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*Australian Journal of Chemistry –
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1. SUBMISSION DETAILS

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_publ_contact_author_address  
;  
  Department of Chemistry  
  University of Western Australia
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    35 Stirling Highway
    Crawley
    Western Australia 6009
    Australia
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_publ_contact_author_email      bws@crystal.uwa.edu.au
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'Skelton, Brian W.' .
; Department of Chemistry,
University of Western Australia,
35 Stirling Highway,
Crawley,
WA 6009,
Australia.
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Sheldrick, G M. (1996). SADABS. Program for Empirical Absorption Correction
  of Area Detector Data. University of Gottingen, Germany.

Siemens (1995). SMART and SAINT. Area-Detector Control and Integration
  Software. Siemens Analytical X-ray Systems Inc., Madison, Wisconsin, USA.

Hall, S.R., King, G.S.D., and Stewart., J.M. (1995).
  The Xtal 3.5 User's Manual. University of Western Australia, Lamb: Perth.
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4. Supplementary data for validation and tables

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C15	.025(4)	.031(4)	.020(3)	-.000(3)	.000(3)	-.001(3)
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C123 .0842(14) .0307(10) .0413(11) -.0058(10) -.0052(11) .0096(10)
C24 .032(4) .034(4) .027(4) .003(3) -.007(3) .001(3)
C25 .024(4) .026(3) .022(3) -.006(3) -.007(3) .004(3)
C26 .035(4) .024(3) .020(3) -.001(3) -.002(3) -.002(3)
C27 .050(4) .032(4) .029(4) -.000(4) -.020(4) .000(3)
C28 .050(5) .035(4) .056(5) -.018(4) -.031(4) .008(4)
O2 .039(3) .040(3) .048(3) -.004(2) -.020(2) .006(2)
C29 .042(4) .036(4) .053(5) -.015(4) -.012(4) .014(4)
C210 .040(4) .025(4) .035(4) -.004(3) -.008(4) .007(3)
Br210 .0429(4) .0350(4) .0420(4) -.0013(4) .0013(4) .0130(3)
C211 .027(3) .030(4) .028(4) .004(3) -.007(3) -.003(3)
C212 .026(4) .043(5) .042(4) .004(3) -.003(3) .005(4)
C213 .061(5) .036(4) .039(4) .009(4) -.002(4) -.010(4)
C214 .083(6) .044(5) .021(4) .004(4) -.019(4) -.006(3)
C215 .042(4) .039(4) .031(4) -.012(3) .001(3) -.005(3)
O216 .034(3) .033(3) .014(2) .000(2) .002(2) -.000(2)
C216 .086(7) .026(4) .024(4) .012(5) .008(5) .002(3)
O217 .056(4) .063(4) .055(4) .021(3) .031(3) .004(3)
C217 .117(8) .061(6) .021(4) .007(6) .001(5) -.004(4)

```

5. Molecular Geometry

#-----

loop_

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_geom_bond_atom_site_label_2

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_geom_bond_site_symmetry_2

_geom_bond_distance

_geom_bond_publ_flag

#<< enter YES for value to be published

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C11 C12 . . 1.534(9) ?
C11 C16 . . 1.542(9) ?
C11 H11a . . .948 ?
C11 H11b . . .972 ?
C12 Br12 . . 1.964(6) ?
C12 C13 . . 1.517(9) ?
C12 H12 . . .971 ?
C13 C113 . . 1.829(6) ?
C13 C14 . . 1.533(9) ?
C13 C115 . . 1.515(9) ?

```

C14	C15	. .	1.524(9)	?
C14	H14a	. .	.952	?
C14	H14b	. .	.965	?
C15	C16	. .	1.552(8)	?
C15	O116	. .	1.443(7)	?
C15	H15	. .	.960	?
C16	C17	. .	1.587(9)	?
C16	C111	. .	1.587(9)	?
C17	O1	. .	1.459(7)	?
C17	C18	. .	1.458(9)	?
C17	C114	. .	1.500(9)	?
O1	C18	. .	1.457(8)	?
C18	C19	. .	1.469(10)	?
C18	H18	. .	.963	?
C19	C110	. .	1.318(9)	?
C19	H19	. .	.968	?
C110	Br110	. .	1.909(6)	?
C110	C111	. .	1.532(9)	?
C111	C112	. .	1.529(9)	?
C111	C113	. .	1.548(9)	?
C112	H112a	. .	.949	?
C112	H112b	. .	.935	?
C112	H112c	. .	.964	?
C113	H113a	. .	.947	?
C113	H113b	. .	.971	?
C113	H113c	. .	.957	?
C114	H114a	. .	.959	?
C114	H114b	. .	.953	?
C114	H114c	. .	.968	?
C115	H115a	. .	.975	?
C115	H115b	. .	.990	?
C115	H115c	. .	.925	?
O116	C116	. .	1.361(8)	?
C116	O117	. .	1.193(9)	?
C116	C117	. .	1.490(10)	?
C117	H117a	. .	.957	?
C117	H117b	. .	.961	?
C117	H117c	. .	.971	?
C21	C22	. .	1.526(9)	?
C21	C26	. .	1.555(9)	?
C21	H21a	. .	.946	?
C21	H21b	. .	.955	?
C22	Br22	. .	1.955(7)	?
C22	C23	. .	1.524(9)	?
C22	H22	. .	.975	?
C23	C123	. .	1.840(7)	?
C23	C24	. .	1.522(9)	?
C23	C215	. .	1.524(9)	?
C24	C25	. .	1.514(9)	?
C24	H24a	. .	.972	?
C24	H24b	. .	.942	?
C25	C26	. .	1.555(8)	?
C25	O216	. .	1.447(7)	?
C25	H25	. .	.960	?
C26	C27	. .	1.564(9)	?
C26	C211	. .	1.591(9)	?
C27	C28	. .	1.454(10)	?

C27 O2 . . 1.462(9) ?
 C27 C214 . . 1.523(9) ?
 C28 O2 . . 1.456(9) ?
 C28 C29 . . 1.476(11) ?
 C28 H28 . . .961 ?
 C29 C210 . . 1.326(10) ?
 C29 H29 . . .997 ?
 C210 Br210 . . 1.904(6) ?
 C210 C211 . . 1.523(9) ?
 C211 C212 . . 1.523(9) ?
 C211 C213 . . 1.559(9) ?
 C212 H212a . . .963 ?
 C212 H212b . . .953 ?
 C212 H212c . . .960 ?
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 C213 H213c . . .958 ?
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 C214 H214b . . .952 ?
 C214 H214c . . .953 ?
 C215 H215a . . .947 ?
 C215 H215b . . .971 ?
 C215 H215c . . .959 ?
 O216 C216 . . 1.361(9) ?
 C216 O217 . . 1.184(12) ?
 C216 C217 . . 1.502(12) ?
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 C217 H217b . . .956 ?
 C217 H217c . . .942) ?

loop_

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_geom_angle_publ_flag

#<< enter YES for value to be published

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 C12 C11 H11a . . . 109.8 ?
 C12 C11 H11b . . . 107.6 ?
 C16 C11 H11a . . . 108.4 ?
 C16 C11 H11b . . . 107.7 ?
 H11a C11 H11b . . . 107.8 ?
 C11 C12 Br12 . . . 107.6(4) ?
 C11 C12 C13 . . . 112.1(5) ?
 C11 C12 H12 . . . 109.1 ?
 Br12 C12 C13 . . . 112.9(4) ?
 Br12 C12 H12 . . . 111.5 ?
 C13 C12 H12 . . . 103.6 ?
 C12 C13 Cl13 . . . 109.2(4) ?
 C12 C13 C14 . . . 106.3(5) ?
 C12 C13 C115 . . . 115.4(5) ?
 Cl13 C13 C14 . . . 105.9(4) ?
 Cl13 C13 C115 . . . 105.4(4) ?
 C14 C13 C115 . . . 114.2(5) ?

C13	C14	C15	.	.	.	115.1(5)	?
C13	C14	H14a	.	.	.	110.0	?
C13	C14	H14b	.	.	.	108.1	?
C15	C14	H14a	.	.	.	107.6	?
C15	C14	H14b	.	.	.	107.8	?
H14a	C14	H14b	.	.	.	108.0	?
C14	C15	C16	.	.	.	112.9(5)	?
C14	C15	O116	.	.	.	109.1(5)	?
C14	C15	H15	.	.	.	108.3	?
C16	C15	O116	.	.	.	109.6(5)	?
C16	C15	H15	.	.	.	105.1	?
O116	C15	H15	.	.	.	111.7(5)	?
C11	C16	C15	.	.	.	110.1(5)	?
C11	C16	C17	.	.	.	112.9(5)	?
C11	C16	C111	.	.	.	108.9(5)	?
C15	C16	C17	.	.	.	106.4(5)	?
C15	C16	C111	.	.	.	114.1(5)	?
C17	C16	C111	.	.	.	104.4(5)	?
C16	C17	O1	.	.	.	115.7(5)	?
C16	C17	C18	.	.	.	114.8(5)	?
C16	C17	C114	.	.	.	119.8(5)	?
O1	C17	C18	.	.	.	59.9(4)	?
O1	C17	C114	.	.	.	112.2(5)	?
C18	C17	C114	.	.	.	119.8(6)	?
C17	O1	C18	.	.	.	60.0(4)	?
C17	C18	O1	.	.	.	60.1(4)	?
C17	C18	C19	.	.	.	119.6(6)	?
C17	C18	H18	.	.	.	132.1	?
O1	C18	C19	.	.	.	118.8(5)	?
O1	C18	H18	.	.	.	138.6	?
C19	C18	H18	.	.	.	90.4	?
C18	C19	C110	.	.	.	118.3(6)	?
C18	C19	H19	.	.	.	121.4	?
C110	C19	H19	.	.	.	120.3	?
C19	C110	Br110	.	.	.	119.3(5)	?
C19	C110	C111	.	.	.	122.0(6)	?
Br110	C110	C111	.	.	.	118.7(4)	?
C16	C111	C110	.	.	.	105.1(5)	?
C16	C111	C112	.	.	.	114.3(5)	?
C16	C111	C113	.	.	.	111.9(5)	?
C110	C111	C112	.	.	.	114.3(5)	?
C110	C111	C113	.	.	.	105.9(5)	?
C112	C111	C113	.	.	.	105.1(5)	?
C111	C112	H112a	.	.	.	109.1	?
C111	C112	H112b	.	.	.	110.4	?
C111	C112	H112c	.	.	.	108.7	?
H112a	C112	H112b	.	.	.	110.8	?
H112a	C112	H112c	.	.	.	108.3	?
H112b	C112	H112c	.	.	.	109.5	?
C111	C113	H113a	.	.	.	111.4	?
C111	C113	H113b	.	.	.	110.4	?
C111	C113	H113c	.	.	.	110.7	?
H113a	C113	H113b	.	.	.	107.9	?
H113a	C113	H113c	.	.	.	109.1	?
H113b	C113	H113c	.	.	.	107.1	?
C17	C114	H114a	.	.	.	111.1	?
C17	C114	H114b	.	.	.	110.9	?

C17	C114	H114c	.	.	.	110.8	?
H114a	C114	H114b	.	.	.	108.4	?
H114a	C114	H114c	.	.	.	107.3	?
H114b	C114	H114c	.	.	.	108.2	?
C13	C115	H115a	.	.	.	110.4	?
C13	C115	H115b	.	.	.	110.5	?
C13	C115	H115c	.	.	.	113.6	?
H115a	C115	H115b	.	.	.	104.3	?
H115a	C115	H115c	.	.	.	109.4	?
H115b	C115	H115c	.	.	.	108.2	?
C15	O116	C116	.	.	.	115.6(5)	?
O116	C116	O117	.	.	.	124.1(6)	?
O116	C116	C117	.	.	.	109.8(6)	?
O117	C116	C117	.	.	.	126.1(7)	?
C116	C117	H117a	.	.	.	114.5	?
C116	C117	H117b	.	.	.	114.3	?
C116	C117	H117c	.	.	.	109.9	?
H117a	C117	H117b	.	.	.	108.0	?
H117a	C117	H117c	.	.	.	106.5	?
H117b	C117	H117c	.	.	.	102.7	?
C22	C21	C26	.	.	.	113.8(5)	?
C22	C21	H21a	.	.	.	109.3	?
C22	C21	H21b	.	.	.	107.4	?
C26	C21	H21a	.	.	.	108.9	?
C26	C21	H21b	.	.	.	107.9	?
H21a	C21	H21b	.	.	.	109.4	?
C21	C22	Br22	.	.	.	108.2(5)	?
C21	C22	C23	.	.	.	112.1(5)	?
C21	C22	H22	.	.	.	109.2	?
Br22	C22	C23	.	.	.	112.5(5)	?
Br22	C22	H22	.	.	.	108.9	?
C23	C22	H22	.	.	.	105.9	?
C22	C23	C123	.	.	.	108.5(4)	?
C22	C23	C24	.	.	.	106.5(5)	?
C22	C23	C215	.	.	.	115.0(6)	?
C123	C23	C24	.	.	.	105.4(4)	?
C123	C23	C215	.	.	.	106.0(4)	?
C24	C23	C215	.	.	.	114.8(5)	?
C23	C24	C25	.	.	.	114.8(5)	?
C23	C24	H24a	.	.	.	107.0	?
C23	C24	H24b	.	.	.	109.0	?
C25	C24	H24a	.	.	.	107.7	?
C25	C24	H24b	.	.	.	109.8	?
H24a	C24	H24b	.	.	.	108.2	?
C24	C25	C26	.	.	.	114.3(5)	?
C24	C25	O216	.	.	.	109.9(5)	?
C24	C25	H25	.	.	.	107.4	?
C26	C25	O216	.	.	.	108.6(5)	?
C26	C25	H25	.	.	.	104.8	?
O216	C25	H25	.	.	.	111.7	?
C21	C26	C25	.	.	.	107.9(5)	?
C21	C26	C27	.	.	.	113.1(5)	?
C21	C26	C211	.	.	.	110.2(5)	?
C25	C26	C27	.	.	.	107.3(5)	?
C25	C26	C211	.	.	.	113.4(5)	?
C27	C26	C211	.	.	.	105.0(5)	?
C26	C27	C28	.	.	.	114.9(6)	?

C26	C27	O2	.	.	.	116.7(5)	?
C26	C27	C214	.	.	.	120.7(6)	?
C28	C27	O2	.	.	.	59.9(4)	?
C28	C27	C214	.	.	.	117.6(6)	?
O2	C27	C214	.	.	.	112.2(5)	?
C27	C28	O2	.	.	.	60.3(4)	?
C27	C28	C29	.	.	.	118.6(6)	?
C27	C28	H28	.	.	.	134.7	?
O2	C28	C29	.	.	.	117.5(6)	?
O2	C28	H28	.	.	.	133.6	?
C29	C28	H28	.	.	.	93.3	?
C27	O2	C28	.	.	.	59.8(4)	?
C28	C29	C210	.	.	.	118.0(6)	?
C28	C29	H29	.	.	.	122.7	?
C210	C29	H29	.	.	.	119.2	?
C29	C210	Br210	.	.	.	119.0(5)	?
C29	C210	C211	.	.	.	121.7(6)	?
Br210	C210	C211	.	.	.	119.3(5)	?
C26	C211	C210	.	.	.	104.6(5)	?
C26	C211	C212	.	.	.	115.1(5)	?
C26	C211	C213	.	.	.	111.5(5)	?
C210	C211	C212	.	.	.	114.1(5)	?
C210	C211	C213	.	.	.	107.1(5)	?
C212	C211	C213	.	.	.	104.4(5)	?
C211	C212	H212a	.	.	.	110.9	?
C211	C212	H212b	.	.	.	110.9	?
C211	C212	H212c	.	.	.	110.8	?
H212a	C212	H212b	.	.	.	108.2	?
H212a	C212	H212c	.	.	.	107.6	?
H212b	C212	H212c	.	.	.	108.4	?
C211	C213	H213a	.	.	.	110.9	?
C211	C213	H213b	.	.	.	109.8	?
C211	C213	H213c	.	.	.	110.5	?
H213a	C213	H213b	.	.	.	108.7	?
H213a	C213	H213c	.	.	.	109.0	?
H213b	C213	H213c	.	.	.	107.8	?
C27	C214	H214a	.	.	.	112.3	?
C27	C214	H214b	.	.	.	113.8	?
C27	C214	H214c	.	.	.	110.7	?
H214a	C214	H214b	.	.	.	107.5	?
H214a	C214	H214c	.	.	.	103.6	?
H214b	C214	H214c	.	.	.	108.4	?
C23	C215	H215a	.	.	.	111.2	?
C23	C215	H215b	.	.	.	110.6	?
C23	C215	H215c	.	.	.	110.9	?
H215a	C215	H215b	.	.	.	107.9	?
H215a	C215	H215c	.	.	.	109.0	?
H215b	C215	H215c	.	.	.	107.0	?
C25	O216	C216	.	.	.	116.2(5)	?
O216	C216	O217	.	.	.	124.1(7)	?
O216	C216	C217	.	.	.	108.6(8)	?
O217	C216	C217	.	.	.	127.3(7)	?
C216	C217	H217a	.	.	.	109.3	?
C216	C217	H217b	.	.	.	109.8	?
C216	C217	H217c	.	.	.	111.6	?
H217a	C217	H217b	.	.	.	107.9	?
H217a	C217	H217c	.	.	.	108.7)	?

H217b C217 H217c . . . 109.6 ?

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_geom_hbond_site_symmetry_A
_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_publ_flag          #<< enter YES for value to be published
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#-----
#       Special items requested by author for inclusion in paper
#-----
```

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_publ_manuscript_incl_extra_item
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#-----
#       Items which are non-mandatory for Acta C submissions
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_geom_special_details              ?
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_cell_special_details
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;
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_exptl_special_details
;      ?
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;      ?
;

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_diffrn_standard_refl_index_l
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_diffrn_attenuator_scale
  ? ?

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_reflns_limit_k_max                22
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_diffrn_ambient_temperature        153
_diffrn_radiation_source            'sealed tube'
_diffrn_radiation_monochromator     graphite
_diffrn_radiation_detector         'CCD area detector'

_refine_ls_extinction_expression   ?
_refine_ls_matrix_type             full
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_refine_ls_goodness_of_fit_all     1.096
_refine_ls_shift/su_mean           .002

#####
#      Structure Factor lists should be submitted as separate files
#####

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