521(21)	1.485(21)	1.517(20)
N(1)–C(2)	1.494(24)	1.490(25)	1.502(25)
N(1)–C(3)	1.520(29)	1.412(34)	1.492(24)
N(1)–C(4)	1.491(20)	1.447(21)	1.553(29)
N(2)–C(5)	1.451(25)	1.448(19)	1.591(20)
N(2)–C(6)	1.545(22)	1.361(33)	1.420(25)
N(2)–C(7)	1.478(21)	1.413(25)	1.451(20)
N(2)–C(8)	1.503(22)	1.464(26)	1.453(25)
Cl(1)–Mn–Cl(2)	112.3(2)	110.8(1)	112.9(2)
Cl(1)–Mn–Cl(3)	110.3(2)	109.4(2)	108.5(3)
Cl(1)–Mn–Cl(4)	108.7(4)	108.7(2)	109.0(2)
Cl(2)–Mn–Cl(3)	108.9(14)	108.0(13)	107.2(9)
Cl(2)–Mn–Cl(4)	106.9(9)	109.5(10)	108.9(13)
Cl(3)–Mn–Cl(4)	109.7(4)	110.5(4)	110.3(5)
C(1)–N(1)–C(2)	103.7(8)	108.6(6)	116.3(7)
C(1)–N(1)–C(3)	111.2(10)	110.5(10)	107.2(9)
C(1)–N(1)–C(4)	112.7(8)	109.4(10)	104.1(9)
C(2)–N(1)–C(3)	107.6(9)	103.2(12)	114.3(16)
C(2)–N(1)–C(4)	105.7(17)	113.2(15)	111.0(10)
C(3)–N(1)–C(4)	115.1(11)	111.8(10)	102.6(12)
C(5)–N(2)–C(6)	111.7(4)	110.4(9)	111.5(6)
C(5)–N(2)–C(7)	109.8(9)	108.8(13)	110.6(12)
C(5)–N(2)–C(8)	108.4(13)	104.0(5)	113.4(10)
C(6)–N(2)–C(7)	108.5(11)	118.7(8)	113.1(9)
C(6)–N(2)–C(8)	102.9(7)	112.0(16)	97.9(11)
C(7)–N(2)–C(8)	115.5(4)	101.7(12)	109.9(7)

**Table 39A-4-008.** [N(CH<sub>3</sub>)<sub>4</sub>]<sub>2</sub>MnCl<sub>4</sub>. Crystal structure [89Mas]. Bond distances [Å] and angles [°] in phase V. *T* = 168 K.

Mn–Cl(1)	2.358(15)	N(1)–C(1)	1.503(15)	N(2)–C(5)	1.509(7)
Mn–Cl(2)	2.356(5)	N(1)–C(2)	1.504(8)	N(2)–C(6)	1.504(18)
Mn–Cl(3)	2.372(13)	N(1)–C(3)	1.519(19)	N(2)–C(7)	1.507(26)
Mn–Cl(4)	2.353(28)	N(1)–C(4)	1.480(11)	N(2)–C(8)	1.481(12)
Cl(1)–Mn–Cl(2)	112.4(3)	Cl(1)–Mn–Cl(3)	110.4(15)		
Cl(1)–Mn–Cl(4)	106.7(13)	Cl(2)–Mn–Cl(3)	107.8(8)		
Cl(2)–Mn–Cl(4)	108.8(7)	Cl(3)–Mn–Cl(4)	110.7(3)		
C(1)–N(1)–C(2)	109.0(3)	C(1)–N(1)–C(3)	109.8(9)		
C(1)–N(1)–C(4)	110.6(17)	C(2)–N(1)–C(3)	109.0(9)		
C(2)–N(1)–C(4)	109.5(8)	C(3)–N(1)–C(4)	108.9(8)		
C(5)–N(2)–C(6)	109.7(4)	C(5)–N(2)–C(7)	109.4(3)		
C(5)–N(2)–C(8)	108.7(5)	C(6)–N(2)–C(7)	108.5(5)		
C(6)–N(2)–C(8)	110.8(13)	C(7)–N(2)–C(8)	109.8(11)		

**Table 39A-4-009.** [N(CH<sub>3</sub>)<sub>4</sub>]<sub>2</sub>MnCl<sub>4</sub>. Transition heat ( $\Delta Q$ ) and transition entropy ( $\Delta S$ ) [88Zub]. *R*: gas constant.

Transition	$\Theta$ [K] <sub>on heating</sub>	$\Theta$ [K] <sub>on cooling</sub>	$\Delta Q/R$ [K]	$\Delta S/R$
I–II	292.60(1)	292.60(1)	250(20)	0.96(10)
II–III	292.30(1)	292.18(1)	0.7(2)	0.0024(6)
III–IV	268.65(1)	266.70(1)	28(5)	0.10(2)
IV–V	175.63(1)	–	37(3)	0.21(2)