# Crystal structure of tetrakis(5,7-dichloroquinolin-8-olato-$\kappa^2$*N*,*O*) zirconium(IV) dimethylformamide disolvate, $C_{42}H_{30}Cl_8N_6O_6Zr$

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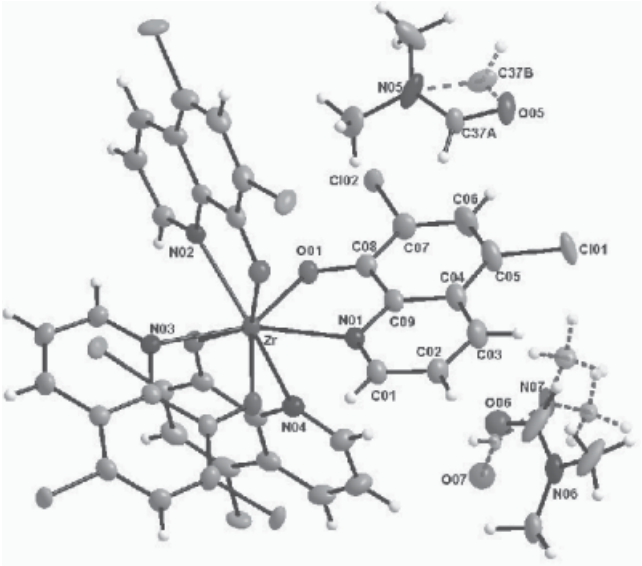
Received May 10, 2013, accepted June 19, 2013, available online August 27, 2013, CCDC no. 900014




**Abstract**

$C_{42}H_{30}Cl_8N_6O_6Zr$, monoclinic, *C*2/*c* (no. 15), $a$ = 30.357(5) Å, $b$ = 13.037(5) Å, $c$ = 26.386(5) Å, $\beta$ = 118.343(5)°, $V$ = 9191 Å$^3$, $Z$ = 8, $R_{gt}(F)$ = 0.042, $wR_{ref}(F^2)$ = 0.1128, $T$ = 100 K.

**Table 1.** Data collection and handling.

| | |
|---|---|
| Crystal: | yellow plates, size 0.086×0.179×0.274 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71073 Å) |
| $\mu$: | 7.58 cm$^{-1}$ |
| Diffractometer, scan mode: | Bruker APEX-II CCD, $\varphi$ and $\omega$ |
| $2\theta_{max}$: | 56° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 59147, 11076 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\,\sigma(I_{obs})$, 8791 |
| $N(param)_{refined}$: | 602 |
| Programs: | SHELX [16], SAINT [17], SIR 97 [18] DIAMOND [19], WinGX [20] |

## Source of material

Chemicals were purchased from Sigma-Aldrich and used as received. $ZrCl_4$ (104.2 mg, 0.447 mmol) and 5,7-dichloro-8-quinolinol (*diClOxH*) (279.7 mg, 1.307 mmol) was separately dissolved in DMF (2.5 ml ea.) and heated to 60 °C. The *diClOx* solution was added drop-wise to the zirconium tetrachloride solution and stirred at 60 °C for 30 minutes. The heating of the reaction solution was then stopped, the solution covered and left to slowly cool, which induced crystallization. Yellow plate-like crystals, suitable for single X-Ray diffraction, formed after 10 days. (Yield: 253 mg, 82%). **UV/Vis**: $\lambda^{DMF}_{max}$ = 396 nm, ε = 191 cm$^{-1}$·M$^{-1}$; **$^1$H NMR** (300 MHz, Acetone-$d_6$): δ = 9.04 (dd, 1H), 8.13 (dd, 1H), 7.72 (q, 1H), 7.62 (s, 1H).

## Experimental details

The aromatic H atoms were placed in geometrically idealized positions (C–H = 0.95 Å) and constrained to ride on their parent atoms with $U_{iso}$(H) = 1.2$U_{eq}$(C) for aromatic. The methyl hydrogen atoms of the solvent molecules were located on the Fourier difference map and refined isotropically. The highest residual electron density was located 2.85 Å from H45B. The DMF solvate molecules show a serious disorder.

## Discussion

Zirconium and hafnium complexes have been a key focus area for many research studies for several decades [1-5]. This study forms part of on-going research of structure reactivity relationships of these metals, aimed at investigating chelation behaviour of *N*- and *O*-donating multidentate ligands [6-11]. The use of these and other *N*- and *O*-donating ligands find application in model catalysts and radiopharmaceutical synthon complexes [12-15]. The asymmetric unit in the title structure consists of a Zr(IV) metal ion coordinated to four bidentate ligands (*diClOx*), as well as two independent *N*,*N*′-dimethylformamide (DMF) solvate molecules. In the complex, the Zr(IV) metal atom lies at the centre of an approximate square antiprismatic coordination polyhedron defined by the *N,O* ligand atoms, with a small distortion towards dodecahedral geometry. The Zr–N and Zr–O bond distances range from 2.415(2) to 2.491(2) Å and 2.075(2) to 2.113(2) Å, respectively. The average N–Zr–O bite angle is 69.77(7)°. The four *diClOx* ligands (group number denoted by $N_x\_O_x$, where $x$ = 1-4) are arranged around the metal centre in a complete space-filling fan-like arrangement. Opposite facing ligands pairs, N1_O1 & N3_O3; N2_O2 & N4_O4, lie across the metal centre at an angle of 29.88(3)° and 28.09(2)°, respectively. The angle between adjacent ligand planes range from 80.18(3) to 86.83(2)°. The title structure displays $\pi$-$\pi$ interactions between the benzene rings of the *diClOx* ligand symmetry generated counterparts of neighbouring molecules, with interplanar and centroid-to-centroid distances of 3.4097(37) Å and 3.6820(11) Å, respectively. Furthermore, a Cl–C interaction is observed between Cl07 and C27 (2–$x$,–$y$,1–$z$), of neighbouring molecules. The effects of the $\pi$-$\pi$ stacking and Cl–C interactions form a network of molecule pairs packing diagonally across the *ab* plane. Both the DMF solvent molecules are disordered over two positions (69%:31% and 52%:48%).

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**Table 2.** continued.

| Atom | Site | Occ. | *x* | *y* | *z* | $U_{iso}$ |
|---|---|---|---|---|---|---|
| H(01) | 8*f* | | 0.7962 | 0.1949 | 0.5208 | 0.031 |
| H(29) | 8*f* | | 0.9550 | 0.0005 | 0.6541 | 0.046 |
| H(33) | 8*f* | | 1.0814 | 0.0939 | 0.5195 | 0.037 |
| H(11) | 8*f* | | 0.9756 | 0.5917 | 0.4218 | 0.033 |
| H(10) | 8*f* | | 0.9662 | 0.4351 | 0.4572 | 0.029 |
| H(19) | 8*f* | | 0.8768 | 0.3716 | 0.3528 | 0.031 |
| H(28) | 8*f* | | 0.8993 | 0.1260 | 0.5972 | 0.038 |
| H(20) | 8*f* | | 0.8396 | 0.3184 | 0.2581 | 0.037 |
| H(02) | 8*f* | | 0.7690 | 0.2061 | 0.5893 | 0.033 |
| H(12) | 8*f* | | 0.9123 | 0.7110 | 0.3908 | 0.036 |
| H(24) | 8*f* | | 0.7346 | –0.0424 | 0.3311 | 0.032 |
| H(06) | 8*f* | | 0.9475 | 0.5344 | 0.7221 | 0.043 |
| H(03) | 8*f* | | 0.8108 | 0.3105 | 0.6683 | 0.040 |
| H(15) | 8*f* | | 0.7544 | 0.7053 | 0.3834 | 0.040 |
| H(21) | 8*f* | | 0.7838 | 0.1839 | 0.2284 | 0.034 |
| H(30) | 8*f* | | 1.0239 | –0.0383 | 0.6430 | 0.040 |
| H(39A) | 8*f* | | 0.8751 | 0.6955 | 0.5358 | 0.179 |
| H(39B) | 8*f* | | 0.8219 | 0.6515 | 0.5193 | 0.179 |
| H(39C) | 8*f* | | 0.8700 | 0.5902 | 0.5613 | 0.179 |

**Table 2.** continued.

| Atom | Site | Occ. | *x* | *y* | *z* | $U_{iso}$ |
|---|---|---|---|---|---|---|
| H(42) | 8*f* | 0.475 | 0.9697 | 0.1154 | 0.7274 | 0.040 |
| H(41A) | 8*f* | 0.475 | 0.8641 | 0.1267 | 0.7471 | 0.080 |
| H(41B) | 8*f* | 0.475 | 0.8715 | 0.2397 | 0.7700 | 0.080 |
| H(41C) | 8*f* | 0.475 | 0.8989 | 0.1493 | 0.8126 | 0.080 |
| H(40A) | 8*f* | 0.475 | 0.9931 | 0.2633 | 0.7900 | 0.087 |
| H(40B) | 8*f* | 0.475 | 0.9813 | 0.2375 | 0.8403 | 0.087 |
| H(40C) | 8*f* | 0.475 | 0.9522 | 0.3259 | 0.7969 | 0.087 |
| H(45A) | 8*f* | 0.525 | 0.8595 | –0.0640 | 0.7298 | 0.145 |
| H(45B) | 8*f* | 0.525 | 0.9179 | –0.0519 | 0.7593 | 0.145 |
| H(45C) | 8*f* | 0.525 | 0.8852 | –0.0273 | 0.6936 | 0.145 |
| H(43) | 8*f* | 0.525 | 0.9113 | 0.2132 | 0.7612 | 0.176 |
| H(44A) | 8*f* | 0.525 | 0.8209 | 0.0399 | 0.7449 | 0.220 |
| H(44B) | 8*f* | 0.525 | 0.8197 | 0.1497 | 0.7201 | 0.220 |
| H(44C) | 8*f* | 0.525 | 0.8498 | 0.1304 | 0.7866 | 0.220 |
| H(37) | 8*f* | 0.687 | 0.8166 | 0.6048 | 0.6049 | 0.052 |
| H(37B) | 8*f* | 0.313 | 0.8592 | 0.7915 | 0.6750 | 0.060 |
| H(38A) | 8*f* | | 0.8852 | 0.8370 | 0.6471 | 0.179 |
| H(38B) | 8*f* | | 0.8732 | 0.8499 | 0.5827 | 0.179 |
| H(38C) | 8*f* | | 0.9203 | 0.7869 | 0.6254 | 0.179 |

**Table 3.** Atomic coordinates and displacement parameters (in $Å^2$).

| Atom | Site | Occ. | *x* | *y* | *z* | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Zr(01) | 8*f* | | 0.882118(9) | 0.30434(2) | 0.48659(1) | 0.0170(1) | 0.0227(1) | 0.0174(1) | 0.0013(1) | 0.00705(9) | 0.00143(9) |
| Cl(02) | 8*f* | | 0.99114(3) | 0.54916(7) | 0.65010(3) | 0.0319(4) | 0.0485(5) | 0.0280(4) | –0.0140(3) | 0.0106(3) | –0.0077(3) |
| Cl(08) | 8*f* | | 1.02465(3) | 0.24999(7) | 0.44255(4) | 0.0357(4) | 0.0452(5) | 0.0452(4) | 0.0108(3) | 0.0275(4) | 0.0109(4) |
| Cl(05) | 8*f* | | 0.72831(3) | 0.01637(7) | 0.22667(3) | 0.0535(5) | 0.0435(4) | 0.0235(4) | –0.0197(4) | 0.0158(3) | –0.0098(3) |
| Cl(06) | 8*f* | | 0.77624(3) | –0.01050(7) | 0.45093(3) | 0.0538(5) | 0.0518(5) | 0.0280(4) | –0.0263(4) | 0.0219(4) | –0.0029(3) |
| Cl(07) | 8*f* | | 1.09534(3) | –0.04033(6) | 0.60716(4) | 0.0281(4) | 0.0283(4) | 0.0436(4) | 0.0108(3) | 0.0048(3) | 0.0009(3) |
| Cl(04) | 8*f* | | 0.72625(3) | 0.52899(7) | 0.42030(4) | 0.0318(4) | 0.0565(5) | 0.0519(5) | 0.0188(4) | 0.0262(4) | 0.0193(4) |
| Cl(01) | 8*f* | | 0.87543(3) | 0.45185(9) | 0.74658(4) | 0.0367(4) | 0.0931(8) | 0.0346(4) | –0.0161(5) | 0.0222(4) | –0.0299(5) |
| Cl(03) | 8*f* | | 0.82366(3) | 0.81099(6) | 0.36295(5) | 0.0391(4) | 0.0263(4) | 0.0697(6) | 0.0068(3) | 0.0122(4) | 0.0150(4) |
| O(01) | 8*f* | | 0.92653(7) | 0.3960(2) | 0.55924(8) | 0.0215(9) | 0.030(1) | 0.0203(9) | –0.0021(8) | 0.0092(8) | –0.0014(8) |
| O(04) | 8*f* | | 0.94415(7) | 0.2708(2) | 0.47576(8) | 0.0216(9) | 0.025(1) | 0.0223(9) | 0.0049(8) | 0.0097(8) | 0.0043(7) |
| O(03) | 8*f* | | 0.83566(7) | 0.1768(2) | 0.46234(8) | 0.025(1) | 0.032(1) | 0.0178(9) | –0.0055(8) | 0.0102(8) | –0.0019(8) |
| N(02) | 8*f* | | 0.89929(8) | 0.4579(2) | 0.44785(9) | 0.019(1) | 0.021(1) | 0.018(1) | 0.0011(9) | 0.0058(8) | –0.0018(8) |
| N(03) | 8*f* | | 0.84624(8) | 0.2720(2) | 0.38166(9) | 0.020(1) | 0.021(1) | 0.020(1) | 0.0029(9) | 0.0076(9) | 0.0023(9) |
| N(04) | 8*f* | | 0.93379(9) | 0.1669(2) | 0.5543(1) | 0.023(1) | 0.024(1) | 0.024(1) | 0.0002(9) | 0.0090(9) | 0.0002(9) |
| O(02) | 8*f* | | 0.81953(7) | 0.4029(2) | 0.45531(8) | 0.0210(9) | 0.029(1) | 0.024(1) | 0.0035(8) | 0.0102(8) | 0.0029(8) |
| C(13) | 8*f* | | 0.8644(1) | 0.6254(2) | 0.4078(1) | 0.026(1) | 0.022(1) | 0.024(1) | 0.000(1) | 0.005(1) | –0.002(1) |
| C(22) | 8*f* | | 0.7898(1) | 0.1528(2) | 0.3073(1) | 0.021(1) | 0.024(1) | 0.021(1) | 0.004(1) | 0.008(1) | 0.001(1) |
| C(01) | 8*f* | | 0.8130(1) | 0.2383(2) | 0.5522(1) | 0.021(1) | 0.034(2) | 0.022(1) | 0.001(1) | 0.010(1) | –0.001(1) |
| C(31) | 8*f* | | 1.0101(1) | 0.0673(2) | 0.5800(1) | 0.027(1) | 0.021(1) | 0.024(1) | 0.001(1) | 0.006(1) | –0.002(1) |
| C(29) | 8*f* | | 0.9608(1) | 0.0356(2) | 0.6271(2) | 0.049(2) | 0.027(2) | 0.042(2) | 0.004(1) | 0.024(2) | 0.010(1) |
| C(25) | 8*f* | | 0.7809(1) | 0.0533(2) | 0.3961(1) | 0.025(1) | 0.033(2) | 0.022(1) | –0.004(1) | 0.012(1) | 0.001(1) |
| C(35) | 8*f* | | 0.9787(1) | 0.2015(2) | 0.5042(1) | 0.020(1) | 0.022(1) | 0.023(1) | 0.001(1) | 0.006(1) | –0.001(1) |
| C(07) | 8*f* | | 0.9423(1) | 0.4768(2) | 0.6479(1) | 0.023(1) | 0.038(2) | 0.026(1) | –0.003(1) | 0.007(1) | –0.002(1) |
| C(33) | 8*f* | | 1.0546(1) | 0.1059(2) | 0.5266(1) | 0.020(1) | 0.031(2) | 0.037(2) | 0.004(1) | 0.010(1) | –0.006(1) |
| C(11) | 8*f* | | 0.9463(1) | 0.5774(2) | 0.4234(1) | 0.025(1) | 0.028(1) | 0.025(1) | –0.006(1) | 0.009(1) | –0.002(1) |
| C(10) | 8*f* | | 0.9403(1) | 0.4826(2) | 0.4447(1) | 0.021(1) | 0.026(1) | 0.023(1) | 0.001(1) | 0.007(1) | –0.001(1) |
| C(08) | 8*f* | | 0.9168(1) | 0.4104(2) | 0.6022(1) | 0.019(1) | 0.028(1) | 0.020(1) | 0.003(1) | 0.006(1) | 0.002(1) |
| N(01) | 8*f* | | 0.85143(8) | 0.2919(2) | 0.55578(9) | 0.019(1) | 0.026(1) | 0.020(1) | 0.0019(9) | 0.0081(9) | –0.0001(9) |
| C(18) | 8*f* | | 0.8613(1) | 0.5276(2) | 0.4296(1) | 0.022(1) | 0.022(1) | 0.017(1) | 0.001(1) | 0.005(1) | –0.002(1) |
| O(05) | 8*f* | | 0.8243(1) | 0.6911(3) | 0.6611(1) | 0.060(2) | 0.099(3) | 0.038(2) | 0.021(2) | 0.032(1) | 0.010(2) |
| C(27) | 8*f* | | 0.81434(9) | 0.1899(2) | 0.3646(1) | 0.016(1) | 0.022(1) | 0.019(1) | 0.005(1) | 0.007(1) | 0.001(1) |
| C(19) | 8*f* | | 0.8548(1) | 0.3165(2) | 0.3418(1) | 0.029(1) | 0.025(1) | 0.022(1) | –0.003(1) | 0.011(1) | 0.001(1) |
| C(32) | 8*f* | | 1.0504(1) | 0.0514(2) | 0.5679(1) | 0.023(1) | 0.021(1) | 0.033(2) | 0.006(1) | 0.004(1) | –0.004(1) |
| N(05) | 8*f* | | 0.8566(1) | 0.7125(4) | 0.6002(2) | 0.044(2) | 0.123(4) | 0.068(2) | 0.000(2) | 0.036(2) | 0.038(2) |
| C(26) | 8*f* | | 0.8101(1) | 0.1398(2) | 0.4098(1) | 0.017(1) | 0.028(1) | 0.020(1) | 0.002(1) | 0.009(1) | –0.000(1) |
| C(34) | 8*f* | | 1.0186(1) | 0.1805(2) | 0.4946(1) | 0.024(1) | 0.027(1) | 0.028(1) | 0.002(1) | 0.012(1) | –0.000(1) |
| C(28) | 8*f* | | 0.9273(1) | 0.1126(2) | 0.5927(1) | 0.035(2) | 0.028(2) | 0.035(2) | 0.002(1) | 0.019(1) | 0.006(1) |
| C(05) | 8*f* | | 0.8906(1) | 0.4348(3) | 0.6913(1) | 0.024(1) | 0.055(2) | 0.022(1) | 0.001(1) | 0.010(1) | –0.009(1) |
| C(04) | 8*f* | | 0.8621(1) | 0.3656(2) | 0.6459(1) | 0.020(1) | 0.039(2) | 0.021(1) | 0.004(1) | 0.008(1) | –0.002(1) |
| C(14) | 8*f* | | 0.8226(1) | 0.6904(2) | 0.3905(1) | 0.032(2) | 0.026(2) | 0.030(2) | 0.005(1) | 0.006(1) | 0.002(1) |
| C(23) | 8*f* | | 0.7595(1) | 0.0648(2) | 0.2965(1) | 0.027(1) | 0.028(1) | 0.021(1) | –0.001(1) | 0.008(1) | –0.004(1) |
| C(20) | 8*f* | | 0.8323(1) | 0.2848(2) | 0.2843(1) | 0.039(2) | 0.030(2) | 0.022(1) | –0.002(1) | 0.014(1) | 0.005(1) |
| C(02) | 8*f* | | 0.7965(1) | 0.2443(2) | 0.5936(1) | 0.021(1) | 0.036(2) | 0.029(1) | –0.000(1) | 0.014(1) | –0.000(1) |
| C(36) | 8*f* | | 0.9746(1) | 0.1439(2) | 0.5474(1) | 0.020(1) | 0.020(1) | 0.023(1) | 0.000(1) | 0.006(1) | –0.002(1) |
| C(12) | 8*f* | | 0.9087(1) | 0.6481(2) | 0.4051(1) | 0.031(2) | 0.022(1) | 0.029(2) | –0.006(1) | 0.008(1) | –0.001(1) |

**Table 3.** continued.

| Atom | Site | Occ. | *x* | *y* | *z* | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C(24) | 8*f* | | 0.7548(1) | 0.0155(2) | 0.3393(1) | 0.024(1) | 0.029(2) | 0.027(1) | –0.007(1) | 0.012(1) | –0.003(1) |
| C(06) | 8*f* | | 0.9295(1) | 0.4890(3) | 0.6921(1) | 0.028(2) | 0.049(2) | 0.024(2) | –0.005(1) | 0.007(1) | –0.013(1) |
| C(03) | 8*f* | | 0.8211(1) | 0.3068(3) | 0.6403(1) | 0.030(1) | 0.046(2) | 0.029(1) | 0.003(1) | 0.018(1) | –0.002(1) |
| C(16) | 8*f* | | 0.7792(1) | 0.5632(2) | 0.4155(1) | 0.023(1) | 0.039(2) | 0.025(1) | 0.008(1) | 0.010(1) | 0.002(1) |
| C(15) | 8*f* | | 0.7813(1) | 0.6606(2) | 0.3946(1) | 0.030(2) | 0.035(2) | 0.028(2) | 0.015(1) | 0.009(1) | 0.002(1) |
| C(21) | 8*f* | | 0.7996(1) | 0.2045(2) | 0.2668(1) | 0.034(2) | 0.029(2) | 0.017(1) | 0.000(1) | 0.009(1) | 0.000(1) |
| C(17) | 8*f* | | 0.8186(1) | 0.4944(2) | 0.4339(1) | 0.024(1) | 0.028(1) | 0.019(1) | 0.005(1) | 0.008(1) | –0.001(1) |
| C(30) | 8*f* | | 1.0018(1) | 0.0127(2) | 0.6207(1) | 0.036(2) | 0.023(1) | 0.034(2) | 0.006(1) | 0.010(1) | 0.005(1) |
| C(09) | 8*f* | | 0.8760(1) | 0.3552(2) | 0.6020(1) | 0.019(1) | 0.028(1) | 0.017(1) | 0.005(1) | 0.006(1) | 0.001(1) |
| C(39) | 8*f* | | 0.8558(3) | 0.6574(7) | 0.5495(3) | 0.099(4) | 0.153(5) | 0.108(4) | –0.013(3) | 0.050(3) | –0.038(3) |
| C(42) | 8*f* | 0.475 | 0.9391(3) | 0.1164(6) | 0.7274(3) | 0.030(1) | 0.046(2) | 0.029(1) | 0.003(1) | 0.018(1) | –0.002(1) |
| N(06) | 8*f* | 0.475 | 0.9289(4) | 0.186(1) | 0.7638(4) | 0.055(6) | 0.14(1) | 0.042(5) | 0.040(6) | 0.022(4) | 0.009(5) |
| C(41) | 8*f* | 0.475 | 0.8875(3) | 0.1745(7) | 0.7742(4) | 0.068(6) | 0.051(5) | 0.039(4) | 0.015(4) | 0.024(4) | 0.009(4) |
| C(40) | 8*f* | 0.475 | 0.9672(3) | 0.2595(7) | 0.8010(4) | 0.053(5) | 0.061(6) | 0.047(5) | 0.015(4) | 0.014(4) | 0.008(4) |
| O(06) | 8*f* | 0.475 | 0.9051(4) | 0.060(1) | 0.6972(5) | 0.125(9) | 0.42(2) | 0.17(1) | –0.16(1) | 0.128(9) | –0.21(1) |
| N(07) | 8*f* | 0.525 | 0.8821(4) | 0.0778(8) | 0.7442(3) | 0.090(5) | 0.148(8) | 0.053(4) | 0.004(6) | 0.035(4) | –0.001(4) |
| C(45) | 8*f* | 0.525 | 0.8865(5) | –0.0244(8) | 0.7307(4) | 0.090(5) | 0.148(8) | 0.053(4) | 0.004(6) | 0.035(4) | –0.001(4) |
| C(43) | 8*f* | 0.525 | 0.9145(7) | 0.150(2) | 0.7467(8) | 0.094(8) | 0.22(2) | 0.14(1) | 0.056(9) | 0.069(8) | 0.13(1) |
| C(44) | 8*f* | 0.525 | 0.8399(5) | 0.101(1) | 0.7493(6) | 0.094(8) | 0.22(2) | 0.14(1) | 0.056(9) | 0.069(8) | 0.13(1) |
| O(07) | 8*f* | 0.525 | 0.9458(8) | 0.145(2) | 0.7334(8) | 0.26(2) | 0.27(2) | 0.23(2) | –0.10(2) | 0.14(2) | –0.17(2) |
| C(37) | 8*f* | 0.687 | 0.8314(2) | 0.6665(5) | 0.6224(2) | 0.035(3) | 0.062(4) | 0.037(3) | –0.006(2) | 0.021(2) | –0.006(3) |
| C(37B) | 8*f* | 0.313 | 0.8450(4) | 0.734(1) | 0.6522(5) | 0.022(6) | 0.047(8) | 0.063(9) | –0.009(5) | 0.006(5) | 0.013(7) |
| C(38) | 8*f* | | 0.8863(3) | 0.8042(6) | 0.6151(3) | 0.099(4) | 0.153(5) | 0.108(4) | –0.013(3) | 0.050(3) | –0.038(3) |

*Acknowledgments.* Financial assistance from the Advanced Metals Initiative (AMI) and the Department of Science and Technology (DST) of South Africa, as well as the New Metals Development Network (NMDN) and the South African Nuclear Energy Corporation Limited (Necsa) is gratefully acknowledged.

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