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*Australian Journal of Chemistry –
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#2    Person making the deposition
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  _publ_contact_author_email  g.gainsford@irl.cri.nz
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#3    Publication details
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  _journal_volume          ?
  _journal_page_first     ?
  _journal_page_last      ?
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#----- TITLE -----#

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  N-Methyldiethanolamine-Modified Titanium iso-Propoxide: X-ray
  Structure
  of [Ti~2~(\m~2~(OCH~2~CH~2~)~2~NCH~3~)(\m~2~-OPr^i^)(OPr^i^)^5~]
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#5    Other data relating to the structure determination and refinement
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Conformational disorder of the isopropyl carbon bound to oxygen in
four isopropoxide groups (1 in one independent molecule, 2 in the
second
independent molecule)
modelled by two site occupancies for C4A, C14A, C16A & associated
hydrogens &
C4B, C14B, C16B & H's with the latter atoms refined
using one common isotropic U (0.042(3)A^2^); final A atom occupancies
are
0.893(8), 0.840(9) & 0.74(1) respectively.
Conformational disorder of one methyl isopropyl carbon (C15) modelled
similarly with final U and occupancies 0.063(1)A^2^, 0.542(9).
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#6      Include your "standard" CIF file here

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  Refinement of F2 against ALL reflections. The weighted R-factor wR
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  goodness of fit S are based on F2, conventional R-factors R are
  based
  on F, with F set to zero for negative F2. The threshold expression
  of
  F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc.
  and is
  not relevant to the choice of reflections for refinement. R-factors
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P=(Fo2+2Fc2)/3'
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H23A H 0.9522 0.2149 0.6221 0.131 Uiso 1 1 calc R . .
H23B H 1.0709 0.2393 0.6647 0.131 Uiso 1 1 calc R . .
H23C H 0.9388 0.2226 0.7037 0.131 Uiso 1 1 calc R . .
C31 C 0.7519(3) 0.04368(7) 0.64685(14) 0.0298(6) Uani 1 1 d . . .
H31 H 0.6884 0.0503 0.6059 0.036 Uiso 1 1 calc R . .
C32 C 0.6648(3) 0.03761(9) 0.70966(17) 0.0486(8) Uani 1 1 d . . .
H32A H 0.6135 0.0621 0.7191 0.068 Uiso 1 1 calc R . .
H32B H 0.7258 0.0310 0.7501 0.068 Uiso 1 1 calc R . .
H32C H 0.5987 0.0158 0.7005 0.068 Uiso 1 1 calc R . .
C33 C 0.8334(3) 0.00650(8) 0.63022(17) 0.0433(7) Uani 1 1 d . . .
H33A H 0.8893 0.0114 0.5895 0.061 Uiso 1 1 calc R . .
H33B H 0.7685 -0.0155 0.6201 0.061 Uiso 1 1 calc R . .
H33C H 0.8951 -0.0005 0.6702 0.061 Uiso 1 1 calc R . .
C42 C 0.6317(3) 0.15820(12) 0.68867(15) 0.0558(9) Uani 1 1 d . . .
H42A H 0.7088 0.1439 0.7125 0.078 Uiso 1 1 calc R A 1
H42B H 0.5464 0.1545 0.7143 0.078 Uiso 1 1 calc R A 1
H42C H 0.6541 0.1866 0.6866 0.078 Uiso 1 1 calc R A 1
C43 C 0.4925(3) 0.16438(10) 0.57731(15) 0.0450(8) Uani 1 1 d . . .
H43A H 0.4814 0.1538 0.5299 0.063 Uiso 1 1 calc R B 1
H43B H 0.5151 0.1928 0.5753 0.063 Uiso 1 1 calc R B 1
H43C H 0.4054 0.1608 0.6015 0.063 Uiso 1 1 calc R B 1
C51 C 0.8090(3) 0.23474(8) 0.46605(16) 0.0372(6) Uani 1 1 d . J .
H51 H 0.9091 0.2341 0.4826 0.045 Uiso 1 1 calc R . .
C52 C 0.7230(4) 0.25333(10) 0.52194(19) 0.0530(9) Uani 1 1 d . . .
H52A H 0.7327 0.2375 0.5646 0.074 Uiso 1 1 calc R J .
H52B H 0.6247 0.2541 0.5060 0.074 Uiso 1 1 calc R . .
H52C H 0.7560 0.2805 0.5313 0.074 Uiso 1 1 calc R . .
C53 C 0.7962(5) 0.25833(11) 0.3997(2) 0.0776(13) Uani 1 1 d . . .
H53A H 0.8526 0.2458 0.3644 0.109 Uiso 1 1 calc R J .
H53B H 0.8294 0.2855 0.4083 0.109 Uiso 1 1 calc R . .
H53C H 0.6983 0.2590 0.3831 0.109 Uiso 1 1 calc R . .
C61 C 0.5272(3) 0.12290(9) 0.37895(14) 0.0372(7) Uani 1 1 d . J .
H61 H 0.5704 0.1147 0.3347 0.045 Uiso 1 1 calc R . .
C62 C 0.4618(4) 0.16359(12) 0.36786(18) 0.0593(10) Uani 1 1 d . . .
H62A H 0.5341 0.1828 0.3561 0.083 Uiso 1 1 calc R J .
H62B H 0.4180 0.1721 0.4106 0.083 Uiso 1 1 calc R . .
H62C H 0.3911 0.1622 0.3297 0.083 Uiso 1 1 calc R . .
C63 C 0.4214(4) 0.09188(13) 0.3973(2) 0.0678(11) Uani 1 1 d . . .
H63A H 0.4680 0.0661 0.4041 0.095 Uiso 1 1 calc R J .
H63B H 0.3503 0.0897 0.3594 0.095 Uiso 1 1 calc R . .
H63C H 0.3770 0.0996 0.4403 0.095 Uiso 1 1 calc R . .
C71 C 1.0902(3) 0.16122(8) 0.49437(13) 0.0319(6) Uani 1 1 d . J .
H71A H 1.1577 0.1398 0.5065 0.038 Uiso 1 1 calc R . .
H71B H 1.1350 0.1871 0.5057 0.038 Uiso 1 1 calc R . .
C72 C 1.0510(3) 0.15950(9) 0.41790(14) 0.0357(6) Uani 1 1 d . J .
H72A H 1.1336 0.1525 0.3912 0.043 Uiso 1 1 calc R . .
H72B H 1.0164 0.1858 0.4017 0.043 Uiso 1 1 calc R . .
C81 C 0.8915(3) 0.06447(8) 0.46213(14) 0.0328(6) Uani 1 1 d . J .
H81A H 0.8138 0.0558 0.4302 0.039 Uiso 1 1 calc R . .
H81B H 0.9367 0.0405 0.4827 0.039 Uiso 1 1 calc R . .
C82 C 0.9968(3) 0.08820(8) 0.42197(15) 0.0377(6) Uani 1 1 d . J .
H82A H 1.0852 0.0907 0.4500 0.045 Uiso 1 1 calc R . .
H82B H 1.0166 0.0743 0.3781 0.045 Uiso 1 1 calc R . .
Ti11 Ti 0.92073(4) 0.110795(12) 1.11644(2) 0.02038(10) Uani 1 1 d . K .
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O11 O 1.08158(18) 0.08164(6) 1.10912(9) 0.0331(4) Uani 1 1 d . . .

O12 O 0.98042(19) 0.15203(5) 1.17007(9) 0.0305(4) Uani 1 1 d . . .
O13 O 0.82918(18) 0.08240(5) 1.18193(9) 0.0270(4) Uani 1 1 d . . .
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O15 O 0.7570(2) 0.17178(5) 0.93071(9) 0.0331(4) Uani 1 1 d . . .
O16 O 0.61181(19) 0.10310(6) 0.94739(10) 0.0369(4) Uani 1 1 d . . .
O17 O 0.95878(17) 0.14332(5) 1.02504(8) 0.0239(4) Uani 1 1 d . . .
O18 O 0.82371(17) 0.07620(4) 1.03779(8) 0.0232(4) Uani 1 1 d . . .
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C112 C 1.2230(4) 0.07749(13) 1.21527(17) 0.0635(11) Uani 1 1 d . . .
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H11F H 1.1885 0.0510 1.2272 0.089 Uiso 1 1 calc R C 1
C113 C 1.3042(3) 0.05131(11) 1.1023(2) 0.0603(10) Uani 1 1 d . . .
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H11I H 1.4021 0.0537 1.1183 0.084 Uiso 1 1 calc R D 1
C121 C 1.0364(3) 0.19107(8) 1.16378(15) 0.0399(7) Uani 1 1 d . K .
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C122 C 1.1724(4) 0.19380(11) 1.2063(2) 0.0610(10) Uani 1 1 d . . .
H2A2 H 1.2375 0.1737 1.1901 0.085 Uiso 1 1 calc R K .
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H2C2 H 1.2129 0.2203 1.2008 0.085 Uiso 1 1 calc R . .
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H12F H 0.9137 0.2171 1.2344 0.112 Uiso 1 1 calc R . .
C131 C 0.7611(3) 0.04482(7) 1.18199(14) 0.0324(6) Uani 1 1 d . K .
H131 H 0.7124 0.0409 1.1355 0.039 Uiso 1 1 calc R . .
C132 C 0.6533(3) 0.04391(9) 1.23685(18) 0.0463(8) Uani 1 1 d . . .
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H13F H 0.6041 0.0183 1.2348 0.065 Uiso 1 1 calc R . .
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H13H H 0.8210 -0.0136 1.1897 0.091 Uiso 1 1 calc R . .
H13I H 0.9153 0.0153 1.2380 0.091 Uiso 1 1 calc R . .
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H14C H 0.6407 0.1833 1.1828 0.058 Uiso 1 1 calc R E 1
C143 C 0.4962(3) 0.16807(10) 1.06488(16) 0.0449(8) Uani 1 1 d . . .
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C151 C 0.8091(3) 0.21049(9) 0.91878(16) 0.0445(7) Uani 1 1 d . K .
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C153 C 0.7980(5) 0.23589(10) 0.9816(2) 0.0691(11) Uani 1 1 d . . .
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H15F H 0.8702 0.2282 1.0165 0.097 Uiso 1 1 calc R . .
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H16E H 0.3454 0.1166 0.8441 0.136 Uiso 1 1 calc R H 1

H16F H 0.5010 0.1094 0.8199 0.136 Uiso 1 1 calc R H 1
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H17B H 1.0713 0.1626 0.9473 0.039 Uiso 1 1 calc R . .
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H15J H 0.7223 0.2502 0.8521 0.088 Uiso 0.458(9) 1 calc PR K 2
C16B C 0.5281(16) 0.0909(4) 0.8863(8) 0.042(3) Uiso 0.257(10) 1 d P K 2
H6B1 H 0.5953 0.0836 0.8500 0.051 Uiso 0.257(10) 1 calc PR K 2

loop_

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_atom_site_aniso_U_11
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_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
Ti1 0.0237(2) 0.0219(2) 0.0186(2) 0.00247(17) 0.00000(16) -0.00218(17)

Ti2 0.0207(2) 0.0228(2) 0.0167(2) 0.00046(16) 0.00128(16) 0.00062(16)
O1 0.0292(10) 0.0387(10) 0.0315(10) 0.0089(8) 0.0003(8) 0.0077(8)
O2 0.0385(10) 0.0308(9) 0.0242(9) 0.0003(7) -0.0051(8) -0.0093(8)
O3 0.0355(10) 0.0250(9) 0.0231(9) 0.0043(7) 0.0012(7) -0.0063(7)
O4 0.0242(9) 0.0322(9) 0.0176(8) -0.0004(7) 0.0038(7) 0.0015(7)
O5 0.0354(10) 0.0234(9) 0.0283(9) 0.0032(7) -0.0010(8) 0.0030(7)
O6 0.0269(9) 0.0349(10) 0.0239(9) -0.0014(7) -0.0026(7) -0.0018(7)
O7 0.0231(8) 0.0252(8) 0.0209(8) 0.0037(7) 0.0025(7) -0.0046(7)
O8 0.0284(9) 0.0205(8) 0.0187(8) -0.0006(6) 0.0023(7) -0.0008(7)
N2 0.0287(11) 0.0343(11) 0.0215(11) 0.0014(9) 0.0055(9) 0.0023(9)
C2' 0.0458(17) 0.0529(18) 0.0205(13) -0.0008(12) 0.0081(12) 0.0021(14)
C11 0.0339(16) 0.0418(16) 0.0478(18) 0.0133(14) -0.0038(13) 0.0047(12)
C12 0.053(2) 0.067(2) 0.0428(19) 0.0114(16) -0.0072(15) 0.0127(17)
C13 0.053(2) 0.067(2) 0.060(2) -0.0071(18) -0.0019(17) 0.0292(18)
C21 0.073(2) 0.0428(17) 0.0375(17) -0.0004(14) -0.0074(16) -0.0257(16)
C22 0.094(3) 0.064(2) 0.083(3) -0.010(2) -0.045(3) -0.016(2)
C23 0.133(4) 0.039(2) 0.105(4) -0.004(2) -0.048(3) -0.009(2)
C31 0.0303(14) 0.0267(13) 0.0325(14) 0.0045(11) 0.0014(11) -0.0057(10)
C32 0.053(2) 0.0408(17) 0.053(2) 0.0048(14) 0.0223(16) -0.0094(14)
C33 0.0514(19) 0.0271(14) 0.0522(19) 0.0010(13) 0.0117(15) -0.0055(13)
C42 0.0479(19) 0.096(3) 0.0247(15) -0.0012(16) 0.0095(13) 0.0234(18)
C43 0.0312(16) 0.070(2) 0.0336(16) 0.0011(15) 0.0062(12) 0.0131(14)
C51 0.0395(16) 0.0262(13) 0.0461(17) 0.0034(12) 0.0044(13) -0.0002(11)
C52 0.053(2) 0.0396(17) 0.066(2) -0.0180(16) 0.0067(17) -0.0002(15)
C53 0.120(4) 0.043(2) 0.071(3) 0.0256(19) 0.018(3) 0.003(2)
C61 0.0314(15) 0.0564(18) 0.0234(13) -0.0065(12) -0.0040(11) -
0.0031(13)
C62 0.049(2) 0.079(3) 0.049(2) 0.0097(18) -0.0095(16) 0.0194(18)
C63 0.053(2) 0.089(3) 0.060(2) -0.004(2) -0.0133(18) -0.032(2)
C71 0.0252(13) 0.0382(14) 0.0327(14) 0.0079(12) 0.0055(11) -0.0068(11)
C72 0.0320(15) 0.0420(15) 0.0336(15) 0.0086(12) 0.0087(12) -0.0027(12)
C81 0.0443(16) 0.0258(13) 0.0286(14) -0.0053(11) 0.0049(12) 0.0023(11)
C82 0.0424(17) 0.0346(15) 0.0369(16) -0.0002(12) 0.0124(13) 0.0104(12)
Ti11 0.0221(2) 0.0212(2) 0.0179(2) 0.00064(16) 0.00065(16) -0.00014(16)
Ti12 0.0249(2) 0.0233(2) 0.0185(2) -0.00060(17) -0.00114(16)
0.00195(17)
O11 0.0269(10) 0.0419(11) 0.0303(10) 0.0023(8) -0.0007(8) 0.0085(8)
O12 0.0410(11) 0.0273(9) 0.0231(9) 0.0015(7) -0.0014(8) -0.0124(8)
O13 0.0342(10) 0.0243(9) 0.0226(9) 0.0018(7) 0.0028(7) -0.0053(7)
O14 0.0235(9) 0.0285(9) 0.0215(8) -0.0019(7) 0.0019(7) 0.0047(7)
O15 0.0428(11) 0.0299(10) 0.0264(9) 0.0047(7) -0.0028(8) 0.0032(8)
O16 0.0335(10) 0.0389(10) 0.0372(11) -0.0019(8) -0.0124(8) -0.0030(8)
O17 0.0241(9) 0.0259(8) 0.0217(8) 0.0012(7) 0.0033(7) -0.0027(7)
O18 0.0290(9) 0.0177(8) 0.0228(9) -0.0022(6) 0.0006(7) 0.0009(7)
N12 0.0359(12) 0.0370(12) 0.0207(11) -0.0043(9) 0.0036(9) 0.0030(10)
C12' 0.063(2) 0.072(2) 0.0227(15) -0.0064(15) 0.0061(14) 0.0069(18)
C112 0.049(2) 0.101(3) 0.0399(19) 0.0061(19) -0.0080(16) 0.023(2)
C113 0.0365(18) 0.070(2) 0.073(2) -0.031(2) -0.0096(17) 0.0208(16)
C121 0.060(2) 0.0328(15) 0.0269(14) 0.0022(11) 0.0018(13) -0.0209(14)
C122 0.058(2) 0.051(2) 0.074(3) -0.0115(18) -0.0019(19) -0.0247(17)
C123 0.081(3) 0.0287(17) 0.130(4) 0.007(2) 0.003(3) -0.0039(18)
C131 0.0395(16) 0.0268(13) 0.0311(14) -0.0001(11) 0.0061(12) -
0.0091(11)
C132 0.0438(18) 0.0404(17) 0.056(2) 0.0050(15) 0.0177(15) -0.0099(14)
C133 0.063(2) 0.0343(17) 0.100(3) 0.0201(18) 0.034(2) 0.0084(16)
C142 0.0429(17) 0.0520(18) 0.0313(15) 0.0018(13) 0.0128(13) 0.0153(14)
C143 0.0332(16) 0.064(2) 0.0379(16) 0.0031(15) 0.0043(13) 0.0190(14)

C151 0.056(2) 0.0338(15) 0.0440(18) 0.0127(13) 0.0070(15) -0.0007(14)
C153 0.099(3) 0.0345(18) 0.074(3) -0.0036(17) 0.010(2) -0.0078(19)
C162 0.063(3) 0.175(6) 0.053(2) 0.021(3) -0.022(2) 0.019(3)
C163 0.075(3) 0.087(3) 0.164(5) -0.051(4) 0.014(3) -0.037(3)
C171 0.0287(14) 0.0404(15) 0.0293(14) 0.0033(11) 0.0077(11) -0.0044(11)
C172 0.0368(17) 0.071(2) 0.0399(17) -0.0082(16) 0.0109(13) 0.0051(15)
C181 0.0484(17) 0.0249(13) 0.0310(14) -0.0081(11) 0.0000(12) 0.0054(12)
C182 0.061(2) 0.0396(16) 0.0388(17) -0.0103(13) 0.0040(15) 0.0092(15)
C4A 0.0274(16) 0.0305(19) 0.0301(16) 0.0041(13) 0.0107(12) 0.0007(13)
C11A 0.0233(16) 0.033(2) 0.0355(18) 0.0003(14) -0.0012(13) 0.0007(14)
C14A 0.0250(15) 0.0288(17) 0.0334(16) 0.0027(12) 0.0071(12) 0.0022(12)
C16A 0.030(2) 0.063(3) 0.037(3) -0.012(2) -0.002(2) -0.0093(19)

_geom_special_details

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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.
;

loop_
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Ti1 O3 1.8193(17) . ?
Ti1 O2 1.8251(17) . ?
Ti1 O1 1.8360(18) . ?
Ti1 O7 2.0844(16) . ?
Ti1 O8 2.1392(16) . ?
Ti1 O4 2.2200(17) . ?
Ti1 Ti2 2.9664(7) . ?
Ti2 O6 1.7917(17) . ?
Ti2 O5 1.8199(17) . ?
Ti2 O4 1.9241(17) . ?
Ti2 O8 2.0421(16) . ?
Ti2 O7 2.0776(17) . ?
Ti2 N2 2.236(2) . ?
O1 C11 1.421(3) . ?
O2 C21 1.420(3) . ?
O3 C31 1.421(3) . ?
O4 C4B 1.34(3) . ?
O4 C4A 1.438(3) . ?
O5 C51 1.419(3) . ?
O6 C61 1.412(3) . ?
O7 C71 1.420(3) . ?
O8 C81 1.407(3) . ?

N2 C2' 1.471(3) . ?
N2 C82 1.491(3) . ?
N2 C72 1.507(3) . ?
C2' H2A 0.9800 . ?
C2' H2B 0.9800 . ?
C2' H2C 0.9800 . ?
C11 C12 1.495(4) . ?
C11 C13 1.505(5) . ?
C11 H11 1.0000 . ?
C12 H12A 0.9800 . ?
C12 H12B 0.9800 . ?
C12 H12C 0.9800 . ?
C13 H13A 0.9800 . ?
C13 H13B 0.9800 . ?
C13 H13C 0.9800 . ?
C21 C23 1.465(5) . ?
C21 C22 1.500(5) . ?
C21 H21 1.0000 . ?
C22 H22A 0.9800 . ?
C22 H22B 0.9800 . ?
C22 H22C 0.9800 . ?
C23 H23A 0.9800 . ?
C23 H23B 0.9800 . ?
C23 H23C 0.9800 . ?
C31 C32 1.510(4) . ?
C31 C33 1.514(4) . ?
C31 H31 1.0000 . ?
C32 H32A 0.9800 . ?
C32 H32B 0.9800 . ?
C32 H32C 0.9800 . ?
C33 H33A 0.9800 . ?
C33 H33B 0.9800 . ?
C33 H33C 0.9800 . ?
C42 C4B 1.35(3) . ?
C42 C4A 1.493(4) . ?
C42 H42A 0.9800 . ?
C42 H42B 0.9800 . ?
C42 H42C 0.9800 . ?
C43 C4A 1.521(3) . ?
C43 C4B 1.66(3) . ?
C43 H43A 0.9800 . ?
C43 H43B 0.9800 . ?
C43 H43C 0.9800 . ?
C51 C53 1.502(4) . ?
C51 C52 1.516(4) . ?
C51 H51 1.0000 . ?
C52 H52A 0.9800 . ?
C52 H52B 0.9800 . ?
C52 H52C 0.9800 . ?
C53 H53A 0.9800 . ?
C53 H53B 0.9800 . ?
C53 H53C 0.9800 . ?
C61 C63 1.507(4) . ?
C61 C62 1.515(5) . ?
C61 H61 1.0000 . ?
C62 H62A 0.9800 . ?
C62 H62B 0.9800 . ?

C62 H62C 0.9800 . ?
C63 H63A 0.9800 . ?
C63 H63B 0.9800 . ?
C63 H63C 0.9800 . ?
C71 C72 1.503(4) . ?
C71 H71A 0.9900 . ?
C71 H71B 0.9900 . ?
C72 H72A 0.9900 . ?
C72 H72B 0.9900 . ?
C81 C82 1.521(4) . ?
C81 H81A 0.9900 . ?
C81 H81B 0.9900 . ?
C82 H82A 0.9900 . ?
C82 H82B 0.9900 . ?
Ti11 O12 1.8058(17) . ?
Ti11 O13 1.8318(17) . ?
Ti11 O11 1.8380(18) . ?
Ti11 O18 2.0946(16) . ?
Ti11 O17 2.1127(17) . ?
Ti11 O14 2.2125(17) . ?
Ti11 Ti12 2.9662(7) . ?
Ti12 O16 1.7964(18) . ?
Ti12 O15 1.8058(18) . ?
Ti12 O14 1.9313(17) . ?
Ti12 O17 2.0588(17) . ?
Ti12 O18 2.0688(16) . ?
Ti12 N12 2.242(2) . ?
O11 C11A 1.407(3) . ?
O11 C11B 1.41(2) . ?
O12 C121 1.424(3) . ?
O13 C131 1.421(3) . ?
O14 C14B 1.38(3) . ?
O14 C14A 1.428(3) . ?
O15 C151 1.415(3) . ?
O16 C16A 1.423(4) . ?
O16 C16B 1.454(13) . ?
O17 C171 1.420(3) . ?
O18 C181 1.412(3) . ?
N12 C172 1.475(4) . ?
N12 C12' 1.476(3) . ?
N12 C182 1.496(3) . ?
C12' H1A 0.9800 . ?
C12' H1B 0.9800 . ?
C12' H1C 0.9800 . ?
C112 C11B 1.41(2) . ?
C112 C11A 1.501(5) . ?
C112 H11D 0.9800 . ?
C112 H11E 0.9800 . ?
C112 H11F 0.9800 . ?
C113 C11A 1.500(4) . ?
C113 C11B 1.54(2) . ?
C113 H11G 0.9800 . ?
C113 H11H 0.9800 . ?
C113 H11I 0.9800 . ?
C121 C123 1.483(5) . ?
C121 C122 1.514(4) . ?
C121 H121 1.0000 . ?

C122 H2A2 0.9800 . ?
C122 H2B2 0.9800 . ?
C122 H2C2 0.9800 . ?
C123 H12D 0.9800 . ?
C123 H12E 0.9800 . ?
C123 H12F 0.9800 . ?
C131 C133 1.503(4) . ?
C131 C132 1.507(4) . ?
C131 H131 1.0000 . ?
C132 H13D 0.9800 . ?
C132 H13E 0.9800 . ?
C132 H13F 0.9800 . ?
C133 H13G 0.9800 . ?
C133 H13H 0.9800 . ?
C133 H13I 0.9800 . ?
C142 C14B 1.49(3) . ?
C142 C14A 1.511(4) . ?
C142 H14A 0.9800 . ?
C142 H14B 0.9800 . ?
C142 H14C 0.9800 . ?
C143 C14A 1.529(4) . ?
C143 C14B 1.57(3) . ?
C143 H14D 0.9800 . ?
C143 H14E 0.9800 . ?
C143 H14F 0.9800 . ?
C151 C15B 1.453(9) . ?
C151 C153 1.485(5) . ?
C151 C15A 1.613(8) . ?
C151 H151 1.0000 . ?
C153 H15D 0.9800 . ?
C153 H15E 0.9800 . ?
C153 H15F 0.9800 . ?
C162 C16B 1.332(13) . ?
C162 C16A 1.507(6) . ?
C162 H16D 0.9800 . ?
C162 H16E 0.9800 . ?
C162 H16F 0.9800 . ?
C163 C16A 1.454(6) . ?
C163 C16B 1.574(14) . ?
C163 H16A 0.9800 . ?
C163 H16B 0.9800 . ?
C163 H16C 0.9800 . ?
C171 C172 1.512(4) . ?
C171 H17A 0.9900 . ?
C171 H17B 0.9900 . ?
C172 H17C 0.9900 . ?
C172 H17D 0.9900 . ?
C181 C182 1.526(3) . ?
C181 H18A 0.9900 . ?
C181 H18B 0.9900 . ?
C182 H18C 0.9900 . ?
C182 H18D 0.9900 . ?
C4A H41 1.0000 . ?
C11A H111 1.0000 . ?
C14A H141 1.0000 . ?
C15A H15A 0.9800 . ?
C15A H15B 0.9800 . ?

C15A H15C 0.9800 . ?
C16A H16I 1.0000 . ?
C4B H4B1 1.0000 . ?
C11B H1B1 1.0000 . ?
C14B H142 1.0000 . ?
C15B H15G 0.9800 . ?
C15B H15H 0.9800 . ?
C15B H15J 0.9800 . ?
C16B H6B1 1.0000 . ?

loop_

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O3 Ti1 O2 98.56(8) . . ?
O3 Ti1 O1 102.18(8) . . ?
O2 Ti1 O1 101.17(9) . . ?
O3 Ti1 O7 160.39(7) . . ?
O2 Ti1 O7 91.88(7) . . ?
O1 Ti1 O7 91.93(7) . . ?
O3 Ti1 O8 89.48(7) . . ?
O2 Ti1 O8 163.65(7) . . ?
O1 Ti1 O8 90.92(7) . . ?
O7 Ti1 O8 76.61(6) . . ?
O3 Ti1 O4 92.93(7) . . ?
O2 Ti1 O4 95.14(7) . . ?
O1 Ti1 O4 155.74(7) . . ?
O7 Ti1 O4 69.52(6) . . ?
O8 Ti1 O4 70.12(6) . . ?
O3 Ti1 Ti2 116.23(6) . . ?
O2 Ti1 Ti2 120.38(6) . . ?
O1 Ti1 Ti2 115.31(6) . . ?
O7 Ti1 Ti2 44.45(5) . . ?
O8 Ti1 Ti2 43.50(4) . . ?
O4 Ti1 Ti2 40.43(4) . . ?
O6 Ti2 O5 96.89(8) . . ?
O6 Ti2 O4 110.84(8) . . ?
O5 Ti2 O4 105.26(8) . . ?
O6 Ti2 O8 92.42(7) . . ?
O5 Ti2 O8 167.98(8) . . ?
O4 Ti2 O8 78.27(7) . . ?
O6 Ti2 O7 168.10(8) . . ?
O5 Ti2 O7 90.74(7) . . ?
O4 Ti2 O7 75.64(7) . . ?
O8 Ti2 O7 78.92(6) . . ?
O6 Ti2 N2 95.49(8) . . ?
O5 Ti2 N2 93.53(8) . . ?
O4 Ti2 N2 145.00(7) . . ?
O8 Ti2 N2 77.97(7) . . ?
O7 Ti2 N2 74.85(7) . . ?
O6 Ti2 Ti1 132.18(6) . . ?
O5 Ti2 Ti1 128.09(6) . . ?
O4 Ti2 Ti1 48.44(5) . . ?

O8 Ti2 Ti1 46.15(4) . . ?
O7 Ti2 Ti1 44.63(4) . . ?
N2 Ti2 Ti1 96.79(6) . . ?
C11 O1 Ti1 136.95(18) . . ?
C21 O2 Ti1 132.36(18) . . ?
C31 O3 Ti1 137.82(15) . . ?
C4B O4 C4A 33.9(16) . . ?
C4B O4 Ti2 136.7(13) . . ?
C4A O4 Ti2 132.91(14) . . ?
C4B O4 Ti1 131.0(12) . . ?
C4A O4 Ti1 125.25(13) . . ?
Ti2 O4 Ti1 91.13(7) . . ?
C51 O5 Ti2 144.04(17) . . ?
C61 O6 Ti2 158.37(18) . . ?
C71 O7 Ti2 120.11(14) . . ?
C71 O7 Ti1 126.85(15) . . ?
Ti2 O7 Ti1 90.92(6) . . ?
C81 O8 Ti2 114.10(14) . . ?
C81 O8 Ti1 132.81(15) . . ?
Ti2 O8 Ti1 90.35(6) . . ?
C2' N2 C82 112.1(2) . . ?
C2' N2 C72 108.6(2) . . ?
C82 N2 C72 109.8(2) . . ?
C2' N2 Ti2 111.95(16) . . ?
C82 N2 Ti2 109.71(16) . . ?
C72 N2 Ti2 104.42(15) . . ?
N2 C2' H2A 109.5 . . ?
N2 C2' H2B 109.5 . . ?
H2A C2' H2B 109.5 . . ?
N2 C2' H2C 109.5 . . ?
H2A C2' H2C 109.5 . . ?
H2B C2' H2C 109.5 . . ?
O1 C11 C12 111.3(3) . . ?
O1 C11 C13 109.3(3) . . ?
C12 C11 C13 112.1(3) . . ?
O1 C11 H11 108.0 . . ?
C12 C11 H11 108.0 . . ?
C13 C11 H11 108.0 . . ?
C11 C12 H12A 109.5 . . ?
C11 C12 H12B 109.5 . . ?
H12A C12 H12B 109.5 . . ?
C11 C12 H12C 109.5 . . ?
H12A C12 H12C 109.5 . . ?
H12B C12 H12C 109.5 . . ?
C11 C13 H13A 109.5 . . ?
C11 C13 H13B 109.5 . . ?
H13A C13 H13B 109.5 . . ?
C11 C13 H13C 109.5 . . ?
H13A C13 H13C 109.5 . . ?
H13B C13 H13C 109.5 . . ?
O2 C21 C23 111.2(3) . . ?
O2 C21 C22 110.5(3) . . ?
C23 C21 C22 113.2(3) . . ?
O2 C21 H21 107.2 . . ?
C23 C21 H21 107.2 . . ?
C22 C21 H21 107.2 . . ?
C21 C22 H22A 109.5 . . ?

C21 C22 H22B 109.5 . . ?
H22A C22 H22B 109.5 . . ?
C21 C22 H22C 109.5 . . ?
H22A C22 H22C 109.5 . . ?
H22B C22 H22C 109.5 . . ?
C21 C23 H23A 109.5 . . ?
C21 C23 H23B 109.5 . . ?
H23A C23 H23B 109.5 . . ?
C21 C23 H23C 109.5 . . ?
H23A C23 H23C 109.5 . . ?
H23B C23 H23C 109.5 . . ?
O3 C31 C32 109.5(2) . . ?
O3 C31 C33 110.0(2) . . ?
C32 C31 C33 111.4(2) . . ?
O3 C31 H31 108.6 . . ?
C32 C31 H31 108.6 . . ?
C33 C31 H31 108.6 . . ?
C31 C32 H32A 109.5 . . ?
C31 C32 H32B 109.5 . . ?
H32A C32 H32B 109.5 . . ?
C31 C32 H32C 109.5 . . ?
H32A C32 H32C 109.5 . . ?
H32B C32 H32C 109.5 . . ?
C31 C33 H33A 109.5 . . ?
C31 C33 H33B 109.5 . . ?
H33A C33 H33B 109.5 . . ?
C31 C33 H33C 109.5 . . ?
H33A C33 H33C 109.5 . . ?
H33B C33 H33C 109.5 . . ?
C4B C42 C4A 32.9(16) . . ?
C4B C42 H42A 114.8 . . ?
C4A C42 H42A 109.5 . . ?
C4B C42 H42B 129.5 . . ?
C4A C42 H42B 109.5 . . ?
H42A C42 H42B 109.5 . . ?
C4B C42 H42C 77.5 . . ?
C4A C42 H42C 109.5 . . ?
H42A C42 H42C 109.5 . . ?
H42B C42 H42C 109.5 . . ?
C4A C43 C4B 29.3(13) . . ?
C4A C43 H43A 109.5 . . ?
C4B C43 H43A 121.0 . . ?
C4A C43 H43B 109.5 . . ?
C4B C43 H43B 80.2 . . ?
H43A C43 H43B 109.5 . . ?
C4A C43 H43C 109.5 . . ?
C4B C43 H43C 121.8 . . ?
H43A C43 H43C 109.5 . . ?
H43B C43 H43C 109.5 . . ?
O5 C51 C53 109.3(3) . . ?
O5 C51 C52 109.5(2) . . ?
C53 C51 C52 110.9(3) . . ?
O5 C51 H51 109.1 . . ?
C53 C51 H51 109.1 . . ?
C52 C51 H51 109.1 . . ?
C51 C52 H52A 109.5 . . ?
C51 C52 H52B 109.5 . . ?

H52A C52 H52B 109.5 . . ?
C51 C52 H52C 109.5 . . ?
H52A C52 H52C 109.5 . . ?
H52B C52 H52C 109.5 . . ?
C51 C53 H53A 109.5 . . ?
C51 C53 H53B 109.5 . . ?
H53A C53 H53B 109.5 . . ?
C51 C53 H53C 109.5 . . ?
H53A C53 H53C 109.5 . . ?
H53B C53 H53C 109.5 . . ?
O6 C61 C63 109.3(2) . . ?
O6 C61 C62 110.4(2) . . ?
C63 C61 C62 112.2(3) . . ?
O6 C61 H61 108.3 . . ?
C63 C61 H61 108.3 . . ?
C62 C61 H61 108.3 . . ?
C61 C62 H62A 109.5 . . ?
C61 C62 H62B 109.5 . . ?
H62A C62 H62B 109.5 . . ?
C61 C62 H62C 109.5 . . ?
H62A C62 H62C 109.5 . . ?
H62B C62 H62C 109.5 . . ?
C61 C63 H63A 109.5 . . ?
C61 C63 H63B 109.5 . . ?
H63A C63 H63B 109.5 . . ?
C61 C63 H63C 109.5 . . ?
H63A C63 H63C 109.5 . . ?
H63B C63 H63C 109.5 . . ?
O7 C71 C72 109.5(2) . . ?
O7 C71 H71A 109.8 . . ?
C72 C71 H71A 109.8 . . ?
O7 C71 H71B 109.8 . . ?
C72 C71 H71B 109.8 . . ?
H71A C71 H71B 108.2 . . ?
C71 C72 N2 108.7(2) . . ?
C71 C72 H72A 109.9 . . ?
N2 C72 H72A 109.9 . . ?
C71 C72 H72B 109.9 . . ?
N2 C72 H72B 109.9 . . ?
H72A C72 H72B 108.3 . . ?
O8 C81 C82 109.2(2) . . ?
O8 C81 H81A 109.8 . . ?
C82 C81 H81A 109.8 . . ?
O8 C81 H81B 109.8 . . ?
C82 C81 H81B 109.8 . . ?
H81A C81 H81B 108.3 . . ?
N2 C82 C81 109.2(2) . . ?
N2 C82 H82A 109.8 . . ?
C81 C82 H82A 109.8 . . ?
N2 C82 H82B 109.8 . . ?
C81 C82 H82B 109.8 . . ?
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O12 Ti11 O11 101.80(9) . . ?
O13 Ti11 O11 101.71(8) . . ?
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O13 Ti11 O18 89.75(7) . . ?

O11 Ti11 O18 89.96(7) . . ?
O12 Ti11 O17 90.94(7) . . ?
O13 Ti11 O17 160.80(7) . . ?
O11 Ti11 O17 92.17(8) . . ?
O18 Ti11 O17 76.92(6) . . ?
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O13 Ti11 O14 94.10(7) . . ?
O11 Ti11 O14 155.41(7) . . ?
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O17 Ti11 O14 68.70(6) . . ?
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O13 Ti11 Ti12 117.17(6) . . ?
O11 Ti11 Ti12 114.81(6) . . ?
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O17 Ti11 Ti12 43.95(5) . . ?
O14 Ti11 Ti12 40.61(4) . . ?
O16 Ti12 O15 98.10(9) . . ?
O16 Ti12 O14 106.77(8) . . ?
O15 Ti12 O14 106.77(8) . . ?
O16 Ti12 O17 169.20(8) . . ?
O15 Ti12 O17 91.25(8) . . ?
O14 Ti12 O17 75.39(7) . . ?
O16 Ti12 O18 91.34(8) . . ?
O15 Ti12 O18 167.76(8) . . ?
O14 Ti12 O18 77.65(7) . . ?
O17 Ti12 O18 78.69(6) . . ?
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O15 Ti12 N12 96.22(9) . . ?
O14 Ti12 N12 144.64(7) . . ?
O17 Ti12 N12 77.65(7) . . ?
O18 Ti12 N12 74.97(7) . . ?
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O15 Ti12 Ti11 130.00(6) . . ?
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O18 Ti12 Ti11 44.91(4) . . ?
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C11B O11 Ti11 141.5(9) . . ?
C121 O12 Ti11 140.33(16) . . ?
C131 O13 Ti11 134.12(16) . . ?
C14B O14 C14A 39.2(13) . . ?
C14B O14 Ti12 135.9(11) . . ?
C14A O14 Ti12 125.35(16) . . ?
C14B O14 Ti11 132.3(11) . . ?
C14A O14 Ti11 126.35(15) . . ?
Ti12 O14 Ti11 91.16(7) . . ?
C151 O15 Ti12 147.70(18) . . ?
C16A O16 C16B 35.2(6) . . ?
C16A O16 Ti12 166.3(2) . . ?
C16B O16 Ti12 148.1(7) . . ?
C171 O17 Ti12 115.49(14) . . ?
C171 O17 Ti11 128.70(15) . . ?
Ti12 O17 Ti11 90.63(6) . . ?
C181 O18 Ti12 119.15(15) . . ?
C181 O18 Ti11 130.26(16) . . ?

Ti12 O18 Ti11 90.87(6) . . ?
 C172 N12 C12' 112.4(2) . . ?
 C172 N12 C182 109.8(2) . . ?
 C12' N12 C182 108.3(2) . . ?
 C172 N12 Ti12 110.10(16) . . ?
 C12' N12 Ti12 112.19(18) . . ?
 C182 N12 Ti12 103.62(14) . . ?
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 N12 C12' H1B 109.5 . . ?
 H1A C12' H1B 109.5 . . ?
 N12 C12' H1C 109.5 . . ?
 H1A C12' H1C 109.5 . . ?
 H1B C12' H1C 109.5 . . ?
 C11B C112 C11A 32.8(11) . . ?
 C11B C112 H11D 119.3 . . ?
 C11A C112 H11D 109.5 . . ?
 C11B C112 H11E 125.4 . . ?
 C11A C112 H11E 109.5 . . ?
 H11D C112 H11E 109.5 . . ?
 C11B C112 H11F 76.8 . . ?
 C11A C112 H11F 109.5 . . ?
 H11D C112 H11F 109.5 . . ?
 H11E C112 H11F 109.5 . . ?
 C11A C113 C11B 31.5(10) . . ?
 C11A C113 H11G 109.5 . . ?
 C11B C113 H11G 122.2 . . ?
 C11A C113 H11H 109.5 . . ?
 C11B C113 H11H 78.0 . . ?
 H11G C113 H11H 109.5 . . ?
 C11A C113 H11I 109.5 . . ?
 C11B C113 H11I 121.9 . . ?
 H11G C113 H11I 109.5 . . ?
 H11H C113 H11I 109.5 . . ?
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 O12 C121 C122 109.3(2) . . ?
 C123 C121 C122 112.2(3) . . ?
 O12 C121 H121 108.4 . . ?
 C123 C121 H121 108.4 . . ?
 C122 C121 H121 108.4 . . ?
 C121 C122 H2A2 109.5 . . ?
 C121 C122 H2B2 109.5 . . ?
 H2A2 C122 H2B2 109.5 . . ?
 C121 C122 H2C2 109.5 . . ?
 H2A2 C122 H2C2 109.5 . . ?
 H2B2 C122 H2C2 109.5 . . ?
 C121 C123 H12D 109.5 . . ?
 C121 C123 H12E 109.5 . . ?
 H12D C123 H12E 109.5 . . ?
 C121 C123 H12F 109.5 . . ?
 H12D C123 H12F 109.5 . . ?
 H12E C123 H12F 109.5 . . ?
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 O13 C131 C132 110.3(2) . . ?
 C133 C131 C132 112.0(3) . . ?
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 C133 C131 H131 108.3 . . ?
 C132 C131 H131 108.3 . . ?

C131 C132 H13D 109.5 . . ?
C131 C132 H13E 109.5 . . ?
H13D C132 H13E 109.5 . . ?
C131 C132 H13F 109.5 . . ?
H13D C132 H13F 109.5 . . ?
H13E C132 H13F 109.5 . . ?
C131 C133 H13G 109.5 . . ?
C131 C133 H13H 109.5 . . ?
H13G C133 H13H 109.5 . . ?
C131 C133 H13I 109.5 . . ?
H13G C133 H13I 109.5 . . ?
H13H C133 H13I 109.5 . . ?
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C14B C142 H14A 119.9 . . ?
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C14B C142 H14B 126.6 . . ?
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H14A C142 H14B 109.5 . . ?
C14B C142 H14C 73.0 . . ?
C14A C142 H14C 109.5 . . ?
H14A C142 H14C 109.5 . . ?
H14B C142 H14C 109.5 . . ?
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C14A C143 H14D 109.5 . . ?
C14B C143 H14D 121.1 . . ?
C14A C143 H14E 109.5 . . ?
C14B C143 H14E 74.1 . . ?
H14D C143 H14E 109.5 . . ?
C14A C143 H14F 109.5 . . ?
C14B C143 H14F 125.0 . . ?
H14D C143 H14F 109.5 . . ?
H14E C143 H14F 109.5 . . ?
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O15 C151 C153 111.0(3) . . ?
C15B C151 C153 122.6(5) . . ?
O15 C151 C15A 104.3(4) . . ?
C15B C151 C15A 29.5(4) . . ?
C153 C151 C15A 103.1(4) . . ?
O15 C151 H151 112.6 . . ?
C15B C151 H151 83.9 . . ?
C153 C151 H151 112.6 . . ?
C15A C151 H151 112.6 . . ?
C151 C153 H15D 109.5 . . ?
C151 C153 H15E 109.5 . . ?
H15D C153 H15E 109.5 . . ?
C151 C153 H15F 109.5 . . ?
H15D C153 H15F 109.5 . . ?
H15E C153 H15F 109.5 . . ?
C16B C162 C16A 35.0(7) . . ?
C16B C162 H16D 117.2 . . ?
C16A C162 H16D 109.5 . . ?
C16B C162 H16E 128.5 . . ?
C16A C162 H16E 109.5 . . ?
H16D C162 H16E 109.5 . . ?
C16B C162 H16F 75.0 . . ?
C16A C162 H16F 109.5 . . ?
H16D C162 H16F 109.5 . . ?

H16E C162 H16F 109.5 . . ?
C16A C163 C16B 33.1(6) . . ?
C16A C163 H16A 109.5 . . ?
C16B C163 H16A 122.9 . . ?
C16A C163 H16B 109.5 . . ?
C16B C163 H16B 76.4 . . ?
H16A C163 H16B 109.5 . . ?
C16A C163 H16C 109.5 . . ?
C16B C163 H16C 122.0 . . ?
H16A C163 H16C 109.5 . . ?
H16B C163 H16C 109.5 . . ?
O17 C171 C172 109.4(2) . . ?
O17 C171 H17A 109.8 . . ?
C172 C171 H17A 109.8 . . ?
O17 C171 H17B 109.8 . . ?
C172 C171 H17B 109.8 . . ?
H17A C171 H17B 108.2 . . ?
N12 C172 C171 110.7(2) . . ?
N12 C172 H17C 109.5 . . ?
C171 C172 H17C 109.5 . . ?
N12 C172 H17D 109.5 . . ?
C171 C172 H17D 109.5 . . ?
H17C C172 H17D 108.1 . . ?
O18 C181 C182 110.3(2) . . ?
O18 C181 H18A 109.6 . . ?
C182 C181 H18A 109.6 . . ?
O18 C181 H18B 109.6 . . ?
C182 C181 H18B 109.6 . . ?
H18A C181 H18B 108.1 . . ?
N12 C182 C181 108.55(19) . . ?
N12 C182 H18C 110.0 . . ?
C181 C182 H18C 110.0 . . ?
N12 C182 H18D 110.0 . . ?
C181 C182 H18D 110.0 . . ?
H18C C182 H18D 108.4 . . ?
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O4 C4A C43 110.58(19) . . ?
C42 C4A C43 111.1(2) . . ?
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C42 C4A H41 108.5 . . ?
C43 C4A H41 108.5 . . ?
O11 C11A C113 109.6(3) . . ?
O11 C11A C112 111.7(3) . . ?
C113 C11A C112 112.6(3) . . ?
O11 C11A H111 107.6 . . ?
C113 C11A H111 107.6 . . ?
C112 C11A H111 107.6 . . ?
O14 C14A C142 110.8(2) . . ?
O14 C14A C143 109.5(2) . . ?
C142 C14A C143 109.3(2) . . ?
O14 C14A H141 109.1 . . ?
C142 C14A H141 109.1 . . ?
C143 C14A H141 109.1 . . ?
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H15A C15A H15B 109.5 . . ?
C151 C15A H15C 109.5 . . ?

H15A C15A H15C 109.5 . . ?
H15B C15A H15C 109.5 . . ?
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O16 C16A C162 107.4(4) . . ?
C163 C16A C162 114.6(4) . . ?
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C163 C16A H161 107.8 . . ?
C162 C16A H161 107.8 . . ?
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O4 C4B C43 108(2) . . ?
C42 C4B C43 111(2) . . ?
O4 C4B H4B1 103.2 . . ?
C42 C4B H4B1 103.2 . . ?
C43 C4B H4B1 103.2 . . ?
C112 C11B O11 117.6(16) . . ?
C112 C11B C113 115.6(15) . . ?
O11 C11B C113 106.9(14) . . ?
C112 C11B H1B1 105.2 . . ?
O11 C11B H1B1 105.2 . . ?
C113 C11B H1B1 105.2 . . ?
O14 C14B C142 114.5(19) . . ?
O14 C14B C143 109.9(18) . . ?
C142 C14B C143 108.1(17) . . ?
O14 C14B H142 108.0 . . ?
C142 C14B H142 108.0 . . ?
C143 C14B H142 108.0 . . ?
C151 C15B H15G 109.5 . . ?
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H15G C15B H15H 109.5 . . ?
C151 C15B H15J 109.5 . . ?
H15G C15B H15J 109.5 . . ?
H15H C15B H15J 109.5 . . ?
C162 C16B O16 115.9(10) . . ?
C162 C16B C163 117.9(10) . . ?
O16 C16B C163 103.2(9) . . ?
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O16 C16B H6B1 106.4 . . ?
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O4 Ti2 O6 C61 125.9(5) ?
O8 Ti2 O6 C61 -155.7(5) ?
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O5 Ti2 O8 C81 -72.2(4) ?

O4 Ti2 O8 C81 179.39(17) ?
O7 Ti2 O8 C81 -103.17(16) ?
N2 Ti2 O8 C81 -26.50(16) ?
Ti1 Ti2 O8 C81 -138.35(18) ?
O6 Ti2 O8 Ti1 -153.04(7) ?
O5 Ti2 O8 Ti1 66.1(4) ?
O4 Ti2 O8 Ti1 -42.26(6) ?
O7 Ti2 O8 Ti1 35.18(6) ?
N2 Ti2 O8 Ti1 111.85(8) ?
O3 Ti1 O8 C81 -105.1(2) ?
O2 Ti1 O8 C81 135.0(3) ?
O1 Ti1 O8 C81 -3.0(2) ?
O7 Ti1 O8 C81 88.8(2) ?
O4 Ti1 O8 C81 161.6(2) ?
Ti2 Ti1 O8 C81 124.2(2) ?
O3 Ti1 O8 Ti2 130.66(7) ?
O2 Ti1 O8 Ti2 10.8(3) ?
O1 Ti1 O8 Ti2 -127.17(7) ?
O7 Ti1 O8 Ti2 -35.40(6) ?
O4 Ti1 O8 Ti2 37.36(6) ?
O6 Ti2 N2 C2' 33.71(19) ?
O5 Ti2 N2 C2' -63.56(19) ?
O4 Ti2 N2 C2' 173.22(17) ?
O8 Ti2 N2 C2' 125.03(19) ?
O7 Ti2 N2 C2' -153.37(19) ?
Ti1 Ti2 N2 C2' 167.41(17) ?
O6 Ti2 N2 C82 -91.43(18) ?
O5 Ti2 N2 C82 171.29(17) ?
O4 Ti2 N2 C82 48.1(2) ?
O8 Ti2 N2 C82 -0.12(17) ?
O7 Ti2 N2 C82 81.49(17) ?
Ti1 Ti2 N2 C82 42.26(17) ?
O6 Ti2 N2 C72 150.98(15) ?
O5 Ti2 N2 C72 53.71(16) ?
O4 Ti2 N2 C72 -69.5(2) ?
O8 Ti2 N2 C72 -117.71(15) ?
O7 Ti2 N2 C72 -36.10(14) ?
Ti1 Ti2 N2 C72 -75.33(15) ?
Ti1 O1 C11 C12 -70.0(4) ?
Ti1 O1 C11 C13 165.6(2) ?
Ti1 O2 C21 C23 91.2(4) ?
Ti1 O2 C21 C22 -142.1(3) ?
Ti1 O3 C31 C32 -152.8(2) ?
Ti1 O3 C31 C33 84.5(3) ?
Ti2 O5 C51 C53 154.8(3) ?
Ti2 O5 C51 C52 -83.6(4) ?
Ti2 O6 C61 C63 -163.0(4) ?
Ti2 O6 C61 C62 -39.2(6) ?
Ti2 O7 C71 C72 5.4(3) ?
Ti1 O7 C71 C72 122.7(2) ?
O7 C71 C72 N2 -38.3(3) ?
C2' N2 C72 C71 170.2(2) ?
C82 N2 C72 C71 -66.9(3) ?
Ti2 N2 C72 C71 50.6(2) ?
Ti2 O8 C81 C82 48.0(2) ?
Ti1 O8 C81 C82 -67.1(3) ?
C2' N2 C82 C81 -101.3(3) ?

C72 N2 C82 C81 137.9(2) ?
Ti2 N2 C82 C81 23.7(3) ?
O8 C81 C82 N2 -45.8(3) ?
O12 Ti11 Ti12 O16 -135.62(11) ?
O13 Ti11 Ti12 O16 -16.14(11) ?
O11 Ti11 Ti12 O16 103.10(11) ?
O18 Ti11 Ti12 O16 41.53(11) ?
O17 Ti11 Ti12 O16 168.30(11) ?
O14 Ti11 Ti12 O16 -77.78(11) ?
O12 Ti11 Ti12 O15 18.00(11) ?
O13 Ti11 Ti12 O15 137.47(10) ?
O11 Ti11 Ti12 O15 -103.29(11) ?
O18 Ti11 Ti12 O15 -164.85(11) ?
O17 Ti11 Ti12 O15 -38.08(10) ?
O14 Ti11 Ti12 O15 75.83(11) ?
O12 Ti11 Ti12 O14 -57.83(10) ?
O13 Ti11 Ti12 O14 61.64(9) ?
O11 Ti11 Ti12 O14 -179.12(10) ?
O18 Ti11 Ti12 O14 119.32(10) ?
O17 Ti11 Ti12 O14 -113.92(10) ?
O12 Ti11 Ti12 O17 56.09(9) ?
O13 Ti11 Ti12 O17 175.56(9) ?
O11 Ti11 Ti12 O17 -65.20(9) ?
O18 Ti11 Ti12 O17 -126.76(9) ?
O14 Ti11 Ti12 O17 113.92(10) ?
O12 Ti11 Ti12 O18 -177.15(10) ?
O13 Ti11 Ti12 O18 -57.68(9) ?
O11 Ti11 Ti12 O18 61.56(9) ?
O17 Ti11 Ti12 O18 126.76(9) ?
O14 Ti11 Ti12 O18 -119.32(10) ?
O12 Ti11 Ti12 N12 121.69(9) ?
O13 Ti11 Ti12 N12 -118.84(9) ?
O11 Ti11 Ti12 N12 0.40(9) ?
O18 Ti11 Ti12 N12 -61.16(9) ?
O17 Ti11 Ti12 N12 65.60(9) ?
O14 Ti11 Ti12 N12 179.52(9) ?
O12 Ti11 O11 C11A 6.9(3) ?
O13 Ti11 O11 C11A -95.1(3) ?
O18 Ti11 O11 C11A 175.2(3) ?
O17 Ti11 O11 C11A 98.3(3) ?
O14 Ti11 O11 C11A 136.0(3) ?
Ti12 Ti11 O11 C11A 137.4(3) ?
O12 Ti11 O11 C11B 60.4(19) ?
O13 Ti11 O11 C11B -41.5(19) ?
O18 Ti11 O11 C11B -131.3(19) ?
O17 Ti11 O11 C11B 151.8(19) ?
O14 Ti11 O11 C11B -170.5(19) ?
Ti12 Ti11 O11 C11B -169.1(19) ?
O13 Ti11 O12 C121 -165.4(3) ?
O11 Ti11 O12 C121 90.5(3) ?
O18 Ti11 O12 C121 -44.1(5) ?
O17 Ti11 O12 C121 -1.9(3) ?
O14 Ti11 O12 C121 -70.6(3) ?
Ti12 Ti11 O12 C121 -37.1(3) ?
O12 Ti11 O13 C131 -175.3(2) ?
O11 Ti11 O13 C131 -71.2(2) ?
O18 Ti11 O13 C131 18.7(2) ?

O17 Ti11 O13 C131 64.3(3) ?
O14 Ti11 O13 C131 89.9(2) ?
Ti12 Ti11 O13 C131 54.9(2) ?
O16 Ti12 O14 C14B -61.9(19) ?
O15 Ti12 O14 C14B 42.3(19) ?
O17 Ti12 O14 C14B 129.1(19) ?
O18 Ti12 O14 C14B -149.5(19) ?
N12 Ti12 O14 C14B 170.6(19) ?
Ti11 Ti12 O14 C14B 171.4(19) ?
O16 Ti12 O14 C14A -11.1(2) ?
O15 Ti12 O14 C14A 93.0(2) ?
O17 Ti12 O14 C14A 179.9(2) ?
O18 Ti12 O14 C14A -98.8(2) ?
N12 Ti12 O14 C14A -138.7(2) ?
Ti11 Ti12 O14 C14A -137.8(2) ?
O16 Ti12 O14 Ti11 126.72(8) ?
O15 Ti12 O14 Ti11 -129.13(7) ?
O17 Ti12 O14 Ti11 -42.29(6) ?
O18 Ti12 O14 Ti11 39.07(6) ?
N12 Ti12 O14 Ti11 -0.82(16) ?
O12 Ti11 O14 C14B -39.6(18) ?
O13 Ti11 O14 C14B 59.8(18) ?
O11 Ti11 O14 C14B -170.0(18) ?
O18 Ti11 O14 C14B 148.1(18) ?
O17 Ti11 O14 C14B -129.0(18) ?
Ti12 Ti11 O14 C14B -171.9(18) ?
O12 Ti11 O14 C14A -90.5(2) ?
O13 Ti11 O14 C14A 8.9(2) ?
O11 Ti11 O14 C14A 139.1(2) ?
O18 Ti11 O14 C14A 97.2(2) ?
O17 Ti11 O14 C14A -179.9(2) ?
Ti12 Ti11 O14 C14A 137.2(2) ?
O12 Ti11 O14 Ti12 132.34(8) ?
O13 Ti11 O14 Ti12 -128.29(7) ?
O11 Ti11 O14 Ti12 1.9(2) ?
O18 Ti11 O14 Ti12 -39.96(6) ?
O17 Ti11 O14 Ti12 42.92(6) ?
O16 Ti12 O15 C151 170.5(4) ?
O14 Ti12 O15 C151 60.1(4) ?
O17 Ti12 O15 C151 -15.0(4) ?
O18 Ti12 O15 C151 -49.4(6) ?
N12 Ti12 O15 C151 -92.7(4) ?
Ti11 Ti12 O15 C151 11.1(4) ?
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O14 Ti12 O16 C16A 65.5(11) ?
O17 Ti12 O16 C16A 165.5(10) ?
O18 Ti12 O16 C16A 143.0(11) ?
N12 Ti12 O16 C16A -141.9(11) ?
Ti11 Ti12 O16 C16A 115.1(11) ?
O15 Ti12 O16 C16B 48.9(11) ?
O14 Ti12 O16 C16B 159.2(10) ?
O17 Ti12 O16 C16B -100.8(11) ?
O18 Ti12 O16 C16B -123.3(11) ?
N12 Ti12 O16 C16B -48.3(11) ?
Ti11 Ti12 O16 C16B -151.2(10) ?
O16 Ti12 O17 C171 76.1(5) ?
O15 Ti12 O17 C171 -73.93(17) ?

O14 Ti12 O17 C171 179.06(17) ?
O18 Ti12 O17 C171 99.04(17) ?
N12 Ti12 O17 C171 22.15(16) ?
Ti11 Ti12 O17 C171 134.27(18) ?
O16 Ti12 O17 Ti11 -58.2(5) ?
O15 Ti12 O17 Ti11 151.80(8) ?
O14 Ti12 O17 Ti11 44.79(7) ?
O18 Ti12 O17 Ti11 -35.23(6) ?
N12 Ti12 O17 Ti11 -112.11(8) ?
O12 Ti11 O17 C171 102.21(19) ?
O13 Ti11 O17 C171 -136.2(2) ?
O11 Ti11 O17 C171 0.37(19) ?
O18 Ti11 O17 C171 -89.08(19) ?
O14 Ti11 O17 C171 -163.8(2) ?
Ti12 Ti11 O17 C171 -124.1(2) ?
O12 Ti11 O17 Ti12 -133.71(8) ?
O13 Ti11 O17 Ti12 -12.1(2) ?
O11 Ti11 O17 Ti12 124.45(8) ?
O18 Ti11 O17 Ti12 35.00(6) ?
O14 Ti11 O17 Ti12 -39.70(6) ?
O16 Ti12 O18 C181 72.92(19) ?
O15 Ti12 O18 C181 -67.7(4) ?
O14 Ti12 O18 C181 179.80(19) ?
O17 Ti12 O18 C181 -102.88(18) ?
N12 Ti12 O18 C181 -22.79(18) ?
Ti11 Ti12 O18 C181 -138.5(2) ?
O16 Ti12 O18 Ti11 -148.61(8) ?
O15 Ti12 O18 Ti11 70.8(4) ?
O14 Ti12 O18 Ti11 -41.73(7) ?
O17 Ti12 O18 Ti11 35.58(6) ?
N12 Ti12 O18 Ti11 115.67(8) ?
O12 Ti11 O18 C181 139.4(3) ?
O13 Ti11 O18 C181 -98.1(2) ?
O11 Ti11 O18 C181 3.6(2) ?
O17 Ti11 O18 C181 95.8(2) ?
O14 Ti11 O18 C181 167.5(2) ?
Ti12 Ti11 O18 C181 130.6(2) ?
O12 Ti11 O18 Ti12 8.8(3) ?
O13 Ti11 O18 Ti12 131.25(7) ?
O11 Ti11 O18 Ti12 -127.04(8) ?
O17 Ti11 O18 Ti12 -34.81(6) ?
O14 Ti11 O18 Ti12 36.83(6) ?
O16 Ti12 N12 C172 -168.3(2) ?
O15 Ti12 N12 C172 92.8(2) ?
O14 Ti12 N12 C172 -38.1(3) ?
O17 Ti12 N12 C172 2.89(19) ?
O18 Ti12 N12 C172 -78.53(19) ?
Ti11 Ti12 N12 C172 -38.71(19) ?
O16 Ti12 N12 C12' 65.7(2) ?
O15 Ti12 N12 C12' -33.2(2) ?
O14 Ti12 N12 C12' -164.07(19) ?
O17 Ti12 N12 C12' -123.1(2) ?
O18 Ti12 N12 C12' 155.5(2) ?
Ti11 Ti12 N12 C12' -164.7(2) ?
O16 Ti12 N12 C182 -50.92(15) ?
O15 Ti12 N12 C182 -149.75(14) ?
O14 Ti12 N12 C182 79.33(19) ?

O17 Ti12 N12 C182 120.32(14) ?
O18 Ti12 N12 C182 38.90(13) ?
Ti11 Ti12 N12 C182 78.72(13) ?
Ti11 O12 C121 C123 111.2(3) ?
Ti11 O12 C121 C122 -125.2(3) ?
Ti11 O13 C131 C133 80.9(3) ?
Ti11 O13 C131 C132 -155.3(2) ?
Ti12 O15 C151 C15B 161.7(6) ?
Ti12 O15 C151 C153 -57.8(5) ?
Ti12 O15 C151 C15A -168.3(4) ?
Ti12 O17 C171 C172 -42.6(3) ?
Ti11 O17 C171 C172 70.8(3) ?
C12' N12 C172 C171 100.7(3) ?
C182 N12 C172 C171 -138.7(2) ?
Ti12 N12 C172 C171 -25.2(3) ?
O17 C171 C172 N12 43.5(3) ?
Ti12 O18 C181 C182 0.6(3) ?
Ti11 O18 C181 C182 -119.1(2) ?
C172 N12 C182 C181 67.2(3) ?
C12' N12 C182 C181 -169.7(2) ?
Ti12 N12 C182 C181 -50.4(2) ?
O18 C181 C182 N12 35.1(3) ?
C4B O4 C4A C42 -48(2) ?
Ti2 O4 C4A C42 -162.0(2) ?
Ti1 O4 C4A C42 64.4(3) ?
C4B O4 C4A C43 74(2) ?
Ti2 O4 C4A C43 -39.2(3) ?
Ti1 O4 C4A C43 -172.82(17) ?
C4B C42 C4A O4 50(2) ?
C4B C42 C4A C43 -73(2) ?
C4B C43 C4A O4 -62(2) ?
C4B C43 C4A C42 60(2) ?
C11B O11 C11A C113 69.4(15) ?
Ti11 O11 C11A C113 -173.9(2) ?
C11B O11 C11A C112 -56.1(15) ?
Ti11 O11 C11A C112 60.6(5) ?
C11B C113 C11A O11 -66.6(14) ?
C11B C113 C11A C112 58.3(14) ?
C11B C112 C11A O11 59.5(15) ?
C11B C112 C11A C113 -64.3(15) ?
C14B O14 C14A C142 -57.5(17) ?
Ti12 O14 C14A C142 -179.17(17) ?
Ti11 O14 C14A C142 57.3(3) ?
C14B O14 C14A C143 63.1(17) ?
Ti12 O14 C14A C143 -58.5(3) ?
Ti11 O14 C14A C143 177.90(17) ?
C14B C142 C14A O14 55.8(17) ?
C14B C142 C14A C143 -65.0(17) ?
C14B C143 C14A O14 -58.9(17) ?
C14B C143 C14A C142 62.6(17) ?
C16B O16 C16A C163 73.6(10) ?
Ti12 O16 C16A C163 -172.5(9) ?
C16B O16 C16A C162 -52.5(9) ?
Ti12 O16 C16A C162 61.3(13) ?
C16B C163 C16A O16 -69.3(9) ?
C16B C163 C16A C162 52.8(9) ?
C16B C162 C16A O16 60.5(10) ?

C16B C162 C16A C163 -63.6(10) ?
C4A O4 C4B C42 74(3) ?
Ti2 O4 C4B C42 175.2(14) ?
Ti1 O4 C4B C42 -21(5) ?
C4A O4 C4B C43 -60(2) ?
Ti2 O4 C4B C43 41(4) ?
Ti1 O4 C4B C43 -154.8(7) ?
C4A C42 C4B O4 -72(3) ?
C4A C42 C4B C43 61(2) ?
C4A C43 C4B O4 70(2) ?
C4A C43 C4B C42 -72(3) ?
C11A C112 C11B O11 -64.4(19) ?
C11A C112 C11B C113 63.5(18) ?
C11A O11 C11B C112 68(2) ?
Ti11 O11 C11B C112 -37(3) ?
C11A O11 C11B C113 -63.5(16) ?
Ti11 O11 C11B C113 -168.8(3) ?
C11A C113 C11B C112 -68.6(19) ?
C11A C113 C11B O11 64.5(16) ?
C14A O14 C14B C142 61.2(18) ?
Ti12 O14 C14B C142 154.1(8) ?
Ti11 O14 C14B C142 -38(3) ?
C14A O14 C14B C143 -60.7(16) ?
Ti12 O14 C14B C143 32(3) ?
Ti11 O14 C14B C143 -159.5(7) ?
C14A C142 C14B O14 -61.5(19) ?
C14A C142 C14B C143 61.4(16) ?
C14A C143 C14B O14 62.6(18) ?
C14A C143 C14B C142 -63.1(17) ?
C16A C162 C16B O16 -64.6(12) ?
C16A C162 C16B C163 58.3(11) ?
C16A O16 C16B C162 72.3(13) ?
Ti12 O16 C16B C162 -83.6(18) ?
C16A O16 C16B C163 -58.1(9) ?
Ti12 O16 C16B C163 146.1(6) ?
C16A C163 C16B C162 -67.9(13) ?
C16A C163 C16B O16 61.2(9) ?