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Volume 55, 2002

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10.1071/CH02040_AC

Accessory Publication: *Aust. J. C*hem., 2002, 55(5), 343-348.

SUPPLEMENTARY DATA

Model compounds related to saquayamycin. Attempts to introduce the *cis* dihydroxyl substitution at the A/B ring junction.

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Table 2. ^{1}H NMR data for bis-epoxide 8

1H ppm	Assignment	Area	Multiplicity/J	COSY	ROESY
3.51	H_{9a}	1	d, 4.5Hz	H_{9b}	H_{9b}, H_{3a}
3.34	H_{8}	1	broad singlet	H_{6up}	CH_{3down}, CH_{3up}
3.15	H_{3a}	1	dd, 7.2, 11.1 Hz	H_{4down}, H_{9b}	H_{4down}, H_{9a}
3.09	H_{9b}	1	dd, 4.5, 11.1 Hz	H_{3a}, H_{9a}	H_{9a}, H_{4down}, H_{6down}
3.04	H_{5}	1	d, 4.2 Hz	H_{4up}	H_{6up}, H_{4up}
2.68	H_{4up}	1	dd, 4.2, 15 Hz	H_{5}, H_{4down}	H_{5}, H_{4down}
2.22	H_{4down}	1	dd, 7.2, 15 Hz	H_{4up}, H_{3a}	H_{up}, H_{3a}
2.12	CH_{3}, Acetate	3	s		
1.94	H_{6down}	1	d 13.8Hz	H_{6up}, CH_{3down}	H_{9b}, CH_{3down}, CH_{3up}
1.45	CH_{3down}	3	s	H_{6down}	CH_{3up}, H_{6down}, H_{6up}
1.09	CH_{3up}	3	s		CH_{3pdown}, H_{6down}, H_{6up}
0.79	H_{6up}	1	d 13.8Hz	H_{6down}, H_{8}	H_{5}, CH_{3down}, CH_{3up}

Table 3. ^{13}C NMR data for bis-epoxide 8

1Hppm	Assignment	HMQC	Assignment	HMBC
3.51	H_{9a}	37.2	C_{9a}	9b, 5, 5a, 8, 9
3.34	H_{8}	67.2	C_{8}	CH_{3up}, 7, 6/9a, 9
3.15	H_{3a}	37.6	C_{3a}	4, 9b, 5
3.09	H_{9b}	39.85	C_{9b}	4, 3a/9a, 5a, 9
3.04	H_{5}	55.2	C_{5}	4, 3a/9a/6, 5a
2.68	H_{4up}	24.1	C_{4}	3a/9a, 9b, 5, 5a

2.22	H_{4down}	24.1	C_4	3a/9a, 5, 5a
2.12	CH_3, Acetate	21.2	Acetate	9
1.94	H_{6down}	37.4	C_6	CH_{3down}, CH_{3up}, 7, 5a, 8
1.45	CH_{3down}	23.17	CH_{3down}	CH_{3up}, 7, 6, 8
1.09	CH_{3up}	27.5	CH_{3up}	CH_{3down}, 7, 6, 8, 9
0.79	H_{6up}	37.4	C_6	CH_{3down}, 7, 9a, 9b, 5, 5a, 8

Table 4. ^{1}H NMR data for mono-epoxide 7

1H ppm	Assignment	Area	Multiplicity/Js	COSY	ROESY
5.62	H_8	1	broad singlet	H_{9a}, H_{6up}	CH_{3down}, CH_{3up}
3.49	H_{9a}	1	dd, 2.4, 6 Hz	H_8, H_{9b}	H_{9b}, H_{3a}, H_{4down}, H_{6down}
3.14	H_{9b}	1	dd, 6, 11.4 Hz	H_{9a}, H_{3a}	H_{9a}, H_{3a},
3.13	H_5	1	d, 4.2 Hz	H_{4up}	H_{4up}, H_{6up}
3.12	H_{3a}	1	ddd, 1.2, 7.8, 11.4 Hz	H_{9b}, H_{4down}	H_{9a}, H_{9b}, H_{4down}
2.73	H_{4up}	1	ddd, 1.2, 4.2, 15.6 Hz	H_{4down}, H_5	H_5, H_{4up}
2.27	H_{4down}	1	dd, 7.8, 15.6 Hz	H_{4up}, H_{3a}	H_{4up}, H_{3a}
2.19	CH_3, Acetate	3	s		
2.12	H_{6down}	1	d, 14.4 Hz	H_{6up}	H_{6up}, CH_{3down}, CH_{3up}, H_{9a}
1.22	H_{6up}	1	d, 14.4 Hz	H_{6down}	H_{6down}, CH_{3down}, CH_{3up}, H_5
1.12	CH_{3down}	3	s		
1.11	CH_{3up}	3	s		

Table 5. ^{13}C NMR data for mono-epoxide 7

1Hppm	Assignment	HMQC	Assignment	HMBC
5.62	H_8	127	C_8	CH_{3down}, 9a, 9b, 9
3.49	H_{9a}	36.5	C_{9a}	3a, 5, 5a, 8, 9, 2
3.14	H_{9b}	38	C_{9b}	1, 2, 5a, 3a/9a
3.13	H_5	53.7	C_5	1, 2, 5a, 6, 3a/9a/9b, 4
3.12	H_{3a}	37.1	C_{3a}	4, 9b, 5
2.73	H_{4up}	24.1	C_4	1, 5a, 5, 3, 9a, 4
2.27	H_{4down}	24.1	C_4	1, 3a, 5a
2.19	CH_3, Acetate	21.2	CH_3, Acetate	
2.12	H_{6down}	41.6	C_6	CH_{3down}, CH_{3up}, 7
1.22	H_{6up}	41.6	C_6	8, 5a, 9b, 7
1.12	CH_{3down}	28.4	CH_{3eq}	CH_{3up}, 7, 6
1.11	CH_{3up}	30.8	CH_{3ax}	CH_{3down}, 7, 6, 9

Table 6. ^{1}H NMR data for bromo-adduct 9

1H ppm	Assignment	Area	Multiplicity/J	COSY	ROESY
5.99	H_5	1	m	H_{9a}, H_{4down}, H_{4up}, H_{6down}	H_{4up}, H_{9a}, H_{6up}
5.65	H_8	1	bs	H_{6up}	Acetate
3.81	H_{3a} and H_{9a}	2	m	H_5, H_{4down}, H_{4up}, H_{6down}	H_{4down}, H_{4up}, H_{6down}
2.77	H_{4up}	1	ddd 2.4, 7.2, 15.6 Hz	H_{3a}, H_5, H_{4down}	H_5, H_{3a}, H_{4down}
2.45	H_{4down}	1	bd 15.6 Hz	H_{4up}, H_{9a}, H_5. H_{6down}	H_{3a}, H_{4up}
2.33	H_{6down}	1	bd 13.8 Hz	H_{4down}, H_{9a}, H_5, H_{6up}	H_{6up}
2.21	Acetate	3	s		H_8
2.11	H_{6up}	1	d 13.8 Hz	H_{6down}, H_8	H_{6down}

1.06	CH_3	3	s		CH_3, H_8
0.83	CH_3	3	s		CH_3, H_8

Table 7. ^{13}C NMR data for bromo-adduct 9

1H ppm	Assignment	HMQC	Assignment	HMBC
5.99	H_5	124.92	C_5	
5.65	H_8	130.97	C_8	9, Acetate
3.81	H_{3a}	55.96	C_{3a}	5, 5a, 1, 2
3.81	H_{9a}	45.06	C_{9a}	5, 5a, 9, 1, Acetate
2.77	H_{4up}	22.72	C_4	5, 5a, 2
2.45	H_{4down}	22.72	C_4	
2.33	H_{6down}	44.89	C_6	5, 5a
2.21	Acetate	21.68	Acetate	9, Acetate
2.11	H_{6up}	44.89	C_6	5, 8, 5a
1.06	CH_3	30.1	CH_3	8
0.83	CH_3	27.36	CH_3	8

Table 8 ^{1}H NMR data for aromatic system 11

1H ppm	Assignment	Area	Multiplicity/Js	COSY	ROESY
7.87	H_4	1	d, 7.8 Hz	H_5	H_4
7.62	H_5	1	d, 7.8 Hz	H_4	H_5, H_6, H_6
6.3	H_9	1	t, 6 Hz	H_8, H_8	H_8, H_8
2.84	H_6	1	d, 11.3 Hz	H_6	H_6, H_5
2.69	H_6	1	d, 11.3 Hz	H_6	H_6, H_5
2.17	H_8	1	dd, 5.8, 13.8 Hz	H_9, H_8	H_9, H_8, H_6, CH_3
2.06	Acetate	3	s		
1.85	H_8	1	dd, 5.2, 13.8 Hz	H_9, H_8	H_9, H_8, H_6, CH_3
1.08	CH_3	3	s		H_8, H_8, H_6, H_6, H_9
1.05	CH_3	3	s		H_8, H_8, H_6, H_6, H_9

Table 9 ^{13}C NMR data for aromatic system 11

1Hppm	Assignment	HMQC	Assignment	HMBC
7.87	H_4	124.79	C_4	9b, 9a, 2
7.62	H_5	137.32	C_5	3a, 5a
6.3	H_9	66.03	C_9	9b, 5a, 9a, 1
2.84	H_6	44.06	C_6	5a, 5, 9a
2.69	H_6	44.06	C_6	5a, 5, 9a
2.17	H_8	41.06	C_8	5a, 1
2.06	Acetate	20.62	Acetate	1
1.85	H_8	41.06	C_8	5a
1.08	CH_3	28.41	CH_3	
1.05	CH_3	27.94	CH_3	

Table 10. ^{1}H NMR data for bromo mono-epoxide 12a

1H ppm	Assignment	Area	Multiplicity/Js	COSY	ROESY
5.65	H_8	1	s		CH_3, CH_3

3.84	H_{9a}	1	s		H_{6down}, H_{4down}
3.54	H_{3a}	1	d, 7.2 Hz	H_{4down}	H_{4down}, H_{4up}
3.16	H_5	1	d, 4.2 Hz	H_{4up}	H_{6down}, H_{6upn}, H_{4down}, H_{4up}
2.75	H_{4up}	1	dd, 4.2, 15 Hz	H_5, H_{4down}	H_5, H_{3a}, H_{4down}
2.56	H_{4down}	1	dd, 7.2, 15 Hz	H_{3a}, H_{4up}	H_5, H_{3a}, H_{4up}
2.2	CH_3, Acetate	3	s		
2.13	H_{6down}	1	d, 14.4 Hz	H_{6up}	H_5, H_{9a}, H_{6up}
1.17	H_{6up}	1	d, 14.4 Hz	H_{6down}	H_{6down}, H_5
1.1	CH_3	3	s		H_{6down}, H_5, H_8
1.08	CH_3	3	s		H_{6down}, H_5, H_8

Table 11. ^{1}H NMR data for bromo mono-epoxide 12b

1H ppm	Assignment	Area	Multiplicity/Js	COSY	ROESY
5.65	H_8	1	s		CH_3, CH_3
3.68	H_{9a}	1	s		H_{6down}, H_{4down}
3.61	H_{3a}	1	d, 7.2 Hz	H_{4down}	H_{4down}, H_{4up}
3.09	H_5	1	d, 4.8 Hz	H_{4up}	H_{6down}, H_{6up}, H_{4down}, H_{4up}
2.7	H_{4up}	1	dd, 4.8, 15 Hz	H_5, H_{4down}	H_5, H_{3a}, H_{4down}
2.5	H_{4down}	1	dd, 7.2, 15 Hz	H_{3a}, H_{4up}	H_5, H_{3a}, H_{4up}
2.2	CH_3, Acetate	3	s		
2.13	H_{6down}	1	d, 14.4 Hz	H_{6up}	H_5, H_{9a}, H_{6up}
1.17	H_{6up}	1	d, 14.4 Hz	H_{6down}	H_{6down}, H_5
1.1	CH_3	3	s		H_{6down}, H_5, H_8
1.08	CH_3	3	s		H_{6down}, H_5, H_8

Table 12. ^{13}C NMR data for bromo mono-epoxides 12a and 12b

1H ppm	Assignment	HMQC	Assignment	HMBC
5.65	H_8	131.05	C_8	9, 9a, CH_3
3.84/3.68	H_{9a}	42.56	C_{9a}	3a, 8, 9, Acetate
3.54/3.61	H_{3a}	53.24	C_{3a}	4, 5, 9b,
3.16/3.09	H_5	54.46	C_5	3a, 4
2.75/2.7	H_{4up}	24.29	C_4	3a, 5, 9a, 9b
2.56/2.5	H_{4down}	24.29	C_4	5, 5a
2.2	CH_3, Acetate	21.83	Acetate	2
2.13	H_{6down}	42.58	C_6	CH_3, CH_3, 1, 7
1.17	H_{6up}	42.58	C_6	CH_3, CH_3, 5a, 9a
1.1	CH_3	27.88	CH_3	CH_3, 8, 9a, 9b
1.08	CH_3	30.87	CH_3	CH_3, 8, 9a, 9b

Table 13. ^{1}H NMR for the aromatic system 13

1H ppm	Assignment	Area	Multiplicity/Js	COSY	ROESY
7.82	H_5	1	d, 7.6 Hz	H_4	H_4
7.64	H_4	1	d, 7.6 Hz	H_5	H_5, H_6
5.88	H_8	1	s		H_6, CH_3
2.92	H_6	2	s		H_4, H_8
2.34	Acetate	3	s		
1.15	2 x CH_3	6	s		H_8

Table 14. ^{13}C NMR for the aromatic system 13

1H ppm	Assignment	HMQC	Assignment	HMBC
7.82	H_5	137.18	C_5	1, 3a, 5a
7.64	H_4	124.57	C_4	3, 3a, 5, 5a, 6, 9a
5.88	H_8	134.31	C_8	6, 7, 9, 9a, CH_3
2.92	H_6	43.79	C_6	3a, 5, 5a, 7, 8, 9a, CH_3
2.34	Acetate	21.08	Acetate	Acetate CO
1.15	2 x CH_3	26.51	2 x CH_3	6, 7, 9a

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  O3  .46148(7)  .83249(9)  .81247(13)  .0416(5)  Uani  ?  ?  1.00000  ?  ?
  C3a  .60109(8)  .94346(11)  .84950(14)  .0258(5)  Uani  ?  ?  1.00000  ?  ?
  C4  .56070(9)  1.05544(12)  .78772(16)  .0299(6)  Uani  ?  ?  1.00000  ?  ?
  C5  .58680(8)  1.08268(10)  .62406(15)  .0262(5)  Uani  ?  ?  1.00000  ?  ?
  O5  .60544(6)  .98825(7)  .52485(10)  .0244(4)  Uani  ?  ?  1.00000  ?  ?
  C5a  .68062(8)  1.06117(9)  .58743(13)  .0221(5)  Uani  ?  ?  1.00000  ?  ?
  C6  .72516(9)  1.12680(10)  .46505(15)  .0270(6)  Uani  ?  ?  1.00000  ?  ?
  C7  .79737(9)  1.06057(11)  .38441(14)  .0271(6)  Uani  ?  ?  1.00000  ?  ?
  C71  .85250(12)  1.13961(14)  .28794(18)  .0387(7)  Uani  ?  ?  1.00000  ?  ?
  C72  .75314(11)  .96927(13)  .27543(17)  .0355(7)  Uani  ?  ?  1.00000  ?  ?
  C8  .86294(9)  1.00506(11)  .51010(14)  .0264(5)  Uani  ?  ?  1.00000  ?  ?
  O8  .89515(6)  1.07454(7)  .64775(10)  .0271(4)  Uani  ?  ?  1.00000  ?  ?
  C91  .91049(8)  .90770(11)  .90947(15)  .0265(6)  Uani  ?  ?  1.00000  ?  ?
  O91  .88501(6)  .89170(7)  .75006(10)  .0262(4)  Uani  ?  ?  1.00000  ?  ?
  O92  .89361(6)  .99172(8)  .97710(11)  .0312(4)  Uani  ?  ?  1.00000  ?  ?
  C92  .95645(11)  .80723(13)  .98388(19)  .0367(7)  Uani  ?  ?  1.00000  ?  ?
  C9  .83786(8)  .98198(10)  .67047(13)  .0222(5)  Uani  ?  ?  1.00000  ?  ?
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  C9a  .74407(8)  1.00956(9)  .72292(13)  .0205(5)  Uani  ?  ?  1.00000  ?  ?
  C9b  .69490(8)  .91208(10)  .79420(14)  .0222(5)  Uani  ?  ?  1.00000  ?  ?
  H3a  .6031(11)  .9415(14)  .966(2)  .040(4)  Uiso  ?  ?  1.00000  ?  ?
  H4A  .4931(12)  1.0520(14)  .787(2)  .042(4)  Uiso  ?  ?  1.00000  ?  ?
  H4B  .5849(11)  1.1130(14)  .862(2)  .039(4)  Uiso  ?  ?  1.00000  ?  ?
  H5  .5520(10)  1.1417(13)  .5674(17)  .028(4)  Uiso  ?  ?  1.00000  ?  ?
  H6A  .6784(11)  1.1525(13)  .3851(19)  .035(4)  Uiso  ?  ?  1.00000  ?  ?
  H6B  .7538(11)  1.1915(14)  .5187(19)  .037(4)  Uiso  ?  ?  1.00000  ?  ?
  H71A  .9035(13)  1.1042(16)  .237(2)  .054(5)  Uiso  ?  ?  1.00000  ?  ?
  H71B  .8111(13)  1.1752(16)  .210(2)  .050(5)  Uiso  ?  ?  1.00000  ?  ?
  H71C  .8782(12)  1.2004(14)  .355(2)  .041(4)  Uiso  ?  ?  1.00000  ?  ?
  H72A  .7985(13)  .9278(15)  .222(2)  .051(5)  Uiso  ?  ?  1.00000  ?  ?
  H72B  .7182(11)  .9167(14)  .332(2)  .038(4)  Uiso  ?  ?  1.00000  ?  ?
  H72C  .7101(13)  1.0025(15)  .191(2)  .052(5)  Uiso  ?  ?  1.00000  ?  ?
  H8  .9126(11)  .9600(13)  .4693(18)  .031(4)  Uiso  ?  ?  1.00000  ?  ?
  H92A  .9884(14)  .7667(17)  .911(2)  .063(6)  Uiso  ?  ?  1.00000  ?  ?
  H92B  .9960(14)  .8283(18)  1.076(3)  .067(6)  Uiso  ?  ?  1.00000  ?  ?
  H92C  .9108(14)  .7618(16)  1.023(2)  .057(6)  Uiso  ?  ?  1.00000  ?  ?
  H9a  .7541(10)  1.0649(12)  .8052(17)  .028(4)  Uiso  ?  ?  1.00000  ?  ?
  H9b  .7326(10)  .8813(11)  .8822(17)  .024(3)  Uiso  ?  ?  1.00000  ?  ?

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  O1  .0498(6)  .0211(4)  .0350(5)  .0003(4)  .0066(4)  -.0033(4)
  O2  .0390(5)  .0257(5)  .0363(5)  -.0115(4)  -.0011(4)  .0019(4)
  C3  .0297(6)  .0330(7)  .0279(6)  -.0057(5)  -.0033(5)  .0090(5)
  O3  .0284(5)  .0460(6)  .0490(6)  -.0088(4)  -.0029(4)  .0168(5)
  C3a  .0236(5)  .0326(6)  .0210(5)  -.0028(5)  .0016(4)  -.0000(5)
  C4  .0269(6)  .0301(6)  .0327(6)  .0026(5)  .0030(5)  -.0052(5)
  C5  .0265(6)  .0204(5)  .0306(6)  .0027(4)  -.0032(5)  -.0026(5)
  O5  .0246(4)  .0213(4)  .0262(4)  -.0033(3)  -.0036(3)  -.0027(3)
  C5a  .0251(5)  .0169(5)  .0230(5)  -.0026(4)  -.0038(4)  -.0014(4)
  C6  .0317(6)  .0211(6)  .0264(6)  -.0056(5)  -.0066(5)  .0040(5)
  C7  .0333(6)  .0272(6)  .0202(5)  -.0100(5)  -.0009(5)  .0025(4)
  C71  .0453(8)  .0407(8)  .0292(7)  -.0177(7)  -.0001(6)  .0082(6)
  C72  .0448(8)  .0370(8)  .0246(6)  -.0149(6)  .0032(6)  -.0054(6)
  C8  .0286(6)  .0279(6)  .0228(5)  -.0049(5)  .0029(4)  -.0016(5)
  O8  .0274(4)  .0284(5)  .0247(4)  -.0077(3)  -.0007(3)  .0002(3)
  C91  .0203(5)  .0325(6)  .0266(6)  -.0003(5)  .0016(4)  .0055(5)
  O91  .0275(4)  .0258(4)  .0250(4)  .0059(3)  .0015(3)  .0030(3)
  O92  .0276(4)  .0386(5)  .0264(4)  .0030(4)  -.0020(3)  -.0017(4)
  C92  .0352(7)  .0356(8)  .0384(8)  .0041(6)  -.0013(6)  .0128(6)
  C9  .0232(5)  .0201(5)  .0227(5)  -.0004(4)  -.0006(4)  .0014(4)
  C9a  .0230(5)  .0181(5)  .0198(5)  -.0005(4)  -.0004(4)  -.0007(4)
  C9b  .0241(5)  .0218(5)  .0204(5)  -.0017(4)  .0006(4)  .0015(4)


# 5. Molecular Geometry
#----------------------

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  C1  O2  .  .  1.3967(16)  ?
  C1  C9b  .  .  1.5167(17)  ?
  O2  C3  .  .  1.3809(17)  ?
  C3  O3  .  .  1.1925(17)  ?
  C3  C3a  .  .  1.5091(18)  ?
  C3a  C4  .  .  1.5393(19)  ?
  C3a  C9b  .  .  1.5403(17)  ?
  C3a  H3a  .  .  .979(17)  ?
  C4  C5  .  .  1.501(2)  ?
  C4  H4A  .  .  .991(18)  ?
  C4  H4B  .  .  .975(16)  ?
  C5  O5  .  .  1.4506(15)  ?
  C5  C5a  .  .  1.4606(17)  ?
  C5  H5  .  .  .971(15)  ?
  O5  C5a  .  .  1.4636(14)  ?
  C5a  C6  .  .  1.4971(18)  ?
  C5a  C9a  .  .  1.5291(15)  ?
  C6  C7  .  .  1.5343(19)  ?
  C6  H6A  .  .  .962(15)  ?
  C6  H6B  .  .  .973(16)  ?
  C7  C71  .  .  1.531(2)  ?
  C7  C72  .  .  1.532(2)  ?
  C7  C8  .  .  1.5115(17)  ?
  C71  H71A  .  .  .99(2)  ?
  C71  H71B  .  .  .951(18)  ?
  C71  H71C  .  .  .977(17)  ?
  C72  H72A  .  .  .98(2)  ?
  C72  H72B  .  .  .969(17)  ?
  C72  H72C  .  .  .987(19)  ?
  C8  O8  .  .  1.4675(15)  ?
  C8  C9  .  .  1.4600(17)  ?
  C8  H8  .  .  .994(16)  ?
  O8  C9  .  .  1.4176(15)  ?
  C91  O91  .  .  1.3699(15)  ?
  C91  O92  .  .  1.1966(16)  ?
  C91  C92  .  .  1.490(2)  ?
  O91  C9  .  .  1.4181(14)  ?
  C92  H92A  .  .  .94(2)  ?
  C92  H92B  .  .  .96(2)  ?
  C92  H92C  .  .  .95(2)  ?
  C9  C9a  .  .  1.5203(17)  ?
  C9a  C9b  .  .  1.5285(16)  ?
  C9a  H9a  .  .  .960(15)  ?
  C9b  H9b  .  .  .953(13)  ?

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_geom_angle_site_symmetry_3
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_geom_angle_publ_flag                #<< enter YES for value to be published
  O1  C1  O2  .  .  .  119.95(11)  ?
  O1  C1  C9b  .  .  .  130.64(12)  ?
  O2  C1  C9b  .  .  .  109.36(10)  ?
```

```
C1  O2  C3  .  .  .  110.18(10)  ?
O2  C3  O3  .  .  .  120.85(12)  ?
O2  C3  C3a  .  .  .  110.87(11)  ?
O3  C3  C3a  .  .  .  128.28(13)  ?
C3  C3a  C4  .  .  .  110.47(10)  ?
C3  C3a  C9b  .  .  .  103.66(10)  ?
C3  C3a  H3a  .  .  .  105.9(10)  ?
C4  C3a  C9b  .  .  .  115.87(10)  ?
C4  C3a  H3a  .  .  .  109.4(10)  ?
C9b  C3a  H3a  .  .  .  111.0(10)  ?
C3a  C4  C5  .  .  .  112.10(11)  ?
C3a  C4  H4A  .  .  .  108.5(10)  ?
C3a  C4  H4B  .  .  .  107.5(9)  ?
C5  C4  H4A  .  .  .  110.2(9)  ?
C5  C4  H4B  .  .  .  108.9(10)  ?
H4A  C4  H4B  .  .  .  109.6(14)  ?
C4  C5  O5  .  .  .  115.91(11)  ?
C4  C5  C5a  .  .  .  119.03(10)  ?
C4  C5  H5  .  .  .  116.2(9)  ?
O5  C5  C5a  .  .  .  60.36(7)  ?
O5  C5  H5  .  .  .  114.1(9)  ?
C5a  C5  H5  .  .  .  119.0(9)  ?
C5  O5  C5a  .  .  .  60.16(7)  ?
C5  C5a  O5  .  .  .  59.48(7)  ?
C5  C5a  C6  .  .  .  122.35(10)  ?
C5  C5a  C9a  .  .  .  115.42(10)  ?
O5  C5a  C6  .  .  .  115.55(9)  ?
O5  C5a  C9a  .  .  .  113.92(9)  ?
C6  C5a  C9a  .  .  .  116.91(10)  ?
C5a  C6  C7  .  .  .  113.42(10)  ?
C5a  C6  H6A  .  .  .  108.7(10)  ?
C5a  C6  H6B  .  .  .  107.4(10)  ?
C7  C6  H6A  .  .  .  109.3(10)  ?
C7  C6  H6B  .  .  .  109.5(10)  ?
H6A  C6  H6B  .  .  .  108.3(13)  ?
C6  C7  C71  .  .  .  109.62(11)  ?
C6  C7  C72  .  .  .  111.54(11)  ?
C6  C7  C8  .  .  .  109.71(10)  ?
C71  C7  C72  .  .  .  109.92(11)  ?
C71  C7  C8  .  .  .  108.25(11)  ?
C72  C7  C8  .  .  .  107.72(11)  ?
C7  C71  H71A  .  .  .  115.0(11)  ?
C7  C71  H71B  .  .  .  108.2(11)  ?
C7  C71  H71C  .  .  .  110.5(10)  ?
H71A  C71  H71B  .  .  .  110.3(16)  ?
H71A  C71  H71C  .  .  .  108.0(15)  ?
H71B  C71  H71C  .  .  .  104.3(15)  ?
C7  C72  H72A  .  .  .  112.1(11)  ?
C7  C72  H72B  .  .  .  112.6(10)  ?
C7  C72  H72C  .  .  .  110.1(11)  ?
H72A  C72  H72B  .  .  .  108.1(15)  ?
H72A  C72  H72C  .  .  .  106.8(16)  ?
H72B  C72  H72C  .  .  .  106.8(15)  ?
C7  C8  O8  .  .  .  115.69(10)  ?
C7  C8  C9  .  .  .  122.02(11)  ?
C7  C8  H8  .  .  .  115.7(8)  ?
O8  C8  C9  .  .  .  57.93(7)  ?
O8  C8  H8  .  .  .  113.2(8)  ?
C9  C8  H8  .  .  .  118.4(9)  ?
C8  O8  C9  .  .  .  60.77(8)  ?
O91  C91  O92  .  .  .  122.36(11)  ?
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```
  O91  C91  C92  .  .  .  111.44(11)  ?
  O92  C91  C92  .  .  .  126.14(12)  ?
  C91  O91  C9  .  .  .  115.32(9)  ?
  C91  C92  H92A  .  .  .  112.1(12)  ?
  C91  C92  H92B  .  .  .  109.8(13)  ?
  C91  C92  H92C  .  .  .  107.9(12)  ?
  H92A  C92  H92B  .  .  .  111.6(17)  ?
  H92A  C92  H92C  .  .  .  109.9(17)  ?
  H92B  C92  H92C  .  .  .  105.3(17)  ?
  C8  C9  O8  .  .  .  61.30(8)  ?
  C8  C9  O91  .  .  .  115.25(10)  ?
  C8  C9  C9a  .  .  .  122.97(10)  ?
  O8  C9  O91  .  .  .  113.38(9)  ?
  O8  C9  C9a  .  .  .  115.59(9)  ?
  O91  C9  C9a  .  .  .  116.20(10)  ?
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  C9b  C9a  H9a  .  .  .  107.0(9)  ?
  C1  C9b  C3a  .  .  .  103.69(9)  ?
  C1  C9b  C9a  .  .  .  113.60(10)  ?
  C1  C9b  H9b  .  .  .  106.5(8)  ?
  C3a  C9b  C9a  .  .  .  113.57(10)  ?
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#------------------------------------------------------------------------
#      Special items requested by author for inclusion in paper
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#       Items which are non-mandatory for Acta C submissions
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;      ?
;

_exptl_special_details
;      ?
;

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;      ?
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#=============================================================================
#       Structure Factor lists should be submitted as separate files
#=============================================================================

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