

**catena-Poly[[tetrakis(hexamethylphosphoramido- $\kappa$ O)bis(nitrato- $\kappa^2$ O, $O'$ )cerium(III)] [silver(I)-di- $\mu$ -sulfido-tungstate(VI)-di- $\mu$ -sulfido]]**

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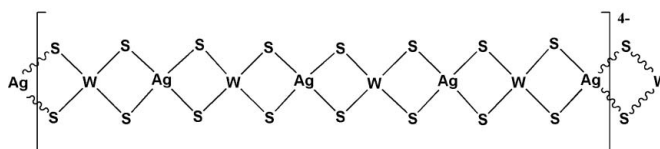
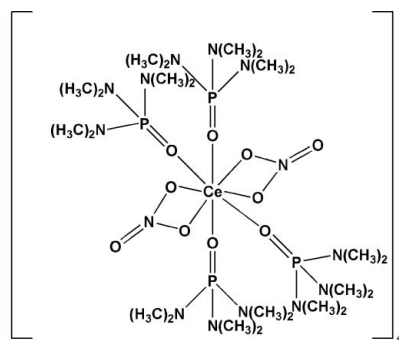
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Key indicators: single-crystal X-ray study;  $T = 153$  K; mean  $\sigma(\text{N}-\text{C}) = 0.011$  Å;  $R$  factor = 0.034;  $wR$  factor = 0.068; data-to-parameter ratio = 15.4.

Hexamethylphosphoramido (hmp), tetrathiotungstate, silver sulfide and cerium nitrate were self-assembled to form a one-dimensional anionic  $[\text{Ag}_4\text{W}_4\text{S}_{16}]_n^{4n-}$  chain in the title compound,  $\{[\text{Ce}(\text{NO}_3)_2(\text{C}_6\text{H}_{18}\text{N}_3\text{OP})_4][\text{AgWS}_4]\}_n$ . The asymmetric unit contains four crystallographically independent  $[\text{Ce}(\text{hmp})_4(\text{NO}_3)_2]^+$  cations, which leads to a one-dimensional polymeric anionic chain having a tetravalent  $[\text{W}_4\text{S}_{16}\text{Ag}_4]$  repeat unit. Each central Ce atom is coordinated by eight O atoms from two chelating nitrate and four hmp ligands, which gives rise to a distorted square-antiprismatic structure. The polymeric chain with average  $\text{W}-\text{Ag}-\text{W}$  and  $\text{Ag}-\text{W}-\text{Ag}$  bond angles of  $163.75$  and  $151.84^\circ$ , respectively, presents a distorted linear configuration. The title complex with a non-centrosymmetric structure, is analogous to the Yb, Y, Eu, Nd, La and Dy isomorphs, which exhibit centrosymmetric structures.

### Related literature

For one-dimensional Mo(W)/S/Ag anionic polymers, see: Niu *et al.* (2004). For their unique properties, see: Zhang, Song *et al.* (2007). For analogous centrosymmetric complexes, see: Cao *et al.* (2007); Zhang, Cao *et al.* (2007); Zhang, Qian *et al.* (2007); Tang, Zhang & Zhang (2008); Tang, Zhang, Zhang & Lu (2008); Wei *et al.* (2010).



### Experimental

#### Crystal data

$[\text{Ce}(\text{NO}_3)_2(\text{C}_6\text{H}_{18}\text{N}_3\text{OP})_4][\text{AgWS}_4]$   
 $M_r = 1400.92$   
 Monoclinic,  $P2_1$   
 $a = 15.639$  (3) Å  
 $b = 30.002$  (6) Å  
 $c = 22.532$  (4) Å  
 $\beta = 90.53$  (3) $^\circ$   
 $V = 10572$  (3) Å<sup>3</sup>  
 $Z = 8$   
 Mo  $K\alpha$  radiation  
 $\mu = 3.72$  mm<sup>-1</sup>  
 $T = 153$  K  
 $0.30 \times 0.22 \times 0.20$  mm

#### Data collection

Rigaku Saturn724+ diffractometer  
 Absorption correction: multi-scan  
 (*CrystalClear*; Rigaku, 2007)  
 $T_{\min} = 0.390$ ,  $T_{\max} = 0.475$   
 49779 measured reflections  
 34142 independent reflections  
 32497 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.024$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$   
 $wR(F^2) = 0.068$   
 $S = 1.06$   
 34142 reflections  
 2221 parameters  
 1 restraint  
 H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.74$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.96$  e Å<sup>-3</sup>  
 Absolute structure: Flack (1983),  
 14534 Friedel pairs  
 Flack parameter: 0.286 (4)

Data collection: *CrystalClear* (Rigaku, 2007); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZQ2066).

## References

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**supplementary materials**

*Acta Cryst.* (2010). E66, m1657-m1658 [ doi:10.1107/S1600536810044260 ]

***catena*-Poly[[tetrakis(hexamethylphosphoramidate- $\kappa O$ )bis(nitrato- $\kappa^2 O, O'$ )cerium(III)] [silver(I)-di- $\mu$ -sulfido-tungstate(VI)-di- $\mu$ -sulfido]]**

**H. Wei, J. Zhang and C. Zhang**

**Comment**

One-dimensional Mo(W)/S/Ag anionic polymers have attracted much attention for their configurational isomerism (Niu *et al.*, 2004) and unique properties as functional materials, such as third-order nonlinear optical (NLO) materials (Zhang, Song & Wang, 2007). Different solvent-coordinated rare-earth cations proved effective to obtain various configurations of anionic chains (Niu *et al.*, 2004). The title compound  $\{4n[\text{Ce}(\text{hmp})_4(\text{NO}_3)_2][\text{Ag}_4\text{W}_4\text{S}_{16}]_n\}$  (hmp = hexamethylphosphoramidate) with a wave-like anionic chain was prepared by following such route using Ce(III)-hmp complex as counterion.

Each  $\text{Ce}^{3+}$  in the cation is coordinated by eight O atoms from two nitrate and four hmp ligands (Fig. 1). Parts of dimethylamine groups from hmp ligands have large librations reflecting a small degree of thermal disorder. The cation in the title compound contains four univalent  $[\text{Ce}(\text{hmp})_4(\text{NO}_3)_2]^+$ , which leads to a 1-D anionic chain having a tetravalent repeat unit. As illustrated in Fig. 2, the anionic chain in the title compound has a distorted linear configuration with average W—Ag—W and Ag—W—Ag angles of 163.75 and 151.84 °, respectively. The title complex is analogous to Yb (Cao *et al.* 2007), Y (Zhang, Cao *et al.* 2007), Eu (Zhang, Qian *et al.* 2007), Nd (Tang, Zhang & Zhang, 2008), La (Tang, Zhang, Zhang & Lu, 2008) and Dy (Wei *et al.* 2010) isomorphs.

**Experimental**

1 mmol  $\text{Ag}_2\text{S}$  was added to a solution of  $[\text{NH}_4]_2\text{WS}_4$  (2 mmol in 30 mL hmp) with thorough stir for 6 h. The solution underwent an additional stir for two minute after 1 mmol  $\text{Ce}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$  was added. After filtration the orange-red filtrate was carefully laid on the surface with 30 ml *i*-PrOH. orange block crystals were obtained after ten days.

**Refinement**

H atoms were positioned geometrically and refined with riding model, with  $U_{\text{iso}} = 1.5U_{\text{eq}}$  for methyl H atoms and 0.96 Å for C—H bonds.

## Figures

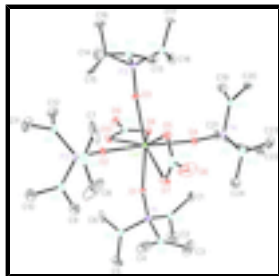


Fig. 1. The molecular structure of one  $[\text{Ce}(\text{hmp})_4(\text{NO}_3)_2]^+$  cation in the title compound, with atom labels and 30% probability displacement ellipsoids. All H atoms have been omitted.



Fig. 2. The molecular structure of a portion of the anionic chain in the title compound, with atom labels and 30% probability displacement ellipsoids.

## **catena-Poly[[tetrakis(hexamethylphosphoramidate-κO)bis(nitrato-κ<sup>2</sup>O,O')cerium(III)] [silver(I)-di-μ-sulfido-tungstate(VI)-di-μ-sulfido]]**

### Crystal data

$[\text{Ce}(\text{NO}_3)_2(\text{C}_6\text{H}_{18}\text{N}_3\text{OP})_4][\text{AgWS}_4]$

$M_r = 1400.92$

Monoclinic,  $P2_1$

$a = 15.639(3) \text{ \AA}$

$b = 30.002(6) \text{ \AA}$

$c = 22.532(4) \text{ \AA}$

$\beta = 90.53(3)^\circ$

$V = 10572(3) \text{ \AA}^3$

$Z = 8$

$F(000) = 5576$

$D_x = 1.760 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 45199 reflections

$\theta = 2.8\text{--}29.0^\circ$

$\mu = 3.72 \text{ mm}^{-1}$

$T = 153 \text{ K}$

Block, orange

$0.3 \times 0.22 \times 0.20 \text{ mm}$

### Data collection

Rigaku Saturn724+ (2x2 bin mode) diffractometer

Radiation source: fine-focus sealed tube graphite

$\omega$  scans

Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2007)

$T_{\min} = 0.390$ ,  $T_{\max} = 0.475$

49779 measured reflections

34142 independent reflections

32497 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.024$

$\theta_{\max} = 25.4^\circ$ ,  $\theta_{\min} = 2.8^\circ$

$h = -12 \rightarrow 18$

$k = -35 \rightarrow 36$

$l = -27 \rightarrow 25$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.034$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

|  |   |
|--|---|
| $wR(F^2) = 0.068$  | $w = 1/[\sigma^2(F_o^2) + (0.0224P)^2 + 4.7571P]$                                   |
| $S = 1.06$   | where $P = (F_o^2 + 2F_c^2)/3$  |
| 34142 reflections  | $(\Delta/\sigma)_{\max} = 0.003$  |
| 2221 parameters  | $\Delta\rho_{\max} = 0.74 \text{ e } \text{\AA}^{-3}$                               |
| 1 restraint  | $\Delta\rho_{\min} = -0.96 \text{ e } \text{\AA}^{-3}$                              |
| Primary atom site location: structure-invariant direct methods | Absolute structure: Flack (1983), 14534 Friedel pairs<br>Flack parameter: 0.286 (4) |

### Special details

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

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

|     | $x$          | $y$           | $z$            | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|---------------|----------------|----------------------------------|
| W1  | 0.70667 (2)  | 0.670558 (10) | 0.635629 (14)  | 0.01653 (8)                      |
| W2  | 0.70710 (2)  | 0.718307 (10) | 0.384943 (14)  | 0.01684 (8)                      |
| W3  | 0.71320 (2)  | 0.680506 (10) | 0.132285 (14)  | 0.01660 (8)                      |
| W4  | 0.71030 (2)  | 0.726819 (9)  | -0.117449 (14) | 0.01602 (8)                      |
| Ag1 | 0.70624 (5)  | 0.70662 (2)   | 0.51475 (3)    | 0.02993 (18)                     |
| Ag2 | 0.71221 (5)  | 0.68628 (2)   | 0.26209 (3)    | 0.03115 (18)                     |
| Ag3 | 0.71502 (5)  | 0.71867 (2)   | 0.01258 (3)    | 0.03065 (18)                     |
| Ag4 | 0.70672 (5)  | 0.68569 (2)   | 0.76465 (3)    | 0.03160 (18)                     |
| S1  | 0.59159 (15) | 0.65587 (8)   | 0.68776 (10)   | 0.0265 (5)                       |
| S2  | 0.82175 (15) | 0.65644 (8)   | 0.68948 (10)   | 0.0244 (5)                       |
| S3  | 0.70493 (16) | 0.74260 (7)   | 0.61376 (10)   | 0.0240 (5)                       |
| S4  | 0.70920 (15) | 0.62697 (7)   | 0.55689 (10)   | 0.0233 (5)                       |
| S5  | 0.59056 (15) | 0.73146 (9)   | 0.43625 (10)   | 0.0304 (6)                       |
| S6  | 0.82233 (15) | 0.73143 (8)   | 0.43943 (10)   | 0.0262 (5)                       |
| S7  | 0.70824 (16) | 0.76450 (7)   | 0.30862 (9)    | 0.0237 (5)                       |
| S8  | 0.70711 (17) | 0.64732 (7)   | 0.35904 (10)   | 0.0279 (5)                       |
| S9  | 0.59795 (15) | 0.66429 (8)   | 0.18283 (10)   | 0.0260 (5)                       |
| S10 | 0.82968 (15) | 0.66679 (7)   | 0.18527 (10)   | 0.0236 (5)                       |
| S11 | 0.70992 (15) | 0.75284 (7)   | 0.11250 (10)   | 0.0214 (5)                       |
| S12 | 0.71504 (15) | 0.63835 (7)   | 0.05201 (9)    | 0.0230 (5)                       |
| S13 | 0.59544 (15) | 0.74205 (7)   | -0.06550 (10)  | 0.0236 (5)                       |
| S14 | 0.82577 (15) | 0.74540 (8)   | -0.06615 (10)  | 0.0266 (5)                       |
| S15 | 0.70532 (15) | 0.76722 (7)   | -0.19945 (10)  | 0.0243 (5)                       |
| S16 | 0.71292 (15) | 0.65425 (7)   | -0.13326 (10)  | 0.0230 (5)                       |

## supplementary materials

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|     |              |               |               |              |
|-----|--------------|---------------|---------------|--------------|
| Ce1 | 0.23943 (3)  | 0.530118 (13) | 0.432688 (18) | 0.01342 (10) |
| P1  | 0.17428 (13) | 0.43188 (7)   | 0.53337 (9)   | 0.0197 (4)   |
| P2  | 0.47960 (13) | 0.52705 (7)   | 0.47157 (9)   | 0.0268 (5)   |
| P3  | 0.30186 (15) | 0.60588 (7)   | 0.30129 (10)  | 0.0229 (5)   |
| P4  | 0.01650 (14) | 0.58453 (7)   | 0.44156 (9)   | 0.0181 (5)   |
| O1  | 0.2087 (3)   | 0.46413 (17)  | 0.4896 (2)    | 0.0179 (12)  |
| O2  | 0.3877 (3)   | 0.52404 (18)  | 0.4519 (2)    | 0.0242 (13)  |
| O3  | 0.2779 (4)   | 0.57219 (17)  | 0.3469 (2)    | 0.0203 (12)  |
| O4  | 0.0975 (3)   | 0.55851 (17)  | 0.4391 (2)    | 0.0208 (13)  |
| O5  | 0.2604 (4)   | 0.6089 (2)    | 0.4817 (3)    | 0.0306 (15)  |
| O6  | 0.2435 (6)   | 0.6213 (3)    | 0.5756 (3)    | 0.071 (3)    |
| O7  | 0.2374 (4)   | 0.55348 (19)  | 0.5427 (3)    | 0.0300 (15)  |
| O8  | 0.1566 (4)   | 0.48881 (18)  | 0.3496 (2)    | 0.0229 (13)  |
| O9  | 0.2122 (4)   | 0.44519 (19)  | 0.2840 (3)    | 0.0328 (16)  |
| O10 | 0.2868 (4)   | 0.46843 (18)  | 0.3593 (2)    | 0.0212 (13)  |
| N1  | 0.0763 (4)   | 0.4198 (2)    | 0.5144 (3)    | 0.0273 (16)  |
| N2  | 0.1759 (5)   | 0.4496 (2)    | 0.6025 (3)    | 0.0328 (17)  |
| N3  | 0.2337 (4)   | 0.3872 (2)    | 0.5358 (3)    | 0.0232 (15)  |
| N4  | 0.5043 (5)   | 0.5670 (3)    | 0.5147 (3)    | 0.051 (2)    |
| N5  | 0.5035 (5)   | 0.4798 (3)    | 0.5038 (3)    | 0.054 (2)    |
| N6  | 0.5411 (4)   | 0.5344 (2)    | 0.4153 (3)    | 0.0337 (16)  |
| N7  | 0.3637 (5)   | 0.6472 (2)    | 0.3233 (3)    | 0.0259 (17)  |
| N8  | 0.3554 (5)   | 0.5809 (2)    | 0.2485 (3)    | 0.0362 (19)  |
| N9  | 0.2145 (5)   | 0.6306 (2)    | 0.2772 (3)    | 0.0238 (16)  |
| N10 | 0.0143 (4)   | 0.6252 (2)    | 0.3931 (3)    | 0.0197 (15)  |
| N11 | -0.0633 (4)  | 0.5508 (2)    | 0.4284 (3)    | 0.0203 (15)  |
| N12 | 0.0054 (5)   | 0.6066 (2)    | 0.5074 (3)    | 0.0285 (18)  |
| N13 | 0.2168 (5)   | 0.4668 (2)    | 0.3295 (3)    | 0.0203 (16)  |
| N14 | 0.2473 (6)   | 0.5946 (3)    | 0.5344 (4)    | 0.039 (2)    |
| C1  | 0.0184 (5)   | 0.4534 (3)    | 0.4900 (4)    | 0.033 (2)    |
| H1A | -0.0202      | 0.4630        | 0.5203        | 0.049*       |
| H1B | -0.0136      | 0.4408        | 0.4575        | 0.049*       |
| H1C | 0.0509       | 0.4784        | 0.4762        | 0.049*       |
| C2  | 0.0327 (6)   | 0.3797 (3)    | 0.5369 (5)    | 0.059 (3)    |
| H2A | -0.0095      | 0.3700        | 0.5085        | 0.089*       |
| H2B | 0.0053       | 0.3866        | 0.5738        | 0.089*       |
| H2C | 0.0738       | 0.3564        | 0.5432        | 0.089*       |
| C3  | 0.1047 (8)   | 0.4672 (5)    | 0.6322 (4)    | 0.105 (6)    |
| H3A | 0.0980       | 0.4981        | 0.6220        | 0.158*       |
| H3B | 0.1133       | 0.4645        | 0.6743        | 0.158*       |
| H3C | 0.0542       | 0.4511        | 0.6206        | 0.158*       |
| C4  | 0.2566 (7)   | 0.4626 (4)    | 0.6307 (4)    | 0.057 (3)    |
| H4A | 0.2553       | 0.4551        | 0.6721        | 0.085*       |
| H4B | 0.2648       | 0.4941        | 0.6263        | 0.085*       |
| H4C | 0.3029       | 0.4470        | 0.6121        | 0.085*       |
| C5  | 0.2358 (6)   | 0.3552 (3)    | 0.5853 (4)    | 0.043 (2)    |
| H5A | 0.2938       | 0.3462        | 0.5929        | 0.065*       |
| H5B | 0.2020       | 0.3296        | 0.5751        | 0.065*       |
| H5C | 0.2130       | 0.3690        | 0.6202        | 0.065*       |

|      |            |            |            |           |
|------|------------|------------|------------|-----------|
| C6   | 0.2675 (5) | 0.3682 (3) | 0.4811 (4) | 0.033 (2) |
| H6A  | 0.2370     | 0.3412     | 0.4717     | 0.049*    |
| H6B  | 0.3271     | 0.3615     | 0.4865     | 0.049*    |
| H6C  | 0.2605     | 0.3891     | 0.4493     | 0.049*    |
| C7   | 0.4995 (7) | 0.6124 (4) | 0.4926 (6) | 0.071 (4) |
| H7A  | 0.5337     | 0.6315     | 0.5175     | 0.106*    |
| H7B  | 0.4412     | 0.6223     | 0.4930     | 0.106*    |
| H7C  | 0.5206     | 0.6134     | 0.4528     | 0.106*    |
| C8   | 0.4866 (8) | 0.5612 (5) | 0.5782 (5) | 0.118 (6) |
| H8A  | 0.4314     | 0.5733     | 0.5870     | 0.177*    |
| H8B  | 0.5295     | 0.5764     | 0.6013     | 0.177*    |
| H8C  | 0.4875     | 0.5300     | 0.5878     | 0.177*    |
| C9   | 0.4446 (6) | 0.4508 (3) | 0.5306 (4) | 0.039 (2) |
| H9A  | 0.4422     | 0.4570     | 0.5723     | 0.059*    |
| H9B  | 0.4624     | 0.4206     | 0.5246     | 0.059*    |
| H9C  | 0.3891     | 0.4552     | 0.5130     | 0.059*    |
| C10  | 0.5930 (6) | 0.4686 (4) | 0.5180 (5) | 0.091 (5) |
| H10A | 0.6010     | 0.4370     | 0.5147     | 0.137*    |
| H10B | 0.6064     | 0.4780     | 0.5577     | 0.137*    |
| H10C | 0.6301     | 0.4836     | 0.4907     | 0.137*    |
| C11  | 0.6314 (6) | 0.5454 (3) | 0.4192 (5) | 0.058 (3) |
| H11A | 0.6464     | 0.5645     | 0.3867     | 0.087*    |
| H11B | 0.6646     | 0.5185     | 0.4174     | 0.087*    |
| H11C | 0.6429     | 0.5604     | 0.4560     | 0.087*    |
| C12  | 0.5168 (6) | 0.5193 (3) | 0.3558 (3) | 0.047 (2) |
| H12A | 0.5483     | 0.4929     | 0.3462     | 0.070*    |
| H12B | 0.5294     | 0.5423     | 0.3276     | 0.070*    |
| H12C | 0.4566     | 0.5130     | 0.3547     | 0.070*    |
| C13  | 0.3310 (6) | 0.6770 (3) | 0.3683 (4) | 0.028 (2) |
| H13A | 0.3592     | 0.7053     | 0.3654     | 0.042*    |
| H13B | 0.3416     | 0.6644     | 0.4069     | 0.042*    |
| H13C | 0.2706     | 0.6809     | 0.3625     | 0.042*    |
| C14  | 0.4561 (5) | 0.6414 (3) | 0.3275 (4) | 0.045 (2) |
| H14A | 0.4694     | 0.6202     | 0.3582     | 0.068*    |
| H14B | 0.4824     | 0.6695     | 0.3368     | 0.068*    |
| H14C | 0.4773     | 0.6307     | 0.2903     | 0.068*    |
| C15  | 0.3602 (6) | 0.5341 (2) | 0.2407 (3) | 0.040 (2) |
| H15A | 0.4189     | 0.5254     | 0.2361     | 0.060*    |
| H15B | 0.3281     | 0.5257     | 0.2060     | 0.060*    |
| H15C | 0.3369     | 0.5194     | 0.2748     | 0.060*    |
| C16  | 0.3807 (7) | 0.6064 (3) | 0.1961 (4) | 0.053 (3) |
| H16A | 0.3372     | 0.6038     | 0.1659     | 0.079*    |
| H16B | 0.4337     | 0.5949     | 0.1813     | 0.079*    |
| H16C | 0.3879     | 0.6372     | 0.2067     | 0.079*    |
| C17  | 0.2135 (6) | 0.6723 (3) | 0.2440 (4) | 0.030 (2) |
| H17A | 0.1635     | 0.6891     | 0.2541     | 0.045*    |
| H17B | 0.2125     | 0.6659     | 0.2022     | 0.045*    |
| H17C | 0.2637     | 0.6892     | 0.2537     | 0.045*    |
| C18  | 0.1435 (6) | 0.6006 (3) | 0.2603 (4) | 0.040 (2) |



## supplementary materials

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|      |              |               |               |              |
|------|--------------|---------------|---------------|--------------|
| H18A | 0.1503       | 0.5913        | 0.2198        | 0.059*       |
| H18B | 0.0902       | 0.6161        | 0.2642        | 0.059*       |
| H18C | 0.1440       | 0.5750        | 0.2858        | 0.059*       |
| C19  | 0.0815 (6)   | 0.6584 (3)    | 0.3958 (4)    | 0.028 (2)    |
| H19A | 0.0605       | 0.6847        | 0.4151        | 0.042*       |
| H19B | 0.0990       | 0.6658        | 0.3563        | 0.042*       |
| H19C | 0.1294       | 0.6467        | 0.4178        | 0.042*       |
| C20  | -0.0589 (6)  | 0.6357 (3)    | 0.3549 (4)    | 0.028 (2)    |
| H20A | -0.0394      | 0.6427        | 0.3158        | 0.043*       |
| H20B | -0.0889      | 0.6609        | 0.3709        | 0.043*       |
| H20C | -0.0967      | 0.6105        | 0.3531        | 0.043*       |
| C21  | -0.0621 (5)  | 0.5211 (3)    | 0.3774 (3)    | 0.0266 (19)  |
| H21A | -0.0906      | 0.5351        | 0.3444        | 0.040*       |
| H21B | -0.0908      | 0.4938        | 0.3871        | 0.040*       |
| H21C | -0.0039      | 0.5147        | 0.3670        | 0.040*       |
| C22  | -0.1502 (6)  | 0.5590 (3)    | 0.4516 (4)    | 0.036 (2)    |
| H22A | -0.1761      | 0.5312        | 0.4622        | 0.054*       |
| H22B | -0.1843      | 0.5734        | 0.4216        | 0.054*       |
| H22C | -0.1464      | 0.5779        | 0.4860        | 0.054*       |
| C23  | -0.0389 (7)  | 0.6479 (3)    | 0.5182 (4)    | 0.037 (2)    |
| H23A | -0.0016      | 0.6681        | 0.5390        | 0.055*       |
| H23B | -0.0886      | 0.6423        | 0.5417        | 0.055*       |
| H23C | -0.0561      | 0.6609        | 0.4810        | 0.055*       |
| C24  | 0.0269 (6)   | 0.5802 (3)    | 0.5609 (4)    | 0.032 (2)    |
| H24A | -0.0248      | 0.5707        | 0.5796        | 0.048*       |
| H24B | 0.0595       | 0.5983        | 0.5880        | 0.048*       |
| H24C | 0.0599       | 0.5547        | 0.5497        | 0.048*       |
| Ce2  | 0.24257 (3)  | 0.535742 (13) | 0.950288 (18) | 0.01308 (10) |
| P5   | 0.20715 (14) | 0.42160 (7)   | 1.02711 (9)   | 0.0202 (4)   |
| P6   | 0.47539 (12) | 0.54651 (6)   | 0.99636 (8)   | 0.0175 (4)   |
| P7   | 0.29820 (14) | 0.60994 (7)   | 0.81644 (9)   | 0.0194 (5)   |
| P8   | 0.01721 (14) | 0.58537 (7)   | 0.96084 (10)  | 0.0189 (5)   |
| O11  | 0.2231 (3)   | 0.46756 (17)  | 1.0052 (2)    | 0.0174 (12)  |
| O12  | 0.3910 (3)   | 0.53180 (18)  | 0.9713 (2)    | 0.0202 (12)  |
| O13  | 0.2741 (4)   | 0.58384 (17)  | 0.8699 (2)    | 0.0206 (13)  |
| O14  | 0.0981 (3)   | 0.55967 (17)  | 0.9588 (2)    | 0.0171 (12)  |
| O15  | 0.1644 (4)   | 0.49599 (19)  | 0.8630 (2)    | 0.0217 (13)  |
| O16  | 0.2289 (5)   | 0.4617 (2)    | 0.7912 (3)    | 0.0419 (18)  |
| O17  | 0.2996 (4)   | 0.48047 (19)  | 0.8704 (3)    | 0.0263 (14)  |
| O18  | 0.2526 (4)   | 0.61465 (19)  | 0.9986 (2)    | 0.0222 (13)  |
| O19  | 0.2197 (5)   | 0.6304 (2)    | 1.0894 (3)    | 0.0455 (19)  |
| O20  | 0.2350 (4)   | 0.56068 (19)  | 1.0601 (2)    | 0.0253 (14)  |
| N15  | 0.1153 (4)   | 0.4051 (2)    | 0.9990 (3)    | 0.0306 (16)  |
| N16  | 0.2127 (4)   | 0.4222 (2)    | 1.1000 (3)    | 0.0289 (16)  |
| N17  | 0.2739 (4)   | 0.3827 (2)    | 1.0084 (3)    | 0.0280 (16)  |
| N18  | 0.4782 (4)   | 0.53218 (19)  | 1.0668 (3)    | 0.0236 (14)  |
| N19  | 0.5490 (4)   | 0.5231 (2)    | 0.9568 (3)    | 0.0342 (17)  |
| N20  | 0.4982 (5)   | 0.5995 (2)    | 0.9978 (3)    | 0.0222 (15)  |
| N21  | 0.3564 (5)   | 0.5802 (2)    | 0.7727 (3)    | 0.0318 (18)  |

|      |             |            |            |             |
|------|-------------|------------|------------|-------------|
| N22  | 0.3521 (5)  | 0.6546 (2) | 0.8353 (3) | 0.0258 (17) |
| N23  | 0.2106 (5)  | 0.6241 (2) | 0.7809 (3) | 0.0306 (18) |
| N24  | 0.0151 (4)  | 0.6245 (2) | 0.9105 (3) | 0.0226 (16) |
| N25  | -0.0618 (4) | 0.5506 (2) | 0.9497 (3) | 0.0275 (17) |
| N26  | 0.0065 (5)  | 0.6085 (2) | 1.0263 (3) | 0.0234 (16) |
| N27  | 0.2304 (5)  | 0.4792 (2) | 0.8397 (3) | 0.0286 (18) |
| N28  | 0.2359 (5)  | 0.6021 (3) | 1.0508 (3) | 0.0317 (19) |
| C25  | 0.0494 (5)  | 0.4383 (3) | 0.9877 (4) | 0.036 (2)   |
| H25A | 0.0289      | 0.4497     | 1.0248     | 0.054*      |
| H25B | 0.0029      | 0.4249     | 0.9660     | 0.054*      |
| H25C | 0.0729      | 0.4623     | 0.9648     | 0.054*      |
| C26  | 0.0806 (6)  | 0.3608 (3) | 1.0119 (5) | 0.059 (3)   |
| H26A | 0.0462      | 0.3509     | 0.9790     | 0.089*      |
| H26B | 0.0461      | 0.3623     | 1.0469     | 0.089*      |
| H26C | 0.1268      | 0.3402     | 1.0183     | 0.089*      |
| C27  | 0.1935 (6)  | 0.3819 (3) | 1.1343 (4) | 0.043 (2)   |
| H27A | 0.1333      | 0.3807     | 1.1421     | 0.065*      |
| H27B | 0.2247      | 0.3826     | 1.1711     | 0.065*      |
| H27C | 0.2100      | 0.3561     | 1.1120     | 0.065*      |
| C28  | 0.1960 (7)  | 0.4630 (3) | 1.1334 (4) | 0.041 (2)   |
| H28A | 0.2343      | 0.4646     | 1.1668     | 0.062*      |
| H28B | 0.1380      | 0.4628     | 1.1470     | 0.062*      |
| H28C | 0.2047      | 0.4883     | 1.1082     | 0.062*      |
| C29  | 0.3532 (6)  | 0.3732 (3) | 1.0395 (4) | 0.044 (2)   |
| H29A | 0.3994      | 0.3881     | 1.0200     | 0.066*      |
| H29B | 0.3633      | 0.3416     | 1.0393     | 0.066*      |
| H29C | 0.3494      | 0.3835     | 1.0797     | 0.066*      |
| C30  | 0.2786 (7)  | 0.3677 (4) | 0.9459 (4) | 0.068 (3)   |
| H30A | 0.2992      | 0.3376     | 0.9446     | 0.102*      |
| H30B | 0.3169      | 0.3868     | 0.9245     | 0.102*      |
| H30C | 0.2227      | 0.3691     | 0.9280     | 0.102*      |
| C31  | 0.4357 (5)  | 0.4912 (3) | 1.0834 (3) | 0.033 (2)   |
| H31A | 0.4236      | 0.4918     | 1.1251     | 0.050*      |
| H31B | 0.4721      | 0.4663     | 1.0748     | 0.050*      |
| H31C | 0.3832      | 0.4884     | 1.0613     | 0.050*      |
| C32  | 0.5563 (5)  | 0.5394 (3) | 1.1024 (3) | 0.038 (2)   |
| H32A | 0.5993      | 0.5184     | 1.0906     | 0.057*      |
| H32B | 0.5437      | 0.5352     | 1.1437     | 0.057*      |
| H32C | 0.5767      | 0.5691     | 1.0963     | 0.057*      |
| C33  | 0.5327 (5)  | 0.4895 (3) | 0.9126 (4) | 0.042 (2)   |
| H33A | 0.5593      | 0.4620     | 0.9245     | 0.062*      |
| H33B | 0.5557      | 0.4989     | 0.8753     | 0.062*      |
| H33C | 0.4721      | 0.4851     | 0.9084     | 0.062*      |
| C34  | 0.6399 (5)  | 0.5338 (3) | 0.9642 (4) | 0.050 (3)   |
| H34A | 0.6644      | 0.5397     | 0.9260     | 0.075*      |
| H34B | 0.6689      | 0.5090     | 0.9823     | 0.075*      |
| H34C | 0.6460      | 0.5596     | 0.9890     | 0.075*      |
| C35  | 0.4626 (5)  | 0.6289 (2) | 1.0424 (4) | 0.032 (2)   |
| H35A | 0.4107      | 0.6420     | 1.0274     | 0.049*      |

## supplementary materials

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|      |             |            |            |           |
|------|-------------|------------|------------|-----------|
| H35B | 0.5030      | 0.6520     | 1.0516     | 0.049*    |
| H35C | 0.4506      | 0.6121     | 1.0776     | 0.049*    |
| C36  | 0.5230 (6)  | 0.6220 (3) | 0.9422 (4) | 0.043 (3) |
| H36A | 0.5594      | 0.6469     | 0.9514     | 0.065*    |
| H36B | 0.4726      | 0.6324     | 0.9218     | 0.065*    |
| H36C | 0.5530      | 0.6014     | 0.9174     | 0.065*    |
| C37  | 0.4301 (6)  | 0.5572 (3) | 0.7973 (4) | 0.053 (3) |
| H37A | 0.4815      | 0.5718     | 0.7847     | 0.079*    |
| H37B | 0.4303      | 0.5269     | 0.7838     | 0.079*    |
| H37C | 0.4275      | 0.5577     | 0.8399     | 0.079*    |
| C38  | 0.3534 (8)  | 0.5825 (4) | 0.7079 (4) | 0.064 (3) |
| H38A | 0.3500      | 0.5529     | 0.6918     | 0.095*    |
| H38B | 0.4042      | 0.5968     | 0.6937     | 0.095*    |
| H38C | 0.3041      | 0.5993     | 0.6955     | 0.095*    |
| C39  | 0.4142 (6)  | 0.6760 (3) | 0.7968 (4) | 0.044 (3) |
| H39A | 0.4643      | 0.6836     | 0.8195     | 0.066*    |
| H39B | 0.3897      | 0.7025     | 0.7800     | 0.066*    |
| H39C | 0.4295      | 0.6559     | 0.7655     | 0.066*    |
| C40  | 0.3224 (6)  | 0.6819 (3) | 0.8827 (4) | 0.037 (2) |
| H40A | 0.2920      | 0.7070     | 0.8667     | 0.055*    |
| H40B | 0.3703      | 0.6921     | 0.9058     | 0.055*    |
| H40C | 0.2850      | 0.6648     | 0.9074     | 0.055*    |
| C41  | 0.1994 (6)  | 0.6669 (3) | 0.7506 (4) | 0.038 (2) |
| H41A | 0.1473      | 0.6806     | 0.7635     | 0.057*    |
| H41B | 0.1967      | 0.6621     | 0.7085     | 0.057*    |
| H41C | 0.2468      | 0.6860     | 0.7599     | 0.057*    |
| C42  | 0.1428 (7)  | 0.5918 (3) | 0.7673 (5) | 0.050 (3) |
| H42A | 0.1355      | 0.5896     | 0.7250     | 0.075*    |
| H42B | 0.0903      | 0.6015     | 0.7848     | 0.075*    |
| H42C | 0.1584      | 0.5631     | 0.7830     | 0.075*    |
| C43  | 0.0837 (6)  | 0.6568 (3) | 0.9081 (4) | 0.030 (2) |
| H43A | 0.0622      | 0.6857     | 0.9186     | 0.044*    |
| H43B | 0.1063      | 0.6578     | 0.8687     | 0.044*    |
| H43C | 0.1282      | 0.6484     | 0.9355     | 0.044*    |
| C44  | -0.0613 (7) | 0.6356 (3) | 0.8744 (5) | 0.045 (3) |
| H44A | -0.0445     | 0.6414     | 0.8343     | 0.067*    |
| H44B | -0.0882     | 0.6617     | 0.8904     | 0.067*    |
| H44C | -0.1007     | 0.6111     | 0.8751     | 0.067*    |
| C45  | -0.0586 (6) | 0.5189 (3) | 0.9002 (4) | 0.033 (2) |
| H45A | -0.0893     | 0.5309     | 0.8668     | 0.050*    |
| H45B | -0.0841     | 0.4912     | 0.9120     | 0.050*    |
| H45C | -0.0001     | 0.5139     | 0.8895     | 0.050*    |
| C46  | -0.1475 (6) | 0.5588 (4) | 0.9741 (5) | 0.046 (3) |
| H46A | -0.1706     | 0.5314     | 0.9890     | 0.069*    |
| H46B | -0.1843     | 0.5703     | 0.9435     | 0.069*    |
| H46C | -0.1433     | 0.5801     | 1.0059     | 0.069*    |
| C47  | -0.0318 (7) | 0.6524 (4) | 1.0354 (5) | 0.052 (3) |
| H47A | 0.0052      | 0.6701     | 1.0602     | 0.077*    |
| H47B | -0.0863     | 0.6491     | 1.0542     | 0.077*    |

|      |              |               |               |              |
|------|--------------|---------------|---------------|--------------|
| H47C | -0.0394      | 0.6669        | 0.9977        | 0.077*       |
| C48  | 0.0185 (7)   | 0.5820 (4)    | 1.0791 (4)    | 0.041 (3)    |
| H48A | -0.0361      | 0.5721        | 1.0931        | 0.061*       |
| H48B | 0.0461       | 0.5996        | 1.1092        | 0.061*       |
| H48C | 0.0534       | 0.5566        | 1.0700        | 0.061*       |
| Ce3  | 0.23763 (3)  | 0.863346 (13) | 0.686301 (18) | 0.01293 (10) |
| P9   | 0.01473 (14) | 0.80796 (7)   | 0.69531 (10)  | 0.0180 (5)   |
| P10  | 0.29502 (15) | 0.78355 (7)   | 0.55792 (9)   | 0.0196 (5)   |
| P11  | 0.47679 (12) | 0.86406 (7)   | 0.72080 (8)   | 0.0199 (4)   |
| P12  | 0.17030 (13) | 0.96496 (6)   | 0.78115 (9)   | 0.0179 (4)   |
| O21  | 0.0972 (4)   | 0.83402 (17)  | 0.6931 (2)    | 0.0201 (12)  |
| O22  | 0.2730 (4)   | 0.81275 (17)  | 0.6093 (2)    | 0.0233 (13)  |
| O23  | 0.3859 (3)   | 0.87277 (18)  | 0.7014 (2)    | 0.0210 (12)  |
| O24  | 0.2046 (3)   | 0.93110 (17)  | 0.7384 (2)    | 0.0194 (13)  |
| O25  | 0.1551 (4)   | 0.90120 (18)  | 0.5999 (2)    | 0.0234 (13)  |
| O26  | 0.2086 (4)   | 0.9464 (2)    | 0.5346 (3)    | 0.0366 (17)  |
| O27  | 0.2877 (4)   | 0.9215 (2)    | 0.6084 (3)    | 0.0260 (14)  |
| O28  | 0.2624 (4)   | 0.78910 (18)  | 0.7428 (3)    | 0.0235 (14)  |
| O29  | 0.2364 (5)   | 0.7803 (2)    | 0.8374 (3)    | 0.052 (2)    |
| O30  | 0.2351 (4)   | 0.8463 (2)    | 0.7985 (3)    | 0.0290 (15)  |
| N29  | 0.0034 (5)   | 0.7856 (2)    | 0.7597 (3)    | 0.0217 (16)  |
| N30  | 0.0141 (4)   | 0.7679 (2)    | 0.6462 (3)    | 0.0227 (16)  |
| N31  | -0.0664 (4)  | 0.8413 (2)    | 0.6819 (3)    | 0.0210 (15)  |
| N32  | 0.3498 (5)   | 0.7412 (2)    | 0.5819 (3)    | 0.0259 (17)  |
| N33  | 0.2078 (5)   | 0.7666 (2)    | 0.5247 (3)    | 0.0267 (17)  |
| N34  | 0.3529 (5)   | 0.8096 (2)    | 0.5093 (3)    | 0.0316 (18)  |
| N35  | 0.4986 (4)   | 0.8159 (2)    | 0.7492 (3)    | 0.0243 (15)  |
| N36  | 0.5008 (4)   | 0.9005 (2)    | 0.7721 (3)    | 0.0343 (17)  |
| N37  | 0.5401 (4)   | 0.8667 (2)    | 0.6626 (3)    | 0.0224 (14)  |
| N38  | 0.1737 (4)   | 0.9510 (2)    | 0.8517 (3)    | 0.0273 (16)  |
| N39  | 0.2289 (4)   | 1.01016 (19)  | 0.7791 (3)    | 0.0248 (15)  |
| N40  | 0.0708 (4)   | 0.9750 (2)    | 0.7634 (3)    | 0.0214 (15)  |
| N41  | 0.2181 (4)   | 0.9240 (2)    | 0.5799 (3)    | 0.0197 (15)  |
| N42  | 0.2433 (5)   | 0.8031 (2)    | 0.7939 (3)    | 0.0237 (17)  |
| C49  | 0.0221 (7)   | 0.8101 (3)    | 0.8150 (4)    | 0.038 (2)    |
| H49A | 0.0658       | 0.7947        | 0.8370        | 0.057*       |
| H49B | -0.0288      | 0.8119        | 0.8383        | 0.057*       |
| H49C | 0.0415       | 0.8396        | 0.8055        | 0.057*       |
| C50  | -0.0419 (6)  | 0.7440 (3)    | 0.7722 (4)    | 0.032 (2)    |
| H50A | -0.0943      | 0.7506        | 0.7922        | 0.048*       |
| H50B | -0.0067      | 0.7254        | 0.7970        | 0.048*       |
| H50C | -0.0543      | 0.7288        | 0.7357        | 0.048*       |
| C51  | 0.0822 (6)   | 0.7340 (3)    | 0.6479 (4)    | 0.026 (2)    |
| H51A | 0.1076       | 0.7316        | 0.6095        | 0.039*       |
| H51B | 0.0581       | 0.7057        | 0.6589        | 0.039*       |
| H51C | 0.1250       | 0.7425        | 0.6766        | 0.039*       |
| C52  | -0.0576 (6)  | 0.7556 (3)    | 0.6091 (4)    | 0.030 (2)    |
| H52A | -0.0774      | 0.7265        | 0.6202        | 0.045*       |
| H52B | -0.0402      | 0.7552        | 0.5683        | 0.045*       |

## supplementary materials

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|      |             |            |            |           |
|------|-------------|------------|------------|-----------|
| H52C | -0.1028     | 0.7769     | 0.6139     | 0.045*    |
| C53  | -0.1515 (5) | 0.8334 (3) | 0.7045 (4) | 0.028 (2) |
| H53A | -0.1845     | 0.8171     | 0.6756     | 0.043*    |
| H53B | -0.1788     | 0.8615     | 0.7123     | 0.043*    |
| H53C | -0.1477     | 0.8165     | 0.7406     | 0.043*    |
| C54  | -0.0633 (5) | 0.8695 (3) | 0.6286 (3) | 0.030 (2) |
| H54A | -0.0912     | 0.8974     | 0.6365     | 0.044*    |
| H54B | -0.0919     | 0.8547     | 0.5963     | 0.044*    |
| H54C | -0.0048     | 0.8749     | 0.6183     | 0.044*    |
| C55  | 0.4142 (6)  | 0.7175 (3) | 0.5472 (4) | 0.057 (3) |
| H55A | 0.3894      | 0.6911     | 0.5304     | 0.085*    |
| H55B | 0.4614      | 0.7095     | 0.5726     | 0.085*    |
| H55C | 0.4341      | 0.7365     | 0.5160     | 0.085*    |
| C56  | 0.3221 (6)  | 0.7151 (3) | 0.6343 (3) | 0.027 (2) |
| H56A | 0.3710      | 0.7013     | 0.6528     | 0.040*    |
| H56B | 0.2823      | 0.6925     | 0.6219     | 0.040*    |
| H56C | 0.2951      | 0.7346     | 0.6622     | 0.040*    |
| C57  | 0.2000 (7)  | 0.7238 (3) | 0.4941 (4) | 0.039 (2) |
| H57A | 0.2013      | 0.7285     | 0.4520     | 0.058*    |
| H57B | 0.1470      | 0.7099     | 0.5045     | 0.058*    |
| H57C | 0.2468      | 0.7048     | 0.5056     | 0.058*    |
| C58  | 0.1435 (6)  | 0.7986 (3) | 0.5087 (4) | 0.041 (3) |
| H58A | 0.0883      | 0.7876     | 0.5200     | 0.061*    |
| H58B | 0.1443      | 0.8034     | 0.4666     | 0.061*    |
| H58C | 0.1547      | 0.8262     | 0.5289     | 0.061*    |
| C59  | 0.3469 (7)  | 0.8029 (4) | 0.4453 (4) | 0.065 (4) |
| H59A | 0.3966      | 0.7872     | 0.4319     | 0.097*    |
| H59B | 0.3434      | 0.8313     | 0.4258     | 0.097*    |
| H59C | 0.2967      | 0.7858     | 0.4360     | 0.097*    |
| C60  | 0.4314 (7)  | 0.8317 (4) | 0.5298 (4) | 0.071 (4) |
| H60A | 0.4360      | 0.8604     | 0.5112     | 0.106*    |
| H60B | 0.4799      | 0.8138     | 0.5196     | 0.106*    |
| H60C | 0.4296      | 0.8354     | 0.5721     | 0.106*    |
| C61  | 0.4952 (6)  | 0.7753 (3) | 0.7119 (4) | 0.036 (2) |
| H61A | 0.4382      | 0.7635     | 0.7118     | 0.054*    |
| H61B | 0.5341      | 0.7534     | 0.7276     | 0.054*    |
| H61C | 0.5111      | 0.7826     | 0.6720     | 0.054*    |
| C62  | 0.4790 (6)  | 0.8062 (3) | 0.8113 (3) | 0.046 (2) |
| H62A | 0.5185      | 0.7844     | 0.8263     | 0.069*    |
| H62B | 0.4218      | 0.7948     | 0.8139     | 0.069*    |
| H62C | 0.4838      | 0.8331     | 0.8342     | 0.069*    |
| C63  | 0.5904 (6)  | 0.9043 (3) | 0.7933 (5) | 0.066 (3) |
| H63A | 0.5913      | 0.9076     | 0.8357     | 0.099*    |
| H63B | 0.6167      | 0.9299     | 0.7755     | 0.099*    |
| H63C | 0.6214      | 0.8779     | 0.7826     | 0.099*    |
| C64  | 0.4474 (6)  | 0.9357 (3) | 0.7886 (5) | 0.066 (3) |
| H64A | 0.4689      | 0.9631     | 0.7725     | 0.098*    |
| H64B | 0.4459      | 0.9378     | 0.8311     | 0.098*    |
| H64C | 0.3907      | 0.9305     | 0.7735     | 0.098*    |

|      |              |               |               |              |
|------|--------------|---------------|---------------|--------------|
| C65  | 0.6288 (5)   | 0.8505 (3)    | 0.6650 (4)    | 0.0317 (19)  |
| H65A | 0.6672       | 0.8755        | 0.6647        | 0.048*       |
| H65B | 0.6395       | 0.8320        | 0.6311        | 0.048*       |
| H65C | 0.6377       | 0.8336        | 0.7006        | 0.048*       |
| C66  | 0.5280 (5)   | 0.9029 (2)    | 0.6201 (3)    | 0.0290 (18)  |
| H66A | 0.5428       | 0.8928        | 0.5811        | 0.043*       |
| H66B | 0.5639       | 0.9276        | 0.6311        | 0.043*       |
| H66C | 0.4693       | 0.9122        | 0.6202        | 0.043*       |
| C67  | 0.1048 (6)   | 0.9256 (3)    | 0.8791 (4)    | 0.049 (3)    |
| H67A | 0.1037       | 0.9318        | 0.9209        | 0.074*       |
| H67B | 0.1143       | 0.8943        | 0.8730        | 0.074*       |
| H67C | 0.0511       | 0.9340        | 0.8614        | 0.074*       |
| C68  | 0.2561 (6)   | 0.9414 (3)    | 0.8794 (4)    | 0.044 (2)    |
| H68A | 0.2700       | 0.9106        | 0.8736        | 0.066*       |
| H68B | 0.2534       | 0.9476        | 0.9211        | 0.066*       |
| H68C | 0.2993       | 0.9597        | 0.8617        | 0.066*       |
| C69  | 0.2304 (6)   | 1.0442 (3)    | 0.8258 (4)    | 0.041 (2)    |
| H69A | 0.1946       | 1.0687        | 0.8142        | 0.061*       |
| H69B | 0.2879       | 1.0545        | 0.8318        | 0.061*       |
| H69C | 0.2095       | 1.0315        | 0.8620        | 0.061*       |
| C70  | 0.2677 (6)   | 1.0235 (3)    | 0.7241 (4)    | 0.042 (2)    |
| H70A | 0.3254       | 1.0330        | 0.7316        | 0.063*       |
| H70B | 0.2357       | 1.0476        | 0.7069        | 0.063*       |
| H70C | 0.2678       | 0.9987        | 0.6971        | 0.063*       |
| C71  | 0.0247 (6)   | 1.0142 (3)    | 0.7858 (4)    | 0.043 (2)    |
| H71A | 0.0027       | 1.0078        | 0.8245        | 0.065*       |
| H71B | -0.0218      | 1.0212        | 0.7593        | 0.065*       |
| H71C | 0.0631       | 1.0391        | 0.7882        | 0.065*       |
| C72  | 0.0136 (5)   | 0.9415 (3)    | 0.7384 (4)    | 0.034 (2)    |
| H72A | -0.0250      | 0.9553        | 0.7106        | 0.052*       |
| H72B | -0.0184      | 0.9278        | 0.7697        | 0.052*       |
| H72C | 0.0465       | 0.9191        | 0.7183        | 0.052*       |
| Ce4  | 0.23742 (3)  | 0.868253 (13) | 0.200816 (19) | 0.01393 (10) |
| P13  | 0.20401 (14) | 0.98002 (7)   | 0.28357 (9)   | 0.0198 (4)   |
| P14  | 0.46704 (12) | 0.85359 (6)   | 0.25212 (8)   | 0.0172 (4)   |
| P15  | 0.30069 (14) | 0.80210 (7)   | 0.06128 (9)   | 0.0204 (5)   |
| P16  | 0.01329 (14) | 0.81818 (7)   | 0.20925 (9)   | 0.0180 (5)   |
| O31  | 0.2193 (4)   | 0.93515 (18)  | 0.2576 (2)    | 0.0232 (13)  |
| O32  | 0.3845 (3)   | 0.86956 (18)  | 0.2254 (2)    | 0.0227 (13)  |
| O33  | 0.2713 (4)   | 0.82408 (18)  | 0.1174 (2)    | 0.0238 (14)  |
| O34  | 0.0944 (4)   | 0.84516 (17)  | 0.2086 (2)    | 0.0244 (13)  |
| O35  | 0.1552 (4)   | 0.9083 (2)    | 0.1148 (3)    | 0.0276 (14)  |
| O36  | 0.2185 (5)   | 0.9425 (2)    | 0.0417 (3)    | 0.0413 (18)  |
| O37  | 0.2903 (4)   | 0.9268 (2)    | 0.1230 (3)    | 0.0278 (15)  |
| O38  | 0.2289 (4)   | 0.83921 (18)  | 0.3096 (3)    | 0.0258 (14)  |
| O39  | 0.2178 (4)   | 0.76932 (19)  | 0.3336 (3)    | 0.0328 (16)  |
| O40  | 0.2506 (4)   | 0.78833 (18)  | 0.2426 (3)    | 0.0251 (14)  |
| N43  | 0.1124 (4)   | 0.9982 (2)    | 0.2576 (3)    | 0.0242 (15)  |
| N44  | 0.2709 (4)   | 1.0200 (2)    | 0.2678 (3)    | 0.0257 (16)  |

## supplementary materials

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|      |             |            |            |             |
|------|-------------|------------|------------|-------------|
| N45  | 0.2122 (4)  | 0.9760 (2) | 0.3557 (3) | 0.0266 (15) |
| N46  | 0.4608 (4)  | 0.8605 (2) | 0.3254 (2) | 0.0235 (14) |
| N47  | 0.5449 (4)  | 0.8810 (2) | 0.2212 (3) | 0.0273 (15) |
| N48  | 0.4928 (4)  | 0.8018 (2) | 0.2459 (3) | 0.0220 (15) |
| N49  | 0.3577 (4)  | 0.8364 (2) | 0.0225 (3) | 0.0328 (17) |
| N50  | 0.3590 (5)  | 0.7588 (2) | 0.0769 (3) | 0.0227 (16) |
| N51  | 0.2195 (5)  | 0.7862 (2) | 0.0203 (3) | 0.0338 (19) |
| N52  | 0.0059 (5)  | 0.7919 (2) | 0.2716 (3) | 0.0261 (17) |
| N53  | 0.0128 (4)  | 0.7823 (2) | 0.1551 (3) | 0.0212 (16) |
| N54  | -0.0679 (4) | 0.8521 (2) | 0.2019 (3) | 0.0242 (16) |
| N55  | 0.2231 (5)  | 0.9268 (2) | 0.0919 (3) | 0.0220 (16) |
| N56  | 0.2327 (4)  | 0.7973 (2) | 0.2963 (3) | 0.0195 (16) |
| C73  | 0.0469 (5)  | 0.9664 (3) | 0.2382 (4) | 0.029 (2)   |
| H73A | 0.0037      | 0.9817     | 0.2156     | 0.043*      |
| H73B | 0.0214      | 0.9527     | 0.2722     | 0.043*      |
| H73C | 0.0726      | 0.9438     | 0.2140     | 0.043*      |
| C74  | 0.0762 (6)  | 1.0408 (3) | 0.2769 (4) | 0.041 (2)   |
| H74A | 0.0372      | 1.0357     | 0.3088     | 0.062*      |
| H74B | 0.0462      | 1.0544     | 0.2442     | 0.062*      |
| H74C | 0.1213      | 1.0601     | 0.2901     | 0.062*      |
| C75  | 0.2670 (7)  | 1.0431 (4) | 0.2111 (4) | 0.059 (3)   |
| H75A | 0.3034      | 1.0283     | 0.1833     | 0.089*      |
| H75B | 0.2859      | 1.0733     | 0.2163     | 0.089*      |
| H75C | 0.2093      | 1.0429     | 0.1964     | 0.089*      |
| C76  | 0.3560 (6)  | 1.0217 (3) | 0.2958 (4) | 0.047 (2)   |
| H76A | 0.3735      | 1.0522     | 0.3001     | 0.070*      |
| H76B | 0.3963      | 1.0061     | 0.2716     | 0.070*      |
| H76C | 0.3538      | 1.0080     | 0.3343     | 0.070*      |
| C77  | 0.2023 (6)  | 1.0147 (3) | 0.3949 (3) | 0.041 (2)   |
| H77A | 0.2377      | 1.0110     | 0.4295     | 0.062*      |
| H77B | 0.1436      | 1.0173     | 0.4065     | 0.062*      |
| H77C | 0.2191      | 1.0412     | 0.3742     | 0.062*      |
| C78  | 0.1899 (6)  | 0.9336 (3) | 0.3846 (4) | 0.034 (2)   |
| H78A | 0.1314      | 0.9345     | 0.3969     | 0.051*      |
| H78B | 0.2263      | 0.9291     | 0.4186     | 0.051*      |
| H78C | 0.1977      | 0.9095     | 0.3571     | 0.051*      |
| C79  | 0.4155 (5)  | 0.9006 (2) | 0.3460 (3) | 0.032 (2)   |
| H79A | 0.4510      | 0.9263     | 0.3403     | 0.049*      |
| H79B | 0.4026      | 0.8975     | 0.3874     | 0.049*      |
| H79C | 0.3633      | 0.9041     | 0.3237     | 0.049*      |
| C80  | 0.5369 (5)  | 0.8506 (2) | 0.3618 (3) | 0.0275 (18) |
| H80A | 0.5202      | 0.8458     | 0.4022     | 0.041*      |
| H80B | 0.5761      | 0.8752     | 0.3600     | 0.041*      |
| H80C | 0.5642      | 0.8242     | 0.3469     | 0.041*      |
| C81  | 0.5308 (6)  | 0.9233 (3) | 0.1934 (6) | 0.091 (5)   |
| H81A | 0.5648      | 0.9254     | 0.1583     | 0.136*      |
| H81B | 0.5467      | 0.9467     | 0.2204     | 0.136*      |
| H81C | 0.4715      | 0.9262     | 0.1829     | 0.136*      |
| C82  | 0.6350 (5)  | 0.8702 (3) | 0.2298 (4) | 0.039 (2)   |

|      |             |            |             |             |
|------|-------------|------------|-------------|-------------|
| H82A | 0.6617      | 0.8929     | 0.2538      | 0.058*      |
| H82B | 0.6627      | 0.8688     | 0.1920      | 0.058*      |
| H82C | 0.6401      | 0.8420     | 0.2495      | 0.058*      |
| C83  | 0.5227 (6)  | 0.7853 (3) | 0.1878 (4)  | 0.038 (2)   |
| H83A | 0.4757      | 0.7721     | 0.1664      | 0.057*      |
| H83B | 0.5665      | 0.7633     | 0.1939      | 0.057*      |
| H83C | 0.5454      | 0.8097     | 0.1653      | 0.057*      |
| C84  | 0.4576 (5)  | 0.7669 (3) | 0.2838 (4)  | 0.0322 (19) |
| H84A | 0.5020      | 0.7462     | 0.2944      | 0.048*      |
| H84B | 0.4128      | 0.7516     | 0.2629      | 0.048*      |
| H84C | 0.4351      | 0.7802     | 0.3192      | 0.048*      |
| C85  | 0.4271 (6)  | 0.8621 (3) | 0.0514 (4)  | 0.050 (3)   |
| H85A | 0.4231      | 0.8928     | 0.0397      | 0.074*      |
| H85B | 0.4814      | 0.8502     | 0.0395      | 0.074*      |
| H85C | 0.4219      | 0.8599     | 0.0937      | 0.074*      |
| C86  | 0.3654 (7)  | 0.8349 (4) | -0.0419 (4) | 0.064 (3)   |
| H86A | 0.4149      | 0.8178     | -0.0523     | 0.096*      |
| H86B | 0.3709      | 0.8646     | -0.0571     | 0.096*      |
| H86C | 0.3153      | 0.8212     | -0.0588     | 0.096*      |
| C87  | 0.4330 (5)  | 0.7455 (3) | 0.0402 (4)  | 0.038 (2)   |
| H87A | 0.4135      | 0.7269     | 0.0081      | 0.057*      |
| H87B | 0.4734      | 0.7293     | 0.0642      | 0.057*      |
| H87C | 0.4598      | 0.7716     | 0.0244      | 0.057*      |
| C88  | 0.3298 (6)  | 0.7254 (3) | 0.1196 (4)  | 0.034 (2)   |
| H88A | 0.3780      | 0.7137     | 0.1412      | 0.051*      |
| H88B | 0.3015      | 0.7015     | 0.0988      | 0.051*      |
| H88C | 0.2906      | 0.7389     | 0.1468      | 0.051*      |
| C89  | 0.1507 (7)  | 0.8183 (4) | 0.0084 (5)  | 0.056 (3)   |
| H89A | 0.0963      | 0.8041     | 0.0136      | 0.084*      |
| H89B | 0.1550      | 0.8290     | -0.0316     | 0.084*      |
| H89C | 0.1557      | 0.8429     | 0.0355      | 0.084*      |
| C90  | 0.2130 (7)  | 0.7446 (3) | -0.0109 (4) | 0.043 (3)   |
| H90A | 0.2112      | 0.7502     | -0.0529     | 0.064*      |
| H90B | 0.1616      | 0.7295     | 0.0006      | 0.064*      |
| H90C | 0.2616      | 0.7264     | -0.0015     | 0.064*      |
| C91  | -0.0344 (7) | 0.7471 (3) | 0.2791 (4)  | 0.038 (3)   |
| H91A | -0.0888     | 0.7504     | 0.2981      | 0.058*      |
| H91B | 0.0021      | 0.7286     | 0.3031      | 0.058*      |
| H91C | -0.0425     | 0.7335     | 0.2408      | 0.058*      |
| C92  | 0.0140 (7)  | 0.8152 (4) | 0.3277 (4)  | 0.045 (3)   |
| H92A | 0.0532      | 0.7994     | 0.3531      | 0.068*      |
| H92B | -0.0409     | 0.8168     | 0.3463      | 0.068*      |
| H92C | 0.0352      | 0.8448     | 0.3209      | 0.068*      |
| C93  | 0.0824 (6)  | 0.7501 (3) | 0.1500 (4)  | 0.040 (3)   |
| H93A | 0.1067      | 0.7521     | 0.1111      | 0.060*      |
| H93B | 0.0606      | 0.7206     | 0.1562      | 0.060*      |
| H93C | 0.1255      | 0.7565     | 0.1793      | 0.060*      |
| C94  | -0.0619 (6) | 0.7700 (3) | 0.1196 (4)  | 0.033 (2)   |
| H94A | -0.0814     | 0.7410     | 0.1314      | 0.049*      |



## supplementary materials

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|      |             |            |            |           |
|------|-------------|------------|------------|-----------|
| H94B | -0.0468     | 0.7694     | 0.0784     | 0.049*    |
| H94C | -0.1066     | 0.7914     | 0.1256     | 0.049*    |
| C95  | -0.1524 (5) | 0.8425 (3) | 0.2243 (4) | 0.040 (3) |
| H95A | -0.1882     | 0.8320     | 0.1924     | 0.060*    |
| H95B | -0.1765     | 0.8692     | 0.2407     | 0.060*    |
| H95C | -0.1485     | 0.8200     | 0.2545     | 0.060*    |
| C96  | -0.0648 (5) | 0.8879 (3) | 0.1576 (4) | 0.038 (2) |
| H96A | -0.0902     | 0.9144     | 0.1737     | 0.056*    |
| H96B | -0.0958     | 0.8790     | 0.1226     | 0.056*    |
| H96C | -0.0064     | 0.8939     | 0.1476     | 0.056*    |

### Atomic displacement parameters ( $\text{\AA}^2$ )

|     | $U^{11}$     | $U^{22}$     | $U^{33}$     | $U^{12}$      | $U^{13}$      | $U^{23}$      |
|-----|--------------|--------------|--------------|---------------|---------------|---------------|
| W1  | 0.01705 (18) | 0.01836 (19) | 0.01421 (16) | -0.00015 (12) | 0.00113 (13)  | -0.00098 (13) |
| W2  | 0.01651 (18) | 0.02086 (19) | 0.01315 (16) | 0.00243 (13)  | 0.00137 (13)  | 0.00264 (13)  |
| W3  | 0.01681 (18) | 0.01789 (19) | 0.01512 (17) | -0.00130 (12) | 0.00127 (13)  | -0.00188 (13) |
| W4  | 0.01607 (18) | 0.01805 (19) | 0.01398 (16) | -0.00043 (12) | 0.00208 (13)  | 0.00047 (13)  |
| Ag1 | 0.0426 (5)   | 0.0317 (4)   | 0.0156 (3)   | 0.0019 (3)    | 0.0014 (3)    | 0.0021 (3)    |
| Ag2 | 0.0432 (5)   | 0.0348 (4)   | 0.0155 (3)   | 0.0027 (3)    | 0.0013 (3)    | -0.0010 (3)   |
| Ag3 | 0.0446 (5)   | 0.0320 (4)   | 0.0154 (3)   | -0.0002 (3)   | 0.0013 (3)    | 0.0000 (3)    |
| Ag4 | 0.0462 (5)   | 0.0337 (4)   | 0.0150 (3)   | -0.0002 (3)   | 0.0013 (3)    | -0.0017 (3)   |
| S1  | 0.0197 (12)  | 0.0375 (12)  | 0.0225 (11)  | -0.0053 (9)   | 0.0052 (9)    | -0.0048 (10)  |
| S2  | 0.0213 (12)  | 0.0328 (11)  | 0.0191 (10)  | 0.0025 (9)    | -0.0006 (8)   | 0.0004 (9)    |
| S3  | 0.0328 (13)  | 0.0169 (10)  | 0.0224 (11)  | 0.0026 (9)    | 0.0010 (9)    | -0.0014 (9)   |
| S4  | 0.0275 (13)  | 0.0220 (11)  | 0.0204 (11)  | 0.0015 (9)    | -0.0002 (9)   | -0.0053 (9)   |
| S5  | 0.0196 (12)  | 0.0491 (14)  | 0.0226 (11)  | 0.0073 (10)   | 0.0047 (9)    | 0.0046 (11)   |
| S6  | 0.0196 (12)  | 0.0343 (12)  | 0.0247 (11)  | 0.0004 (9)    | -0.0025 (9)   | 0.0025 (10)   |
| S7  | 0.0307 (13)  | 0.0216 (10)  | 0.0188 (10)  | 0.0024 (9)    | -0.0001 (9)   | 0.0048 (9)    |
| S8  | 0.0366 (14)  | 0.0225 (11)  | 0.0246 (12)  | 0.0028 (9)    | -0.0016 (10)  | 0.0053 (10)   |
| S9  | 0.0209 (12)  | 0.0370 (12)  | 0.0202 (11)  | -0.0084 (9)   | 0.0055 (9)    | -0.0019 (10)  |
| S10 | 0.0217 (11)  | 0.0280 (11)  | 0.0211 (10)  | -0.0009 (9)   | -0.0004 (8)   | 0.0008 (9)    |
| S11 | 0.0254 (12)  | 0.0159 (10)  | 0.0230 (11)  | 0.0006 (8)    | 0.0013 (9)    | -0.0010 (9)   |
| S12 | 0.0275 (12)  | 0.0218 (10)  | 0.0196 (10)  | -0.0014 (9)   | 0.0015 (9)    | -0.0074 (9)   |
| S13 | 0.0214 (12)  | 0.0288 (11)  | 0.0207 (11)  | 0.0057 (9)    | 0.0061 (9)    | 0.0018 (9)    |
| S14 | 0.0221 (12)  | 0.0349 (12)  | 0.0227 (11)  | -0.0067 (9)   | -0.0009 (9)   | -0.0012 (10)  |
| S15 | 0.0262 (12)  | 0.0240 (11)  | 0.0229 (11)  | -0.0002 (9)   | 0.0039 (9)    | 0.0058 (9)    |
| S16 | 0.0277 (12)  | 0.0238 (11)  | 0.0176 (10)  | 0.0011 (9)    | 0.0028 (8)    | 0.0004 (9)    |
| Ce1 | 0.0114 (2)   | 0.0133 (2)   | 0.0156 (2)   | -0.00090 (16) | -0.00033 (16) | 0.00136 (19)  |
| P1  | 0.0173 (11)  | 0.0195 (10)  | 0.0222 (10)  | -0.0007 (8)   | 0.0019 (8)    | 0.0046 (9)    |
| P2  | 0.0174 (11)  | 0.0353 (12)  | 0.0277 (11)  | -0.0073 (9)   | -0.0052 (8)   | 0.0077 (10)   |
| P3  | 0.0264 (12)  | 0.0208 (10)  | 0.0215 (11)  | 0.0007 (9)    | 0.0057 (9)    | 0.0032 (9)    |
| P4  | 0.0156 (11)  | 0.0182 (10)  | 0.0205 (11)  | 0.0002 (8)    | 0.0005 (8)    | -0.0034 (9)   |
| O1  | 0.020 (3)    | 0.015 (3)    | 0.019 (3)    | -0.002 (2)    | 0.003 (2)     | 0.006 (2)     |
| O2  | 0.013 (3)    | 0.025 (3)    | 0.034 (3)    | -0.002 (2)    | -0.004 (2)    | 0.003 (3)     |
| O3  | 0.024 (3)    | 0.019 (3)    | 0.018 (3)    | -0.004 (2)    | 0.005 (2)     | 0.005 (2)     |
| O4  | 0.008 (3)    | 0.022 (3)    | 0.032 (3)    | -0.002 (2)    | -0.004 (2)    | 0.005 (2)     |
| O5  | 0.036 (4)    | 0.026 (3)    | 0.030 (3)    | -0.006 (3)    | 0.000 (3)     | 0.002 (3)     |

|     |             |             |             |               |              |              |
|-----|-------------|-------------|-------------|---------------|--------------|--------------|
| O6  | 0.127 (8)   | 0.041 (4)   | 0.046 (4)   | -0.028 (5)    | 0.015 (5)    | -0.023 (4)   |
| O7  | 0.042 (4)   | 0.019 (3)   | 0.029 (3)   | -0.006 (3)    | -0.007 (3)   | 0.008 (3)    |
| O8  | 0.016 (3)   | 0.024 (3)   | 0.029 (3)   | -0.003 (2)    | 0.001 (2)    | -0.001 (2)   |
| O9  | 0.039 (4)   | 0.026 (3)   | 0.033 (4)   | -0.007 (3)    | 0.002 (3)    | -0.006 (3)   |
| O10 | 0.019 (3)   | 0.018 (3)   | 0.027 (3)   | 0.003 (2)     | -0.003 (2)   | -0.003 (2)   |
| N1  | 0.014 (4)   | 0.030 (4)   | 0.038 (4)   | -0.007 (3)    | 0.000 (3)    | 0.014 (3)    |
| N2  | 0.047 (5)   | 0.029 (4)   | 0.023 (4)   | -0.008 (3)    | 0.010 (3)    | -0.008 (3)   |
| N3  | 0.023 (4)   | 0.023 (3)   | 0.024 (3)   | 0.006 (3)     | -0.002 (3)   | 0.000 (3)    |
| N4  | 0.036 (5)   | 0.070 (6)   | 0.049 (5)   | -0.008 (4)    | 0.001 (4)    | -0.018 (5)   |
| N5  | 0.018 (4)   | 0.079 (6)   | 0.064 (5)   | 0.008 (4)     | 0.000 (4)    | 0.045 (5)    |
| N6  | 0.012 (4)   | 0.039 (4)   | 0.050 (4)   | -0.005 (3)    | 0.005 (3)    | 0.002 (4)    |
| N7  | 0.024 (4)   | 0.023 (3)   | 0.030 (4)   | -0.003 (3)    | 0.001 (3)    | -0.004 (3)   |
| N8  | 0.050 (5)   | 0.036 (4)   | 0.023 (4)   | 0.014 (3)     | 0.023 (3)    | 0.010 (3)    |
| N9  | 0.023 (4)   | 0.026 (4)   | 0.023 (4)   | 0.000 (3)     | 0.005 (3)    | -0.002 (3)   |
| N10 | 0.015 (4)   | 0.018 (3)   | 0.026 (4)   | 0.001 (3)     | -0.004 (3)   | 0.003 (3)    |
| N11 | 0.018 (4)   | 0.019 (3)   | 0.023 (3)   | 0.000 (3)     | -0.001 (3)   | -0.002 (3)   |
| N12 | 0.032 (4)   | 0.021 (4)   | 0.033 (4)   | 0.002 (3)     | 0.002 (3)    | -0.008 (3)   |
| N13 | 0.026 (4)   | 0.014 (3)   | 0.021 (4)   | -0.005 (3)    | -0.001 (3)   | -0.002 (3)   |
| N14 | 0.045 (6)   | 0.028 (4)   | 0.045 (5)   | -0.002 (4)    | -0.002 (4)   | -0.021 (4)   |
| C1  | 0.019 (5)   | 0.037 (5)   | 0.042 (5)   | 0.004 (4)     | 0.004 (4)    | -0.002 (4)   |
| C2  | 0.033 (6)   | 0.059 (6)   | 0.085 (8)   | -0.019 (5)    | 0.000 (5)    | 0.038 (6)    |
| C3  | 0.078 (10)  | 0.212 (17)  | 0.026 (6)   | 0.052 (10)    | 0.006 (6)    | -0.031 (8)   |
| C4  | 0.063 (8)   | 0.083 (8)   | 0.024 (5)   | -0.025 (6)    | -0.006 (5)   | -0.015 (5)   |
| C5  | 0.051 (6)   | 0.024 (4)   | 0.055 (6)   | -0.001 (4)    | -0.008 (5)   | 0.014 (4)    |
| C6  | 0.026 (5)   | 0.026 (4)   | 0.046 (5)   | 0.008 (4)     | -0.006 (4)   | -0.013 (4)   |
| C7  | 0.036 (6)   | 0.066 (8)   | 0.110 (10)  | 0.028 (5)     | -0.040 (6)   | -0.060 (8)   |
| C8  | 0.098 (11)  | 0.209 (17)  | 0.048 (7)   | -0.080 (11)   | 0.030 (7)    | -0.065 (9)   |
| C9  | 0.034 (5)   | 0.029 (4)   | 0.055 (6)   | -0.004 (4)    | -0.011 (4)   | 0.004 (4)    |
| C10 | 0.026 (6)   | 0.146 (12)  | 0.103 (9)   | 0.008 (7)     | 0.001 (6)    | 0.080 (9)    |
| C11 | 0.034 (6)   | 0.063 (7)   | 0.078 (7)   | -0.015 (5)    | 0.012 (5)    | -0.003 (6)   |
| C12 | 0.048 (6)   | 0.053 (6)   | 0.039 (5)   | -0.002 (5)    | 0.014 (4)    | -0.001 (5)   |
| C13 | 0.038 (6)   | 0.016 (4)   | 0.030 (5)   | -0.009 (4)    | 0.005 (4)    | -0.008 (4)   |
| C14 | 0.035 (5)   | 0.033 (5)   | 0.069 (6)   | -0.004 (4)    | 0.006 (5)    | 0.004 (5)    |
| C15 | 0.061 (6)   | 0.033 (4)   | 0.027 (4)   | -0.014 (4)    | 0.033 (4)    | -0.008 (4)   |
| C16 | 0.073 (8)   | 0.043 (5)   | 0.042 (5)   | 0.018 (5)     | 0.029 (5)    | 0.016 (5)    |
| C17 | 0.035 (5)   | 0.031 (5)   | 0.024 (4)   | 0.002 (4)     | -0.005 (4)   | 0.004 (4)    |
| C18 | 0.038 (6)   | 0.041 (6)   | 0.039 (5)   | 0.004 (5)     | -0.008 (4)   | -0.004 (5)   |
| C19 | 0.031 (5)   | 0.019 (4)   | 0.035 (5)   | -0.005 (4)    | 0.000 (4)    | 0.000 (4)    |
| C20 | 0.030 (5)   | 0.032 (5)   | 0.023 (4)   | 0.001 (4)     | -0.007 (4)   | 0.005 (4)    |
| C21 | 0.026 (5)   | 0.021 (4)   | 0.033 (4)   | -0.001 (3)    | -0.004 (4)   | -0.011 (4)   |
| C22 | 0.018 (5)   | 0.042 (5)   | 0.048 (6)   | 0.003 (4)     | -0.004 (4)   | 0.009 (5)    |
| C23 | 0.036 (6)   | 0.035 (5)   | 0.039 (5)   | -0.001 (4)    | 0.006 (4)    | -0.019 (4)   |
| C24 | 0.037 (6)   | 0.033 (5)   | 0.028 (5)   | 0.001 (4)     | -0.001 (4)   | -0.005 (4)   |
| Ce2 | 0.0105 (2)  | 0.0135 (2)  | 0.0153 (2)  | -0.00026 (16) | 0.00115 (16) | 0.00153 (18) |
| P5  | 0.0228 (12) | 0.0178 (10) | 0.0198 (10) | -0.0028 (8)   | -0.0006 (8)  | 0.0031 (9)   |
| P6  | 0.0131 (10) | 0.0177 (10) | 0.0217 (10) | -0.0017 (7)   | -0.0006 (8)  | -0.0003 (8)  |
| P7  | 0.0211 (11) | 0.0218 (10) | 0.0155 (10) | 0.0000 (8)    | 0.0037 (8)   | 0.0041 (9)   |
| P8  | 0.0109 (11) | 0.0202 (10) | 0.0258 (11) | 0.0000 (8)    | 0.0018 (8)   | -0.0042 (9)  |
| O11 | 0.023 (3)   | 0.016 (3)   | 0.014 (3)   | 0.001 (2)     | 0.002 (2)    | 0.001 (2)    |

## supplementary materials

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|     |             |             |             |              |              |               |
|-----|-------------|-------------|-------------|--------------|--------------|---------------|
| O12 | 0.011 (3)   | 0.026 (3)   | 0.024 (3)   | -0.004 (2)   | -0.007 (2)   | 0.002 (2)     |
| O13 | 0.020 (3)   | 0.019 (3)   | 0.023 (3)   | -0.002 (2)   | 0.001 (2)    | 0.006 (2)     |
| O14 | 0.007 (3)   | 0.023 (3)   | 0.022 (3)   | -0.001 (2)   | 0.004 (2)    | -0.001 (2)    |
| O15 | 0.012 (3)   | 0.026 (3)   | 0.027 (3)   | -0.004 (2)   | 0.008 (2)    | -0.004 (2)    |
| O16 | 0.055 (5)   | 0.048 (4)   | 0.023 (3)   | -0.007 (3)   | 0.009 (3)    | -0.019 (3)    |
| O17 | 0.021 (3)   | 0.026 (3)   | 0.032 (3)   | 0.008 (2)    | 0.001 (3)    | -0.005 (3)    |
| O18 | 0.023 (3)   | 0.024 (3)   | 0.020 (3)   | 0.002 (2)    | 0.001 (2)    | 0.002 (3)     |
| O19 | 0.071 (5)   | 0.036 (4)   | 0.030 (4)   | -0.018 (3)   | 0.011 (3)    | -0.027 (3)    |
| O20 | 0.032 (4)   | 0.022 (3)   | 0.021 (3)   | -0.001 (3)   | 0.004 (3)    | 0.005 (3)     |
| N15 | 0.023 (4)   | 0.021 (3)   | 0.047 (4)   | -0.007 (3)   | -0.009 (3)   | 0.007 (3)     |
| N16 | 0.029 (4)   | 0.024 (3)   | 0.034 (4)   | -0.004 (3)   | 0.002 (3)    | 0.012 (3)     |
| N17 | 0.021 (4)   | 0.023 (4)   | 0.040 (4)   | 0.003 (3)    | -0.005 (3)   | -0.004 (3)    |
| N18 | 0.021 (3)   | 0.022 (3)   | 0.028 (3)   | -0.004 (3)   | -0.005 (3)   | 0.009 (3)     |
| N19 | 0.013 (4)   | 0.041 (4)   | 0.048 (4)   | 0.000 (3)    | -0.004 (3)   | -0.030 (4)    |
| N20 | 0.028 (4)   | 0.014 (3)   | 0.025 (3)   | -0.004 (3)   | -0.007 (3)   | 0.000 (3)     |
| N21 | 0.040 (5)   | 0.038 (4)   | 0.017 (3)   | 0.001 (3)    | 0.013 (3)    | -0.007 (3)    |
| N22 | 0.030 (4)   | 0.024 (4)   | 0.024 (4)   | -0.007 (3)   | 0.003 (3)    | -0.001 (3)    |
| N23 | 0.026 (4)   | 0.035 (4)   | 0.031 (4)   | -0.006 (3)   | -0.002 (3)   | 0.009 (3)     |
| N24 | 0.018 (4)   | 0.019 (3)   | 0.030 (4)   | 0.005 (3)    | -0.009 (3)   | -0.001 (3)    |
| N25 | 0.015 (4)   | 0.028 (4)   | 0.040 (4)   | 0.002 (3)    | 0.001 (3)    | -0.010 (3)    |
| N26 | 0.025 (4)   | 0.026 (4)   | 0.019 (4)   | 0.002 (3)    | 0.005 (3)    | -0.006 (3)    |
| N27 | 0.045 (5)   | 0.021 (4)   | 0.020 (4)   | -0.007 (3)   | 0.010 (3)    | -0.003 (3)    |
| N28 | 0.027 (5)   | 0.044 (5)   | 0.025 (4)   | -0.007 (4)   | 0.006 (3)    | -0.007 (4)    |
| C25 | 0.013 (5)   | 0.050 (6)   | 0.045 (5)   | 0.004 (4)    | 0.004 (4)    | 0.005 (5)     |
| C26 | 0.036 (6)   | 0.038 (5)   | 0.103 (8)   | -0.019 (5)   | -0.027 (6)   | 0.015 (6)     |
| C27 | 0.054 (6)   | 0.042 (5)   | 0.034 (5)   | -0.006 (4)   | 0.004 (4)    | 0.012 (4)     |
| C28 | 0.064 (7)   | 0.036 (5)   | 0.023 (5)   | -0.002 (5)   | 0.005 (5)    | -0.005 (4)    |
| C29 | 0.043 (6)   | 0.038 (5)   | 0.051 (5)   | 0.014 (4)    | -0.009 (4)   | -0.004 (5)    |
| C30 | 0.064 (8)   | 0.077 (8)   | 0.063 (7)   | 0.022 (6)    | -0.015 (6)   | -0.037 (7)    |
| C31 | 0.031 (5)   | 0.035 (4)   | 0.034 (4)   | -0.011 (4)   | -0.009 (4)   | 0.018 (4)     |
| C32 | 0.035 (5)   | 0.043 (5)   | 0.036 (4)   | 0.000 (4)    | -0.011 (4)   | 0.010 (4)     |
| C33 | 0.017 (4)   | 0.042 (5)   | 0.064 (6)   | 0.008 (4)    | -0.008 (4)   | -0.034 (5)    |
| C34 | 0.025 (5)   | 0.071 (7)   | 0.054 (5)   | 0.003 (5)    | -0.003 (4)   | -0.037 (5)    |
| C35 | 0.030 (5)   | 0.017 (4)   | 0.050 (5)   | -0.001 (3)   | -0.005 (4)   | -0.007 (4)    |
| C36 | 0.056 (7)   | 0.034 (5)   | 0.039 (5)   | -0.018 (5)   | -0.004 (5)   | 0.018 (4)     |
| C37 | 0.035 (6)   | 0.042 (5)   | 0.081 (7)   | 0.015 (4)    | 0.028 (5)    | -0.020 (5)    |
| C38 | 0.075 (9)   | 0.079 (8)   | 0.037 (6)   | -0.010 (6)   | 0.011 (5)    | -0.027 (6)    |
| C39 | 0.057 (7)   | 0.036 (5)   | 0.038 (5)   | -0.015 (4)   | 0.020 (5)    | -0.003 (4)    |
| C40 | 0.039 (6)   | 0.031 (5)   | 0.041 (5)   | -0.003 (4)   | 0.009 (4)    | 0.000 (4)     |
| C41 | 0.043 (6)   | 0.040 (5)   | 0.030 (5)   | 0.010 (4)    | 0.004 (4)    | 0.014 (4)     |
| C42 | 0.044 (7)   | 0.042 (5)   | 0.064 (7)   | -0.022 (5)   | -0.018 (5)   | 0.014 (5)     |
| C43 | 0.022 (5)   | 0.024 (4)   | 0.043 (5)   | -0.006 (3)   | 0.002 (4)    | 0.012 (4)     |
| C44 | 0.035 (6)   | 0.029 (5)   | 0.069 (7)   | 0.013 (4)    | -0.025 (5)   | 0.002 (5)     |
| C45 | 0.037 (5)   | 0.017 (4)   | 0.046 (5)   | 0.002 (3)    | -0.011 (4)   | -0.006 (4)    |
| C46 | 0.026 (6)   | 0.047 (6)   | 0.065 (7)   | 0.000 (4)    | 0.008 (5)    | -0.008 (5)    |
| C47 | 0.040 (7)   | 0.067 (7)   | 0.048 (6)   | -0.012 (5)   | 0.019 (5)    | -0.019 (6)    |
| C48 | 0.029 (6)   | 0.060 (6)   | 0.033 (5)   | 0.000 (5)    | 0.013 (4)    | 0.005 (5)     |
| Ce3 | 0.0116 (2)  | 0.0123 (2)  | 0.0149 (2)  | 0.00061 (16) | 0.00046 (16) | -0.00151 (18) |
| P9  | 0.0115 (10) | 0.0173 (10) | 0.0251 (11) | -0.0015 (8)  | 0.0010 (8)   | 0.0005 (9)    |

## supplementary materials

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|     |             |             |             |             |             |             |
|-----|-------------|-------------|-------------|-------------|-------------|-------------|
| P10 | 0.0236 (12) | 0.0197 (10) | 0.0156 (10) | -0.0034 (9) | 0.0041 (8)  | -0.0046 (9) |
| P11 | 0.0144 (10) | 0.0231 (10) | 0.0221 (10) | 0.0019 (8)  | -0.0021 (8) | -0.0052 (9) |
| P12 | 0.0200 (11) | 0.0144 (9)  | 0.0192 (10) | 0.0026 (8)  | 0.0024 (8)  | -0.0029 (8) |
| O21 | 0.018 (3)   | 0.021 (3)   | 0.022 (3)   | -0.001 (2)  | 0.002 (2)   | 0.002 (2)   |
| O22 | 0.029 (3)   | 0.016 (3)   | 0.025 (3)   | 0.000 (2)   | 0.003 (2)   | -0.004 (2)  |
| O23 | 0.007 (3)   | 0.031 (3)   | 0.025 (3)   | -0.001 (2)  | -0.003 (2)  | -0.003 (3)  |
| O24 | 0.018 (3)   | 0.018 (3)   | 0.023 (3)   | 0.003 (2)   | 0.000 (2)   | -0.008 (2)  |
| O25 | 0.022 (3)   | 0.018 (3)   | 0.030 (3)   | -0.007 (2)  | -0.006 (2)  | 0.008 (2)   |
| O26 | 0.034 (4)   | 0.050 (4)   | 0.026 (3)   | 0.004 (3)   | -0.001 (3)  | 0.022 (3)   |
| O27 | 0.020 (3)   | 0.033 (3)   | 0.025 (3)   | -0.006 (2)  | 0.003 (3)   | 0.002 (3)   |
| O28 | 0.032 (4)   | 0.017 (3)   | 0.021 (3)   | 0.011 (2)   | 0.005 (2)   | -0.001 (2)  |
| O29 | 0.087 (6)   | 0.040 (4)   | 0.030 (4)   | 0.020 (4)   | 0.012 (4)   | 0.018 (3)   |
| O30 | 0.041 (4)   | 0.023 (3)   | 0.024 (3)   | 0.006 (3)   | 0.005 (3)   | 0.000 (3)   |
| N29 | 0.026 (4)   | 0.027 (4)   | 0.012 (3)   | -0.002 (3)  | 0.005 (3)   | 0.002 (3)   |
| N30 | 0.010 (4)   | 0.031 (4)   | 0.027 (4)   | 0.000 (3)   | -0.002 (3)  | -0.004 (3)  |
| N31 | 0.015 (4)   | 0.019 (3)   | 0.029 (4)   | 0.001 (3)   | 0.005 (3)   | 0.004 (3)   |
| N32 | 0.028 (4)   | 0.025 (4)   | 0.025 (4)   | 0.008 (3)   | 0.007 (3)   | -0.012 (3)  |
| N33 | 0.027 (4)   | 0.024 (4)   | 0.028 (4)   | -0.002 (3)  | -0.003 (3)  | -0.014 (3)  |
| N34 | 0.034 (4)   | 0.040 (4)   | 0.020 (3)   | -0.021 (3)  | 0.003 (3)   | -0.006 (3)  |
| N35 | 0.029 (4)   | 0.021 (3)   | 0.023 (3)   | 0.002 (3)   | 0.007 (3)   | 0.002 (3)   |
| N36 | 0.014 (3)   | 0.043 (4)   | 0.046 (4)   | 0.009 (3)   | -0.013 (3)  | -0.030 (3)  |
| N37 | 0.017 (3)   | 0.023 (3)   | 0.027 (3)   | 0.001 (3)   | -0.003 (3)  | 0.006 (3)   |
| N38 | 0.026 (4)   | 0.037 (4)   | 0.019 (3)   | 0.001 (3)   | 0.005 (3)   | -0.004 (3)  |
| N39 | 0.026 (4)   | 0.011 (3)   | 0.037 (4)   | 0.001 (3)   | 0.002 (3)   | -0.009 (3)  |
| N40 | 0.024 (4)   | 0.015 (3)   | 0.025 (3)   | 0.007 (3)   | -0.002 (3)  | -0.003 (3)  |
| N41 | 0.018 (4)   | 0.023 (3)   | 0.019 (4)   | 0.002 (3)   | 0.002 (3)   | 0.001 (3)   |
| N42 | 0.034 (4)   | 0.021 (4)   | 0.016 (3)   | 0.009 (3)   | -0.003 (3)  | 0.002 (3)   |
| C49 | 0.053 (7)   | 0.037 (5)   | 0.024 (5)   | -0.009 (5)  | -0.001 (4)  | 0.001 (4)   |
| C50 | 0.039 (6)   | 0.014 (4)   | 0.043 (5)   | -0.005 (4)  | 0.017 (4)   | 0.011 (4)   |
| C51 | 0.023 (5)   | 0.019 (4)   | 0.037 (5)   | 0.000 (3)   | -0.001 (4)  | -0.003 (4)  |
| C52 | 0.013 (4)   | 0.031 (5)   | 0.047 (5)   | 0.000 (3)   | 0.000 (4)   | -0.005 (4)  |
| C53 | 0.017 (5)   | 0.027 (4)   | 0.041 (5)   | 0.007 (3)   | 0.009 (4)   | -0.006 (4)  |
| C54 | 0.017 (4)   | 0.031 (5)   | 0.040 (5)   | 0.006 (3)   | -0.011 (4)  | -0.006 (4)  |
| C55 | 0.041 (6)   | 0.070 (7)   | 0.059 (6)   | 0.023 (5)   | 0.017 (5)   | -0.020 (6)  |
| C56 | 0.044 (6)   | 0.013 (4)   | 0.023 (4)   | -0.010 (4)  | -0.005 (4)  | 0.001 (4)   |
| C57 | 0.043 (6)   | 0.033 (5)   | 0.040 (5)   | -0.006 (4)  | 0.003 (4)   | -0.030 (5)  |
| C58 | 0.031 (6)   | 0.049 (6)   | 0.043 (6)   | 0.001 (5)   | -0.001 (4)  | -0.008 (5)  |
| C59 | 0.080 (9)   | 0.095 (9)   | 0.019 (5)   | -0.053 (7)  | 0.003 (5)   | -0.003 (5)  |
| C60 | 0.088 (9)   | 0.092 (8)   | 0.032 (5)   | -0.058 (7)  | 0.007 (5)   | -0.005 (5)  |
| C61 | 0.037 (5)   | 0.026 (4)   | 0.046 (5)   | 0.001 (4)   | -0.003 (4)  | 0.002 (4)   |
| C62 | 0.051 (6)   | 0.057 (6)   | 0.030 (5)   | 0.021 (5)   | 0.004 (4)   | 0.025 (4)   |
| C63 | 0.035 (6)   | 0.072 (7)   | 0.090 (8)   | 0.007 (5)   | -0.025 (5)  | -0.060 (6)  |
| C64 | 0.035 (6)   | 0.078 (8)   | 0.083 (8)   | 0.009 (5)   | -0.017 (5)  | -0.049 (7)  |
| C65 | 0.021 (5)   | 0.031 (4)   | 0.044 (5)   | 0.003 (4)   | 0.006 (4)   | 0.005 (4)   |
| C66 | 0.018 (4)   | 0.032 (4)   | 0.037 (4)   | -0.001 (3)  | 0.000 (3)   | 0.012 (4)   |
| C67 | 0.046 (6)   | 0.063 (6)   | 0.038 (5)   | -0.020 (5)  | 0.000 (4)   | 0.010 (5)   |
| C68 | 0.058 (7)   | 0.050 (6)   | 0.023 (5)   | 0.002 (5)   | -0.007 (4)  | 0.001 (4)   |
| C69 | 0.043 (6)   | 0.024 (4)   | 0.055 (5)   | 0.000 (4)   | -0.007 (4)  | -0.014 (4)  |
| C70 | 0.032 (6)   | 0.037 (5)   | 0.057 (6)   | -0.010 (4)  | -0.001 (5)  | 0.009 (5)   |

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## supplementary materials

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|     |             |             |             |              |              |               |
|-----|-------------|-------------|-------------|--------------|--------------|---------------|
| C71 | 0.025 (5)   | 0.037 (5)   | 0.068 (6)   | 0.008 (4)    | 0.000 (4)    | -0.024 (5)    |
| C72 | 0.026 (5)   | 0.039 (5)   | 0.038 (5)   | 0.008 (4)    | -0.001 (4)   | 0.003 (4)     |
| Ce4 | 0.0111 (2)  | 0.0124 (2)  | 0.0183 (2)  | 0.00022 (16) | 0.00083 (16) | -0.00175 (18) |
| P13 | 0.0233 (12) | 0.0144 (10) | 0.0216 (10) | 0.0010 (8)   | 0.0041 (8)   | -0.0045 (9)   |
| P14 | 0.0120 (10) | 0.0173 (9)  | 0.0222 (10) | -0.0002 (7)  | -0.0003 (8)  | 0.0010 (8)    |
| P15 | 0.0228 (11) | 0.0171 (10) | 0.0215 (10) | 0.0014 (8)   | 0.0036 (8)   | -0.0009 (9)   |
| P16 | 0.0119 (11) | 0.0187 (10) | 0.0234 (11) | -0.0017 (8)  | 0.0018 (8)   | 0.0004 (9)    |
| O31 | 0.026 (3)   | 0.020 (3)   | 0.023 (3)   | 0.004 (2)    | 0.006 (2)    | -0.004 (2)    |
| O32 | 0.014 (3)   | 0.024 (3)   | 0.030 (3)   | 0.002 (2)    | -0.004 (2)   | 0.000 (3)     |
| O33 | 0.026 (3)   | 0.028 (3)   | 0.018 (3)   | 0.006 (2)    | 0.005 (2)    | -0.015 (2)    |
| O34 | 0.022 (3)   | 0.017 (3)   | 0.034 (3)   | -0.006 (2)   | -0.002 (2)   | -0.002 (2)    |
| O35 | 0.016 (3)   | 0.033 (3)   | 0.034 (3)   | 0.001 (2)    | 0.004 (2)    | 0.012 (3)     |
| O36 | 0.051 (5)   | 0.040 (4)   | 0.033 (4)   | 0.001 (3)    | 0.005 (3)    | 0.016 (3)     |
| O37 | 0.027 (4)   | 0.029 (3)   | 0.027 (3)   | -0.009 (3)   | 0.006 (3)    | 0.000 (3)     |
| O38 | 0.030 (4)   | 0.017 (3)   | 0.030 (3)   | 0.003 (2)    | -0.003 (3)   | 0.002 (3)     |
| O39 | 0.054 (4)   | 0.018 (3)   | 0.026 (3)   | -0.002 (3)   | 0.001 (3)    | 0.007 (3)     |
| O40 | 0.033 (4)   | 0.013 (3)   | 0.029 (3)   | 0.007 (2)    | 0.000 (3)    | -0.007 (3)    |
| N43 | 0.027 (4)   | 0.018 (3)   | 0.028 (3)   | 0.005 (3)    | -0.001 (3)   | -0.007 (3)    |
| N44 | 0.036 (4)   | 0.014 (3)   | 0.027 (4)   | -0.001 (3)   | 0.007 (3)    | 0.006 (3)     |
| N45 | 0.040 (4)   | 0.019 (3)   | 0.021 (3)   | -0.002 (3)   | 0.009 (3)    | -0.007 (3)    |
| N46 | 0.016 (3)   | 0.030 (3)   | 0.024 (3)   | 0.008 (3)    | -0.006 (2)   | -0.011 (3)    |
| N47 | 0.009 (3)   | 0.034 (4)   | 0.039 (4)   | 0.001 (3)    | 0.001 (3)    | 0.023 (3)     |
| N48 | 0.025 (4)   | 0.020 (3)   | 0.021 (3)   | -0.002 (3)   | 0.007 (3)    | 0.003 (3)     |
| N49 | 0.033 (4)   | 0.036 (4)   | 0.029 (4)   | 0.003 (3)    | 0.010 (3)    | 0.003 (3)     |
| N50 | 0.029 (4)   | 0.019 (3)   | 0.021 (3)   | -0.002 (3)   | 0.012 (3)    | 0.001 (3)     |
| N51 | 0.037 (5)   | 0.035 (4)   | 0.029 (4)   | 0.000 (3)    | -0.005 (3)   | -0.012 (3)    |
| N52 | 0.028 (4)   | 0.029 (4)   | 0.021 (4)   | -0.006 (3)   | -0.004 (3)   | 0.004 (3)     |
| N53 | 0.017 (4)   | 0.028 (4)   | 0.020 (3)   | 0.000 (3)    | 0.001 (3)    | -0.003 (3)    |
| N54 | 0.015 (4)   | 0.022 (3)   | 0.036 (4)   | 0.003 (3)    | 0.003 (3)    | 0.002 (3)     |
| N55 | 0.024 (4)   | 0.017 (3)   | 0.025 (4)   | 0.003 (3)    | -0.001 (3)   | -0.001 (3)    |
| N56 | 0.017 (4)   | 0.014 (3)   | 0.027 (4)   | 0.002 (3)    | -0.010 (3)   | -0.001 (3)    |
| C73 | 0.018 (5)   | 0.032 (5)   | 0.035 (5)   | 0.009 (4)    | 0.000 (4)    | 0.003 (4)     |
| C74 | 0.046 (6)   | 0.028 (5)   | 0.051 (5)   | 0.019 (4)    | -0.004 (4)   | -0.007 (4)    |
| C75 | 0.057 (7)   | 0.066 (7)   | 0.055 (6)   | -0.015 (6)   | 0.004 (5)    | 0.035 (6)     |
| C76 | 0.031 (5)   | 0.036 (5)   | 0.073 (6)   | -0.008 (4)   | -0.008 (5)   | 0.010 (5)     |
| C77 | 0.059 (7)   | 0.030 (5)   | 0.035 (5)   | 0.006 (4)    | -0.002 (4)   | -0.013 (4)    |
| C78 | 0.048 (6)   | 0.027 (5)   | 0.028 (5)   | 0.004 (4)    | 0.010 (4)    | 0.001 (4)     |
| C79 | 0.031 (5)   | 0.033 (4)   | 0.033 (4)   | 0.011 (4)    | 0.003 (4)    | -0.017 (4)    |
| C80 | 0.023 (4)   | 0.026 (4)   | 0.034 (4)   | 0.006 (3)    | -0.008 (3)   | 0.000 (4)     |
| C81 | 0.033 (6)   | 0.061 (7)   | 0.179 (13)  | -0.001 (5)   | 0.014 (7)    | 0.081 (8)     |
| C82 | 0.007 (4)   | 0.044 (5)   | 0.065 (6)   | 0.002 (4)    | 0.001 (4)    | 0.027 (5)     |
| C83 | 0.043 (6)   | 0.036 (5)   | 0.037 (5)   | 0.013 (4)    | 0.002 (4)    | -0.012 (4)    |
| C84 | 0.026 (5)   | 0.028 (4)   | 0.043 (5)   | -0.001 (4)   | -0.004 (4)   | 0.006 (4)     |
| C85 | 0.046 (6)   | 0.040 (5)   | 0.063 (6)   | -0.022 (4)   | 0.029 (5)    | -0.012 (5)    |
| C86 | 0.066 (8)   | 0.092 (9)   | 0.034 (5)   | 0.012 (6)    | 0.015 (5)    | 0.025 (6)     |
| C87 | 0.033 (5)   | 0.036 (5)   | 0.045 (5)   | 0.009 (4)    | 0.010 (4)    | 0.000 (4)     |
| C88 | 0.042 (6)   | 0.021 (5)   | 0.039 (5)   | -0.003 (4)   | 0.010 (4)    | -0.005 (4)    |
| C89 | 0.040 (6)   | 0.068 (8)   | 0.059 (7)   | 0.008 (5)    | -0.021 (5)   | -0.017 (6)    |
| C90 | 0.058 (7)   | 0.043 (6)   | 0.028 (5)   | -0.006 (5)   | 0.005 (4)    | -0.017 (5)    |

|     |           |           |           |            |            |            |
|-----|-----------|-----------|-----------|------------|------------|------------|
| C91 | 0.047 (7) | 0.022 (5) | 0.046 (6) | -0.023 (4) | 0.010 (5)  | 0.005 (4)  |
| C92 | 0.056 (7) | 0.049 (6) | 0.031 (5) | -0.013 (5) | 0.000 (5)  | 0.003 (5)  |
| C93 | 0.041 (6) | 0.042 (6) | 0.036 (5) | -0.004 (5) | -0.011 (4) | -0.008 (5) |
| C94 | 0.026 (5) | 0.038 (5) | 0.034 (5) | -0.009 (4) | -0.004 (4) | -0.003 (4) |
| C95 | 0.007 (4) | 0.050 (6) | 0.064 (7) | 0.008 (4)  | 0.007 (4)  | 0.004 (5)  |
| C96 | 0.014 (4) | 0.041 (5) | 0.057 (6) | 0.005 (4)  | -0.015 (4) | -0.001 (5) |

*Geometric parameters (Å)*

|                       |            |          |           |
|-----------------------|------------|----------|-----------|
| W1—S2                 | 2.202 (2)  | C42—H42A | 0.9600    |
| W1—S1                 | 2.203 (2)  | C42—H42B | 0.9600    |
| W1—S4                 | 2.205 (2)  | C42—H42C | 0.9600    |
| W1—S3                 | 2.217 (2)  | C43—H43A | 0.9600    |
| W1—Ag1                | 2.9307 (9) | C43—H43B | 0.9600    |
| W1—Ag4                | 2.9424 (9) | C43—H43C | 0.9600    |
| W2—S5                 | 2.203 (2)  | C44—H44A | 0.9600    |
| W2—S6                 | 2.206 (2)  | C44—H44B | 0.9600    |
| W2—S8                 | 2.208 (2)  | C44—H44C | 0.9600    |
| W2—S7                 | 2.209 (2)  | C45—H45A | 0.9600    |
| W2—Ag2                | 2.9320 (9) | C45—H45B | 0.9600    |
| W2—Ag1                | 2.9458 (9) | C45—H45C | 0.9600    |
| W3—S9                 | 2.196 (2)  | C46—H46A | 0.9600    |
| W3—S12                | 2.207 (2)  | C46—H46B | 0.9600    |
| W3—S10                | 2.207 (2)  | C46—H46C | 0.9600    |
| W3—S11                | 2.216 (2)  | C47—H47A | 0.9600    |
| W3—Ag2                | 2.9300 (9) | C47—H47B | 0.9600    |
| W3—Ag3                | 2.9307 (9) | C47—H47C | 0.9600    |
| W4—S13                | 2.201 (2)  | C48—H48A | 0.9600    |
| W4—S14                | 2.207 (2)  | C48—H48B | 0.9600    |
| W4—S16                | 2.207 (2)  | C48—H48C | 0.9600    |
| W4—S15                | 2.211 (2)  | Ce3—O23  | 2.358 (5) |
| W4—Ag4 <sup>i</sup>   | 2.9292 (9) | Ce3—O21  | 2.372 (6) |
| W4—Ag3                | 2.9402 (9) | Ce3—O22  | 2.375 (5) |
| Ag1—S3                | 2.479 (2)  | Ce3—O24  | 2.406 (5) |
| Ag1—S4                | 2.572 (2)  | Ce3—O30  | 2.580 (6) |
| Ag1—S6                | 2.605 (3)  | Ce3—O25  | 2.589 (5) |
| Ag1—S5                | 2.626 (3)  | Ce3—O28  | 2.593 (6) |
| Ag2—S8                | 2.480 (2)  | Ce3—O27  | 2.599 (6) |
| Ag2—S7                | 2.571 (2)  | Ce3—N41  | 3.023 (7) |
| Ag2—S9                | 2.600 (3)  | Ce3—N42  | 3.025 (7) |
| Ag2—S10               | 2.602 (2)  | P9—O21   | 1.510 (6) |
| Ag3—S11               | 2.476 (2)  | P9—N29   | 1.610 (7) |
| Ag3—S12               | 2.568 (2)  | P9—N30   | 1.633 (7) |
| Ag3—S14               | 2.616 (2)  | P9—N31   | 1.641 (7) |
| Ag3—S13               | 2.650 (3)  | P10—O22  | 1.494 (6) |
| Ag4—S16 <sup>ii</sup> | 2.487 (2)  | P10—N32  | 1.624 (7) |
| Ag4—S15 <sup>ii</sup> | 2.577 (2)  | P10—N34  | 1.627 (7) |
| Ag4—S2                | 2.633 (2)  | P10—N33  | 1.630 (7) |

## supplementary materials

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|                      |            |          |            |
|----------------------|------------|----------|------------|
| Ag4—S1               | 2.643 (3)  | P11—O23  | 1.506 (5)  |
| Ag4—W4 <sup>ii</sup> | 2.9292 (9) | P11—N35  | 1.615 (6)  |
| S15—Ag4 <sup>i</sup> | 2.577 (2)  | P11—N36  | 1.632 (6)  |
| S16—Ag4 <sup>i</sup> | 2.487 (2)  | P11—N37  | 1.653 (6)  |
| Ce1—O2               | 2.363 (5)  | P12—O24  | 1.502 (5)  |
| Ce1—O4               | 2.382 (5)  | P12—N40  | 1.631 (7)  |
| Ce1—O3               | 2.391 (5)  | P12—N39  | 1.638 (6)  |
| Ce1—O1               | 2.409 (5)  | P12—N38  | 1.645 (7)  |
| Ce1—O7               | 2.576 (6)  | O25—N41  | 1.284 (9)  |
| Ce1—O8               | 2.583 (6)  | O26—N41  | 1.230 (9)  |
| Ce1—O10              | 2.595 (5)  | O27—N41  | 1.262 (9)  |
| Ce1—O5               | 2.628 (6)  | O28—N42  | 1.264 (9)  |
| Ce1—N14              | 3.002 (8)  | O29—N42  | 1.199 (9)  |
| Ce1—N13              | 3.021 (7)  | O30—N42  | 1.306 (9)  |
| P1—O1                | 1.486 (5)  | N29—C50  | 1.463 (10) |
| P1—N1                | 1.628 (7)  | N29—C49  | 1.473 (11) |
| P1—N3                | 1.631 (6)  | N30—C52  | 1.441 (10) |
| P1—N2                | 1.647 (7)  | N30—C51  | 1.474 (10) |
| P2—O2                | 1.502 (6)  | N31—C53  | 1.450 (10) |
| P2—N4                | 1.589 (8)  | N31—C54  | 1.471 (10) |
| P2—N6                | 1.614 (7)  | N32—C55  | 1.463 (10) |
| P2—N5                | 1.634 (7)  | N32—C56  | 1.485 (10) |
| P3—O3                | 1.491 (5)  | N33—C58  | 1.434 (12) |
| P3—N8                | 1.641 (7)  | N33—C57  | 1.464 (10) |
| P3—N9                | 1.642 (7)  | N34—C59  | 1.459 (10) |
| P3—N7                | 1.645 (7)  | N34—C60  | 1.466 (11) |
| P4—O4                | 1.490 (6)  | N35—C62  | 1.464 (10) |
| P4—N11               | 1.632 (7)  | N35—C61  | 1.480 (10) |
| P4—N12               | 1.635 (7)  | N36—C64  | 1.400 (10) |
| P4—N10               | 1.637 (7)  | N36—C63  | 1.481 (10) |
| O5—N14               | 1.282 (10) | N37—C66  | 1.459 (9)  |
| O6—N14               | 1.228 (10) | N37—C65  | 1.470 (9)  |
| O7—N14               | 1.258 (10) | N38—C68  | 1.455 (11) |
| O8—N13               | 1.240 (9)  | N38—C67  | 1.461 (10) |
| O9—N13               | 1.214 (9)  | N39—C70  | 1.441 (10) |
| O10—N13              | 1.279 (9)  | N39—C69  | 1.466 (9)  |
| N1—C1                | 1.458 (10) | N40—C72  | 1.456 (10) |
| N1—C2                | 1.476 (10) | N40—C71  | 1.471 (9)  |
| N2—C3                | 1.407 (12) | C49—H49A | 0.9600     |
| N2—C4                | 1.460 (11) | C49—H49B | 0.9600     |
| N3—C6                | 1.462 (9)  | C49—H49C | 0.9600     |
| N3—C5                | 1.473 (9)  | C50—H50A | 0.9600     |
| N4—C7                | 1.449 (13) | C50—H50B | 0.9600     |
| N4—C8                | 1.471 (12) | C50—H50C | 0.9600     |
| N5—C9                | 1.406 (10) | C51—H51A | 0.9600     |
| N5—C10               | 1.472 (11) | C51—H51B | 0.9600     |
| N6—C11               | 1.452 (10) | C51—H51C | 0.9600     |
| N6—C12               | 1.460 (10) | C52—H52A | 0.9600     |

|          |            |          |        |
|----------|------------|----------|--------|
| N7—C13   | 1.449 (10) | C52—H52B | 0.9600 |
| N7—C14   | 1.458 (11) | C52—H52C | 0.9600 |
| N8—C15   | 1.419 (10) | C53—H53A | 0.9600 |
| N8—C16   | 1.465 (10) | C53—H53B | 0.9600 |
| N9—C17   | 1.458 (10) | C53—H53C | 0.9600 |
| N9—C18   | 1.475 (11) | C54—H54A | 0.9600 |
| N10—C19  | 1.448 (11) | C54—H54B | 0.9600 |
| N10—C20  | 1.461 (10) | C54—H54C | 0.9600 |
| N11—C21  | 1.454 (9)  | C55—H55A | 0.9600 |
| N11—C22  | 1.481 (11) | C55—H55B | 0.9600 |
| N12—C23  | 1.443 (11) | C55—H55C | 0.9600 |
| N12—C24  | 1.476 (11) | C56—H56A | 0.9600 |
| C1—H1A   | 0.9600     | C56—H56B | 0.9600 |
| C1—H1B   | 0.9600     | C56—H56C | 0.9600 |
| C1—H1C   | 0.9600     | C57—H57A | 0.9600 |
| C2—H2A   | 0.9600     | C57—H57B | 0.9600 |
| C2—H2B   | 0.9600     | C57—H57C | 0.9600 |
| C2—H2C   | 0.9600     | C58—H58A | 0.9600 |
| C3—H3A   | 0.9600     | C58—H58B | 0.9600 |
| C3—H3B   | 0.9600     | C58—H58C | 0.9600 |
| C3—H3C   | 0.9600     | C59—H59A | 0.9600 |
| C4—H4A   | 0.9600     | C59—H59B | 0.9600 |
| C4—H4B   | 0.9600     | C59—H59C | 0.9600 |
| C4—H4C   | 0.9600     | C60—H60A | 0.9600 |
| C5—H5A   | 0.9600     | C60—H60B | 0.9600 |
| C5—H5B   | 0.9600     | C60—H60C | 0.9600 |
| C5—H5C   | 0.9600     | C61—H61A | 0.9600 |
| C6—H6A   | 0.9600     | C61—H61B | 0.9600 |
| C6—H6B   | 0.9600     | C61—H61C | 0.9600 |
| C6—H6C   | 0.9600     | C62—H62A | 0.9600 |
| C7—H7A   | 0.9600     | C62—H62B | 0.9600 |
| C7—H7B   | 0.9600     | C62—H62C | 0.9600 |
| C7—H7C   | 0.9600     | C63—H63A | 0.9600 |
| C8—H8A   | 0.9600     | C63—H63B | 0.9600 |
| C8—H8B   | 0.9600     | C63—H63C | 0.9600 |
| C8—H8C   | 0.9600     | C64—H64A | 0.9600 |
| C9—H9A   | 0.9600     | C64—H64B | 0.9600 |
| C9—H9B   | 0.9600     | C64—H64C | 0.9600 |
| C9—H9C   | 0.9600     | C65—H65A | 0.9600 |
| C10—H10A | 0.9600     | C65—H65B | 0.9600 |
| C10—H10B | 0.9600     | C65—H65C | 0.9600 |
| C10—H10C | 0.9600     | C66—H66A | 0.9600 |
| C11—H11A | 0.9600     | C66—H66B | 0.9600 |
| C11—H11B | 0.9600     | C66—H66C | 0.9600 |
| C11—H11C | 0.9600     | C67—H67A | 0.9600 |
| C12—H12A | 0.9600     | C67—H67B | 0.9600 |
| C12—H12B | 0.9600     | C67—H67C | 0.9600 |
| C12—H12C | 0.9600     | C68—H68A | 0.9600 |
| C13—H13A | 0.9600     | C68—H68B | 0.9600 |



## supplementary materials

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|          |           |          |            |
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| C13—H13B | 0.9600    | C68—H68C | 0.9600     |
| C13—H13C | 0.9600    | C69—H69A | 0.9600     |
| C14—H14A | 0.9600    | C69—H69B | 0.9600     |
| C14—H14B | 0.9600    | C69—H69C | 0.9600     |
| C14—H14C | 0.9600    | C70—H70A | 0.9600     |
| C15—H15A | 0.9600    | C70—H70B | 0.9600     |
| C15—H15B | 0.9600    | C70—H70C | 0.9600     |
| C15—H15C | 0.9600    | C71—H71A | 0.9600     |
| C16—H16A | 0.9600    | C71—H71B | 0.9600     |
| C16—H16B | 0.9600    | C71—H71C | 0.9600     |
| C16—H16C | 0.9600    | C72—H72A | 0.9600     |
| C17—H17A | 0.9600    | C72—H72B | 0.9600     |
| C17—H17B | 0.9600    | C72—H72C | 0.9600     |
| C17—H17C | 0.9600    | Ce4—O34  | 2.350 (6)  |
| C18—H18A | 0.9600    | Ce4—O32  | 2.360 (5)  |
| C18—H18B | 0.9600    | Ce4—O33  | 2.365 (5)  |
| C18—H18C | 0.9600    | Ce4—O31  | 2.398 (5)  |
| C19—H19A | 0.9600    | Ce4—O40  | 2.583 (6)  |
| C19—H19B | 0.9600    | Ce4—O38  | 2.606 (6)  |
| C19—H19C | 0.9600    | Ce4—O35  | 2.609 (6)  |
| C20—H20A | 0.9600    | Ce4—O37  | 2.620 (6)  |
| C20—H20B | 0.9600    | Ce4—N55  | 3.025 (7)  |
| C20—H20C | 0.9600    | Ce4—N56  | 3.028 (7)  |
| C21—H21A | 0.9600    | P13—O31  | 1.488 (6)  |
| C21—H21B | 0.9600    | P13—N44  | 1.633 (7)  |
| C21—H21C | 0.9600    | P13—N45  | 1.634 (6)  |
| C22—H22A | 0.9600    | P13—N43  | 1.635 (7)  |
| C22—H22B | 0.9600    | P14—O32  | 1.499 (5)  |
| C22—H22C | 0.9600    | P14—N48  | 1.612 (7)  |
| C23—H23A | 0.9600    | P14—N47  | 1.631 (6)  |
| C23—H23B | 0.9600    | P14—N46  | 1.668 (6)  |
| C23—H23C | 0.9600    | P15—O33  | 1.501 (5)  |
| C24—H24A | 0.9600    | P15—N49  | 1.623 (7)  |
| C24—H24B | 0.9600    | P15—N50  | 1.625 (7)  |
| C24—H24C | 0.9600    | P15—N51  | 1.634 (8)  |
| Ce2—O12  | 2.368 (5) | P16—O34  | 1.504 (6)  |
| Ce2—O13  | 2.372 (5) | P16—N52  | 1.617 (7)  |
| Ce2—O14  | 2.380 (5) | P16—N53  | 1.626 (7)  |
| Ce2—O11  | 2.411 (5) | P16—N54  | 1.633 (7)  |
| Ce2—O20  | 2.588 (6) | O35—N55  | 1.309 (9)  |
| Ce2—O15  | 2.596 (6) | O36—N55  | 1.228 (9)  |
| Ce2—O18  | 2.610 (6) | O37—N55  | 1.257 (9)  |
| Ce2—O17  | 2.610 (6) | O38—N56  | 1.294 (9)  |
| Ce2—N28  | 3.018 (8) | O39—N56  | 1.213 (9)  |
| Ce2—N27  | 3.019 (7) | O40—N56  | 1.275 (9)  |
| P5—O11   | 1.487 (5) | N43—C73  | 1.464 (10) |
| P5—N17   | 1.624 (7) | N43—C74  | 1.466 (9)  |
| P5—N15   | 1.642 (7) | N44—C75  | 1.453 (10) |
| P5—N16   | 1.644 (7) | N44—C76  | 1.469 (10) |

|          |            |          |            |
|----------|------------|----------|------------|
| P6—O12   | 1.497 (5)  | N45—C77  | 1.468 (9)  |
| P6—N19   | 1.623 (7)  | N45—C78  | 1.473 (10) |
| P6—N20   | 1.630 (6)  | N46—C80  | 1.469 (8)  |
| P6—N18   | 1.645 (6)  | N46—C79  | 1.473 (9)  |
| P7—O13   | 1.488 (6)  | N47—C81  | 1.432 (10) |
| P7—N21   | 1.617 (7)  | N47—C82  | 1.457 (9)  |
| P7—N23   | 1.635 (8)  | N48—C84  | 1.461 (10) |
| P7—N22   | 1.637 (7)  | N48—C83  | 1.479 (10) |
| P8—O14   | 1.483 (6)  | N49—C86  | 1.459 (10) |
| P8—N24   | 1.633 (7)  | N49—C85  | 1.476 (10) |
| P8—N25   | 1.635 (7)  | N50—C88  | 1.465 (10) |
| P8—N26   | 1.640 (7)  | N50—C87  | 1.483 (10) |
| O15—N27  | 1.268 (9)  | N51—C90  | 1.436 (10) |
| O16—N27  | 1.212 (9)  | N51—C89  | 1.468 (12) |
| O17—N27  | 1.279 (9)  | N52—C92  | 1.449 (11) |
| O18—N28  | 1.266 (9)  | N52—C91  | 1.495 (11) |
| O19—N28  | 1.242 (9)  | N53—C94  | 1.457 (10) |
| O20—N28  | 1.260 (10) | N53—C93  | 1.461 (11) |
| N15—C25  | 1.454 (10) | N54—C95  | 1.447 (10) |
| N15—C26  | 1.465 (10) | N54—C96  | 1.470 (10) |
| N16—C28  | 1.459 (10) | C73—H73A | 0.9600     |
| N16—C27  | 1.467 (10) | C73—H73B | 0.9600     |
| N17—C29  | 1.446 (10) | C73—H73C | 0.9600     |
| N17—C30  | 1.481 (11) | C74—H74A | 0.9600     |
| N18—C31  | 1.448 (9)  | C74—H74B | 0.9600     |
| N18—C32  | 1.470 (9)  | C74—H74C | 0.9600     |
| N19—C33  | 1.438 (9)  | C75—H75A | 0.9600     |
| N19—C34  | 1.465 (10) | C75—H75B | 0.9600     |
| N20—C35  | 1.451 (10) | C75—H75C | 0.9600     |
| N20—C36  | 1.476 (10) | C76—H76A | 0.9600     |
| N21—C37  | 1.449 (11) | C76—H76B | 0.9600     |
| N21—C38  | 1.462 (11) | C76—H76C | 0.9600     |
| N22—C40  | 1.427 (11) | C77—H77A | 0.9600     |
| N22—C39  | 1.457 (10) | C77—H77B | 0.9600     |
| N23—C41  | 1.465 (11) | C77—H77C | 0.9600     |
| N23—C42  | 1.467 (12) | C78—H78A | 0.9600     |
| N24—C43  | 1.448 (11) | C78—H78B | 0.9600     |
| N24—C44  | 1.476 (11) | C78—H78C | 0.9600     |
| N25—C45  | 1.467 (10) | C79—H79A | 0.9600     |
| N25—C46  | 1.473 (11) | C79—H79B | 0.9600     |
| N26—C48  | 1.441 (11) | C79—H79C | 0.9600     |
| N26—C47  | 1.462 (13) | C80—H80A | 0.9600     |
| C25—H25A | 0.9600     | C80—H80B | 0.9600     |
| C25—H25B | 0.9600     | C80—H80C | 0.9600     |
| C25—H25C | 0.9600     | C81—H81A | 0.9600     |
| C26—H26A | 0.9600     | C81—H81B | 0.9600     |
| C26—H26B | 0.9600     | C81—H81C | 0.9600     |
| C26—H26C | 0.9600     | C82—H82A | 0.9600     |
| C27—H27A | 0.9600     | C82—H82B | 0.9600     |

## supplementary materials

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| C27—H27B | 0.9600 | C82—H82C | 0.9600 |
| C27—H27C | 0.9600 | C83—H83A | 0.9600 |
| C28—H28A | 0.9600 | C83—H83B | 0.9600 |
| C28—H28B | 0.9600 | C83—H83C | 0.9600 |
| C28—H28C | 0.9600 | C84—H84A | 0.9600 |
| C29—H29A | 0.9600 | C84—H84B | 0.9600 |
| C29—H29B | 0.9600 | C84—H84C | 0.9600 |
| C29—H29C | 0.9600 | C85—H85A | 0.9600 |
| C30—H30A | 0.9600 | C85—H85B | 0.9600 |
| C30—H30B | 0.9600 | C85—H85C | 0.9600 |
| C30—H30C | 0.9600 | C86—H86A | 0.9600 |
| C31—H31A | 0.9600 | C86—H86B | 0.9600 |
| C31—H31B | 0.9600 | C86—H86C | 0.9600 |
| C31—H31C | 0.9600 | C87—H87A | 0.9600 |
| C32—H32A | 0.9600 | C87—H87B | 0.9600 |
| C32—H32B | 0.9600 | C87—H87C | 0.9600 |
| C32—H32C | 0.9600 | C88—H88A | 0.9600 |
| C33—H33A | 0.9600 | C88—H88B | 0.9600 |
| C33—H33B | 0.9600 | C88—H88C | 0.9600 |
| C33—H33C | 0.9600 | C89—H89A | 0.9600 |
| C34—H34A | 0.9600 | C89—H89B | 0.9600 |
| C34—H34B | 0.9600 | C89—H89C | 0.9600 |
| C34—H34C | 0.9600 | C90—H90A | 0.9600 |
| C35—H35A | 0.9600 | C90—H90B | 0.9600 |
| C35—H35B | 0.9600 | C90—H90C | 0.9600 |
| C35—H35C | 0.9600 | C91—H91A | 0.9600 |
| C36—H36A | 0.9600 | C91—H91B | 0.9600 |
| C36—H36B | 0.9600 | C91—H91C | 0.9600 |
| C36—H36C | 0.9600 | C92—H92A | 0.9600 |
| C37—H37A | 0.9600 | C92—H92B | 0.9600 |
| C37—H37B | 0.9600 | C92—H92C | 0.9600 |
| C37—H37C | 0.9600 | C93—H93A | 0.9600 |
| C38—H38A | 0.9600 | C93—H93B | 0.9600 |
| C38—H38B | 0.9600 | C93—H93C | 0.9600 |
| C38—H38C | 0.9600 | C94—H94A | 0.9600 |
| C39—H39A | 0.9600 | C94—H94B | 0.9600 |
| C39—H39B | 0.9600 | C94—H94C | 0.9600 |
| C39—H39C | 0.9600 | C95—H95A | 0.9600 |
| C40—H40A | 0.9600 | C95—H95B | 0.9600 |
| C40—H40B | 0.9600 | C95—H95C | 0.9600 |
| C40—H40C | 0.9600 | C96—H96A | 0.9600 |
| C41—H41A | 0.9600 | C96—H96B | 0.9600 |
| C41—H41B | 0.9600 | C96—H96C | 0.9600 |
| C41—H41C | 0.9600 |          |        |

Symmetry codes: (i)  $x, y, z-1$ ; (ii)  $x, y, z+1$ .

Fig. 1

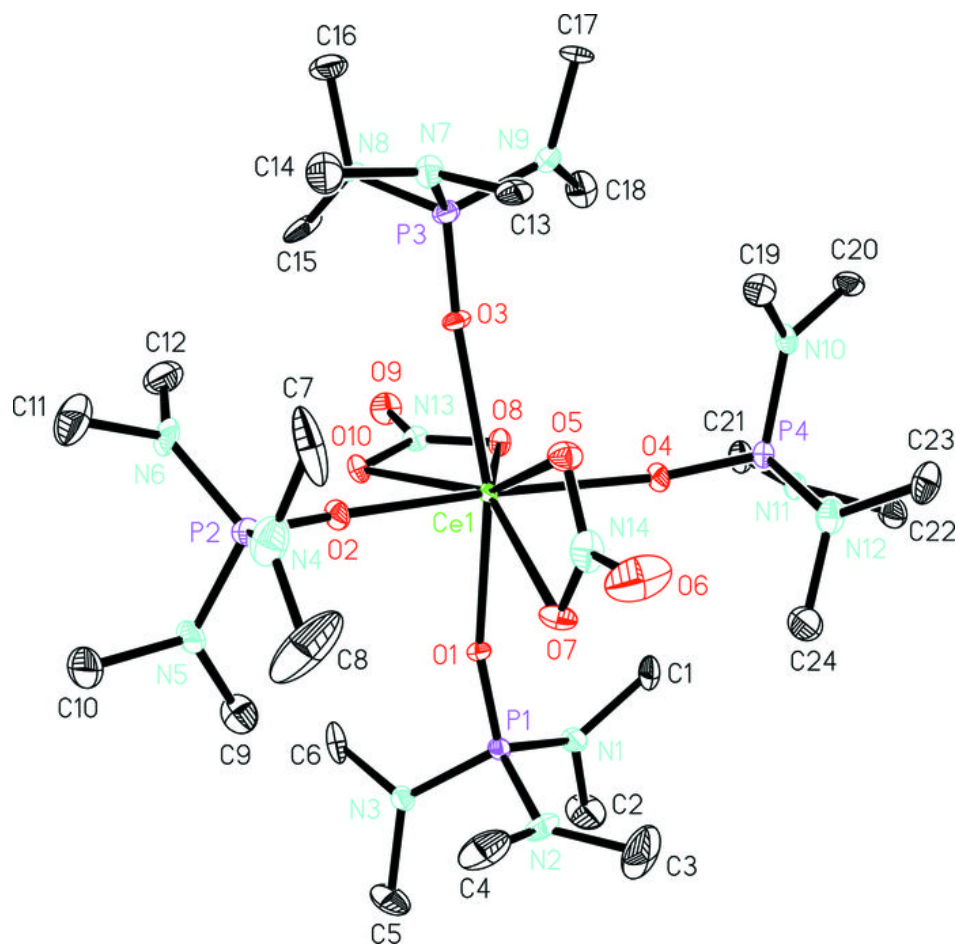


Fig. 2

