RSC Advances

# Isolation and enantiostability of the B-chiral bis(salicylato)borate anions [$B_R(Sal)_2$] and [$B_S(Sal)_2$]

Lawrence W-Y. Wong, Alex S-F. Au Yeung, Gemma S-S. Tam, Jack W-H. Kan, Herman H-Y. Sung, Fu Kit Sheong, Zhenyang Lin and Ian D. Williams*

*Department of Chemistry, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, China.*

## Supporting Information

1. **Supplemental Figures**
   - **S1. Sparteinium Monocation in 2**
   - **S2. 2D energy surface for 'hinged' [$BSal_2$]$^-$ conformations**
2. **Circular Dichroism Spectra**
3. **Powder X-ray Diffractograms**
4. **Structure Determination Summaries for 1-5**

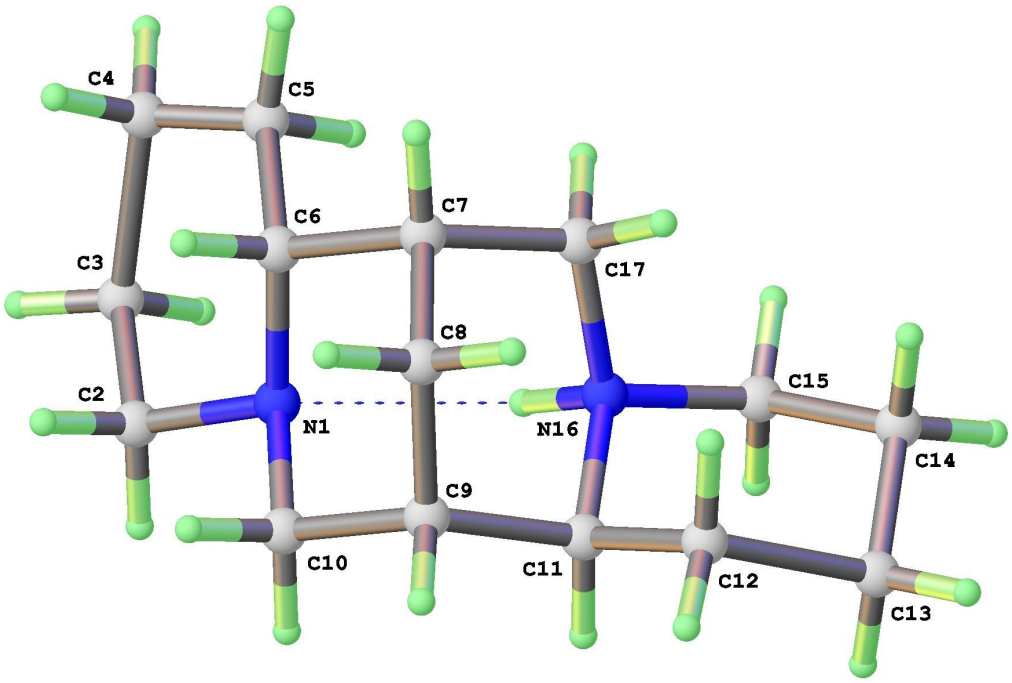


**Figure S1.** [HSpa]$^{+}$ monocation in **2** with labelling scheme and chiral centres 6R, 7S, 9S, 11S.

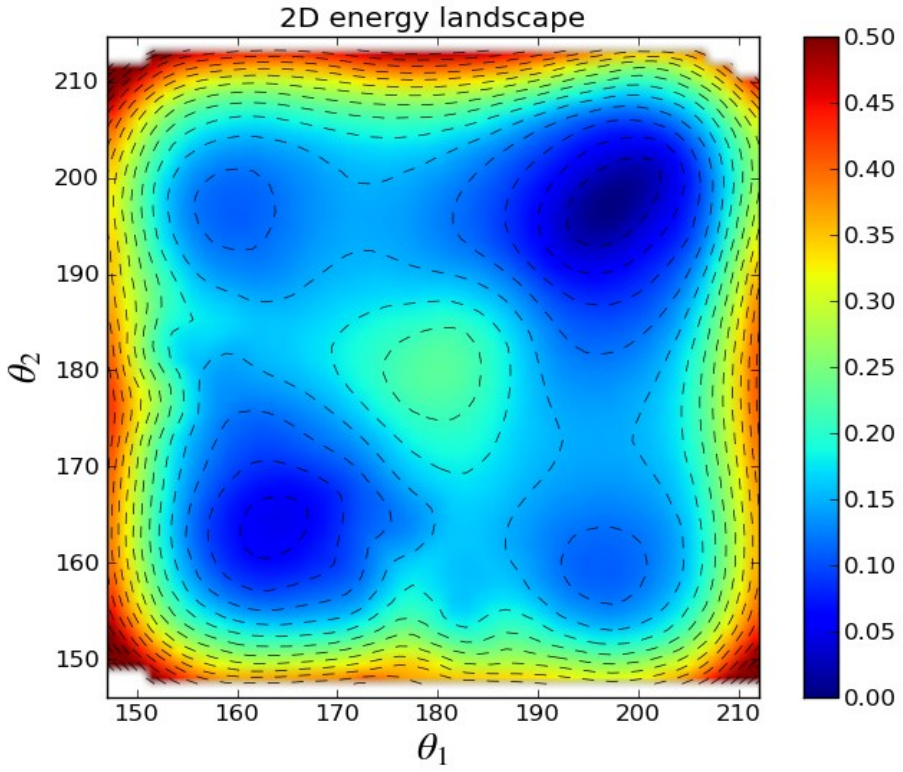


**Figure S2.** 2D energy landscape with θ1 and θ2 being the two dihedral angles. The dihedral angle on one chelate ring is varied, whilst other held fixed to obtain a 2D potential energy surface.

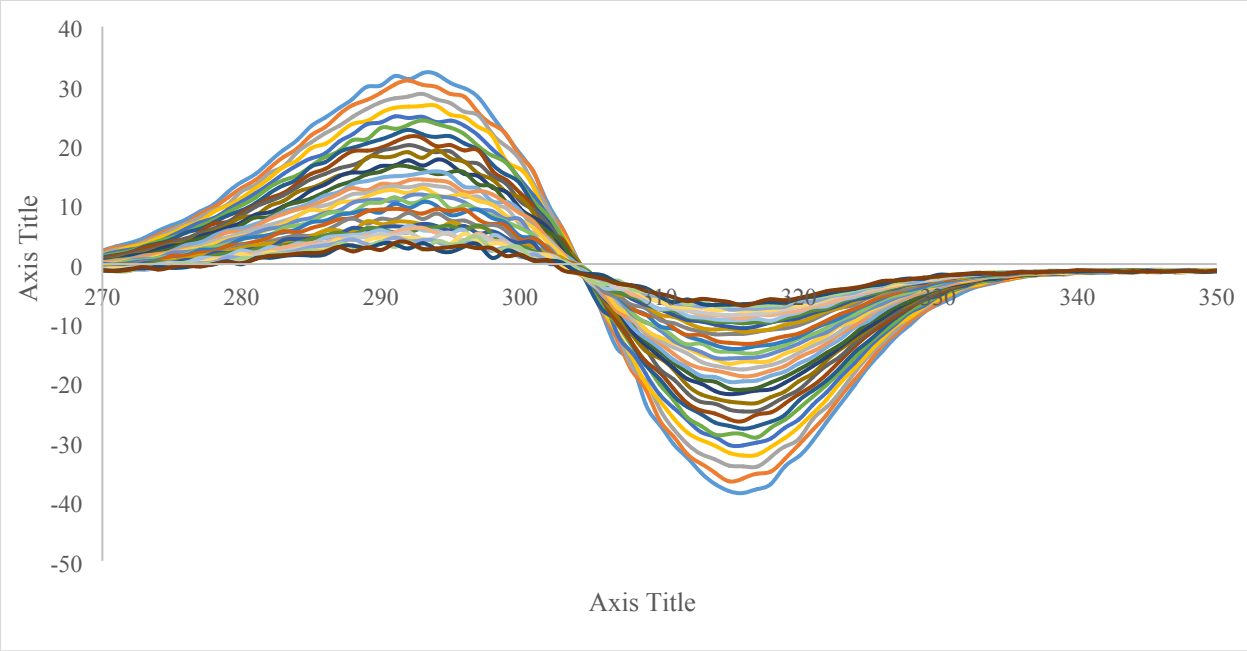


**Figure S3.** CD spectrum showing racemization of [HSpa][$B_S(Sal)_2$] in pure water (10min intervals).

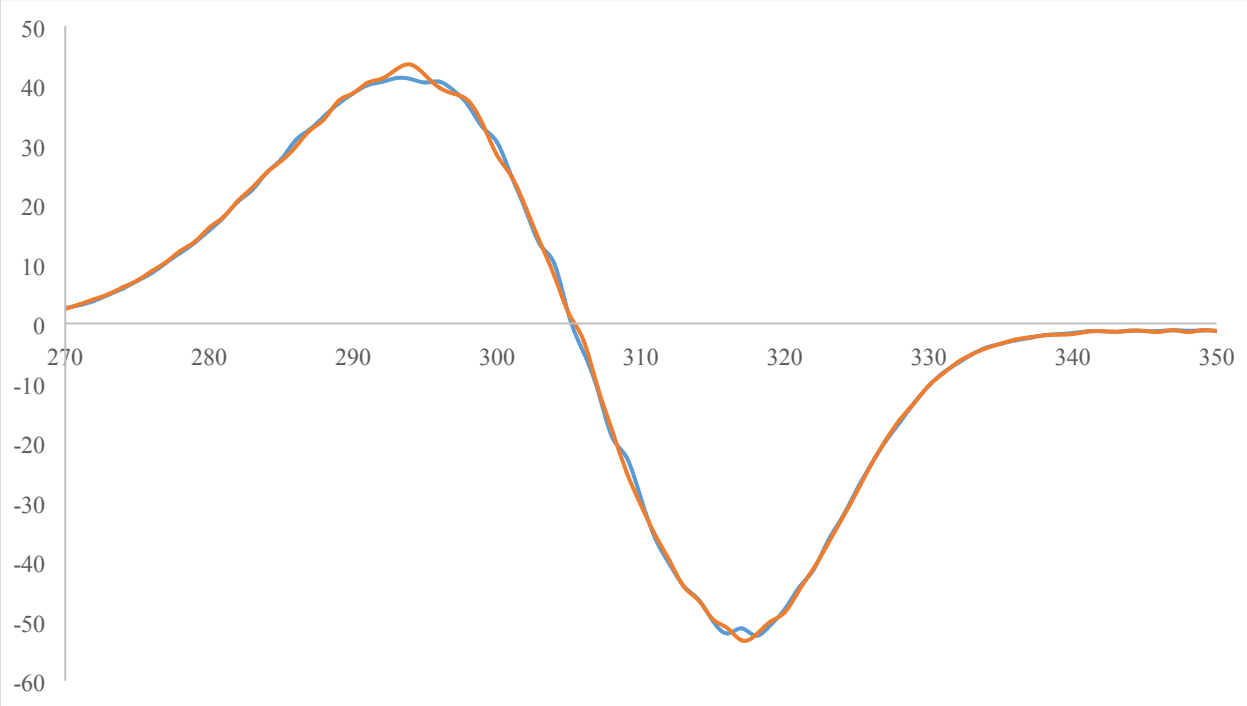


**Figure S4.** CD spectrum showing enantiostability [HSpa][$B_S(Sal)_2$] in DMF/$H_2O$ (4:1) solution (1 week).

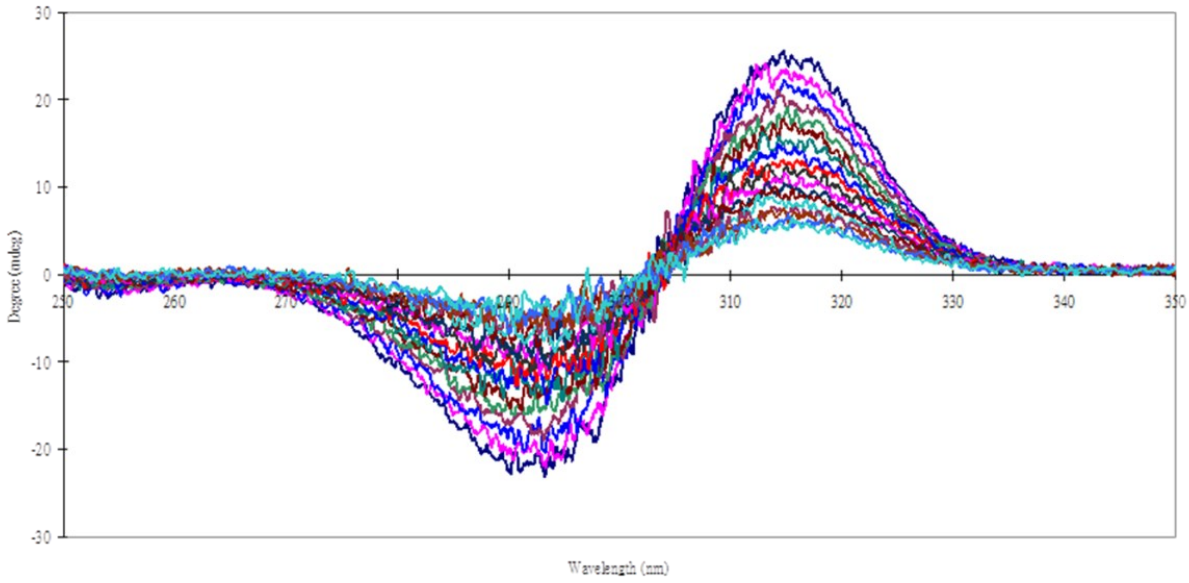


**Figure S5.** CD spectrum showing racemization of $[H_2Spa][B_R(Sal)_2]_2$ in pure water (5min intervals). Note sparteinium ion has little spectral contribution in range 250-350nm and can be ignored

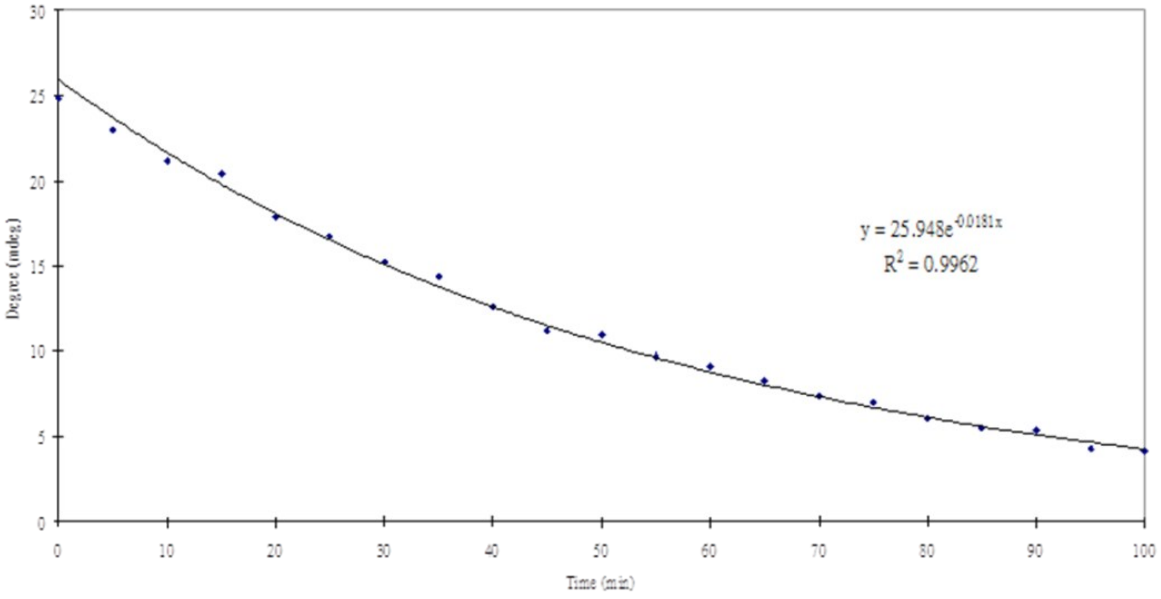


**Figure S6.** Plot showing kinetics of racemization at boron for $[H_2Spa][B_R(Sal)_2]_2$ in aqueous solution from CD trough at 282nm. Half-life $t_{1/2}$ = 40 mins

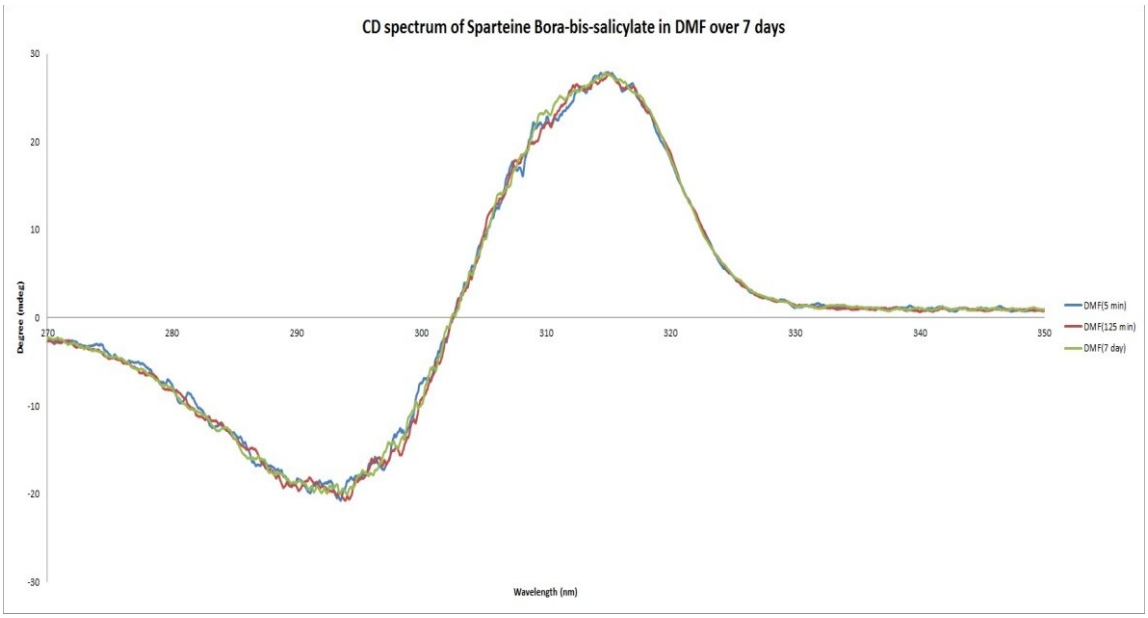


**Figure S7.** CD spectrum showing enantiostability $[H_2Spa][B_R(Sal)_2]_2$ in pure DMF solution (1 week).

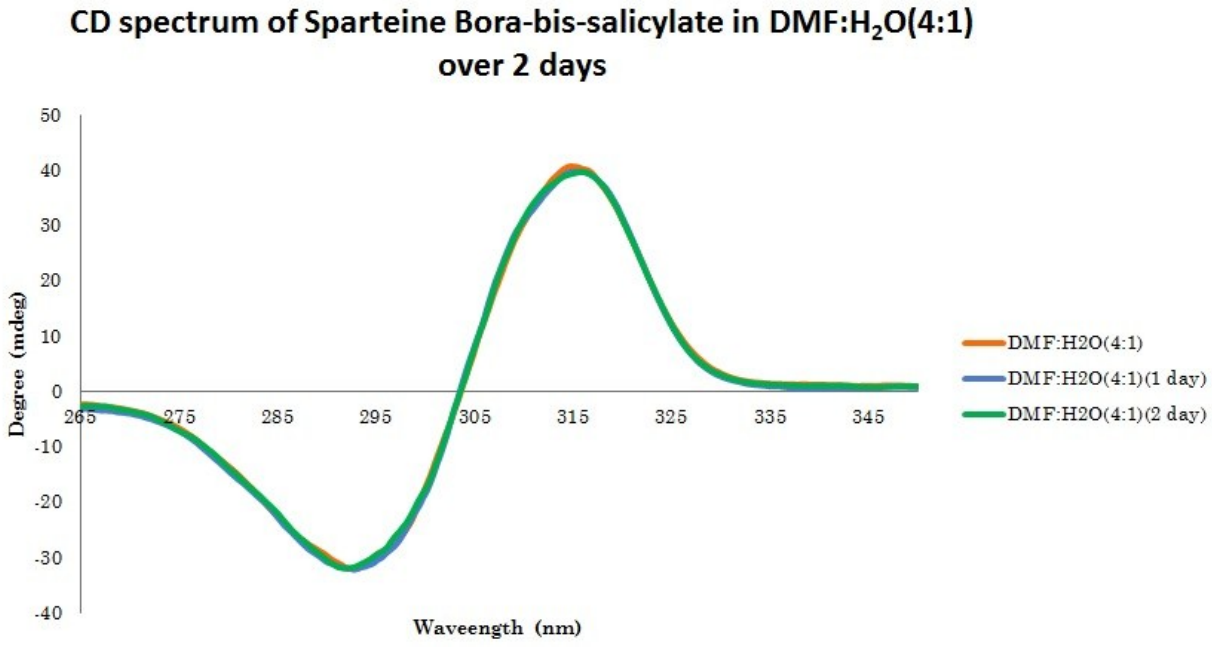


**Figure S8.** CD spectrum showing enantiostability $[H_2Spa][B_R(Sal)_2]_2$ solution in DMF/$H_2O$ (4:1) mixture over 2 days.

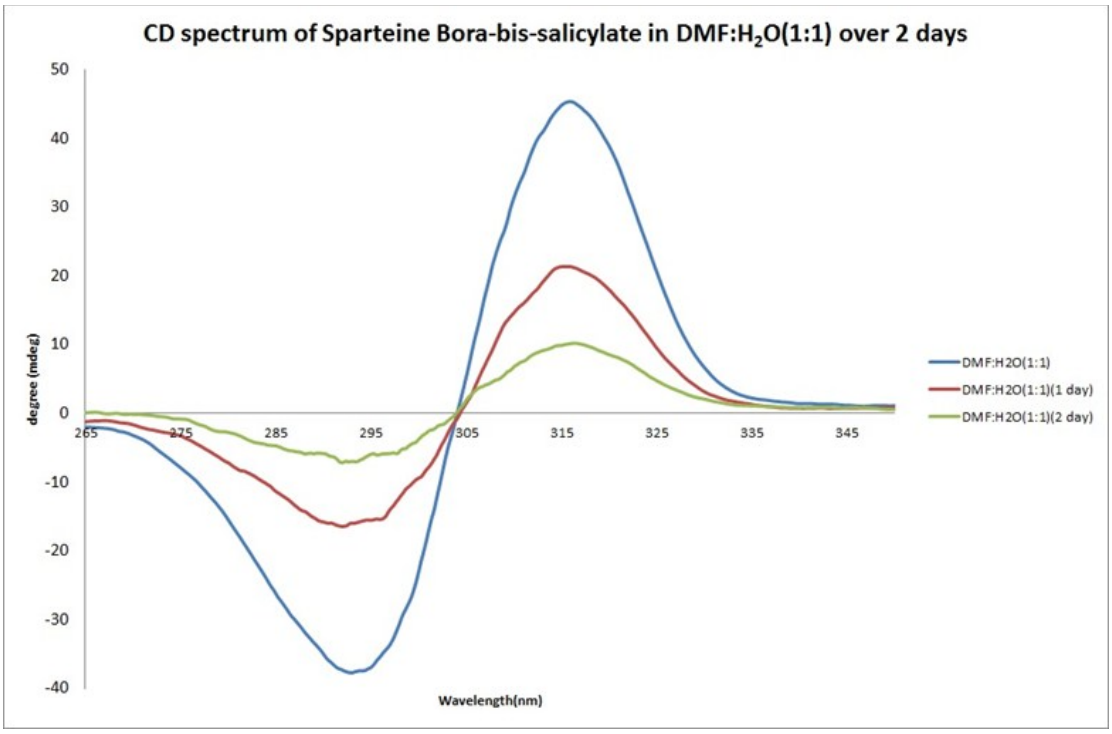


**Figure S9.** CD spectra showing $B_R$ racemization of $[H_2Spa][B_R(Sal)_2]_2$ DMF/$H_2O$ (1:1) solution ($t_{1/2}$ = ca. 18h)

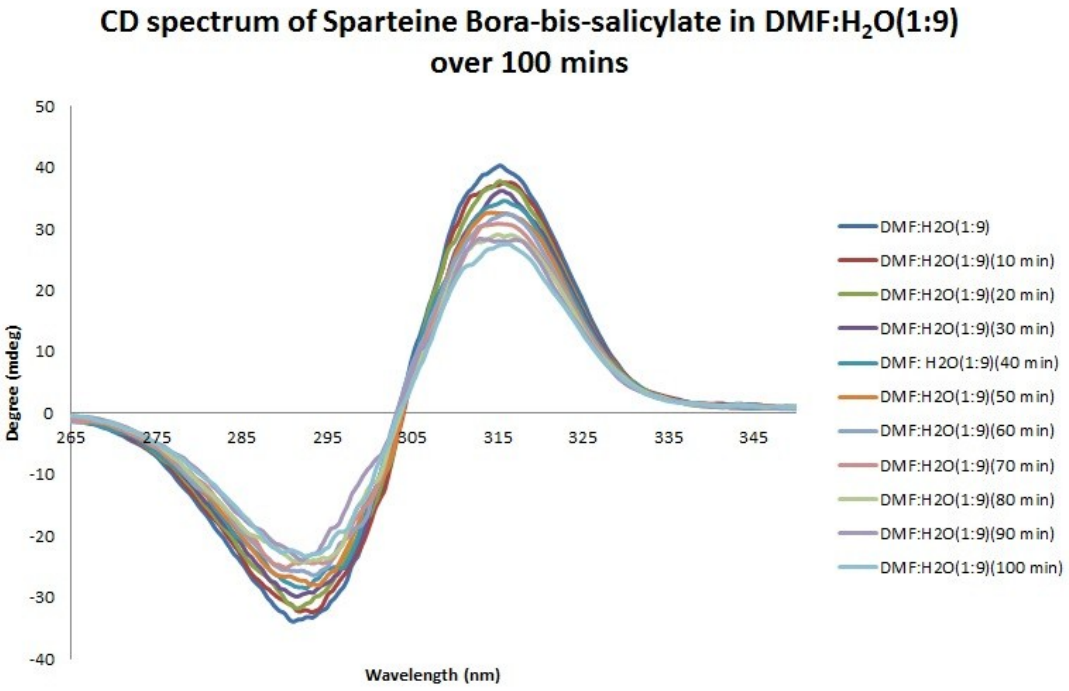


**Figure S10.** CD spectra showing $B_R$ racemization of **3** $[H_2Spa][B_R(Sal)_2]_2$ in DMF/$H_2O$ (1:9) soln ($t_{1/2}$ = ca. 2h)

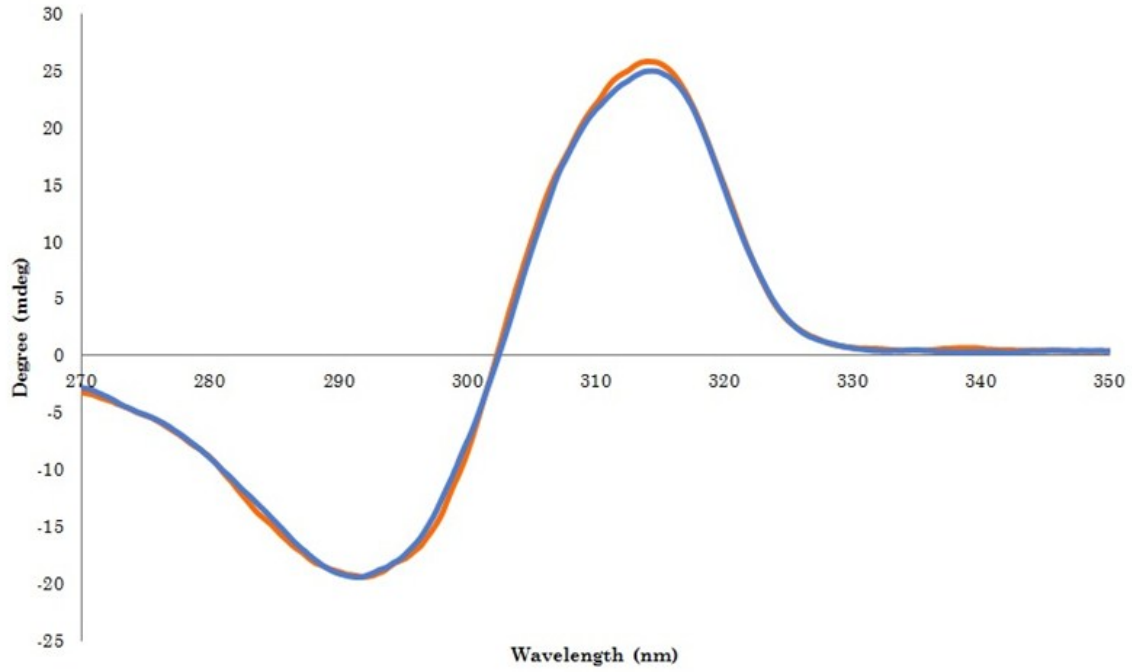


**Figure S11.** CD spectra showing retention of $B_R$ chirality in $[H_2Spa][B_R(Sal)_2]_2$ **3** (red) after metathesis crystallization to $[NBu_4][B_R(Sal)_2]_2$ **4** (blue)

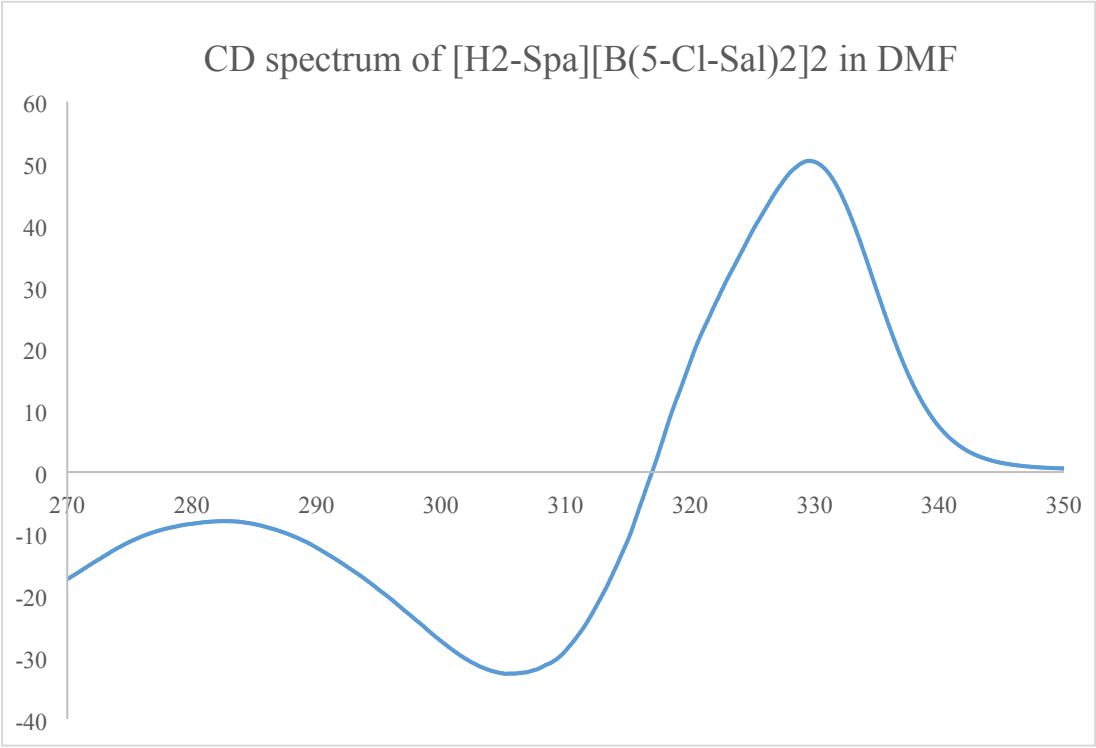


**Figure S12.** CD spectrum of $[H_2\text{-Spa}][B(5\text{-Cl-Sal})_2]_2$ **5** (after dehydration) in DMF.

## Powder X-ray Diffractograms

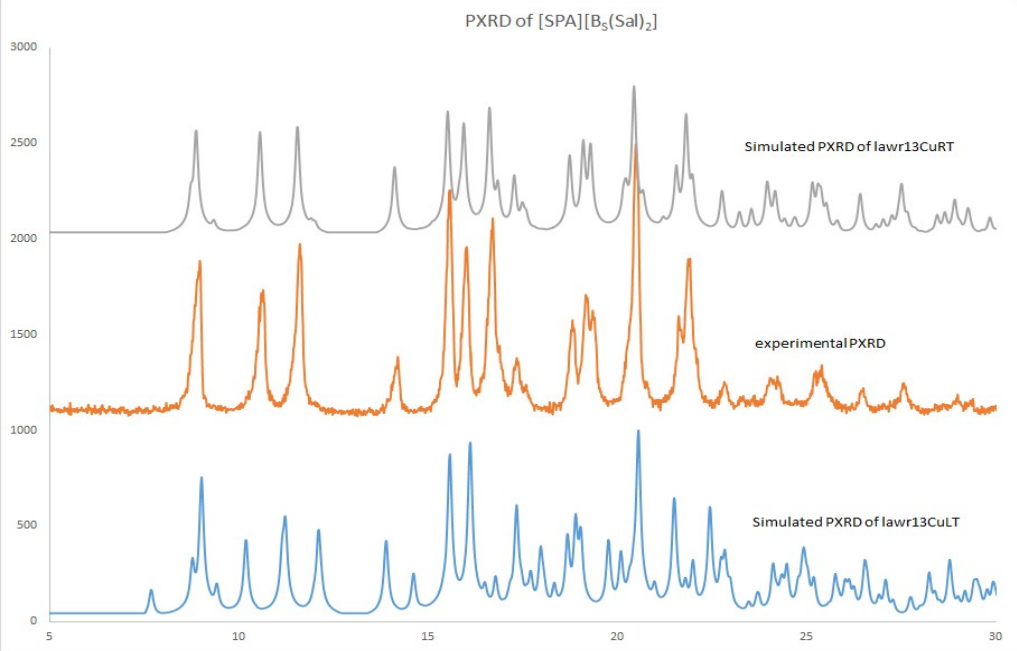


**Figure S13.** Powder X-ray diffractograms of isolated compound [H-Spa][$B_5$(Sal)$_2$] **2** with those simulated from single crystal structures **2** and **2-RT** - the powder pattern at RT is different from the low T structure of **2** due to an orthorhombic-monoclinic phase transition upon cooling.

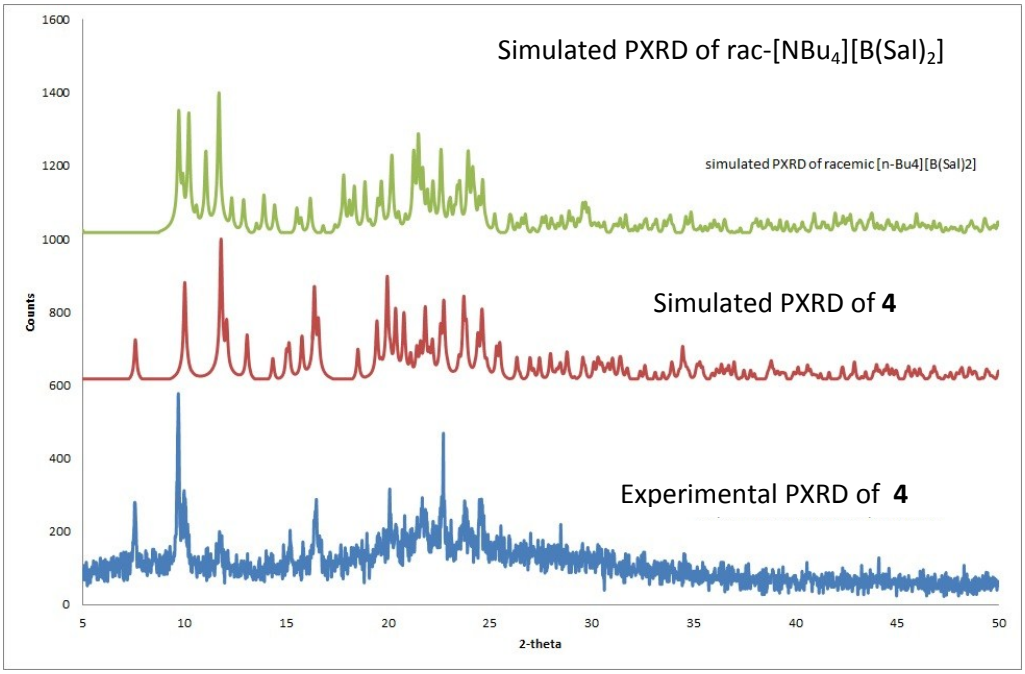


**Figure S14**. Powder diffractogram of **4** [$NBu_4$][$B_R$(Sal)$_2$] matches S-XRD of **4** (rather than rac-[$NBu_4$][B(Sal)$_2$] crystal structure ).

## Structure Determination Summaries and Tables for Compounds 1-5.

**Table 1 Crystal data and structure refinement for compound 1.**

| | |
|---|---|
| Identification code | alex316a |
| Empirical formula | $C_{34}H_{33}BN_2O_8$ |
| Formula weight | 608.43 |
| Temperature/K | 99.9(2) |
| Crystal system | triclinic |
| Space group | P1 |
| a/Å | 7.9518(3) |
| b/Å | 9.5337(5) |
| c/Å | 10.5702(3) |
| α/° | 89.020(3) |
| β/° | 76.831(3) |
| γ/° | 65.860(4) |
| Volume/Å$^3$ | 709.41(6) |
| Z | 1 |
| $\rho_{calc}$g/cm$^3$ | 1.424 |
| μ/mm$^{-1}$ | 0.831 |
| F(000) | 320.0 |
| Crystal size/mm$^3$ | 0.25 × 0.2 × 0.2 |
| Radiation | CuKα (λ = 1.54184) |
| 2Θ range for data collection/° | 8.624 to 134.982 |
| Index ranges | $-9 \leq h \leq 9$, $-10 \leq k \leq 11$, $-12 \leq l \leq 12$ |
| Reflections collected | 10175 |
| Independent reflections | 4775 [$R_{int}$ = 0.0175, $R_{sigma}$ = 0.0192] |
| Data/restraints/parameters | 4775/3/415 |
| Completeness to theta = 66.5° | 99.8% |
| Goodness-of-fit on F$^2$ | 1.012 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0252, $wR_2$ = 0.0661 |
| Final R indexes [all data] | $R_1$ = 0.0256, $wR_2$ = 0.0664 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.17/-0.18 |
| Flack parameter | 0.07(5) |

**Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for compound 1. $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| O1 | 4744.2(19) | 8238.0(16) | 4268.4(14) | 21.0(3) |
| O2 | 10974.0(19) | 1158.6(16) | 4750.7(14) | 23.1(3) |
| N1 | 7885(2) | 6522.3(19) | 7993.7(15) | 19.3(3) |
| N2 | 7884(2) | 6669.6(18) | 1803.4(15) | 14.6(3) |
| C30 | 10662(3) | 1121(2) | 3479(2) | 25.3(5) |
| C31 | 6785(3) | 7837(2) | 7624.3(19) | 20.8(4) |
| C32 | 6318(3) | 8015(2) | 6404.7(19) | 18.7(4) |
| C33 | 7000(2) | 6757(2) | 5524.7(18) | 16.4(4) |
| C34 | 8215(3) | 5301(2) | 5868.9(18) | 15.6(4) |
| C35 | 9009(3) | 3912(2) | 5043.6(18) | 17.1(4) |
| C36 | 10169(3) | 2557(2) | 5443.6(19) | 18.5(4) |
| C37 | 10612(3) | 2529(2) | 6672.2(19) | 20.7(4) |
| C38 | 9856(3) | 3839(2) | 7487.5(19) | 20.3(4) |
| C39 | 8622(3) | 5260(2) | 7117.6(18) | 17.0(4) |
| C40 | 6447(2) | 6904(2) | 4227.3(18) | 15.7(4) |
| C41 | 8031(2) | 7032(2) | 3155.5(17) | 14.4(4) |
| C42 | 8090(2) | 8634(2) | 3184.4(17) | 16.0(4) |
| C43 | 7788(2) | 9353(2) | 1904.0(17) | 15.7(4) |
| C44 | 5920(3) | 9430(2) | 1672.4(19) | 18.2(4) |
| C45 | 6092(3) | 7781(2) | 1459.2(18) | 16.9(4) |
| C46 | 9564(3) | 6694(2) | 803.7(17) | 16.8(4) |
| C47 | 9425(3) | 8352(2) | 749.2(17) | 16.2(4) |
| C48 | 11277(3) | 8419(2) | 772.7(18) | 19.2(4) |
| C49 | 11920(3) | 9354(3) | 110(2) | 27.1(4) |
| B1 | 3596(3) | 4276(3) | 3020(2) | 16.5(4) |
| O10 | 5433(2) | 1934.4(17) | 5447.8(14) | 27.4(3) |
| O11 | 4287.7(18) | 2918.0(15) | 3751.8(13) | 18.8(3) |
| O12 | 2186.8(18) | 5647.8(15) | 3816.2(13) | 18.0(3) |
| O20 | 8078.4(18) | 3827.0(16) | 990.9(13) | 19.9(3) |
| O21 | 5291.8(18) | 4603.7(15) | 2407.0(13) | 18.3(3) |
| O22 | 2755.9(17) | 3948.1(15) | 2043.9(13) | 17.5(3) |
| C10 | 4550(3) | 3056(2) | 4941.1(18) | 19.0(4) |
| C11 | 3624(3) | 4646(2) | 5590.6(19) | 17.9(4) |
| C12 | 2397(2) | 5860(2) | 5021.2(18) | 16.5(4) |
| C13 | 1376(3) | 7315(2) | 5702.1(19) | 19.4(4) |
| C14 | 1624(3) | 7565(2) | 6920.8(19) | 22.3(4) |
| C15 | 2888(3) | 6381(3) | 7477(2) | 24.0(4) |
| C16 | 3868(3) | 4933(2) | 6810.9(19) | 21.3(4) |

| | | | | |
|---|---|---|---|---|
| C20 | 6499(2) | 3818(2) | 1319.3(18) | 16.0(4) |
| C21 | 5792(3) | 3047(2) | 504.2(18) | 16.2(4) |
| C22 | 3903(3) | 3221(2) | 884.0(18) | 15.5(4) |
| C23 | 3156(3) | 2664(2) | 38.5(19) | 17.9(4) |
| C24 | 4309(3) | 1913(2) | -1162.1(18) | 19.7(4) |
| C25 | 6212(3) | 1686(2) | -1529.5(18) | 20.5(4) |
| C26 | 6937(3) | 2258(2) | -699.7(19) | 18.2(4) |

**Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for compound 1. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.**

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| O1 | 13.5(6) | 23.8(8) | 21.6(7) | 4.2(6) | -2.0(5) | -4.9(6) |
| O2 | 26.7(7) | 16.6(7) | 23.8(7) | -1.0(6) | -7.0(6) | -6.1(6) |
| N1 | 23.2(8) | 22.5(9) | 13.9(7) | 0.5(6) | -1.9(6) | -12.7(7) |
| N2 | 16.1(7) | 13.5(8) | 15.9(7) | 2.1(6) | -6.1(6) | -6.7(6) |
| C30 | 28.3(10) | 21.9(11) | 24(1) | -4.6(8) | -4.6(8) | -9.4(9) |
| C31 | 23.7(9) | 20.9(10) | 17.1(9) | -4.8(7) | 0.3(7) | -11.2(8) |
| C32 | 18.4(9) | 17.1(9) | 19.5(9) | 1.5(7) | -1.1(7) | -8.3(7) |
| C33 | 15.4(8) | 19.4(9) | 15.7(9) | 2.0(7) | -1.1(7) | -10.0(7) |
| C34 | 15.1(8) | 20.2(10) | 14.3(8) | 2.7(7) | -1.7(6) | -11.0(7) |
| C35 | 18.7(9) | 20.2(10) | 13.9(9) | 1.4(7) | -3.4(7) | -9.7(7) |
| C36 | 19.4(9) | 18.4(10) | 18.7(9) | 0.3(8) | -2.4(7) | -9.9(8) |
| C37 | 21.5(9) | 20.8(10) | 21.6(9) | 6.0(8) | -7.6(8) | -9.3(8) |
| C38 | 25.0(9) | 24.2(10) | 16.2(9) | 5.7(8) | -7.3(7) | -13.6(8) |
| C39 | 18.9(9) | 21.5(10) | 13.4(8) | 0.3(7) | -1.3(7) | -12.5(8) |
| C40 | 14.7(8) | 14.5(9) | 17.8(9) | 2.8(7) | -4.1(7) | -5.9(7) |
| C41 | 15.7(8) | 15.7(9) | 12.2(8) | 0.9(6) | -5.2(6) | -6.0(7) |
| C42 | 18.8(9) | 15.6(9) | 15.3(8) | 0.2(7) | -4.5(7) | -8.5(7) |
| C43 | 17.5(9) | 14.0(9) | 16.4(8) | 1.6(7) | -5.3(7) | -6.7(7) |
| C44 | 17.0(9) | 17.0(9) | 21.5(9) | 4.2(7) | -8.3(7) | -6.0(7) |
| C45 | 16.5(8) | 19.2(9) | 17.1(9) | 4.1(7) | -9.1(6) | -7.0(7) |
| C46 | 18.2(9) | 17.8(9) | 13.5(8) | -0.6(7) | -2.6(7) | -7.3(7) |
| C47 | 18.7(9) | 18.3(9) | 14.0(8) | 3.1(7) | -5.9(7) | -9.1(7) |
| C48 | 19.8(9) | 21.8(9) | 17.2(9) | 0.4(7) | -6.1(7) | -9.0(7) |
| C49 | 26.3(10) | 30.5(11) | 30.3(11) | 6.0(9) | -8.8(8) | -16.7(9) |
| B1 | 15.8(9) | 17.3(10) | 17.1(10) | 0.0(8) | -3.6(7) | -7.5(8) |
| O10 | 35.7(8) | 19.7(7) | 24.3(7) | 3.4(6) | -13.3(6) | -6.1(6) |
| O11 | 21.4(6) | 17.4(7) | 16.8(6) | 0.0(5) | -6.2(5) | -6.5(5) |
| O12 | 17.0(6) | 18.9(7) | 16.1(6) | -1.0(5) | -4.7(5) | -5.1(5) |
| O20 | 18.5(7) | 19.6(7) | 23.4(7) | -1.5(5) | -3.6(5) | -10.2(5) |
| O21 | 18.6(6) | 19.4(7) | 18.0(6) | -2.5(5) | -4.0(5) | -8.9(5) |
| O22 | 15.4(6) | 20.2(7) | 16.6(6) | -1.2(5) | -4.2(5) | -6.8(5) |
| C10 | 19.3(9) | 21.1(10) | 17.5(9) | 2.3(8) | -5.4(7) | -8.9(8) |
| C11 | 17.6(8) | 20.2(10) | 16.8(9) | 2.6(7) | -1.8(7) | -10.1(7) |
| C12 | 15.2(8) | 21.3(10) | 14.7(9) | 1.2(7) | -1.2(7) | -10.4(7) |
| C13 | 16.8(9) | 18.6(9) | 20.8(9) | 0.4(7) | 0.2(7) | -7.7(7) |
| C14 | 24.1(10) | 22.6(10) | 17.8(9) | -4.4(8) | 2.6(7) | -11.1(8) |
| C15 | 30(1) | 29.7(11) | 14.8(9) | -0.1(8) | -2.3(7) | -16.6(9) |
| C16 | 26.8(10) | 23.3(10) | 17.8(10) | 4.5(8) | -6.3(8) | -13.9(8) |
| C20 | 17.6(9) | 14.0(9) | 17.0(9) | 3.4(7) | -6.2(7) | -6.2(7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C21 | 18.9(9) | 13.2(9) | 18.4(9) | 4.6(7) | -6.3(7) | -7.8(7) |
| C22 | 19.1(9) | 10.9(8) | 17.0(9) | 3.2(7) | -6.5(7) | -5.6(7) |
| C23 | 18.8(8) | 17.1(9) | 20.2(9) | 3.7(7) | -9.1(7) | -7.5(7) |
| C24 | 26.9(10) | 17.0(9) | 19.6(9) | 3.5(7) | -13.7(8) | -9.3(8) |
| C25 | 27.3(10) | 16.6(9) | 15.6(9) | 1.8(7) | -4.4(7) | -7.8(8) |
| C26 | 19.5(9) | 15.5(9) | 19.7(9) | 3.5(7) | -4.2(7) | -7.6(7) |

**Bond Lengths for compound 1.**

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| O1 | C40 | 1.421(2) | C48 | C49 | 1.317(3) |
| O2 | C30 | 1.425(2) | B1 | O11 | 1.468(3) |
| O2 | C36 | 1.359(2) | B1 | O12 | 1.443(2) |
| N1 | C31 | 1.316(3) | B1 | O21 | 1.508(3) |
| N1 | C39 | 1.365(3) | B1 | O22 | 1.451(2) |
| N2 | C41 | 1.517(2) | O10 | C10 | 1.209(3) |
| N2 | C45 | 1.508(2) | O11 | C10 | 1.338(2) |
| N2 | C46 | 1.511(2) | O12 | C12 | 1.351(2) |
| C31 | C32 | 1.410(3) | O20 | C20 | 1.228(2) |
| C32 | C33 | 1.369(3) | O21 | C20 | 1.320(2) |
| C33 | C34 | 1.427(3) | O22 | C22 | 1.348(2) |
| C33 | C40 | 1.520(2) | C10 | C11 | 1.484(3) |
| C34 | C35 | 1.421(3) | C11 | C12 | 1.405(3) |
| C34 | C39 | 1.425(2) | C11 | C16 | 1.395(3) |
| C35 | C36 | 1.372(3) | C12 | C13 | 1.395(3) |
| C36 | C37 | 1.418(3) | C13 | C14 | 1.385(3) |
| C37 | C38 | 1.361(3) | C14 | C15 | 1.396(3) |
| C38 | C39 | 1.421(3) | C15 | C16 | 1.383(3) |
| C40 | C41 | 1.535(3) | C20 | C21 | 1.476(3) |
| C41 | C42 | 1.547(3) | C21 | C22 | 1.403(3) |
| C42 | C43 | 1.530(3) | C21 | C26 | 1.400(3) |
| C43 | C44 | 1.532(2) | C22 | C23 | 1.396(3) |
| C43 | C47 | 1.548(2) | C23 | C24 | 1.388(3) |
| C44 | C45 | 1.538(3) | C24 | C25 | 1.399(3) |
| C46 | C47 | 1.540(3) | C25 | C26 | 1.380(3) |
| C47 | C48 | 1.506(3) | | | |

**Bond Angles for compound 1.**

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| C36 | O2 | C30 | 116.90(15) | C49 | C48 | C47 | 124.03(19) |
| C31 | N1 | C39 | 116.73(16) | O11 | B1 | O21 | 106.61(15) |
| C45 | N2 | C41 | 113.74(13) | O12 | B1 | O11 | 114.05(16) |
| C45 | N2 | C46 | 108.33(14) | O12 | B1 | O21 | 107.55(16) |
| C46 | N2 | C41 | 109.23(13) | O12 | B1 | O22 | 107.65(15) |
| N1 | C31 | C32 | 124.52(17) | O22 | B1 | O11 | 109.33(16) |
| C33 | C32 | C31 | 119.72(18) | O22 | B1 | O21 | 111.70(16) |
| C32 | C33 | C34 | 118.19(17) | C10 | O11 | B1 | 120.76(15) |
| C32 | C33 | C40 | 120.77(17) | C12 | O12 | B1 | 116.98(14) |
| C34 | C33 | C40 | 121.03(16) | C20 | O21 | B1 | 120.87(15) |
| C35 | C34 | C33 | 123.57(17) | C22 | O22 | B1 | 118.59(15) |
| C35 | C34 | C39 | 119.10(17) | O10 | C10 | O11 | 120.89(17) |
| C39 | C34 | C33 | 117.33(17) | O10 | C10 | C11 | 123.56(17) |
| C36 | C35 | C34 | 120.12(17) | O11 | C10 | C11 | 115.49(16) |
| O2 | C36 | C35 | 125.28(17) | C12 | C11 | C10 | 120.31(17) |
| O2 | C36 | C37 | 114.10(17) | C16 | C11 | C10 | 120.32(18) |
| C35 | C36 | C37 | 120.62(17) | C16 | C11 | C12 | 119.24(18) |
| C38 | C37 | C36 | 120.47(18) | O12 | C12 | C11 | 121.09(16) |
| C37 | C38 | C39 | 120.56(18) | O12 | C12 | C13 | 119.01(17) |
| N1 | C39 | C34 | 123.47(18) | C13 | C12 | C11 | 119.90(17) |
| N1 | C39 | C38 | 117.44(17) | C14 | C13 | C12 | 119.71(18) |
| C38 | C39 | C34 | 119.08(17) | C13 | C14 | C15 | 120.89(18) |
| O1 | C40 | C33 | 111.66(15) | C16 | C15 | C14 | 119.23(19) |
| O1 | C40 | C41 | 108.03(15) | C15 | C16 | C11 | 120.97(19) |
| C33 | C40 | C41 | 109.58(14) | O20 | C20 | O21 | 120.22(17) |
| N2 | C41 | C40 | 111.93(14) | O20 | C20 | C21 | 123.12(17) |
| N2 | C41 | C42 | 107.62(14) | O21 | C20 | C21 | 116.52(16) |
| C40 | C41 | C42 | 114.02(14) | C22 | C21 | C20 | 119.69(16) |
| C43 | C42 | C41 | 109.90(14) | C26 | C21 | C20 | 120.48(17) |
| C42 | C43 | C44 | 109.48(15) | C26 | C21 | C22 | 119.59(17) |
| C42 | C43 | C47 | 110.16(14) | O22 | C22 | C21 | 121.72(17) |
| C44 | C43 | C47 | 108.27(15) | O22 | C22 | C23 | 118.36(17) |
| C43 | C44 | C45 | 109.11(14) | C23 | C22 | C21 | 119.90(17) |
| N2 | C45 | C44 | 108.48(14) | C24 | C23 | C22 | 119.42(18) |
| N2 | C46 | C47 | 109.92(14) | C23 | C24 | C25 | 121.06(17) |
| C46 | C47 | C43 | 107.49(14) | C26 | C25 | C24 | 119.33(17) |
| C48 | C47 | C43 | 112.22(15) | C25 | C26 | C21 | 120.64(18) |
| C48 | C47 | C46 | 111.97(15) | | | | |

**Hydrogen Bonds for compound 1.**

| D | H | A | d(D-H)/Å | d(H-A)/Å | d(D-A)/Å | D-H-A/° |
|---|---|---|---|---|---|---|
| N2 | H2 | O20 | 0.91(3) | 1.91(3) | 2.790(2) | 160(2) |

**Torsion Angles for compound 1.**

| A | B | C | D | Angle/° | A | B | C | D | Angle/° |
|---|---|---|---|---|---|---|---|---|---|
| O1 | C40 | C41 | N2 | -76.48(18) | C46 | N2 | C45 | C44 | -68.16(17) |
| O1 | C40 | C41 | C42 | 45.98(19) | C46 | C47 | C48 | C49 | 143.28(19) |
| O2 | C36 | C37 | C38 | -178.00(17) | C47 | C43 | C44 | C45 | 54.52(19) |
| N1 | C31 | C32 | C33 | 1.3(3) | B1 | O11 | C10 | O10 | -166.43(18) |
| N2 | C41 | C42 | C43 | 5.48(18) | B1 | O11 | C10 | C11 | 16.1(2) |
| N2 | C46 | C47 | C43 | 9.34(18) | B1 | O12 | C12 | C11 | -15.3(2) |
| N2 | C46 | C47 | C48 | 133.02(15) | B1 | O12 | C12 | C13 | 164.47(17) |
| C30 | O2 | C36 | C35 | 3.5(3) | B1 | O21 | C20 | O20 | -163.05(17) |
| C30 | O2 | C36 | C37 | -176.96(16) | B1 | O21 | C20 | C21 | 21.2(2) |
| C31 | N1 | C39 | C34 | -1.8(3) | B1 | O22 | C22 | C21 | -12.6(3) |
| C31 | N1 | C39 | C38 | 178.30(17) | B1 | O22 | C22 | C23 | 168.82(17) |
| C31 | C32 | C33 | C34 | -1.7(3) | O10 | C10 | C11 | C12 | -170.76(19) |
| C31 | C32 | C33 | C40 | 177.24(16) | O10 | C10 | C11 | C16 | 5.2(3) |
| C32 | C33 | C34 | C35 | 179.85(17) | O11 | B1 | O12 | C12 | 36.2(2) |
| C32 | C33 | C34 | C39 | 0.5(3) | O11 | B1 | O21 | C20 | 80.74(19) |
| C32 | C33 | C40 | O1 | -21.1(2) | O11 | B1 | O22 | C22 | -84.8(2) |
| C32 | C33 | C40 | C41 | 98.57(19) | O11 | C10 | C11 | C12 | 6.7(3) |
| C33 | C34 | C35 | C36 | 179.89(17) | O11 | C10 | C11 | C16 | -177.40(16) |
| C33 | C34 | C39 | N1 | 1.3(3) | O12 | B1 | O11 | C10 | -37.7(2) |
| C33 | C34 | C39 | C38 | -178.78(16) | O12 | B1 | O21 | C20 | -156.54(15) |
| C33 | C40 | C41 | N2 | 161.67(15) | O12 | B1 | O22 | C22 | 150.85(15) |
| C33 | C40 | C41 | C42 | -75.87(18) | O12 | C12 | C13 | C14 | -177.87(17) |
| C34 | C33 | C40 | O1 | 157.83(16) | O20 | C20 | C21 | C22 | -173.46(18) |
| C34 | C33 | C40 | C41 | -82.5(2) | O20 | C20 | C21 | C26 | 0.9(3) |
| C34 | C35 | C36 | O2 | 178.60(17) | O21 | B1 | O11 | C10 | 80.88(19) |
| C34 | C35 | C36 | C37 | -0.9(3) | O21 | B1 | O12 | C12 | -81.82(19) |
| C35 | C34 | C39 | N1 | -178.08(16) | O21 | B1 | O22 | C22 | 33.0(2) |
| C35 | C34 | C39 | C38 | 1.8(3) | O21 | C20 | C21 | C22 | 2.2(2) |
| C35 | C36 | C37 | C38 | 1.6(3) | O21 | C20 | C21 | C26 | 176.54(16) |
| C36 | C37 | C38 | C39 | -0.5(3) | O22 | B1 | O11 | C10 | -158.23(15) |
| C37 | C38 | C39 | N1 | 178.70(17) | O22 | B1 | O12 | C12 | 157.68(15) |
| C37 | C38 | C39 | C34 | -1.2(3) | O22 | B1 | O21 | C20 | -38.6(2) |
| C39 | N1 | C31 | C32 | 0.5(3) | O22 | C22 | C23 | C24 | 179.94(16) |
| C39 | C34 | C35 | C36 | -0.8(3) | C10 | C11 | C12 | O12 | -7.0(3) |
| C40 | C33 | C34 | C35 | 0.9(3) | C10 | C11 | C12 | C13 | 173.18(17) |
| C40 | C33 | C34 | C39 | -178.44(16) | C10 | C11 | C16 | C15 | -174.44(18) |
| C40 | C41 | C42 | C43 | -119.31(16) | C11 | C12 | C13 | C14 | 1.9(3) |
| C41 | N2 | C45 | C44 | 53.50(19) | C12 | C11 | C16 | C15 | 1.5(3) |
| C41 | N2 | C46 | C47 | -68.07(17) | C12 | C13 | C14 | C15 | 0.3(3) |
| C41 | C42 | C43 | C44 | 55.84(18) | C13 | C14 | C15 | C16 | -1.5(3) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C41 | C42 | C43 | C47 | -63.11(18) | C14 | C15 | C16 | C11 | 0.6(3) |
| C42 | C43 | C44 | C45 | -65.59(19) | C16 | C11 | C12 | O12 | 176.98(17) |
| C42 | C43 | C47 | C46 | 53.80(18) | C16 | C11 | C12 | C13 | -2.8(3) |
| C42 | C43 | C47 | C48 | -69.7(2) | C20 | C21 | C22 | O22 | -6.8(3) |
| C43 | C44 | C45 | N2 | 10.6(2) | C20 | C21 | C22 | C23 | 171.74(17) |
| C43 | C47 | C48 | C49 | -95.7(2) | C20 | C21 | C26 | C25 | -172.65(17) |
| C44 | C43 | C47 | C46 | -65.89(18) | C21 | C22 | C23 | C24 | 1.3(3) |
| C44 | C43 | C47 | C48 | 170.58(15) | C22 | C21 | C26 | C25 | 1.7(3) |
| C45 | N2 | C41 | C40 | 63.24(19) | C22 | C23 | C24 | C25 | 1.0(3) |
| C45 | N2 | C41 | C42 | -62.80(18) | C23 | C24 | C25 | C26 | -1.9(3) |
| C45 | N2 | C46 | C47 | 56.31(18) | C24 | C25 | C26 | C21 | 0.6(3) |
| C46 | N2 | C41 | C40 | -175.61(15) | C26 | C21 | C22 | O22 | 178.80(17) |
| C46 | N2 | C41 | C42 | 58.36(17) | C26 | C21 | C22 | C23 | -2.7(3) |

**Hydrogen Atom Coordinates (Å×10$^4$) and Isotropic Displacement Parameters (Å$^2$×10$^3$) for compound 1.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| H1 | 3850(50) | 8150(40) | 4800(40) | 51(9) |
| H2 | 7910(40) | 5700(30) | 1740(20) | 24(6) |
| H30A | 11068 | 1842 | 2966 | 38 |
| H30B | 9308 | 1419 | 3547 | 38 |
| H30C | 11396 | 75 | 3048 | 38 |
| H31 | 6269 | 8728 | 8221 | 25 |
| H32 | 5534 | 9004 | 6194 | 22 |
| H35 | 8737 | 3922 | 4213 | 21 |
| H37 | 11442 | 1588 | 6928 | 25 |
| H38 | 10156 | 3804 | 8311 | 24 |
| H40 | 6268 | 5967 | 4006 | 19 |
| H41 | 9272 | 6254 | 3282 | 17 |
| H42A | 7086 | 9316 | 3924 | 19 |
| H42B | 9334 | 8523 | 3310 | 19 |
| H43 | 7738 | 10417 | 1950 | 19 |
| H44A | 5647 | 9995 | 897 | 22 |
| H44B | 4863 | 9987 | 2435 | 22 |
| H45A | 4976 | 7673 | 2017 | 20 |
| H45B | 6141 | 7555 | 537 | 20 |
| H46A | 9587 | 6301 | -64 | 20 |
| H46B | 10757 | 6013 | 1038 | 20 |
| H47 | 9085 | 8746 | -82 | 19 |
| H48 | 12029 | 7746 | 1298 | 23 |
| H49A | 11201 | 10041 | -425 | 33 |
| H49B | 13101 | 9341 | 166 | 33 |
| H13 | 516 | 8130 | 5331 | 23 |
| H14 | 924 | 8555 | 7384 | 27 |
| H15 | 3072 | 6568 | 8304 | 29 |
| H16 | 4720 | 4121 | 7190 | 26 |
| H23 | 1870 | 2798 | 283 | 22 |
| H24 | 3796 | 1548 | -1743 | 24 |
| H25 | 6998 | 1143 | -2342 | 25 |
| H26 | 8226 | 2115 | -948 | 22 |

**Table 2 Crystal data and structure refinement for Compound 2.**

| | |
|---|---|
| Identification code | lawr13CuLT3 |
| Empirical formula | $C_{29}H_{35}BN_2O_6$ |
| Formula weight | 518.40 |
| Temperature/K | 100.15 |
| Crystal system | monoclinic |
| Space group | $P2_1$ |
| a/Å | 11.5542(4) |
| b/Å | 18.7836(5) |
| c/Å | 11.9810(4) |
| α/° | 90 |
| β/° | 95.040(3) |
| γ/° | 90 |
| Volume/Å$^3$ | 2590.18(14) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.329 |
| μ/mm$^{-1}$ | 0.748 |
| F(000) | 1104.0 |
| Crystal size/mm$^3$ | 0.1 × 0.1 × 0.1 |
| Radiation | CuKα (λ = 1.54184) |
| 2Θ range for data collection/° | 7.408 to 134.946 |
| Index ranges | $-13 \leq h \leq 13$, $-22 \leq k \leq 22$, $-14 \leq l \leq 14$ |
| Reflections collected | 14696 |
| Independent reflections | 14696 [$R_{int}$ = ?, $R_{sigma}$ = 0.0286] |
| Data/restraints/parameters | 14696/1/694 |
| Completeness to theta = 66.5° | 100% |
| Goodness-of-fit on $F^2$ | 1.012 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0305, $wR_2$ = 0.0811 |
| Final R indexes [all data] | $R_1$ = 0.0342, $wR_2$ = 0.0826 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.17/-0.13 |
| Flack parameter | -0.01(8) |

**Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for compound 2. $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| N1 | 3444(2) | 6223.1(14) | 171.7(19) | 24.0(5) |
| N16 | 2001(2) | 6212.3(13) | 1883.2(19) | 22.7(5) |
| C31 | 3894(3) | 5799.2(18) | -765(2) | 30.5(7) |
| C32 | 4943(3) | 6146.7(19) | -1218(3) | 34.2(8) |
| C33 | 5907(3) | 6266(2) | -292(3) | 36.3(8) |
| C34 | 5453(3) | 6724.6(19) | 629(3) | 31.3(7) |
| C35 | 4401(3) | 6382.3(18) | 1102(2) | 26.8(7) |
| C36 | 2764(3) | 6870.3(16) | -240(2) | 25.5(6) |
| C37 | 2293(3) | 7277.6(17) | 726(3) | 25.4(6) |
| C38 | 3315(3) | 7506.3(17) | 1538(3) | 29.9(7) |
| C39 | 3900(3) | 6828.8(18) | 2020(2) | 27.4(6) |
| C40 | 3016(3) | 6413.1(17) | 2638(2) | 26.9(7) |
| C41 | 1206(3) | 5793.6(18) | 2517(2) | 27.6(7) |
| C42 | 136(3) | 5560.0(17) | 1784(3) | 28.9(7) |
| C43 | -508(3) | 6198.6(18) | 1267(3) | 28.7(7) |
| C44 | 327(3) | 6647.7(17) | 642(3) | 27.5(7) |
| C45 | 1423(3) | 6848.3(16) | 1373(2) | 23.7(6) |
| N1A | 899(3) | 3830.7(15) | 5162(2) | 26.5(6) |
| N16A | 2768(3) | 3900.5(14) | 6752(2) | 31.0(6) |
| C31A | 346(3) | 4140.9(19) | 4089(2) | 33.3(8) |
| C32A | -887(3) | 3881(2) | 3815(3) | 35.8(8) |
| C33A | -1628(4) | 4056(2) | 4776(3) | 42.3(9) |
| C34A | -1093(4) | 3730(2) | 5853(3) | 44.1(9) |
| C35A | 162(4) | 3970.5(18) | 6137(3) | 34.2(8) |
| C36A | 1224(3) | 3060.6(18) | 5055(3) | 33.9(7) |
| C37A | 1815(3) | 2774.0(18) | 6154(3) | 36.4(8) |
| C38A | 985(4) | 2850(2) | 7064(3) | 46.2(10) |
| C39A | 765(4) | 3645(2) | 7210(3) | 43.6(10) |
| C40A | 1919(4) | 3996(2) | 7577(3) | 41.8(9) |
| C41A | 3855(4) | 4264(2) | 7135(3) | 45.1(10) |
| C42A | 4757(4) | 4196(2) | 6304(3) | 46.6(10) |
| C43A | 5010(4) | 3420(2) | 6073(3) | 46.2(10) |
| C44A | 3866(3) | 3047(2) | 5690(3) | 39.9(8) |
| C45A | 2971(3) | 3136.9(18) | 6537(3) | 33.3(8) |
| O10 | 2118(2) | 4801.0(11) | 154.2(16) | 26.5(5) |
| O11 | 3717.6(19) | 4163.1(11) | 555.5(16) | 22.9(4) |
| O12 | 3659.7(19) | 2978.0(11) | 1393.4(17) | 24.0(5) |
| O20 | 7219(2) | 3776.5(13) | 597(2) | 35.1(5) |

| | | | | |
|---|---|---|---|---|
| O21 | 5427(2) | 3448.1(12) | 879.6(17) | 25.9(5) |
| O22 | 4486.3(19) | 3944.7(11) | 2447.4(16) | 22.3(4) |
| C10 | 2587(3) | 4255.2(16) | 545(2) | 21.0(6) |
| C11 | 1917(3) | 3662.0(15) | 983(2) | 21.5(6) |
| C12 | 2504(3) | 3051.3(16) | 1411(2) | 21.3(6) |
| C13 | 1866(3) | 2498.6(17) | 1841(2) | 25.9(6) |
| C14 | 672(3) | 2551.8(17) | 1842(2) | 27.6(7) |
| C15 | 86(3) | 3149.3(18) | 1401(2) | 28.2(7) |
| C16 | 710(3) | 3698.9(16) | 977(2) | 23.8(6) |
| C20 | 6340(3) | 3878.6(17) | 1062(2) | 25.5(6) |
| C21 | 6231(3) | 4459.0(17) | 1882(2) | 23.5(6) |
| C22 | 5313(3) | 4451.6(16) | 2569(2) | 22.0(6) |
| C23 | 5251(3) | 4968.8(17) | 3401(2) | 26.0(6) |
| C24 | 6108(3) | 5488.1(18) | 3540(3) | 30.9(7) |
| C25 | 7019(3) | 5508.0(19) | 2846(3) | 32.5(7) |
| C26 | 7076(3) | 4992.1(18) | 2027(3) | 28.4(6) |
| B1 | 4325(3) | 3625.6(18) | 1330(3) | 22.0(7) |
| O10A | 2558.2(19) | 5091.5(11) | 4921.1(16) | 23.7(4) |
| O11A | 1109.5(18) | 5668.6(11) | 5585.8(17) | 23.9(4) |
| O12A | 1360.9(19) | 6864.1(11) | 6390.9(19) | 26.5(5) |
| O20A | -2390(2) | 6355.9(12) | 5450.1(18) | 28.6(5) |
| O21A | -485.1(19) | 6446.5(11) | 5745.1(17) | 24.7(4) |
| O22A | 560.7(18) | 5934.3(11) | 7420.0(17) | 24.2(4) |
| C10A | 2216(3) | 5609.4(15) | 5410(2) | 19.2(6) |
| C11A | 2984(3) | 6207.9(16) | 5807(2) | 18.8(6) |
| C12A | 2500(3) | 6814.3(15) | 6262(2) | 19.9(6) |
| C13A | 3220(3) | 7394.4(15) | 6574(2) | 22.0(6) |
| C14A | 4392(3) | 7365.1(17) | 6440(2) | 25.2(7) |
| C15A | 4883(3) | 6754.2(17) | 6003(2) | 24.1(6) |
| C16A | 4171(3) | 6181.4(16) | 5690(2) | 22.9(6) |
| C20A | -1499(3) | 6189.2(16) | 5994(2) | 23.0(6) |
| C21A | -1461(3) | 5697.7(15) | 6966(2) | 20.5(6) |
| C22A | -425(3) | 5597.5(16) | 7648(2) | 21.7(6) |
| C23A | -412(3) | 5159.3(16) | 8588(2) | 24.7(6) |
| C24A | -1425(3) | 4825.8(18) | 8840(2) | 28.8(7) |
| C25A | -2465(3) | 4920.6(18) | 8164(3) | 29.7(7) |
| C26A | -2476(3) | 5355.8(18) | 7236(2) | 26.2(6) |
| B2 | 642(3) | 6230.8(18) | 6304(3) | 22.9(7) |

**Anisotropic Displacement Parameters ($Å^2×10^3$) for compound 2. The Anisotropic**

**displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.**

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| N1 | 28.4(15) | 19.4(14) | 24.3(11) | 2.3(10) | 4(1) | -2.1(10) |
| N16 | 24.5(14) | 19.0(13) | 25.0(11) | 1.9(9) | 3.6(10) | -0.5(10) |
| C31 | 40(2) | 27.0(17) | 25.7(14) | -0.3(12) | 9.2(13) | 2.2(14) |
| C32 | 43(2) | 30.0(19) | 32.3(15) | 6.6(13) | 16.3(14) | 4.8(15) |
| C33 | 34(2) | 35(2) | 41.7(17) | 12.0(15) | 12.5(15) | 2.1(15) |
| C34 | 26.2(18) | 28.7(18) | 39.5(16) | 3.8(14) | 5.3(13) | -2.4(14) |
| C35 | 25.9(17) | 26.3(17) | 28.3(14) | 5.1(12) | 2.2(12) | -1.8(13) |
| C36 | 28.9(17) | 22.7(16) | 25.0(13) | 8.2(11) | 3.2(12) | -0.8(12) |
| C37 | 25.8(17) | 19.2(15) | 31.0(14) | 2.4(11) | 1.6(12) | 1.1(12) |
| C38 | 29.2(18) | 23.5(17) | 36.9(15) | -1.4(12) | 2.9(13) | -4.5(13) |
| C39 | 26.7(17) | 27.1(17) | 28.3(14) | -3.7(12) | 0.7(12) | -1.7(13) |
| C40 | 28.1(17) | 30.2(17) | 22.0(13) | 2.6(11) | -0.3(12) | 3.7(13) |
| C41 | 28.4(17) | 27.1(17) | 28.5(14) | 7.7(12) | 8.6(12) | 1.7(13) |
| C42 | 29.9(18) | 21.5(16) | 36.7(15) | 0.6(12) | 10.5(13) | -3.7(13) |
| C43 | 26.9(18) | 24.6(18) | 34.8(14) | -0.5(12) | 4.0(12) | -2.5(13) |
| C44 | 29.2(17) | 20.9(16) | 32.0(14) | 4.1(12) | 0.0(13) | -1.3(12) |
| C45 | 28.6(17) | 17.8(15) | 24.8(13) | -0.3(11) | 2.9(12) | -0.3(12) |
| N1A | 32.7(16) | 21.8(14) | 26.3(11) | -5.5(10) | 9.8(11) | -6.5(11) |
| N16A | 52.1(19) | 17.6(14) | 23.0(11) | -1.5(9) | 0.7(12) | -1.7(13) |
| C31A | 41(2) | 32.5(19) | 26.1(14) | -1.9(13) | 1.8(13) | -12.3(15) |
| C32A | 33(2) | 32.1(19) | 43.2(17) | -11.2(14) | 6.8(15) | -8.1(15) |
| C33A | 38(2) | 34(2) | 56(2) | -10.8(16) | 13.4(17) | -4.2(17) |
| C34A | 53(3) | 28.9(19) | 55(2) | -1.8(16) | 31.7(19) | -1.3(17) |
| C35A | 53(2) | 19.9(16) | 32.9(15) | -3.3(12) | 19.4(15) | 2.5(14) |
| C36A | 32.3(19) | 24.7(18) | 46.5(17) | -15.4(14) | 13.3(15) | -6.9(14) |
| C37A | 46(2) | 13.9(16) | 51.5(19) | -3.5(13) | 18.0(17) | -2.3(14) |
| C38A | 57(3) | 27(2) | 58(2) | 13.5(16) | 27(2) | 3.2(18) |
| C39A | 68(3) | 32(2) | 34.9(16) | 7.0(14) | 26.7(18) | 11.0(18) |
| C40A | 72(3) | 29.4(19) | 23.6(14) | -3.7(12) | 3.8(16) | 10.1(18) |
| C41A | 69(3) | 25.2(19) | 36.7(17) | -4.2(14) | -21.4(18) | -2.5(18) |
| C42A | 42(2) | 37(2) | 56(2) | 13.8(17) | -20.5(18) | -13.1(17) |
| C43A | 44(2) | 45(2) | 48(2) | 2.4(17) | -8.0(17) | -3.3(18) |
| C44A | 37(2) | 40(2) | 42.3(18) | -11.5(15) | 4.2(16) | -3.9(16) |
| C45A | 47(2) | 20.1(18) | 33.1(15) | -0.7(12) | 6.0(15) | 1.5(15) |
| O10 | 30.0(12) | 18.9(11) | 30.1(10) | 3.9(8) | -1.1(9) | 1.1(9) |
| O11 | 23.8(11) | 19.2(11) | 25.7(9) | 4.2(8) | 2.7(8) | -1.5(8) |
| O12 | 21.8(12) | 16.9(11) | 33(1) | 2.9(8) | 0.8(8) | 0.6(8) |
| O20 | 27.9(13) | 32.8(14) | 47.1(12) | -7.8(10) | 16.1(11) | -0.6(10) |
| O21 | 24.1(12) | 21.6(11) | 32.4(10) | -3.6(8) | 5.4(9) | -0.4(9) |
| O22 | 22.9(11) | 19.4(10) | 25.3(9) | 2.2(7) | 5.7(8) | 0.0(8) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C10 | 27.1(16) | 15.9(14) | 19.8(12) | -3.2(10) | 0.5(11) | -1.8(11) |
| C11 | 29.9(17) | 15.2(15) | 19.4(11) | -2.5(10) | 3.1(11) | -3.1(12) |
| C12 | 27.3(17) | 16.2(14) | 20.6(12) | -1.2(10) | 3.2(11) | -0.7(12) |
| C13 | 34.1(19) | 17.3(15) | 26.7(13) | 1.0(11) | 4.3(12) | -2.8(13) |
| C14 | 32.5(19) | 22.6(16) | 28.5(13) | -2.7(12) | 8.0(12) | -9.1(14) |
| C15 | 25.2(18) | 30.8(18) | 29.5(14) | -7.5(12) | 7.2(12) | -4.8(13) |
| C16 | 27.3(17) | 18.5(15) | 25.4(13) | -4.6(11) | 0.3(11) | 2.2(12) |
| C20 | 22.0(17) | 22.3(17) | 32.7(14) | 0.6(12) | 5.5(12) | 1.6(12) |
| C21 | 21.1(16) | 22.5(16) | 27.1(13) | -0.1(11) | 2.9(11) | 1.3(12) |
| C22 | 19.4(15) | 20.6(15) | 25.8(13) | 3.2(11) | -0.1(11) | 1.2(12) |
| C23 | 25.7(16) | 26.4(17) | 26.2(13) | 0.3(11) | 4.9(12) | 1.1(13) |
| C24 | 31.3(18) | 28.7(18) | 32.3(15) | -7.7(12) | 0.0(13) | -0.8(14) |
| C25 | 27.6(17) | 29.2(18) | 40.3(16) | -4.0(13) | 1.1(13) | -5.6(14) |
| C26 | 22.6(16) | 28.6(17) | 34.8(14) | -0.8(12) | 7.0(12) | -3.2(13) |
| B1 | 22.1(18) | 16.9(17) | 26.9(15) | 1.5(12) | 1.8(13) | -0.5(13) |
| O10A | 27.0(12) | 17.7(10) | 26.7(9) | -3.2(8) | 3.5(8) | 0.8(8) |
| O11A | 21.1(11) | 17.1(11) | 34(1) | -3.6(8) | 5.0(8) | -2.9(8) |
| O12A | 19.8(12) | 15.3(11) | 45.6(12) | -4.3(9) | 8.9(9) | 0.3(8) |
| O20A | 19.8(11) | 30.4(13) | 34.9(11) | 6.3(9) | -0.4(9) | 1.0(9) |
| O21A | 18.7(11) | 21.7(11) | 34(1) | 4.7(8) | 4.2(9) | -0.9(8) |
| O22A | 16.9(10) | 23.5(12) | 32(1) | -0.9(8) | 0.4(8) | -0.7(8) |
| C10A | 22.8(15) | 15.8(14) | 18.7(12) | 2.3(10) | 0.2(10) | -0.1(11) |
| C11A | 22.9(15) | 16.8(14) | 17.0(11) | 1.5(10) | 3.6(10) | -1.5(11) |
| C12A | 20.8(16) | 15.7(14) | 23.2(12) | 1.4(10) | 1.9(11) | -0.4(12) |
| C13A | 24.1(16) | 15.6(15) | 26.3(13) | -1.3(10) | 2.8(12) | 0.5(11) |
| C14A | 26.0(17) | 20.3(16) | 28.9(14) | 0.5(11) | -0.3(12) | -6.4(12) |
| C15A | 16.6(15) | 25.3(16) | 30.8(14) | 1.3(12) | 3.3(11) | -2.2(12) |
| C16A | 26.0(16) | 20.2(16) | 23.0(12) | -0.6(11) | 4.2(11) | 3.0(12) |
| C20A | 22.5(17) | 17.7(15) | 28.9(13) | -5.2(11) | 3.1(12) | 0.8(12) |
| C21A | 20.6(15) | 16.1(14) | 24.9(12) | -2.4(10) | 1.9(11) | 1.3(11) |
| C22A | 22.6(16) | 16.2(14) | 26.9(13) | -6.3(10) | 4.8(11) | -0.5(11) |
| C23A | 27.2(17) | 23.5(17) | 23.0(13) | -3.4(11) | -0.3(12) | 5.6(12) |
| C24A | 33.8(19) | 27.4(17) | 25.9(13) | 2.4(11) | 7.0(12) | 2.2(14) |
| C25A | 22.2(17) | 34.0(19) | 33.9(15) | 1.4(13) | 8.7(13) | -6.0(13) |
| C26A | 18.8(15) | 28.2(17) | 31.1(15) | -0.9(12) | -0.3(12) | 0.3(12) |
| B2 | 18.4(18) | 16.7(17) | 34.3(16) | -2.7(13) | 6.3(13) | -2.9(13) |

**Bond Lengths for compound 2.**

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| N1 | C31 | 1.506(4) | O12 | B1 | 1.445(4) |
| N1 | C35 | 1.529(4) | O20 | C20 | 1.216(4) |
| N1 | C36 | 1.506(4) | O21 | C20 | 1.332(4) |
| N16 | C40 | 1.466(4) | O21 | B1 | 1.464(4) |
| N16 | C41 | 1.470(4) | O22 | C22 | 1.347(4) |
| N16 | C45 | 1.475(4) | O22 | B1 | 1.463(4) |
| C31 | C32 | 1.518(5) | C10 | C11 | 1.479(4) |
| C32 | C33 | 1.518(5) | C11 | C12 | 1.406(4) |
| C33 | C34 | 1.529(5) | C11 | C16 | 1.395(5) |
| C34 | C35 | 1.527(4) | C12 | C13 | 1.398(4) |
| C35 | C39 | 1.536(4) | C13 | C14 | 1.383(5) |
| C36 | C37 | 1.528(4) | C14 | C15 | 1.390(5) |
| C37 | C38 | 1.525(4) | C15 | C16 | 1.382(5) |
| C37 | C45 | 1.548(4) | C20 | C21 | 1.480(4) |
| C38 | C39 | 1.530(5) | C21 | C22 | 1.400(4) |
| C39 | C40 | 1.528(4) | C21 | C26 | 1.399(5) |
| C41 | C42 | 1.517(5) | C22 | C23 | 1.398(4) |
| C42 | C43 | 1.515(5) | C23 | C24 | 1.390(5) |
| C43 | C44 | 1.526(4) | C24 | C25 | 1.398(5) |
| C44 | C45 | 1.523(4) | C25 | C26 | 1.385(5) |
| N1A | C31A | 1.502(4) | O10A | C10A | 1.219(4) |
| N1A | C35A | 1.528(4) | O11A | C10A | 1.318(4) |
| N1A | C36A | 1.503(4) | O11A | B2 | 1.493(4) |
| N16A | C40A | 1.463(5) | O12A | C12A | 1.342(4) |
| N16A | C41A | 1.466(5) | O12A | B2 | 1.449(4) |
| N16A | C45A | 1.480(4) | O20A | C20A | 1.211(4) |
| C31A | C32A | 1.515(5) | O21A | C20A | 1.325(4) |
| C32A | C33A | 1.530(5) | O21A | B2 | 1.468(4) |
| C33A | C34A | 1.511(6) | O22A | C22A | 1.352(4) |
| C34A | C35A | 1.529(6) | O22A | B2 | 1.459(4) |
| C35A | C39A | 1.535(5) | C10A | C11A | 1.485(4) |
| C36A | C37A | 1.527(5) | C11A | C12A | 1.400(4) |
| C37A | C38A | 1.521(5) | C11A | C16A | 1.392(4) |
| C37A | C45A | 1.533(5) | C12A | C13A | 1.402(4) |
| C38A | C39A | 1.527(5) | C13A | C14A | 1.378(5) |
| C39A | C40A | 1.518(6) | C14A | C15A | 1.402(4) |
| C41A | C42A | 1.509(6) | C15A | C16A | 1.386(4) |
| C42A | C43A | 1.518(6) | C20A | C21A | 1.483(4) |
| C43A | C44A | 1.530(5) | C21A | C22A | 1.402(4) |
| C44A | C45A | 1.520(5) | C21A | C26A | 1.400(4) |

| | | | | | |
|---|---|---|---|---|---|
| O10 | C10 | 1.233(4) | C22A | C23A | 1.394(4) |
| O11 | C10 | 1.316(4) | C23A | C24A | 1.385(5) |
| O11 | B1 | 1.503(4) | C24A | C25A | 1.401(5) |
| O12 | C12 | 1.344(4) | C25A | C26A | 1.379(5) |

**Bond Angles for compound 2.**

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| C31 | N1 | C35 | 111.8(3) | C12 | C11 | C10 | 119.5(3) |
| C31 | N1 | C36 | 112.7(2) | C16 | C11 | C10 | 121.0(3) |
| C36 | N1 | C35 | 113.8(2) | C16 | C11 | C12 | 119.5(3) |
| C40 | N16 | C41 | 108.7(2) | O12 | C12 | C11 | 121.7(3) |
| C40 | N16 | C45 | 110.9(2) | O12 | C12 | C13 | 119.1(3) |
| C41 | N16 | C45 | 111.5(2) | C13 | C12 | C11 | 119.1(3) |
| N1 | C31 | C32 | 112.2(3) | C14 | C13 | C12 | 120.3(3) |
| C31 | C32 | C33 | 111.1(3) | C13 | C14 | C15 | 120.7(3) |
| C32 | C33 | C34 | 109.5(3) | C16 | C15 | C14 | 119.4(3) |
| C35 | C34 | C33 | 111.4(3) | C15 | C16 | C11 | 121.0(3) |
| N1 | C35 | C39 | 109.6(3) | O20 | C20 | O21 | 120.7(3) |
| C34 | C35 | N1 | 111.1(2) | O20 | C20 | C21 | 122.9(3) |
| C34 | C35 | C39 | 113.4(3) | O21 | C20 | C21 | 116.3(3) |
| N1 | C36 | C37 | 111.5(2) | C22 | C21 | C20 | 119.7(3) |
| C36 | C37 | C45 | 114.2(3) | C26 | C21 | C20 | 120.7(3) |
| C38 | C37 | C36 | 108.5(3) | C26 | C21 | C22 | 119.4(3) |
| C38 | C37 | C45 | 109.1(2) | O22 | C22 | C21 | 120.7(3) |
| C37 | C38 | C39 | 107.3(3) | O22 | C22 | C23 | 119.2(3) |
| C38 | C39 | C35 | 111.4(2) | C23 | C22 | C21 | 120.1(3) |
| C40 | C39 | C35 | 112.2(3) | C24 | C23 | C22 | 119.5(3) |
| C40 | C39 | C38 | 108.4(3) | C23 | C24 | C25 | 120.9(3) |
| N16 | C40 | C39 | 111.4(2) | C26 | C25 | C24 | 119.2(3) |
| N16 | C41 | C42 | 111.7(2) | C25 | C26 | C21 | 120.9(3) |
| C43 | C42 | C41 | 110.7(3) | O12 | B1 | O11 | 112.1(3) |
| C42 | C43 | C44 | 109.2(3) | O12 | B1 | O21 | 108.1(3) |
| C45 | C44 | C43 | 112.6(2) | O12 | B1 | O22 | 108.8(2) |
| N16 | C45 | C37 | 109.8(3) | O21 | B1 | O11 | 107.4(2) |
| N16 | C45 | C44 | 111.2(3) | O22 | B1 | O11 | 107.7(2) |
| C44 | C45 | C37 | 112.6(2) | O22 | B1 | O21 | 112.7(3) |
| C31A | N1A | C35A | 111.3(3) | C10A | O11A | B2 | 123.8(2) |
| C36A | N1A | C31A | 113.0(3) | C12A | O12A | B2 | 119.8(2) |
| C36A | N1A | C35A | 113.0(2) | C20A | O21A | B2 | 124.3(2) |
| C40A | N16A | C41A | 109.7(3) | C22A | O22A | B2 | 119.1(2) |
| C40A | N16A | C45A | 111.3(3) | O10A | C10A | O11A | 120.3(3) |
| C41A | N16A | C45A | 111.2(3) | O10A | C10A | C11A | 123.2(3) |
| N1A | C31A | C32A | 112.4(3) | O11A | C10A | C11A | 116.5(2) |
| C31A | C32A | C33A | 110.2(3) | C12A | C11A | C10A | 119.5(3) |
| C34A | C33A | C32A | 110.0(3) | C16A | C11A | C10A | 120.5(3) |
| C33A | C34A | C35A | 112.3(3) | C16A | C11A | C12A | 119.9(3) |
| N1A | C35A | C34A | 111.1(3) | O12A | C12A | C11A | 122.1(3) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N1A | C35A | C39A | 109.2(3) | O12A | C12A | C13A | 118.7(3) |
| C34A | C35A | C39A | 114.9(3) | C11A | C12A | C13A | 119.2(3) |
| N1A | C36A | C37A | 111.2(3) | C14A | C13A | C12A | 120.3(3) |
| C36A | C37A | C45A | 114.4(3) | C13A | C14A | C15A | 120.7(3) |
| C38A | C37A | C36A | 108.8(3) | C16A | C15A | C14A | 119.1(3) |
| C38A | C37A | C45A | 109.4(3) | C15A | C16A | C11A | 120.8(3) |
| C37A | C38A | C39A | 107.2(3) | O20A | C20A | O21A | 120.8(3) |
| C38A | C39A | C35A | 111.2(3) | O20A | C20A | C21A | 123.2(3) |
| C40A | C39A | C35A | 113.1(3) | O21A | C20A | C21A | 116.0(3) |
| C40A | C39A | C38A | 107.9(4) | C22A | C21A | C20A | 120.4(3) |
| N16A | C40A | C39A | 112.0(3) | C26A | C21A | C20A | 120.0(3) |
| N16A | C41A | C42A | 112.1(3) | C26A | C21A | C22A | 119.5(3) |
| C41A | C42A | C43A | 110.8(3) | O22A | C22A | C21A | 120.7(3) |
| C42A | C43A | C44A | 108.7(3) | O22A | C22A | C23A | 119.3(3) |
| C45A | C44A | C43A | 111.6(3) | C23A | C22A | C21A | 119.9(3) |
| N16A | C45A | C37A | 109.6(3) | C24A | C23A | C22A | 119.6(3) |
| N16A | C45A | C44A | 110.6(3) | C23A | C24A | C25A | 121.0(3) |
| C44A | C45A | C37A | 112.1(3) | C26A | C25A | C24A | 119.2(3) |
| C10 | O11 | B1 | 120.2(2) | C25A | C26A | C21A | 120.7(3) |
| C12 | O12 | B1 | 116.7(2) | O12A | B2 | O11A | 112.8(3) |
| C20 | O21 | B1 | 120.2(2) | O12A | B2 | O21A | 106.6(3) |
| C22 | O22 | B1 | 114.9(2) | O12A | B2 | O22A | 109.3(3) |
| O10 | C10 | O11 | 121.0(3) | O21A | B2 | O11A | 106.5(2) |
| O10 | C10 | C11 | 122.3(3) | O22A | B2 | O11A | 108.3(3) |
| O11 | C10 | C11 | 116.6(3) | O22A | B2 | O21A | 113.4(3) |

**Hydrogen Bonds for compound 2.**

| D | H | A | d(D-H)/Å | d(H-A)/Å | d(D-A)/Å | D-H-A/° |
|---|---|---|---|---|---|---|
| N1 | H1 | N16 | 1.01(5) | 2.01(5) | 2.754(3) | 128(4) |
| N1A | H1A | N16A | 0.96(4) | 2.07(4) | 2.754(4) | 127(3) |

**Torsion Angles for compound 2.**

| A | B | C | D | Angle/° | A | B | C | D | Angle/° |
|---|---|---|---|---|---|---|---|---|---|
| N1 | C31 | C32 | C33 | 56.3(4) | O21 | C20 | C21 | C26 | -171.8(3) |
| N1 | C35 | C39 | C38 | -55.1(3) | O22 | C22 | C23 | C24 | 179.3(3) |
| N1 | C35 | C39 | C40 | 66.8(3) | C10 | O11 | B1 | O12 | 40.4(4) |
| N1 | C36 | C37 | C38 | 59.4(3) | C10 | O11 | B1 | O21 | 159.0(2) |
| N1 | C36 | C37 | C45 | -62.5(3) | C10 | O11 | B1 | O22 | -79.3(3) |
| N16 | C41 | C42 | C43 | -58.1(3) | C10 | C11 | C12 | O12 | -2.7(4) |
| C31 | N1 | C35 | C34 | 52.6(3) | C10 | C11 | C12 | C13 | 178.9(2) |
| C31 | N1 | C35 | C39 | 178.7(2) | C10 | C11 | C16 | C15 | -179.0(2) |
| C31 | N1 | C36 | C37 | 178.5(3) | C11 | C12 | C13 | C14 | 0.2(4) |
| C31 | C32 | C33 | C34 | -57.6(4) | C12 | O12 | B1 | O11 | -39.6(3) |
| C32 | C33 | C34 | C35 | 57.6(4) | C12 | O12 | B1 | O21 | -157.8(2) |
| C33 | C34 | C35 | N1 | -55.2(4) | C12 | O12 | B1 | O22 | 79.5(3) |
| C33 | C34 | C35 | C39 | -179.1(3) | C12 | C11 | C16 | C15 | 1.1(4) |
| C34 | C35 | C39 | C38 | 69.7(3) | C12 | C13 | C14 | C15 | 1.0(4) |
| C34 | C35 | C39 | C40 | -168.5(3) | C13 | C14 | C15 | C16 | -1.1(4) |
| C35 | N1 | C31 | C32 | -53.4(3) | C14 | C15 | C16 | C11 | 0.1(4) |
| C35 | N1 | C36 | C37 | -52.8(3) | C16 | C11 | C12 | O12 | 177.2(2) |
| C35 | C39 | C40 | N16 | -63.2(3) | C16 | C11 | C12 | C13 | -1.2(4) |
| C36 | N1 | C31 | C32 | 76.4(3) | C20 | O21 | B1 | O11 | 80.5(3) |
| C36 | N1 | C35 | C34 | -76.6(3) | C20 | O21 | B1 | O12 | -158.4(2) |
| C36 | N1 | C35 | C39 | 49.5(3) | C20 | O21 | B1 | O22 | -38.1(4) |
| C36 | C37 | C38 | C39 | -63.8(3) | C20 | C21 | C22 | O22 | -4.0(4) |
| C36 | C37 | C45 | N16 | 61.6(3) | C20 | C21 | C22 | C23 | 175.4(3) |
| C36 | C37 | C45 | C44 | -62.9(4) | C20 | C21 | C26 | C25 | -175.5(3) |
| C37 | C38 | C39 | C35 | 63.2(3) | C21 | C22 | C23 | C24 | -0.1(5) |
| C37 | C38 | C39 | C40 | -60.8(3) | C22 | O22 | B1 | O11 | -73.3(3) |
| C38 | C37 | C45 | N16 | -60.0(3) | C22 | O22 | B1 | O12 | 164.9(2) |
| C38 | C37 | C45 | C44 | 175.5(3) | C22 | O22 | B1 | O21 | 45.0(3) |
| C38 | C39 | C40 | N16 | 60.3(3) | C22 | C21 | C26 | C25 | 0.5(5) |
| C40 | N16 | C41 | C42 | -179.4(3) | C22 | C23 | C24 | C25 | 1.2(5) |
| C40 | N16 | C45 | C37 | 58.1(3) | C23 | C24 | C25 | C26 | -1.4(5) |
| C40 | N16 | C45 | C44 | -176.6(2) | C24 | C25 | C26 | C21 | 0.5(5) |
| C41 | N16 | C40 | C39 | 178.0(3) | C26 | C21 | C22 | O22 | 179.9(3) |
| C41 | N16 | C45 | C37 | 179.4(2) | C26 | C21 | C22 | C23 | -0.7(4) |
| C41 | N16 | C45 | C44 | -55.3(3) | B1 | O11 | C10 | O10 | 160.9(2) |
| C41 | C42 | C43 | C44 | 54.7(3) | B1 | O11 | C10 | C11 | -21.4(4) |
| C42 | C43 | C44 | C45 | -53.4(3) | B1 | O12 | C12 | C11 | 23.0(4) |
| C43 | C44 | C45 | N16 | 53.9(3) | B1 | O12 | C12 | C13 | -158.6(3) |
| C43 | C44 | C45 | C37 | 177.6(3) | B1 | O21 | C20 | O20 | -172.3(3) |
| C45 | N16 | C40 | C39 | -59.1(3) | B1 | O21 | C20 | C21 | 9.9(4) |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C45 | N16 | C41 | C42 | 58.0(3) | B1 | O22 | C22 | C21 | -25.1(4) |
| C45 | C37 | C38 | C39 | 61.1(3) | B1 | O22 | C22 | C23 | 155.6(3) |
| N1A | C31A | C32A | C33A | 57.3(4) | O10A | C10A | C11A | C12A | 173.7(3) |
| N1A | C35A | C39A | C38A | -56.6(4) | O10A | C10A | C11A | C16A | -3.8(4) |
| N1A | C35A | C39A | C40A | 65.0(4) | O11A | C10A | C11A | C12A | -4.6(3) |
| N1A | C36A | C37A | C38A | 59.7(4) | O11A | C10A | C11A | C16A | 177.9(2) |
| N1A | C36A | C37A | C45A | -63.0(4) | O12A | C12A | C13A | C14A | -179.2(3) |
| N16A | C41A | C42A | C43A | -57.5(4) | O20A | C20A | C21A | C22A | -171.7(3) |
| C31A | N1A | C35A | C34A | 52.3(4) | O20A | C20A | C21A | C26A | 5.3(4) |
| C31A | N1A | C35A | C39A | -179.9(3) | O21A | C20A | C21A | C22A | 8.0(4) |
| C31A | N1A | C36A | C37A | 178.3(3) | O21A | C20A | C21A | C26A | -175.0(3) |
| C31A | C32A | C33A | C34A | -57.1(4) | O22A | C22A | C23A | C24A | 178.5(3) |
| C32A | C33A | C34A | C35A | 56.4(4) | C10A | O11A | B2 | O12A | 25.2(4) |
| C33A | C34A | C35A | N1A | -54.1(4) | C10A | O11A | B2 | O21A | 141.8(2) |
| C33A | C34A | C35A | C39A | -178.7(3) | C10A | O11A | B2 | O22A | -95.9(3) |
| C34A | C35A | C39A | C38A | 69.0(4) | C10A | C11A | C12A | O12A | 2.5(4) |
| C34A | C35A | C39A | C40A | -169.4(3) | C10A | C11A | C12A | C13A | -176.3(2) |
| C35A | N1A | C31A | C32A | -54.9(4) | C10A | C11A | C16A | C15A | 176.5(2) |
| C35A | N1A | C36A | C37A | -54.2(4) | C11A | C12A | C13A | C14A | -0.4(4) |
| C35A | C39A | C40A | N16A | -63.5(4) | C12A | O12A | B2 | O11A | -26.4(4) |
| C36A | N1A | C31A | C32A | 73.5(4) | C12A | O12A | B2 | O21A | -143.0(2) |
| C36A | N1A | C35A | C34A | -76.1(4) | C12A | O12A | B2 | O22A | 94.1(3) |
| C36A | N1A | C35A | C39A | 51.7(4) | C12A | C11A | C16A | C15A | -1.1(4) |
| C36A | C37A | C38A | C39A | -63.2(4) | C12A | C13A | C14A | C15A | -0.7(4) |
| C36A | C37A | C45A | N16A | 62.5(3) | C13A | C14A | C15A | C16A | 1.0(4) |
| C36A | C37A | C45A | C44A | -60.8(4) | C14A | C15A | C16A | C11A | -0.1(4) |
| C37A | C38A | C39A | C35A | 63.2(5) | C16A | C11A | C12A | O12A | -179.9(3) |
| C37A | C38A | C39A | C40A | -61.3(4) | C16A | C11A | C12A | C13A | 1.3(4) |
| C38A | C37A | C45A | N16A | -59.8(4) | C20A | O21A | B2 | O11A | 96.1(3) |
| C38A | C37A | C45A | C44A | 176.9(3) | C20A | O21A | B2 | O12A | -143.2(3) |
| C38A | C39A | C40A | N16A | 60.0(4) | C20A | O21A | B2 | O22A | -22.9(4) |
| C40A | N16A | C41A | C42A | -178.7(3) | C20A | C21A | C22A | O22A | -1.4(4) |
| C40A | N16A | C45A | C37A | 56.6(3) | C20A | C21A | C22A | C23A | 177.1(3) |
| C40A | N16A | C45A | C44A | -179.3(3) | C20A | C21A | C26A | C25A | -177.3(3) |
| C41A | N16A | C40A | C39A | 178.7(3) | C21A | C22A | C23A | C24A | 0.0(4) |
| C41A | N16A | C45A | C37A | 179.2(3) | C22A | O22A | B2 | O11A | -89.1(3) |
| C41A | N16A | C45A | C44A | -56.6(4) | C22A | O22A | B2 | O12A | 147.7(2) |
| C41A | C42A | C43A | C44A | 55.1(4) | C22A | O22A | B2 | O21A | 28.9(4) |
| C42A | C43A | C44A | C45A | -55.4(4) | C22A | C21A | C26A | C25A | -0.2(4) |
| C43A | C44A | C45A | N16A | 56.5(4) | C22A | C23A | C24A | C25A | 0.1(5) |
| C43A | C44A | C45A | C37A | 179.2(3) | C23A | C24A | C25A | C26A | -0.3(5) |
| C45A | N16A | C40A | C39A | -57.8(4) | C24A | C25A | C26A | C21A | 0.3(5) |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C45A | N16A | C41A | C42A | 57.7(4) | C26A | C21A | C22A | O22A | -178.5(3) |
| C45A | C37A | C38A | C39A | 62.4(4) | C26A | C21A | C22A | C23A | 0.1(4) |
| O10 | C10 | C11 | C12 | 179.5(3) | B2 | O11A | C10A | O10A | 171.6(3) |
| O10 | C10 | C11 | C16 | -0.4(4) | B2 | O11A | C10A | C11A | -10.1(4) |
| O11 | C10 | C11 | C12 | 1.9(4) | B2 | O12A | C12A | C11A | 14.3(4) |
| O11 | C10 | C11 | C16 | -178.0(2) | B2 | O12A | C12A | C13A | -167.0(3) |
| O12 | C12 | C13 | C14 | -178.3(3) | B2 | O21A | C20A | O20A | -175.1(3) |
| O20 | C20 | C21 | C22 | -165.5(3) | B2 | O21A | C20A | C21A | 5.2(4) |
| O20 | C20 | C21 | C26 | 10.5(5) | B2 | O22A | C22A | C21A | -17.9(4) |
| O21 | C20 | C21 | C22 | 12.2(4) | B2 | O22A | C22A | C23A | 163.5(3) |

**Hydrogen Atom Coordinates (Å×10$^4$) and Isotropic Displacement Parameters (Å$^2$×10$^3$) for compound 2.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| H1 | 2840(40) | 5940(30) | 540(40) | 53(13) |
| H31A | 3269 | 5749 | -1381 | 37 |
| H31B | 4110 | 5316 | -489 | 37 |
| H32A | 4711 | 6609 | -1566 | 41 |
| H32B | 5233 | 5839 | -1804 | 41 |
| H33A | 6571 | 6507 | -600 | 44 |
| H33B | 6180 | 5802 | 24 | 44 |
| H34A | 6077 | 6791 | 1241 | 38 |
| H34B | 5233 | 7199 | 321 | 38 |
| H35 | 4660 | 5917 | 1445 | 32 |
| H36A | 2109 | 6721 | -778 | 31 |
| H36B | 3273 | 7188 | -640 | 31 |
| H37 | 1891 | 7715 | 415 | 30 |
| H38A | 3040 | 7800 | 2147 | 36 |
| H38B | 3873 | 7791 | 1141 | 36 |
| H39 | 4555 | 6971 | 2576 | 33 |
| H40A | 3388 | 5978 | 2970 | 32 |
| H40B | 2762 | 6708 | 3256 | 32 |
| H41A | 964 | 6083 | 3147 | 33 |
| H41B | 1619 | 5368 | 2837 | 33 |
| H42A | 371 | 5244 | 1182 | 35 |
| H42B | -385 | 5288 | 2239 | 35 |
| H43A | -824 | 6487 | 1861 | 34 |
| H43B | -1164 | 6037 | 741 | 34 |
| H44A | 547 | 6379 | -18 | 33 |
| H44B | -75 | 7088 | 367 | 33 |
| H45 | 1186 | 7156 | 1995 | 28 |
| H1A | 1630(40) | 4060(20) | 5340(30) | 36(10) |
| H31C | 817 | 4012 | 3468 | 40 |
| H31D | 341 | 4666 | 4151 | 40 |
| H32C | -884 | 3360 | 3691 | 43 |
| H32D | -1225 | 4111 | 3118 | 43 |
| H33C | -1681 | 4579 | 4863 | 51 |
| H33D | -2424 | 3867 | 4603 | 51 |
| H34C | -1114 | 3205 | 5784 | 53 |
| H34D | -1562 | 3865 | 6473 | 53 |
| H35A | 145 | 4498 | 6251 | 41 |
| H36C | 1755 | 3009 | 4456 | 41 |
| H36D | 516 | 2778 | 4841 | 41 |

| | | | | |
|---|---|---|---|---|
| H37A | 1970 | 2255 | 6053 | 44 |
| H38C | 1333 | 2642 | 7776 | 55 |
| H38D | 246 | 2600 | 6843 | 55 |
| H39A | 241 | 3704 | 7825 | 52 |
| H40C | 1793 | 4512 | 7691 | 50 |
| H40D | 2233 | 3791 | 8302 | 50 |
| H41C | 4166 | 4058 | 7861 | 54 |
| H41D | 3692 | 4774 | 7256 | 54 |
| H42C | 5482 | 4436 | 6604 | 56 |
| H42D | 4475 | 4435 | 5595 | 56 |
| H43C | 5372 | 3190 | 6761 | 55 |
| H43D | 5555 | 3383 | 5484 | 55 |
| H44C | 3553 | 3246 | 4960 | 48 |
| H44D | 4015 | 2533 | 5584 | 48 |
| H45A | 3286 | 2912 | 7256 | 40 |
| H13 | 2254 | 2084 | 2134 | 31 |
| H14 | 248 | 2176 | 2147 | 33 |
| H15 | -735 | 3179 | 1393 | 34 |
| H16 | 312 | 4108 | 676 | 29 |
| H23 | 4627 | 4965 | 3868 | 31 |
| H24 | 6074 | 5835 | 4114 | 37 |
| H25 | 7593 | 5871 | 2936 | 39 |
| H26 | 7697 | 5000 | 1557 | 34 |
| H13A | 2900 | 7809 | 6879 | 26 |
| H14A | 4871 | 7763 | 6645 | 30 |
| H15A | 5693 | 6733 | 5923 | 29 |
| H16A | 4498 | 5766 | 5393 | 28 |
| H23A | 288 | 5090 | 9052 | 30 |
| H24A | -1415 | 4528 | 9482 | 35 |
| H25A | -3155 | 4688 | 8342 | 36 |
| H26A | -3179 | 5424 | 6776 | 31 |

**Table 3 Crystal data and structure refinement for compound 2-RT.**

| | |
|---|---|
| Identification code | lawr13CuRT3 |
| Empirical formula | $C_{29}H_{35}BN_2O_6$ |
| Formula weight | 518.40 |
| Temperature/K | 281(12) |
| Crystal system | orthorhombic |
| Space group | $P2_12_12_1$ |
| a/Å | 11.70439(17) |
| b/Å | 11.96490(18) |
| c/Å | 18.9233(2) |
| α/° | 90 |
| β/° | 90 |
| γ/° | 90 |
| Volume/Å$^3$ | 2650.06(6) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.299 |
| μ/mm$^{-1}$ | 0.731 |
| F(000) | 1104.0 |
| Crystal size/mm$^3$ | 0.1 × 0.1 × 0.1 |
| Radiation | CuKα (λ = 1.54184) |
| 2Θ range for data collection/° | 8.744 to 134.972 |
| Index ranges | $-14 \leq h \leq 10$, $-13 \leq k \leq 14$, $-22 \leq l \leq 19$ |
| Reflections collected | 14561 |
| Independent reflections | 4763 [$R_{int}$ = 0.0157, $R_{sigma}$ = 0.0151] |
| Data/restraints/parameters | 4763/213/482 |
| Completeness to theta = 66.5° | 99.8% |
| Goodness-of-fit on $F^2$ | 1.014 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0285, $wR_2$ = 0.0751 |
| Final R indexes [all data] | $R_1$ = 0.0310, $wR_2$ = 0.0770 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.11/-0.10 |
| Flack parameter | 0.00(6) |

**Fractional Atomic Coordinates (×10$^4$) and Equivalent Isotropic Displacement Parameters (Å$^2$×10$^3$) for compound 2-RT. $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| B1 | 3055.9(18) | 6384(2) | 1216.6(11) | 54.6(4) |
| O10 | 5061.6(13) | 5047.7(13) | 2352.4(6) | 64.3(3) |
| O11 | 3558.0(11) | 5631.2(12) | 1761.3(6) | 58.5(3) |
| O12 | 3725.4(12) | 6435.7(14) | 578.7(7) | 64.7(4) |
| O20 | 114.6(14) | 5691.6(17) | 1262.7(9) | 84.7(5) |
| O21 | 1939.4(12) | 5924.3(13) | 1027.9(7) | 63.1(3) |
| O22 | 2973.0(11) | 7503.8(11) | 1515.9(7) | 56.9(3) |
| C10 | 4669.8(15) | 5504.2(14) | 1831.6(8) | 49.0(4) |
| C11 | 5380.1(15) | 5907.5(14) | 1237.7(8) | 47.8(4) |
| C12 | 4865.3(16) | 6361.8(15) | 640.1(8) | 50.2(4) |
| C13 | 5546.3(19) | 6726.1(18) | 82.2(10) | 61.3(5) |
| C14 | 6713(2) | 6632.4(19) | 121.4(11) | 68.3(5) |
| C15 | 7231.6(18) | 6173(2) | 711.5(12) | 69.5(5) |
| C16 | 6563.3(17) | 5819.2(18) | 1266.1(11) | 60.4(4) |
| C20 | 1007.3(16) | 6156.1(17) | 1393.8(10) | 57.7(4) |
| C21 | 1119.3(15) | 7025.6(16) | 1940.5(10) | 55.4(4) |
| C22 | 2103.0(15) | 7690.2(15) | 1963.6(10) | 52.0(4) |
| C23 | 2177(2) | 8565.1(19) | 2444.3(12) | 67.8(5) |
| C24 | 1283(2) | 8759(2) | 2901.5(15) | 85.7(7) |
| C25 | 321(2) | 8096(3) | 2891.5(17) | 93.4(8) |
| C26 | 237.1(19) | 7236(2) | 2412.4(13) | 75.1(6) |
| N1 | 3575.5(18) | 5181.9(15) | 3705.0(9) | 65.6(4) |
| N16 | 5246.1(18) | 6852.4(15) | 3707.0(9) | 69.1(5) |
| C31 | 2986(18) | 4248(16) | 3278(9) | 116(6) |
| C31A | 3065(11) | 4219(8) | 3334(5) | 65(2) |
| C32 | 1843(14) | 3940(14) | 3656(10) | 78(3) |
| C32A | 1996(19) | 3767(18) | 3612(14) | 106(6) |
| C33 | 1028(12) | 4743(12) | 3550(6) | 96(3) |
| C33A | 1163(12) | 4890(12) | 3796(6) | 91(3) |
| C34 | 1503(10) | 5703(12) | 3978(6) | 97(3) |
| C34A | 1743(10) | 5798(10) | 4234(5) | 87(2) |
| C35 | 2836(13) | 6185(13) | 3892(7) | 72(2) |
| C35A | 2684(13) | 6116(13) | 3715(7) | 76(3) |
| C36 | 4316(11) | 4804(12) | 4382(7) | 71(2) |
| C36A | 3978(11) | 4819(15) | 4359(9) | 78(3) |
| C37 | 4892(8) | 5730(8) | 4745(6) | 69.1(19) |
| C37A | 4487(9) | 5836(11) | 4772(6) | 86(3) |
| C38 | 3993(8) | 6527(9) | 5006(5) | 83(2) |

| | | | | |
|---|---|---|---|---|
| C38A | 3618(10) | 6714(10) | 4869(6) | 100(3) |
| C39 | 3446(10) | 7056(10) | 4355(5) | 75(2) |
| C39A | 3241(12) | 7090(12) | 4125(6) | 94(3) |
| C40 | 4349(13) | 7680(13) | 3951(5) | 72(2) |
| C40A | 4294(15) | 7585(14) | 3732(6) | 91(3) |
| C41 | 6095(14) | 7549(13) | 3364(9) | 83(3) |
| C41A | 6212(13) | 7351(13) | 3279(11) | 98(4) |
| C42 | 7089(10) | 6821(10) | 3062(6) | 76.4(19) |
| C42A | 7176(13) | 6545(13) | 3259(7) | 109(4) |
| C43 | 7683(8) | 6250(8) | 3670(5) | 74.5(17) |
| C43A | 7496(11) | 6025(11) | 3925(6) | 107(3) |
| C44 | 6790(9) | 5608(9) | 4100(5) | 75(2) |
| C44A | 6474(10) | 5501(14) | 4283(7) | 105(3) |
| C45 | 5809(9) | 6365(12) | 4326(8) | 62(2) |
| C45A | 5514(11) | 6315(15) | 4394(9) | 79(3) |

**Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for compound 2-RT. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.**

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| B1 | 52.7(10) | 67.7(12) | 43.2(9) | 4.9(9) | -0.7(8) | 0.1(9) |
| O10 | 70.0(8) | 76.8(8) | 46.1(6) | 15.9(6) | -2.8(6) | 2.6(7) |
| O11 | 56.5(7) | 71.4(8) | 47.7(7) | 14.0(6) | 5.3(5) | 3.0(6) |
| O12 | 59.9(8) | 94.2(10) | 40.0(6) | 11.9(6) | 0.6(5) | 6.9(7) |
| O20 | 64.4(9) | 108.9(12) | 80.7(10) | -11.9(9) | -3.8(8) | -29.0(9) |
| O21 | 58.8(7) | 77.7(9) | 52.8(7) | -6.9(6) | -3.8(6) | -5.6(6) |
| O22 | 50.6(6) | 64.1(7) | 56.1(7) | 4.7(5) | 1.8(5) | -5.3(5) |
| C10 | 57.8(9) | 49.1(8) | 40.0(8) | 0.1(6) | 0.1(7) | 0.7(7) |
| C11 | 56.3(9) | 48.3(8) | 38.9(7) | -3.3(7) | 2.6(7) | -1.0(7) |
| C12 | 58.7(10) | 53.3(9) | 38.6(7) | -2.6(7) | 2.8(7) | 0.4(7) |
| C13 | 73.8(12) | 68.1(11) | 42.0(9) | 4.6(8) | 7.7(8) | -1.7(9) |
| C14 | 76.6(13) | 73.5(12) | 54.9(10) | -0.9(9) | 20.7(10) | -10.9(10) |
| C15 | 54.8(11) | 84.7(14) | 68.9(12) | -4.7(11) | 9.3(9) | -3.5(10) |
| C16 | 58.8(10) | 69.2(11) | 53.3(9) | -2.1(9) | -1.0(8) | 2.9(8) |
| C20 | 54.3(10) | 66.6(11) | 52.3(9) | 6.1(8) | -5.9(8) | -7.0(8) |
| C21 | 48.3(9) | 61(1) | 57(1) | 5.0(8) | -3.5(8) | 0.3(8) |
| C22 | 50.4(9) | 54.7(9) | 50.9(9) | 8.5(7) | -4.1(8) | 2.6(7) |
| C23 | 65.6(12) | 61.1(11) | 76.7(13) | -5(1) | -1.6(10) | -2.9(9) |
| C24 | 82.7(16) | 80.6(15) | 93.8(17) | -27.9(13) | 9.2(13) | 3.7(13) |
| C25 | 73.0(15) | 107.3(19) | 100(2) | -24.1(16) | 25.7(14) | 7.8(14) |
| C26 | 54.5(12) | 85.6(14) | 85.1(15) | -6.1(12) | 10.8(11) | -3.8(10) |
| N1 | 87.0(11) | 63.7(9) | 46.1(8) | 12.2(7) | 17.6(8) | 6.8(9) |
| N16 | 86.0(12) | 65.3(10) | 55.9(9) | 5.0(8) | -2.8(9) | 6.8(9) |
| C31 | 112(10) | 124(11) | 111(9) | -24(7) | -4(7) | -28(8) |
| C31A | 86(6) | 61(4) | 46(3) | 12(3) | 27(3) | -3(4) |
| C32 | 77(5) | 78(6) | 79(5) | 20(4) | 23(4) | -13(5) |
| C32A | 114(10) | 87(6) | 117(9) | 23(5) | 29(7) | 14(5) |
| C33 | 82(4) | 105(6) | 100(7) | 25(5) | 5(5) | 6(4) |
| C33A | 86(5) | 98(5) | 88(7) | 19(5) | 18(4) | -25(4) |
| C34 | 86(5) | 102(5) | 103(8) | 9(5) | 16(4) | 25(4) |
| C34A | 90(5) | 87(4) | 85(5) | 10(4) | 27(4) | 3(3) |
| C35 | 86(4) | 66(4) | 64(5) | 20(3) | 10(3) | 5(3) |
| C35A | 86(4) | 67(4) | 75(6) | 10(4) | 6(4) | 24(3) |
| C36 | 97(6) | 65(3) | 50(3) | 22(2) | 3(4) | 15(4) |
| C36A | 86(6) | 78(4) | 71(4) | 22(3) | -11(4) | 16(4) |
| C37 | 97(5) | 71(3) | 40(3) | 7(2) | 7(3) | 26(3) |
| C37A | 104(6) | 111(6) | 44(3) | 6(3) | 2(4) | 28(4) |
| C38 | 103(5) | 93(4) | 53(3) | 0(3) | 12(3) | 31(4) |
| C38A | 114(6) | 107(6) | 79(5) | -20(4) | 8(4) | 33(4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C39 | 90(4) | 62(3) | 73(5) | 4(3) | 8(3) | 23(3) |
| C39A | 106(5) | 77(4) | 100(7) | -3(5) | 0(4) | 40(4) |
| C40 | 94(4) | 55(4) | 67(4) | 1(3) | -3(4) | 12(3) |
| C40A | 113(5) | 58(4) | 102(8) | 1(6) | -10(6) | 14(3) |
| C41 | 88(5) | 86(5) | 75(4) | 12(4) | -3(3) | 12(4) |
| C41A | 87(6) | 104(7) | 104(7) | -3(5) | 9(5) | -35(5) |
| C42 | 65(3) | 99(5) | 65(4) | 7(3) | -9(3) | -7(3) |
| C42A | 93(6) | 139(9) | 95(8) | -21(6) | -3(6) | -17(6) |
| C43 | 66(3) | 90(4) | 67(4) | -9(3) | -10(3) | 8(3) |
| C43A | 94(5) | 118(7) | 109(8) | -19(5) | -6(5) | -8(4) |
| C44 | 84(5) | 75(4) | 68(4) | 4(3) | 1(3) | 25(4) |
| C44A | 88(5) | 113(6) | 113(8) | -6(6) | -4(4) | 14(4) |
| C45 | 78(4) | 63(3) | 45(3) | -5(2) | -4(3) | 12(3) |
| C45A | 100(6) | 85(5) | 51(5) | -11(3) | -13(4) | 10(4) |

**Bond Lengths for compound 2-RT.**

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| B1 | O11 | 1.490(2) | N16 | C41 | 1.450(17) |
| B1 | O12 | 1.441(2) | N16 | C41A | 1.513(16) |
| B1 | O21 | 1.462(3) | N16 | C45 | 1.466(15) |
| B1 | O22 | 1.457(3) | N16 | C45A | 1.484(17) |
| O10 | C10 | 1.216(2) | C31 | C32 | 1.56(3) |
| O11 | C10 | 1.317(2) | C31A | C32A | 1.46(3) |
| O12 | C12 | 1.342(2) | C32 | C33A | 1.41(2) |
| O20 | C20 | 1.209(2) | C32A | C33 | 1.63(3) |
| O21 | C20 | 1.322(2) | C33 | C34 | 1.511(15) |
| O22 | C22 | 1.343(2) | C33A | C34A | 1.527(14) |
| C10 | C11 | 1.479(2) | C34 | C35A | 1.55(2) |
| C11 | C12 | 1.392(2) | C34A | C35 | 1.506(17) |
| C11 | C16 | 1.390(3) | C35 | C39 | 1.539(16) |
| C12 | C13 | 1.393(3) | C35A | C39A | 1.545(18) |
| C13 | C14 | 1.372(3) | C36 | C37 | 1.467(17) |
| C14 | C15 | 1.385(3) | C36A | C37A | 1.56(2) |
| C15 | C16 | 1.376(3) | C37 | C38 | 1.504(10) |
| C20 | C21 | 1.473(3) | C37 | C45 | 1.536(13) |
| C21 | C22 | 1.400(3) | C37A | C38A | 1.474(12) |
| C21 | C26 | 1.388(3) | C37A | C45A | 1.512(15) |
| C22 | C23 | 1.390(3) | C38 | C39 | 1.525(10) |
| C23 | C24 | 1.377(4) | C38A | C39A | 1.542(12) |
| C24 | C25 | 1.377(4) | C39 | C40 | 1.503(17) |
| C25 | C26 | 1.375(4) | C39A | C40A | 1.56(2) |
| N1 | C31 | 1.541(19) | C41 | C42 | 1.561(19) |
| N1 | C31A | 1.475(13) | C41A | C42A | 1.49(2) |
| N1 | C35 | 1.521(17) | C42 | C43 | 1.508(10) |
| N1 | C35A | 1.529(15) | C42A | C43A | 1.455(14) |
| N1 | C36 | 1.612(13) | C43 | C44 | 1.531(11) |
| N1 | C36A | 1.394(16) | C43A | C44A | 1.511(13) |
| N16 | C40 | 1.516(16) | C44 | C45 | 1.523(13) |
| N16 | C40A | 1.419(18) | C44A | C45A | 1.501(17) |

**Bond Angles for compound 2-RT.**

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| O12 | B1 | O11 | 113.01(17) | C45A | N16 | C41A | 118.8(8) |
| O12 | B1 | O21 | 107.31(15) | N1 | C31 | C32 | 108.4(12) |
| O12 | B1 | O22 | 108.82(17) | C32A | C31A | N1 | 117.6(11) |
| O21 | B1 | O11 | 107.09(16) | C33A | C32 | C31 | 112.3(12) |
| O22 | B1 | O11 | 108.26(15) | C31A | C32A | C33 | 107.7(15) |
| O22 | B1 | O21 | 112.42(17) | C34 | C33 | C32A | 104.5(12) |
| C10 | O11 | B1 | 121.97(14) | C32 | C33A | C34A | 115.1(12) |
| C12 | O12 | B1 | 117.74(14) | C33 | C34 | C35A | 113.4(10) |
| C20 | O21 | B1 | 122.06(15) | C35 | C34A | C33A | 111.3(9) |
| C22 | O22 | B1 | 116.62(15) | N1 | C35 | C39 | 113.7(10) |
| O10 | C10 | O11 | 120.41(16) | C34A | C35 | N1 | 109.9(10) |
| O10 | C10 | C11 | 123.39(17) | C34A | C35 | C39 | 110.9(10) |
| O11 | C10 | C11 | 116.17(15) | N1 | C35A | C34 | 112.3(11) |
| C12 | C11 | C10 | 120.10(16) | N1 | C35A | C39A | 105.7(9) |
| C16 | C11 | C10 | 120.39(16) | C39A | C35A | C34 | 117.1(12) |
| C16 | C11 | C12 | 119.50(16) | C37 | C36 | N1 | 114.1(10) |
| O12 | C12 | C11 | 121.76(15) | N1 | C36A | C37A | 109.2(12) |
| O12 | C12 | C13 | 118.86(16) | C36 | C37 | C38 | 108.1(9) |
| C11 | C12 | C13 | 119.36(17) | C36 | C37 | C45 | 117.0(10) |
| C14 | C13 | C12 | 120.20(19) | C38 | C37 | C45 | 110.2(8) |
| C13 | C14 | C15 | 120.81(19) | C38A | C37A | C36A | 110.8(9) |
| C16 | C15 | C14 | 119.22(19) | C38A | C37A | C45A | 109.8(11) |
| C15 | C16 | C11 | 120.9(2) | C45A | C37A | C36A | 111.2(11) |
| O20 | C20 | O21 | 120.62(19) | C37 | C38 | C39 | 107.0(8) |
| O20 | C20 | C21 | 123.07(19) | C37A | C38A | C39A | 106.9(9) |
| O21 | C20 | C21 | 116.28(16) | C38 | C39 | C35 | 112.0(9) |
| C22 | C21 | C20 | 119.75(17) | C40 | C39 | C35 | 111.9(9) |
| C26 | C21 | C20 | 120.90(18) | C40 | C39 | C38 | 108.8(9) |
| C26 | C21 | C22 | 119.26(19) | C35A | C39A | C40A | 112.4(11) |
| O22 | C22 | C21 | 120.63(17) | C38A | C39A | C35A | 111.0(10) |
| O22 | C22 | C23 | 119.39(17) | C38A | C39A | C40A | 108.7(10) |
| C23 | C22 | C21 | 119.97(18) | C39 | C40 | N16 | 108.5(10) |
| C24 | C23 | C22 | 119.4(2) | N16 | C40A | C39A | 113.8(11) |
| C23 | C24 | C25 | 121.0(2) | N16 | C41 | C42 | 110.7(10) |
| C26 | C25 | C24 | 119.9(2) | C42A | C41A | N16 | 109.0(11) |
| C25 | C26 | C21 | 120.4(2) | C43 | C42 | C41 | 108.5(9) |
| C31 | N1 | C36 | 117.0(9) | C43A | C42A | C41A | 116.8(13) |
| C31A | N1 | C35A | 107.5(7) | C42 | C43 | C44 | 108.5(7) |
| C35 | N1 | C31 | 116.0(9) | C42A | C43A | C44A | 111.2(10) |
| C35 | N1 | C36 | 110.0(7) | C45 | C44 | C43 | 111.5(8) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C36A | N1 | C31A | 108.4(8) | C45A | C44A | C43A | 112.7(12) |
| C36A | N1 | C35A | 116.6(9) | N16 | C45 | C37 | 107.2(8) |
| C40A | N16 | C41A | 111.2(9) | N16 | C45 | C44 | 110.5(10) |
| C40A | N16 | C45A | 113.9(8) | C44 | C45 | C37 | 112.2(9) |
| C41 | N16 | C40 | 103.6(8) | N16 | C45A | C37A | 114.2(10) |
| C41 | N16 | C45 | 106.2(7) | N16 | C45A | C44A | 108.5(11) |
| C45 | N16 | C40 | 109.1(7) | C44A | C45A | C37A | 114.6(12) |

**Hydrogen Bonds for compound 2-RT.**

| D | H | A | d(D-H)/Å | d(H-A)/Å | d(D-A)/Å | D-H-A/° |
|---|---|---|---|---|---|---|
| N1 | H1 | N16 | 0.89(3) | 2.20(2) | 2.796(3) | 124(2) |

**Torsion Angles for compound 2-RT.**

| A | B | C | D | Angle/° | A | B | C | D | Angle/° |
|---|---|---|---|---|---|---|---|---|---|
| B1 | O11 | C10 | O10 | 166.94(17) | C31A | N1 | C35A | C39A | 178.5(8) |
| B1 | O11 | C10 | C11 | -15.2(2) | C31A | N1 | C36A | C37A | -178.2(8) |
| B1 | O12 | C12 | C11 | 20.0(3) | C31A | C32A | C33 | C34 | -58.8(18) |
| B1 | O12 | C12 | C13 | -161.53(18) | C32 | C33A | C34A | C35 | 56.5(15) |
| B1 | O21 | C20 | O20 | -173.7(2) | C32A | C33 | C34 | C35A | 58.3(15) |
| B1 | O21 | C20 | C21 | 8.3(3) | C33 | C34 | C35A | N1 | -57.0(13) |
| B1 | O22 | C22 | C21 | -23.1(2) | C33 | C34 | C35A | C39A | -179.5(10) |
| B1 | O22 | C22 | C23 | 158.09(18) | C33A | C34A | C35 | N1 | -50.4(12) |
| O10 | C10 | C11 | C12 | 176.14(17) | C33A | C34A | C35 | C39 | -177.0(10) |
| O10 | C10 | C11 | C16 | -2.8(3) | C34 | C35A | C39A | C38A | 69.2(14) |
| O11 | B1 | O12 | C12 | -34.2(3) | C34 | C35A | C39A | C40A | -168.8(11) |
| O11 | B1 | O21 | C20 | 85.3(2) | C34A | C35 | C39 | C38 | 73.1(13) |
| O11 | B1 | O22 | C22 | -77.95(19) | C34A | C35 | C39 | C40 | -164.5(11) |
| O11 | C10 | C11 | C12 | -1.7(2) | C35 | N1 | C31 | C32 | -50.2(14) |
| O11 | C10 | C11 | C16 | 179.40(17) | C35 | N1 | C36 | C37 | -47.3(12) |
| O12 | B1 | O11 | C10 | 33.0(3) | C35 | C39 | C40 | N16 | -62.0(12) |
| O12 | B1 | O21 | C20 | -153.05(18) | C35A | N1 | C31A | C32A | -57.2(14) |
| O12 | B1 | O22 | C22 | 158.87(14) | C35A | N1 | C36A | C37A | -56.8(13) |
| O12 | C12 | C13 | C14 | -178.18(19) | C35A | C39A | C40A | N16 | -68.8(12) |
| O20 | C20 | C21 | C22 | -166.5(2) | C36 | N1 | C31 | C32 | 82.4(14) |
| O20 | C20 | C21 | C26 | 10.2(3) | C36 | N1 | C35 | C34A | -84.3(9) |
| O21 | B1 | O11 | C10 | 150.94(16) | C36 | N1 | C35 | C39 | 40.8(11) |
| O21 | B1 | O12 | C12 | -152.01(17) | C36 | C37 | C38 | C39 | -67.5(11) |
| O21 | B1 | O22 | C22 | 40.1(2) | C36 | C37 | C45 | N16 | 60.9(12) |
| O21 | C20 | C21 | C22 | 11.4(3) | C36 | C37 | C45 | C44 | -60.6(14) |
| O21 | C20 | C21 | C26 | -171.94(19) | C36A | N1 | C31A | C32A | 69.6(14) |
| O22 | B1 | O11 | C10 | -87.6(2) | C36A | N1 | C35A | C34 | -72.2(12) |
| O22 | B1 | O12 | C12 | 86.1(2) | C36A | N1 | C35A | C39A | 56.6(13) |
| O22 | B1 | O21 | C20 | -33.4(2) | C36A | C37A | C38A | C39A | -60.5(14) |
| O22 | C22 | C23 | C24 | 179.8(2) | C36A | C37A | C45A | N16 | 67.3(14) |
| C10 | C11 | C12 | O12 | -0.8(3) | C36A | C37A | C45A | C44A | -58.8(16) |
| C10 | C11 | C12 | C13 | -179.28(16) | C37 | C38 | C39 | C35 | 63.1(12) |
| C10 | C11 | C16 | C15 | 178.81(18) | C37 | C38 | C39 | C40 | -61.1(12) |
| C11 | C12 | C13 | C14 | 0.3(3) | C37A | C38A | C39A | C35A | 62.4(14) |
| C12 | C11 | C16 | C15 | -0.1(3) | C37A | C38A | C39A | C40A | -61.8(14) |
| C12 | C13 | C14 | C15 | 0.2(3) | C38 | C37 | C45 | N16 | -63.0(12) |
| C13 | C14 | C15 | C16 | -0.7(4) | C38 | C37 | C45 | C44 | 175.5(10) |
| C14 | C15 | C16 | C11 | 0.6(3) | C38 | C39 | C40 | N16 | 62.3(10) |
| C16 | C11 | C12 | O12 | 178.07(18) | C38A | C37A | C45A | N16 | -55.6(15) |
| C16 | C11 | C12 | C13 | -0.4(3) | C38A | C37A | C45A | C44A | 178.3(11) |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C20 | C21 | C22 | O22 | -3.6(3) | C38A | C39A | C40A | N16 | 54.5(13) |
| C20 | C21 | C22 | C23 | 175.23(18) | C40 | N16 | C41 | C42 | -178.9(10) |
| C20 | C21 | C26 | C25 | -175.9(2) | C40 | N16 | C45 | C37 | 62.6(11) |
| C21 | C22 | C23 | C24 | 0.9(3) | C40 | N16 | C45 | C44 | -174.8(9) |
| C22 | C21 | C26 | C25 | 0.8(4) | C40A | N16 | C41A | C42A | -179.0(11) |
| C22 | C23 | C24 | C25 | 0.3(4) | C40A | N16 | C45A | C37A | 46.6(15) |
| C23 | C24 | C25 | C26 | -1.0(5) | C40A | N16 | C45A | C44A | 175.8(11) |
| C24 | C25 | C26 | C21 | 0.4(5) | C41 | N16 | C40 | C39 | -176.9(9) |
| C26 | C21 | C22 | O22 | 179.70(18) | C41 | N16 | C45 | C37 | 173.8(10) |
| C26 | C21 | C22 | C23 | -1.5(3) | C41 | N16 | C45 | C44 | -63.7(12) |
| N1 | C31 | C32 | C33A | 51.4(17) | C41 | C42 | C43 | C44 | 54.3(12) |
| N1 | C31A | C32A | C33 | 63.0(19) | C41A | N16 | C40A | C39A | 176.4(10) |
| N1 | C35 | C39 | C38 | -51.4(13) | C41A | N16 | C45A | C37A | -179.4(11) |
| N1 | C35 | C39 | C40 | 71.0(12) | C41A | N16 | C45A | C44A | -50.3(15) |
| N1 | C35A | C39A | C38A | -56.7(13) | C41A | C42A | C43A | C44A | 52.5(18) |
| N1 | C35A | C39A | C40A | 65.4(13) | C42 | C43 | C44 | C45 | -54.0(13) |
| N1 | C36 | C37 | C38 | 61.1(11) | C42A | C43A | C44A | C45A | -55.4(17) |
| N1 | C36 | C37 | C45 | -63.9(12) | C43 | C44 | C45 | N16 | 59.2(12) |
| N1 | C36A | C37A | C38A | 58.5(13) | C43 | C44 | C45 | C37 | 178.8(9) |
| N1 | C36A | C37A | C45A | -63.9(13) | C43A | C44A | C45A | N16 | 52.9(15) |
| N16 | C41 | C42 | C43 | -63.3(13) | C43A | C44A | C45A | C37A | -178.2(11) |
| N16 | C41A | C42A | C43A | -46.0(18) | C45 | N16 | C40 | C39 | -64.1(10) |
| C31 | N1 | C35 | C34A | 51.4(11) | C45 | N16 | C41 | C42 | 66.1(13) |
| C31 | N1 | C35 | C39 | 176.5(9) | C45 | C37 | C38 | C39 | 61.4(12) |
| C31 | N1 | C36 | C37 | 177.5(10) | C45A | N16 | C40A | C39A | -46.3(12) |
| C31 | C32 | C33A | C34A | -56.6(17) | C45A | N16 | C41A | C42A | 46.0(17) |
| C31A | N1 | C35A | C34 | 49.7(10) | C45A | C37A | C38A | C39A | 62.7(14) |

**Hydrogen Atom Coordinates (Å×10$^4$) and Isotropic Displacement Parameters (Å$^2$×10$^3$) for compound 2-RT.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| H13 | 5209 | 7034 | -318 | 74 |
| H14 | 7161 | 6880 | -253 | 82 |
| H15 | 8022 | 6104 | 733 | 83 |
| H16 | 6908 | 5517 | 1666 | 73 |
| H23 | 2824 | 9016 | 2457 | 81 |
| H24 | 1330 | 9346 | 3222 | 103 |
| H25 | -271 | 8230 | 3208 | 112 |
| H26 | -415 | 6792 | 2404 | 90 |
| H1 | 4160(20) | 5410(20) | 3442(13) | 67(6) |
| H31A | 3479 | 3597 | 3253 | 139 |
| H31B | 2834 | 4503 | 2801 | 139 |
| H31C | 2935 | 4436 | 2846 | 77 |
| H31D | 3624 | 3621 | 3329 | 77 |
| H32A | 1417 | 3425 | 3361 | 93 |
| H32B | 2014 | 3563 | 4097 | 93 |
| H32C | 2093 | 3547 | 4102 | 128 |
| H32D | 1767 | 3115 | 3342 | 128 |
| H33A | 917 | 4961 | 3061 | 115 |
| H33B | 305 | 4490 | 3742 | 115 |
| H33C | 478 | 4649 | 4042 | 109 |
| H33D | 926 | 5212 | 3349 | 109 |
| H34A | 1572 | 5469 | 4467 | 116 |
| H34B | 966 | 6320 | 3961 | 116 |
| H34C | 1228 | 6429 | 4285 | 105 |
| H34D | 1909 | 5510 | 4702 | 105 |
| H35 | 2629 | 6555 | 3448 | 86 |
| H35A | 2584 | 6367 | 3226 | 91 |
| H36A | 3815 | 4431 | 4716 | 85 |
| H36B | 4886 | 4267 | 4231 | 85 |
| H36C | 4563 | 4254 | 4292 | 94 |
| H36D | 3358 | 4489 | 4628 | 94 |
| H37 | 5268 | 5414 | 5163 | 83 |
| H37A | 4731 | 5576 | 5239 | 103 |
| H38A | 4335 | 7098 | 5302 | 99 |
| H38B | 3423 | 6131 | 5281 | 99 |
| H38C | 3936 | 7339 | 5129 | 120 |
| H38D | 2970 | 6423 | 5131 | 120 |
| H39 | 2875 | 7598 | 4517 | 90 |
| H39A | 2671 | 7685 | 4178 | 113 |

| | | | | |
|---|---|---|---|---|
| H40A | 4697 | 8243 | 4252 | 86 |
| H40B | 4011 | 8052 | 3547 | 86 |
| H40C | 4072 | 7773 | 3253 | 109 |
| H40D | 4522 | 8271 | 3966 | 109 |
| H41A | 6399 | 8082 | 3701 | 99 |
| H41B | 5739 | 7965 | 2982 | 99 |
| H41C | 5953 | 7509 | 2803 | 118 |
| H41D | 6461 | 8047 | 3493 | 118 |
| H42A | 6788 | 6268 | 2737 | 92 |
| H42B | 7626 | 7290 | 2808 | 92 |
| H42C | 6982 | 5956 | 2927 | 131 |
| H42D | 7841 | 6929 | 3073 | 131 |
| H43A | 8058 | 6800 | 3966 | 89 |
| H43B | 8258 | 5738 | 3492 | 89 |
| H43C | 7827 | 6584 | 4235 | 129 |
| H43D | 8069 | 5456 | 3839 | 129 |
| H44A | 6492 | 4998 | 3818 | 90 |
| H44B | 7150 | 5292 | 4516 | 90 |
| H44C | 6202 | 4883 | 3998 | 125 |
| H44D | 6708 | 5203 | 4738 | 125 |
| H45 | 6113 | 6969 | 4621 | 75 |
| H45A | 5816 | 6906 | 4700 | 95 |

**Atomic Occupancy for compound 2-RT.**

| Atom | *Occupancy* | Atom | *Occupancy* | Atom | *Occupancy* |
|---|---|---|---|---|---|
| C31 | 0.5 | H31A | 0.5 | H31B | 0.5 |
| C31A | 0.5 | H31C | 0.5 | H31D | 0.5 |
| C32 | 0.5 | H32A | 0.5 | H32B | 0.5 |
| C32A | 0.5 | H32C | 0.5 | H32D | 0.5 |
| C33 | 0.5 | H33A | 0.5 | H33B | 0.5 |
| C33A | 0.5 | H33C | 0.5 | H33D | 0.5 |
| C34 | 0.5 | H34A | 0.5 | H34B | 0.5 |
| C34A | 0.5 | H34C | 0.5 | H34D | 0.5 |
| C35 | 0.5 | H35 | 0.5 | C35A | 0.5 |
| H35A | 0.5 | C36 | 0.5 | H36A | 0.5 |
| H36B | 0.5 | C36A | 0.5 | H36C | 0.5 |
| H36D | 0.5 | C37 | 0.5 | H37 | 0.5 |
| C37A | 0.5 | H37A | 0.5 | C38 | 0.5 |
| H38A | 0.5 | H38B | 0.5 | C38A | 0.5 |
| H38C | 0.5 | H38D | 0.5 | C39 | 0.5 |
| H39 | 0.5 | C39A | 0.5 | H39A | 0.5 |
| C40 | 0.5 | H40A | 0.5 | H40B | 0.5 |
| C40A | 0.5 | H40C | 0.5 | H40D | 0.5 |
| C41 | 0.5 | H41A | 0.5 | H41B | 0.5 |
| C41A | 0.5 | H41C | 0.5 | H41D | 0.5 |
| C42 | 0.5 | H42A | 0.5 | H42B | 0.5 |
| C42A | 0.5 | H42C | 0.5 | H42D | 0.5 |
| C43 | 0.5 | H43A | 0.5 | H43B | 0.5 |
| C43A | 0.5 | H43C | 0.5 | H43D | 0.5 |
| C44 | 0.5 | H44A | 0.5 | H44B | 0.5 |
| C44A | 0.5 | H44C | 0.5 | H44D | 0.5 |
| C45 | 0.5 | H45 | 0.5 | C45A | 0.5 |
| H45A | 0.5 | | | | |

**Table 4 Crystal data and structure refinement for compound 3.**

| | |
|---|---|
| Identification code | lawr12f |
| Empirical formula | $C_{86}H_{88}B_4N_4O_{24}$ |
| Formula weight | 1604.84 |
| Temperature/K | 100.00(10) |
| Crystal system | monoclinic |
| Space group | $P2_1$ |
| a/Å | 12.29380(10) |
| b/Å | 19.4089(2) |
| c/Å | 16.2958(2) |
| α/° | 90 |
| β/° | 90.4770(10) |
| γ/° | 90 |
| Volume/Å$^3$ | 3888.19(7) |
| Z | 2 |
| $\rho_{calc}$g/cm$^3$ | 1.371 |
| μ/mm$^{-1}$ | 0.820 |
| F(000) | 1688.0 |
| Crystal size/mm$^3$ | 0.4 × 0.2 × 0.2 |
| Radiation | CuKα (λ = 1.54184) |
| 2Θ range for data collection/° | 7.084 to 134.994 |
| Index ranges | $-14 \leq h \leq 14$, $-23 \leq k \leq 23$, $-13 \leq l \leq 19$ |
| Reflections collected | 22164 |
| Independent reflections | 13854 [$R_{int}$ = 0.0242, $R_{sigma}$ = 0.0368] |
| Data/restraints/parameters | 13854/3/1159 |
| Completeness to theta = 66.5° | 99.6% |
| Goodness-of-fit on $F^2$ | 1.018 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0490, $wR_2$ = 0.1269 |
| Final R indexes [all data] | $R_1$ = 0.0501, $wR_2$ = 0.1278 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.33/-0.22 |
| Flack parameter | -0.20(10) |

**Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for compound 3. $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| B1 | 1187(4) | 6035(2) | 6660(3) | 33.5(9) |
| O10 | -926(2) | 5123.2(14) | 5588.5(18) | 37.2(6) |
| O11 | 575(2) | 5477.8(14) | 6212.8(18) | 37.0(6) |
| O12 | 483(2) | 6418.5(15) | 7202.0(18) | 38.5(6) |
| O20 | 2921(3) | 6899.3(17) | 5238.8(19) | 53.8(8) |
| O21 | 1618(2) | 6502.9(15) | 6029.7(18) | 40.3(6) |
| O22 | 2000(2) | 5695.2(16) | 7153.5(18) | 39.7(7) |
| C10 | -446(3) | 5561.3(18) | 5987(2) | 27.7(7) |
| C11 | -1006(3) | 6186.6(17) | 6291(2) | 25.6(7) |
| C12 | -524(3) | 6573.0(19) | 6919(2) | 28.9(7) |
| C13 | -1087(3) | 7119(2) | 7262(2) | 34.7(8) |
| C14 | -2106(3) | 7292(2) | 6956(2) | 36.3(9) |
| C15 | -2572(3) | 6924(2) | 6319(2) | 35.2(8) |
| C16 | -2030(3) | 6366(2) | 5994(2) | 30.0(7) |
| C20 | 2648(4) | 6522(2) | 5794(2) | 37.4(9) |
| C21 | 3405(3) | 6079(2) | 6250(2) | 33.3(8) |
| C22 | 3052(3) | 5686.6(19) | 6914(2) | 30.1(7) |
| C23 | 3775(3) | 5285(2) | 7354(3) | 37.5(9) |
| C24 | 4860(4) | 5271(2) | 7128(3) | 46.9(11) |
| C25 | 5220(4) | 5657(3) | 6475(4) | 57.1(13) |
| C26 | 4503(4) | 6065(3) | 6051(3) | 52.2(12) |
| B2 | 6206(4) | 3850(2) | 8352(3) | 38.1(10) |
| O10A | 4179(3) | 4799.6(15) | 9448(2) | 51.5(8) |
| O11A | 5640(2) | 4419.8(14) | 8807(2) | 42.4(7) |
| O12A | 5462(2) | 3480.3(15) | 7826(2) | 43.2(7) |
| O20A | 7975(3) | 2998.1(19) | 9780(2) | 60.5(10) |
| O21A | 6648(3) | 3380.7(15) | 8984(2) | 44.8(7) |
| O22A | 7009(2) | 4165.2(16) | 7842.9(18) | 41.4(7) |
| C10A | 4624(3) | 4355(2) | 9046(3) | 36.7(9) |
| C11A | 4024(3) | 3746.8(19) | 8745(2) | 31.5(8) |
| C12A | 4457(3) | 3349.2(19) | 8116(2) | 33.6(8) |
| C13A | 3856(4) | 2821(2) | 7769(3) | 42.0(9) |
| C14A | 2838(4) | 2666(2) | 8077(3) | 44.2(10) |
| C15A | 2419(3) | 3041(2) | 8723(3) | 46.2(11) |
| C16A | 2997(3) | 3585(2) | 9049(3) | 39.6(9) |
| C20A | 7686(4) | 3376(2) | 9237(2) | 41.5(10) |
| C21A | 8423(3) | 3821(2) | 8780(2) | 34.3(8) |
| C22A | 8059(3) | 4193.4(19) | 8102(2) | 29.7(7) |

| | | | | |
|---|---|---|---|---|
| C23A | 8775(3) | 4597(2) | 7655(3) | 36.7(8) |
| C24A | 9858(4) | 4627(2) | 7896(3) | 45.6(10) |
| C25A | 10220(4) | 4265(3) | 8563(4) | 60.0(14) |
| C26A | 9514(4) | 3861(3) | 8999(3) | 53.6(12) |
| B3 | 3970(4) | 3749(3) | 2008(3) | 41.3(11) |
| O10B | 2419(2) | 2603.7(14) | 722.4(18) | 39.8(6) |
| O11B | 3627(2) | 3147.4(15) | 1483.1(18) | 39.9(6) |
| O12B | 3053(4) | 4049(2) | 2414(3) | 42.4(9) |
| O12D | 3318(7) | 4436(5) | 1844(5) | 32.3(18) |
| O20B | 5949(4) | 4546(2) | 802(3) | 40.0(9) |
| O20D | 4693(8) | 3053(5) | 3850(6) | 40(2) |
| O21B | 4490(4) | 4209(2) | 1483(2) | 36.3(9) |
| O21D | 3959(8) | 3617(5) | 2798(5) | 27.7(17) |
| O22B | 4655(4) | 3449(2) | 2674(3) | 42.2(10) |
| O22D | 5092(9) | 4038(5) | 1698(7) | 35(2) |
| C10B | 2647(3) | 3094.5(19) | 1165(2) | 31.3(8) |
| C11B | 1858(3) | 3640(2) | 1371(2) | 31.8(8) |
| C12B | 2092(5) | 4074(3) | 1996(4) | 37.8(13) |
| C12D | 2249(11) | 4303(8) | 1731(9) | 29(3) |
| C13B | 1324(6) | 4576(4) | 2215(4) | 47.9(16) |
| C13D | 1503(13) | 4838(9) | 1910(10) | 40(3) |
| C14B | 363(4) | 4645(3) | 1799(3) | 57.7(13) |
| C15B | 81(4) | 4140(3) | 1240(4) | 60.1(13) |
| C16B | 832(4) | 3638(3) | 1030(4) | 53.3(12) |
| C20B | 5532(5) | 4165(3) | 1304(4) | 33.9(12) |
| C20D | 4788(10) | 3289(6) | 3167(9) | 29(2) |
| C21B | 6169(9) | 3662(4) | 1784(5) | 32(2) |
| C21D | 5807(16) | 3256(12) | 2709(12) | 25(5) |
| C22B | 5711(6) | 3333(4) | 2454(7) | 33(2) |
| C22D | 5926(16) | 3617(13) | 1997(15) | 24(5) |
| C23B | 6346(11) | 2885(4) | 2964(6) | 39(2) |
| C23D | 6850(20) | 3623(13) | 1534(16) | 42(6) |
| C24B | 7433(9) | 2772(4) | 2733(7) | 40(2) |
| C24D | 7682(19) | 3209(14) | 1808(14) | 37(5) |
| C25B | 7875(6) | 3094(4) | 2070(7) | 41(2) |
| C25D | 7630(20) | 2842(17) | 2476(18) | 45(7) |
| C26B | 7236(9) | 3539(3) | 1598(4) | 34.6(16) |
| C26D | 6710(20) | 2859(17) | 2924(19) | 40(8) |
| B4 | 8932(4) | 6230(3) | 2974(3) | 41.3(11) |
| O10C | 7468(2) | 7334.3(14) | 4346.4(17) | 35.3(6) |
| O11C | 8612(2) | 6832.8(15) | 3498.3(18) | 37.9(6) |
| O12C | 8000(3) | 5916.5(18) | 2581(2) | 46.2(8) |

| | | | | |
|---|---|---|---|---|
| O12E | 8300(20) | 5521(16) | 3155(18) | 41(6) |
| O20C | 10916(3) | 5396.6(18) | 4215(2) | 43.2(8) |
| O20E | 9760(20) | 6897(14) | 1225(16) | 61(6) |
| O21C | 9454(3) | 5734.1(16) | 3508(2) | 35.2(7) |
| O21E | 8960(20) | 6349(14) | 2253(15) | 54(6) |
| O22C | 9625(3) | 6503.2(18) | 2333(2) | 40.5(8) |
| O22E | 10060(30) | 5891(17) | 3400(20) | 62(7) |
| C10C | 7664(3) | 6865.6(19) | 3871(2) | 30.1(7) |
| C10H | 9760(30) | 6656(17) | 1870(20) | 46(7) |
| C11C | 6854(3) | 6331(2) | 3652(2) | 33.7(8) |
| C12C | 7055(5) | 5892(3) | 3004(3) | 40.3(12) |
| C12E | 7220(40) | 5690(30) | 3250(30) | 37(12) |
| C13C | 6266(5) | 5408(3) | 2778(3) | 50.7(13) |
| C13E | 6480(40) | 5130(30) | 3080(30) | 48(11) |
| C14C | 5310(5) | 5363(3) | 3203(3) | 60.3(14) |
| C15C | 5092(4) | 5821(3) | 3832(4) | 59.4(13) |
| C16C | 5864(4) | 6308(3) | 4054(3) | 48.2(11) |
| C20C | 10510(5) | 5774(2) | 3705(3) | 34.5(10) |
| C21C | 11133(4) | 6275(2) | 3208(3) | 40.3(10) |
| C22C | 10693(4) | 6607(2) | 2533(3) | 40.7(9) |
| C23C | 11342(5) | 7037(2) | 2059(3) | 55.3(13) |
| C24C | 12408(5) | 7140(2) | 2268(4) | 61.3(16) |
| C25C | 12853(4) | 6810(3) | 2936(4) | 55.1(12) |
| C26C | 12227(4) | 6377(2) | 3409(3) | 49.7(11) |
| N1 | -1391(3) | 3985.1(16) | 4699(2) | 30.4(6) |
| N16 | 1251(3) | 3512.9(16) | 5653(2) | 31.9(7) |
| C31 | -2427(3) | 4317(2) | 4387(3) | 42.8(10) |
| C32 | -3233(4) | 4427(2) | 5075(4) | 52.0(12) |
| C33 | -3466(4) | 3766(3) | 5530(4) | 56.3(13) |
| C34 | -2395(4) | 3442(3) | 5840(3) | 45.1(10) |
| C35 | -1625(3) | 3315.8(19) | 5128(3) | 34.8(8) |
| C36 | -605(3) | 3910.6(19) | 4006(2) | 33.0(8) |
| C37 | 413(3) | 3503.5(19) | 4242(2) | 31.2(8) |
| C38 | 81(3) | 2810.8(19) | 4589(2) | 33.8(8) |
| C39 | -563(3) | 2953.0(18) | 5375(2) | 32.5(8) |
| C40 | 152(3) | 3365(2) | 5992(2) | 33.9(8) |
| C41 | 1962(4) | 3894(2) | 6254(3) | 43.7(10) |
| C42 | 3091(4) | 3974(2) | 5926(4) | 54.0(13) |
| C43 | 3065(4) | 4351(2) | 5103(4) | 56.5(13) |
| C44 | 2309(4) | 3982(2) | 4502(3) | 43.5(10) |
| C45 | 1169(3) | 3895.1(18) | 4844(2) | 29.7(7) |
| N1A | 3687(3) | 5958.1(18) | 10267(2) | 35.9(7) |

| | | | | |
|---|---|---|---|---|
| N16A | 6301(3) | 6419.5(18) | 9290(2) | 36.3(7) |
| C31A | 2659(4) | 5635(3) | 10593(3) | 49.1(11) |
| C32A | 1845(4) | 5494(3) | 9915(4) | 57.7(13) |
| C33A | 1594(4) | 6139(3) | 9421(4) | 65.8(15) |
| C34A | 2643(4) | 6469(3) | 9104(3) | 56.0(12) |
| C35A | 3432(4) | 6612(2) | 9818(3) | 46(1) |
| C36A | 4484(4) | 6057(2) | 10953(2) | 39.7(9) |
| C37A | 5495(4) | 6458(2) | 10699(2) | 39.0(9) |
| C38A | 5148(4) | 7135(2) | 10331(3) | 44.3(10) |
| C39A | 4489(4) | 6979(2) | 9550(3) | 43.6(10) |
| C40A | 5206(4) | 6557(2) | 8940(3) | 40.3(9) |
| C41A | 6244(3) | 6056(2) | 10109(2) | 34.4(8) |
| C42A | 7388(4) | 5973(2) | 10450(3) | 45.3(10) |
| C43A | 8120(4) | 5590(2) | 9858(3) | 53.9(12) |
| C44A | 8136(4) | 5955(2) | 9035(3) | 51.9(12) |
| C45A | 7000(4) | 6026(2) | 8702(3) | 46.1(11) |

**Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for compound 3. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.**

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| B1 | 30(2) | 26(2) | 44(2) | 4.5(18) | -7.7(17) | 0.6(16) |
| O10 | 41.7(15) | 24.8(13) | 45.0(15) | -7.0(11) | -5.9(12) | -2.2(11) |
| O11 | 33.0(14) | 24.8(13) | 53.1(16) | -4.5(12) | -7.4(12) | 7.3(11) |
| O12 | 35.4(14) | 34.2(15) | 45.8(15) | -6.7(12) | -11.0(12) | 0.1(11) |
| O20 | 84(3) | 38.3(17) | 38.9(16) | 7.9(13) | 6.2(15) | -2.7(16) |
| O21 | 44.1(16) | 32.4(14) | 44.3(15) | 10.4(12) | -11.7(12) | -2.1(12) |
| O22 | 27.8(13) | 46.3(16) | 44.8(15) | 17.0(13) | -3.8(11) | -0.3(12) |
| C10 | 31.2(18) | 17.5(16) | 34.3(18) | -0.8(13) | -2.7(14) | -0.5(13) |
| C11 | 30.2(17) | 16.4(15) | 30.1(16) | 3.8(12) | 4.4(13) | -2.7(13) |
| C12 | 31.2(18) | 23.2(17) | 32.2(17) | 4.1(14) | -0.3(14) | -3.9(14) |
| C13 | 48(2) | 24.6(18) | 31.2(18) | -2.5(14) | 6.5(16) | -2.1(16) |
| C14 | 44(2) | 28.6(19) | 37(2) | 1.1(16) | 17.0(17) | 6.1(16) |
| C15 | 31.4(19) | 31(2) | 43(2) | 5.1(16) | 7.7(15) | 5.4(15) |
| C16 | 29.4(18) | 28.2(18) | 32.4(17) | 4.2(14) | -0.3(14) | -3.5(14) |
| C20 | 57(3) | 26.2(19) | 29.1(18) | -2.5(15) | -2.9(17) | -3.9(17) |
| C21 | 38(2) | 28.1(18) | 33.8(18) | -6.7(15) | 2.2(15) | -2.6(15) |
| C22 | 30.4(18) | 27.2(18) | 32.6(18) | -2.7(14) | -3.1(14) | -2.5(14) |
| C23 | 34(2) | 38(2) | 40(2) | -1.6(17) | -7.1(16) | 1.4(16) |
| C24 | 33(2) | 46(3) | 61(3) | -12(2) | -9.0(19) | 4.1(18) |
| C25 | 33(2) | 58(3) | 80(4) | -14(3) | 14(2) | -1(2) |
| C26 | 49(3) | 49(3) | 60(3) | -1(2) | 19(2) | -7(2) |
| B2 | 34(2) | 32(2) | 49(3) | 2.5(19) | 17.0(19) | -2.7(18) |
| O10A | 60(2) | 25.6(15) | 69(2) | -7.0(14) | 21.9(16) | 5.9(13) |
| O11A | 35.6(15) | 27.9(14) | 63.8(19) | -3.2(13) | 16.0(13) | -8.0(11) |
| O12A | 38.6(15) | 32.9(15) | 58.4(18) | -8.2(13) | 16.0(13) | -1.7(12) |
| O20A | 89(3) | 47(2) | 45.7(18) | 17.1(16) | 4.1(17) | 6.2(18) |
| O21A | 44.3(16) | 36.4(16) | 54.1(17) | 13.5(13) | 20.7(14) | 3.0(13) |
| O22A | 30.7(14) | 48.1(17) | 45.5(16) | 16.4(13) | 4.6(12) | -2.4(12) |
| C10A | 37(2) | 23.2(18) | 50(2) | 5.6(16) | 11.1(17) | 1.3(15) |
| C11A | 29.4(18) | 23.1(17) | 42(2) | 12.0(15) | 1.2(15) | 3.2(14) |
| C12A | 32.2(19) | 25.0(18) | 44(2) | 8.9(16) | 2.9(16) | 3.2(15) |
| C13A | 51(2) | 34(2) | 41(2) | 5.0(17) | -8.0(18) | -0.5(18) |
| C14A | 44(2) | 40(2) | 49(2) | 11.9(19) | -17.1(19) | -10.8(19) |
| C15A | 27.6(19) | 48(3) | 63(3) | 20(2) | -9.0(18) | -9.2(18) |
| C16A | 35(2) | 38(2) | 46(2) | 11.8(18) | 5.2(17) | 3.8(17) |
| C20A | 60(3) | 30(2) | 34(2) | 3.3(16) | 12.5(18) | 2.6(19) |
| C21A | 39(2) | 28.4(18) | 35.7(19) | -1.7(15) | 3.7(15) | 4.4(16) |
| C22A | 28.2(18) | 28.1(18) | 32.8(18) | 0.0(14) | 7.4(14) | 3.6(14) |
| C23A | 35(2) | 37(2) | 38(2) | -0.3(16) | 7.5(16) | -2.5(16) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C24A | 34(2) | 40(2) | 63(3) | -2(2) | 10.2(19) | -5.3(18) |
| C25A | 33(2) | 55(3) | 91(4) | -5(3) | -13(2) | -1(2) |
| C26A | 52(3) | 47(3) | 62(3) | 7(2) | -18(2) | 7(2) |
| B3 | 44(3) | 41(3) | 39(2) | -11(2) | -5(2) | 3(2) |
| O10B | 47.0(16) | 22.4(13) | 49.9(16) | -1.6(12) | -7.7(13) | 5.7(12) |
| O11B | 39.1(15) | 40.0(15) | 40.7(15) | -11.6(12) | -4.2(12) | 6.8(12) |
| O12B | 53(3) | 37(2) | 37(2) | -8.7(17) | 2.5(18) | 0.7(19) |
| O20B | 47(2) | 33(2) | 40(2) | 13.3(17) | -4.9(17) | -7.8(18) |
| O21B | 42(2) | 27.6(19) | 39(2) | 6.6(16) | -4.8(18) | -1.2(17) |
| O22B | 58(3) | 35(2) | 33(2) | 6.3(18) | -5(2) | -7(2) |
| C10B | 42(2) | 25.3(18) | 26.2(17) | 5.7(14) | 1.8(14) | 0.8(15) |
| C11B | 41(2) | 27.5(18) | 26.8(17) | 6.3(14) | 5.0(15) | 4.2(15) |
| C12B | 47(4) | 28(3) | 39(3) | 2(3) | 15(3) | 1(3) |
| C13B | 64(4) | 37(3) | 43(3) | -10(3) | 18(3) | 12(3) |
| C14B | 58(3) | 59(3) | 56(3) | 2(2) | 18(2) | 27(3) |
| C15B | 45(3) | 54(3) | 82(4) | 8(3) | -2(2) | 13(2) |
| C16B | 50(3) | 36(2) | 74(3) | -3(2) | -9(2) | 5(2) |
| C20B | 48(3) | 19(2) | 34(3) | 0(2) | -10(3) | -2(2) |
| C21B | 53(5) | 21(3) | 21(4) | -1(3) | -5(4) | -5(3) |
| C22B | 49(4) | 20(3) | 31(4) | 2(3) | -10(4) | -7(2) |
| C23B | 59(7) | 21(4) | 38(4) | 1(2) | -5(5) | -13(5) |
| C24B | 53(6) | 22(3) | 42(5) | 9(3) | -22(4) | -3(3) |
| C25B | 46(4) | 33(4) | 44(4) | 5(3) | -15(4) | 3(3) |
| C26B | 48(5) | 19(3) | 36(3) | 0(2) | -15(3) | 1(3) |
| B4 | 53(3) | 31(2) | 40(2) | -3.3(19) | 9(2) | -1(2) |
| O10C | 43.2(15) | 25.8(13) | 37.1(14) | -4.2(11) | 4.3(11) | -8.7(11) |
| O11C | 38.9(15) | 31.5(14) | 43.5(15) | -6.1(12) | 3.5(12) | -5.5(12) |
| O12C | 66(2) | 33.5(17) | 38.9(17) | -9.7(14) | 1.1(15) | -2.2(16) |
| O20C | 51(2) | 32.9(17) | 45.7(19) | 14.4(15) | 8.6(15) | 5.4(15) |
| O21C | 45(2) | 26.2(16) | 34.6(17) | 5.4(12) | 6.6(14) | -0.3(14) |
| O22C | 56(2) | 31.6(17) | 33.7(18) | 8.3(14) | 10.2(16) | 5.4(16) |
| C10C | 35.8(19) | 25.3(18) | 29.0(17) | 3.2(14) | -1.4(14) | -6.6(15) |
| C11C | 45(2) | 24.9(18) | 31.5(18) | 5.3(14) | -8.1(15) | -10.3(16) |
| C12C | 61(3) | 30(2) | 30(2) | 4(2) | -10(2) | -3(2) |
| C13C | 75(4) | 36(3) | 41(3) | -3(2) | -21(3) | -13(3) |
| C14C | 70(3) | 53(3) | 57(3) | 3(2) | -21(3) | -33(3) |
| C15C | 53(3) | 59(3) | 67(3) | 6(3) | -3(2) | -27(2) |
| C16C | 47(2) | 45(2) | 53(2) | -3(2) | -1(2) | -16(2) |
| C20C | 49(3) | 20(2) | 34(2) | 1.4(18) | 9(2) | 4(2) |
| C21C | 59(3) | 20.3(18) | 42(2) | -4.5(15) | 18.9(19) | 1.6(17) |
| C22C | 56(3) | 20.4(18) | 46(2) | -3.5(16) | 11.9(19) | 5.2(17) |
| C23C | 87(4) | 29(2) | 50(3) | 7.0(19) | 22(3) | 9(2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C24C | 82(4) | 28(2) | 74(3) | 2(2) | 42(3) | 1(2) |
| C25C | 56(3) | 37(2) | 73(3) | -10(2) | 17(2) | -6(2) |
| C26C | 71(3) | 36(2) | 42(2) | -6.4(19) | 8(2) | 10(2) |
| N1 | 31.8(16) | 20.2(14) | 39.1(17) | -5.7(13) | -4.3(13) | -0.7(12) |
| N16 | 35.1(17) | 21.7(15) | 38.9(16) | -6.2(13) | -2.4(13) | 6.9(13) |
| C31 | 36(2) | 33(2) | 59(3) | -9.1(19) | -15.9(19) | 3.4(17) |
| C32 | 33(2) | 42(2) | 81(3) | -15(2) | -8(2) | 6.1(18) |
| C33 | 33(2) | 54(3) | 81(4) | -15(3) | 8(2) | -4(2) |
| C34 | 37(2) | 43(2) | 56(3) | -4(2) | 11.1(19) | -3.3(18) |
| C35 | 35.2(19) | 24.0(18) | 45(2) | -5.1(15) | 5.1(16) | -5.5(15) |
| C36 | 45(2) | 25.7(18) | 28.4(17) | -2.1(14) | -2.1(15) | -1.8(16) |
| C37 | 39(2) | 23.7(18) | 30.8(17) | -6.9(14) | 4.0(15) | -2.2(15) |
| C38 | 39(2) | 21.1(17) | 41(2) | -6.0(15) | -1.0(16) | 0.5(15) |
| C39 | 38(2) | 17.7(16) | 42(2) | 2.6(14) | 4.9(16) | 0.7(14) |
| C40 | 41(2) | 26.9(18) | 34.0(18) | 3.2(15) | 3.2(16) | 8.6(16) |
| C41 | 49(2) | 31(2) | 50(2) | -10.7(18) | -17.9(19) | 13.2(18) |
| C42 | 40(2) | 34(2) | 87(4) | -20(2) | -19(2) | 7.6(19) |
| C43 | 38(2) | 34(2) | 98(4) | -14(2) | 2(2) | -5.7(19) |
| C44 | 38(2) | 30(2) | 63(3) | -7.0(19) | 10.3(19) | -1.4(17) |
| C45 | 33.6(19) | 17.9(16) | 37.6(19) | -1.1(14) | 0.9(15) | 0.6(14) |
| N1A | 39.0(18) | 30.3(17) | 38.5(17) | -8.2(14) | 1.9(14) | 1.7(13) |
| N16A | 42.7(18) | 30.0(17) | 36.1(17) | -2.7(14) | 0.1(14) | -2.5(14) |
| C31A | 39(2) | 55(3) | 54(3) | -15(2) | 13.6(19) | -5(2) |
| C32A | 40(2) | 51(3) | 82(4) | -19(3) | 5(2) | -2(2) |
| C33A | 40(3) | 60(3) | 97(4) | -18(3) | -16(3) | 8(2) |
| C34A | 47(3) | 55(3) | 66(3) | -5(3) | -12(2) | 10(2) |
| C35A | 42(2) | 30(2) | 66(3) | -10.3(19) | -10(2) | 9.2(17) |
| C36A | 43(2) | 43(2) | 32.8(19) | -8.6(17) | 3.1(16) | 3.3(18) |
| C37A | 45(2) | 38(2) | 34.2(19) | -10.0(17) | -0.9(16) | -0.2(18) |
| C38A | 40(2) | 37(2) | 56(3) | -15.8(19) | 2.4(19) | -2.7(18) |
| C39A | 48(2) | 22.8(19) | 60(3) | 7.0(18) | -6(2) | 4.4(16) |
| C40A | 55(3) | 27.9(19) | 38(2) | 8.4(16) | -13.0(18) | -10.8(18) |
| C41A | 41(2) | 25.8(18) | 35.8(19) | -1.1(15) | -0.2(16) | -0.2(15) |
| C42A | 49(2) | 37(2) | 50(2) | -2.0(19) | -4.7(19) | -2.8(19) |
| C43A | 50(3) | 35(2) | 76(3) | -6(2) | 5(2) | 11(2) |
| C44A | 45(3) | 37(2) | 74(3) | -12(2) | 20(2) | -2.0(19) |
| C45A | 56(3) | 30(2) | 52(2) | -10.5(18) | 16(2) | -14.0(19) |

**Bond Lengths for compound 3.**

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| B1 | O11 | 1.503(5) | C22D | C23D | 1.37(3) |
| B1 | O12 | 1.448(5) | C23B | C24B | 1.409(16) |
| B1 | O21 | 1.473(5) | C23D | C24D | 1.38(3) |
| B1 | O22 | 1.437(5) | C24B | C25B | 1.365(14) |
| O10 | C10 | 1.219(5) | C24D | C25D | 1.30(3) |
| O11 | C10 | 1.315(5) | C25B | C26B | 1.394(11) |
| O12 | C12 | 1.352(5) | C25D | C26D | 1.36(3) |
| O20 | C20 | 1.214(5) | B4 | O11C | 1.503(5) |
| O21 | C20 | 1.327(5) | B4 | O12C | 1.443(7) |
| O22 | C22 | 1.354(5) | B4 | O12E | 1.61(3) |
| C10 | C11 | 1.482(5) | B4 | O21C | 1.445(6) |
| C11 | C12 | 1.397(5) | B4 | O21E | 1.20(2) |
| C11 | C16 | 1.389(5) | B4 | O22C | 1.453(6) |
| C12 | C13 | 1.385(5) | B4 | O22E | 1.67(4) |
| C13 | C14 | 1.385(6) | O10C | C10C | 1.221(5) |
| C14 | C15 | 1.382(6) | O11C | C10C | 1.320(5) |
| C15 | C16 | 1.379(6) | O12C | C12C | 1.357(7) |
| C20 | C21 | 1.465(6) | O12E | C12E | 1.37(6) |
| C21 | C22 | 1.395(5) | O20C | C20C | 1.212(7) |
| C21 | C26 | 1.391(6) | O20E | C10H | 1.15(5) |
| C22 | C23 | 1.379(6) | O21C | C20C | 1.337(7) |
| C23 | C24 | 1.388(6) | O21E | C10H | 1.32(4) |
| C24 | C25 | 1.378(8) | O22C | C22C | 1.365(6) |
| C25 | C26 | 1.367(8) | O22E | C21C | 1.55(3) |
| B2 | O11A | 1.506(5) | C10C | C11C | 1.479(5) |
| B2 | O12A | 1.440(6) | C10H | C22C | 1.57(3) |
| B2 | O21A | 1.475(6) | C11C | C12C | 1.379(6) |
| B2 | O22A | 1.433(5) | C11C | C12E | 1.47(5) |
| O10A | C10A | 1.215(5) | C11C | C16C | 1.388(6) |
| O11A | C10A | 1.318(5) | C12C | C13C | 1.398(7) |
| O12A | C12A | 1.351(5) | C12E | C13E | 1.45(7) |
| O20A | C20A | 1.200(6) | C13C | C14C | 1.372(9) |
| O21A | C20A | 1.338(6) | C13E | C14C | 1.53(5) |
| O22A | C22A | 1.355(5) | C14C | C15C | 1.383(8) |
| C10A | C11A | 1.474(6) | C15C | C16C | 1.386(7) |
| C11A | C12A | 1.392(6) | C20C | C21C | 1.484(6) |
| C11A | C16A | 1.396(6) | C21C | C22C | 1.382(6) |
| C12A | C13A | 1.383(6) | C21C | C26C | 1.395(7) |
| C13A | C14A | 1.385(7) | C22C | C23C | 1.391(7) |
| C14A | C15A | 1.384(7) | C23C | C24C | 1.366(8) |

| | | | | | |
|---|---|---|---|---|---|
| C15A | C16A | 1.377(7) | C24C | C25C | 1.373(8) |
| C20A | C21A | 1.461(6) | C25C | C26C | 1.379(7) |
| C21A | C22A | 1.392(5) | N1 | C31 | 1.512(5) |
| C21A | C26A | 1.386(6) | N1 | C35 | 1.504(5) |
| C22A | C23A | 1.388(5) | N1 | C36 | 1.500(5) |
| C23A | C24A | 1.386(6) | N16 | C40 | 1.492(5) |
| C24A | C25A | 1.365(8) | N16 | C41 | 1.501(5) |
| C25A | C26A | 1.374(8) | N16 | C45 | 1.516(5) |
| B3 | O11B | 1.506(5) | C31 | C32 | 1.518(7) |
| B3 | O12B | 1.434(7) | C32 | C33 | 1.509(8) |
| B3 | O12D | 1.577(10) | C33 | C34 | 1.540(7) |
| B3 | O21B | 1.395(7) | C34 | C35 | 1.523(6) |
| B3 | O21D | 1.314(10) | C35 | C39 | 1.534(6) |
| B3 | O22B | 1.487(7) | C36 | C37 | 1.526(5) |
| B3 | O22D | 1.576(12) | C37 | C38 | 1.515(5) |
| O10B | C10B | 1.226(5) | C37 | C45 | 1.546(5) |
| O11B | C10B | 1.312(5) | C38 | C39 | 1.538(5) |
| O12B | C12B | 1.360(8) | C39 | C40 | 1.551(5) |
| O12D | C12D | 1.350(17) | C41 | C42 | 1.500(7) |
| O20B | C20B | 1.219(7) | C42 | C43 | 1.528(8) |
| O20D | C20D | 1.209(18) | C43 | C44 | 1.523(7) |
| O21B | C20B | 1.319(8) | C44 | C45 | 1.522(5) |
| O21D | C20D | 1.340(16) | N1A | C31A | 1.511(6) |
| O22B | C22B | 1.368(9) | N1A | C35A | 1.496(6) |
| O22D | C22D | 1.40(3) | N1A | C36A | 1.492(5) |
| C10B | C11B | 1.477(5) | N16A | C40A | 1.481(5) |
| C11B | C12B | 1.351(7) | N16A | C41A | 1.511(5) |
| C11B | C12D | 1.492(15) | N16A | C45A | 1.501(5) |
| C11B | C16B | 1.374(6) | C31A | C32A | 1.510(7) |
| C12B | C13B | 1.404(9) | C32A | C33A | 1.519(9) |
| C12D | C13D | 1.42(2) | C33A | C34A | 1.533(8) |
| C13B | C14B | 1.364(10) | C34A | C35A | 1.535(7) |
| C13D | C14B | 1.460(17) | C35A | C39A | 1.549(7) |
| C14B | C15B | 1.380(8) | C36A | C37A | 1.526(6) |
| C15B | C16B | 1.387(7) | C37A | C38A | 1.506(7) |
| C20B | C21B | 1.473(9) | C37A | C41A | 1.548(5) |
| C20D | C21D | 1.47(2) | C38A | C39A | 1.534(7) |
| C21B | C22B | 1.388(12) | C39A | C40A | 1.565(6) |
| C21B | C26B | 1.370(14) | C41A | C42A | 1.516(6) |
| C21D | C22D | 1.36(3) | C42A | C43A | 1.519(7) |
| C21D | C26D | 1.39(3) | C43A | C44A | 1.517(8) |
| C22B | C23B | 1.431(13) | C44A | C45A | 1.499(7) |

**Bond Angles for compound 3.**

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| O12 | B1 | O11 | 111.5(3) | C21D | C22D | C23D | 125(2) |
| O12 | B1 | O21 | 109.2(3) | C23D | C22D | O22D | 114(3) |
| O21 | B1 | O11 | 106.7(3) | C24B | C23B | C22B | 117.0(9) |
| O22 | B1 | O11 | 106.5(3) | C22D | C23D | C24D | 116(3) |
| O22 | B1 | O12 | 108.1(3) | C25B | C24B | C23B | 121.7(7) |
| O22 | B1 | O21 | 114.9(3) | C25D | C24D | C23D | 123(2) |
| C10 | O11 | B1 | 121.4(3) | C24B | C25B | C26B | 119.6(8) |
| C12 | O12 | B1 | 117.2(3) | C24D | C25D | C26D | 119(3) |
| C20 | O21 | B1 | 124.6(3) | C21B | C26B | C25B | 121.5(8) |
| C22 | O22 | B1 | 120.3(3) | C25D | C26D | C21D | 123(3) |
| O10 | C10 | O11 | 121.3(3) | O11C | B4 | O12E | 115.5(11) |
| O10 | C10 | C11 | 121.7(3) | O11C | B4 | O22E | 107.0(11) |
| O11 | C10 | C11 | 116.9(3) | O12C | B4 | O11C | 111.7(4) |
| C12 | C11 | C10 | 119.3(3) | O12C | B4 | O21C | 109.5(4) |
| C16 | C11 | C10 | 120.7(3) | O12C | B4 | O22C | 107.7(4) |
| C16 | C11 | C12 | 119.9(3) | O12E | B4 | O22E | 89.3(16) |
| O12 | C12 | C11 | 120.8(3) | O21C | B4 | O11C | 107.1(4) |
| O12 | C12 | C13 | 119.4(3) | O21C | B4 | O22C | 114.6(4) |
| C13 | C12 | C11 | 119.7(4) | O21E | B4 | O11C | 114.6(13) |
| C12 | C13 | C14 | 119.6(4) | O21E | B4 | O12E | 111.1(18) |
| C15 | C14 | C13 | 120.8(4) | O21E | B4 | O22E | 116.8(17) |
| C16 | C15 | C14 | 119.8(4) | O22C | B4 | O11C | 106.4(4) |
| C15 | C16 | C11 | 120.2(4) | C10C | O11C | B4 | 122.4(3) |
| O20 | C20 | O21 | 120.2(4) | C12C | O12C | B4 | 118.0(4) |
| O20 | C20 | C21 | 123.6(4) | C12E | O12E | B4 | 106(3) |
| O21 | C20 | C21 | 116.2(3) | C20C | O21C | B4 | 122.1(4) |
| C22 | C21 | C20 | 120.8(4) | B4 | O21E | C10H | 125(3) |
| C26 | C21 | C20 | 120.4(4) | C22C | O22C | B4 | 116.8(4) |
| C26 | C21 | C22 | 118.7(4) | C21C | O22E | B4 | 116(2) |
| O22 | C22 | C21 | 121.4(3) | O10C | C10C | O11C | 120.5(3) |
| O22 | C22 | C23 | 118.0(3) | O10C | C10C | C11C | 122.7(4) |
| C23 | C22 | C21 | 120.6(4) | O11C | C10C | C11C | 116.8(3) |
| C22 | C23 | C24 | 119.3(4) | O20E | C10H | O21E | 128(3) |
| C25 | C24 | C23 | 120.7(4) | O20E | C10H | C22C | 131(3) |
| C26 | C25 | C24 | 119.7(4) | O21E | C10H | C22C | 101(3) |
| C25 | C26 | C21 | 121.1(5) | C12C | C11C | C10C | 119.6(4) |
| O12A | B2 | O11A | 111.5(4) | C12C | C11C | C16C | 120.3(4) |
| O12A | B2 | O21A | 109.7(4) | C12E | C11C | C10C | 119.3(19) |

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|---|---|---|---|---|---|---|---|
| O21A | B2 | O11A | 106.1(4) | C16C | C11C | C10C | 120.0(4) |
| O22A | B2 | O11A | 107.1(3) | C16C | C11C | C12E | 117(2) |
| O22A | B2 | O12A | 107.8(4) | O12C | C12C | C11C | 121.8(4) |
| O22A | B2 | O21A | 114.6(4) | O12C | C12C | C13C | 118.9(5) |
| C10A | O11A | B2 | 121.2(3) | C11C | C12C | C13C | 119.3(5) |
| C12A | O12A | B2 | 117.6(3) | O12E | C12E | C11C | 124(4) |
| C20A | O21A | B2 | 124.3(3) | O12E | C12E | C13E | 113(4) |
| C22A | O22A | B2 | 119.8(3) | C13E | C12E | C11C | 122(4) |
| O10A | C10A | O11A | 121.6(4) | C14C | C13C | C12C | 120.3(5) |
| O10A | C10A | C11A | 121.5(4) | C12E | C13E | C14C | 110(4) |
| O11A | C10A | C11A | 116.8(3) | C13C | C14C | C15C | 120.4(4) |
| C12A | C11A | C10A | 119.8(3) | C15C | C14C | C13E | 118(2) |
| C12A | C11A | C16A | 119.3(4) | C14C | C15C | C16C | 119.6(5) |
| C16A | C11A | C10A | 120.9(4) | C15C | C16C | C11C | 120.0(5) |
| O12A | C12A | C11A | 120.7(4) | O20C | C20C | O21C | 121.6(4) |
| O12A | C12A | C13A | 118.9(4) | O20C | C20C | C21C | 124.0(5) |
| C13A | C12A | C11A | 120.4(4) | O21C | C20C | C21C | 114.3(4) |
| C12A | C13A | C14A | 119.6(4) | C22C | C21C | O22E | 92.9(13) |
| C15A | C14A | C13A | 120.3(4) | C22C | C21C | C20C | 122.7(5) |
| C16A | C15A | C14A | 120.2(4) | C22C | C21C | C26C | 119.4(4) |
| C15A | C16A | C11A | 120.1(4) | C26C | C21C | O22E | 147.6(14) |
| O20A | C20A | O21A | 120.4(4) | C26C | C21C | C20C | 117.8(4) |
| O20A | C20A | C21A | 123.7(5) | O22C | C22C | C21C | 119.4(4) |
| O21A | C20A | C21A | 115.7(4) | O22C | C22C | C23C | 120.7(4) |
| C22A | C21A | C20A | 121.0(4) | C21C | C22C | C10H | 148.8(14) |
| C26A | C21A | C20A | 120.3(4) | C21C | C22C | C23C | 119.9(5) |
| C26A | C21A | C22A | 118.7(4) | C23C | C22C | C10H | 89.8(14) |
| O22A | C22A | C21A | 121.7(3) | C24C | C23C | C22C | 120.2(5) |
| O22A | C22A | C23A | 117.7(3) | C23C | C24C | C25C | 120.3(5) |
| C23A | C22A | C21A | 120.5(4) | C24C | C25C | C26C | 120.4(5) |
| C24A | C23A | C22A | 119.1(4) | C25C | C26C | C21C | 119.8(5) |
| C25A | C24A | C23A | 120.7(4) | C35 | N1 | C31 | 111.2(3) |
| C24A | C25A | C26A | 120.2(4) | C36 | N1 | C31 | 109.5(3) |
| C25A | C26A | C21A | 120.8(4) | C36 | N1 | C35 | 113.1(3) |
| O11B | B3 | O12D | 114.9(5) | C40 | N16 | C41 | 112.2(3) |
| O11B | B3 | O22D | 109.6(5) | C40 | N16 | C45 | 111.3(3) |
| O12B | B3 | O11B | 111.0(4) | C41 | N16 | C45 | 111.1(3) |
| O12B | B3 | O22B | 105.3(4) | N1 | C31 | C32 | 111.4(4) |
| O21B | B3 | O11B | 106.0(4) | C33 | C32 | C31 | 111.8(4) |
| O21B | B3 | O12B | 113.0(4) | C32 | C33 | C34 | 110.1(4) |
| O21B | B3 | O22B | 116.0(4) | C35 | C34 | C33 | 110.6(4) |
| O21D | B3 | O11B | 113.6(5) | N1 | C35 | C34 | 109.7(3) |

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|---|---|---|---|---|---|---|---|
| O21D | B3 | O12D | 108.8(6) | N1 | C35 | C39 | 110.7(3) |
| O21D | B3 | O22D | 113.5(7) | C34 | C35 | C39 | 114.0(4) |
| O22B | B3 | O11B | 105.3(4) | N1 | C36 | C37 | 113.1(3) |
| O22D | B3 | O12D | 95.2(6) | C36 | C37 | C45 | 113.1(3) |
| C10B | O11B | B3 | 122.5(3) | C38 | C37 | C36 | 109.3(3) |
| C12B | O12B | B3 | 117.8(4) | C38 | C37 | C45 | 111.2(3) |
| C12D | O12D | B3 | 110.7(9) | C37 | C38 | C39 | 107.1(3) |
| C20B | O21B | B3 | 123.1(4) | C35 | C39 | C38 | 107.8(3) |
| B3 | O21D | C20D | 121.3(10) | C35 | C39 | C40 | 114.2(3) |
| C22B | O22B | B3 | 114.0(6) | C38 | C39 | C40 | 109.8(3) |
| C22D | O22D | B3 | 108.9(13) | N16 | C40 | C39 | 111.7(3) |
| O10B | C10B | O11B | 119.9(4) | C42 | C41 | N16 | 110.7(4) |
| O10B | C10B | C11B | 122.9(4) | C41 | C42 | C43 | 110.4(4) |
| O11B | C10B | C11B | 117.2(3) | C44 | C43 | C42 | 110.3(4) |
| C10B | C11B | C12D | 119.9(6) | C45 | C44 | C43 | 112.1(4) |
| C12B | C11B | C10B | 118.9(4) | N16 | C45 | C37 | 110.3(3) |
| C12B | C11B | C16B | 119.7(4) | N16 | C45 | C44 | 108.6(3) |
| C16B | C11B | C10B | 120.5(4) | C44 | C45 | C37 | 112.0(3) |
| C16B | C11B | C12D | 116.9(6) | C35A | N1A | C31A | 110.6(4) |
| O12B | C12B | C13B | 118.8(6) | C36A | N1A | C31A | 109.7(3) |
| C11B | C12B | O12B | 122.2(5) | C36A | N1A | C35A | 113.0(3) |
| C11B | C12B | C13B | 119.0(6) | C40A | N16A | C41A | 112.1(3) |
| O12D | C12D | C11B | 121.9(11) | C40A | N16A | C45A | 111.7(3) |
| O12D | C12D | C13D | 117.6(13) | C45A | N16A | C41A | 110.9(3) |
| C13D | C12D | C11B | 120.4(12) | C32A | C31A | N1A | 111.6(4) |
| C14B | C13B | C12B | 121.5(6) | C31A | C32A | C33A | 111.6(4) |
| C12D | C13D | C14B | 114.1(13) | C32A | C33A | C34A | 110.8(4) |
| C13B | C14B | C15B | 118.1(5) | C33A | C34A | C35A | 110.3(5) |
| C15B | C14B | C13D | 120.0(7) | N1A | C35A | C34A | 110.3(4) |
| C14B | C15B | C16B | 119.8(5) | N1A | C35A | C39A | 110.8(3) |
| C11B | C16B | C15B | 120.6(5) | C34A | C35A | C39A | 113.3(4) |
| O20B | C20B | O21B | 121.6(5) | N1A | C36A | C37A | 113.3(3) |
| O20B | C20B | C21B | 122.3(7) | C36A | C37A | C41A | 113.7(3) |
| O21B | C20B | C21B | 116.0(7) | C38A | C37A | C36A | 108.9(4) |
| O20D | C20D | O21D | 121.0(11) | C38A | C37A | C41A | 111.1(3) |
| O20D | C20D | C21D | 122.7(14) | C37A | C38A | C39A | 107.7(3) |
| O21D | C20D | C21D | 116.3(14) | C35A | C39A | C40A | 114.7(4) |
| C22B | C21B | C20B | 120.3(10) | C38A | C39A | C35A | 107.2(4) |
| C26B | C21B | C20B | 120.3(9) | C38A | C39A | C40A | 109.5(4) |
| C26B | C21B | C22B | 119.3(8) | N16A | C40A | C39A | 111.4(3) |
| C22D | C21D | C20D | 121(2) | N16A | C41A | C37A | 110.3(3) |
| C22D | C21D | C26D | 114(2) | N16A | C41A | C42A | 108.9(3) |

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|---|---|---|---|
| C26D C21D C20D | 125(2) | C42A C41A C37A | 112.3(3) |
| O22B C22B C21B | 121.5(9) | C41A C42A C43A | 111.8(4) |
| O22B C22B C23B | 117.6(10) | C44A C43A C42A | 110.2(4) |
| C21B C22B C23B | 120.9(9) | C45A C44A C43A | 110.1(4) |
| C21D C22D O22D | 120.9(19) | C44A C45A N16A | 110.7(4) |

**Hydrogen Bonds for compound 3.**

| D | H | A | d(D-H)/Å | d(H-A)/Å | d(D-A)/Å | D-H-A/° |
|---|---|---|---|---|---|---|
| N1A | H1A | O10A | 1.00(5) | 1.76(5) | 2.687(4) | 152(4) |
| N16 | H16 | O10C[1] | 0.88(5) | 1.94(5) | 2.777(4) | 159(4) |
| N1 | H1 | O10 | 0.91(5) | 1.84(5) | 2.700(4) | 158(4) |
| N16A | H16A | O10B[2] | 0.96(6) | 1.85(6) | 2.786(4) | 167(5) |

[1]1-X,-1/2+Y,1-Z; [2]1-X,1/2+Y,1-Z

**Torsion Angles for compound 3.**

| A | B | C | D | Angle/° | A | B | C | D | Angle/° |
|---|---|---|---|---|---|---|---|---|---|
| B1 | O11 | C10 | O10 | 176.3(4) | C22B | C23B | C24B | C25B | 2.2(11) |
| B1 | O11 | C10 | C11 | -8.1(5) | C22D | C21D | C26D | C25D | 1(4) |
| B1 | O12 | C12 | C11 | 22.6(5) | C22D | C23D | C24D | C25D | -2(4) |
| B1 | O12 | C12 | C13 | -157.9(3) | C23B | C24B | C25B | C26B | -0.9(11) |
| B1 | O21 | C20 | O20 | 176.1(4) | C23D | C24D | C25D | C26D | 1(4) |
| B1 | O21 | C20 | C21 | -5.0(5) | C24B | C25B | C26B | C21B | 0.0(10) |
| B1 | O22 | C22 | C21 | 8.8(5) | C24D | C25D | C26D | C21D | -1(5) |
| B1 | O22 | C22 | C23 | -172.3(4) | C26B | C21B | C22B | O22B | 178.7(6) |
| O10 | C10 | C11 | C12 | 162.6(3) | C26B | C21B | C22B | C23B | 1.7(10) |
| O10 | C10 | C11 | C16 | -13.4(5) | C26D | C21D | C22D | O22D | 179.8(19) |
| O11 | B1 | O12 | C12 | -40.8(5) | C26D | C21D | C22D | C23D | -2(3) |
| O11 | B1 | O21 | C20 | -104.1(4) | B4 | O11C | C10C | O10C | 173.8(4) |
| O11 | B1 | O22 | C22 | 102.8(4) | B4 | O11C | C10C | C11C | -8.9(5) |
| O11 | C10 | C11 | C12 | -13.0(5) | B4 | O12C | C12C | C11C | 21.1(8) |
| O11 | C10 | C11 | C16 | 171.0(3) | B4 | O12C | C12C | C13C | -158.8(5) |
| O12 | B1 | O11 | C10 | 34.2(5) | B4 | O12E | C12E | C11C | -37(5) |
| O12 | B1 | O21 | C20 | 135.3(4) | B4 | O12E | C12E | C13E | 156(4) |
| O12 | B1 | O22 | C22 | -137.3(3) | B4 | O21C | C20C | O20C | 172.6(4) |
| O12 | C12 | C13 | C14 | 178.0(3) | B4 | O21C | C20C | C21C | -11.5(6) |
| O20 | C20 | C21 | C22 | 176.3(4) | B4 | O21E | C10H | O20E | -164(3) |
| O20 | C20 | C21 | C26 | -0.9(6) | B4 | O21E | C10H | C22C | 15(4) |
| O21 | B1 | O11 | C10 | -84.9(4) | B4 | O22C | C22C | C21C | 19.0(5) |
| O21 | B1 | O12 | C12 | 76.8(4) | B4 | O22C | C22C | C23C | -161.8(4) |
| O21 | B1 | O22 | C22 | -15.1(5) | B4 | O22E | C21C | C22C | -19.2(18) |
| O21 | C20 | C21 | C22 | -2.6(5) | B4 | O22E | C21C | C26C | 164.5(8) |
| O21 | C20 | C21 | C26 | -179.8(4) | O10C | C10C | C11C | C12C | 168.3(4) |
| O22 | B1 | O11 | C10 | 151.9(3) | O10C | C10C | C11C | C12E | -165(3) |
| O22 | B1 | O12 | C12 | -157.5(3) | O10C | C10C | C11C | C16C | -6.6(6) |
| O22 | B1 | O21 | C20 | 13.7(6) | O11C | B4 | O12C | C12C | -35.8(6) |
| O22 | C22 | C23 | C24 | -179.4(4) | O11C | B4 | O12E | C12E | 43(3) |
| C10 | C11 | C12 | O12 | 5.8(5) | O11C | B4 | O21C | C20C | -84.4(5) |
| C10 | C11 | C12 | C13 | -173.8(3) | O11C | B4 | O21E | C10H | 81(3) |
| C10 | C11 | C16 | C15 | 175.8(3) | O11C | B4 | O22C | C22C | 81.8(5) |
| C11 | C12 | C13 | C14 | -2.5(5) | O11C | B4 | O22E | C21C | -79.3(18) |
| C12 | C11 | C16 | C15 | -0.2(5) | O11C | C10C | C11C | C12C | -8.9(6) |
| C12 | C13 | C14 | C15 | 0.6(6) | O11C | C10C | C11C | C12E | 18(3) |
| C13 | C14 | C15 | C16 | 1.5(6) | O11C | C10C | C11C | C16C | 176.1(4) |
| C14 | C15 | C16 | C11 | -1.7(6) | O12C | B4 | O11C | C10C | 30.7(5) |
| C16 | C11 | C12 | O12 | -178.2(3) | O12C | B4 | O21C | C20C | 154.4(4) |
| C16 | C11 | C12 | C13 | 2.2(5) | O12C | B4 | O22C | C22C | -158.3(4) |

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|---|---|---|---|---|---|---|---|---|---|
| C20 | C21 | C22 | O22 | 0.7(5) | O12C | C12C | C13C | C14C | 178.9(5) |
| C20 | C21 | C22 | C23 | -178.2(4) | O12E | B4 | O11C | C10C | -22.4(13) |
| C20 | C21 | C26 | C25 | 179.6(4) | O12E | B4 | O21E | C10H | -146(3) |
| C21 | C22 | C23 | C24 | -0.5(6) | O12E | B4 | O22E | C21C | 164(2) |
| C22 | C21 | C26 | C25 | 2.3(7) | O12E | C12E | C13E | C14C | 180(4) |
| C22 | C23 | C24 | C25 | 0.6(7) | O20C | C20C | C21C | C22C | 167.9(4) |
| C23 | C24 | C25 | C26 | 0.7(7) | O20C | C20C | C21C | C26C | -8.0(7) |
| C24 | C25 | C26 | C21 | -2.2(8) | O20E | C10H | C22C | C21C | -156(3) |
| C26 | C21 | C22 | O22 | 177.9(4) | O20E | C10H | C22C | C23C | 7(4) |
| C26 | C21 | C22 | C23 | -1.0(6) | O21C | B4 | O11C | C10C | -89.1(5) |
| B2 | O11A | C10A | O10A | 176.4(4) | O21C | B4 | O12C | C12C | 82.5(5) |
| B2 | O11A | C10A | C11A | -8.6(6) | O21C | B4 | O22C | C22C | -36.3(5) |
| B2 | O12A | C12A | C11A | 22.2(5) | O21C | C20C | C21C | C22C | -7.8(6) |
| B2 | O12A | C12A | C13A | -158.9(4) | O21C | C20C | C21C | C26C | 176.2(4) |
| B2 | O21A | C20A | O20A | 176.8(4) | O21E | B4 | O11C | C10C | 108.9(16) |
| B2 | O21A | C20A | C21A | -6.6(6) | O21E | B4 | O12E | C12E | -90(3) |
| B2 | O22A | C22A | C21A | 11.5(6) | O21E | B4 | O22E | C21C | 51(3) |
| B2 | O22A | C22A | C23A | -169.9(4) | O21E | C10H | C22C | C21C | 25(4) |
| O10A | C10A | C11A | C12A | 162.8(4) | O21E | C10H | C22C | C23C | -171(2) |
| O10A | C10A | C11A | C16A | -13.6(6) | O22C | B4 | O11C | C10C | 147.9(4) |
| O11A | B2 | O12A | C12A | -40.1(5) | O22C | B4 | O12C | C12C | -152.3(4) |
| O11A | B2 | O21A | C20A | -100.2(4) | O22C | B4 | O21C | C20C | 33.3(6) |
| O11A | B2 | O22A | C22A | 97.8(4) | O22C | C22C | C23C | C24C | 179.6(4) |
| O11A | C10A | C11A | C12A | -12.3(6) | O22E | B4 | O11C | C10C | -120.0(13) |
| O11A | C10A | C11A | C16A | 171.4(4) | O22E | B4 | O12E | C12E | 152(3) |
| O12A | B2 | O11A | C10A | 33.9(6) | O22E | B4 | O21E | C10H | -46(3) |
| O12A | B2 | O21A | C20A | 139.3(4) | O22E | C21C | C22C | C10H | -17(3) |
| O12A | B2 | O22A | C22A | -142.1(4) | O22E | C21C | C22C | C23C | -177.4(12) |
| O12A | C12A | C13A | C14A | 178.0(4) | O22E | C21C | C26C | C25C | 176(2) |
| O20A | C20A | C21A | C22A | 173.3(4) | C10C | C11C | C12C | O12C | 2.9(8) |
| O20A | C20A | C21A | C26A | -4.5(7) | C10C | C11C | C12C | C13C | -177.2(5) |
| O21A | B2 | O11A | C10A | -85.5(5) | C10C | C11C | C12E | O12E | 9(6) |
| O21A | B2 | O12A | C12A | 77.2(4) | C10C | C11C | C12E | C13E | 175(4) |
| O21A | B2 | O22A | C22A | -19.6(6) | C10C | C11C | C16C | C15C | 178.0(4) |
| O21A | C20A | C21A | C22A | -3.2(6) | C10H | C22C | C23C | C24C | -171.3(13) |
| O21A | C20A | C21A | C26A | 179.1(4) | C11C | C12C | C13C | C14C | -1.0(9) |
| O22A | B2 | O11A | C10A | 151.6(4) | C11C | C12E | C13E | C14C | 12(7) |
| O22A | B2 | O12A | C12A | -157.4(3) | C12C | C11C | C16C | C15C | 3.1(7) |
| O22A | B2 | O21A | C20A | 17.8(6) | C12C | C13C | C14C | C15C | 3.5(9) |
| O22A | C22A | C23A | C24A | -178.9(4) | C12E | C11C | C16C | C15C | -24(3) |
| C10A | C11A | C12A | O12A | 5.6(5) | C12E | C13E | C14C | C15C | -37(5) |
| C10A | C11A | C12A | C13A | -173.3(4) | C13C | C14C | C15C | C16C | -2.7(9) |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| C10A | C11A | C16A | C15A | 175.8(4) | C13E | C14C | C15C | C16C | 33(3) |
| C11A | C12A | C13A | C14A | -3.1(6) | C14C | C15C | C16C | C11C | -0.6(8) |
| C12A | C11A | C16A | C15A | -0.6(6) | C16C | C11C | C12C | O12C | 177.8(5) |
| C12A | C13A | C14A | C15A | 0.5(6) | C16C | C11C | C12C | C13C | -2.3(8) |
| C13A | C14A | C15A | C16A | 2.0(6) | C16C | C11C | C12E | O12E | -150(4) |
| C14A | C15A | C16A | C11A | -2.0(6) | C16C | C11C | C12E | C13E | 16(6) |
| C16A | C11A | C12A | O12A | -178.0(4) | C20C | C21C | C22C | O22C | 3.6(6) |
| C16A | C11A | C12A | C13A | 3.1(6) | C20C | C21C | C22C | C23C | -175.6(4) |
| C20A | C21A | C22A | O22A | 0.7(6) | C20C | C21C | C26C | C25C | 176.5(4) |
| C20A | C21A | C22A | C23A | -177.8(4) | C21C | C22C | C23C | C24C | -1.1(7) |
| C20A | C21A | C26A | C25A | 178.5(5) | C22C | C21C | C26C | C25C | 0.4(6) |
| C21A | C22A | C23A | C24A | -0.3(6) | C22C | C23C | C24C | C25C | 1.3(7) |
| C22A | C21A | C26A | C25A | 0.7(7) | C23C | C24C | C25C | C26C | -0.7(7) |
| C22A | C23A | C24A | C25A | 0.0(7) | C24C | C25C | C26C | C21C | -0.2(7) |
| C23A | C24A | C25A | C26A | 0.6(8) | C26C | C21C | C22C | O22C | 179.5(4) |
| C24A | C25A | C26A | C21A | -1.0(8) | C26C | C21C | C22C | C10H | 161(2) |
| C26A | C21A | C22A | O22A | 178.5(4) | C26C | C21C | C22C | C23C | 0.2(6) |
| C26A | C21A | C22A | C23A | -0.1(6) | N1 | C31 | C32 | C33 | -54.6(5) |
| B3 | O11B | C10B | O10B | 177.9(4) | N1 | C35 | C39 | C38 | -60.2(4) |
| B3 | O11B | C10B | C11B | -2.7(5) | N1 | C35 | C39 | C40 | 62.2(4) |
| B3 | O12B | C12B | C11B | 23.5(9) | N1 | C36 | C37 | C38 | 54.7(4) |
| B3 | O12B | C12B | C13B | -155.5(6) | N1 | C36 | C37 | C45 | -69.9(4) |
| B3 | O12D | C12D | C11B | -30.0(16) | N16 | C41 | C42 | C43 | 57.8(5) |
| B3 | O12D | C12D | C13D | 154.7(13) | C31 | N1 | C35 | C34 | -58.3(4) |
| B3 | O21B | C20B | O20B | 175.1(5) | C31 | N1 | C35 | C39 | 175.0(3) |
| B3 | O21B | C20B | C21B | -8.6(7) | C31 | N1 | C36 | C37 | -173.2(3) |
| B3 | O21D | C20D | O20D | -165.8(10) | C31 | C32 | C33 | C34 | 54.7(6) |
| B3 | O21D | C20D | C21D | 16.1(17) | C32 | C33 | C34 | C35 | -57.0(5) |
| B3 | O22B | C22B | C21B | 19.3(8) | C33 | C34 | C35 | N1 | 58.8(5) |
| B3 | O22B | C22B | C23B | -163.6(6) | C33 | C34 | C35 | C39 | -176.5(4) |
| B3 | O22D | C22D | C21D | -27(2) | C34 | C35 | C39 | C38 | 175.6(3) |
| B3 | O22D | C22D | C23D | 154.5(17) | C34 | C35 | C39 | C40 | -62.0(4) |
| O10B | C10B | C11B | C12B | 165.6(5) | C35 | N1 | C31 | C32 | 56.3(4) |
| O10B | C10B | C11B | C12D | -164.7(8) | C35 | N1 | C36 | C37 | -48.6(4) |
| O10B | C10B | C11B | C16B | -3.8(6) | C35 | C39 | C40 | N16 | -120.8(3) |
| O11B | B3 | O12B | C12B | -36.8(7) | C36 | N1 | C31 | C32 | -177.9(3) |
| O11B | B3 | O12D | C12D | 40.9(10) | C36 | N1 | C35 | C34 | 177.9(3) |
| O11B | B3 | O21B | C20B | -85.9(5) | C36 | N1 | C35 | C39 | 51.3(4) |
| O11B | B3 | O21D | C20D | 81.6(10) | C36 | C37 | C38 | C39 | -63.2(4) |
| O11B | B3 | O22B | C22B | 82.0(5) | C36 | C37 | C45 | N16 | 116.5(3) |
| O11B | B3 | O22D | C22D | -79.4(11) | C36 | C37 | C45 | C44 | -122.6(4) |
| O11B | C10B | C11B | C12B | -13.8(6) | C37 | C38 | C39 | C35 | 66.4(4) |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| O11B | C10B | C11B | C12D | 15.9(9) | C37 | C38 | C39 | C40 | -58.7(4) |
| O11B | C10B | C11B | C16B | 176.8(4) | C38 | C37 | C45 | N16 | -7.0(4) |
| O12B | B3 | O11B | C10B | 27.1(6) | C38 | C37 | C45 | C44 | 114.0(4) |
| O12B | B3 | O21B | C20B | 152.3(5) | C38 | C39 | C40 | N16 | 0.5(4) |
| O12B | B3 | O22B | C22B | -160.5(5) | C40 | N16 | C41 | C42 | 174.5(3) |
| O12B | C12B | C13B | C14B | 177.4(6) | C40 | N16 | C45 | C37 | -52.9(4) |
| O12D | B3 | O11B | C10B | -25.6(7) | C40 | N16 | C45 | C44 | -175.9(3) |
| O12D | B3 | O21D | C20D | -149.1(9) | C41 | N16 | C40 | C39 | -178.4(3) |
| O12D | B3 | O22D | C22D | 161.8(10) | C41 | N16 | C45 | C37 | -178.6(3) |
| O12D | C12D | C13D | C14B | -178.0(12) | C41 | N16 | C45 | C44 | 58.4(4) |
| O20B | C20B | C21B | C22B | 167.6(6) | C41 | C42 | C43 | C44 | -55.2(5) |
| O20B | C20B | C21B | C26B | -9.1(9) | C42 | C43 | C44 | C45 | 55.5(5) |
| O20D | C20D | C21D | C22D | -170.1(16) | C43 | C44 | C45 | N16 | -56.5(4) |
| O20D | C20D | C21D | C26D | 12(3) | C43 | C44 | C45 | C37 | -178.5(4) |
| O21B | B3 | O11B | C10B | -95.9(5) | C45 | N16 | C40 | C39 | 56.4(4) |
| O21B | B3 | O12B | C12B | 82.2(6) | C45 | N16 | C41 | C42 | -60.2(4) |
| O21B | B3 | O22B | C22B | -34.9(6) | C45 | C37 | C38 | C39 | 62.5(4) |
| O21B | C20B | C21B | C22B | -8.7(8) | N1A | C31A | C32A | C33A | -54.9(6) |
| O21B | C20B | C21B | C26B | 174.6(6) | N1A | C35A | C39A | C38A | -59.8(4) |
| O21D | B3 | O11B | C10B | 100.5(6) | N1A | C35A | C39A | C40A | 62.0(5) |
| O21D | B3 | O12D | C12D | -87.7(10) | N1A | C36A | C37A | C38A | 55.2(4) |
| O21D | B3 | O22D | C22D | 48.8(12) | N1A | C36A | C37A | C41A | -69.2(5) |
| O21D | C20D | C21D | C22D | 8(2) | N16A | C41A | C42A | C43A | -56.5(5) |
| O21D | C20D | C21D | C26D | -170(2) | C31A | N1A | C35A | C34A | -58.8(5) |
| O22B | B3 | O11B | C10B | 140.6(4) | C31A | N1A | C35A | C39A | 175.0(4) |
| O22B | B3 | O12B | C12B | -150.3(5) | C31A | N1A | C36A | C37A | -173.2(3) |
| O22B | B3 | O21B | C20B | 30.6(7) | C31A | C32A | C33A | C34A | 53.8(6) |
| O22B | C22B | C23B | C24B | -179.7(7) | C32A | C33A | C34A | C35A | -55.2(6) |
| O22D | B3 | O11B | C10B | -131.4(6) | C33A | C34A | C35A | N1A | 58.0(5) |
| O22D | B3 | O12D | C12D | 155.3(9) | C33A | C34A | C35A | C39A | -177.2(4) |
| O22D | B3 | O21D | C20D | -44.5(12) | C34A | C35A | C39A | C38A | 175.7(4) |
| O22D | C22D | C23D | C24D | -179.5(16) | C34A | C35A | C39A | C40A | -62.5(5) |
| C10B | C11B | C12B | O12B | 3.5(9) | C35A | N1A | C31A | C32A | 57.4(5) |
| C10B | C11B | C12B | C13B | -177.5(6) | C35A | N1A | C36A | C37A | -49.4(5) |
| C10B | C11B | C12D | O12D | 3.0(17) | C35A | C39A | C40A | N16A | -119.6(4) |
| C10B | C11B | C12D | C13D | 178.1(12) | C36A | N1A | C31A | C32A | -177.3(4) |
| C10B | C11B | C16B | C15B | 178.3(5) | C36A | N1A | C35A | C34A | 177.9(4) |
| C11B | C12B | C13B | C14B | -1.6(11) | C36A | N1A | C35A | C39A | 51.6(5) |
| C11B | C12D | C13D | C14B | 7(2) | C36A | C37A | C38A | C39A | -63.6(4) |
| C12B | C11B | C16B | C15B | 9.1(8) | C36A | C37A | C41A | N16A | 116.3(4) |
| C12B | C13B | C14B | C15B | 10.2(11) | C36A | C37A | C41A | C42A | -122.0(4) |
| C12D | C11B | C16B | C15B | -20.2(10) | C37A | C38A | C39A | C35A | 66.2(4) |

| | | | |
|---|---|---|---|
| C12D C13D C14B C15B | -27.7(18) | C37A C38A C39A C40A | -58.8(5) |
| C13B C14B C15B C16B | -9.1(9) | C37A C41A C42A C43A | -179.0(4) |
| C13D C14B C15B C16B | 25.7(12) | C38A C37A C41A N16A | -7.0(5) |
| C14B C15B C16B C11B | -0.3(8) | C38A C37A C41A C42A | 114.7(4) |
| C16B C11B C12B O12B | 172.9(5) | C38A C39A C40A N16A | 0.9(5) |
| C16B C11B C12B C13B | -8.1(9) | C40A N16A C41A C37A | -52.9(4) |
| C16B C11B C12D O12D | -158.6(11) | C40A N16A C41A C42A | -176.6(3) |
| C16B C11B C12D C13D | 16.5(18) | C40A N16A C45A C44A | 174.4(4) |
| C20B C21B C22B O22B | 2.0(10) | C41A N16A C40A C39A | 55.9(4) |
| C20B C21B C22B C23B | -175.0(6) | C41A N16A C45A C44A | -59.8(5) |
| C20B C21B C26B C25B | 176.3(6) | C41A C37A C38A C39A | 62.4(5) |
| C20D C21D C22D O22D | 1(3) | C41A C42A C43A C44A | 56.3(5) |
| C20D C21D C22D C23D | 179(2) | C42A C43A C44A C45A | -56.3(5) |
| C20D C21D C26D C25D | 180(2) | C43A C44A C45A N16A | 58.4(5) |
| C21B C22B C23B C24B | -2.6(11) | C45A N16A C40A C39A | -178.9(3) |
| C21D C22D C23D C24D | 2(3) | C45A N16A C41A C37A | -178.5(3) |
| C22B C21B C26B C25B | -0.4(10) | C45A N16A C41A C42A | 57.8(4) |

**Hydrogen Atom Coordinates (Å×10$^4$) and Isotropic Displacement Parameters (Å$^2$×10$^3$) for compound 3.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| H13 | -776 | 7373 | 7704 | 42 |
| H14 | -2489 | 7670 | 7188 | 44 |
| H15 | -3263 | 7054 | 6105 | 42 |
| H16D | -2357 | 6105 | 5565 | 36 |
| H23 | 3532 | 5021 | 7808 | 45 |
| H24 | 5360 | 4992 | 7426 | 56 |
| H25 | 5963 | 5641 | 6319 | 69 |
| H26 | 4759 | 6343 | 5613 | 63 |
| H13A | 4140 | 2565 | 7322 | 50 |
| H14E | 2426 | 2300 | 7843 | 53 |
| H15A | 1730 | 2923 | 8943 | 55 |
| H16E | 2697 | 3850 | 9482 | 48 |
| H23A | 8525 | 4849 | 7191 | 44 |
| H24A | 10353 | 4902 | 7594 | 55 |
| H25A | 10962 | 4293 | 8725 | 72 |
| H26A | 9775 | 3605 | 9457 | 64 |
| H13B | 1478 | 4874 | 2664 | 57 |
| H13D | 1725 | 5283 | 2086 | 48 |
| H14B | -98 | 5029 | 1891 | 69 |
| H14A | -184 | 4867 | 2111 | 69 |
| H15B | -625 | 4137 | 999 | 72 |
| H16B | 635 | 3290 | 647 | 64 |
| H23B | 6048 | 2672 | 3437 | 47 |
| H23D | 6906 | 3895 | 1052 | 51 |
| H24B | 7870 | 2464 | 3047 | 47 |
| H24D | 8329 | 3190 | 1495 | 45 |
| H25B | 8613 | 3015 | 1931 | 49 |
| H25D | 8231 | 2567 | 2646 | 54 |
| H26B | 7548 | 3761 | 1137 | 41 |
| H26D | 6672 | 2587 | 3407 | 48 |
| H13C | 6392 | 5109 | 2327 | 61 |
| H13E | 6699 | 4677 | 2921 | 58 |
| H14C | 4795 | 5016 | 3065 | 72 |
| H14D | 4743 | 5200 | 2855 | 72 |
| H15C | 4416 | 5801 | 4110 | 71 |
| H16C | 5716 | 6626 | 4482 | 58 |
| H23C | 11042 | 7258 | 1589 | 66 |
| H24C | 12843 | 7441 | 1949 | 74 |
| H25C | 13597 | 6881 | 3074 | 66 |

| | | | | |
|---|---|---|---|---|
| H26C | 12539 | 6149 | 3869 | 60 |
| H31A | -2761 | 4020 | 3960 | 51 |
| H31B | -2253 | 4766 | 4132 | 51 |
| H32A | -2938 | 4772 | 5464 | 62 |
| H32B | -3921 | 4611 | 4843 | 62 |
| H33A | -3847 | 3439 | 5161 | 68 |
| H33B | -3945 | 3863 | 6001 | 68 |
| H34A | -2044 | 3754 | 6243 | 54 |
| H34B | -2552 | 3001 | 6118 | 54 |
| H35 | -2011 | 3011 | 4726 | 42 |
| H36A | -386 | 4375 | 3818 | 40 |
| H36B | -974 | 3676 | 3542 | 40 |
| H37 | 831 | 3416 | 3729 | 37 |
| H38A | 733 | 2530 | 4715 | 41 |
| H38B | -376 | 2558 | 4187 | 41 |
| H39 | -751 | 2501 | 5632 | 39 |
| H40A | -214 | 3804 | 6126 | 41 |
| H40B | 233 | 3097 | 6506 | 41 |
| H41A | 1647 | 4354 | 6361 | 52 |
| H41B | 1990 | 3639 | 6779 | 52 |
| H42A | 3425 | 3513 | 5854 | 65 |
| H42B | 3542 | 4236 | 6323 | 65 |
| H43A | 2809 | 4830 | 5186 | 68 |
| H43B | 3808 | 4370 | 4874 | 68 |
| H44A | 2268 | 4249 | 3985 | 52 |
| H44B | 2614 | 3523 | 4374 | 52 |
| H45 | 854 | 4362 | 4947 | 36 |
| H31C | 2842 | 5198 | 10875 | 59 |
| H31D | 2328 | 5948 | 11001 | 59 |
| H32C | 1165 | 5315 | 10156 | 69 |
| H32D | 2139 | 5136 | 9545 | 69 |
| H33C | 1203 | 6473 | 9771 | 79 |
| H33D | 1115 | 6019 | 8951 | 79 |
| H34C | 2467 | 6906 | 8819 | 67 |
| H34D | 2991 | 6156 | 8705 | 67 |
| H35A | 3052 | 6925 | 10211 | 55 |
| H36C | 4709 | 5600 | 11164 | 48 |
| H36D | 4123 | 6306 | 11405 | 48 |
| H37A | 5925 | 6560 | 11209 | 47 |
| H38C | 5794 | 7417 | 10197 | 53 |
| H38D | 4697 | 7395 | 10725 | 53 |
| H39A | 4288 | 7425 | 9283 | 52 |

| | | | | |
|---|---|---|---|---|
| H40C | 4843 | 6114 | 8813 | 48 |
| H40D | 5280 | 6817 | 8421 | 48 |
| H41C | 5928 | 5587 | 10019 | 41 |
| H42C | 7359 | 5718 | 10975 | 54 |
| H42D | 7700 | 6434 | 10563 | 54 |
| H43C | 8867 | 5567 | 10087 | 65 |
| H43D | 7850 | 5113 | 9784 | 65 |
| H44C | 8467 | 6417 | 9100 | 62 |
| H44D | 8583 | 5688 | 8644 | 62 |
| H45A | 6685 | 5563 | 8609 | 55 |
| H45B | 7018 | 6270 | 8169 | 55 |
| H1A | 4040(40) | 5620(30) | 9880(30) | 43(13) |
| H16 | 1550(40) | 3110(30) | 5540(30) | 36(12) |
| H1 | -1130(30) | 4290(20) | 5080(30) | 24(10) |
| H16A | 6670(40) | 6850(30) | 9360(30) | 49(14) |

**Atomic Occupancy for compound 3.**

| Atom | *Occupancy* | Atom | *Occupancy* | Atom | *Occupancy* |
|---|---|---|---|---|---|
| O12B | 0.7 | O12D | 0.3 | O20B | 0.7 |
| O20D | 0.3 | O21B | 0.7 | O21D | 0.3 |
| O22B | 0.7 | O22D | 0.3 | C12B | 0.7 |
| C12D | 0.3 | C13B | 0.7 | H13B | 0.7 |
| C13D | 0.3 | H13D | 0.3 | H14B | 0.7 |
| H14A | 0.3 | C20B | 0.7 | C20D | 0.3 |
| C21B | 0.7 | C21D | 0.3 | C22B | 0.7 |
| C22D | 0.3 | C23B | 0.7 | H23B | 0.7 |
| C23D | 0.3 | H23D | 0.3 | C24B | 0.7 |
| H24B | 0.7 | C24D | 0.3 | H24D | 0.3 |
| C25B | 0.7 | H25B | 0.7 | C25D | 0.3 |
| H25D | 0.3 | C26B | 0.7 | H26B | 0.7 |
| C26D | 0.3 | H26D | 0.3 | O12C | 0.9 |
| O12E | 0.1 | O20C | 0.85 | O20E | 0.15 |
| O21C | 0.85 | O21E | 0.15 | O22C | 0.85 |
| O22E | 0.15 | C10H | 0.15 | C12C | 0.9 |
| C12E | 0.1 | C13C | 0.9 | H13C | 0.9 |
| C13E | 0.1 | H13E | 0.1 | H14C | 0.9 |
| H14D | 0.1 | C20C | 0.85 | | |

**Table 5 Crystal data and structure refinement for compound 4.**

| | |
|---|---|
| Identification code | lawr111b |
| Empirical formula | $C_{30}H_{44}BNO_6$ |
| Formula weight | 525.47 |
| Temperature/K | 100.00(10) |
| Crystal system | monoclinic |
| Space group | $P2_1$ |
| a/Å | 9.49961(15) |
| b/Å | 13.42524(18) |
| c/Å | 12.0837(2) |
| α/° | 90 |
| β/° | 110.1708(19) |
| γ/° | 90 |
| Volume/Å$^3$ | 1446.58(4) |
| Z | 2 |
| $\rho_{calc}$g/cm$^3$ | 1.206 |
| μ/mm$^{-1}$ | 0.659 |
| F(000) | 568.0 |
| Crystal size/mm$^3$ | 0.03 × 0.02 × 0.02 |
| Radiation | CuKα (λ = 1.54184) |
| 2Θ range for data collection/° | 7.794 to 135 |
| Index ranges | $-11 \leq h \leq 11$, $-16 \leq k \leq 16$, $-14 \leq l \leq 14$ |
| Reflections collected | 21442 |
| Independent reflections | 5215 [$R_{int}$ = 0.0393, $R_{sigma}$ = 0.0330] |
| Data/restraints/parameters | 5215/1/347 |
| Goodness-of-fit on $F^2$ | 1.036 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0281, $wR_2$ = 0.0640 |
| Final R indexes [all data] | $R_1$ = 0.0309, $wR_2$ = 0.0652 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.13/-0.15 |
| Flack parameter | -0.03(7) |

**Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for compound 4. $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| O20 | 2415.1(16) | 4091.0(11) | 5070.2(13) | 22.2(3) |
| O21 | 2272.8(15) | 4424.3(10) | 3244.7(12) | 18.7(3) |
| O22 | 3273.2(15) | 3281.9(10) | 2124.7(12) | 19.0(3) |
| O30 | 4647.6(16) | 6531.0(11) | 2046.1(14) | 25.9(3) |
| O31 | 3920.9(14) | 5005.3(10) | 2272.2(12) | 18.1(3) |
| O32 | 1399.9(14) | 4414.4(10) | 1143.1(12) | 19.0(3) |
| C20 | 2747(2) | 3873.2(13) | 4212.9(17) | 15.7(4) |
| C21 | 3646(2) | 2982.9(13) | 4164.2(18) | 15.2(4) |
| C22 | 3861(2) | 2735.5(14) | 3106.7(17) | 15.4(4) |
| C23 | 4683(2) | 1883.5(15) | 3053.2(18) | 18.7(4) |
| C24 | 5283(2) | 1288.8(14) | 4040(2) | 20.8(4) |
| C25 | 5067(2) | 1527.2(15) | 5092(2) | 21.5(4) |
| C26 | 4257(2) | 2369.4(15) | 5149.6(18) | 18.6(4) |
| C30 | 3663(2) | 5906.9(15) | 1797.9(17) | 17.1(4) |
| C31 | 2134(2) | 6091.3(14) | 948.6(17) | 16.5(4) |
| C32 | 1087(2) | 5320.5(14) | 648.6(17) | 16.0(4) |
| C33 | -334(2) | 5488.3(16) | -193.1(18) | 20.3(4) |
| C34 | -696(2) | 6415.1(18) | -700.6(18) | 24.9(4) |
| C35 | 336(3) | 7197.2(16) | -395(2) | 26.3(5) |
| C36 | 1753(2) | 7027.8(15) | 422.9(18) | 21.7(4) |
| B1 | 2714(2) | 4273.6(16) | 2186.4(19) | 17.0(4) |
| N1 | 9335.0(17) | 7038.1(12) | 3325.5(15) | 16.0(3) |
| C1 | 9267(2) | 6938.0(15) | 4559.3(18) | 16.9(4) |
| C2 | 10613(2) | 6432.8(15) | 5453.3(18) | 18.6(4) |
| C3 | 10367(2) | 6327.4(15) | 6627.3(18) | 20.7(4) |
| C4 | 11696(2) | 5804.3(15) | 7535.5(19) | 22.3(4) |
| C5 | 7926(2) | 7604.0(14) | 2598.2(17) | 16.7(4) |
| C6 | 7836(2) | 7895.5(17) | 1356.3(19) | 23.7(4) |
| C7 | 6202(2) | 8088.2(17) | 568.6(19) | 24.6(4) |
| C8 | 5459(2) | 8948.0(18) | 971(2) | 32.5(5) |
| C9 | 10741(2) | 7580.8(14) | 3341.6(18) | 18.2(4) |
| C10 | 10911(2) | 8635.2(14) | 3839(2) | 22.9(4) |
| C11 | 12532(2) | 8999.6(15) | 4147.4(19) | 21.7(4) |
| C12 | 13069(3) | 9029.4(18) | 3104(2) | 30.6(5) |
| C13 | 9389(2) | 6013.9(14) | 2801.0(18) | 17.2(4) |
| C14 | 8220(2) | 5272.8(14) | 2881.7(19) | 19.2(4) |
| C15 | 8210(2) | 4360.8(15) | 2126(2) | 23.5(4) |
| C16 | 7142(2) | 3558.6(14) | 2247(2) | 23.6(4) |

**Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for compound 4. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.**

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| O20 | 28.3(7) | 19.5(7) | 22.7(7) | -0.6(6) | 14.0(6) | -0.5(6) |
| O21 | 19.8(6) | 16.8(6) | 20.0(7) | 2.0(5) | 7.7(5) | 4.2(5) |
| O22 | 25.8(7) | 16.0(6) | 15.5(7) | 3.4(5) | 7.3(6) | 4.8(5) |
| O30 | 21.0(7) | 25.8(8) | 28.4(8) | 0.8(6) | 5.4(6) | -8.2(6) |
| O31 | 13.7(6) | 19.4(7) | 19.2(7) | 2.7(5) | 3.2(5) | 0.6(5) |
| O32 | 17.4(6) | 15.9(7) | 20.3(7) | 2.9(5) | 2.0(5) | -2.8(5) |
| C20 | 14.3(8) | 14.4(9) | 18.8(10) | -0.5(7) | 6.2(7) | -3.7(7) |
| C21 | 12.8(8) | 13.4(8) | 18.8(10) | 0.0(7) | 4.6(7) | -3.9(6) |
| C22 | 13.2(8) | 15.4(8) | 17.2(9) | 1.6(7) | 4.6(7) | -3.3(7) |
| C23 | 17.6(8) | 17.6(9) | 21.6(10) | -1.8(8) | 7.6(7) | -1.0(7) |
| C24 | 15.7(9) | 14.3(9) | 30.5(11) | 1.7(8) | 5.5(8) | 0.6(7) |
| C25 | 17.1(9) | 18.8(9) | 24.8(11) | 7.7(8) | 2.5(8) | -0.1(8) |
| C26 | 15.4(8) | 20.8(9) | 18.5(10) | 1.1(7) | 4.5(7) | -4.5(7) |
| C30 | 18.6(9) | 18.6(9) | 15.8(9) | -1.9(7) | 8.3(7) | -0.7(8) |
| C31 | 20.1(9) | 16.6(9) | 14.7(9) | -0.4(7) | 8.2(7) | 1.3(7) |
| C32 | 17.1(9) | 18.5(9) | 13.4(9) | -0.1(7) | 6.6(7) | 2.0(7) |
| C33 | 16.2(9) | 27.3(10) | 16.2(10) | 1.8(8) | 4.1(7) | -0.4(8) |
| C34 | 20.2(10) | 36.3(11) | 17.2(10) | 6.5(9) | 5.1(8) | 9.4(9) |
| C35 | 34.2(11) | 22.2(10) | 24.7(11) | 7.0(8) | 12.9(9) | 11.6(8) |
| C36 | 29.5(10) | 18.2(10) | 19.2(10) | 1.1(8) | 10.6(8) | 0.6(8) |
| B1 | 16.5(9) | 16.1(10) | 17.7(10) | 2.1(8) | 4.8(8) | 1.3(8) |
| N1 | 14.1(7) | 14.8(7) | 19.1(8) | -1.3(6) | 5.8(6) | 0.7(6) |
| C1 | 15.5(8) | 17.6(9) | 18.7(10) | -3.2(7) | 7.3(7) | 0.9(7) |
| C2 | 15.8(9) | 18.1(9) | 21.2(10) | -2.6(8) | 5.3(7) | 1.0(7) |
| C3 | 19.5(10) | 20.5(10) | 21.9(10) | -1.1(8) | 6.9(8) | -0.9(8) |
| C4 | 21.4(9) | 21(1) | 23.2(11) | 1.5(8) | 6.0(8) | -0.4(8) |
| C5 | 13.1(8) | 18.7(9) | 17.6(10) | -0.5(8) | 4.3(7) | 1.2(7) |
| C6 | 22.2(10) | 28.8(11) | 21.7(11) | 3.6(8) | 9.6(8) | 1.7(8) |
| C7 | 23.4(10) | 31.2(11) | 17.3(10) | 2.2(8) | 4.9(8) | -1.1(9) |
| C8 | 22.6(10) | 37.1(13) | 30.7(12) | 0.5(10) | 0.2(9) | 4.8(9) |
| C9 | 13.1(8) | 18.5(9) | 23.1(10) | -1.8(8) | 6.3(7) | -1.5(7) |
| C10 | 16.5(9) | 17.8(10) | 33.4(12) | -4.8(8) | 7.2(9) | 0.0(7) |
| C11 | 17.8(9) | 19.9(10) | 24.8(10) | -3.5(8) | 3.9(8) | -1.1(8) |
| C12 | 30.2(11) | 31.2(12) | 31.9(12) | -1.3(9) | 12.6(9) | -9.9(9) |
| C13 | 16.8(8) | 15.0(9) | 20.4(9) | -4.5(7) | 7.1(7) | 0.3(7) |
| C14 | 17.9(8) | 16.6(9) | 24.1(11) | -2.6(8) | 8.6(8) | -0.9(7) |
| C15 | 21.1(9) | 20.5(10) | 30.9(11) | -8.5(9) | 11.7(8) | -4.6(8) |

| | | | | | |
|---|---|---|---|---|---|
| C16 | 22.0(9) | 16.2(9) | 30.8(12) | -1.3(8) | 7.0(9) | -2.6(7) |

**Bond Lengths for compound 4.**

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| O20 | C20 | 1.218(3) | C32 | C33 | 1.401(3) |
| O21 | C20 | 1.325(2) | C33 | C34 | 1.377(3) |
| O21 | B1 | 1.491(3) | C34 | C35 | 1.397(3) |
| O22 | C22 | 1.342(2) | C35 | C36 | 1.387(3) |
| O22 | B1 | 1.445(3) | N1 | C1 | 1.520(3) |
| O30 | C30 | 1.214(3) | N1 | C5 | 1.527(2) |
| O31 | C30 | 1.325(2) | N1 | C9 | 1.516(2) |
| O31 | B1 | 1.486(2) | N1 | C13 | 1.522(2) |
| O32 | C32 | 1.343(2) | C1 | C2 | 1.520(2) |
| O32 | B1 | 1.449(2) | C2 | C3 | 1.522(3) |
| C20 | C21 | 1.482(3) | C3 | C4 | 1.528(3) |
| C21 | C22 | 1.402(3) | C5 | C6 | 1.525(3) |
| C21 | C26 | 1.399(3) | C6 | C7 | 1.537(3) |
| C22 | C23 | 1.399(3) | C7 | C8 | 1.517(3) |
| C23 | C24 | 1.384(3) | C9 | C10 | 1.525(3) |
| C24 | C25 | 1.393(3) | C10 | C11 | 1.534(3) |
| C25 | C26 | 1.383(3) | C11 | C12 | 1.515(3) |
| C30 | C31 | 1.482(3) | C13 | C14 | 1.519(3) |
| C31 | C32 | 1.394(3) | C14 | C15 | 1.526(3) |
| C31 | C36 | 1.399(3) | C15 | C16 | 1.521(3) |

**Bond Angles for compound 4.**

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| C20 | O21 | B1 | 124.84(15) | C33 | C34 | C35 | 121.11(18) |
| C22 | O22 | B1 | 120.43(16) | C36 | C35 | C34 | 119.06(19) |
| C30 | O31 | B1 | 123.40(15) | C35 | C36 | C31 | 120.4(2) |
| C32 | O32 | B1 | 119.84(15) | O22 | B1 | O21 | 112.73(16) |
| O20 | C20 | O21 | 120.55(17) | O22 | B1 | O31 | 108.93(16) |
| O20 | C20 | C21 | 123.30(18) | O22 | B1 | O32 | 107.29(16) |
| O21 | C20 | C21 | 116.12(17) | O31 | B1 | O21 | 106.79(15) |
| C22 | C21 | C20 | 119.64(17) | O32 | B1 | O21 | 108.41(16) |
| C26 | C21 | C20 | 121.12(18) | O32 | B1 | O31 | 112.78(16) |
| C26 | C21 | C22 | 119.22(17) | C1 | N1 | C5 | 106.44(14) |
| O22 | C22 | C21 | 121.95(17) | C1 | N1 | C13 | 110.33(15) |
| O22 | C22 | C23 | 118.36(18) | C9 | N1 | C1 | 111.42(15) |
| C23 | C22 | C21 | 119.68(18) | C9 | N1 | C5 | 111.24(14) |
| C24 | C23 | C22 | 120.16(19) | C9 | N1 | C13 | 106.46(14) |
| C23 | C24 | C25 | 120.49(18) | C13 | N1 | C5 | 111.01(14) |
| C26 | C25 | C24 | 119.55(18) | C2 | C1 | N1 | 115.24(15) |
| C25 | C26 | C21 | 120.90(19) | C1 | C2 | C3 | 109.99(16) |
| O30 | C30 | O31 | 120.78(18) | C2 | C3 | C4 | 110.97(17) |
| O30 | C30 | C31 | 122.93(18) | C6 | C5 | N1 | 115.76(16) |
| O31 | C30 | C31 | 116.28(17) | C5 | C6 | C7 | 110.76(17) |
| C32 | C31 | C30 | 119.81(17) | C8 | C7 | C6 | 114.30(18) |
| C32 | C31 | C36 | 120.00(18) | N1 | C9 | C10 | 115.12(16) |
| C36 | C31 | C30 | 120.17(18) | C9 | C10 | C11 | 110.65(16) |
| O32 | C32 | C31 | 121.90(17) | C12 | C11 | C10 | 113.85(18) |
| O32 | C32 | C33 | 118.62(17) | C14 | C13 | N1 | 115.74(16) |
| C31 | C32 | C33 | 119.48(18) | C13 | C14 | C15 | 109.91(17) |
| C34 | C33 | C32 | 119.92(19) | C16 | C15 | C14 | 112.15(18) |

**Torsion Angles for compound 4.**

| A | B | C | D | Angle/° | A | B | C | D | Angle/° |
|---|---|---|---|---|---|---|---|---|---|
| O20 | C20 | C21 | C22 | 174.16(17) | C32 | O32 | B1 | O31 | -26.8(2) |
| O20 | C20 | C21 | C26 | -4.4(3) | C32 | C31 | C36 | C35 | 0.2(3) |
| O21 | C20 | C21 | C22 | -4.1(2) | C32 | C33 | C34 | C35 | 0.3(3) |
| O21 | C20 | C21 | C26 | 177.34(16) | C33 | C34 | C35 | C36 | 0.8(3) |
| O22 | C22 | C23 | C24 | -178.69(17) | C34 | C35 | C36 | C31 | -1.0(3) |
| O30 | C30 | C31 | C32 | 175.91(19) | C36 | C31 | C32 | O32 | -179.14(18) |
| O30 | C30 | C31 | C36 | -2.2(3) | C36 | C31 | C32 | C33 | 0.9(3) |
| O31 | C30 | C31 | C32 | -3.1(3) | B1 | O21 | C20 | O20 | 174.72(17) |
| O31 | C30 | C31 | C36 | 178.74(18) | B1 | O21 | C20 | C21 | -6.9(2) |
| O32 | C32 | C33 | C34 | 178.89(19) | B1 | O22 | C22 | C21 | 15.5(3) |
| C20 | O21 | B1 | O22 | 20.6(2) | B1 | O22 | C22 | C23 | -165.99(16) |
| C20 | O21 | B1 | O31 | -99.04(19) | B1 | O31 | C30 | O30 | 168.19(19) |
| C20 | O21 | B1 | O32 | 139.17(16) | B1 | O31 | C30 | C31 | -12.8(3) |
| C20 | C21 | C22 | O22 | -0.1(3) | B1 | O32 | C32 | C31 | 13.5(3) |
| C20 | C21 | C22 | C23 | -178.65(16) | B1 | O32 | C32 | C33 | -166.54(18) |
| C20 | C21 | C26 | C25 | 178.54(18) | N1 | C1 | C2 | C3 | -176.83(16) |
| C21 | C22 | C23 | C24 | -0.1(3) | N1 | C5 | C6 | C7 | 158.58(17) |
| C22 | O22 | B1 | O21 | -24.2(2) | N1 | C9 | C10 | C11 | 163.65(17) |
| C22 | O22 | B1 | O31 | 94.17(19) | N1 | C13 | C14 | C15 | 169.29(16) |
| C22 | O22 | B1 | O32 | -143.46(16) | C1 | N1 | C5 | C6 | 173.41(16) |
| C22 | C21 | C26 | C25 | 0.0(3) | C1 | N1 | C9 | C10 | -59.7(2) |
| C22 | C23 | C24 | C25 | 0.4(3) | C1 | N1 | C13 | C14 | 49.3(2) |
| C23 | C24 | C25 | C26 | -0.5(3) | C1 | C2 | C3 | C4 | 178.99(16) |
| C24 | C25 | C26 | C21 | 0.3(3) | C5 | N1 | C1 | C2 | -177.31(15) |
| C26 | C21 | C22 | O22 | 178.41(17) | C5 | N1 | C9 | C10 | 58.9(2) |
| C26 | C21 | C22 | C23 | -0.1(3) | C5 | N1 | C13 | C14 | -68.5(2) |
| C30 | O31 | B1 | O21 | -91.7(2) | C5 | C6 | C7 | C8 | 62.7(2) |
| C30 | O31 | B1 | O22 | 146.31(17) | C9 | N1 | C1 | C2 | -55.9(2) |
| C30 | O31 | B1 | O32 | 27.3(3) | C9 | N1 | C5 | C6 | 51.9(2) |
| C30 | C31 | C32 | O32 | 2.7(3) | C9 | N1 | C13 | C14 | 170.32(16) |
| C30 | C31 | C32 | C33 | -177.22(18) | C9 | C10 | C11 | C12 | 60.1(2) |
| C30 | C31 | C36 | C35 | 178.3(2) | C13 | N1 | C1 | C2 | 62.2(2) |
| C31 | C32 | C33 | C34 | -1.2(3) | C13 | N1 | C5 | C6 | -66.5(2) |
| C32 | O32 | B1 | O21 | 91.2(2) | C13 | N1 | C9 | C10 | 179.96(17) |
| C32 | O32 | B1 | O22 | -146.80(17) | C13 | C14 | C15 | C16 | 175.65(17) |

**Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for compound 4.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| H23 | 4830 | 1713 | 2338 | 22 |
| H24 | 5845 | 714 | 3999 | 25 |
| H25 | 5473 | 1114 | 5765 | 26 |
| H26 | 4114 | 2534 | 5868 | 22 |
| H33 | -1048 | 4963 | -414 | 24 |
| H34 | -1665 | 6524 | -1268 | 30 |
| H35 | 72 | 7836 | -743 | 32 |
| H36 | 2470 | 7551 | 628 | 26 |
| H1A | 9161 | 7612 | 4855 | 20 |
| H1B | 8355 | 6556 | 4508 | 20 |
| H2A | 11527 | 6833 | 5562 | 22 |
| H2B | 10761 | 5767 | 5159 | 22 |
| H3A | 9441 | 5940 | 6512 | 25 |
| H3B | 10235 | 6996 | 6924 | 25 |
| H4A | 11863 | 5159 | 7223 | 33 |
| H4B | 11480 | 5702 | 8264 | 33 |
| H4C | 12596 | 6217 | 7701 | 33 |
| H5A | 7042 | 7188 | 2538 | 20 |
| H5B | 7857 | 8218 | 3031 | 20 |
| H6A | 8261 | 7355 | 1011 | 28 |
| H6B | 8439 | 8504 | 1392 | 28 |
| H7A | 6176 | 8225 | -243 | 29 |
| H7B | 5611 | 7476 | 543 | 29 |
| H8A | 4419 | 9014 | 438 | 49 |
| H8B | 6005 | 9566 | 960 | 49 |
| H8C | 5475 | 8820 | 1773 | 49 |
| H9A | 10749 | 7612 | 2525 | 22 |
| H9B | 11624 | 7185 | 3813 | 22 |
| H10A | 10630 | 8646 | 4556 | 28 |
| H10B | 10226 | 9089 | 3251 | 28 |
| H11A | 12615 | 9676 | 4489 | 26 |
| H11B | 13202 | 8556 | 4758 | 26 |
| H12A | 12422 | 9474 | 2498 | 46 |
| H12B | 13031 | 8357 | 2778 | 46 |
| H12C | 14103 | 9276 | 3361 | 46 |
| H13A | 9270 | 6099 | 1960 | 21 |
| H13B | 10395 | 5725 | 3204 | 21 |
| H14A | 7217 | 5590 | 2606 | 23 |
| H14B | 8450 | 5067 | 3712 | 23 |

| | | | | |
|---|---|---|---|---|
| H15A | 7911 | 4566 | 1290 | 28 |
| H15B | 9237 | 4082 | 2363 | 28 |
| H16A | 6131 | 3838 | 2043 | 35 |
| H16B | 7480 | 3316 | 3062 | 35 |
| H16C | 7127 | 3005 | 1715 | 35 |

**Table 6 Crystal data and structure refinement for Compound 5.**

| | |
|---|---|
| Identification code | gem39CuLT |
| Empirical formula | $C_{43}H_{42}B_2Cl_4N_2O_{13}$ |
| Formula weight | 958.20 |
| Temperature/K | 99.9(3) |
| Crystal system | monoclinic |
| Space group | $P2_1$ |
| a/Å | 12.1841(4) |
| b/Å | 10.7394(3) |
| c/Å | 16.5166(7) |
| α/° | 90 |
| β/° | 98.350(3) |
| γ/° | 90 |
| Volume/Å$^3$ | 2138.29(13) |
| Z | 2 |
| $\rho_{calc}$g/cm$^3$ | 1.488 |
| μ/mm$^{-1}$ | 3.108 |
| F(000) | 992.0 |
| Crystal size/mm$^3$ | 0.35 × 0.03 × 0.02 |
| Radiation | CuKα (λ = 1.54178) |
| 2Θ range for data collection/° | 8.458 to 134.998 |
| Index ranges | $-14 \leq h \leq 14$, $-12 \leq k \leq 12$, $-19 \leq l \leq 19$ |
| Reflections collected | 13467 |
| Independent reflections | 13467 [$R_{int}$ = ?, $R_{sigma}$ = 0.0285] |
| Data/restraints/parameters | 13467/2/594 |
| Completeness to theta = 66.5° | 99.9% |
| Goodness-of-fit on $F^2$ | 1.022 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0520, $wR_2$ = 0.1421 |
| Final R indexes [all data] | $R_1$ = 0.0564, $wR_2$ = 0.1445 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.45/-0.35 |
| Flack parameter | 0.019(12) |

**Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Compound 5. $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| B1 | 2507(6) | 3045(7) | 4409(4) | 20.2(14) |
| Cl1 | 7209.2(13) | 887.2(15) | 3318.4(9) | 26.0(3) |
| Cl2 | -2845.1(14) | 4667.3(18) | 3907.9(12) | 36.8(4) |
| O10 | 4154(4) | 4519(5) | 3047(3) | 25.3(10) |
| O11 | 2964(4) | 4009(4) | 3887(3) | 20.2(9) |
| O12 | 3393(4) | 2354(4) | 4895(3) | 22(1) |
| O20 | 267(4) | 1462(4) | 3173(3) | 22.3(9) |
| O21 | 1854(4) | 2155(4) | 3845(3) | 21.0(9) |
| O22 | 1874(4) | 3665(4) | 4954(3) | 23(1) |
| C10 | 3861(5) | 3803(6) | 3554(4) | 19.3(13) |
| C11 | 4532(5) | 2697(6) | 3850(4) | 19.5(12) |
| C12 | 4264(5) | 2041(6) | 4537(4) | 19.1(12) |
| C13 | 4957(6) | 1046(6) | 4848(4) | 23.0(13) |
| C14 | 5855(5) | 705(6) | 4480(4) | 21.6(13) |
| C15 | 6084(5) | 1353(6) | 3786(4) | 20.7(12) |
| C16 | 5435(5) | 2343(6) | 3478(4) | 19.4(13) |
| C20 | 761(5) | 2217(6) | 3639(4) | 17.0(12) |
| C21 | 187(5) | 3203(6) | 4049(4) | 18.2(12) |
| C22 | 793(6) | 3862(6) | 4713(4) | 19.6(12) |
| C23 | 220(6) | 4710(6) | 5144(4) | 23.4(13) |
| C24 | -887(6) | 4937(7) | 4901(4) | 26.0(14) |
| C25 | -1455(6) | 4322(7) | 4223(4) | 25.3(14) |
| C26 | -930(5) | 3446(6) | 3806(4) | 22.0(13) |
| B2 | 2666(6) | 2344(7) | 673(4) | 18.9(14) |
| Cl1A | 7883.6(13) | 4396.6(16) | 1620.1(10) | 29.8(4) |
| Cl2A | -2367.3(15) | 332.6(18) | 1198.9(11) | 33.3(4) |
| O10A | 4959(4) | 698(4) | 1819(3) | 24.3(10) |
| O11A | 3370(4) | 1347(4) | 1138(3) | 21.0(9) |
| O12A | 3319(4) | 3138(5) | 219(3) | 24.3(10) |
| O20A | 839(4) | 3733(4) | 1938(3) | 23.8(10) |
| O21A | 2211(4) | 3121(4) | 1288(3) | 20.4(9) |
| O22A | 1831(4) | 1732(5) | 105(3) | 25.4(10) |
| C10A | 4416(5) | 1504(6) | 1397(4) | 18.3(12) |
| C11A | 4966(5) | 2652(6) | 1144(4) | 17.0(12) |
| C12A | 4360(5) | 3417(6) | 553(4) | 18.2(12) |
| C13A | 4872(6) | 4477(7) | 279(4) | 22.8(13) |
| C14A | 5953(5) | 4760(6) | 598(4) | 21.5(13) |
| C15A | 6534(5) | 3998(6) | 1198(4) | 19.7(12) |

| | | | | |
|---|---|---|---|---|
| C16A | 6047(6) | 2939(6) | 1465(4) | 20.3(13) |
| C20A | 1197(6) | 3015(6) | 1460(4) | 19.0(12) |
| C21A | 503(5) | 2015(6) | 1033(4) | 18.4(13) |
| C22A | 851(5) | 1441(7) | 352(4) | 21.7(13) |
| C23A | 149(6) | 580(7) | -97(4) | 29.7(16) |
| C24A | -842(6) | 266(8) | 150(4) | 31.1(16) |
| C25A | -1161(5) | 809(7) | 847(4) | 24.3(13) |
| C26A | -502(5) | 1699(6) | 1282(4) | 19.8(13) |
| N1 | 1700(5) | 7494(6) | 3187(4) | 25.0(12) |
| N16 | 3926(5) | 8427(5) | 2021(3) | 23.1(12) |
| C31 | 807(7) | 6842(7) | 3576(5) | 35.4(18) |
| C32 | -191(6) | 6537(8) | 2941(6) | 40.3(19) |
| C33 | -646(7) | 7697(9) | 2486(7) | 52(2) |
| C34 | 274(7) | 8352(9) | 2111(7) | 47(2) |
| C35 | 1248(6) | 8670(7) | 2759(6) | 34.0(17) |
| C36 | 2698(6) | 7719(7) | 3814(4) | 30.2(15) |
| C37 | 3589(6) | 8507(7) | 3495(4) | 26.8(15) |
| C38 | 3077(6) | 9714(7) | 3152(5) | 33.5(17) |
| C39 | 2195(6) | 9381(7) | 2434(5) | 33.4(16) |
| C40 | 2709(6) | 8631(6) | 1770(4) | 26.8(15) |
| C41 | 4195(5) | 7822(6) | 2859(4) | 19.7(13) |
| C42 | 5439(6) | 7799(7) | 3087(5) | 29.4(15) |
| C43 | 6013(6) | 7110(7) | 2466(5) | 32.9(17) |
| C44 | 5666(6) | 7671(7) | 1617(5) | 32.6(16) |
| C45 | 4420(7) | 7697(7) | 1398(4) | 31.2(16) |
| O1W | 2293(4) | 5675(4) | 2207(3) | 23.1(10) |

**Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Compound 5. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.**

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| B1 | 15(3) | 22(4) | 24(3) | 3(3) | 2(3) | 0(3) |
| Cl1 | 19.0(7) | 25.7(8) | 33.2(7) | 2.4(6) | 4.0(6) | 3.7(6) |
| Cl2 | 19.5(8) | 32.8(10) | 56.2(10) | -13.2(8) | -0.6(7) | 4.6(7) |
| O10 | 23(2) | 18(2) | 34(2) | 5.5(19) | 3.3(18) | 0(2) |
| O11 | 19(2) | 13(2) | 28(2) | 2.2(17) | 0.6(17) | 0.1(17) |
| O12 | 19(2) | 23(2) | 23(2) | 0.9(16) | 0.5(17) | 2.7(18) |
| O20 | 23(2) | 17(2) | 26(2) | -4.3(17) | -1.6(17) | 0.9(19) |
| O21 | 20(2) | 16(2) | 26(2) | -4.2(16) | 2.4(18) | 2.3(18) |
| O22 | 20(2) | 24(2) | 25(2) | -5.6(17) | 0.1(17) | 0.8(19) |
| C10 | 16(3) | 15(3) | 26(3) | -3(2) | -2(2) | -5(2) |
| C11 | 18(3) | 17(3) | 22(3) | 0(2) | -3(2) | -5(2) |
| C12 | 13(3) | 21(3) | 22(3) | -2(2) | -2(2) | -3(2) |
| C13 | 22(3) | 24(3) | 21(3) | 5(2) | -4(2) | -1(3) |
| C14 | 18(3) | 21(3) | 23(3) | 2(2) | -4(2) | 2(3) |
| C15 | 15(3) | 20(3) | 26(3) | -1(2) | 0(2) | -1(3) |
| C16 | 18(3) | 17(3) | 23(3) | 0(2) | 1(2) | -3(2) |
| C20 | 16(3) | 16(3) | 18(3) | 0(2) | 1(2) | -1(2) |
| C21 | 20(3) | 11(3) | 23(3) | 1(2) | 3(2) | -1(2) |
| C22 | 22(3) | 17(3) | 19(3) | -2(2) | 1(2) | -3(3) |
| C23 | 26(3) | 20(3) | 24(3) | -4(2) | 5(2) | 0(3) |
| C24 | 25(4) | 24(4) | 30(3) | -5(3) | 10(3) | -3(3) |
| C25 | 19(3) | 20(4) | 36(3) | 1(3) | 3(3) | -3(3) |
| C26 | 20(3) | 23(3) | 23(3) | -2(2) | 2(2) | -2(3) |
| B2 | 9(3) | 21(4) | 26(3) | 0(3) | 0(3) | -2(3) |
| Cl1A | 19.7(8) | 31.4(9) | 37.0(8) | 4.7(7) | -0.9(6) | -9.2(7) |
| Cl2A | 22.3(8) | 37.8(10) | 40.9(9) | -13.0(7) | 8.0(7) | -12.9(7) |
| O10A | 21(2) | 14(2) | 37(2) | 5.4(18) | 3.3(18) | -0.2(19) |
| O11A | 16(2) | 13(2) | 34(2) | 0.3(17) | 3.2(17) | -3.0(18) |
| O12A | 17(2) | 30(3) | 25(2) | 5.2(18) | -0.5(17) | -5(2) |
| O20A | 23(2) | 17(2) | 31(2) | -6.5(18) | 4.8(18) | -2.2(19) |
| O21A | 16(2) | 17(2) | 27(2) | -3.9(16) | 0.5(17) | -2.8(17) |
| O22A | 19(2) | 31(3) | 26(2) | -9.0(19) | 3.5(18) | -7(2) |
| C10A | 16(3) | 13(3) | 27(3) | 1(2) | 6(2) | 0(2) |
| C11A | 16(3) | 10(3) | 26(3) | 2(2) | 7(2) | -1(2) |
| C12A | 15(3) | 18(3) | 21(3) | 1(2) | 3(2) | -2(2) |
| C13A | 25(3) | 22(3) | 21(3) | 6(2) | 3(2) | 1(3) |
| C14A | 24(3) | 15(3) | 26(3) | 3(2) | 6(2) | -3(3) |
| C15A | 16(3) | 18(3) | 25(3) | 0(2) | 4(2) | -3(2) |
| C16A | 21(3) | 17(3) | 23(3) | 1(2) | 3(2) | 0(2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C20A | 24(3) | 10(3) | 22(3) | 3(2) | 0(2) | 1(2) |
| C21A | 17(3) | 16(3) | 20(3) | 0(2) | -3(2) | 1(2) |
| C22A | 15(3) | 25(3) | 24(3) | -2(2) | -1(2) | 1(3) |
| C23A | 24(4) | 35(4) | 30(3) | -14(3) | 4(3) | -9(3) |
| C24A | 24(4) | 34(4) | 34(3) | -14(3) | 2(3) | -8(3) |
| C25A | 17(3) | 28(4) | 29(3) | -4(3) | 4(2) | -5(3) |
| C26A | 20(3) | 18(3) | 20(3) | 0(2) | -1(2) | 0(3) |
| N1 | 22(3) | 16(3) | 40(3) | -2(2) | 13(2) | 0(2) |
| N16 | 25(3) | 15(3) | 30(3) | 3(2) | 4(2) | -7(2) |
| C31 | 34(4) | 25(4) | 52(4) | 2(3) | 22(3) | -6(3) |
| C32 | 22(4) | 28(4) | 74(5) | 3(4) | 17(4) | -8(3) |
| C33 | 21(4) | 33(5) | 104(8) | 12(5) | 12(5) | 3(4) |
| C34 | 18(4) | 31(5) | 91(7) | 22(4) | 3(4) | -1(3) |
| C35 | 20(4) | 15(3) | 70(5) | 7(3) | 15(3) | 4(3) |
| C36 | 33(4) | 31(4) | 29(3) | -7(3) | 11(3) | -5(3) |
| C37 | 25(3) | 25(4) | 31(3) | -11(3) | 7(3) | -6(3) |
| C38 | 28(4) | 17(4) | 60(5) | -10(3) | 20(3) | -8(3) |
| C39 | 20(3) | 15(3) | 66(5) | 10(3) | 10(3) | 4(3) |
| C40 | 22(3) | 15(3) | 42(4) | 10(3) | -2(3) | -5(3) |
| C41 | 20(3) | 15(3) | 25(3) | -1(2) | 2(2) | -1(2) |
| C42 | 23(4) | 24(4) | 40(4) | 3(3) | 0(3) | -4(3) |
| C43 | 19(4) | 23(4) | 59(5) | 10(3) | 10(3) | 6(3) |
| C44 | 33(4) | 22(4) | 47(4) | 1(3) | 20(3) | 1(3) |
| C45 | 41(4) | 26(4) | 28(3) | 0(3) | 8(3) | -9(3) |
| O1W | 21(2) | 12(2) | 34(2) | -0.3(17) | -3(2) | -3.2(19) |

**Bond Lengths for Compound 5.**

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| B1 | O11 | 1.505(8) | O21A | C20A | 1.313(8) |
| B1 | O12 | 1.453(8) | O22A | C22A | 1.354(8) |
| B1 | O21 | 1.482(8) | C10A | C11A | 1.492(8) |
| B1 | O22 | 1.432(8) | C11A | C12A | 1.401(9) |
| Cl1 | C15 | 1.743(7) | C11A | C16A | 1.381(9) |
| Cl2 | C25 | 1.738(7) | C12A | C13A | 1.404(9) |
| O10 | C10 | 1.227(8) | C13A | C14A | 1.380(9) |
| O11 | C10 | 1.312(8) | C14A | C15A | 1.397(9) |
| O12 | C12 | 1.331(8) | C15A | C16A | 1.384(9) |
| O20 | C20 | 1.216(8) | C20A | C21A | 1.481(9) |
| O21 | C20 | 1.327(8) | C21A | C22A | 1.401(9) |
| O22 | C22 | 1.336(8) | C21A | C26A | 1.390(9) |
| C10 | C11 | 1.484(9) | C22A | C23A | 1.397(9) |
| C11 | C12 | 1.415(9) | C23A | C24A | 1.372(10) |
| C11 | C16 | 1.389(9) | C24A | C25A | 1.395(10) |
| C12 | C13 | 1.411(9) | C25A | C26A | 1.381(9) |
| C13 | C14 | 1.375(9) | N1 | C31 | 1.513(9) |
| C14 | C15 | 1.403(9) | N1 | C35 | 1.512(9) |
| C15 | C16 | 1.377(9) | N1 | C36 | 1.498(9) |
| C20 | C21 | 1.485(9) | N16 | C40 | 1.497(9) |
| C21 | C22 | 1.420(8) | N16 | C41 | 1.520(8) |
| C21 | C26 | 1.386(9) | N16 | C45 | 1.490(9) |
| C22 | C23 | 1.403(9) | C31 | C32 | 1.522(12) |
| C23 | C24 | 1.372(10) | C32 | C33 | 1.517(12) |
| C24 | C25 | 1.394(10) | C33 | C34 | 1.529(12) |
| C25 | C26 | 1.377(10) | C34 | C35 | 1.518(12) |
| B2 | O11A | 1.511(8) | C35 | C39 | 1.544(10) |
| B2 | O12A | 1.447(9) | C36 | C37 | 1.529(10) |
| B2 | O21A | 1.483(8) | C37 | C38 | 1.512(11) |
| B2 | O22A | 1.438(8) | C37 | C41 | 1.554(9) |
| Cl1A | C15A | 1.743(6) | C38 | C39 | 1.522(11) |
| Cl2A | C25A | 1.735(7) | C39 | C40 | 1.564(11) |
| O10A | C10A | 1.241(8) | C41 | C42 | 1.508(9) |
| O11A | C10A | 1.295(8) | C42 | C43 | 1.517(11) |
| O12A | C12A | 1.341(7) | C43 | C44 | 1.528(11) |
| O20A | C20A | 1.227(8) | C44 | C45 | 1.509(11) |

**Bond Angles for Compound 5.**

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| O12 | B1 | O11 | 111.1(5) | C16A | C11A | C12A | 121.0(6) |
| O12 | B1 | O21 | 107.8(6) | O12A | C12A | C11A | 121.8(6) |
| O21 | B1 | O11 | 107.0(5) | O12A | C12A | C13A | 119.1(6) |
| O22 | B1 | O11 | 108.5(6) | C11A | C12A | C13A | 119.0(6) |
| O22 | B1 | O12 | 108.4(5) | C14A | C13A | C12A | 120.0(6) |
| O22 | B1 | O21 | 114.0(6) | C13A | C14A | C15A | 119.9(6) |
| C10 | O11 | B1 | 121.6(5) | C14A | C15A | Cl1A | 119.4(5) |
| C12 | O12 | B1 | 117.4(5) | C16A | C15A | Cl1A | 119.9(5) |
| C20 | O21 | B1 | 123.7(5) | C16A | C15A | C14A | 120.7(6) |
| C22 | O22 | B1 | 118.9(5) | C11A | C16A | C15A | 119.3(6) |
| O10 | C10 | O11 | 121.6(6) | O20A | C20A | O21A | 121.2(6) |
| O10 | C10 | C11 | 121.7(6) | O20A | C20A | C21A | 122.1(6) |
| O11 | C10 | C11 | 116.7(5) | O21A | C20A | C21A | 116.7(6) |
| C12 | C11 | C10 | 118.9(6) | C22A | C21A | C20A | 118.9(6) |
| C16 | C11 | C10 | 120.5(6) | C26A | C21A | C20A | 120.2(6) |
| C16 | C11 | C12 | 120.6(6) | C26A | C21A | C22A | 120.8(6) |
| O12 | C12 | C11 | 121.5(6) | O22A | C22A | C21A | 121.5(6) |
| O12 | C12 | C13 | 120.2(6) | O22A | C22A | C23A | 119.4(6) |
| C13 | C12 | C11 | 118.2(6) | C23A | C22A | C21A | 119.0(6) |
| C14 | C13 | C12 | 120.9(6) | C24A | C23A | C22A | 120.1(6) |
| C13 | C14 | C15 | 119.6(6) | C23A | C24A | C25A | 120.4(6) |
| C14 | C15 | Cl1 | 118.8(5) | C24A | C25A | Cl2A | 120.3(5) |
| C16 | C15 | Cl1 | 120.2(5) | C26A | C25A | Cl2A | 119.1(5) |
| C16 | C15 | C14 | 120.9(6) | C26A | C25A | C24A | 120.5(6) |
| C15 | C16 | C11 | 119.7(6) | C25A | C26A | C21A | 119.0(6) |
| O20 | C20 | O21 | 121.0(6) | C35 | N1 | C31 | 110.4(6) |
| O20 | C20 | C21 | 122.8(6) | C36 | N1 | C31 | 110.1(6) |
| O21 | C20 | C21 | 116.1(5) | C36 | N1 | C35 | 113.1(6) |
| C22 | C21 | C20 | 118.8(6) | C40 | N16 | C41 | 112.9(5) |
| C26 | C21 | C20 | 120.7(6) | C45 | N16 | C40 | 111.6(6) |
| C26 | C21 | C22 | 120.5(6) | C45 | N16 | C41 | 110.4(5) |
| O22 | C22 | C21 | 122.0(6) | N1 | C31 | C32 | 111.0(6) |
| O22 | C22 | C23 | 119.6(6) | C33 | C32 | C31 | 111.3(7) |
| C23 | C22 | C21 | 118.3(6) | C32 | C33 | C34 | 110.0(7) |
| C24 | C23 | C22 | 120.5(6) | C35 | C34 | C33 | 111.2(8) |
| C23 | C24 | C25 | 120.2(6) | N1 | C35 | C34 | 109.7(6) |
| C24 | C25 | Cl2 | 119.2(6) | N1 | C35 | C39 | 109.6(6) |
| C26 | C25 | Cl2 | 120.0(5) | C34 | C35 | C39 | 114.4(7) |
| C26 | C25 | C24 | 120.9(6) | N1 | C36 | C37 | 113.4(6) |
| C25 | C26 | C21 | 119.5(6) | C36 | C37 | C41 | 113.7(6) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| O12A | B2 | O11A | 111.5(5) | C38 | C37 | C36 | 109.2(6) |
| O12A | B2 | O21A | 108.2(5) | C38 | C37 | C41 | 111.3(6) |
| O21A | B2 | O11A | 106.9(5) | C37 | C38 | C39 | 107.3(6) |
| O22A | B2 | O11A | 107.6(5) | C35 | C39 | C40 | 112.6(6) |
| O22A | B2 | O12A | 108.8(5) | C38 | C39 | C35 | 108.9(7) |
| O22A | B2 | O21A | 113.9(5) | C38 | C39 | C40 | 110.9(6) |
| C10A | O11A | B2 | 122.3(5) | N16 | C40 | C39 | 111.3(6) |
| C12A | O12A | B2 | 118.5(5) | N16 | C41 | C37 | 110.6(5) |
| C20A | O21A | B2 | 123.8(5) | C42 | C41 | N16 | 108.1(5) |
| C22A | O22A | B2 | 118.7(5) | C42 | C41 | C37 | 113.4(6) |
| O10A | C10A | O11A | 120.9(6) | C41 | C42 | C43 | 112.6(6) |
| O10A | C10A | C11A | 120.6(6) | C42 | C43 | C44 | 109.6(6) |
| O11A | C10A | C11A | 118.4(5) | C45 | C44 | C43 | 111.3(6) |
| C12A | C11A | C10A | 117.8(6) | N16 | C45 | C44 | 109.7(6) |
| C16A | C11A | C10A | 121.2(6) | | | | |

**Hydrogen Bonds for Compound 5.**

| D | H | A | d(D-H)/Å | d(H-A)/Å | d(D-A)/Å | D-H-A/° |
|---|---|---|---|---|---|---|
| N1 | H1 | O1W | 0.78(11) | 1.94(12) | 2.701(8) | 167(12) |
| N16 | H16 | O10A[1] | 0.79(10) | 2.01(10) | 2.787(7) | 166(8) |
| O1W | H1WA | O20A | 0.81(8) | 1.96(9) | 2.730(7) | 157(12) |
| O1W | H1WB | O10 | 0.81(7) | 1.96(7) | 2.774(6) | 177(10) |

[1]+X,1+Y,+Z

**Hydrogen Atom Coordinates (Å×10$^4$) and Isotropic Displacement Parameters (Å$^2$×10$^3$) for Compound 5.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| H13 | 4802 | 606 | 5317 | 28 |
| H14 | 6317 | 35 | 4695 | 26 |
| H16A | 5605 | 2782 | 3012 | 23 |
| H23 | 601 | 5131 | 5608 | 28 |
| H24 | -1268 | 5515 | 5196 | 31 |
| H26 | -1329 | 3012 | 3356 | 26 |
| H13A | 4473 | 4999 | -126 | 27 |
| H14A | 6302 | 5473 | 409 | 26 |
| H16B | 6452 | 2415 | 1865 | 24 |
| H23A | 359 | 212 | -575 | 36 |
| H24A | -1313 | -324 | -155 | 37 |
| H26A | -732 | 2089 | 1745 | 24 |
| H1 | 1880(90) | 7060(110) | 2860(70) | 60(30) |
| H16 | 4230(70) | 9090(90) | 2050(50) | 30(20) |
| H31A | 572 | 7383 | 4005 | 42 |
| H31B | 1111 | 6063 | 3841 | 42 |
| H32A | 29 | 5926 | 2545 | 48 |
| H32B | -778 | 6154 | 3215 | 48 |
| H33A | -949 | 8269 | 2869 | 63 |
| H33B | -1256 | 7465 | 2049 | 63 |
| H34A | 529 | 7804 | 1694 | 57 |
| H34B | -23 | 9125 | 1835 | 57 |
| H35 | 963 | 9211 | 3176 | 41 |
| H36A | 3024 | 6907 | 4003 | 36 |
| H36B | 2461 | 8144 | 4292 | 36 |
| H37 | 4158 | 8721 | 3973 | 32 |
| H38A | 3650 | 10253 | 2966 | 40 |
| H38B | 2738 | 10165 | 3576 | 40 |
| H39 | 1883 | 10174 | 2179 | 40 |
| H40A | 2331 | 7815 | 1684 | 32 |
| H40B | 2588 | 9091 | 1246 | 32 |
| H41 | 3924 | 6942 | 2815 | 24 |
| H42A | 5629 | 7394 | 3628 | 35 |
| H42B | 5719 | 8665 | 3136 | 35 |
| H43A | 5809 | 6218 | 2460 | 40 |
| H43B | 6828 | 7175 | 2617 | 40 |
| H44A | 5959 | 8530 | 1606 | 39 |
| H44B | 5990 | 7174 | 1206 | 39 |
| H45A | 4215 | 8080 | 851 | 37 |

| | | | | |
|---|---|---|---|---|
| H45B | 4126 | 6836 | 1375 | 37 |
| H1WA | 1760(80) | 5240(110) | 2040(70) | 70(40) |
| H1WB | 2840(70) | 5360(100) | 2460(50) | 50(30) |