

Crystal structure of the formal 20 electron zirconocene pentafulvene complex $\text{Cp}_2\text{Zr}(\eta^5, \eta^1\text{-adamantylidenepentafulvene})$: toluene:*n*-hexane = 1:0.125:0.125

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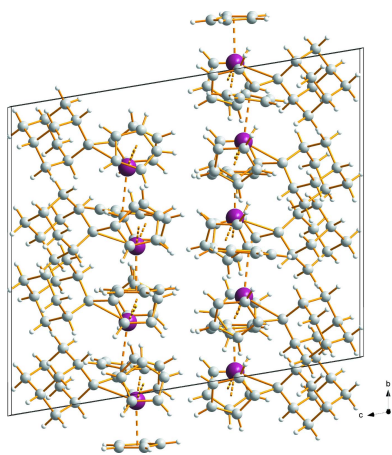
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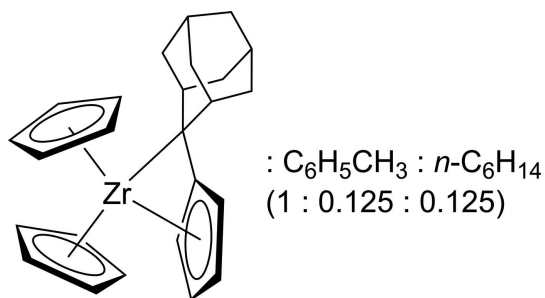
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The crystal structure of a solvated zirconocene pentafulvene complex with a bulky adamantylidene substitution pattern, namely $(\eta^5, \eta^1\text{-adamantylidenepentafulvene})\text{bis}(\eta^5\text{-cyclopentadienyl})\text{zirconium(IV)-toluene-}n\text{-hexane}$ (8/1/1), $[\text{Zr}(\text{C}_{15}\text{H}_{18})(\text{C}_5\text{H}_5)_2] \cdot 0.125\text{C}_7\text{H}_8 \cdot 0.125\text{C}_6\text{H}_{14}$, is reported. Reducing zirconocene dichloride with magnesium results in the formation of a low-valent zirconocene reagent that reacts readily with adamantylidenepentafulvene to give the aforementioned complex. Single crystal X-ray diffraction proves the dianion-like $\eta^5:\eta^1$ binding mode of the fulvene ligand to the central Zr^{IV} atom. The asymmetric unit contains four independent molecules of $[\eta^5:\eta^1\text{-adamantylidenepentafulvene}]\text{bis}[(\eta^5)\text{-cyclopentadienyl}]\text{zirconium(IV)}$, together with half a molecule of toluene disordered with half a molecule of *n*-hexane (the solvent molecules have no direct influence on the complex). In each of the four complex molecules, the central Zr^{IV} atom has a distorted tetrahedral coordination environment. The measured crystal consisted of two domains with a refined ratio of 0.77:0.23.

1. Chemical context

Over the last few decades, pentafulvenes have found plenty of applications in organometallic chemistry (Preethalayam *et al.*, 2017; Neuenschwander, 1989), one of which is their use as versatile ligands for a variety of early and late transition metals featuring a multitude of coordination modes and reactivity patterns (Preethalayam *et al.*, 2017; Kreindlin & Rybinskaya, 2004). Whereas for late transition metals $\eta^2\text{-}$ and $\eta^4\text{-}$ binding modes are known (Kim *et al.*, 2000; Rais & Bergman, 2004), most metals are bound in an $\eta^6\text{-}$ manner, either in a neutral olefinic $\eta^2:\eta^2:\eta^2$ (Konietzny *et al.*, 2010) or in a dianionic $\eta^5:\eta^1$ fashion (Ebert *et al.*, 2014). The change of polarity at the exocyclic carbon atom of the pentafulvene ligand, resulting from its bonding to the central metal atom, enables a multitude of insertion reactions and C–H-activation reactions that are of great interest to our research group (Ebert *et al.*, 2014; Manssen *et al.*, 2015, 2017; Oswald *et al.*, 2016). In this context we have recently reported the syntheses of the first zirconocene-based pentafulvene complexes and their reactivities (Jaroschik *et al.*, 2017). Here we report the synthesis and crystal structure of the solvated title compound, $(\eta^5, \eta^1\text{-adamantylidenepentafulvene})\text{bis}(\eta^5\text{-cyclopentadienyl})\text{-zirconium(IV)}$, **1**.





2. Structural commentary

Compound **1** crystallizes in the triclinic space group $P\bar{1}$ with four formula units per asymmetric unit together with one disordered solvent molecule (ratio toluene:*n*-hexane = 1:1). Fig. 1 shows one of the complex molecules present in the crystal of **1**. As a result of the high similarities with respect to structural parameters (bond lengths and angles) of the four complexes in the asymmetric unit, only this complex (Zr1) is discussed in detail. The molecular structure shows the zirconium(IV) atom to be in a distorted tetrahedral coordination environment. The zirconium atom lies 0.21 Å above the plane defined by the three centroids of the pentafulvene and cyclopentadienyl ligands, which is in good agreement with related complexes, *e.g.* 0.20 Å for the analogous complex with a 6,6'-di-*para*-tolylfulvene substitution pattern (Jaroschik *et al.*, 2017) and 0.20 Å for Cp₃ZrH (Edelbach *et al.*, 1999). The molecular structure of **1** in the solid state clearly confirms the $\pi\text{-}\eta^5\text{:}\sigma\text{-}\eta^1$ binding mode of the fulvene moiety to the central metal atom. Characteristic parameters for this coordination mode are the deviation (bend angle θ) of the C_{exo}–C_{ipso} bond

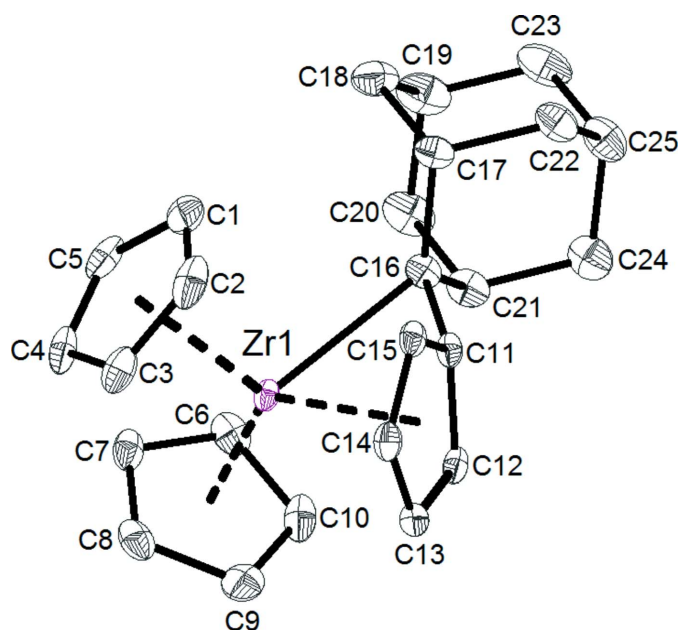


Figure 1
One of the four independent complex molecules in the crystal structure of **1**. Displacement ellipsoids are drawn at the 50% probability level. H atoms and solvent molecules have been omitted for clarity.

toward the central zirconium(IV) atom (29.4°) as well as the ring slippage (Δ) toward the C_{ipso} atom of the five-membered ring of the pentafulvene ligand (0.318 Å). The bond between the zirconium(IV) atom and the exocyclic carbon atom [Zr1–C16 = 2.605 (3) Å] is considerably longer than those of other zirconium complexes [Kraft *et al.*, 2002 (2.37 Å); Novarino *et al.*, 2011 (2.37 Å)], indicating a weak Zr–C_{exo} contact, but in good agreement with [$\pi\text{-}\eta^5\text{:}\sigma\text{-}\eta^1\text{-C}_5\text{H}_4\text{=C}(\textit{para}\text{-tolyl})_2$]-Zr(THF) (2.70 and 2.71 Å) reported previously by our group (Ebert *et al.*, 2014). Regarding the fulvene moiety, the coordination to the zirconocene fragment leads to the loss of the alternating single- and double-bond pattern of free pentafulvene. This is indicated by the narrow range of the C–C bond lengths within the five-membered ring of the fulvene ligand [1.406 (4) to 1.437 (4) Å] in comparison with free fulvene [1.327 (3) to 1.459 (2) Å] (Garcia *et al.*, 1989). Hence, the hybridization of the exocyclic carbon atom lies between *sp*² and *sp*³, which is further confirmed by the sum of angles around the C16 carbon atom [C11–C16–C17 = 116.9 (2)°, C17–C16–C21 = 109.4 (2)°, C11–C16–C21 = 118.7 (3)° = 345°].

3. Supramolecular features

No significant supramolecular features between the complex molecules or between the complex molecules and the solvent

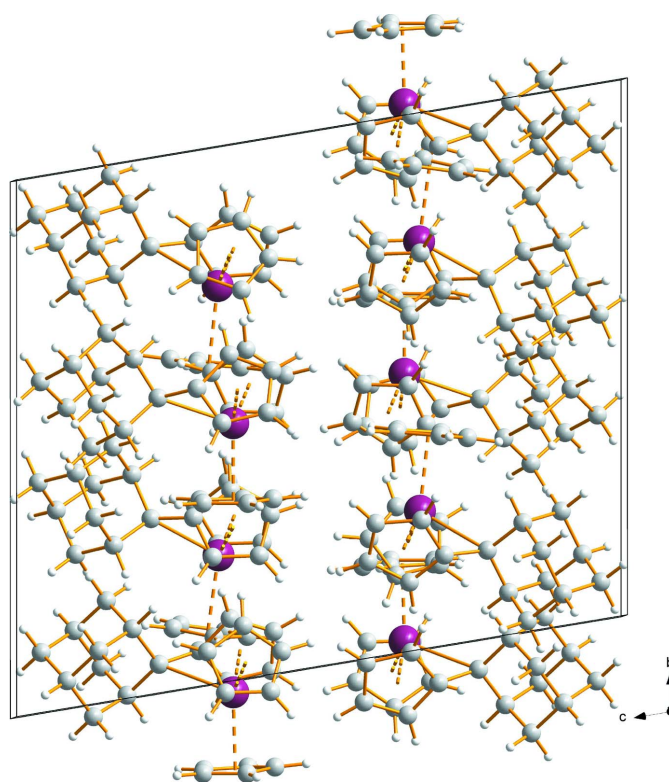


Figure 2
A view along the *a* axis showing the packing of molecules in the crystal structure of compound **1**. Solvent molecules have been omitted for clarity. No significant supramolecular features can be observed. Color code: C grey, H white, Zr plum spheres.

Table 1
Experimental details.

| | |
|--|--|
| Crystal data | |
| Chemical formula | $[\text{Zr}(\text{C}_{15}\text{H}_{18})(\text{C}_5\text{H}_5)_2] \cdot 0.125\text{C}_7\text{H}_8 \cdot 0.125\text{C}_6\text{H}_{14}$ |
| M_r | 441.98 |
| Crystal system, space group | Triclinic, $P\bar{1}$ |
| Temperature (K) | 105 |
| a, b, c (Å) | 13.6751 (6), 16.0733 (7), 19.5889 (9) |
| α, β, γ (°) | 98.6919 (18), 109.4236 (16), 90.5484 (16) |
| V (Å ³) | 4005.8 (3) |
| Z | 8 |
| Radiation type | Mo $K\alpha$ |
| μ (mm ⁻¹) | 0.56 |
| Crystal size (mm) | 0.28 × 0.24 × 0.04 |
| Data collection | |
| Diffractometer | Bruker APEXII CCD |
| Absorption correction | Multi-scan (TWINABS; Bruker, 2013) |
| $T_{\text{min}}, T_{\text{max}}$ | 0.900, 1.000 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 67120, 67120, 48102 |
| $(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹) | 0.746 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)], wR(F^2), S$ | 0.044, 0.110, 1.01 |
| No. of reflections | 67120 |
| No. of parameters | 1058 |
| No. of restraints | 72 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³) | 1.04, -0.91 |

Computer programs: APEX2 and SAINT (Bruker, 2013), SHELXS2013 (Sheldrick, 2015a), SHELXL2014 (Sheldrick, 2015b), DIAMOND (Brandenburg & Putz, 2006) and publCIF (Westrip, 2010).

molecules are observed. Hence the intermolecular forces appear to be dominated by van der Waals interactions only. In the crystal structure of **1**, the solvent molecules are located in the voids resulting from the packing arrangements of the complex molecules. Fig. 2 shows the packing without solvent molecules and Fig. 3 the packing with the contribution of the solvents.

4. Synthesis and crystallization

All reactions were carried out under a dry nitrogen atmosphere using Schlenk techniques or in a glove box. Zirconocene dichloride was purchased from Strem Chemicals and used as received. Adamantylidenepentafulvene was prepared according to a published procedure (Miller & Bercaw, 2006). Solvents were dried according to standard procedures over Na/K alloy with benzophenone as indicator and distilled under a nitrogen atmosphere.

Zirconocene dichloride (1.000 g, 3.421 mmol), magnesium (0.083 g, 3.421 mmol) and adamantylidenepentafulvene (0.884 g, 3.421 mmol) were added to a Schlenk tube under argon. THF (40 ml) was added, and the reaction was stirred for 16 h at room temperature. THF was evaporated under vacuum and 40 ml of toluene were added to the crude product. After filtration, toluene was evaporated under vacuum to give **1** as a yellow solid in 81% yield.

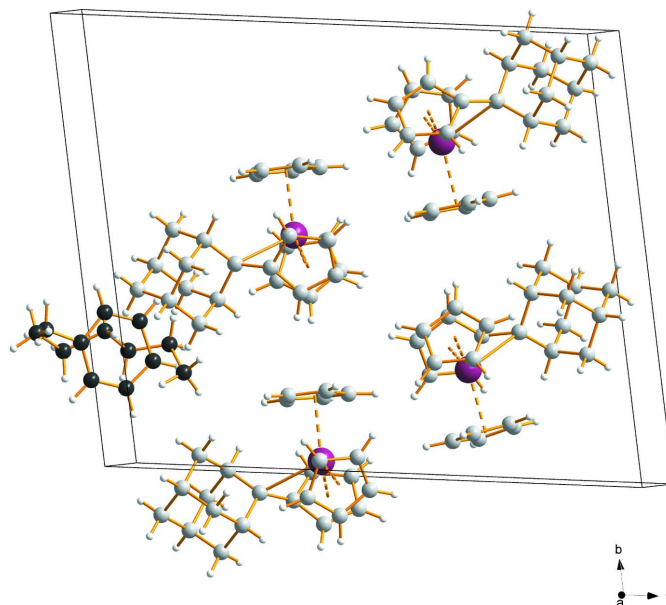


Figure 3
A view along the a axis showing the packing of molecules in the asymmetric unit. Color code: C grey, H white, Zr plum spheres. Solvent molecules are highlighted in black.

Crystals suitable for single crystal X-ray diffraction were obtained from a saturated solution of **1** in toluene, layered with n -hexane at room temperature.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

The measured crystal consisted of two domains. TWINABS was therefore used to model the absorption correction and to generate a reflection file in the HKLF5 format. The refined ratio of the two domains was 0.77:0.23. Hydrogen atoms bonded to the carbon atoms were located from difference-Fourier maps but were subsequently fixed to idealized positions using appropriate riding models with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. Reflections (001) and (00 $\bar{1}$) were obstructed from the primary beam stop and consequently omitted from the refinement. The solvent molecules toluene and n -hexane were located from difference maps and refined with RIGU commands, with site occupancies fixed to 0.50 each.

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supporting information

Acta Cryst. (2017). E73, 1823-1826 [https://doi.org/10.1107/S2056989017015560]

Crystal structure of the formal 20 electron zirconocene pentafulvene complex Cp₂Zr(η^5, η^1 -adamantylidenepentafulvene):toluene:*n*-hexane = 1:0.125:0.125

Malte Fischer, Marc Schmidtman and Rüdiger Beckhaus

Computing details

Data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINTE* (Bruker, 2013); data reduction: *SAINTE* (Bruker, 2013); program(s) used to solve structure: *SHELXS2013* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015b); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

(η^5, η^1 -Adamantylidenepentafulvene)bis(η^5 -cyclopentadienyl)zirconium(IV)-toluene-*n*-hexane (8/1/1)

Crystal data

[Zr(C₁₅H₁₈)(C₅H₅)₂]·0.125C₇H₈·0.125C₆H₁₄

M_r = 441.98

Triclinic, *P* $\bar{1}$

a = 13.6751 (6) Å

b = 16.0733 (7) Å

c = 19.5889 (9) Å

α = 98.6919 (18)°

β = 109.4236 (16)°

γ = 90.5484 (16)°

V = 4005.8 (3) Å³

Z = 8

F(000) = 1844

D_x = 1.466 Mg m⁻³

Mo *K* α radiation, λ = 0.71073 Å

Cell parameters from 6013 reflections

θ = 2.2–31.9°

μ = 0.56 mm⁻¹

T = 105 K

Plate, yellow

0.28 × 0.24 × 0.04 mm

Data collection

Bruker APEXII CCD

diffractometer

Radiation source: sealed tube

φ and ω scans

Absorption correction: multi-scan

(*TWINABS*; Bruker, 2013)

T_{min} = 0.900, *T_{max}* = 1.000

67120 measured reflections

67120 independent reflections

48102 reflections with *I* > 2 σ (*I*)

θ_{\max} = 32.0°, θ_{\min} = 1.3°

h = -20→20

k = -23→23

l = -29→29

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2 σ (*F*²)] = 0.044

wR(*F*²) = 0.110

S = 1.01

67120 reflections

1058 parameters

72 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: difference Fourier map

H-atom parameters constrained

w = 1/[$\sigma^2(F_o^2) + (0.040P)^2 + 4.P$]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/σ)_{max} = 0.002

$\Delta\rho_{\max}$ = 1.04 e Å⁻³

$\Delta\rho_{\min}$ = -0.91 e Å⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refined as a 2-component twin

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. (<1) |
|------|--------------|--------------|--------------|----------------------------------|-----------|
| Zr1 | 0.34828 (2) | 0.23916 (2) | 0.66261 (2) | 0.01264 (6) | |
| C1 | 0.4036 (2) | 0.11710 (19) | 0.7380 (2) | 0.0277 (7) | |
| H1 | 0.4576 | 0.1313 | 0.7840 | 0.033* | |
| C2 | 0.4159 (2) | 0.08779 (19) | 0.6707 (2) | 0.0295 (8) | |
| H2 | 0.4799 | 0.0757 | 0.6634 | 0.035* | |
| C3 | 0.3174 (2) | 0.07918 (17) | 0.61545 (19) | 0.0239 (6) | |
| H3 | 0.3034 | 0.0645 | 0.5641 | 0.029* | |
| C4 | 0.2435 (2) | 0.09648 (18) | 0.65087 (19) | 0.0236 (6) | |
| H4 | 0.1702 | 0.0916 | 0.6276 | 0.028* | |
| C5 | 0.2957 (2) | 0.12171 (19) | 0.72507 (19) | 0.0260 (7) | |
| H5 | 0.2645 | 0.1391 | 0.7612 | 0.031* | |
| C6 | 0.2160 (2) | 0.33703 (19) | 0.69904 (18) | 0.0222 (6) | |
| H6 | 0.2347 | 0.3591 | 0.7498 | 0.027* | |
| C7 | 0.15621 (19) | 0.26119 (18) | 0.66255 (18) | 0.0211 (6) | |
| H7 | 0.1248 | 0.2244 | 0.6841 | 0.025* | |
| C8 | 0.1513 (2) | 0.24974 (19) | 0.58924 (18) | 0.0232 (6) | |
| H8 | 0.1178 | 0.2029 | 0.5527 | 0.028* | |
| C9 | 0.2046 (2) | 0.3198 (2) | 0.57885 (19) | 0.0258 (6) | |
| H9 | 0.2131 | 0.3286 | 0.5342 | 0.031* | |
| C10 | 0.2429 (2) | 0.37398 (18) | 0.6462 (2) | 0.0251 (7) | |
| H10 | 0.2805 | 0.4267 | 0.6550 | 0.030* | |
| C11 | 0.50795 (18) | 0.31699 (16) | 0.70541 (16) | 0.0149 (5) | |
| C12 | 0.45190 (19) | 0.35608 (17) | 0.64371 (16) | 0.0162 (5) | |
| H12 | 0.4286 | 0.4116 | 0.6464 | 0.019* | |
| C13 | 0.43710 (19) | 0.29892 (18) | 0.57876 (16) | 0.0175 (5) | |
| H13 | 0.3993 | 0.3081 | 0.5305 | 0.021* | |
| C14 | 0.48798 (19) | 0.22570 (18) | 0.59757 (16) | 0.0175 (5) | |
| H14 | 0.4904 | 0.1769 | 0.5642 | 0.021* | |
| C15 | 0.53463 (18) | 0.23734 (17) | 0.67431 (16) | 0.0158 (5) | |
| H15 | 0.5770 | 0.1987 | 0.7013 | 0.019* | |
| C16 | 0.48953 (19) | 0.32835 (18) | 0.77477 (16) | 0.0175 (5) | |
| C17 | 0.5652 (2) | 0.29025 (19) | 0.83666 (16) | 0.0202 (6) | |
| H17 | 0.5805 | 0.2326 | 0.8171 | 0.024* | |
| C18 | 0.5207 (2) | 0.2850 (2) | 0.89840 (18) | 0.0282 (7) | |
| H18A | 0.4553 | 0.2488 | 0.8790 | 0.034* | |
| H18B | 0.5707 | 0.2595 | 0.9377 | 0.034* | |
| C19 | 0.4996 (2) | 0.3735 (2) | 0.92980 (19) | 0.0327 (8) | |
| H19 | 0.4703 | 0.3698 | 0.9698 | 0.039* | |

| | | | | |
|------|--------------|--------------|--------------|-------------|
| C20 | 0.4203 (2) | 0.4103 (2) | 0.86754 (18) | 0.0304 (7) |
| H20A | 0.3550 | 0.3740 | 0.8482 | 0.036* |
| H20B | 0.4044 | 0.4672 | 0.8868 | 0.036* |
| C21 | 0.4643 (2) | 0.41597 (19) | 0.80549 (17) | 0.0225 (6) |
| H21 | 0.4128 | 0.4405 | 0.7654 | 0.027* |
| C22 | 0.6668 (2) | 0.3476 (2) | 0.86836 (18) | 0.0243 (6) |
| H22A | 0.7178 | 0.3233 | 0.9080 | 0.029* |
| H22B | 0.6971 | 0.3510 | 0.8294 | 0.029* |
| C23 | 0.5999 (3) | 0.4300 (2) | 0.96032 (19) | 0.0333 (8) |
| H23A | 0.6512 | 0.4062 | 1.0003 | 0.040* |
| H23B | 0.5857 | 0.4869 | 0.9808 | 0.040* |
| C24 | 0.5656 (2) | 0.4735 (2) | 0.83771 (19) | 0.0281 (7) |
| H24A | 0.5949 | 0.4790 | 0.7986 | 0.034* |
| H24B | 0.5504 | 0.5305 | 0.8574 | 0.034* |
| C25 | 0.6443 (2) | 0.4363 (2) | 0.89874 (19) | 0.0286 (7) |
| H25 | 0.7101 | 0.4731 | 0.9187 | 0.034* |
| Zr2 | 0.33274 (2) | 0.74120 (2) | 0.66375 (2) | 0.01197 (5) |
| C26 | 0.4932 (2) | 0.8472 (3) | 0.6977 (2) | 0.0361 (9) |
| H26 | 0.5029 | 0.8891 | 0.7395 | 0.043* |
| C27 | 0.4365 (2) | 0.8540 (2) | 0.6258 (2) | 0.0276 (7) |
| H27 | 0.4031 | 0.9024 | 0.6094 | 0.033* |
| C28 | 0.4371 (2) | 0.7770 (2) | 0.58141 (18) | 0.0273 (7) |
| H28 | 0.4010 | 0.7625 | 0.5302 | 0.033* |
| C29 | 0.5009 (3) | 0.7261 (2) | 0.6268 (2) | 0.0380 (10) |
| H29 | 0.5188 | 0.6713 | 0.6111 | 0.046* |
| C30 | 0.5334 (2) | 0.7678 (3) | 0.6977 (2) | 0.0423 (10) |
| H30 | 0.5760 | 0.7464 | 0.7396 | 0.051* |
| C31 | 0.3605 (3) | 0.6196 (2) | 0.7418 (2) | 0.0377 (8) |
| H31 | 0.3838 | 0.6372 | 0.7934 | 0.045* |
| C32 | 0.4224 (3) | 0.6016 (2) | 0.6991 (3) | 0.0407 (10) |
| H32 | 0.4961 | 0.6020 | 0.7167 | 0.049* |
| C33 | 0.3600 (4) | 0.5831 (2) | 0.6271 (3) | 0.0476 (12) |
| H33 | 0.3828 | 0.5697 | 0.5861 | 0.057* |
| C34 | 0.2572 (3) | 0.5873 (2) | 0.6246 (3) | 0.0499 (12) |
| H34 | 0.1973 | 0.5780 | 0.5817 | 0.060* |
| C35 | 0.2586 (3) | 0.6076 (2) | 0.6958 (3) | 0.0417 (11) |
| H35 | 0.1992 | 0.6124 | 0.7106 | 0.050* |
| C36 | 0.22181 (19) | 0.83159 (16) | 0.70249 (15) | 0.0148 (5) |
| C37 | 0.15190 (18) | 0.75914 (17) | 0.66475 (16) | 0.0166 (5) |
| H37 | 0.1218 | 0.7226 | 0.6872 | 0.020* |
| C38 | 0.13525 (19) | 0.75110 (19) | 0.58924 (16) | 0.0194 (6) |
| H38 | 0.0946 | 0.7070 | 0.5524 | 0.023* |
| C39 | 0.1891 (2) | 0.81971 (18) | 0.57744 (16) | 0.0195 (5) |
| H39 | 0.1915 | 0.8296 | 0.5314 | 0.023* |
| C40 | 0.2386 (2) | 0.87093 (17) | 0.64555 (15) | 0.0162 (5) |
| H40 | 0.2770 | 0.9230 | 0.6529 | 0.019* |
| C41 | 0.30012 (19) | 0.83558 (17) | 0.77373 (16) | 0.0165 (5) |
| C42 | 0.3601 (2) | 0.92080 (19) | 0.80907 (17) | 0.0222 (6) |

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|------|-------------|---------------|--------------|-------------|
| H42 | 0.3795 | 0.9464 | 0.7715 | 0.027* |
| C43 | 0.4583 (2) | 0.9108 (2) | 0.87292 (18) | 0.0302 (7) |
| H43A | 0.4959 | 0.9665 | 0.8950 | 0.036* |
| H43B | 0.5048 | 0.8737 | 0.8547 | 0.036* |
| C44 | 0.4288 (2) | 0.8724 (2) | 0.93092 (18) | 0.0316 (7) |
| H44 | 0.4932 | 0.8655 | 0.9723 | 0.038* |
| C45 | 0.3719 (2) | 0.7856 (2) | 0.89559 (18) | 0.0280 (7) |
| H45A | 0.4182 | 0.7482 | 0.8775 | 0.034* |
| H45B | 0.3532 | 0.7596 | 0.9326 | 0.034* |
| C46 | 0.2733 (2) | 0.79519 (19) | 0.83160 (16) | 0.0195 (6) |
| H46 | 0.2361 | 0.7387 | 0.8090 | 0.023* |
| C47 | 0.2898 (2) | 0.97955 (19) | 0.83913 (18) | 0.0265 (7) |
| H47A | 0.3271 | 1.0354 | 0.8615 | 0.032* |
| H47B | 0.2263 | 0.9877 | 0.7985 | 0.032* |
| C48 | 0.3582 (3) | 0.9296 (2) | 0.96019 (19) | 0.0323 (8) |
| H48A | 0.3393 | 0.9044 | 0.9976 | 0.039* |
| H48B | 0.3951 | 0.9853 | 0.9837 | 0.039* |
| C49 | 0.2023 (2) | 0.85360 (19) | 0.86180 (17) | 0.0226 (6) |
| H49A | 0.1377 | 0.8602 | 0.8214 | 0.027* |
| H49B | 0.1831 | 0.8281 | 0.8989 | 0.027* |
| C50 | 0.2600 (2) | 0.9406 (2) | 0.89689 (18) | 0.0266 (7) |
| H50 | 0.2139 | 0.9784 | 0.9159 | 0.032* |
| Zr3 | 0.17259 (2) | 0.02164 (2) | 0.35641 (2) | 0.01183 (5) |
| C51 | 0.2177 (3) | 0.15654 (19) | 0.3091 (2) | 0.0295 (7) |
| H51 | 0.2407 | 0.1475 | 0.2680 | 0.035* |
| C52 | 0.2799 (2) | 0.16506 (18) | 0.3813 (2) | 0.0263 (7) |
| H52 | 0.3535 | 0.1650 | 0.3987 | 0.032* |
| C53 | 0.2165 (2) | 0.17380 (18) | 0.42502 (18) | 0.0233 (6) |
| H53 | 0.2390 | 0.1769 | 0.4768 | 0.028* |
| C54 | 0.1140 (2) | 0.17722 (18) | 0.3784 (2) | 0.0243 (7) |
| H54 | 0.0552 | 0.1871 | 0.3934 | 0.029* |
| C55 | 0.1135 (2) | 0.16350 (19) | 0.3063 (2) | 0.0286 (7) |
| H55 | 0.0541 | 0.1596 | 0.2632 | 0.034* |
| C56 | -0.0062 (2) | -0.0617 (2) | 0.3120 (2) | 0.0342 (9) |
| H56 | -0.0303 | -0.0868 | 0.2617 | 0.041* |
| C57 | -0.0243 (2) | 0.02045 (19) | 0.34153 (19) | 0.0242 (7) |
| H57 | -0.0646 | 0.0602 | 0.3148 | 0.029* |
| C58 | 0.0274 (2) | 0.0321 (2) | 0.41629 (19) | 0.0266 (7) |
| H58 | 0.0281 | 0.0816 | 0.4498 | 0.032* |
| C59 | 0.0777 (3) | -0.0391 (2) | 0.4347 (2) | 0.0337 (8) |
| H59 | 0.1209 | -0.0462 | 0.4825 | 0.040* |
| C60 | 0.0545 (2) | -0.09897 (19) | 0.3716 (2) | 0.0370 (10) |
| H60 | 0.0758 | -0.1551 | 0.3691 | 0.044* |
| C61 | 0.2692 (2) | -0.06680 (17) | 0.30162 (17) | 0.0183 (6) |
| C62 | 0.2524 (2) | -0.11713 (18) | 0.35200 (17) | 0.0202 (6) |
| H62 | 0.2097 | -0.1680 | 0.3385 | 0.024* |
| C63 | 0.3090 (2) | -0.0795 (2) | 0.42394 (19) | 0.0248 (6) |
| H63 | 0.3086 | -0.0989 | 0.4673 | 0.030* |

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|------|-------------|---------------|--------------|-------------|
| C64 | 0.3669 (2) | -0.0073 (2) | 0.42099 (19) | 0.0249 (6) |
| H64 | 0.4116 | 0.0303 | 0.4619 | 0.030* |
| C65 | 0.3463 (2) | -0.00141 (19) | 0.34688 (18) | 0.0224 (6) |
| H65 | 0.3783 | 0.0394 | 0.3292 | 0.027* |
| C66 | 0.1889 (2) | -0.05370 (18) | 0.23524 (17) | 0.0196 (6) |
| C67 | 0.2210 (3) | -0.0062 (2) | 0.18306 (19) | 0.0269 (7) |
| H67 | 0.2693 | 0.0435 | 0.2120 | 0.032* |
| C68 | 0.1258 (3) | 0.0237 (2) | 0.1271 (2) | 0.0364 (8) |
| H68A | 0.0898 | 0.0635 | 0.1530 | 0.044* |
| H68B | 0.1482 | 0.0538 | 0.0938 | 0.044* |
| C69 | 0.0517 (3) | -0.0514 (3) | 0.0829 (2) | 0.0415 (9) |
| H69 | -0.0107 | -0.0314 | 0.0470 | 0.050* |
| C70 | 0.0179 (3) | -0.0972 (2) | 0.1348 (2) | 0.0365 (8) |
| H70A | -0.0307 | -0.1460 | 0.1063 | 0.044* |
| H70B | -0.0188 | -0.0587 | 0.1610 | 0.044* |
| C71 | 0.1129 (2) | -0.1280 (2) | 0.19077 (18) | 0.0257 (6) |
| H71 | 0.0901 | -0.1583 | 0.2244 | 0.031* |
| C72 | 0.2770 (3) | -0.0669 (2) | 0.1411 (2) | 0.0370 (9) |
| H72A | 0.3000 | -0.0370 | 0.1079 | 0.044* |
| H72B | 0.3391 | -0.0866 | 0.1764 | 0.044* |
| C73 | 0.1075 (4) | -0.1122 (3) | 0.0413 (2) | 0.0483 (11) |
| H73A | 0.0593 | -0.1610 | 0.0119 | 0.058* |
| H73B | 0.1296 | -0.0828 | 0.0074 | 0.058* |
| C74 | 0.1684 (3) | -0.1886 (2) | 0.1486 (2) | 0.0331 (8) |
| H74A | 0.2301 | -0.2088 | 0.1838 | 0.040* |
| H74B | 0.1208 | -0.2381 | 0.1205 | 0.040* |
| C75 | 0.2020 (3) | -0.1429 (2) | 0.0962 (2) | 0.0401 (9) |
| H75 | 0.2381 | -0.1823 | 0.0694 | 0.048* |
| Zr4 | 0.16561 (2) | 0.52009 (2) | 0.35633 (2) | 0.01146 (5) |
| C76 | 0.2956 (2) | 0.41870 (19) | 0.3221 (2) | 0.0279 (7) |
| H76 | 0.2749 | 0.3925 | 0.2722 | 0.034* |
| C77 | 0.2735 (2) | 0.38672 (19) | 0.3785 (2) | 0.0290 (7) |
| H77 | 0.2381 | 0.3340 | 0.3739 | 0.035* |
| C78 | 0.3130 (2) | 0.4463 (2) | 0.44286 (19) | 0.0263 (7) |
| H78 | 0.3061 | 0.4424 | 0.4890 | 0.032* |
| C79 | 0.3649 (2) | 0.51291 (19) | 0.42664 (18) | 0.0223 (6) |
| H79 | 0.4011 | 0.5610 | 0.4606 | 0.027* |
| C80 | 0.3538 (2) | 0.49636 (19) | 0.35210 (19) | 0.0241 (6) |
| H80 | 0.3807 | 0.5311 | 0.3265 | 0.029* |
| C81 | 0.2010 (3) | 0.65239 (19) | 0.30234 (18) | 0.0259 (7) |
| H81 | 0.2182 | 0.6415 | 0.2588 | 0.031* |
| C82 | 0.2712 (2) | 0.66405 (17) | 0.37391 (18) | 0.0216 (6) |
| H82 | 0.3447 | 0.6655 | 0.3877 | 0.026* |
| C83 | 0.2138 (2) | 0.67337 (17) | 0.42211 (17) | 0.0201 (6) |
| H83 | 0.2415 | 0.6782 | 0.4740 | 0.024* |
| C84 | 0.1083 (2) | 0.67435 (18) | 0.37968 (19) | 0.0237 (6) |
| H84 | 0.0525 | 0.6834 | 0.3981 | 0.028* |
| C85 | 0.0999 (2) | 0.65966 (19) | 0.30595 (19) | 0.0267 (7) |

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|------|---------------|--------------|--------------|-------------|-----|
| H85 | 0.0373 | 0.6553 | 0.2653 | 0.032* | |
| C86 | 0.00649 (18) | 0.44439 (17) | 0.29543 (16) | 0.0164 (5) | |
| C87 | -0.02264 (19) | 0.51655 (18) | 0.33577 (16) | 0.0178 (5) | |
| H87 | -0.0615 | 0.5607 | 0.3150 | 0.021* | |
| C88 | 0.0155 (2) | 0.5111 (2) | 0.41062 (17) | 0.0226 (6) | |
| H88 | 0.0103 | 0.5523 | 0.4493 | 0.027* | |
| C89 | 0.0627 (2) | 0.4343 (2) | 0.41867 (17) | 0.0223 (6) | |
| H89 | 0.0945 | 0.4144 | 0.4637 | 0.027* | |
| C90 | 0.0549 (2) | 0.39190 (17) | 0.34873 (17) | 0.0195 (6) | |
| H90 | 0.0779 | 0.3373 | 0.3384 | 0.023* | |
| C91 | 0.0358 (2) | 0.44995 (18) | 0.23175 (16) | 0.0194 (6) | |
| C92 | 0.0661 (2) | 0.36983 (19) | 0.19246 (18) | 0.0241 (6) | |
| H92 | 0.1139 | 0.3387 | 0.2292 | 0.029* | |
| C93 | 0.1192 (3) | 0.3925 (2) | 0.1394 (2) | 0.0361 (9) | |
| H93A | 0.1837 | 0.4282 | 0.1672 | 0.043* | |
| H93B | 0.1383 | 0.3404 | 0.1142 | 0.043* | |
| C94 | 0.0470 (3) | 0.4397 (3) | 0.0825 (2) | 0.0421 (10) | |
| H94 | 0.0828 | 0.4544 | 0.0485 | 0.051* | |
| C95 | 0.0195 (3) | 0.5201 (2) | 0.12220 (19) | 0.0365 (8) | |
| H95A | -0.0272 | 0.5515 | 0.0859 | 0.044* | |
| H95B | 0.0834 | 0.5565 | 0.1499 | 0.044* | |
| C96 | -0.0342 (2) | 0.4987 (2) | 0.17498 (18) | 0.0259 (6) | |
| H96 | -0.0525 | 0.5518 | 0.2005 | 0.031* | |
| C97 | -0.0340 (2) | 0.3136 (2) | 0.1473 (2) | 0.0322 (8) | |
| H97A | -0.0157 | 0.2611 | 0.1220 | 0.039* | |
| H97B | -0.0695 | 0.2979 | 0.1806 | 0.039* | |
| C98 | -0.0529 (3) | 0.3835 (3) | 0.0383 (2) | 0.0464 (10) | |
| H98A | -0.1002 | 0.4138 | 0.0014 | 0.056* | |
| H98B | -0.0352 | 0.3313 | 0.0122 | 0.056* | |
| C99 | -0.1345 (3) | 0.4425 (2) | 0.1305 (2) | 0.0351 (8) | |
| H99A | -0.1706 | 0.4285 | 0.1638 | 0.042* | |
| H99B | -0.1819 | 0.4735 | 0.0941 | 0.042* | |
| C100 | -0.1066 (3) | 0.3612 (2) | 0.0908 (2) | 0.0380 (9) | |
| H100 | -0.1714 | 0.3250 | 0.0624 | 0.046* | |
| C101 | 0.2208 (8) | 0.2642 (6) | -0.0633 (9) | 0.050 (2) | 0.5 |
| C102 | 0.2427 (5) | 0.1823 (5) | -0.0513 (6) | 0.0411 (18) | 0.5 |
| H102 | 0.2244 | 0.1372 | -0.0915 | 0.049* | 0.5 |
| C103 | 0.2883 (7) | 0.1677 (6) | 0.0150 (6) | 0.057 (2) | 0.5 |
| H103 | 0.2962 | 0.1109 | 0.0229 | 0.068* | 0.5 |
| C104 | 0.3251 (10) | 0.2308 (9) | 0.0735 (9) | 0.077 (4) | 0.5 |
| H104 | 0.3608 | 0.2203 | 0.1218 | 0.092* | 0.5 |
| C105 | 0.3052 (7) | 0.3174 (6) | 0.0563 (7) | 0.062 (3) | 0.5 |
| H105 | 0.3317 | 0.3638 | 0.0950 | 0.074* | 0.5 |
| C106 | 0.2523 (10) | 0.3332 (6) | -0.0101 (9) | 0.058 (3) | 0.5 |
| H106 | 0.2376 | 0.3887 | -0.0198 | 0.070* | 0.5 |
| C107 | 0.1697 (15) | 0.2892 (17) | -0.1291 (12) | 0.126 (7) | 0.5 |
| H10F | 0.1629 | 0.3503 | -0.1213 | 0.189* | 0.5 |
| H10G | 0.1005 | 0.2600 | -0.1506 | 0.189* | 0.5 |

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|------|-------------|-------------|-------------|-----------|-----|
| H10H | 0.2092 | 0.2754 | -0.1624 | 0.189* | 0.5 |
| C108 | 0.2677 (9) | 0.2072 (9) | 0.1250 (9) | 0.107 (5) | 0.5 |
| H10A | 0.2311 | 0.2368 | 0.1559 | 0.160* | 0.5 |
| H10B | 0.3106 | 0.1656 | 0.1509 | 0.160* | 0.5 |
| H10C | 0.2169 | 0.1784 | 0.0790 | 0.160* | 0.5 |
| C109 | 0.3356 (8) | 0.2694 (8) | 0.1086 (7) | 0.065 (3) | 0.5 |
| H10D | 0.3155 | 0.3273 | 0.1208 | 0.078* | 0.5 |
| H10E | 0.4089 | 0.2656 | 0.1390 | 0.078* | 0.5 |
| C110 | 0.3242 (14) | 0.2513 (13) | 0.0296 (10) | 0.115 (6) | 0.5 |
| H11A | 0.3894 | 0.2704 | 0.0234 | 0.138* | 0.5 |
| H11B | 0.3132 | 0.1896 | 0.0126 | 0.138* | 0.5 |
| C111 | 0.2397 (13) | 0.2919 (13) | -0.0149 (9) | 0.092 (5) | 0.5 |
| H11C | 0.2572 | 0.3530 | -0.0095 | 0.111* | 0.5 |
| H11D | 0.1763 | 0.2840 | -0.0022 | 0.111* | 0.5 |
| C112 | 0.2243 (10) | 0.2438 (11) | -0.0980 (8) | 0.083 (4) | 0.5 |
| H11E | 0.2881 | 0.2525 | -0.1100 | 0.100* | 0.5 |
| H11F | 0.2098 | 0.1825 | -0.1019 | 0.100* | 0.5 |
| C113 | 0.1355 (10) | 0.2802 (9) | -0.1492 (6) | 0.046 (2) | 0.5 |
| H11G | 0.0781 | 0.2844 | -0.1297 | 0.069* | 0.5 |
| H11H | 0.1127 | 0.2437 | -0.1972 | 0.069* | 0.5 |
| H11I | 0.1572 | 0.3365 | -0.1544 | 0.069* | 0.5 |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|--------------|--------------|--------------|
| Zr1 | 0.01101 (10) | 0.00916 (11) | 0.01929 (14) | 0.00180 (8) | 0.00651 (10) | 0.00375 (10) |
| C1 | 0.0270 (14) | 0.0175 (15) | 0.037 (2) | 0.0013 (11) | 0.0042 (13) | 0.0142 (14) |
| C2 | 0.0225 (13) | 0.0138 (14) | 0.061 (2) | 0.0082 (10) | 0.0222 (15) | 0.0144 (15) |
| C3 | 0.0317 (15) | 0.0100 (12) | 0.0349 (18) | 0.0012 (10) | 0.0178 (13) | 0.0030 (11) |
| C4 | 0.0185 (12) | 0.0142 (13) | 0.043 (2) | -0.0006 (10) | 0.0150 (13) | 0.0071 (13) |
| C5 | 0.0326 (15) | 0.0188 (15) | 0.0362 (19) | 0.0034 (11) | 0.0209 (14) | 0.0128 (13) |
| C6 | 0.0154 (11) | 0.0207 (14) | 0.0286 (17) | 0.0068 (10) | 0.0069 (11) | -0.0012 (12) |
| C7 | 0.0126 (11) | 0.0178 (14) | 0.0348 (18) | 0.0027 (9) | 0.0092 (11) | 0.0077 (12) |
| C8 | 0.0135 (11) | 0.0214 (15) | 0.0298 (17) | 0.0037 (10) | 0.0021 (11) | 0.0016 (13) |
| C9 | 0.0187 (12) | 0.0278 (16) | 0.0337 (18) | 0.0105 (11) | 0.0080 (12) | 0.0145 (14) |
| C10 | 0.0153 (11) | 0.0129 (13) | 0.048 (2) | 0.0046 (9) | 0.0106 (13) | 0.0084 (13) |
| C11 | 0.0108 (10) | 0.0124 (12) | 0.0214 (14) | 0.0000 (8) | 0.0056 (10) | 0.0024 (10) |
| C12 | 0.0142 (11) | 0.0112 (12) | 0.0247 (15) | -0.0008 (8) | 0.0082 (10) | 0.0039 (10) |
| C13 | 0.0156 (11) | 0.0185 (13) | 0.0178 (14) | -0.0023 (9) | 0.0046 (10) | 0.0033 (11) |
| C14 | 0.0150 (11) | 0.0169 (13) | 0.0223 (15) | -0.0014 (9) | 0.0097 (10) | 0.0010 (11) |
| C15 | 0.0107 (10) | 0.0146 (12) | 0.0239 (15) | 0.0010 (8) | 0.0081 (10) | 0.0036 (11) |
| C16 | 0.0154 (11) | 0.0191 (13) | 0.0181 (14) | 0.0041 (9) | 0.0063 (10) | 0.0016 (11) |
| C17 | 0.0198 (12) | 0.0227 (15) | 0.0173 (14) | 0.0052 (10) | 0.0050 (11) | 0.0032 (11) |
| C18 | 0.0286 (15) | 0.0373 (19) | 0.0205 (16) | 0.0072 (13) | 0.0085 (13) | 0.0095 (14) |
| C19 | 0.0316 (16) | 0.048 (2) | 0.0198 (17) | 0.0105 (15) | 0.0118 (13) | 0.0015 (15) |
| C20 | 0.0266 (15) | 0.0396 (19) | 0.0239 (17) | 0.0113 (13) | 0.0100 (13) | -0.0023 (14) |
| C21 | 0.0227 (13) | 0.0214 (15) | 0.0216 (16) | 0.0072 (11) | 0.0064 (11) | 0.0001 (12) |
| C22 | 0.0192 (12) | 0.0288 (17) | 0.0217 (16) | 0.0049 (11) | 0.0045 (11) | -0.0005 (13) |

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|-----|--------------|--------------|--------------|--------------|--------------|--------------|
| C23 | 0.0331 (16) | 0.039 (2) | 0.0194 (17) | 0.0084 (14) | 0.0029 (13) | -0.0061 (15) |
| C24 | 0.0315 (15) | 0.0203 (15) | 0.0277 (18) | 0.0040 (12) | 0.0071 (13) | -0.0034 (13) |
| C25 | 0.0254 (14) | 0.0284 (18) | 0.0258 (18) | 0.0015 (12) | 0.0045 (13) | -0.0049 (14) |
| Zr2 | 0.01016 (10) | 0.00995 (11) | 0.01683 (13) | 0.00053 (8) | 0.00541 (9) | 0.00342 (10) |
| C26 | 0.0283 (15) | 0.051 (2) | 0.0274 (19) | -0.0275 (15) | 0.0169 (14) | -0.0126 (16) |
| C27 | 0.0225 (13) | 0.0207 (15) | 0.048 (2) | 0.0009 (11) | 0.0193 (14) | 0.0150 (14) |
| C28 | 0.0214 (13) | 0.0385 (19) | 0.0226 (16) | -0.0117 (12) | 0.0111 (12) | -0.0015 (14) |
| C29 | 0.0312 (16) | 0.0276 (17) | 0.075 (3) | 0.0058 (13) | 0.040 (2) | 0.0155 (18) |
| C30 | 0.0115 (12) | 0.073 (3) | 0.050 (2) | -0.0005 (15) | 0.0089 (14) | 0.038 (2) |
| C31 | 0.069 (3) | 0.0175 (15) | 0.033 (2) | 0.0068 (15) | 0.0220 (19) | 0.0119 (14) |
| C32 | 0.0271 (16) | 0.0268 (18) | 0.079 (3) | 0.0139 (13) | 0.0219 (19) | 0.029 (2) |
| C33 | 0.101 (4) | 0.0120 (15) | 0.056 (3) | 0.0115 (18) | 0.059 (3) | 0.0083 (16) |
| C34 | 0.054 (2) | 0.0108 (16) | 0.061 (3) | -0.0111 (15) | -0.013 (2) | 0.0071 (17) |
| C35 | 0.0412 (19) | 0.0165 (15) | 0.091 (4) | 0.0084 (13) | 0.048 (2) | 0.0222 (19) |
| C36 | 0.0141 (10) | 0.0109 (12) | 0.0195 (14) | 0.0013 (8) | 0.0066 (10) | 0.0006 (10) |
| C37 | 0.0109 (10) | 0.0165 (13) | 0.0222 (15) | 0.0016 (9) | 0.0062 (10) | 0.0014 (11) |
| C38 | 0.0138 (11) | 0.0226 (14) | 0.0176 (14) | 0.0033 (10) | 0.0019 (10) | -0.0017 (11) |
| C39 | 0.0204 (12) | 0.0201 (14) | 0.0186 (14) | 0.0098 (10) | 0.0060 (11) | 0.0051 (11) |
| C40 | 0.0190 (11) | 0.0128 (12) | 0.0183 (14) | 0.0054 (9) | 0.0075 (10) | 0.0043 (10) |
| C41 | 0.0157 (11) | 0.0155 (13) | 0.0179 (14) | -0.0033 (9) | 0.0060 (10) | 0.0012 (10) |
| C42 | 0.0256 (13) | 0.0209 (14) | 0.0188 (15) | -0.0105 (11) | 0.0085 (11) | -0.0022 (12) |
| C43 | 0.0242 (14) | 0.042 (2) | 0.0197 (16) | -0.0152 (13) | 0.0050 (12) | -0.0020 (14) |
| C44 | 0.0265 (15) | 0.045 (2) | 0.0178 (16) | -0.0069 (14) | 0.0018 (12) | 0.0026 (15) |
| C45 | 0.0320 (15) | 0.0330 (18) | 0.0203 (16) | 0.0007 (13) | 0.0084 (13) | 0.0097 (14) |
| C46 | 0.0220 (12) | 0.0194 (14) | 0.0178 (14) | -0.0039 (10) | 0.0078 (11) | 0.0025 (11) |
| C47 | 0.0362 (16) | 0.0173 (14) | 0.0244 (17) | -0.0071 (12) | 0.0110 (13) | -0.0031 (12) |
| C48 | 0.0362 (17) | 0.039 (2) | 0.0190 (17) | -0.0152 (14) | 0.0099 (14) | -0.0044 (15) |
| C49 | 0.0242 (13) | 0.0226 (15) | 0.0220 (16) | -0.0065 (11) | 0.0120 (12) | -0.0029 (12) |
| C50 | 0.0316 (15) | 0.0217 (16) | 0.0257 (17) | -0.0086 (12) | 0.0141 (13) | -0.0077 (13) |
| Zr3 | 0.01074 (10) | 0.00897 (11) | 0.01757 (13) | 0.00172 (8) | 0.00685 (9) | 0.00275 (9) |
| C51 | 0.0496 (19) | 0.0124 (14) | 0.036 (2) | -0.0010 (12) | 0.0284 (17) | 0.0020 (13) |
| C52 | 0.0173 (12) | 0.0122 (13) | 0.050 (2) | -0.0018 (10) | 0.0132 (13) | 0.0039 (14) |
| C53 | 0.0305 (14) | 0.0122 (13) | 0.0247 (17) | -0.0042 (11) | 0.0081 (13) | -0.0013 (12) |
| C54 | 0.0213 (13) | 0.0104 (13) | 0.047 (2) | 0.0022 (10) | 0.0197 (14) | 0.0032 (13) |
| C55 | 0.0314 (15) | 0.0122 (14) | 0.0326 (19) | -0.0019 (11) | -0.0032 (13) | 0.0073 (13) |
| C56 | 0.0212 (14) | 0.042 (2) | 0.039 (2) | -0.0178 (13) | 0.0184 (14) | -0.0141 (16) |
| C57 | 0.0123 (11) | 0.0239 (15) | 0.042 (2) | 0.0035 (10) | 0.0122 (12) | 0.0133 (14) |
| C58 | 0.0259 (14) | 0.0272 (16) | 0.0342 (19) | -0.0019 (12) | 0.0219 (14) | 0.0007 (14) |
| C59 | 0.0302 (16) | 0.044 (2) | 0.040 (2) | 0.0052 (14) | 0.0217 (15) | 0.0230 (17) |
| C60 | 0.0292 (15) | 0.0121 (14) | 0.085 (3) | 0.0031 (11) | 0.0368 (19) | 0.0135 (17) |
| C61 | 0.0165 (11) | 0.0135 (12) | 0.0295 (16) | 0.0053 (9) | 0.0148 (11) | 0.0010 (11) |
| C62 | 0.0189 (12) | 0.0144 (13) | 0.0314 (17) | 0.0070 (10) | 0.0122 (12) | 0.0072 (12) |
| C63 | 0.0219 (13) | 0.0240 (15) | 0.0307 (18) | 0.0106 (11) | 0.0085 (12) | 0.0112 (13) |
| C64 | 0.0150 (12) | 0.0263 (16) | 0.0308 (18) | 0.0064 (10) | 0.0038 (12) | 0.0058 (13) |
| C65 | 0.0132 (11) | 0.0202 (14) | 0.0377 (19) | 0.0033 (10) | 0.0133 (12) | 0.0058 (13) |
| C66 | 0.0243 (13) | 0.0161 (13) | 0.0221 (15) | 0.0063 (10) | 0.0135 (12) | 0.0014 (11) |
| C67 | 0.0404 (17) | 0.0208 (15) | 0.0267 (17) | 0.0073 (12) | 0.0206 (14) | 0.0041 (13) |
| C68 | 0.057 (2) | 0.035 (2) | 0.0243 (18) | 0.0160 (16) | 0.0213 (17) | 0.0064 (15) |

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| C69 | 0.056 (2) | 0.045 (2) | 0.0195 (18) | 0.0146 (18) | 0.0081 (17) | 0.0051 (16) |
| C70 | 0.0372 (18) | 0.040 (2) | 0.0255 (19) | 0.0024 (15) | 0.0056 (15) | -0.0041 (16) |
| C71 | 0.0312 (15) | 0.0217 (15) | 0.0236 (16) | -0.0004 (12) | 0.0111 (13) | -0.0027 (12) |
| C72 | 0.057 (2) | 0.0297 (19) | 0.040 (2) | 0.0103 (16) | 0.0371 (19) | 0.0060 (16) |
| C73 | 0.080 (3) | 0.041 (2) | 0.028 (2) | 0.008 (2) | 0.026 (2) | -0.0011 (18) |
| C74 | 0.048 (2) | 0.0225 (17) | 0.0300 (19) | 0.0049 (14) | 0.0192 (16) | -0.0050 (14) |
| C75 | 0.065 (2) | 0.032 (2) | 0.032 (2) | 0.0141 (17) | 0.0308 (19) | -0.0003 (16) |
| Zr4 | 0.01103 (10) | 0.00883 (11) | 0.01512 (13) | 0.00078 (8) | 0.00556 (9) | 0.00119 (9) |
| C76 | 0.0174 (12) | 0.0202 (15) | 0.042 (2) | 0.0051 (10) | 0.0097 (13) | -0.0080 (14) |
| C77 | 0.0152 (12) | 0.0145 (14) | 0.056 (2) | 0.0041 (10) | 0.0095 (14) | 0.0077 (14) |
| C78 | 0.0182 (12) | 0.0272 (16) | 0.0357 (19) | 0.0060 (11) | 0.0073 (12) | 0.0160 (14) |
| C79 | 0.0137 (11) | 0.0221 (15) | 0.0281 (17) | 0.0006 (10) | 0.0032 (11) | 0.0033 (12) |
| C80 | 0.0142 (11) | 0.0229 (15) | 0.0384 (19) | 0.0026 (10) | 0.0136 (12) | 0.0037 (13) |
| C81 | 0.0452 (18) | 0.0130 (14) | 0.0231 (16) | -0.0045 (12) | 0.0168 (14) | 0.0020 (12) |
| C82 | 0.0210 (12) | 0.0116 (13) | 0.0348 (18) | -0.0014 (10) | 0.0135 (12) | 0.0022 (12) |
| C83 | 0.0232 (13) | 0.0134 (13) | 0.0212 (15) | -0.0016 (10) | 0.0068 (11) | -0.0026 (11) |
| C84 | 0.0202 (12) | 0.0118 (13) | 0.0387 (19) | 0.0015 (10) | 0.0114 (13) | -0.0003 (12) |
| C85 | 0.0286 (14) | 0.0130 (14) | 0.0289 (18) | -0.0022 (11) | -0.0039 (13) | 0.0067 (13) |
| C86 | 0.0102 (10) | 0.0137 (12) | 0.0246 (15) | -0.0031 (8) | 0.0051 (10) | 0.0029 (11) |
| C87 | 0.0123 (10) | 0.0184 (13) | 0.0260 (16) | 0.0025 (9) | 0.0090 (10) | 0.0072 (11) |
| C88 | 0.0195 (12) | 0.0271 (16) | 0.0270 (16) | 0.0031 (11) | 0.0149 (12) | 0.0054 (13) |
| C89 | 0.0195 (12) | 0.0282 (16) | 0.0251 (16) | 0.0027 (11) | 0.0106 (11) | 0.0146 (13) |
| C90 | 0.0167 (11) | 0.0134 (12) | 0.0319 (17) | 0.0002 (9) | 0.0108 (11) | 0.0080 (11) |
| C91 | 0.0189 (12) | 0.0178 (14) | 0.0201 (15) | -0.0058 (10) | 0.0066 (11) | -0.0009 (11) |
| C92 | 0.0249 (14) | 0.0213 (15) | 0.0239 (16) | -0.0087 (11) | 0.0102 (12) | -0.0069 (12) |
| C93 | 0.0405 (18) | 0.040 (2) | 0.0284 (19) | -0.0181 (15) | 0.0214 (16) | -0.0151 (16) |
| C94 | 0.059 (2) | 0.046 (2) | 0.0190 (18) | -0.0270 (18) | 0.0164 (17) | -0.0082 (16) |
| C95 | 0.047 (2) | 0.037 (2) | 0.0199 (17) | -0.0193 (16) | 0.0041 (15) | 0.0050 (15) |
| C96 | 0.0285 (14) | 0.0235 (16) | 0.0192 (16) | -0.0075 (12) | -0.0004 (12) | 0.0035 (12) |
| C97 | 0.0335 (16) | 0.0238 (17) | 0.033 (2) | -0.0135 (13) | 0.0094 (15) | -0.0082 (15) |
| C98 | 0.060 (2) | 0.047 (2) | 0.0222 (19) | -0.0241 (19) | 0.0063 (18) | -0.0071 (17) |
| C99 | 0.0296 (16) | 0.036 (2) | 0.0288 (19) | -0.0106 (14) | -0.0046 (14) | 0.0076 (15) |
| C100 | 0.0388 (18) | 0.036 (2) | 0.0271 (19) | -0.0216 (15) | 0.0002 (15) | -0.0054 (16) |
| C101 | 0.041 (4) | 0.032 (4) | 0.093 (7) | 0.004 (3) | 0.044 (5) | 0.013 (5) |
| C102 | 0.028 (3) | 0.020 (3) | 0.074 (5) | 0.006 (2) | 0.019 (3) | 0.000 (3) |
| C103 | 0.050 (5) | 0.036 (5) | 0.071 (6) | 0.004 (4) | 0.010 (4) | -0.008 (4) |
| C104 | 0.066 (7) | 0.067 (7) | 0.067 (7) | 0.026 (5) | -0.006 (6) | -0.015 (5) |
| C105 | 0.048 (5) | 0.040 (5) | 0.095 (7) | -0.002 (4) | 0.034 (5) | -0.017 (5) |
| C106 | 0.055 (5) | 0.020 (4) | 0.107 (8) | -0.008 (4) | 0.042 (5) | 0.001 (4) |
| C107 | 0.090 (13) | 0.167 (17) | 0.145 (12) | -0.007 (11) | 0.045 (9) | 0.083 (11) |
| C108 | 0.072 (8) | 0.101 (11) | 0.146 (13) | -0.006 (7) | 0.015 (8) | 0.067 (10) |
| C109 | 0.038 (5) | 0.063 (7) | 0.088 (8) | -0.005 (5) | 0.009 (5) | 0.023 (6) |
| C110 | 0.114 (11) | 0.130 (15) | 0.104 (9) | 0.010 (9) | 0.028 (8) | 0.049 (9) |
| C111 | 0.079 (9) | 0.152 (16) | 0.058 (7) | 0.031 (10) | 0.035 (6) | 0.025 (9) |
| C112 | 0.052 (6) | 0.133 (13) | 0.083 (8) | 0.016 (7) | 0.045 (6) | 0.021 (8) |
| C113 | 0.057 (6) | 0.048 (5) | 0.034 (5) | -0.009 (4) | 0.019 (4) | 0.003 (4) |

Geometric parameters (Å, °)

| | | | |
|---------|-----------|----------|-----------|
| Zr1—C11 | 2.334 (2) | C51—C55 | 1.413 (4) |
| Zr1—C15 | 2.482 (2) | C51—H51 | 0.9500 |
| Zr1—C12 | 2.487 (2) | C52—C53 | 1.401 (4) |
| Zr1—C3 | 2.578 (3) | C52—H52 | 0.9500 |
| Zr1—C1 | 2.601 (3) | C53—C54 | 1.403 (4) |
| Zr1—C9 | 2.604 (3) | C53—H53 | 0.9500 |
| Zr1—C16 | 2.605 (3) | C54—C55 | 1.395 (5) |
| Zr1—C6 | 2.613 (3) | C54—H54 | 0.9500 |
| Zr1—C5 | 2.614 (3) | C55—H55 | 0.9500 |
| Zr1—C10 | 2.615 (3) | C56—C60 | 1.410 (6) |
| Zr1—C8 | 2.619 (3) | C56—C57 | 1.418 (5) |
| Zr1—C2 | 2.620 (3) | C56—H56 | 0.9500 |
| Zr1—C14 | 2.620 (2) | C57—C58 | 1.380 (5) |
| Zr1—C13 | 2.623 (3) | C57—H57 | 0.9500 |
| Zr1—C4 | 2.631 (3) | C58—C59 | 1.373 (5) |
| Zr1—C7 | 2.653 (2) | C58—H58 | 0.9500 |
| C1—C2 | 1.397 (5) | C59—C60 | 1.389 (5) |
| C1—C5 | 1.415 (4) | C59—H59 | 0.9500 |
| C1—H1 | 0.9500 | C60—H60 | 0.9500 |
| C2—C3 | 1.409 (5) | C61—C62 | 1.439 (4) |
| C2—H2 | 0.9500 | C61—C65 | 1.441 (4) |
| C3—C4 | 1.412 (4) | C61—C66 | 1.442 (4) |
| C3—H3 | 0.9500 | C62—C63 | 1.400 (5) |
| C4—C5 | 1.383 (5) | C62—H62 | 0.9500 |
| C4—H4 | 0.9500 | C63—C64 | 1.417 (4) |
| C5—H5 | 0.9500 | C63—H63 | 0.9500 |
| C6—C10 | 1.411 (4) | C64—C65 | 1.402 (5) |
| C6—C7 | 1.412 (4) | C64—H64 | 0.9500 |
| C6—H6 | 0.9500 | C65—H65 | 0.9500 |
| C7—C8 | 1.399 (4) | C66—C71 | 1.524 (4) |
| C7—H7 | 0.9500 | C66—C67 | 1.532 (4) |
| C8—C9 | 1.412 (4) | C67—C68 | 1.533 (5) |
| C8—H8 | 0.9500 | C67—C72 | 1.551 (4) |
| C9—C10 | 1.400 (5) | C67—H67 | 1.0000 |
| C9—H9 | 0.9500 | C68—C69 | 1.520 (5) |
| C10—H10 | 0.9500 | C68—H68A | 0.9900 |
| C11—C15 | 1.437 (4) | C68—H68B | 0.9900 |
| C11—C12 | 1.437 (4) | C69—C70 | 1.524 (5) |
| C11—C16 | 1.448 (4) | C69—C73 | 1.546 (5) |
| C12—C13 | 1.406 (4) | C69—H69 | 1.0000 |
| C12—H12 | 0.9500 | C70—C71 | 1.537 (5) |
| C13—C14 | 1.408 (4) | C70—H70A | 0.9900 |
| C13—H13 | 0.9500 | C70—H70B | 0.9900 |
| C14—C15 | 1.406 (4) | C71—C74 | 1.547 (4) |
| C14—H14 | 0.9500 | C71—H71 | 1.0000 |
| C15—H15 | 0.9500 | C72—C75 | 1.538 (5) |

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| C16—C17 | 1.523 (4) | C72—H72A | 0.9900 |
| C16—C21 | 1.535 (4) | C72—H72B | 0.9900 |
| C17—C18 | 1.536 (4) | C73—C75 | 1.522 (6) |
| C17—C22 | 1.547 (4) | C73—H73A | 0.9900 |
| C17—H17 | 1.0000 | C73—H73B | 0.9900 |
| C18—C19 | 1.531 (5) | C74—C75 | 1.528 (5) |
| C18—H18A | 0.9900 | C74—H74A | 0.9900 |
| C18—H18B | 0.9900 | C74—H74B | 0.9900 |
| C19—C23 | 1.527 (5) | C75—H75 | 1.0000 |
| C19—C20 | 1.538 (5) | Zr4—C86 | 2.329 (2) |
| C19—H19 | 1.0000 | Zr4—C87 | 2.468 (2) |
| C20—C21 | 1.538 (4) | Zr4—C90 | 2.502 (3) |
| C20—H20A | 0.9900 | Zr4—C83 | 2.571 (3) |
| C20—H20B | 0.9900 | Zr4—C91 | 2.574 (3) |
| C21—C24 | 1.547 (4) | Zr4—C78 | 2.594 (3) |
| C21—H21 | 1.0000 | Zr4—C76 | 2.605 (3) |
| C22—C25 | 1.534 (4) | Zr4—C88 | 2.619 (2) |
| C22—H22A | 0.9900 | Zr4—C81 | 2.622 (3) |
| C22—H22B | 0.9900 | Zr4—C77 | 2.623 (3) |
| C23—C25 | 1.534 (5) | Zr4—C79 | 2.625 (3) |
| C23—H23A | 0.9900 | Zr4—C84 | 2.628 (3) |
| C23—H23B | 0.9900 | Zr4—C82 | 2.631 (3) |
| C24—C25 | 1.523 (5) | Zr4—C80 | 2.632 (2) |
| C24—H24A | 0.9900 | Zr4—C85 | 2.633 (3) |
| C24—H24B | 0.9900 | Zr4—C89 | 2.643 (3) |
| C25—H25 | 1.0000 | C76—C77 | 1.402 (5) |
| Zr2—C36 | 2.337 (2) | C76—C80 | 1.409 (4) |
| Zr2—C40 | 2.470 (3) | C76—H76 | 0.9500 |
| Zr2—C37 | 2.499 (2) | C77—C78 | 1.404 (5) |
| Zr2—C34 | 2.573 (3) | C77—H77 | 0.9500 |
| Zr2—C33 | 2.600 (3) | C78—C79 | 1.410 (4) |
| Zr2—C28 | 2.602 (3) | C78—H78 | 0.9500 |
| Zr2—C26 | 2.603 (3) | C79—C80 | 1.400 (4) |
| Zr2—C39 | 2.606 (3) | C79—H79 | 0.9500 |
| Zr2—C41 | 2.609 (3) | C80—H80 | 0.9500 |
| Zr2—C35 | 2.612 (3) | C81—C82 | 1.394 (5) |
| Zr2—C31 | 2.613 (3) | C81—C85 | 1.413 (4) |
| Zr2—C30 | 2.614 (3) | C81—H81 | 0.9500 |
| Zr2—C38 | 2.628 (3) | C82—C83 | 1.407 (4) |
| Zr2—C27 | 2.630 (3) | C82—H82 | 0.9500 |
| Zr2—C29 | 2.633 (3) | C83—C84 | 1.408 (4) |
| Zr2—C32 | 2.641 (3) | C83—H83 | 0.9500 |
| C26—C27 | 1.385 (5) | C84—C85 | 1.393 (5) |
| C26—C30 | 1.394 (6) | C84—H84 | 0.9500 |
| C26—H26 | 0.9500 | C85—H85 | 0.9500 |
| C27—C28 | 1.402 (5) | C86—C90 | 1.434 (4) |
| C27—H27 | 0.9500 | C86—C87 | 1.439 (4) |
| C28—C29 | 1.392 (5) | C86—C91 | 1.446 (4) |

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| C28—H28 | 0.9500 | C87—C88 | 1.400 (4) |
| C29—C30 | 1.371 (6) | C87—H87 | 0.9500 |
| C29—H29 | 0.9500 | C88—C89 | 1.405 (4) |
| C30—H30 | 0.9500 | C88—H88 | 0.9500 |
| C31—C35 | 1.377 (6) | C89—C90 | 1.404 (4) |
| C31—C32 | 1.379 (5) | C89—H89 | 0.9500 |
| C31—H31 | 0.9500 | C90—H90 | 0.9500 |
| C32—C33 | 1.369 (6) | C91—C96 | 1.529 (4) |
| C32—H32 | 0.9500 | C91—C92 | 1.531 (4) |
| C33—C34 | 1.393 (6) | C92—C93 | 1.534 (4) |
| C33—H33 | 0.9500 | C92—C97 | 1.549 (4) |
| C34—C35 | 1.376 (6) | C92—H92 | 1.0000 |
| C34—H34 | 0.9500 | C93—C94 | 1.526 (6) |
| C35—H35 | 0.9500 | C93—H93A | 0.9900 |
| C36—C37 | 1.437 (4) | C93—H93B | 0.9900 |
| C36—C41 | 1.441 (4) | C94—C95 | 1.521 (5) |
| C36—C40 | 1.442 (4) | C94—C98 | 1.545 (5) |
| C37—C38 | 1.405 (4) | C94—H94 | 1.0000 |
| C37—H37 | 0.9500 | C95—C96 | 1.527 (4) |
| C38—C39 | 1.410 (4) | C95—H95A | 0.9900 |
| C38—H38 | 0.9500 | C95—H95B | 0.9900 |
| C39—C40 | 1.405 (4) | C96—C99 | 1.548 (4) |
| C39—H39 | 0.9500 | C96—H96 | 1.0000 |
| C40—H40 | 0.9500 | C97—C100 | 1.529 (5) |
| C41—C46 | 1.528 (4) | C97—H97A | 0.9900 |
| C41—C42 | 1.531 (4) | C97—H97B | 0.9900 |
| C42—C43 | 1.530 (5) | C98—C100 | 1.527 (5) |
| C42—C47 | 1.546 (4) | C98—H98A | 0.9900 |
| C42—H42 | 1.0000 | C98—H98B | 0.9900 |
| C43—C44 | 1.532 (5) | C99—C100 | 1.535 (5) |
| C43—H43A | 0.9900 | C99—H99A | 0.9900 |
| C43—H43B | 0.9900 | C99—H99B | 0.9900 |
| C44—C48 | 1.528 (5) | C100—H100 | 1.0000 |
| C44—C45 | 1.535 (5) | C101—C106 | 1.357 (18) |
| C44—H44 | 1.0000 | C101—C107 | 1.37 (2) |
| C45—C46 | 1.533 (4) | C101—C102 | 1.390 (12) |
| C45—H45A | 0.9900 | C102—C103 | 1.298 (14) |
| C45—H45B | 0.9900 | C102—H102 | 0.9500 |
| C46—C49 | 1.551 (4) | C103—C104 | 1.360 (15) |
| C46—H46 | 1.0000 | C103—H103 | 0.9500 |
| C47—C50 | 1.535 (4) | C104—C105 | 1.488 (19) |
| C47—H47A | 0.9900 | C104—H104 | 0.9500 |
| C47—H47B | 0.9900 | C105—C106 | 1.33 (2) |
| C48—C50 | 1.528 (5) | C105—H105 | 0.9500 |
| C48—H48A | 0.9900 | C106—H106 | 0.9500 |
| C48—H48B | 0.9900 | C107—H10F | 0.9800 |
| C49—C50 | 1.541 (4) | C107—H10G | 0.9800 |
| C49—H49A | 0.9900 | C107—H10H | 0.9800 |

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| C49—H49B | 0.9900 | C108—C109 | 1.498 (15) |
| C50—H50 | 1.0000 | C108—H10A | 0.9800 |
| Zr3—C61 | 2.332 (2) | C108—H10B | 0.9800 |
| Zr3—C65 | 2.471 (2) | C108—H10C | 0.9800 |
| Zr3—C62 | 2.495 (3) | C109—C110 | 1.49 (2) |
| Zr3—C53 | 2.567 (3) | C109—H10D | 0.9900 |
| Zr3—C66 | 2.577 (3) | C109—H10E | 0.9900 |
| Zr3—C56 | 2.588 (3) | C110—C111 | 1.43 (2) |
| Zr3—C59 | 2.597 (3) | C110—H11A | 0.9900 |
| Zr3—C57 | 2.610 (2) | C110—H11B | 0.9900 |
| Zr3—C52 | 2.612 (3) | C111—C112 | 1.64 (2) |
| Zr3—C58 | 2.616 (3) | C111—H11C | 0.9900 |
| Zr3—C64 | 2.616 (3) | C111—H11D | 0.9900 |
| Zr3—C60 | 2.625 (3) | C112—C113 | 1.48 (2) |
| Zr3—C51 | 2.627 (3) | C112—H11E | 0.9900 |
| Zr3—C63 | 2.634 (3) | C112—H11F | 0.9900 |
| Zr3—C55 | 2.646 (3) | C113—H11G | 0.9800 |
| Zr3—C54 | 2.650 (3) | C113—H11H | 0.9800 |
| C51—C52 | 1.371 (5) | C113—H11I | 0.9800 |
| | | | |
| C11—Zr1—C15 | 34.54 (9) | C62—Zr3—C52 | 122.63 (9) |
| C11—Zr1—C12 | 34.50 (9) | C53—Zr3—C52 | 31.38 (9) |
| C15—Zr1—C12 | 54.73 (9) | C66—Zr3—C52 | 103.48 (10) |
| C11—Zr1—C3 | 126.33 (9) | C56—Zr3—C52 | 149.13 (11) |
| C15—Zr1—C3 | 92.23 (9) | C59—Zr3—C52 | 130.06 (12) |
| C12—Zr1—C3 | 135.13 (9) | C57—Zr3—C52 | 119.87 (9) |
| C11—Zr1—C1 | 98.03 (10) | C61—Zr3—C58 | 146.65 (10) |
| C15—Zr1—C1 | 79.87 (9) | C65—Zr3—C58 | 157.88 (11) |
| C12—Zr1—C1 | 131.46 (9) | C62—Zr3—C58 | 115.14 (10) |
| C3—Zr1—C1 | 52.17 (11) | C53—Zr3—C58 | 81.23 (10) |
| C11—Zr1—C9 | 110.83 (10) | C66—Zr3—C58 | 135.81 (10) |
| C15—Zr1—C9 | 127.83 (9) | C56—Zr3—C58 | 51.37 (10) |
| C12—Zr1—C9 | 77.99 (9) | C59—Zr3—C58 | 30.55 (10) |
| C3—Zr1—C9 | 110.24 (11) | C57—Zr3—C58 | 30.64 (10) |
| C1—Zr1—C9 | 150.55 (10) | C52—Zr3—C58 | 112.24 (10) |
| C11—Zr1—C16 | 33.52 (9) | C61—Zr3—C64 | 55.60 (10) |
| C15—Zr1—C16 | 59.31 (8) | C65—Zr3—C64 | 31.85 (10) |
| C12—Zr1—C16 | 60.17 (9) | C62—Zr3—C64 | 52.98 (10) |
| C3—Zr1—C16 | 132.33 (10) | C53—Zr3—C64 | 87.56 (10) |
| C1—Zr1—C16 | 83.66 (10) | C66—Zr3—C64 | 87.85 (10) |
| C9—Zr1—C16 | 117.42 (10) | C56—Zr3—C64 | 137.06 (12) |
| C11—Zr1—C6 | 106.60 (9) | C59—Zr3—C64 | 103.17 (11) |
| C15—Zr1—C6 | 141.11 (9) | C57—Zr3—C64 | 154.31 (10) |
| C12—Zr1—C6 | 94.71 (9) | C52—Zr3—C64 | 73.56 (10) |
| C3—Zr1—C6 | 125.77 (9) | C58—Zr3—C64 | 126.11 (11) |
| C1—Zr1—C6 | 115.03 (10) | C61—Zr3—C60 | 96.13 (10) |
| C9—Zr1—C6 | 51.85 (10) | C65—Zr3—C60 | 122.75 (10) |
| C16—Zr1—C6 | 85.69 (9) | C62—Zr3—C60 | 68.12 (9) |

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| C11—Zr1—C5 | 125.43 (10) | C53—Zr3—C60 | 129.84 (10) |
| C15—Zr1—C5 | 111.34 (9) | C66—Zr3—C60 | 95.70 (11) |
| C12—Zr1—C5 | 159.73 (10) | C56—Zr3—C60 | 31.37 (12) |
| C3—Zr1—C5 | 51.83 (10) | C59—Zr3—C60 | 30.85 (12) |
| C1—Zr1—C5 | 31.50 (9) | C57—Zr3—C60 | 51.40 (10) |
| C9—Zr1—C5 | 119.68 (10) | C52—Zr3—C60 | 160.80 (12) |
| C16—Zr1—C5 | 100.67 (10) | C58—Zr3—C60 | 50.58 (10) |
| C6—Zr1—C5 | 89.99 (10) | C64—Zr3—C60 | 108.34 (11) |
| C11—Zr1—C10 | 92.94 (9) | C61—Zr3—C51 | 94.79 (10) |
| C15—Zr1—C10 | 123.24 (9) | C65—Zr3—C51 | 76.03 (10) |
| C12—Zr1—C10 | 69.00 (8) | C62—Zr3—C51 | 127.84 (9) |
| C3—Zr1—C10 | 137.93 (10) | C53—Zr3—C51 | 51.35 (10) |
| C1—Zr1—C10 | 146.14 (10) | C66—Zr3—C51 | 82.54 (10) |
| C9—Zr1—C10 | 31.11 (10) | C56—Zr3—C51 | 126.29 (13) |
| C16—Zr1—C10 | 88.26 (9) | C59—Zr3—C51 | 146.06 (11) |
| C6—Zr1—C10 | 31.31 (10) | C57—Zr3—C51 | 107.42 (10) |
| C5—Zr1—C10 | 120.21 (9) | C52—Zr3—C51 | 30.34 (11) |
| C11—Zr1—C8 | 141.75 (10) | C58—Zr3—C51 | 117.02 (10) |
| C15—Zr1—C8 | 153.01 (10) | C64—Zr3—C51 | 94.32 (11) |
| C12—Zr1—C8 | 109.33 (9) | C60—Zr3—C51 | 157.22 (12) |
| C3—Zr1—C8 | 86.62 (10) | C61—Zr3—C63 | 55.18 (10) |
| C1—Zr1—C8 | 119.21 (10) | C65—Zr3—C63 | 52.87 (10) |
| C9—Zr1—C8 | 31.38 (9) | C62—Zr3—C63 | 31.52 (10) |
| C16—Zr1—C8 | 136.36 (9) | C53—Zr3—C63 | 110.49 (10) |
| C6—Zr1—C8 | 51.55 (10) | C66—Zr3—C63 | 87.45 (10) |
| C5—Zr1—C8 | 88.99 (10) | C56—Zr3—C63 | 105.99 (12) |
| C10—Zr1—C8 | 51.39 (9) | C59—Zr3—C63 | 78.33 (10) |
| C11—Zr1—C2 | 98.90 (9) | C57—Zr3—C63 | 126.84 (10) |
| C15—Zr1—C2 | 68.29 (9) | C52—Zr3—C63 | 104.08 (10) |
| C12—Zr1—C2 | 121.92 (9) | C58—Zr3—C63 | 107.37 (10) |
| C3—Zr1—C2 | 31.45 (10) | C64—Zr3—C63 | 31.31 (9) |
| C1—Zr1—C2 | 31.05 (11) | C60—Zr3—C63 | 77.23 (10) |
| C9—Zr1—C2 | 141.18 (11) | C51—Zr3—C63 | 125.18 (10) |
| C16—Zr1—C2 | 101.20 (10) | C61—Zr3—C55 | 119.01 (11) |
| C6—Zr1—C2 | 141.32 (10) | C65—Zr3—C55 | 106.90 (10) |
| C5—Zr1—C2 | 51.35 (9) | C62—Zr3—C55 | 153.18 (10) |
| C10—Zr1—C2 | 168.14 (9) | C53—Zr3—C55 | 51.44 (11) |
| C8—Zr1—C2 | 117.29 (10) | C66—Zr3—C55 | 94.64 (10) |
| C11—Zr1—C14 | 55.37 (9) | C56—Zr3—C55 | 99.36 (12) |
| C15—Zr1—C14 | 31.84 (9) | C59—Zr3—C55 | 119.17 (11) |
| C12—Zr1—C14 | 52.94 (9) | C57—Zr3—C55 | 76.46 (10) |
| C3—Zr1—C14 | 82.72 (9) | C52—Zr3—C55 | 50.86 (10) |
| C1—Zr1—C14 | 97.79 (10) | C58—Zr3—C55 | 88.63 (11) |
| C9—Zr1—C14 | 103.26 (9) | C64—Zr3—C55 | 123.40 (10) |
| C16—Zr1—C14 | 87.24 (8) | C60—Zr3—C55 | 127.48 (10) |
| C6—Zr1—C14 | 145.34 (9) | C51—Zr3—C55 | 31.09 (10) |
| C5—Zr1—C14 | 124.67 (9) | C63—Zr3—C55 | 154.65 (10) |
| C10—Zr1—C14 | 114.65 (9) | C61—Zr3—C54 | 145.55 (9) |

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| C8—Zr1—C14 | 121.68 (10) | C65—Zr3—C54 | 119.91 (9) |
| C2—Zr1—C14 | 73.34 (9) | C62—Zr3—C54 | 171.19 (10) |
| C11—Zr1—C13 | 55.30 (9) | C53—Zr3—C54 | 31.14 (10) |
| C15—Zr1—C13 | 52.91 (9) | C66—Zr3—C54 | 125.18 (10) |
| C12—Zr1—C13 | 31.79 (9) | C56—Zr3—C54 | 99.94 (10) |
| C3—Zr1—C13 | 105.38 (9) | C59—Zr3—C54 | 95.31 (10) |
| C1—Zr1—C13 | 128.67 (9) | C57—Zr3—C54 | 69.09 (9) |
| C9—Zr1—C13 | 75.52 (9) | C52—Zr3—C54 | 50.89 (8) |
| C16—Zr1—C13 | 87.61 (9) | C58—Zr3—C54 | 67.01 (9) |
| C6—Zr1—C13 | 114.57 (9) | C64—Zr3—C54 | 118.49 (10) |
| C5—Zr1—C13 | 154.74 (9) | C60—Zr3—C54 | 116.25 (9) |
| C10—Zr1—C13 | 83.54 (9) | C51—Zr3—C54 | 50.77 (9) |
| C8—Zr1—C13 | 101.47 (9) | C63—Zr3—C54 | 140.09 (11) |
| C2—Zr1—C13 | 103.79 (9) | C55—Zr3—C54 | 30.54 (11) |
| C14—Zr1—C13 | 31.15 (9) | C52—C51—C55 | 108.4 (3) |
| C11—Zr1—C4 | 148.27 (10) | C52—C51—Zr3 | 74.22 (18) |
| C15—Zr1—C4 | 119.31 (9) | C55—C51—Zr3 | 75.18 (18) |
| C12—Zr1—C4 | 165.27 (10) | C52—C51—H51 | 125.8 |
| C3—Zr1—C4 | 31.43 (9) | C55—C51—H51 | 125.8 |
| C1—Zr1—C4 | 51.37 (10) | Zr3—C51—H51 | 116.8 |
| C9—Zr1—C4 | 100.62 (10) | C51—C52—C53 | 108.6 (3) |
| C16—Zr1—C4 | 130.95 (10) | C51—C52—Zr3 | 75.44 (17) |
| C6—Zr1—C4 | 95.81 (9) | C53—C52—Zr3 | 72.53 (16) |
| C5—Zr1—C4 | 30.58 (10) | C51—C52—H52 | 125.7 |
| C10—Zr1—C4 | 117.07 (9) | C53—C52—H52 | 125.7 |
| C8—Zr1—C4 | 69.97 (10) | Zr3—C52—H52 | 118.2 |
| C2—Zr1—C4 | 51.17 (9) | C52—C53—C54 | 107.5 (3) |
| C14—Zr1—C4 | 114.13 (9) | C52—C53—Zr3 | 76.09 (17) |
| C13—Zr1—C4 | 133.51 (9) | C54—C53—Zr3 | 77.70 (17) |
| C11—Zr1—C7 | 137.70 (9) | C52—C53—H53 | 126.3 |
| C15—Zr1—C7 | 172.12 (9) | C54—C53—H53 | 126.3 |
| C12—Zr1—C7 | 120.17 (9) | Zr3—C53—H53 | 112.5 |
| C3—Zr1—C7 | 95.22 (9) | C55—C54—C53 | 108.0 (3) |
| C1—Zr1—C7 | 102.75 (9) | C55—C54—Zr3 | 74.56 (17) |
| C9—Zr1—C7 | 51.36 (9) | C53—C54—Zr3 | 71.16 (16) |
| C16—Zr1—C7 | 113.32 (9) | C55—C54—H54 | 126.0 |
| C6—Zr1—C7 | 31.10 (9) | C53—C54—H54 | 126.0 |
| C5—Zr1—C7 | 71.72 (9) | Zr3—C54—H54 | 120.1 |
| C10—Zr1—C7 | 51.17 (9) | C54—C55—C51 | 107.3 (3) |
| C8—Zr1—C7 | 30.76 (10) | C54—C55—Zr3 | 74.90 (18) |
| C2—Zr1—C7 | 117.66 (9) | C51—C55—Zr3 | 73.74 (19) |
| C14—Zr1—C7 | 152.20 (10) | C54—C55—H55 | 126.3 |
| C13—Zr1—C7 | 126.86 (9) | C51—C55—H55 | 126.3 |
| C4—Zr1—C7 | 67.17 (9) | Zr3—C55—H55 | 117.1 |
| C2—C1—C5 | 107.4 (3) | C60—C56—C57 | 106.8 (3) |
| C2—C1—Zr1 | 75.22 (18) | C60—C56—Zr3 | 75.73 (17) |
| C5—C1—Zr1 | 74.78 (18) | C57—C56—Zr3 | 75.00 (16) |
| C2—C1—H1 | 126.3 | C60—C56—H56 | 126.6 |

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| C5—C1—H1 | 126.3 | C57—C56—H56 | 126.6 |
| Zr1—C1—H1 | 115.9 | Zr3—C56—H56 | 115.1 |
| C1—C2—C3 | 108.5 (3) | C58—C57—C56 | 107.4 (3) |
| C1—C2—Zr1 | 73.73 (17) | C58—C57—Zr3 | 74.91 (15) |
| C3—C2—Zr1 | 72.64 (16) | C56—C57—Zr3 | 73.34 (15) |
| C1—C2—H2 | 125.8 | C58—C57—H57 | 126.3 |
| C3—C2—H2 | 125.8 | C56—C57—H57 | 126.3 |
| Zr1—C2—H2 | 119.7 | Zr3—C57—H57 | 117.5 |
| C2—C3—C4 | 107.0 (3) | C59—C58—C57 | 109.5 (3) |
| C2—C3—Zr1 | 75.91 (17) | C59—C58—Zr3 | 73.97 (16) |
| C4—C3—Zr1 | 76.36 (16) | C57—C58—Zr3 | 74.45 (15) |
| C2—C3—H3 | 126.5 | C59—C58—H58 | 125.3 |
| C4—C3—H3 | 126.5 | C57—C58—H58 | 125.3 |
| Zr1—C3—H3 | 113.8 | Zr3—C58—H58 | 118.1 |
| C5—C4—C3 | 108.6 (3) | C58—C59—C60 | 108.3 (3) |
| C5—C4—Zr1 | 74.04 (17) | C58—C59—Zr3 | 75.48 (17) |
| C3—C4—Zr1 | 72.21 (15) | C60—C59—Zr3 | 75.68 (18) |
| C5—C4—H4 | 125.7 | C58—C59—H59 | 125.9 |
| C3—C4—H4 | 125.7 | C60—C59—H59 | 125.9 |
| Zr1—C4—H4 | 119.8 | Zr3—C59—H59 | 115.2 |
| C4—C5—C1 | 108.3 (3) | C59—C60—C56 | 107.9 (3) |
| C4—C5—Zr1 | 75.38 (17) | C59—C60—Zr3 | 73.47 (17) |
| C1—C5—Zr1 | 73.72 (17) | C56—C60—Zr3 | 72.90 (17) |
| C4—C5—H5 | 125.9 | C59—C60—H60 | 126.0 |
| C1—C5—H5 | 125.9 | C56—C60—H60 | 126.0 |
| Zr1—C5—H5 | 117.0 | Zr3—C60—H60 | 119.5 |
| C10—C6—C7 | 107.4 (3) | C62—C61—C65 | 104.9 (3) |
| C10—C6—Zr1 | 74.42 (15) | C62—C61—C66 | 123.3 (2) |
| C7—C6—Zr1 | 76.01 (15) | C65—C61—C66 | 122.7 (3) |
| C10—C6—H6 | 126.3 | C62—C61—Zr3 | 78.99 (15) |
| C7—C6—H6 | 126.3 | C65—C61—Zr3 | 77.91 (15) |
| Zr1—C6—H6 | 115.5 | C66—C61—Zr3 | 82.49 (15) |
| C8—C7—C6 | 108.1 (3) | C63—C62—C61 | 109.3 (3) |
| C8—C7—Zr1 | 73.28 (15) | C63—C62—Zr3 | 79.71 (17) |
| C6—C7—Zr1 | 72.89 (14) | C61—C62—Zr3 | 66.55 (14) |
| C8—C7—H7 | 126.0 | C63—C62—H62 | 125.3 |
| C6—C7—H7 | 126.0 | C61—C62—H62 | 125.3 |
| Zr1—C7—H7 | 119.7 | Zr3—C62—H62 | 119.9 |
| C7—C8—C9 | 108.3 (3) | C62—C63—C64 | 108.3 (3) |
| C7—C8—Zr1 | 75.97 (16) | C62—C63—Zr3 | 68.77 (16) |
| C9—C8—Zr1 | 73.71 (16) | C64—C63—Zr3 | 73.64 (17) |
| C7—C8—H8 | 125.8 | C62—C63—H63 | 125.9 |
| C9—C8—H8 | 125.8 | C64—C63—H63 | 125.9 |
| Zr1—C8—H8 | 116.5 | Zr3—C63—H63 | 123.3 |
| C10—C9—C8 | 107.6 (3) | C65—C64—C63 | 107.8 (3) |
| C10—C9—Zr1 | 74.90 (17) | C65—C64—Zr3 | 68.40 (15) |
| C8—C9—Zr1 | 74.91 (17) | C63—C64—Zr3 | 75.05 (16) |
| C10—C9—H9 | 126.2 | C65—C64—H64 | 126.1 |

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| C8—C9—H9 | 126.2 | C63—C64—H64 | 126.1 |
| Zr1—C9—H9 | 116.2 | Zr3—C64—H64 | 122.1 |
| C9—C10—C6 | 108.5 (3) | C64—C65—C61 | 109.4 (3) |
| C9—C10—Zr1 | 73.99 (16) | C64—C65—Zr3 | 79.75 (15) |
| C6—C10—Zr1 | 74.27 (16) | C61—C65—Zr3 | 67.32 (13) |
| C9—C10—H10 | 125.8 | C64—C65—H65 | 125.3 |
| C6—C10—H10 | 125.8 | C61—C65—H65 | 125.3 |
| Zr1—C10—H10 | 117.9 | Zr3—C65—H65 | 119.2 |
| C15—C11—C12 | 105.3 (2) | C61—C66—C71 | 118.2 (3) |
| C15—C11—C16 | 121.7 (2) | C61—C66—C67 | 117.3 (2) |
| C12—C11—C16 | 124.6 (2) | C71—C66—C67 | 109.4 (3) |
| C15—C11—Zr1 | 78.38 (14) | C61—C66—Zr3 | 63.80 (14) |
| C12—C11—Zr1 | 78.57 (14) | C71—C66—Zr3 | 119.42 (18) |
| C16—C11—Zr1 | 83.55 (15) | C67—C66—Zr3 | 122.33 (19) |
| C13—C12—C11 | 109.0 (2) | C66—C67—C68 | 111.0 (3) |
| C13—C12—Zr1 | 79.43 (15) | C66—C67—C72 | 108.5 (3) |
| C11—C12—Zr1 | 66.92 (13) | C68—C67—C72 | 108.7 (3) |
| C13—C12—H12 | 125.5 | C66—C67—H67 | 109.6 |
| C11—C12—H12 | 125.5 | C68—C67—H67 | 109.6 |
| Zr1—C12—H12 | 119.7 | C72—C67—H67 | 109.6 |
| C12—C13—C14 | 108.2 (3) | C69—C68—C67 | 110.0 (3) |
| C12—C13—Zr1 | 68.78 (14) | C69—C68—H68A | 109.7 |
| C14—C13—Zr1 | 74.31 (15) | C67—C68—H68A | 109.7 |
| C12—C13—H13 | 125.9 | C69—C68—H68B | 109.7 |
| C14—C13—H13 | 125.9 | C67—C68—H68B | 109.7 |
| Zr1—C13—H13 | 122.6 | H68A—C68—H68B | 108.2 |
| C15—C14—C13 | 108.1 (2) | C68—C69—C70 | 109.2 (3) |
| C15—C14—Zr1 | 68.68 (13) | C68—C69—C73 | 109.4 (3) |
| C13—C14—Zr1 | 74.54 (14) | C70—C69—C73 | 109.4 (3) |
| C15—C14—H14 | 126.0 | C68—C69—H69 | 109.6 |
| C13—C14—H14 | 126.0 | C70—C69—H69 | 109.6 |
| Zr1—C14—H14 | 122.5 | C73—C69—H69 | 109.6 |
| C14—C15—C11 | 109.1 (2) | C69—C70—C71 | 110.3 (3) |
| C14—C15—Zr1 | 79.47 (14) | C69—C70—H70A | 109.6 |
| C11—C15—Zr1 | 67.08 (13) | C71—C70—H70A | 109.6 |
| C14—C15—H15 | 125.5 | C69—C70—H70B | 109.6 |
| C11—C15—H15 | 125.5 | C71—C70—H70B | 109.6 |
| Zr1—C15—H15 | 119.5 | H70A—C70—H70B | 108.1 |
| C11—C16—C17 | 116.9 (2) | C66—C71—C70 | 110.4 (3) |
| C11—C16—C21 | 118.7 (3) | C66—C71—C74 | 108.5 (2) |
| C17—C16—C21 | 109.4 (2) | C70—C71—C74 | 108.6 (3) |
| C11—C16—Zr1 | 62.92 (14) | C66—C71—H71 | 109.8 |
| C17—C16—Zr1 | 123.48 (19) | C70—C71—H71 | 109.8 |
| C21—C16—Zr1 | 118.71 (18) | C74—C71—H71 | 109.8 |
| C16—C17—C18 | 111.1 (2) | C75—C72—C67 | 109.3 (3) |
| C16—C17—C22 | 108.3 (2) | C75—C72—H72A | 109.8 |
| C18—C17—C22 | 108.6 (3) | C67—C72—H72A | 109.8 |
| C16—C17—H17 | 109.6 | C75—C72—H72B | 109.8 |

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| C18—C17—H17 | 109.6 | C67—C72—H72B | 109.8 |
| C22—C17—H17 | 109.6 | H72A—C72—H72B | 108.3 |
| C19—C18—C17 | 109.8 (3) | C75—C73—C69 | 109.4 (3) |
| C19—C18—H18A | 109.7 | C75—C73—H73A | 109.8 |
| C17—C18—H18A | 109.7 | C69—C73—H73A | 109.8 |
| C19—C18—H18B | 109.7 | C75—C73—H73B | 109.8 |
| C17—C18—H18B | 109.7 | C69—C73—H73B | 109.8 |
| H18A—C18—H18B | 108.2 | H73A—C73—H73B | 108.2 |
| C23—C19—C18 | 110.3 (3) | C75—C74—C71 | 109.9 (3) |
| C23—C19—C20 | 109.7 (3) | C75—C74—H74A | 109.7 |
| C18—C19—C20 | 108.1 (3) | C71—C74—H74A | 109.7 |
| C23—C19—H19 | 109.6 | C75—C74—H74B | 109.7 |
| C18—C19—H19 | 109.6 | C71—C74—H74B | 109.7 |
| C20—C19—H19 | 109.6 | H74A—C74—H74B | 108.2 |
| C21—C20—C19 | 110.1 (2) | C73—C75—C74 | 110.1 (3) |
| C21—C20—H20A | 109.6 | C73—C75—C72 | 109.5 (3) |
| C19—C20—H20A | 109.6 | C74—C75—C72 | 108.9 (3) |
| C21—C20—H20B | 109.6 | C73—C75—H75 | 109.5 |
| C19—C20—H20B | 109.6 | C74—C75—H75 | 109.5 |
| H20A—C20—H20B | 108.2 | C72—C75—H75 | 109.5 |
| C16—C21—C20 | 110.5 (3) | C86—Zr4—C87 | 34.75 (9) |
| C16—C21—C24 | 108.8 (2) | C86—Zr4—C90 | 34.31 (10) |
| C20—C21—C24 | 108.1 (3) | C87—Zr4—C90 | 54.72 (9) |
| C16—C21—H21 | 109.8 | C86—Zr4—C83 | 132.39 (9) |
| C20—C21—H21 | 109.8 | C87—Zr4—C83 | 98.55 (9) |
| C24—C21—H21 | 109.8 | C90—Zr4—C83 | 142.17 (9) |
| C25—C22—C17 | 110.0 (2) | C86—Zr4—C91 | 33.84 (9) |
| C25—C22—H22A | 109.7 | C87—Zr4—C91 | 60.07 (9) |
| C17—C22—H22A | 109.7 | C90—Zr4—C91 | 59.99 (10) |
| C25—C22—H22B | 109.7 | C83—Zr4—C91 | 134.28 (10) |
| C17—C22—H22B | 109.7 | C86—Zr4—C78 | 118.07 (10) |
| H22A—C22—H22B | 108.2 | C87—Zr4—C78 | 130.64 (9) |
| C19—C23—C25 | 109.5 (3) | C90—Zr4—C78 | 84.54 (10) |
| C19—C23—H23A | 109.8 | C83—Zr4—C78 | 99.37 (10) |
| C25—C23—H23A | 109.8 | C91—Zr4—C78 | 125.61 (10) |
| C19—C23—H23B | 109.8 | C86—Zr4—C76 | 102.33 (9) |
| C25—C23—H23B | 109.8 | C87—Zr4—C76 | 136.89 (10) |
| H23A—C23—H23B | 108.2 | C90—Zr4—C76 | 87.52 (9) |
| C25—C24—C21 | 109.9 (3) | C83—Zr4—C76 | 124.43 (9) |
| C25—C24—H24A | 109.7 | C91—Zr4—C76 | 84.50 (10) |
| C21—C24—H24A | 109.7 | C78—Zr4—C76 | 51.81 (11) |
| C25—C24—H24B | 109.7 | C86—Zr4—C88 | 55.31 (10) |
| C21—C24—H24B | 109.7 | C87—Zr4—C88 | 31.78 (9) |
| H24A—C24—H24B | 108.2 | C90—Zr4—C88 | 52.75 (9) |
| C24—C25—C23 | 109.6 (3) | C83—Zr4—C88 | 90.09 (9) |
| C24—C25—C22 | 109.6 (3) | C91—Zr4—C88 | 87.66 (9) |
| C23—C25—C22 | 108.9 (3) | C78—Zr4—C88 | 102.87 (10) |
| C24—C25—H25 | 109.6 | C76—Zr4—C88 | 137.11 (10) |

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| C23—C25—H25 | 109.6 | C86—Zr4—C81 | 116.39 (10) |
| C22—C25—H25 | 109.6 | C87—Zr4—C81 | 104.40 (10) |
| C36—Zr2—C40 | 34.76 (9) | C90—Zr4—C81 | 150.47 (10) |
| C36—Zr2—C37 | 34.37 (9) | C83—Zr4—C81 | 51.73 (10) |
| C40—Zr2—C37 | 54.85 (9) | C91—Zr4—C81 | 92.22 (10) |
| C36—Zr2—C34 | 112.54 (13) | C78—Zr4—C81 | 122.70 (10) |
| C40—Zr2—C34 | 127.93 (12) | C76—Zr4—C81 | 100.41 (10) |
| C37—Zr2—C34 | 79.37 (12) | C88—Zr4—C81 | 122.02 (10) |
| C36—Zr2—C33 | 143.00 (11) | C86—Zr4—C77 | 95.22 (9) |
| C40—Zr2—C33 | 153.28 (14) | C87—Zr4—C77 | 122.33 (9) |
| C37—Zr2—C33 | 110.60 (12) | C90—Zr4—C77 | 67.66 (9) |
| C34—Zr2—C33 | 31.23 (13) | C83—Zr4—C77 | 128.99 (10) |
| C36—Zr2—C28 | 124.58 (10) | C91—Zr4—C77 | 94.62 (10) |
| C40—Zr2—C28 | 90.57 (10) | C78—Zr4—C77 | 31.22 (11) |
| C37—Zr2—C28 | 135.72 (10) | C76—Zr4—C77 | 31.12 (11) |
| C34—Zr2—C28 | 110.53 (14) | C88—Zr4—C77 | 108.44 (10) |
| C33—Zr2—C28 | 87.93 (11) | C81—Zr4—C77 | 129.29 (10) |
| C36—Zr2—C26 | 98.65 (10) | C86—Zr4—C79 | 146.40 (10) |
| C40—Zr2—C26 | 81.99 (12) | C87—Zr4—C79 | 158.15 (10) |
| C37—Zr2—C26 | 132.45 (11) | C90—Zr4—C79 | 115.10 (9) |
| C34—Zr2—C26 | 148.09 (14) | C83—Zr4—C79 | 79.20 (9) |
| C33—Zr2—C26 | 116.88 (14) | C91—Zr4—C79 | 135.54 (9) |
| C28—Zr2—C26 | 51.39 (10) | C78—Zr4—C79 | 31.35 (9) |
| C36—Zr2—C39 | 55.56 (9) | C76—Zr4—C79 | 51.33 (10) |
| C40—Zr2—C39 | 31.98 (9) | C88—Zr4—C79 | 126.45 (10) |
| C37—Zr2—C39 | 53.04 (9) | C81—Zr4—C79 | 91.35 (10) |
| C34—Zr2—C39 | 102.03 (12) | C77—Zr4—C79 | 51.26 (9) |
| C33—Zr2—C39 | 121.60 (13) | C86—Zr4—C84 | 101.91 (9) |
| C28—Zr2—C39 | 82.82 (10) | C87—Zr4—C84 | 70.22 (9) |
| C26—Zr2—C39 | 101.06 (12) | C90—Zr4—C84 | 122.99 (9) |
| C36—Zr2—C41 | 33.30 (9) | C83—Zr4—C84 | 31.40 (9) |
| C40—Zr2—C41 | 59.52 (9) | C91—Zr4—C84 | 105.97 (10) |
| C37—Zr2—C41 | 59.62 (8) | C78—Zr4—C84 | 128.28 (11) |
| C34—Zr2—C41 | 119.76 (13) | C76—Zr4—C84 | 149.17 (9) |
| C33—Zr2—C41 | 137.08 (10) | C88—Zr4—C84 | 73.21 (9) |
| C28—Zr2—C41 | 129.71 (9) | C81—Zr4—C84 | 51.25 (10) |
| C26—Zr2—C41 | 82.96 (9) | C77—Zr4—C84 | 159.41 (11) |
| C39—Zr2—C41 | 87.35 (9) | C79—Zr4—C84 | 110.55 (9) |
| C36—Zr2—C35 | 94.17 (10) | C86—Zr4—C82 | 144.70 (10) |
| C40—Zr2—C35 | 123.59 (9) | C87—Zr4—C82 | 120.51 (9) |
| C37—Zr2—C35 | 68.87 (10) | C90—Zr4—C82 | 173.47 (9) |
| C34—Zr2—C35 | 30.77 (14) | C83—Zr4—C82 | 31.36 (9) |
| C33—Zr2—C35 | 50.69 (11) | C91—Zr4—C82 | 122.81 (10) |
| C28—Zr2—C35 | 138.38 (11) | C78—Zr4—C82 | 97.21 (10) |
| C26—Zr2—C35 | 145.22 (14) | C76—Zr4—C82 | 98.52 (9) |
| C39—Zr2—C35 | 112.79 (11) | C88—Zr4—C82 | 120.75 (9) |
| C41—Zr2—C35 | 90.63 (11) | C81—Zr4—C82 | 30.78 (10) |
| C36—Zr2—C31 | 106.40 (11) | C77—Zr4—C82 | 116.71 (9) |

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| C40—Zr2—C31 | 141.15 (10) | C79—Zr4—C82 | 67.60 (9) |
| C37—Zr2—C31 | 92.85 (11) | C84—Zr4—C82 | 51.24 (8) |
| C34—Zr2—C31 | 51.07 (13) | C86—Zr4—C80 | 132.47 (9) |
| C33—Zr2—C31 | 50.71 (12) | C87—Zr4—C80 | 166.93 (10) |
| C28—Zr2—C31 | 127.68 (11) | C90—Zr4—C80 | 117.13 (9) |
| C26—Zr2—C31 | 114.70 (13) | C83—Zr4—C80 | 93.28 (9) |
| C39—Zr2—C31 | 142.67 (11) | C91—Zr4—C80 | 107.43 (9) |
| C41—Zr2—C31 | 86.75 (10) | C78—Zr4—C80 | 51.76 (10) |
| C35—Zr2—C31 | 30.57 (13) | C76—Zr4—C80 | 31.21 (9) |
| C36—Zr2—C30 | 126.34 (12) | C88—Zr4—C80 | 154.62 (10) |
| C40—Zr2—C30 | 112.79 (11) | C81—Zr4—C80 | 78.66 (10) |
| C37—Zr2—C30 | 160.27 (12) | C77—Zr4—C80 | 51.40 (9) |
| C34—Zr2—C30 | 117.50 (14) | C79—Zr4—C80 | 30.90 (10) |
| C33—Zr2—C30 | 86.64 (15) | C84—Zr4—C80 | 119.65 (9) |
| C28—Zr2—C30 | 51.07 (11) | C82—Zr4—C80 | 68.43 (9) |
| C26—Zr2—C30 | 30.99 (12) | C86—Zr4—C85 | 93.83 (10) |
| C39—Zr2—C30 | 126.36 (11) | C87—Zr4—C85 | 73.93 (9) |
| C41—Zr2—C30 | 101.33 (12) | C90—Zr4—C85 | 126.30 (9) |
| C35—Zr2—C30 | 119.82 (12) | C83—Zr4—C85 | 51.63 (10) |
| C31—Zr2—C30 | 90.93 (12) | C91—Zr4—C85 | 82.80 (10) |
| C36—Zr2—C38 | 55.18 (9) | C78—Zr4—C85 | 147.88 (10) |
| C40—Zr2—C38 | 53.00 (9) | C76—Zr4—C85 | 128.56 (11) |
| C37—Zr2—C38 | 31.69 (9) | C88—Zr4—C85 | 91.87 (10) |
| C34—Zr2—C38 | 75.14 (11) | C81—Zr4—C85 | 31.19 (10) |
| C33—Zr2—C38 | 102.14 (13) | C77—Zr4—C85 | 159.46 (11) |
| C28—Zr2—C38 | 106.89 (10) | C79—Zr4—C85 | 118.55 (9) |
| C26—Zr2—C38 | 131.84 (12) | C84—Zr4—C85 | 30.72 (10) |
| C39—Zr2—C38 | 31.24 (9) | C82—Zr4—C85 | 51.11 (9) |
| C41—Zr2—C38 | 87.14 (8) | C80—Zr4—C85 | 109.85 (10) |
| C35—Zr2—C38 | 81.55 (11) | C86—Zr4—C89 | 54.90 (10) |
| C31—Zr2—C38 | 111.60 (11) | C87—Zr4—C89 | 52.66 (9) |
| C30—Zr2—C38 | 156.48 (10) | C90—Zr4—C89 | 31.52 (10) |
| C36—Zr2—C27 | 97.99 (9) | C83—Zr4—C89 | 112.14 (9) |
| C40—Zr2—C27 | 68.36 (9) | C91—Zr4—C89 | 87.38 (9) |
| C37—Zr2—C27 | 122.77 (9) | C78—Zr4—C89 | 77.98 (9) |
| C34—Zr2—C27 | 141.41 (14) | C76—Zr4—C89 | 106.43 (10) |
| C33—Zr2—C27 | 117.66 (11) | C88—Zr4—C89 | 30.96 (9) |
| C28—Zr2—C27 | 31.10 (10) | C81—Zr4—C89 | 152.98 (9) |
| C26—Zr2—C27 | 30.68 (11) | C77—Zr4—C89 | 77.60 (9) |
| C39—Zr2—C27 | 75.71 (10) | C79—Zr4—C89 | 107.72 (9) |
| C41—Zr2—C27 | 98.76 (9) | C84—Zr4—C89 | 103.01 (9) |
| C35—Zr2—C27 | 167.76 (10) | C82—Zr4—C89 | 142.69 (10) |
| C31—Zr2—C27 | 141.62 (12) | C80—Zr4—C89 | 127.12 (10) |
| C30—Zr2—C27 | 50.70 (11) | C85—Zr4—C89 | 122.44 (10) |
| C38—Zr2—C27 | 106.61 (10) | C77—C76—C80 | 108.3 (3) |
| C36—Zr2—C29 | 147.40 (10) | C77—C76—Zr4 | 75.14 (16) |
| C40—Zr2—C29 | 118.25 (10) | C80—C76—Zr4 | 75.47 (15) |
| C37—Zr2—C29 | 165.16 (12) | C77—C76—H76 | 125.8 |

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| C34—Zr2—C29 | 99.56 (14) | C80—C76—H76 | 125.8 |
| C33—Zr2—C29 | 69.59 (12) | Zr4—C76—H76 | 115.7 |
| C28—Zr2—C29 | 30.84 (11) | C76—C77—C78 | 108.1 (3) |
| C26—Zr2—C29 | 50.63 (11) | C76—C77—Zr4 | 73.74 (17) |
| C39—Zr2—C29 | 113.48 (11) | C78—C77—Zr4 | 73.26 (17) |
| C41—Zr2—C29 | 130.91 (11) | C76—C77—H77 | 126.0 |
| C35—Zr2—C29 | 117.27 (10) | C78—C77—H77 | 126.0 |
| C31—Zr2—C29 | 97.94 (12) | Zr4—C77—H77 | 118.9 |
| C30—Zr2—C29 | 30.30 (12) | C77—C78—C79 | 107.5 (3) |
| C38—Zr2—C29 | 133.58 (12) | C77—C78—Zr4 | 75.53 (18) |
| C27—Zr2—C29 | 50.49 (10) | C79—C78—Zr4 | 75.56 (17) |
| C36—Zr2—C32 | 136.79 (11) | C77—C78—H78 | 126.2 |
| C40—Zr2—C32 | 171.54 (11) | C79—C78—H78 | 126.2 |
| C37—Zr2—C32 | 118.85 (10) | Zr4—C78—H78 | 115.0 |
| C34—Zr2—C32 | 50.65 (13) | C80—C79—C78 | 108.5 (3) |
| C33—Zr2—C32 | 30.26 (14) | C80—C79—Zr4 | 74.83 (16) |
| C28—Zr2—C32 | 97.63 (11) | C78—C79—Zr4 | 73.09 (16) |
| C26—Zr2—C32 | 101.53 (13) | C80—C79—H79 | 125.7 |
| C39—Zr2—C32 | 151.19 (12) | C78—C79—H79 | 125.7 |
| C41—Zr2—C32 | 112.99 (12) | Zr4—C79—H79 | 118.2 |
| C35—Zr2—C32 | 50.05 (10) | C79—C80—C76 | 107.5 (3) |
| C31—Zr2—C32 | 30.43 (11) | C79—C80—Zr4 | 74.28 (15) |
| C30—Zr2—C32 | 71.45 (12) | C76—C80—Zr4 | 73.32 (14) |
| C38—Zr2—C32 | 125.53 (11) | C79—C80—H80 | 126.3 |
| C27—Zr2—C32 | 118.36 (10) | C76—C80—H80 | 126.3 |
| C29—Zr2—C32 | 69.27 (11) | Zr4—C80—H80 | 118.1 |
| C27—C26—C30 | 107.8 (3) | C82—C81—C85 | 108.0 (3) |
| C27—C26—Zr2 | 75.73 (17) | C82—C81—Zr4 | 74.95 (17) |
| C30—C26—Zr2 | 74.96 (18) | C85—C81—Zr4 | 74.82 (18) |
| C27—C26—H26 | 126.1 | C82—C81—H81 | 126.0 |
| C30—C26—H26 | 126.1 | C85—C81—H81 | 126.0 |
| Zr2—C26—H26 | 115.4 | Zr4—C81—H81 | 116.3 |
| C26—C27—C28 | 108.1 (3) | C81—C82—C83 | 108.0 (3) |
| C26—C27—Zr2 | 73.59 (17) | C81—C82—Zr4 | 74.27 (16) |
| C28—C27—Zr2 | 73.35 (16) | C83—C82—Zr4 | 71.97 (15) |
| C26—C27—H27 | 125.9 | C81—C82—H82 | 126.0 |
| C28—C27—H27 | 125.9 | C83—C82—H82 | 126.0 |
| Zr2—C27—H27 | 119.0 | Zr4—C82—H82 | 119.6 |
| C29—C28—C27 | 106.9 (3) | C82—C83—C84 | 107.8 (3) |
| C29—C28—Zr2 | 75.84 (17) | C82—C83—Zr4 | 76.66 (16) |
| C27—C28—Zr2 | 75.55 (16) | C84—C83—Zr4 | 76.52 (16) |
| C29—C28—H28 | 126.6 | C82—C83—H83 | 126.1 |
| C27—C28—H28 | 126.6 | C84—C83—H83 | 126.1 |
| Zr2—C28—H28 | 114.5 | Zr4—C83—H83 | 113.2 |
| C30—C29—C28 | 108.9 (3) | C85—C84—C83 | 108.0 (3) |
| C30—C29—Zr2 | 74.08 (17) | C85—C84—Zr4 | 74.84 (17) |
| C28—C29—Zr2 | 73.31 (16) | C83—C84—Zr4 | 72.08 (16) |
| C30—C29—H29 | 125.6 | C85—C84—H84 | 126.0 |

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| C28—C29—H29 | 125.6 | C83—C84—H84 | 126.0 |
| Zr2—C29—H29 | 118.9 | Zr4—C84—H84 | 119.0 |
| C29—C30—C26 | 108.1 (3) | C84—C85—C81 | 108.0 (3) |
| C29—C30—Zr2 | 75.62 (18) | C84—C85—Zr4 | 74.44 (18) |
| C26—C30—Zr2 | 74.04 (17) | C81—C85—Zr4 | 73.99 (18) |
| C29—C30—H30 | 125.9 | C84—C85—H85 | 126.0 |
| C26—C30—H30 | 125.9 | C81—C85—H85 | 126.0 |
| Zr2—C30—H30 | 116.5 | Zr4—C85—H85 | 117.6 |
| C35—C31—C32 | 107.4 (4) | C90—C86—C87 | 105.3 (3) |
| C35—C31—Zr2 | 74.7 (2) | C90—C86—C91 | 123.6 (2) |
| C32—C31—Zr2 | 75.9 (2) | C87—C86—C91 | 122.2 (3) |
| C35—C31—H31 | 126.3 | C90—C86—Zr4 | 79.46 (15) |
| C32—C31—H31 | 126.3 | C87—C86—Zr4 | 77.95 (15) |
| Zr2—C31—H31 | 115.4 | C91—C86—Zr4 | 82.42 (15) |
| C33—C32—C31 | 108.7 (3) | C88—C87—C86 | 109.0 (3) |
| C33—C32—Zr2 | 73.2 (2) | C88—C87—Zr4 | 80.04 (15) |
| C31—C32—Zr2 | 73.68 (19) | C86—C87—Zr4 | 67.31 (13) |
| C33—C32—H32 | 125.7 | C88—C87—H87 | 125.5 |
| C31—C32—H32 | 125.7 | C86—C87—H87 | 125.5 |
| Zr2—C32—H32 | 119.2 | Zr4—C87—H87 | 118.7 |
| C32—C33—C34 | 107.8 (3) | C87—C88—C89 | 108.2 (3) |
| C32—C33—Zr2 | 76.5 (2) | C87—C88—Zr4 | 68.18 (14) |
| C34—C33—Zr2 | 73.3 (2) | C89—C88—Zr4 | 75.48 (15) |
| C32—C33—H33 | 126.1 | C87—C88—H88 | 125.9 |
| C34—C33—H33 | 126.1 | C89—C88—H88 | 125.9 |
| Zr2—C33—H33 | 116.2 | Zr4—C88—H88 | 122.1 |
| C35—C34—C33 | 107.4 (4) | C90—C89—C88 | 108.3 (3) |
| C35—C34—Zr2 | 76.2 (2) | C90—C89—Zr4 | 68.67 (15) |
| C33—C34—Zr2 | 75.4 (2) | C88—C89—Zr4 | 73.56 (15) |
| C35—C34—H34 | 126.3 | C90—C89—H89 | 125.8 |
| C33—C34—H34 | 126.3 | C88—C89—H89 | 125.8 |
| Zr2—C34—H34 | 114.5 | Zr4—C89—H89 | 123.5 |
| C34—C35—C31 | 108.6 (3) | C89—C90—C86 | 108.9 (2) |
| C34—C35—Zr2 | 73.1 (2) | C89—C90—Zr4 | 79.80 (16) |
| C31—C35—Zr2 | 74.76 (19) | C86—C90—Zr4 | 66.23 (14) |
| C34—C35—H35 | 125.7 | C89—C90—H90 | 125.6 |
| C31—C35—H35 | 125.7 | C86—C90—H90 | 125.6 |
| Zr2—C35—H35 | 118.3 | Zr4—C90—H90 | 119.9 |
| C37—C36—C41 | 124.0 (3) | C86—C91—C96 | 116.4 (2) |
| C37—C36—C40 | 105.3 (2) | C86—C91—C92 | 118.5 (3) |
| C41—C36—C40 | 122.2 (2) | C96—C91—C92 | 109.5 (3) |
| C37—C36—Zr2 | 78.98 (14) | C86—C91—Zr4 | 63.74 (15) |
| C41—C36—Zr2 | 83.75 (15) | C96—C91—Zr4 | 123.97 (19) |
| C40—C36—Zr2 | 77.67 (14) | C92—C91—Zr4 | 118.07 (19) |
| C38—C37—C36 | 109.0 (2) | C91—C92—C93 | 110.1 (3) |
| C38—C37—Zr2 | 79.23 (14) | C91—C92—C97 | 108.7 (2) |
| C36—C37—Zr2 | 66.65 (13) | C93—C92—C97 | 108.3 (3) |
| C38—C37—H37 | 125.5 | C91—C92—H92 | 109.9 |

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| C36—C37—H37 | 125.5 | C93—C92—H92 | 109.9 |
| Zr2—C37—H37 | 120.1 | C97—C92—H92 | 109.9 |
| C37—C38—C39 | 108.3 (3) | C94—C93—C92 | 110.6 (3) |
| C37—C38—Zr2 | 69.08 (14) | C94—C93—H93A | 109.5 |
| C39—C38—Zr2 | 73.52 (15) | C92—C93—H93A | 109.5 |
| C37—C38—H38 | 125.9 | C94—C93—H93B | 109.5 |
| C39—C38—H38 | 125.9 | C92—C93—H93B | 109.5 |
| Zr2—C38—H38 | 123.2 | H93A—C93—H93B | 108.1 |
| C40—C39—C38 | 108.2 (3) | C95—C94—C93 | 108.7 (3) |
| C40—C39—Zr2 | 68.67 (15) | C95—C94—C98 | 109.7 (3) |
| C38—C39—Zr2 | 75.23 (16) | C93—C94—C98 | 109.4 (3) |
| C40—C39—H39 | 125.9 | C95—C94—H94 | 109.6 |
| C38—C39—H39 | 125.9 | C93—C94—H94 | 109.6 |
| Zr2—C39—H39 | 121.8 | C98—C94—H94 | 109.6 |
| C39—C40—C36 | 108.9 (2) | C94—C95—C96 | 110.2 (3) |
| C39—C40—Zr2 | 79.35 (16) | C94—C95—H95A | 109.6 |
| C36—C40—Zr2 | 67.57 (14) | C96—C95—H95A | 109.6 |
| C39—C40—H40 | 125.5 | C94—C95—H95B | 109.6 |
| C36—C40—H40 | 125.5 | C96—C95—H95B | 109.6 |
| Zr2—C40—H40 | 119.2 | H95A—C95—H95B | 108.1 |
| C36—C41—C46 | 118.4 (2) | C95—C96—C91 | 111.0 (3) |
| C36—C41—C42 | 116.8 (2) | C95—C96—C99 | 108.7 (3) |
| C46—C41—C42 | 109.7 (2) | C91—C96—C99 | 108.3 (3) |
| C36—C41—Zr2 | 62.95 (14) | C95—C96—H96 | 109.6 |
| C46—C41—Zr2 | 120.21 (18) | C91—C96—H96 | 109.6 |
| C42—C41—Zr2 | 121.86 (16) | C99—C96—H96 | 109.6 |
| C43—C42—C41 | 111.0 (3) | C100—C97—C92 | 109.8 (3) |
| C43—C42—C47 | 108.4 (3) | C100—C97—H97A | 109.7 |
| C41—C42—C47 | 108.7 (2) | C92—C97—H97A | 109.7 |
| C43—C42—H42 | 109.6 | C100—C97—H97B | 109.7 |
| C41—C42—H42 | 109.6 | C92—C97—H97B | 109.7 |
| C47—C42—H42 | 109.6 | H97A—C97—H97B | 108.2 |
| C42—C43—C44 | 109.7 (2) | C100—C98—C94 | 109.2 (3) |
| C42—C43—H43A | 109.7 | C100—C98—H98A | 109.8 |
| C44—C43—H43A | 109.7 | C94—C98—H98A | 109.8 |
| C42—C43—H43B | 109.7 | C100—C98—H98B | 109.8 |
| C44—C43—H43B | 109.7 | C94—C98—H98B | 109.8 |
| H43A—C43—H43B | 108.2 | H98A—C98—H98B | 108.3 |
| C48—C44—C43 | 110.2 (3) | C100—C99—C96 | 109.6 (3) |
| C48—C44—C45 | 109.7 (3) | C100—C99—H99A | 109.7 |
| C43—C44—C45 | 108.7 (3) | C96—C99—H99A | 109.7 |
| C48—C44—H44 | 109.4 | C100—C99—H99B | 109.7 |
| C43—C44—H44 | 109.4 | C96—C99—H99B | 109.7 |
| C45—C44—H44 | 109.4 | H99A—C99—H99B | 108.2 |
| C46—C45—C44 | 109.9 (3) | C98—C100—C97 | 109.8 (3) |
| C46—C45—H45A | 109.7 | C98—C100—C99 | 109.4 (3) |
| C44—C45—H45A | 109.7 | C97—C100—C99 | 109.4 (3) |
| C46—C45—H45B | 109.7 | C98—C100—H100 | 109.4 |

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| C44—C45—H45B | 109.7 | C97—C100—H100 | 109.4 |
| H45A—C45—H45B | 108.2 | C99—C100—H100 | 109.4 |
| C41—C46—C45 | 110.7 (2) | C106—C101—C107 | 109.2 (14) |
| C41—C46—C49 | 108.4 (2) | C106—C101—C102 | 123.9 (14) |
| C45—C46—C49 | 108.4 (3) | C107—C101—C102 | 126.8 (17) |
| C41—C46—H46 | 109.8 | C103—C102—C101 | 119.8 (10) |
| C45—C46—H46 | 109.8 | C103—C102—H102 | 120.1 |
| C49—C46—H46 | 109.8 | C101—C102—H102 | 120.1 |
| C50—C47—C42 | 109.7 (3) | C102—C103—C104 | 122.4 (11) |
| C50—C47—H47A | 109.7 | C102—C103—H103 | 118.8 |
| C42—C47—H47A | 109.7 | C104—C103—H103 | 118.8 |
| C50—C47—H47B | 109.7 | C103—C104—C105 | 115.0 (14) |
| C42—C47—H47B | 109.7 | C103—C104—H104 | 122.5 |
| H47A—C47—H47B | 108.2 | C105—C104—H104 | 122.5 |
| C50—C48—C44 | 109.4 (3) | C106—C105—C104 | 123.4 (11) |
| C50—C48—H48A | 109.8 | C106—C105—H105 | 118.3 |
| C44—C48—H48A | 109.8 | C104—C105—H105 | 118.3 |
| C50—C48—H48B | 109.8 | C105—C106—C101 | 115.1 (11) |
| C44—C48—H48B | 109.8 | C105—C106—H106 | 122.4 |
| H48A—C48—H48B | 108.2 | C101—C106—H106 | 122.4 |
| C50—C49—C46 | 109.6 (2) | C101—C107—H10F | 109.5 |
| C50—C49—H49A | 109.7 | C101—C107—H10G | 109.5 |
| C46—C49—H49A | 109.7 | H10F—C107—H10G | 109.5 |
| C50—C49—H49B | 109.7 | C101—C107—H10H | 109.5 |
| C46—C49—H49B | 109.7 | H10F—C107—H10H | 109.5 |
| H49A—C49—H49B | 108.2 | H10G—C107—H10H | 109.5 |
| C48—C50—C47 | 109.5 (3) | C109—C108—H10A | 109.5 |
| C48—C50—C49 | 109.2 (3) | C109—C108—H10B | 109.5 |
| C47—C50—C49 | 109.4 (3) | H10A—C108—H10B | 109.5 |
| C48—C50—H50 | 109.6 | C109—C108—H10C | 109.5 |
| C47—C50—H50 | 109.6 | H10A—C108—H10C | 109.5 |
| C49—C50—H50 | 109.6 | H10B—C108—H10C | 109.5 |
| C61—Zr3—C65 | 34.77 (10) | C110—C109—C108 | 109.6 (13) |
| C61—Zr3—C62 | 34.46 (10) | C110—C109—H10D | 109.7 |
| C65—Zr3—C62 | 54.74 (9) | C108—C109—H10D | 109.7 |
| C61—Zr3—C53 | 129.88 (9) | C110—C109—H10E | 109.7 |
| C65—Zr3—C53 | 96.00 (9) | C108—C109—H10E | 109.7 |
| C62—Zr3—C53 | 140.09 (10) | H10D—C109—H10E | 108.2 |
| C61—Zr3—C66 | 33.70 (10) | C111—C110—C109 | 112.4 (15) |
| C65—Zr3—C66 | 60.12 (10) | C111—C110—H11A | 109.1 |
| C62—Zr3—C66 | 59.95 (10) | C109—C110—H11A | 109.1 |
| C53—Zr3—C66 | 133.08 (9) | C111—C110—H11B | 109.1 |
| C61—Zr3—C56 | 102.48 (10) | C109—C110—H11B | 109.1 |
| C65—Zr3—C56 | 137.01 (10) | H11A—C110—H11B | 107.9 |
| C62—Zr3—C56 | 87.42 (11) | C110—C111—C112 | 102.9 (14) |
| C53—Zr3—C56 | 126.91 (10) | C110—C111—H11C | 111.2 |
| C66—Zr3—C56 | 84.74 (10) | C112—C111—H11C | 111.2 |
| C61—Zr3—C59 | 119.11 (11) | C110—C111—H11D | 111.2 |

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| C65—Zr3—C59 | 131.17 (11) | C112—C111—H11D | 111.2 |
| C62—Zr3—C59 | 85.40 (10) | H11C—C111—H11D | 109.1 |
| C53—Zr3—C59 | 100.06 (11) | C113—C112—C111 | 107.4 (11) |
| C66—Zr3—C59 | 126.39 (11) | C113—C112—H11E | 110.2 |
| C56—Zr3—C59 | 51.76 (12) | C111—C112—H11E | 110.2 |
| C61—Zr3—C57 | 133.05 (10) | C113—C112—H11F | 110.2 |
| C65—Zr3—C57 | 167.57 (10) | C111—C112—H11F | 110.2 |
| C62—Zr3—C57 | 117.43 (9) | H11E—C112—H11F | 108.5 |
| C53—Zr3—C57 | 95.31 (10) | C112—C113—H11G | 109.5 |
| C66—Zr3—C57 | 108.03 (10) | C112—C113—H11H | 109.5 |
| C56—Zr3—C57 | 31.66 (10) | H11G—C113—H11H | 109.5 |
| C59—Zr3—C57 | 51.17 (11) | C112—C113—H11I | 109.5 |
| C61—Zr3—C52 | 100.23 (9) | H11G—C113—H11I | 109.5 |
| C65—Zr3—C52 | 69.21 (9) | H11H—C113—H11I | 109.5 |
| | | | |
| C5—C1—C2—C3 | 3.6 (3) | C52—C53—C54—C55 | 4.9 (3) |
| Zr1—C1—C2—C3 | -64.8 (2) | Zr3—C53—C54—C55 | -66.0 (2) |
| C5—C1—C2—Zr1 | 68.4 (2) | C52—C53—C54—Zr3 | 70.9 (2) |
| C1—C2—C3—C4 | -5.1 (3) | C53—C54—C55—C51 | -3.4 (3) |
| Zr1—C2—C3—C4 | -70.7 (2) | Zr3—C54—C55—C51 | -67.2 (2) |
| C1—C2—C3—Zr1 | 65.6 (2) | C53—C54—C55—Zr3 | 63.8 (2) |
| C2—C3—C4—C5 | 4.7 (3) | C52—C51—C55—C54 | 0.5 (4) |
| Zr1—C3—C4—C5 | -65.6 (2) | Zr3—C51—C55—C54 | 67.9 (2) |
| C2—C3—C4—Zr1 | 70.4 (2) | C52—C51—C55—Zr3 | -67.4 (2) |
| C3—C4—C5—C1 | -2.5 (3) | C60—C56—C57—C58 | 1.9 (3) |
| Zr1—C4—C5—C1 | -67.0 (2) | Zr3—C56—C57—C58 | -67.75 (19) |
| C3—C4—C5—Zr1 | 64.4 (2) | C60—C56—C57—Zr3 | 69.68 (19) |
| C2—C1—C5—C4 | -0.7 (3) | C56—C57—C58—C59 | 0.4 (3) |
| Zr1—C1—C5—C4 | 68.1 (2) | Zr3—C57—C58—C59 | -66.3 (2) |
| C2—C1—C5—Zr1 | -68.7 (2) | C56—C57—C58—Zr3 | 66.69 (18) |
| C10—C6—C7—C8 | 3.0 (3) | C57—C58—C59—C60 | -2.6 (3) |
| Zr1—C6—C7—C8 | -65.35 (19) | Zr3—C58—C59—C60 | -69.2 (2) |
| C10—C6—C7—Zr1 | 68.39 (18) | C57—C58—C59—Zr3 | 66.6 (2) |
| C6—C7—C8—C9 | -2.1 (3) | C58—C59—C60—C56 | 3.8 (3) |
| Zr1—C7—C8—C9 | -67.22 (19) | Zr3—C59—C60—C56 | -65.3 (2) |
| C6—C7—C8—Zr1 | 65.09 (19) | C58—C59—C60—Zr3 | 69.1 (2) |
| C7—C8—C9—C10 | 0.4 (3) | C57—C56—C60—C59 | -3.5 (3) |
| Zr1—C8—C9—C10 | -68.36 (19) | Zr3—C56—C60—C59 | 65.6 (2) |
| C7—C8—C9—Zr1 | 68.7 (2) | C57—C56—C60—Zr3 | -69.17 (18) |
| C8—C9—C10—C6 | 1.5 (3) | C65—C61—C62—C63 | 5.2 (3) |
| Zr1—C9—C10—C6 | -66.8 (2) | C66—C61—C62—C63 | -142.3 (3) |
| C8—C9—C10—Zr1 | 68.37 (19) | Zr3—C61—C62—C63 | -68.98 (19) |
| C7—C6—C10—C9 | -2.8 (3) | C65—C61—C62—Zr3 | 74.18 (16) |
| Zr1—C6—C10—C9 | 66.66 (19) | C66—C61—C62—Zr3 | -73.3 (2) |
| C7—C6—C10—Zr1 | -69.49 (19) | C61—C62—C63—C64 | -3.0 (3) |
| C15—C11—C12—C13 | 5.4 (3) | Zr3—C62—C63—C64 | -63.5 (2) |
| C16—C11—C12—C13 | -142.9 (3) | C61—C62—C63—Zr3 | 60.50 (17) |
| Zr1—C11—C12—C13 | -69.05 (17) | C62—C63—C64—C65 | -0.6 (3) |

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| C15—C11—C12—Zr1 | 74.44 (16) | Zr3—C63—C64—C65 | -60.95 (19) |
| C16—C11—C12—Zr1 | -73.8 (2) | C62—C63—C64—Zr3 | 60.38 (19) |
| C11—C12—C13—C14 | -3.4 (3) | C63—C64—C65—C61 | 3.9 (3) |
| Zr1—C12—C13—C14 | -64.32 (18) | Zr3—C64—C65—C61 | -61.37 (17) |
| C11—C12—C13—Zr1 | 60.92 (16) | C63—C64—C65—Zr3 | 65.3 (2) |
| C12—C13—C14—C15 | -0.1 (3) | C62—C61—C65—C64 | -5.6 (3) |
| Zr1—C13—C14—C15 | -60.85 (17) | C66—C61—C65—C64 | 142.2 (3) |
| C12—C13—C14—Zr1 | 60.76 (17) | Zr3—C61—C65—C64 | 69.4 (2) |
| C13—C14—C15—C11 | 3.5 (3) | C62—C61—C65—Zr3 | -74.98 (16) |
| Zr1—C14—C15—C11 | -61.09 (16) | C66—C61—C65—Zr3 | 72.8 (2) |
| C13—C14—C15—Zr1 | 64.62 (17) | C62—C61—C66—C71 | -39.4 (4) |
| C12—C11—C15—C14 | -5.5 (3) | C65—C61—C66—C71 | 178.7 (2) |
| C16—C11—C15—C14 | 144.0 (2) | Zr3—C61—C66—C71 | -110.9 (2) |
| Zr1—C11—C15—C14 | 69.13 (18) | C62—C61—C66—C67 | -173.9 (2) |
| C12—C11—C15—Zr1 | -74.59 (16) | C65—C61—C66—C67 | 44.2 (4) |
| C16—C11—C15—Zr1 | 74.8 (2) | Zr3—C61—C66—C67 | 114.6 (2) |
| C15—C11—C16—C17 | 43.8 (4) | C62—C61—C66—Zr3 | 71.5 (2) |
| C12—C11—C16—C17 | -172.9 (2) | C65—C61—C66—Zr3 | -70.4 (2) |
| Zr1—C11—C16—C17 | 115.8 (2) | C61—C66—C67—C68 | -164.5 (3) |
| C15—C11—C16—C21 | 178.4 (2) | C71—C66—C67—C68 | 57.4 (3) |
| C12—C11—C16—C21 | -38.3 (4) | Zr3—C66—C67—C68 | -89.6 (3) |
| Zr1—C11—C16—C21 | -109.6 (2) | C61—C66—C67—C72 | 76.2 (3) |
| C15—C11—C16—Zr1 | -72.1 (2) | C71—C66—C67—C72 | -62.0 (3) |
| C12—C11—C16—Zr1 | 71.3 (2) | Zr3—C66—C67—C72 | 151.0 (2) |
| C11—C16—C17—C18 | -164.1 (3) | C66—C67—C68—C69 | -58.8 (3) |
| C21—C16—C17—C18 | 57.3 (3) | C72—C67—C68—C69 | 60.4 (4) |
| Zr1—C16—C17—C18 | -90.2 (3) | C67—C68—C69—C70 | 59.2 (4) |
| C11—C16—C17—C22 | 76.6 (3) | C67—C68—C69—C73 | -60.5 (4) |
| C21—C16—C17—C22 | -61.9 (3) | C68—C69—C70—C71 | -59.6 (4) |
| Zr1—C16—C17—C22 | 150.59 (18) | C73—C69—C70—C71 | 60.1 (4) |
| C16—C17—C18—C19 | -60.0 (3) | C61—C66—C71—C70 | 165.1 (2) |
| C22—C17—C18—C19 | 59.0 (3) | C67—C66—C71—C70 | -57.2 (3) |
| C17—C18—C19—C23 | -59.6 (4) | Zr3—C66—C71—C70 | 90.9 (3) |
| C17—C18—C19—C20 | 60.3 (3) | C61—C66—C71—C74 | -76.0 (3) |
| C23—C19—C20—C21 | 59.9 (3) | C67—C66—C71—C74 | 61.7 (3) |
| C18—C19—C20—C21 | -60.4 (4) | Zr3—C66—C71—C74 | -150.2 (2) |
| C11—C16—C21—C20 | 165.5 (2) | C69—C70—C71—C66 | 59.2 (3) |
| C17—C16—C21—C20 | -56.9 (3) | C69—C70—C71—C74 | -59.7 (4) |
| Zr1—C16—C21—C20 | 92.4 (3) | C66—C67—C72—C75 | 60.9 (4) |
| C11—C16—C21—C24 | -76.0 (3) | C68—C67—C72—C75 | -59.9 (4) |
| C17—C16—C21—C24 | 61.7 (3) | C68—C69—C73—C75 | 60.1 (4) |
| Zr1—C16—C21—C24 | -149.0 (2) | C70—C69—C73—C75 | -59.5 (4) |
| C19—C20—C21—C16 | 59.3 (3) | C66—C71—C74—C75 | -60.9 (4) |
| C19—C20—C21—C24 | -59.7 (3) | C70—C71—C74—C75 | 59.1 (4) |
| C16—C17—C22—C25 | 60.6 (3) | C69—C73—C75—C74 | 59.6 (4) |
| C18—C17—C22—C25 | -60.2 (3) | C69—C73—C75—C72 | -60.1 (4) |
| C18—C19—C23—C25 | 59.9 (4) | C71—C74—C75—C73 | -59.9 (4) |
| C20—C19—C23—C25 | -59.1 (3) | C71—C74—C75—C72 | 60.1 (4) |

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| C16—C21—C24—C25 | -59.8 (3) | C67—C72—C75—C73 | 60.3 (4) |
| C20—C21—C24—C25 | 60.3 (3) | C67—C72—C75—C74 | -60.1 (4) |
| C21—C24—C25—C23 | -60.8 (3) | C80—C76—C77—C78 | 3.1 (3) |
| C21—C24—C25—C22 | 58.6 (3) | Zr4—C76—C77—C78 | -65.7 (2) |
| C19—C23—C25—C24 | 59.9 (4) | C80—C76—C77—Zr4 | 68.8 (2) |
| C19—C23—C25—C22 | -60.0 (4) | C76—C77—C78—C79 | -3.3 (3) |
| C17—C22—C25—C24 | -59.2 (3) | Zr4—C77—C78—C79 | -69.4 (2) |
| C17—C22—C25—C23 | 60.7 (3) | C76—C77—C78—Zr4 | 66.1 (2) |
| C30—C26—C27—C28 | 3.0 (3) | C77—C78—C79—C80 | 2.4 (3) |
| Zr2—C26—C27—C28 | -65.75 (19) | Zr4—C78—C79—C80 | -67.0 (2) |
| C30—C26—C27—Zr2 | 68.7 (2) | C77—C78—C79—Zr4 | 69.4 (2) |
| C26—C27—C28—C29 | -4.1 (3) | C78—C79—C80—C76 | -0.5 (3) |
| Zr2—C27—C28—C29 | -70.00 (19) | Zr4—C79—C80—C76 | -66.35 (19) |
| C26—C27—C28—Zr2 | 65.91 (19) | C78—C79—C80—Zr4 | 65.88 (19) |
| C27—C28—C29—C30 | 3.7 (3) | C77—C76—C80—C79 | -1.6 (3) |
| Zr2—C28—C29—C30 | -66.1 (2) | Zr4—C76—C80—C79 | 67.0 (2) |
| C27—C28—C29—Zr2 | 69.80 (19) | C77—C76—C80—Zr4 | -68.6 (2) |
| C28—C29—C30—C26 | -1.9 (3) | C85—C81—C82—C83 | 3.6 (3) |
| Zr2—C29—C30—C26 | -67.5 (2) | Zr4—C81—C82—C83 | -64.6 (2) |
| C28—C29—C30—Zr2 | 65.6 (2) | C85—C81—C82—Zr4 | 68.1 (2) |
| C27—C26—C30—C29 | -0.7 (3) | C81—C82—C83—C84 | -4.8 (3) |
| Zr2—C26—C30—C29 | 68.6 (2) | Zr4—C82—C83—C84 | -70.89 (19) |
| C27—C26—C30—Zr2 | -69.24 (19) | C81—C82—C83—Zr4 | 66.1 (2) |
| C35—C31—C32—C33 | 3.2 (4) | C82—C83—C84—C85 | 4.2 (3) |
| Zr2—C31—C32—C33 | -65.4 (3) | Zr4—C83—C84—C85 | -66.8 (2) |
| C35—C31—C32—Zr2 | 68.6 (2) | C82—C83—C84—Zr4 | 70.98 (19) |
| C31—C32—C33—C34 | -1.6 (4) | C83—C84—C85—C81 | -2.0 (3) |
| Zr2—C32—C33—C34 | -67.2 (3) | Zr4—C84—C85—C81 | -67.0 (2) |
| C31—C32—C33—Zr2 | 65.7 (2) | C83—C84—C85—Zr4 | 64.9 (2) |
| C32—C33—C34—C35 | -0.7 (4) | C82—C81—C85—C84 | -1.0 (4) |
| Zr2—C33—C34—C35 | -70.1 (2) | Zr4—C81—C85—C84 | 67.3 (2) |
| C32—C33—C34—Zr2 | 69.4 (3) | C82—C81—C85—Zr4 | -68.2 (2) |
| C33—C34—C35—C31 | 2.7 (4) | C90—C86—C87—C88 | 5.4 (3) |
| Zr2—C34—C35—C31 | -66.9 (2) | C91—C86—C87—C88 | -142.9 (3) |
| C33—C34—C35—Zr2 | 69.6 (3) | Zr4—C86—C87—C88 | -70.01 (19) |
| C32—C31—C35—C34 | -3.7 (4) | C90—C86—C87—Zr4 | 75.38 (16) |
| Zr2—C31—C35—C34 | 65.8 (2) | C91—C86—C87—Zr4 | -72.9 (2) |
| C32—C31—C35—Zr2 | -69.4 (2) | C86—C87—C88—C89 | -3.7 (3) |
| C41—C36—C37—C38 | -143.3 (2) | Zr4—C87—C88—C89 | -65.40 (19) |
| C40—C36—C37—C38 | 5.1 (3) | C86—C87—C88—Zr4 | 61.68 (16) |
| Zr2—C36—C37—C38 | -68.67 (19) | C87—C88—C89—C90 | 0.5 (3) |
| C41—C36—C37—Zr2 | -74.6 (2) | Zr4—C88—C89—C90 | -60.19 (18) |
| C40—C36—C37—Zr2 | 73.81 (16) | C87—C88—C89—Zr4 | 60.69 (18) |
| C36—C37—C38—C39 | -3.0 (3) | C88—C89—C90—C86 | 2.9 (3) |
| Zr2—C37—C38—C39 | -63.50 (19) | Zr4—C89—C90—C86 | -60.38 (16) |
| C36—C37—C38—Zr2 | 60.52 (17) | C88—C89—C90—Zr4 | 63.30 (19) |
| C37—C38—C39—C40 | -0.5 (3) | C87—C86—C90—C89 | -5.0 (3) |
| Zr2—C38—C39—C40 | -61.15 (18) | C91—C86—C90—C89 | 142.7 (3) |

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| C37—C38—C39—Zr2 | 60.66 (18) | Zr4—C86—C90—C89 | 69.21 (19) |
| C38—C39—C40—C36 | 3.8 (3) | C87—C86—C90—Zr4 | -74.26 (16) |
| Zr2—C39—C40—C36 | -61.64 (17) | C91—C86—C90—Zr4 | 73.5 (2) |
| C38—C39—C40—Zr2 | 65.41 (19) | C90—C86—C91—C96 | 171.3 (2) |
| C37—C36—C40—C39 | -5.4 (3) | C87—C86—C91—C96 | -46.2 (4) |
| C41—C36—C40—C39 | 143.7 (2) | Zr4—C86—C91—C96 | -116.8 (2) |
| Zr2—C36—C40—C39 | 69.33 (18) | C90—C86—C91—C92 | 37.3 (4) |
| C37—C36—C40—Zr2 | -74.77 (17) | C87—C86—C91—C92 | 179.8 (2) |
| C41—C36—C40—Zr2 | 74.4 (2) | Zr4—C86—C91—C92 | 109.2 (2) |
| C37—C36—C41—C46 | -39.3 (4) | C90—C86—C91—Zr4 | -71.9 (2) |
| C40—C36—C41—C46 | 177.4 (2) | C87—C86—C91—Zr4 | 70.6 (2) |
| Zr2—C36—C41—C46 | -111.5 (2) | C86—C91—C92—C93 | -166.3 (3) |
| C37—C36—C41—C42 | -173.9 (2) | C96—C91—C92—C93 | 56.8 (3) |
| C40—C36—C41—C42 | 42.8 (3) | Zr4—C91—C92—C93 | -92.6 (3) |
| Zr2—C36—C41—C42 | 113.9 (2) | C86—C91—C92—C97 | 75.3 (3) |
| C37—C36—C41—Zr2 | 72.2 (2) | C96—C91—C92—C97 | -61.6 (3) |
| C40—C36—C41—Zr2 | -71.2 (2) | Zr4—C91—C92—C97 | 149.0 (2) |
| C36—C41—C42—C43 | -164.6 (2) | C91—C92—C93—C94 | -59.1 (3) |
| C46—C41—C42—C43 | 57.1 (3) | C97—C92—C93—C94 | 59.6 (4) |
| Zr2—C41—C42—C43 | -91.2 (3) | C92—C93—C94—C95 | 59.8 (3) |
| C36—C41—C42—C47 | 76.3 (3) | C92—C93—C94—C98 | -60.0 (4) |
| C46—C41—C42—C47 | -62.0 (3) | C93—C94—C95—C96 | -59.5 (4) |
| Zr2—C41—C42—C47 | 149.7 (2) | C98—C94—C95—C96 | 60.2 (4) |
| C41—C42—C43—C44 | -59.4 (3) | C94—C95—C96—C91 | 59.2 (4) |
| C47—C42—C43—C44 | 59.9 (3) | C94—C95—C96—C99 | -59.8 (4) |
| C42—C43—C44—C48 | -60.1 (3) | C86—C91—C96—C95 | 164.8 (3) |
| C42—C43—C44—C45 | 60.1 (4) | C92—C91—C96—C95 | -57.3 (3) |
| C48—C44—C45—C46 | 60.4 (3) | Zr4—C91—C96—C95 | 89.9 (3) |
| C43—C44—C45—C46 | -60.2 (3) | C86—C91—C96—C99 | -75.9 (3) |
| C36—C41—C46—C45 | 165.6 (2) | C92—C91—C96—C99 | 62.0 (3) |
| C42—C41—C46—C45 | -56.9 (3) | Zr4—C91—C96—C99 | -150.8 (2) |
| Zr2—C41—C46—C45 | 92.1 (3) | C91—C92—C97—C100 | 60.0 (4) |
| C36—C41—C46—C49 | -75.6 (3) | C93—C92—C97—C100 | -59.6 (4) |
| C42—C41—C46—C49 | 61.9 (3) | C95—C94—C98—C100 | -59.8 (5) |
| Zr2—C41—C46—C49 | -149.14 (18) | C93—C94—C98—C100 | 59.4 (4) |
| C44—C45—C46—C41 | 59.1 (3) | C95—C96—C99—C100 | 59.9 (4) |
| C44—C45—C46—C49 | -59.7 (3) | C91—C96—C99—C100 | -60.8 (4) |
| C43—C42—C47—C50 | -60.4 (3) | C94—C98—C100—C97 | -60.1 (4) |
| C41—C42—C47—C50 | 60.3 (3) | C94—C98—C100—C99 | 60.0 (4) |
| C43—C44—C48—C50 | 59.3 (3) | C92—C97—C100—C98 | 60.8 (4) |
| C45—C44—C48—C50 | -60.3 (4) | C92—C97—C100—C99 | -59.3 (3) |
| C41—C46—C49—C50 | -60.3 (3) | C96—C99—C100—C98 | -60.5 (4) |
| C45—C46—C49—C50 | 59.9 (3) | C96—C99—C100—C97 | 59.8 (4) |
| C44—C48—C50—C47 | -59.3 (3) | C106—C101—C102—C103 | 6.1 (14) |
| C44—C48—C50—C49 | 60.5 (3) | C107—C101—C102—C103 | -177.2 (13) |
| C42—C47—C50—C48 | 60.4 (3) | C101—C102—C103—C104 | -6.5 (15) |
| C42—C47—C50—C49 | -59.2 (3) | C102—C103—C104—C105 | 2.5 (17) |
| C46—C49—C50—C48 | -60.6 (3) | C103—C104—C105—C106 | 2.4 (18) |

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| C46—C49—C50—C47 | 59.2 (4) | C104—C105—C106—C101 | -2.8 (17) |
| C55—C51—C52—C53 | 2.5 (4) | C107—C101—C106—C105 | -178.5 (13) |
| Zr3—C51—C52—C53 | -65.5 (2) | C102—C101—C106—C105 | -1.4 (16) |
| C55—C51—C52—Zr3 | 68.0 (2) | C108—C109—C110—C111 | 86.9 (18) |
| C51—C52—C53—C54 | -4.6 (3) | C109—C110—C111—C112 | -165.7 (13) |
| Zr3—C52—C53—C54 | -72.0 (2) | C110—C111—C112—C113 | 178.6 (14) |
| C51—C52—C53—Zr3 | 67.4 (2) | | |
