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##############################################################################
#                                                                            #
#                                                                            #
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#                                                                            #
#                                                                            #
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#                                                                            #
#    This Supplementary Material is written in the Crystallographic          #
#    Information File (CIF) format. For further details see: S.R. Hall,      #
#    F.H. Allen and I.D. Brown, Acta Cryst. (1991) A47, 655-685.             #
#                                                                            #
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Neodymium(III) complexes with bulky ansa-bis(cyclopentadienyl) ligands:
Synthesis and use in olefin oligomerization
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      'Jean-Francois Carpentier, Stéphane Bogaert,
      Thomas Chenal, André Mortreux, Guy Nowogrocki'
      Laboratoire de Catalyse
      Groupe de Chimie Organique Appliquee
      URA CNRS 402
      USTL - ENSCL - Batiment C7
      F-59652 Villeneuve D'ASCQ
      France
;
      'Christian W. Lehmann'
;     Max-Planck-Institut f\"ur Kohlenforschung
      Kaiser-Wilhelm-Platz 1
      D-45470 M\"ulheim an der Ruhr
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      Germany
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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
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Cl2 Cl 0.9397(7) 0.8433(9) 0.0248(7) 0.132(6) Uani 0.70 1 d P . .
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C1 C 0.7468(19) 0.4519(14) 0.0364(13) 0.072(8) Uani 1 1 d . . .
C2 C 0.585(2) 0.5109(16) 0.1138(12) 0.081(8) Uani 1 1 d . . .
C11 C 0.8184(19) 0.6293(15) 0.1380(12) 0.053(7) Uani 1 1 d . . .
C12 C 0.8175(19) 0.6947(14) 0.1943(11) 0.044(6) Uani 1 1 d . . .
C13 C 0.9195(19) 0.7538(17) 0.2082(14) 0.064(8) Uani 1 1 d . . .
C14 C 0.9764(18) 0.7160(14) 0.1662(13) 0.043(6) Uani 1 1 d . . .
C15 C 0.9126(17) 0.6384(15) 0.1224(12) 0.050(7) Uani 1 1 d . . .
Si12 Si 0.7272(6) 0.7203(5) 0.2542(3) 0.066(2) Uani 1 1 d . . .
C121 C 0.5979(19) 0.7382(16) 0.2131(14) 0.092(10) Uani 1 1 d . . .
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C123 C 0.697(3) 0.634(2) 0.2997(14) 0.111(11) Uani 1 1 d . . .
C141 C 1.094(2) 0.749(2) 0.1713(16) 0.090(10) Uani 1 1 d . . .
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C143 C 1.130(2) 0.721(2) 0.1031(16) 0.113(11) Uani 1 1 d . . .
C144 C 1.154(2) 0.717(2) 0.2309(18) 0.117(12) Uani 1 1 d . . .
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C22 C 0.7127(17) 0.6275(17) -0.0354(13) 0.060(7) Uani 1 1 d . . .
C23 C 0.684(2) 0.7009(19) -0.0520(12) 0.078(9) Uani 1 1 d . . .
C24 C 0.6142(17) 0.7176(17) -0.0089(13) 0.059(8) Uani 1 1 d . . .
C25 C 0.6039(17) 0.6621(14) 0.0305(12) 0.045(7) Uani 1 1 d . . .
Si22 Si 0.7870(7) 0.5745(6) -0.1008(4) 0.091(3) Uani 1 1 d . . .
C221 C 0.917(2) 0.555(2) -0.0601(14) 0.110(12) Uani 1 1 d . . .
C222 C 0.818(2) 0.639(3) -0.1656(16) 0.139(15) Uani 1 1 d . . .
C223 C 0.690(2) 0.462(2) -0.1500(16) 0.137(15) Uani 1 1 d . . .
C241 C 0.551(2) 0.7859(17) -0.0164(12) 0.072(9) Uani 1 1 d . . .
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C243 C 0.507(2) 0.8065(17) 0.0469(13) 0.083(10) Uani 1 1 d . . .
C244 C 0.614(2) 0.8614(16) -0.0284(16) 0.103(12) Uani 1 1 d . . .
Li1 Li 0.909(5) 0.974(4) 0.117(4) 0.09(2) Uani 0.70 1 d P . .
O3 O 1.035(2) 1.0445(16) 0.1927(17) 0.098(10) Uani 0.70 1 d P . .
C31 C 1.034(5) 1.065(3) 0.263(3) 0.13(2) Uani 0.70 1 d P . .
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O4 O 0.865(3) 1.070(2) 0.080(2) 0.130(13) Uani 0.70 1 d P . .
C41 C 0.801(5) 1.069(4) 0.013(3) 0.16(3) Uani 0.70 1 d P . .
C42 C 0.768(5) 1.133(5) 0.018(3) 0.14(3) Uani 0.70 1 d P . .
C43 C 0.821(4) 1.201(4) 0.076(4) 0.14(2) Uani 0.70 1 d P . .
C44 C 0.878(4) 1.149(5) 0.120(2) 0.12(2) Uani 0.70 1 d P . .
Nd2 Nd 1.30838(10) 0.77464(9) 0.59618(7) 0.0516(5) Uani 1 1 d . . .
Cl3 Cl 1.1610(5) 0.7932(5) 0.6724(4) 0.086(2) Uani 1 1 d . . .
Cl4 Cl 1.1799(5) 0.6178(4) 0.5428(3) 0.077(2) Uani 1 1 d . . .
Si4 Si 1.5361(5) 0.8959(5) 0.5780(4) 0.061(2) Uani 1 1 d . . .
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Si52 Si 1.4584(6) 0.9622(5) 0.7618(4) 0.069(2) Uani 1 1 d . . .
C521 C 1.399(2) 0.9356(15) 0.8353(12) 0.085(9) Uani 1 1 d . . .
C522 C 1.372(3) 1.0214(17) 0.7159(14) 0.110(12) Uani 1 1 d . . .
C523 C 1.596(2) 1.034(2) 0.7957(16) 0.122(12) Uani 1 1 d . . .
C541 C 1.451(2) 0.6346(17) 0.6870(14) 0.074(9) Uani 1 1 d . . .
C542 C 1.443(3) 0.5699(17) 0.6170(16) 0.114(12) Uani 1 1 d . . .
C543 C 1.550(2) 0.6333(19) 0.7330(16) 0.106(11) Uani 1 1 d . . .
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C622 C 1.462(3) 0.630(2) 0.4529(15) 0.134(15) Uani 1 1 d . . .
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C643 C 1.111(2) 0.916(2) 0.4259(15) 0.106(11) Uani 1 1 d . . .
C644 C 1.131(2) 0.955(2) 0.5614(17) 0.147(17) Uani 1 1 d . . .
Li2 Li 1.072(4) 0.654(3) 0.620(3) 0.079(14) Uani 1 1 d . . .
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C74 C 1.054(3) 0.491(4) 0.660(2) 0.103(15) Uani 0.70 1 d P . .
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C81 C 0.872(4) 0.614(3) 0.513(2) 0.102(16) Uani 0.70 1 d P . .
C82 C 0.772(4) 0.625(5) 0.522(4) 0.20(4) Uani 0.70 1 d P . .
C83 C 0.748(5) 0.639(5) 0.580(3) 0.18(3) Uani 0.70 1 d P . .
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C32 0.28(12) 0.11(7) 0.25(11) -0.03(6) -0.24(10) 0.04(7)
C33 0.09(4) 0.09(6) 0.23(10) -0.05(5) 0.03(6) -0.04(4)
C34 0.06(3) 0.11(5) 0.20(6) -0.02(4) -0.06(4) -0.01(3)
O4 0.10(3) 0.11(3) 0.15(4) 0.07(3) 0.00(3) -0.06(2)
C41 0.13(6) 0.17(7) 0.12(5) 0.08(5) -0.06(5) -0.07(5)
C42 0.08(4) 0.19(7) 0.13(5) -0.02(5) 0.00(3) 0.08(5)
C43 0.08(4) 0.13(5) 0.25(8) 0.10(5) 0.01(4) 0.03(4)
C44 0.08(3) 0.20(6) 0.08(4) 0.01(4) 0.03(3) 0.06(4)
Nd2 0.0438(10) 0.0616(11) 0.0483(9) 0.0158(8) 0.0061(7) 0.0134(8)
Cl3 0.063(4) 0.107(6) 0.083(5) 0.008(4) 0.033(4) 0.019(4)
Cl4 0.078(5) 0.064(5) 0.076(5) 0.008(4) 0.013(4) 0.004(4)
```

```
Si4 0.053(5) 0.081(6) 0.055(5) 0.028(4) 0.016(4) 0.015(4)
C3 0.11(2) 0.038(18) 0.12(2) 0.034(16) 0.050(19) -0.010(16)
C4 0.041(15) 0.13(3) 0.079(19) 0.035(17) 0.027(14) 0.040(17)
C51 0.020(12) 0.06(2) 0.033(15) -0.005(13) 0.008(11) -0.009(13)
C52 0.034(15) 0.07(2) 0.052(18) 0.011(15) -0.016(13) 0.014(15)
C53 0.07(2) 0.05(2) 0.066(19) 0.003(17) -0.022(16) 0.028(18)
C54 0.028(15) 0.07(2) 0.055(18) 0.011(16) -0.010(13) 0.026(15)
C55 0.045(15) 0.025(17) 0.09(2) 0.016(15) 0.002(15) 0.014(13)
Si52 0.075(5) 0.059(6) 0.061(5) -0.002(4) 0.015(4) 0.017(5)
C521 0.14(3) 0.061(19) 0.056(17) -0.004(14) 0.039(18) 0.026(18)
C522 0.17(3) 0.09(2) 0.08(2) 0.003(17) 0.01(2) 0.10(2)
C523 0.07(2) 0.11(3) 0.13(3) -0.01(2) -0.02(2) -0.029(19)
C541 0.08(2) 0.05(2) 0.08(2) 0.007(16) -0.035(17) 0.019(17)
C542 0.15(3) 0.06(2) 0.11(3) -0.01(2) -0.01(2) 0.06(2)
C543 0.09(2) 0.11(3) 0.16(3) 0.10(2) 0.01(2) 0.04(2)
C544 0.08(2) 0.09(2) 0.17(3) 0.10(2) 0.05(2) 0.027(19)
C61 0.002(12) 0.075(19) 0.070(18) 0.037(16) -0.002(12) -0.004(13)
C62 0.062(18) 0.062(19) 0.044(16) 0.032(14) 0.002(14) 0.032(16)
C63 0.061(18) 0.057(19) 0.035(15) 0.002(13) 0.010(13) 0.019(15)
C64 0.034(15) 0.043(17) 0.054(16) 0.017(13) 0.026(13) -0.011(13)
C65 0.048(16) 0.071(19) 0.055(16) 0.048(14) 0.031(14) 0.017(16)
Si62 0.082(6) 0.098(7) 0.053(5) 0.007(5) 0.009(5) 0.041(6)
C621 0.12(3) 0.09(3) 0.09(2) -0.01(2) 0.02(2) 0.02(2)
C622 0.17(3) 0.13(3) 0.09(2) -0.04(2) -0.01(2) 0.10(3)
C623 0.13(3) 0.14(3) 0.08(2) 0.03(2) 0.06(2) 0.04(2)
C641 0.035(17) 0.12(3) 0.10(2) 0.02(2) 0.005(16) 0.034(19)
C642 0.05(2) 0.11(3) 0.19(4) 0.06(3) 0.00(2) 0.03(2)
C643 0.07(2) 0.18(3) 0.11(3) 0.11(2) 0.012(18) 0.04(2)
C644 0.09(2) 0.17(3) 0.15(3) -0.07(3) -0.02(2) 0.10(2)
Li2 0.08(3) 0.06(3) 0.11(4) 0.03(3) 0.04(3) 0.02(3)
O7 0.056(15) 0.10(2) 0.054(18) 0.054(16) 0.024(13) 0.014(16)
C71 0.13(4) 0.14(5) 0.08(4) 0.04(3) 0.07(3) 0.04(4)
C72 0.26(8) 0.23(8) 0.11(5) 0.17(5) 0.14(6) 0.13(7)
C73 0.12(4) 0.18(7) 0.12(5) 0.11(5) 0.08(4) 0.04(4)
C74 0.08(3) 0.10(4) 0.10(4) 0.03(3) 0.00(3) -0.03(3)
O8 0.040(15) 0.12(2) 0.09(2) 0.035(18) 0.004(16) 0.035(16)
C81 0.08(3) 0.12(4) 0.06(3) -0.02(3) -0.01(3) 0.00(3)
C82 0.07(4) 0.29(8) 0.15(6) -0.08(6) -0.08(4) 0.08(5)
C83 0.09(4) 0.31(9) 0.12(5) 0.02(6) -0.02(4) 0.10(5)
C84 0.17(6) 0.52(13) 0.07(4) 0.06(6) 0.00(4) 0.22(8)

_geom_special_details
;
 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.
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Nd1 C22 2.66(2) . ?
Nd1 Cl2 2.658(11) . ?
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Nd1 C11 2.701(7) . ?
Nd1 C13 2.73(2) . ?
Nd1 C15 2.74(2) . ?
Nd1 C25 2.75(2) . ?
Nd1 C23 2.76(2) . ?
Nd1 C24 2.81(2) . ?
Nd1 C14 2.82(2) . ?
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Cl2 Li1 2.69(7) . ?
Si1 C21 1.84(2) . ?
Si1 C1 1.87(2) . ?
Si1 C11 1.89(2) . ?
Si1 C2 1.91(3) . ?
C11 C15 1.34(3) . ?
C11 C12 1.39(3) . ?
C12 C13 1.46(3) . ?
C12 Si12 1.89(2) . ?
C13 C14 1.37(3) . ?
C14 C15 1.41(3) . ?
C14 C141 1.53(3) . ?
Si12 C121 1.91(2) . ?
Si12 C123 1.91(3) . ?
Si12 C122 1.91(3) . ?
C141 C143 1.54(4) . ?
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C141 C144 1.60(4) . ?
C21 C22 1.34(3) . ?
C21 C25 1.39(3) . ?
C22 C23 1.46(3) . ?
C22 Si22 1.94(3) . ?
C23 C24 1.40(3) . ?
C24 C25 1.37(3) . ?
C24 C241 1.59(3) . ?
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Si22 C222 1.93(3) . ?
Si22 C223 1.99(3) . ?
C241 C244 1.47(4) . ?
C241 C243 1.49(3) . ?
C241 C242 1.59(3) . ?
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Li1 O4 2.09(8) . ?
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O3 C34 1.41(6) . ?
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C33 C34 1.39(9) . ?
O4 C44 1.34(5) . ?
O4 C41 1.47(6) . ?
C41 C42 1.24(7) . ?
C42 C43 1.41(7) . ?
C43 C44 1.60(6) . ?
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Nd2 C52 2.69(2) . ?
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Nd2 Cl3 2.717(7) . ?
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Nd2 C55 2.74(2) . ?
Nd2 C65 2.74(2) . ?
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C63 C64 1.40(3) . ?
C64 C65 1.45(3) . ?
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Si62 C623 1.89(3) . ?
Si62 C621 1.90(3) . ?
Si62 C622 1.94(3) . ?
C641 C644 1.55(3) . ?
C641 C643 1.56(4) . ?
C641 C642 1.57(4) . ?
Li2 O8 1.91(5) . ?
Li2 O7 1.98(5) . ?
O7 C71 1.36(4) . ?
O7 C74 1.44(5) . ?
C71 C72 1.52(7) . ?
C72 C73 1.17(7) . ?
C73 C74 1.31(6) . ?
O8 C84 1.25(6) . ?
O8 C81 1.40(4) . ?
C81 C82 1.42(6) . ?
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C82 C84 1.98(7) . ?
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Cl1 Nd1 C22 85.5(8) . . ?
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Cl1 Nd1 Cl2 136.4(6) . . ?
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C11 Nd1 C13 81.9(6) . . ?
C11 Nd1 C15 28.9(6) . . ?
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Cl2 Nd1 C15 107.6(6) . . ?
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C22 Nd1 C25 48.0(7) . . ?
Cl2 Nd1 C25 131.0(6) . . ?
C12 Nd1 C25 90.4(8) . . ?
C11 Nd1 C25 100.6(5) . . ?
C13 Nd1 C25 121.4(8) . . ?
C15 Nd1 C25 105.8(7) . . ?
C11 Nd1 C23 115.0(8) . . ?
C21 Nd1 C23 50.6(8) . . ?
C22 Nd1 C23 31.3(7) . . ?
Cl2 Nd1 C23 83.6(7) . . ?
C12 Nd1 C23 136.2(9) . . ?
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Cl2 Nd1 C24 103.7(7) . . ?
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C25 Nd1 C24 28.4(6) . . ?
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C11 Nd1 C14 48.1(7) . . ?
C21 Nd1 C14 109.7(7) . . ?
C22 Nd1 C14 116.2(7) . . ?
Cl2 Nd1 C14 93.5(5) . . ?
C12 Nd1 C14 48.6(7) . . ?
C11 Nd1 C14 104.8(5) . . ?
C13 Nd1 C14 28.5(6) . . ?
C15 Nd1 C14 29.3(6) . . ?
C25 Nd1 C14 130.9(7) . . ?
C23 Nd1 C14 144.8(8) . . ?
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C24 Nd1 C14 158.0(8) . . ?
Li1 C11 Nd1 96.0(18) . . ?
Nd1 C12 Li1 85.1(16) . . ?
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C21 Si1 C11 98.6(10) . . ?
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C11 C12 Si12 138(2) . . ?
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C141 C14 Nd1 126.2(18) . . ?
C11 C15 C14 107(2) . . ?
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C121 Si12 C123 108.3(14) . . ?
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C143 C141 C144 110(2) . . ?
C142 C141 C144 108(2) . . ?
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Si1 C21 Nd1 97.5(9) . . ?
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C21 C22 Si22 136(2) . . ?
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C23 C22 Nd1 78.2(13) . . ?
Si22 C22 Nd1 122.5(10) . . ?
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C22 C23 Nd1 70.5(12) . . ?
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C241 C24 Nd1 125.3(15) . . ?
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C24 C25 Nd1 77.9(14) . . ?
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C51 Nd2 Cl3 125.0(5) . . ?
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Cl4 Nd2 C63 81.0(5) . . ?
Cl3 Nd2 C63 112.2(5) . . ?
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C51 Nd2 C55 30.7(6) . . ?
C62 Nd2 C55 86.3(8) . . ?
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Cl3 Nd2 C55 132.4(6) . . ?
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C51 Nd2 C65 80.8(7) . . ?
C62 Nd2 C65 50.5(7) . . ?
C52 Nd2 C65 91.7(8) . . ?
Cl4 Nd2 C65 129.1(5) . . ?
Cl3 Nd2 C65 105.5(5) . . ?
C63 Nd2 C65 49.2(7) . . ?
C55 Nd2 C65 105.0(8) . . ?
C61 Nd2 C53 115.3(8) . . ?
C51 Nd2 C53 52.0(8) . . ?
C62 Nd2 C53 135.0(8) . . ?
C52 Nd2 C53 30.3(7) . . ?
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Cl4 Nd2 C64 100.6(5) . . ?
Cl3 Nd2 C64 94.0(4) . . ?
C63 Nd2 C64 29.1(5) . . ?
C55 Nd2 C64 128.9(7) . . ?
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Cl3 Nd2 C54 104.4(6) . . ?
C63 Nd2 C54 141.3(7) . . ?
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Li2 Cl3 Nd2 89.8(11) . . ?
Li2 Cl4 Nd2 89.0(12) . . ?
C51 Si4 C61 97.4(10) . . ?
C51 Si4 C4 109.4(11) . . ?
C61 Si4 C4 113.6(11) . . ?
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C61 Si4 C3 110.1(12) . . ?
C4 Si4 C3 110.2(13) . . ?
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C55 C51 C52 106(2) . . ?
C55 C51 Si4 119.6(18) . . ?
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C55 C51 Nd2 78.1(12) . . ?
C52 C51 Nd2 75.4(11) . . ?
Si4 C51 Nd2 98.2(8) . . ?
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Si62 C62 Nd2 125.5(10) . . ?
C62 C63 C64 112(2) . . ?
C62 C63 Nd2 72.7(13) . . ?
C64 C63 Nd2 79.5(13) . . ?
C63 C64 C65 106.2(19) . . ?
C63 C64 C641 127(2) . . ?
C65 C64 C641 126(2) . . ?
C63 C64 Nd2 71.4(13) . . ?
C65 C64 Nd2 71.8(13) . . ?
C641 C64 Nd2 128.8(16) . . ?
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C61 C65 Nd2 68.0(13) . . ?
C64 C65 Nd2 78.1(13) . . ?
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C644 C641 C642 112(3) . . ?
C643 C641 C642 107(2) . . ?
C644 C641 C64 108.4(19) . . ?
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C642 C641 C64 108(2) . . ?
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Cl3 Li2 Cl4 99.3(18) . . ?
O8 Li2 Nd2 134(2) . . ?
O7 Li2 Nd2 123(2) . . ?
Cl3 Li2 Nd2 49.8(9) . . ?
Cl4 Li2 Nd2 49.6(9) . . ?
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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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H1A H 0.1166 1.0415 0.6403 0.040 Uiso 1 1 calc R . .
H1B H -0.0069 1.0024 0.6368 0.040 Uiso 1 1 calc R . .
H1C H 0.0423 1.0419 0.5727 0.040 Uiso 1 1 calc R . .
C2 C 0.2785(3) 0.95798(18) 0.54257(17) 0.0280(8) Uani 1 1 d . . .
H2A H 0.2612 0.9896 0.5056 0.042 Uiso 1 1 calc R . .
H2B H 0.3171 0.9162 0.5255 0.042 Uiso 1 1 calc R . .
H2C H 0.3303 0.9813 0.5745 0.042 Uiso 1 1 calc R . .
C11 C 0.0389(3) 0.87963(15) 0.53069(14) 0.0181(6) Uani 1 1 d . . .
C12 C 0.0614(3) 0.82201(17) 0.48564(14) 0.0199(7) Uani 1 1 d . . .
C13 C -0.0480(3) 0.78688(16) 0.47789(14) 0.0194(6) Uani 1 1 d . . .
H13 H -0.0595 0.7470 0.4507 0.023 Uiso 1 1 calc R . .
C14 C -0.1368(3) 0.81890(17) 0.51567(15) 0.0197(6) Uani 1 1 d . . .
C15 C -0.0813(3) 0.87569(16) 0.54808(15) 0.0192(6) Uani 1 1 d . . .
H15 H -0.1195 0.9069 0.5775 0.023 Uiso 1 1 calc R . .
C21 C 0.1677(3) 0.86972(15) 0.65440(15) 0.0190(6) Uani 1 1 d . . .
C22 C 0.0961(3) 0.84813(16) 0.71059(14) 0.0189(6) Uani 1 1 d . . .
C23 C 0.1387(3) 0.78184(16) 0.73039(14) 0.0197(7) Uani 1 1 d . . .
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C24 C 0.2322(3) 0.76006(16) 0.68935(15) 0.0204(7) Uani 1 1 d . . .
C25 C 0.2480(3) 0.81476(16) 0.64264(15) 0.0200(7) Uani 1 1 d . . .
H25 H 0.3047 0.8146 0.6082 0.024 Uiso 1 1 calc R . .
C31 C 0.0216(5) 0.4586(2) 0.6766(2) 0.0422(10) Uani 1 1 d . . .
H31A H 0.1022 0.4698 0.6622 0.051 Uiso 1 1 calc R . .
H31B H -0.0183 0.4327 0.6406 0.051 Uiso 1 1 calc R . .
C32 C 0.0236(5) 0.4161(2) 0.7404(2) 0.0542(13) Uani 1 1 d . . .
H32A H -0.0468 0.3864 0.7441 0.065 Uiso 1 1 calc R . .
H32B H 0.0944 0.3866 0.7430 0.065 Uiso 1 1 calc R . .
C33 C 0.0249(5) 0.4716(3) 0.7931(2) 0.0547(14) Uani 1 1 d . . .
H33A H -0.0062 0.4539 0.8357 0.066 Uiso 1 1 calc R . .
H33B H 0.1049 0.4899 0.8003 0.066 Uiso 1 1 calc R . .
C34 C -0.0539(4) 0.5261(2) 0.76413(18) 0.0407(10) Uani 1 1 d . . .
H34A H -0.1360 0.5177 0.7775 0.049 Uiso 1 1 calc R . .
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H34B H -0.0303 0.5728 0.7798 0.049 Uiso 1 1 calc R . .
C41 C -0.1648(3) 0.54030(19) 0.49279(16) 0.0283(8) Uani 1 1 d . . .
H41A H -0.1014 0.5076 0.4808 0.034 Uiso 1 1 calc R . .
H41B H -0.1473 0.5863 0.4731 0.034 Uiso 1 1 calc R . .
C42 C -0.2818(4) 0.5137(2) 0.46818(18) 0.0334(9) Uani 1 1 d . . .
H42A H -0.2725 0.4845 0.4280 0.040 Uiso 1 1 calc R . .
H42B H -0.3360 0.5525 0.4581 0.040 Uiso 1 1 calc R . .
C43 C -0.3253(4) 0.4706(2) 0.5271(2) 0.0415(10) Uani 1 1 d . . .
H43A H -0.4118 0.4669 0.5270 0.050 Uiso 1 1 calc R . .
H43B H -0.2909 0.4234 0.5269 0.050 Uiso 1 1 calc R . .
C44 C -0.2825(4) 0.5122(3) 0.5855(2) 0.0470(11) Uani 1 1 d . . .
H44A H -0.3415 0.5473 0.5986 0.056 Uiso 1 1 calc R . .
H44B H -0.2673 0.4814 0.6241 0.056 Uiso 1 1 calc R . .
C121 C 0.1428(4) 0.7161(2) 0.38442(17) 0.0307(8) Uani 1 1 d . . .
H12A H 0.0693 0.7250 0.3606 0.046 Uiso 1 1 calc R . .
H12B H 0.1316 0.6776 0.4157 0.046 Uiso 1 1 calc R . .
H12C H 0.2040 0.7037 0.3524 0.046 Uiso 1 1 calc R . .
C122 C 0.2219(4) 0.8681(2) 0.37158(17) 0.0344(9) Uani 1 1 d . . .
H12D H 0.2848 0.8533 0.3417 0.052 Uiso 1 1 calc R . .
H12E H 0.2470 0.9093 0.3964 0.052 Uiso 1 1 calc R . .
H12F H 0.1518 0.8791 0.3455 0.052 Uiso 1 1 calc R . .
C123 C 0.3260(3) 0.7709(2) 0.47618(17) 0.0302(8) Uani 1 1 d . . .
H12G H 0.3840 0.7547 0.4439 0.045 Uiso 1 1 calc R . .
H12H H 0.3089 0.7336 0.5079 0.045 Uiso 1 1 calc R . .
H12I H 0.3570 0.8113 0.5001 0.045 Uiso 1 1 calc R . .
C141 C -0.3751(4) 0.8395(3) 0.5820(2) 0.0466(11) Uani 1 1 d . . .
H14A H -0.4598 0.8345 0.5758 0.070 Uiso 1 1 calc R . .
H14B H -0.3551 0.8889 0.5853 0.070 Uiso 1 1 calc R . .
H14C H -0.3513 0.8157 0.6230 0.070 Uiso 1 1 calc R . .
C142 C -0.3247(4) 0.70478(19) 0.50598(19) 0.0326(8) Uani 1 1 d . . .
H14D H -0.2997 0.6832 0.5478 0.049 Uiso 1 1 calc R . .
H14E H -0.2803 0.6847 0.4690 0.049 Uiso 1 1 calc R . .
H14F H -0.4084 0.6963 0.4991 0.049 Uiso 1 1 calc R . .
C143 C -0.3516(4) 0.8392(2) 0.4301(2) 0.0389(10) Uani 1 1 d . . .
H14G H -0.4341 0.8270 0.4237 0.058 Uiso 1 1 calc R . .
H14H H -0.3054 0.8211 0.3929 0.058 Uiso 1 1 calc R . .
H14I H -0.3436 0.8899 0.4320 0.058 Uiso 1 1 calc R . .
C221 C -0.1634(3) 0.9044(2) 0.72547(18) 0.0327(8) Uani 1 1 d . . .
H22A H -0.2183 0.9212 0.7592 0.049 Uiso 1 1 calc R . .
H22B H -0.1910 0.8599 0.7078 0.049 Uiso 1 1 calc R . .
H22C H -0.1583 0.9384 0.6893 0.049 Uiso 1 1 calc R . .
C222 C 0.0393(4) 0.97900(19) 0.79338(18) 0.0347(9) Uani 1 1 d . . .
H22D H 0.1179 0.9736 0.8124 0.052 Uiso 1 1 calc R . .
H22E H -0.0137 0.9973 0.8274 0.052 Uiso 1 1 calc R . .
H22F H 0.0424 1.0114 0.7558 0.052 Uiso 1 1 calc R . .
C223 C -0.0367(4) 0.8363(2) 0.83904(17) 0.0321(8) Uani 1 1 d . . .
H22G H 0.0383 0.8300 0.8619 0.048 Uiso 1 1 calc R . .
H22H H -0.0673 0.7909 0.8252 0.048 Uiso 1 1 calc R . .
H22I H -0.0926 0.8585 0.8692 0.048 Uiso 1 1 calc R . .
C241 C 0.4340(4) 0.6999(2) 0.7688(2) 0.0385(9) Uani 1 1 d . . .
H24A H 0.4785 0.6577 0.7791 0.058 Uiso 1 1 calc R . .
H24B H 0.3945 0.7164 0.8090 0.058 Uiso 1 1 calc R . .
H24C H 0.4874 0.7360 0.7526 0.058 Uiso 1 1 calc R . .
C242 C 0.4017(4) 0.65492(19) 0.62606(18) 0.0321(8) Uani 1 1 d . . .
H24D H 0.4515 0.6934 0.6115 0.048 Uiso 1 1 calc R . .
H24E H 0.3447 0.6440 0.5911 0.048 Uiso 1 1 calc R . .
H24F H 0.4503 0.6140 0.6350 0.048 Uiso 1 1 calc R . .
C243 C 0.2236(3) 0.61037(17) 0.73430(17) 0.0258(7) Uani 1 1 d . . .
H24G H 0.2699 0.5690 0.7452 0.039 Uiso 1 1 calc R . .
H24H H 0.1663 0.5987 0.6997 0.039 Uiso 1 1 calc R . .
H24I H 0.1826 0.6266 0.7741 0.039 Uiso 1 1 calc R . .
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Si12 Si 0.18776(9) 0.79617(5) 0.43133(4) 0.02200(19) Uani 1 1 d . . .
Si14 Si -0.29724(9) 0.80026(5) 0.50986(4) 0.02141(19) Uani 1 1 d . . .
Si22 Si -0.01517(9) 0.89262(5) 0.76399(4) 0.02116(19) Uani 1 1 d . . .
Si24 Si 0.32267(9) 0.68038(5) 0.70345(4) 0.02195(19) Uani 1 1 d . . .
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Cl2 Cl -0.14321(8) 0.69887(4) 0.67553(4) 0.02836(19) Uani 1 1 d . . .
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C2      0.029(2)    0.0280(17)  0.0269(16)  0.0021(14) -0.0015(14) -0.0075(15)
C11     0.0207(18)  0.0163(14)  0.0173(14)  0.0048(11) -0.0012(12) -0.0014(12)
C12     0.0202(18)  0.0241(16)  0.0153(13)  0.0029(12)  0.0008(12)  0.0019(13)
C13     0.0219(19)  0.0205(15)  0.0158(13) -0.0003(12) -0.0027(12)  0.0009(13)
C14     0.0167(18)  0.0233(15)  0.0189(14)  0.0017(12) -0.0033(12) -0.0012(13)
C15     0.0220(19)  0.0175(14)  0.0182(14)  0.0016(11) -0.0027(12)  0.0023(13)
C21     0.0226(19)  0.0155(14)  0.0190(14)  0.0002(11) -0.0028(12) -0.0030(13)
C22     0.0196(18)  0.0203(15)  0.0170(14) -0.0017(11) -0.0027(12) -0.0030(13)
C23     0.0249(19)  0.0196(15)  0.0144(13)  0.0024(11) -0.0050(12) -0.0005(13)
C24     0.0226(19)  0.0189(15)  0.0196(14)  0.0006(12) -0.0052(12) -0.0006(13)
C25     0.0214(19)  0.0204(14)  0.0181(14)  0.0001(12) -0.0044(12) -0.0021(13)
C31     0.058(3)    0.0271(19)  0.041(2)     0.0010(16)  0.000(2)     0.0002(19)
C32     0.060(4)    0.036(2)    0.067(3)     0.020(2)   -0.016(3)   -0.008(2)
C33     0.065(4)    0.065(3)    0.034(2)     0.027(2)   -0.011(2)   -0.025(3)
C34     0.048(3)    0.048(2)    0.0260(18) -0.0023(16)  0.0052(17) -0.018(2)
C41     0.033(2)    0.0272(17)  0.0249(16) -0.0018(14) -0.0024(14)  0.0019(15)
C42     0.035(2)    0.0317(19)  0.0333(18) -0.0009(15) -0.0086(16) -0.0011(17)
C43     0.038(3)    0.045(2)    0.041(2)     0.0015(18) -0.0011(18) -0.012(2)
C44     0.048(3)    0.055(3)    0.039(2)     0.0028(19)  0.0087(19) -0.022(2)
C121    0.027(2)    0.037(2)    0.0273(17) -0.0092(15) -0.0030(15)  0.0053(16)
C122    0.037(2)    0.041(2)    0.0252(17)  0.0042(15)  0.0055(16) -0.0026(18)
C123    0.023(2)    0.042(2)    0.0250(16) -0.0080(15) -0.0003(14)  0.0061(16)
C141    0.024(2)    0.068(3)    0.048(2)    -0.031(2)    0.0022(18) 0.000(2)
C142    0.031(2)    0.0289(18)  0.0378(19)  0.0037(15) -0.0045(16) -0.0035(16)
C143    0.032(2)    0.038(2)    0.046(2)     0.0136(18) -0.0156(18) -0.0050(18)
C221    0.028(2)    0.039(2)    0.0305(18) -0.0062(16)  0.0020(15)  0.0072(17)
C222    0.047(3)    0.0272(18)  0.0301(18) -0.0100(15)  0.0076(17) -0.0086(17)
C223    0.038(2)    0.0323(19)  0.0259(17)  0.0031(14)  0.0073(15) -0.0011(17)
C241    0.032(2)    0.040(2)    0.044(2)     0.0034(18) -0.0164(18) -0.0015(18)
C242    0.028(2)    0.0283(18)  0.040(2)     0.0066(15)  0.0065(16)  0.0066(16)
C243    0.028(2)    0.0222(16)  0.0268(16)  0.0029(13) -0.0021(14)  0.0017(14)
Li      0.031(4)    0.023(3)    0.029(3)     0.001(2)   -0.001(2)   -0.006(3)
O3      0.0448(18)  0.0285(13)  0.0239(12)  0.0019(10) -0.0011(11) -0.0009(12)
O4      0.0340(17)  0.0375(14)  0.0257(12)  0.0011(10) -0.0001(11) -0.0150(12)
Si1     0.0217(5)   0.0163(4)   0.0183(4)   0.0016(3)  -0.0021(3)  -0.0015(3)
Si12    0.0205(5)   0.0275(5)   0.0179(4)  -0.0018(3)  -0.0002(3)   0.0012(4)
Si14    0.0173(5)   0.0223(4)   0.0246(4)  -0.0024(3)  -0.0020(3)   0.0002(4)
Si22    0.0247(5)   0.0195(4)   0.0193(4)  -0.0023(3)   0.0015(4)  -0.0009(4)
Si24    0.0214(5)   0.0191(4)   0.0253(4)   0.0022(3)  -0.0039(4)   0.0011(4)
Cl1     0.0294(5)   0.0186(3)   0.0278(4)  -0.0029(3)   0.0012(3)   0.0020(3)
```

```
Cl2     0.0294(5)   0.0259(4)   0.0299(4)  0.0000(3)    0.0077(3)  -0.0035(4)
Nd      0.01881(10) 0.01453(9)  0.01775(9) -0.00003(6) -0.00210(6) -0.00059(7)

_geom_special_details
;
 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.
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C1      Si1    1.866(3) . ?
C1      H1A    0.9800 . ?
C1      H1B    0.9800 . ?
C1      H1C    0.9800 . ?
C2      Si1    1.868(4) . ?
C2      H2A    0.9800 . ?
C2      H2B    0.9800 . ?
C2      H2C    0.9800 . ?
C11     C15    1.419(5) . ?
C11     C12    1.455(4) . ?
C11     Si1    1.883(3) . ?
C11     Nd     2.687(3) . ?
C12     C13    1.429(5) . ?
C12     Si12   1.880(3) . ?
C12     Nd     2.710(3) . ?
C13     C14    1.410(5) . ?
C13     Nd     2.790(3) . ?
C13     H13    0.9500 . ?
C14     C15    1.421(4) . ?
C14     Si14   1.871(4) . ?
C14     Nd     2.847(3) . ?
C15     Nd     2.745(3) . ?
C15     H15    0.9500 . ?
C21     C25    1.420(5) . ?
C21     C22    1.457(4) . ?
C21     Si1    1.885(3) . ?
C21     Nd     2.709(3) . ?
C22     C23    1.422(4) . ?
C22     Si22   1.873(3) . ?
C22     Nd     2.709(3) . ?
C23     C24    1.415(5) . ?
C23     Nd     2.773(3) . ?
C23     H23    0.9500 . ?
C24     C25    1.423(4) . ?
C24     Si24   1.870(3) . ?
C24     Nd     2.829(3) . ?
C25     Nd     2.750(3) . ?
C25     H25    0.9500 . ?
C31     O3     1.446(5) . ?
C31     C32    1.520(6) . ?
C31     H31A   0.9900 . ?
C31     H31B   0.9900 . ?
```

C32	C33	1.505(7)	.	?
C32	H32A	0.9900	.	?
C32	H32B	0.9900	.	?
C33	C34	1.498(7)	.	?
C33	H33A	0.9900	.	?
C33	H33B	0.9900	.	?
C34	O3	1.446(4)	.	?
C34	H34A	0.9900	.	?
C34	H34B	0.9900	.	?
C41	O4	1.449(4)	.	?
C41	C42	1.513(5)	.	?
C41	H41A	0.9900	.	?
C41	H41B	0.9900	.	?
C42	C43	1.530(5)	.	?
C42	H42A	0.9900	.	?
C42	H42B	0.9900	.	?
C43	C44	1.502(6)	.	?
C43	H43A	0.9900	.	?
C43	H43B	0.9900	.	?
C44	O4	1.447(5)	.	?
C44	H44A	0.9900	.	?
C44	H44B	0.9900	.	?
C121	Si12	1.878(4)	.	?
C121	H12A	0.9800	.	?
C121	H12B	0.9800	.	?
C121	H12C	0.9800	.	?
C122	Si12	1.874(4)	.	?
C122	H12D	0.9800	.	?
C122	H12E	0.9800	.	?
C122	H12F	0.9800	.	?
C123	Si12	1.880(4)	.	?
C123	H12G	0.9800	.	?
C123	H12H	0.9800	.	?
C123	H12I	0.9800	.	?
C141	Si14	1.864(4)	.	?
C141	H14A	0.9800	.	?
C141	H14B	0.9800	.	?
C141	H14C	0.9800	.	?
C142	Si14	1.865(4)	.	?
C142	H14D	0.9800	.	?
C142	H14E	0.9800	.	?
C142	H14F	0.9800	.	?
C143	Si14	1.875(4)	.	?
C143	H14G	0.9800	.	?
C143	H14H	0.9800	.	?
C143	H14I	0.9800	.	?
C221	Si22	1.873(4)	.	?
C221	H22A	0.9800	.	?
C221	H22B	0.9800	.	?
C221	H22C	0.9800	.	?
C222	Si22	1.870(4)	.	?
C222	H22D	0.9800	.	?
C222	H22E	0.9800	.	?
C222	H22F	0.9800	.	?
C223	Si22	1.875(3)	.	?
C223	H22G	0.9800	.	?
C223	H22H	0.9800	.	?
C223	H22I	0.9800	.	?
C241	Si24	1.865(4)	.	?
C241	H24A	0.9800	.	?
C241	H24B	0.9800	.	?

```
C241   H24C  0.9800 . ?
C242   Si24  1.866(4) . ?
C242   H24D  0.9800 . ?
C242   H24E  0.9800 . ?
C242   H24F  0.9800 . ?
C243   Si24  1.866(4) . ?
C243   H24G  0.9800 . ?
C243   H24H  0.9800 . ?
C243   H24I  0.9800 . ?
Li     O3    1.921(6) . ?
Li     O4    1.929(6) . ?
Li     Cl2   2.396(6) . ?
Li     Cl1   2.409(6) . ?
Li     Nd    3.580(6) . ?
Cl1    Nd    2.7250(8) . ?
Cl2    Nd    2.7287(9) . ?

loop_
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Si1    C1     H1A   109.5 . . ?
Si1    C1     H1B   109.5 . . ?
H1A    C1     H1B   109.5 . . ?
Si1    C1     H1C   109.5 . . ?
H1A    C1     H1C   109.5 . . ?
H1B    C1     H1C   109.5 . . ?
Si1    C2     H2A   109.5 . . ?
Si1    C2     H2B   109.5 . . ?
H2A    C2     H2B   109.5 . . ?
Si1    C2     H2C   109.5 . . ?
H2A    C2     H2C   109.5 . . ?
H2B    C2     H2C   109.5 . . ?
C15    C11    C12   106.5(3) . . ?
C15    C11    Si1   118.3(2) . . ?
C12    C11    Si1   131.9(3) . . ?
C15    C11    Nd     77.11(17) . . ?
C12    C11    Nd     75.23(16) . . ?
Si1    C11    Nd     97.78(12) . . ?
C13    C12    C11   105.8(3) . . ?
C13    C12    Si12  119.0(2) . . ?
C11    C12    Si12  134.5(3) . . ?
C13    C12    Nd     78.06(17) . . ?
C11    C12    Nd     73.49(16) . . ?
Si12   C12    Nd    121.62(15) . . ?
C14    C13    C12   111.4(3) . . ?
C14    C13    Nd     77.75(17) . . ?
C12    C13    Nd     71.87(17) . . ?
C14    C13    H13   124.3 . . ?
C12    C13    H13   124.3 . . ?
Nd     C13    H13   117.7 . . ?
C13    C14    C15   105.2(3) . . ?
C13    C14    Si14  126.0(2) . . ?
C15    C14    Si14  127.7(3) . . ?
C13    C14    Nd     73.31(18) . . ?
C15    C14    Nd     71.34(17) . . ?
Si14   C14    Nd    128.78(14) . . ?
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C14    C15    C11   111.0(3) . . ?
C14    C15    Nd     79.29(18) . . ?
C11    C15    Nd     72.62(17) . . ?
C14    C15    H15   124.5 . . ?
C11    C15    H15   124.5 . . ?
Nd     C15    H15   115.3 . . ?
C25    C21    C22   106.3(3) . . ?
C25    C21    Si1   118.0(2) . . ?
C22    C21    Si1   131.6(3) . . ?
C25    C21    Nd     76.51(18) . . ?
C22    C21    Nd     74.42(17) . . ?
Si1    C21    Nd     97.01(12) . . ?
C23    C22    C21   106.3(3) . . ?
C23    C22    Si22  118.8(2) . . ?
C21    C22    Si22  134.2(2) . . ?
C23    C22    Nd     77.46(17) . . ?
C21    C22    Nd     74.38(17) . . ?
Si22   C22    Nd    121.13(16) . . ?
C24    C23    C22   111.1(3) . . ?
C24    C23    Nd     77.58(18) . . ?
C22    C23    Nd     72.51(17) . . ?
C24    C23    H23   124.4 . . ?
C22    C23    H23   124.4 . . ?
Nd     C23    H23   117.1 . . ?
C23    C24    C25   105.3(3) . . ?
C23    C24    Si24  124.9(2) . . ?
C25    C24    Si24  129.5(3) . . ?
C23    C24    Nd     73.17(19) . . ?
C25    C24    Nd     72.14(19) . . ?
Si24   C24    Nd    124.69(14) . . ?
C21    C25    C24   111.0(3) . . ?
C21    C25    Nd     73.34(19) . . ?
C24    C25    Nd     78.4(2) . . ?
C21    C25    H25   124.5 . . ?
C24    C25    H25   124.5 . . ?
Nd     C25    H25   115.5 . . ?
O3     C31    C32   105.5(3) . . ?
O3     C31    H31A  110.6 . . ?
C32    C31    H31A  110.6 . . ?
O3     C31    H31B  110.6 . . ?
C32    C31    H31B  110.6 . . ?
H31A   C31    H31B  108.8 . . ?
C33    C32    C31   102.2(3) . . ?
C33    C32    H32A  111.3 . . ?
C31    C32    H32A  111.3 . . ?
C33    C32    H32B  111.3 . . ?
C31    C32    H32B  111.3 . . ?
H32A   C32    H32B  109.2 . . ?
C34    C33    C32   102.6(3) . . ?
C34    C33    H33A  111.2 . . ?
C32    C33    H33A  111.2 . . ?
C34    C33    H33B  111.2 . . ?
C32    C33    H33B  111.2 . . ?
H33A   C33    H33B  109.2 . . ?
O3     C34    C33   106.5(4) . . ?
O3     C34    H34A  110.4 . . ?
C33    C34    H34A  110.4 . . ?
O3     C34    H34B  110.4 . . ?
C33    C34    H34B  110.4 . . ?
H34A   C34    H34B  108.6 . . ?
O4     C41    C42   105.8(3) . . ?
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O4	C41	H41A	110.6	.	.	?
C42	C41	H41A	110.6	.	.	?
O4	C41	H41B	110.6	.	.	?
C42	C41	H41B	110.6	.	.	?
H41A	C41	H41B	108.7	.	.	?
C41	C42	C43	102.6(3)	.	.	?
C41	C42	H42A	111.2	.	.	?
C43	C42	H42A	111.2	.	.	?
C41	C42	H42B	111.2	.	.	?
C43	C42	H42B	111.2	.	.	?
H42A	C42	H42B	109.2	.	.	?
C44	C43	C42	102.3(3)	.	.	?
C44	C43	H43A	111.3	.	.	?
C42	C43	H43A	111.3	.	.	?
C44	C43	H43B	111.3	.	.	?
C42	C43	H43B	111.3	.	.	?
H43A	C43	H43B	109.2	.	.	?
O4	C44	C43	106.3(3)	.	.	?
O4	C44	H44A	110.5	.	.	?
C43	C44	H44A	110.5	.	.	?
O4	C44	H44B	110.5	.	.	?
C43	C44	H44B	110.5	.	.	?
H44A	C44	H44B	108.7	.	.	?
Si12	C121	H12A	109.5	.	.	?
Si12	C121	H12B	109.5	.	.	?
H12A	C121	H12B	109.5	.	.	?
Si12	C121	H12C	109.5	.	.	?
H12A	C121	H12C	109.5	.	.	?
H12B	C121	H12C	109.5	.	.	?
Si12	C122	H12D	109.5	.	.	?
Si12	C122	H12E	109.5	.	.	?
H12D	C122	H12E	109.5	.	.	?
Si12	C122	H12F	109.5	.	.	?
H12D	C122	H12F	109.5	.	.	?
H12E	C122	H12F	109.5	.	.	?
Si12	C123	H12G	109.5	.	.	?
Si12	C123	H12H	109.5	.	.	?
H12G	C123	H12H	109.5	.	.	?
Si12	C123	H12I	109.5	.	.	?
H12G	C123	H12I	109.5	.	.	?
H12H	C123	H12I	109.5	.	.	?
Si14	C141	H14A	109.5	.	.	?
Si14	C141	H14B	109.5	.	.	?
H14A	C141	H14B	109.5	.	.	?
Si14	C141	H14C	109.5	.	.	?
H14A	C141	H14C	109.5	.	.	?
H14B	C141	H14C	109.5	.	.	?
Si14	C142	H14D	109.5	.	.	?
Si14	C142	H14E	109.5	.	.	?
H14D	C142	H14E	109.5	.	.	?
Si14	C142	H14F	109.5	.	.	?
H14D	C142	H14F	109.5	.	.	?
H14E	C142	H14F	109.5	.	.	?
Si14	C143	H14G	109.5	.	.	?
Si14	C143	H14H	109.5	.	.	?
H14G	C143	H14H	109.5	.	.	?
Si14	C143	H14I	109.5	.	.	?
H14G	C143	H14I	109.5	.	.	?
H14H	C143	H14I	109.5	.	.	?
Si22	C221	H22A	109.5	.	.	?
Si22	C221	H22B	109.5	.	.	?

H22A	C221	H22B	109.5	.	.	?
Si22	C221	H22C	109.5	.	.	?
H22A	C221	H22C	109.5	.	.	?
H22B	C221	H22C	109.5	.	.	?
Si22	C222	H22D	109.5	.	.	?
Si22	C222	H22E	109.5	.	.	?
H22D	C222	H22E	109.5	.	.	?
Si22	C222	H22F	109.5	.	.	?
H22D	C222	H22F	109.5	.	.	?
H22E	C222	H22F	109.5	.	.	?
Si22	C223	H22G	109.5	.	.	?
Si22	C223	H22H	109.5	.	.	?
H22G	C223	H22H	109.5	.	.	?
Si22	C223	H22I	109.5	.	.	?
H22G	C223	H22I	109.5	.	.	?
H22H	C223	H22I	109.5	.	.	?
Si24	C241	H24A	109.5	.	.	?
Si24	C241	H24B	109.5	.	.	?
H24A	C241	H24B	109.5	.	.	?
Si24	C241	H24C	109.5	.	.	?
H24A	C241	H24C	109.5	.	.	?
H24B	C241	H24C	109.5	.	.	?
Si24	C242	H24D	109.5	.	.	?
Si24	C242	H24E	109.5	.	.	?
H24D	C242	H24E	109.5	.	.	?
Si24	C242	H24F	109.5	.	.	?
H24D	C242	H24F	109.5	.	.	?
H24E	C242	H24F	109.5	.	.	?
Si24	C243	H24G	109.5	.	.	?
Si24	C243	H24H	109.5	.	.	?
H24G	C243	H24H	109.5	.	.	?
Si24	C243	H24I	109.5	.	.	?
H24G	C243	H24I	109.5	.	.	?
H24H	C243	H24I	109.5	.	.	?
O3	Li	O4	103.8(3)	.	.	?
O3	Li	Cl2	113.7(3)	.	.	?
O4	Li	Cl2	118.2(3)	.	.	?
O3	Li	Cl1	117.6(3)	.	.	?
O4	Li	Cl1	104.7(3)	.	.	?
Cl2	Li	Cl1	99.2(2)	.	.	?
O3	Li	Nd	132.2(3)	.	.	?
O4	Li	Nd	123.8(2)	.	.	?
Cl2	Li	Nd	49.63(11)	.	.	?
Cl1	Li	Nd	49.54(10)	.	.	?
C34	O3	C31	108.9(3)	.	.	?
C34	O3	Li	127.5(3)	.	.	?
C31	O3	Li	122.7(3)	.	.	?
C41	O4	C44	109.5(3)	.	.	?
C41	O4	Li	129.9(3)	.	.	?
C44	O4	Li	120.5(3)	.	.	?
C1	Si1	C2	108.18(17)	.	.	?
C1	Si1	C11	110.26(16)	.	.	?
C2	Si1	C11	113.28(15)	.	.	?
C1	Si1	C21	113.84(14)	.	.	?
C2	Si1	C21	110.93(16)	.	.	?
C11	Si1	C21	100.33(13)	.	.	?
C122	Si12	C121	109.93(17)	.	.	?
C122	Si12	C12	109.80(17)	.	.	?
C121	Si12	C12	107.43(17)	.	.	?
C122	Si12	C123	108.83(19)	.	.	?
C121	Si12	C123	104.89(17)	.	.	?

C12	Si12	C123	115.77(15)	.	?
C141	Si14	C142	110.6(2)	.	?
C141	Si14	C14	110.05(17)	.	?
C142	Si14	C14	110.84(17)	.	?
C141	Si14	C143	110.3(2)	.	?
C142	Si14	C143	107.63(18)	.	?
C14	Si14	C143	107.39(17)	.	?
C222	Si22	C22	111.19(17)	.	?
C222	Si22	C221	108.83(19)	.	?
C22	Si22	C221	115.59(15)	.	?
C222	Si22	C223	107.68(17)	.	?
C22	Si22	C223	106.74(16)	.	?
C221	Si22	C223	106.41(19)	.	?
C241	Si24	C242	108.1(2)	.	?
C241	Si24	C243	108.92(18)	.	?
C242	Si24	C243	112.49(17)	.	?
C241	Si24	C24	108.46(17)	.	?
C242	Si24	C24	110.90(15)	.	?
C243	Si24	C24	107.89(16)	.	?
Li	Cl1	Nd	88.20(14)	.	?
Li	Cl2	Nd	88.39(15)	.	?
C11	Nd	C22	87.30(9)	.	?
C11	Nd	C12	31.28(9)	.	?
C22	Nd	C12	114.91(10)	.	?
C11	Nd	C21	64.86(9)	.	?
C22	Nd	C21	31.20(9)	.	?
C12	Nd	C21	86.62(9)	.	?
C11	Nd	Cl1	123.21(7)	.	?
C22	Nd	Cl1	136.32(7)	.	?
C12	Nd	Cl1	92.08(7)	.	?
C21	Nd	Cl1	131.05(8)	.	?
C11	Nd	Cl2	134.48(8)	.	?
C22	Nd	Cl2	95.52(7)	.	?
C12	Nd	Cl2	137.56(8)	.	?
C21	Nd	Cl2	126.65(7)	.	?
Cl1	Nd	Cl2	84.24(3)	.	?
C11	Nd	C15	30.27(10)	.	?
C22	Nd	C15	90.62(9)	.	?
C12	Nd	C15	49.97(10)	.	?
C21	Nd	C15	81.38(10)	.	?
Cl1	Nd	C15	131.92(7)	.	?
Cl2	Nd	C15	104.21(7)	.	?
C11	Nd	C25	80.36(10)	.	?
C22	Nd	C25	49.90(10)	.	?
C12	Nd	C25	88.45(10)	.	?
C21	Nd	C25	30.15(10)	.	?
Cl1	Nd	C25	100.93(7)	.	?
Cl2	Nd	C25	133.82(7)	.	?
C15	Nd	C25	105.41(10)	.	?
C11	Nd	C23	113.91(9)	.	?
C22	Nd	C23	30.03(9)	.	?
C12	Nd	C23	134.60(10)	.	?
C21	Nd	C23	49.69(9)	.	?
Cl1	Nd	C23	107.00(7)	.	?
Cl2	Nd	C23	86.14(7)	.	?
C15	Nd	C23	120.60(9)	.	?
C25	Nd	C23	48.21(10)	.	?
C11	Nd	C13	49.64(9)	.	?
C22	Nd	C13	135.81(9)	.	?
C12	Nd	C13	30.07(10)	.	?
C21	Nd	C13	113.59(9)	.	?

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 Cl1     Nd      C13     84.15(7) . . ?
 Cl2     Nd      C13    107.75(7) . . ?
 C15     Nd      C13     47.95(9) . . ?
 C25     Nd      C13    118.42(10) . . ?
 C23     Nd      C13    163.28(10) . . ?
 Cl1     Nd      C24    109.57(10) . . ?
 C22     Nd      C24     49.93(10) . . ?
 Cl2     Nd      C24    115.60(10) . . ?
 C21     Nd      C24     49.99(9) . . ?
 Cl1     Nd      C24     88.15(7) . . ?
 Cl2     Nd      C24    106.55(7) . . ?
 C15     Nd      C24    131.34(9) . . ?
 C25     Nd      C24     29.50(9) . . ?
 C23     Nd      C24     29.25(10) . . ?
 C13     Nd      C24    143.83(10) . . ?
 Cl1     Nd      C14     49.95(10) . . ?
 C22     Nd      C14    118.10(9) . . ?
 Cl2     Nd      C14     49.84(10) . . ?
 C21     Nd      C14    110.29(9) . . ?
 Cl1     Nd      C14    105.57(7) . . ?
 Cl2     Nd      C14     90.48(7) . . ?
 C15     Nd      C14     29.37(9) . . ?
 C25     Nd      C14    130.31(9) . . ?
 C23     Nd      C14    146.72(9) . . ?
 C13     Nd      C14     28.95(9) . . ?
 C24     Nd      C14    159.30(9) . . ?

 loop_
  _geom_torsion_atom_site_label_1
  _geom_torsion_atom_site_label_2
  _geom_torsion_atom_site_label_3
  _geom_torsion_atom_site_label_4
  _geom_torsion
  _geom_torsion_site_symmetry_1
  _geom_torsion_site_symmetry_2
  _geom_torsion_site_symmetry_3
  _geom_torsion_site_symmetry_4
  _geom_torsion_publ_flag
 C15   Cl1   Cl2   C13          0.7(3) . . . . ?
 Si1   Cl1   Cl2   C13        159.3(2) . . . . ?
 Nd    Cl1   Cl2   C13         72.0(2) . . . . ?
 C15   Cl1   Cl2   Si12       170.2(3) . . . . ?
 Si1   Cl1   Cl2   Si12       -31.2(5) . . . . ?
 Nd    Cl1   Cl2   Si12      -118.4(3) . . . . ?
 C15   Cl1   Cl2   Nd         -71.4(2) . . . . ?
 Si1   Cl1   Cl2   Nd          87.2(2) . . . . ?
 Cl1   Cl2   C13   C14         -0.4(3) . . . . ?
 Si12  Cl2   C13   C14       -171.9(2) . . . . ?
 Nd    Cl2   C13   C14         68.4(2) . . . . ?
 Cl1   Cl2   C13   Nd         -68.78(19) . . . . ?
 Si12  Cl2   C13   Nd         119.7(2) . . . . ?
 Cl2   C13   C14   C15         -0.1(3) . . . . ?
 Nd    C13   C14   C15         64.7(2) . . . . ?
 Cl2   C13   C14   Si14       169.1(2) . . . . ?
 Nd    C13   C14   Si14      -126.2(2) . . . . ?
 Cl2   C13   C14   Nd         -64.7(2) . . . . ?
 C13   C14   C15   Cl1          0.5(3) . . . . ?
 Si14  C14   C15   Cl1       -168.4(2) . . . . ?
 Nd    C14   C15   Cl1         66.5(2) . . . . ?
 C13   C14   C15   Nd         -66.0(2) . . . . ?
 Si14  C14   C15   Nd         125.1(2) . . . . ?
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Cl2	Cl1	C15	C14	-0.7(3)	.	.	.	?
Si1	Cl1	C15	C14	-162.8(2)	.	.	.	?
Nd	Cl1	C15	C14	-70.8(2)	.	.	.	?
Cl2	Cl1	C15	Nd	70.1(2)	.	.	.	?
Si1	Cl1	C15	Nd	-91.98(18)	.	.	.	?
C25	C21	C22	C23	1.0(3)	.	.	.	?
Si1	C21	C22	C23	157.0(3)	.	.	.	?
Nd	C21	C22	C23	71.5(2)	.	.	.	?
C25	C21	C22	Si22	171.0(3)	.	.	.	?
Si1	C21	C22	Si22	-33.0(5)	.	.	.	?
Nd	C21	C22	Si22	-118.5(3)	.	.	.	?
C25	C21	C22	Nd	-70.5(2)	.	.	.	?
Si1	C21	C22	Nd	85.5(3)	.	.	.	?
C21	C22	C23	C24	-0.7(4)	.	.	.	?
Si22	C22	C23	C24	-172.5(2)	.	.	.	?
Nd	C22	C23	C24	68.7(2)	.	.	.	?
C21	C22	C23	Nd	-69.4(2)	.	.	.	?
Si22	C22	C23	Nd	118.8(2)	.	.	.	?
C22	C23	C24	C25	0.0(4)	.	.	.	?
Nd	C23	C24	C25	65.5(2)	.	.	.	?
C22	C23	C24	Si24	173.6(2)	.	.	.	?
Nd	C23	C24	Si24	-120.9(2)	.	.	.	?
C22	C23	C24	Nd	-65.5(2)	.	.	.	?
C22	C21	C25	C24	-1.1(4)	.	.	.	?
Si1	C21	C25	C24	-160.9(2)	.	.	.	?
Nd	C21	C25	C24	-70.1(2)	.	.	.	?
C22	C21	C25	Nd	69.0(2)	.	.	.	?
Si1	C21	C25	Nd	-90.8(2)	.	.	.	?
C23	C24	C25	C21	0.7(4)	.	.	.	?
Si24	C24	C25	C21	-172.5(2)	.	.	.	?
Nd	C24	C25	C21	66.9(2)	.	.	.	?
C23	C24	C25	Nd	-66.2(2)	.	.	.	?
Si24	C24	C25	Nd	120.6(3)	.	.	.	?
O3	C31	C32	C33	-31.6(5)	.	.	.	?
C31	C32	C33	C34	37.4(5)	.	.	.	?
C32	C33	C34	O3	-30.5(5)	.	.	.	?
O4	C41	C42	C43	-29.2(4)	.	.	.	?
C41	C42	C43	C44	36.4(4)	.	.	.	?
C42	C43	C44	O4	-30.9(5)	.	.	.	?
C33	C34	O3	C31	10.9(4)	.	.	.	?
C33	C34	O3	Li	-157.9(4)	.	.	.	?
C32	C31	O3	C34	13.2(5)	.	.	.	?
C32	C31	O3	Li	-177.4(4)	.	.	.	?
O4	Li	O3	C34	-129.2(4)	.	.	.	?
Cl2	Li	O3	C34	0.5(5)	.	.	.	?
Cl1	Li	O3	C34	115.7(4)	.	.	.	?
Nd	Li	O3	C34	56.7(5)	.	.	.	?
O4	Li	O3	C31	63.4(5)	.	.	.	?
Cl2	Li	O3	C31	-166.9(3)	.	.	.	?
Cl1	Li	O3	C31	-51.7(5)	.	.	.	?
Nd	Li	O3	C31	-110.7(4)	.	.	.	?
C42	C41	O4	C44	10.5(4)	.	.	.	?
C42	C41	O4	Li	-166.4(3)	.	.	.	?
C43	C44	O4	C41	13.2(5)	.	.	.	?
C43	C44	O4	Li	-169.5(3)	.	.	.	?
O3	Li	O4	C41	-127.4(3)	.	.	.	?
Cl2	Li	O4	C41	105.6(4)	.	.	.	?
Cl1	Li	O4	C41	-3.5(5)	.	.	.	?
Nd	Li	O4	C41	47.3(5)	.	.	.	?
O3	Li	O4	C44	56.0(5)	.	.	.	?
Cl2	Li	O4	C44	-71.0(4)	.	.	.	?

Cl1	Li	O4	C44	179.9(3)	.	.	?
Nd	Li	O4	C44	-129.3(3)	.	.	?
C15	C11	Si1	C1	-39.4(3)	.	.	?
C12	C11	Si1	C1	163.9(3)	.	.	?
Nd	C11	Si1	C1	-118.94(14)	.	.	?
C15	C11	Si1	C2	-160.8(2)	.	.	?
C12	C11	Si1	C2	42.6(3)	.	.	?
Nd	C11	Si1	C2	119.67(15)	.	.	?
C15	C11	Si1	C21	80.9(3)	.	.	?
C12	C11	Si1	C21	-75.7(3)	.	.	?
Nd	C11	Si1	C21	1.40(15)	.	.	?
C25	C21	Si1	C1	-165.2(3)	.	.	?
C22	C21	Si1	C1	41.0(3)	.	.	?
Nd	C21	Si1	C1	116.35(16)	.	.	?
C25	C21	Si1	C2	-43.0(3)	.	.	?
C22	C21	Si1	C2	163.3(3)	.	.	?
Nd	C21	Si1	C2	-121.37(14)	.	.	?
C25	C21	Si1	C11	77.0(3)	.	.	?
C22	C21	Si1	C11	-76.7(3)	.	.	?
Nd	C21	Si1	C11	-1.39(15)	.	.	?
C13	C12	Si12	C122	111.3(3)	.	.	?
C11	C12	Si12	C122	-57.3(4)	.	.	?
Nd	C12	Si12	C122	-155.11(18)	.	.	?
C13	C12	Si12	C121	-8.3(3)	.	.	?
C11	C12	Si12	C121	-176.8(3)	.	.	?
Nd	C12	Si12	C121	85.4(2)	.	.	?
C13	C12	Si12	C123	-125.0(3)	.	.	?
C11	C12	Si12	C123	66.4(4)	.	.	?
Nd	C12	Si12	C123	-31.4(2)	.	.	?
C13	C14	Si14	C141	166.9(3)	.	.	?
C15	C14	Si14	C141	-26.4(4)	.	.	?
Nd	C14	Si14	C141	69.5(3)	.	.	?
C13	C14	Si14	C142	44.3(3)	.	.	?
C15	C14	Si14	C142	-149.0(3)	.	.	?
Nd	C14	Si14	C142	-53.1(2)	.	.	?
C13	C14	Si14	C143	-73.0(3)	.	.	?
C15	C14	Si14	C143	93.7(3)	.	.	?
Nd	C14	Si14	C143	-170.4(2)	.	.	?
C23	C22	Si22	C222	121.0(3)	.	.	?
C21	C22	Si22	C222	-48.0(4)	.	.	?
Nd	C22	Si22	C222	-146.52(17)	.	.	?
C23	C22	Si22	C221	-114.2(3)	.	.	?
C21	C22	Si22	C221	76.7(4)	.	.	?
Nd	C22	Si22	C221	-21.8(2)	.	.	?
C23	C22	Si22	C223	3.9(3)	.	.	?
C21	C22	Si22	C223	-165.2(3)	.	.	?
Nd	C22	Si22	C223	96.30(19)	.	.	?
C23	C24	Si24	C241	-79.8(3)	.	.	?
C25	C24	Si24	C241	92.1(3)	.	.	?
Nd	C24	Si24	C241	-172.87(19)	.	.	?
C23	C24	Si24	C242	161.6(3)	.	.	?
C25	C24	Si24	C242	-26.4(4)	.	.	?
Nd	C24	Si24	C242	68.6(2)	.	.	?
C23	C24	Si24	C243	38.0(3)	.	.	?
C25	C24	Si24	C243	-150.0(3)	.	.	?
Nd	C24	Si24	C243	-55.0(2)	.	.	?
O3	Li	Cl1	Nd	-123.3(3)	.	.	?
O4	Li	Cl1	Nd	122.1(2)	.	.	?
Cl2	Li	Cl1	Nd	-0.31(17)	.	.	?
O3	Li	Cl2	Nd	126.1(3)	.	.	?
O4	Li	Cl2	Nd	-111.9(3)	.	.	?

Cl1	Li	Cl2	Nd	0.31(17)	.	.	.	?
C15	C11	Nd	C22	-95.89(18)	.	.	.	?
C12	C11	Nd	C22	152.9(2)	.	.	.	?
Si1	C11	Nd	C22	21.46(13)	.	.	.	?
C15	C11	Nd	C12	111.3(3)	.	.	.	?
Si1	C11	Nd	C12	-131.4(3)	.	.	.	?
C15	C11	Nd	C21	-118.4(2)	.	.	.	?
C12	C11	Nd	C21	130.3(2)	.	.	.	?
Si1	C11	Nd	C21	-1.06(12)	.	.	.	?
C15	C11	Nd	Cl1	117.55(16)	.	.	.	?
C12	C11	Nd	Cl1	6.3(2)	.	.	.	?
Si1	C11	Nd	Cl1	-125.10(10)	.	.	.	?
C15	C11	Nd	Cl2	-0.8(2)	.	.	.	?
C12	C11	Nd	Cl2	-112.06(19)	.	.	.	?
Si1	C11	Nd	Cl2	116.55(11)	.	.	.	?
C12	C11	Nd	C15	-111.3(3)	.	.	.	?
Si1	C11	Nd	C15	117.3(2)	.	.	.	?
C15	C11	Nd	C25	-145.64(19)	.	.	.	?
C12	C11	Nd	C25	103.1(2)	.	.	.	?
Si1	C11	Nd	C25	-28.29(13)	.	.	.	?
C15	C11	Nd	C23	-110.19(18)	.	.	.	?
C12	C11	Nd	C23	138.55(19)	.	.	.	?
Si1	C11	Nd	C23	7.15(17)	.	.	.	?
C15	C11	Nd	C13	73.29(19)	.	.	.	?
C12	C11	Nd	C13	-37.96(19)	.	.	.	?
Si1	C11	Nd	C13	-169.4(2)	.	.	.	?
C15	C11	Nd	C24	-141.40(17)	.	.	.	?
C12	C11	Nd	C24	107.3(2)	.	.	.	?
Si1	C11	Nd	C24	-24.05(15)	.	.	.	?
C15	C11	Nd	C14	35.09(17)	.	.	.	?
C12	C11	Nd	C14	-76.2(2)	.	.	.	?
Si1	C11	Nd	C14	152.44(19)	.	.	.	?
C23	C22	Nd	Cl1	-153.2(2)	.	.	.	?
C21	C22	Nd	Cl1	-42.01(19)	.	.	.	?
Si22	C22	Nd	Cl1	90.60(17)	.	.	.	?
C23	C22	Nd	Cl2	-138.03(19)	.	.	.	?
C21	C22	Nd	Cl2	-26.9(2)	.	.	.	?
Si22	C22	Nd	Cl2	105.74(17)	.	.	.	?
C23	C22	Nd	C21	-111.2(3)	.	.	.	?
Si22	C22	Nd	C21	132.6(3)	.	.	.	?
C23	C22	Nd	Cl1	-15.0(2)	.	.	.	?
C21	C22	Nd	Cl1	96.11(18)	.	.	.	?
Si22	C22	Nd	Cl1	-131.28(13)	.	.	.	?
C23	C22	Nd	Cl2	72.4(2)	.	.	.	?
C21	C22	Nd	Cl2	-176.45(17)	.	.	.	?
Si22	C22	Nd	Cl2	-43.84(16)	.	.	.	?
C23	C22	Nd	C15	176.7(2)	.	.	.	?
C21	C22	Nd	C15	-72.11(19)	.	.	.	?
Si22	C22	Nd	C15	60.50(17)	.	.	.	?
C23	C22	Nd	C25	-73.5(2)	.	.	.	?
C21	C22	Nd	C25	37.66(18)	.	.	.	?
Si22	C22	Nd	C25	170.3(2)	.	.	.	?
C21	C22	Nd	C23	111.2(3)	.	.	.	?
Si22	C22	Nd	C23	-116.2(3)	.	.	.	?
C23	C22	Nd	C13	-165.00(18)	.	.	.	?
C21	C22	Nd	C13	-53.9(2)	.	.	.	?
Si22	C22	Nd	C13	78.8(2)	.	.	.	?
C23	C22	Nd	C24	-34.61(19)	.	.	.	?
C21	C22	Nd	C24	76.5(2)	.	.	.	?
Si22	C22	Nd	C24	-150.9(2)	.	.	.	?
C23	C22	Nd	C14	165.90(19)	.	.	.	?

C21	C22	Nd	C14	-82.9(2)	. . . .	?
Si22	C22	Nd	C14	49.66(19)	. . . .	?
C13	C12	Nd	C11	-110.7(3)	. . . .	?
Si12	C12	Nd	C11	132.5(3)	. . . .	?
C13	C12	Nd	C22	-140.87(18)	. . . .	?
C11	C12	Nd	C22	-30.2(2)	. . . .	?
Si12	C12	Nd	C22	102.32(18)	. . . .	?
C13	C12	Nd	C21	-154.4(2)	. . . .	?
C11	C12	Nd	C21	-43.7(2)	. . . .	?
Si12	C12	Nd	C21	88.75(18)	. . . .	?
C13	C12	Nd	C11	74.56(18)	. . . .	?
C11	C12	Nd	C11	-174.74(19)	. . . .	?
Si12	C12	Nd	C11	-42.26(17)	. . . .	?
C13	C12	Nd	C12	-9.2(2)	. . . .	?
C11	C12	Nd	C12	101.52(19)	. . . .	?
Si12	C12	Nd	C12	-126.00(14)	. . . .	?
C13	C12	Nd	C15	-72.9(2)	. . . .	?
C11	C12	Nd	C15	37.85(18)	. . . .	?
Si12	C12	Nd	C15	170.3(2)	. . . .	?
C13	C12	Nd	C25	175.44(19)	. . . .	?
C11	C12	Nd	C25	-73.9(2)	. . . .	?
Si12	C12	Nd	C25	58.63(18)	. . . .	?
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Si12	C12	Nd	C14	-151.0(2)	. . . .	?
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C22	C21	Nd	C11	132.4(2)	. . . .	?
Si1	C21	Nd	C11	1.06(11)	. . . .	?
C25	C21	Nd	C22	111.5(3)	. . . .	?
Si1	C21	Nd	C22	-131.3(3)	. . . .	?
C25	C21	Nd	C12	-92.74(18)	. . . .	?
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Si1	C21	Nd	C12	24.41(13)	. . . .	?
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Si1	C21	Nd	C11	114.24(11)	. . . .	?
C25	C21	Nd	C12	115.92(16)	. . . .	?
C22	C21	Nd	C12	4.4(2)	. . . .	?
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C22	C21	Nd	C25	-111.5(3)	. . . .	?
Si1	C21	Nd	C25	117.1(2)	. . . .	?
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Si1	C21	Nd	C24	152.34(19)	. . . .	?

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C21	C25	Nd	C13	88.54(19)	. . . . ?

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C25	C24	Nd	C12	-160.32(17)	.	.	.	?

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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
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Nd Nd 0.24432(5) 0.50671(6) 0.20433(4) 0.0534(3) Uani 1 1 d . . .
Si1 Si 0.3005(3) 0.5550(3) 0.0462(2) 0.0633(12) Uani 1 1 d . . .
Si12 Si 0.4799(2) 0.4959(3) 0.2116(3) 0.0720(13) Uani 1 1 d . . .
Si14 Si 0.2322(3) 0.1995(3) 0.1830(2) 0.0642(12) Uani 1 1 d . . .
Si23 Si 0.0123(2) 0.6077(3) 0.1339(3) 0.0648(12) Uani 1 1 d . . .
Si24 Si 0.1729(3) 0.7942(3) 0.2411(2) 0.0660(12) Uani 1 1 d . . .
Cl1 Cl 0.1564(2) 0.4193(3) 0.2848(2) 0.0745(12) Uani 1 1 d . . .
Cl2 Cl 0.3292(3) 0.5758(3) 0.3315(2) 0.0785(12) Uani 1 1 d . . .
Li Li 0.2586(12) 0.4851(14) 0.3887(11) 0.040(5) Uiso 1 1 d . . .
C1 C 0.2504(10) 0.5040(11) -0.0447(8) 0.076(5) Uani 1 1 d . . .
C2 C 0.3832(10) 0.6417(13) 0.0369(11) 0.095(6) Uani 1 1 d . . .
C11 C 0.3272(8) 0.4457(10) 0.1115(8) 0.052(4) Uani 1 1 d . . .
C12 C 0.3820(9) 0.4371(11) 0.1779(9) 0.064(4) Uani 1 1 d . . .
C13 C 0.3535(9) 0.3555(10) 0.2125(8) 0.060(4) Uani 1 1 d . . .
C14 C 0.2853(9) 0.3166(10) 0.1685(8) 0.059(4) Uani 1 1 d . . .
C15 C 0.2646(8) 0.3758(10) 0.1054(8) 0.057(4) Uani 1 1 d . . .
C21 C 0.2280(9) 0.6203(11) 0.0865(7) 0.058(4) Uani 1 1 d . . .
C22 C 0.1513(8) 0.5817(9) 0.0821(7) 0.046(3) Uani 1 1 d . . .
C23 C 0.1177(8) 0.6278(10) 0.1359(7) 0.054(4) Uani 1 1 d . . .
C24 C 0.1769(8) 0.6954(10) 0.1747(8) 0.054(4) Uani 1 1 d . . .
C25 C 0.2454(9) 0.6898(10) 0.1436(8) 0.056(4) Uani 1 1 d . . .
C121 C 0.5392(10) 0.4742(14) 0.1455(12) 0.097(6) Uani 1 1 d . . .
C122 C 0.4776(10) 0.6335(12) 0.2310(12) 0.105(7) Uani 1 1 d . . .
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C123 C 0.5260(11) 0.4297(14) 0.2978(11) 0.103(6) Uani 1 1 d . . .
C141 C 0.2522(10) 0.1678(14) 0.2798(10) 0.088(5) Uiso 1 1 d . . .
C142 C 0.2724(12) 0.0986(12) 0.1358(10) 0.095(6) Uani 1 1 d . . .
C143 C 0.1217(9) 0.2113(13) 0.1416(10) 0.084(5) Uani 1 1 d . . .
C231 C -0.0148(11) 0.6305(14) 0.2207(10) 0.095(6) Uani 1 1 d . . .
C232 C -0.0097(10) 0.4732(13) 0.1121(10) 0.085(5) Uani 1 1 d . . .
C233 C -0.0489(10) 0.6906(14) 0.0618(11) 0.102(7) Uani 1 1 d . . .
C241 C 0.2722(12) 0.8584(13) 0.2654(11) 0.102(6) Uani 1 1 d . . .
C242 C 0.0943(11) 0.8859(13) 0.2027(10) 0.097(6) Uani 1 1 d . . .
C243 C 0.1515(11) 0.7448(13) 0.3257(9) 0.089(6) Uani 1 1 d . . .
O3 O 0.1938(8) 0.5297(9) 0.4495(7) 0.098(4) Uani 1 1 d . . .
C31 C 0.1090(13) 0.5059(16) 0.4426(12) 0.112(8) Uani 1 1 d . . .
C32 C 0.0740(14) 0.5839(19) 0.4766(15) 0.146(10) Uani 1 1 d . . .
C33 C 0.1388(17) 0.6581(17) 0.5041(12) 0.125(8) Uani 1 1 d . . .
C34 C 0.2162(13) 0.6154(15) 0.4951(10) 0.099(6) Uani 1 1 d . . .
O4 O 0.3311(8) 0.3809(10) 0.4472(8) 0.112(5) Uani 1 1 d . . .
C41 C 0.3242(18) 0.2832(17) 0.4656(14) 0.138(9) Uani 1 1 d . . .
C42 C 0.405(2) 0.251(2) 0.504(2) 0.209(17) Uani 1 1 d . . .
C43 C 0.4541(17) 0.337(2) 0.5151(18) 0.186(14) Uani 1 1 d . . .
C44 C 0.4090(13) 0.418(2) 0.4826(17) 0.162(12) Uani 1 1 d . . .

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Si1 0.064(3) 0.057(3) 0.073(3) 0.009(2) 0.026(2) 0.008(2)
Si12 0.045(2) 0.061(3) 0.108(4) 0.001(3) 0.014(2) -0.001(2)
Si14 0.072(3) 0.045(2) 0.073(3) 0.003(2) 0.015(2) -0.003(2)
Si23 0.048(3) 0.066(3) 0.080(3) 0.002(2) 0.014(2) 0.003(2)
Si24 0.081(3) 0.043(2) 0.074(3) -0.007(2) 0.019(3) -0.001(2)
Cl1 0.072(3) 0.076(3) 0.078(3) 0.004(2) 0.023(2) -0.013(2)
Cl2 0.080(3) 0.076(3) 0.073(3) 0.001(2) 0.006(2) -0.014(2)
C1 0.096(13) 0.072(11) 0.063(10) 0.006(9) 0.027(9) 0.018(9)
C2 0.063(11) 0.097(14) 0.140(18) 0.041(12) 0.054(12) -0.002(10)
C11 0.037(8) 0.045(8) 0.082(12) -0.010(8) 0.031(8) -0.001(7)
C12 0.052(10) 0.058(10) 0.080(12) 0.007(9) 0.012(9) 0.008(8)
C13 0.058(10) 0.036(8) 0.080(11) -0.010(8) 0.006(9) 0.009(7)
C14 0.075(11) 0.039(8) 0.065(10) 0.004(8) 0.019(9) 0.009(8)
C15 0.054(9) 0.043(8) 0.078(11) -0.012(8) 0.025(8) 0.003(7)
C21 0.068(11) 0.061(10) 0.050(9) 0.031(8) 0.023(8) 0.013(8)
C22 0.060(9) 0.043(8) 0.042(8) 0.012(6) 0.024(7) 0.013(7)
C23 0.054(9) 0.052(9) 0.055(9) 0.006(7) 0.011(8) 0.011(7)
C24 0.056(9) 0.044(8) 0.064(10) 0.008(7) 0.020(8) 0.021(7)
C25 0.072(11) 0.044(8) 0.054(9) 0.013(7) 0.021(8) 0.012(7)
C121 0.053(11) 0.095(14) 0.144(19) -0.001(12) 0.024(11) 0.004(9)
C122 0.075(13) 0.048(10) 0.18(2) -0.019(12) 0.008(13) -0.007(9)
C123 0.075(13) 0.100(15) 0.113(16) 0.008(12) -0.016(11) -0.012(11)
C142 0.148(18) 0.058(11) 0.093(14) -0.020(10) 0.055(13) 0.001(11)
C143 0.061(11) 0.082(12) 0.103(14) 0.000(10) 0.011(10) -0.016(9)
C231 0.085(13) 0.112(15) 0.101(15) -0.025(12) 0.047(12) -0.012(11)
C232 0.082(13) 0.082(13) 0.087(13) -0.009(10) 0.016(10) -0.007(10)
C233 0.069(12) 0.088(13) 0.136(18) 0.047(12) -0.001(12) 0.021(10)
C241 0.106(15) 0.068(12) 0.124(17) -0.014(11) 0.012(13) -0.008(11)
C242 0.116(16) 0.082(13) 0.096(14) 0.018(11) 0.034(12) 0.053(11)
C243 0.116(15) 0.076(12) 0.071(12) -0.002(9) 0.014(11) 0.006(11)
O3 0.106(10) 0.104(10) 0.092(9) -0.021(8) 0.040(8) -0.014(8)
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C31 0.101(16) 0.138(19) 0.120(17) -0.047(14) 0.071(14) -0.041(14)
C32 0.114(19) 0.14(2) 0.19(3) -0.09(2) 0.055(18) -0.028(16)
C33 0.17(2) 0.109(18) 0.101(17) -0.035(13) 0.041(17) -0.034(17)
C34 0.103(16) 0.090(14) 0.081(14) -0.012(11) -0.021(12) -0.017(12)
O4 0.097(10) 0.101(11) 0.128(12) 0.051(9) 0.009(9) -0.002(8)
C41 0.18(3) 0.080(17) 0.15(2) 0.012(15) 0.024(19) 0.014(17)
C42 0.18(3) 0.11(2) 0.33(5) 0.09(3) 0.05(3) 0.02(2)
C43 0.12(2) 0.15(3) 0.24(4) 0.07(3) -0.03(2) 0.00(2)
C44 0.068(15) 0.14(2) 0.24(3) 0.06(2) -0.037(18) -0.024(15)

_geom_special_details
;
 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.
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Nd C15 2.701(13) . ?
Nd C11 2.713(12) . ?
Nd C21 2.715(12) . ?
Nd C12 2.720(4) . ?
Nd C11 2.724(4) . ?
Nd C22 2.727(13) . ?
Nd C25 2.740(13) . ?
Nd C12 2.756(15) . ?
Nd C13 2.775(13) . ?
Nd C14 2.797(13) . ?
Nd C24 2.804(12) . ?
Nd C23 2.814(13) . ?
Si1 C21 1.872(15) . ?
Si1 C1 1.900(17) . ?
Si1 C2 1.907(16) . ?
Si1 C11 1.926(15) . ?
Si12 C12 1.858(16) . ?
Si12 C121 1.87(2) . ?
Si12 C122 1.896(17) . ?
Si12 C123 1.90(2) . ?
Si14 C142 1.874(16) . ?
Si14 C141 1.878(18) . ?
Si14 C14 1.890(15) . ?
Si14 C143 1.914(17) . ?
Si23 C23 1.860(15) . ?
Si23 C232 1.880(17) . ?
Si23 C231 1.890(18) . ?
Si23 C233 1.906(17) . ?
Si24 C242 1.865(17) . ?
Si24 C24 1.870(14) . ?
Si24 C243 1.900(18) . ?
Si24 C241 1.899(19) . ?
Cl1 Li 2.51(2) . ?
Cl2 Li 2.22(2) . ?
Li O3 1.93(2) . ?
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