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# Hexa-$\mu$-chlorido-hexachlorido($\eta^6$-hexamethylbenzene)trialuminium(III)-lanthanum(III) benzene solvate

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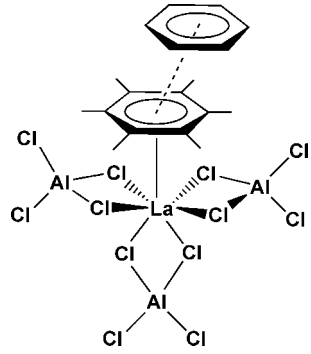
Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.005 Å; disorder in main residue; $R$ factor = 0.025; $wR$ factor = 0.063; data-to-parameter ratio = 22.5.

In the title compound, $[Al_3LaCl_{12}(C_{12}H_{18})]\cdot C_6H_6$, all molecules are located on a mirror plane. Three chloridoaluminate groups and a hexamethylbenzene molecule are bound to the central lanthanum(III) ion, forming a distorted pentagonal bipyramid with the $\eta^6$-coordinated arene located at the apical position. The hexamethylbenzene ligand disordered between two orientations in a 1:1 ratio is also involved in parallel-slipped $\pi$–$\pi$ stacking intermolecular interactions with a benzene solvent molecule [centroid–centroid distance 3.612 (4) Å].

## Related literature

For the previously characterized lanthanum chloroaluminate and chlorogallate complexes, see: Filatov *et al.* (2008). For a recent review of other lanthanide chloroaluminate complexes, see: Bochkarev (2002). For complexes of lanthanide chlorogallates with polycyclic aromatic systems, see: Gorlov *et al.* (2008).




## Experimental

### Crystal data

$[Al_3LaCl_{12}(C_{12}H_{18})]\cdot C_6H_6$
$M_r$ = 885.62
Orthorhombic, *Pnma*
$a$ = 12.2127 (6) Å
$b$ = 16.4205 (8) Å
$c$ = 16.9790 (8) Å
$V$ = 3404.9 (3) Å$^3$
$Z$ = 4
Mo- $K\alpha$ radiation
$\mu$ = 2.28 mm$^{-1}$
$T$ = 173 K
0.22 × 0.20 × 0.16 mm

### Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
$T_{min}$ = 0.613, $T_{max}$ = 0.697
28535 measured reflections
4250 independent reflections
3911 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.018

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.063
$S$ = 1.05
4250 reflections
189 parameters
H-atom parameters not refined
$\Delta\rho_{max}$ = 0.89 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.99 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| La1—C1 | 2.945 (3) | La1—Cl4 | 2.9298 (6) |
| La1—C2 | 2.965 (2) | La1—Cl5 | 2.9083 (7) |
| La1—C3 | 2.957 (3) | La1—Cl6 | 2.9097 (7) |
| La1—C4 | 2.941 (4) | La1—*Cg*1 | 2.613 (3) |
| La1—Cl3 | 2.9128 (5) | | |

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL* and *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2516).

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# supplementary materials

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# Hexa-$\mu$-chlorido-hexachlorido($\eta^6$-hexamethylbenzene)trialuminium(III)lanthanum(III) benzene solvate

**A. S. Filatov, S. N. Gifford, D. K. Kumar and M. A. Petrukhina**

## Comment

We have recently reported X-ray structural characterization of the first two lanthanum(III) chloroaluminate complexes with neutral arenes, [La($\eta^6$-$C_6H_5Me$)($AlCl_4$)$_3$] and [La($\eta^6$-$C_6Me_6$)($AlCl_4$)$_3$], as well as of the first lanthanum(III) chlorogallate complex, [La($\eta^6$-$C_6Me_6$)($GaCl_4$)$_3$] (Filatov *et al.*, 2008). The [La($\eta^6$-$C_6Me_6$)($AlCl_4$)$_3$]·0.5$C_6H_6$ complex crystallizes in the monoclinic $P2_1/c$ space group with the $\beta$ angle being close to 90° ($\beta$ = 90.27°). We later found that under slightly different experimental conditions, namely at a higher temperature (285 *versus* 273 K), the lanthanum complex with hexamethylbenzene, [La($\eta^6$-$C_6Me_6$)($AlCl_4$)$_3$]·$C_6H_6$ (I), is crystallized.

The molecular structure of (I) is comprised of the three chloroaluminate groups and a hexamethylbenzene molecule bound to the central lanthanum(III) ion (Fig.1). The coordination polyhedron is a distorted pentagonal bipyramid with the $\eta^6$-arene located at the apical position. The La–C bond distances span from 2.941 (4) to 2.965 (2) Å with a La–centroid distance being 2.613 (3) Å. These distances are comparable to those found in the previously reported complex [La($\eta^6$-$C_6Me_6$)($AlCl_4$)$_3$]·0.5$C_6H_6$ (II) [La—C 2.927 (7)–3.035 (7)Å; La–centroid 2.633 (7)Å].

In (I), coordinated hexamethylbenzene is engaged into π-π stacking interactions with a solvent benzene molecule. The intercentroid distance between their 6-membered rings is 3.612 (4) Å. The two ring planes are not parallel and the dihedral angle is 12.7° (Fig.2). In the above hemisolvate (II), on the contrary, both benzene faces are involved in π-π stacking interactions as benzene is sandwiched between two hexamethylbenzene molecules. The distance between the centroids of the hexamethylbenzene and benzene rings (3.688 (4) Å) is noticeably longer than that found in (I).

## Experimental

$LaCl_3$ (100 mg, 0.41 mmol), $AlCl_3$ (163 mg, 1.22 mmol), hexamethylbenzene (66 mg, 0.41 mmol) and an excess of aluminium foil were placed into a Schlenk flask inside the glove box. Benzene (10 ml) was added to the flask and the mixture was refluxed for two hours. The $LaCl_3$, $AlCl_3$, and hexamethylbenzene dissolved completely to give a yellow solution. The solution was filtered while hot through a pad of Celite and then kept at 12°C under argon for 2 days to afford a yellow crystalline material. Yield: 240 mg (65%). IR data ($cm^{-1}$): 3091 (w), 3071 (w), 3036 (w), 1598 (*m*), 1531 (w), 1478 (*m*), 1423 (*s*), 1382 (*m*), 1332 (*m*), 1272 (*m*), 1180 (w), 1076 (w), 983 (w), 824 (w), 677 (*s*).

## Refinement

All C—H atoms were refined using the riding model approximation, with C—H = 0.95–0.98Å [$U_{iso}$(H) = 1.2 or 1.5Ueq(C)]. All other atoms were refined anisotropically. Large anisotropy of the carbon atoms of hexamethylbenzene suggests the

presence of disorder. It was modeled over two rotational orientations in a 1:1 ratio. The C5 and C8 carbon atoms lie on a mirror plane and are constrained to have identical anisotropic displacement parameters (EADP command in the *SHELXL* realm).

## Figures

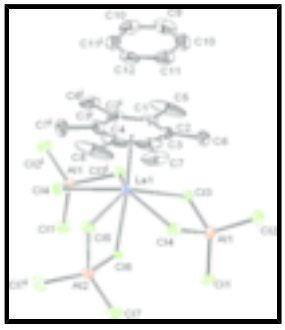


Fig. 1. A view of the molecular structure of (I), along with the atom numbering scheme [symmetry code: (i) *x*, -*y* + 1/2, *z*]. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen atoms and disordered parts are omitted for clarity.

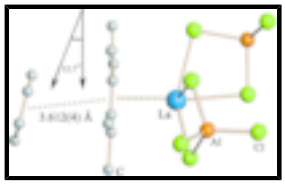


Fig. 2. A view of the molecular structure of (I) showing π-π stacking interactions between co-ordinated $C_6Me_6$ and benzene rings.

## Hexa-μ-chlorido-hexachlorido(η$^6$- hexamethylbenzene)trialuminium(III)lanthanum(III) benzene solvate

*Crystal data*

| | |
|---|---|
| $[Al_3LaCl_{12}(C_{12}H_{18})]\cdot C_6H_6$ | $F_{000}$ = 1728 |
| $M_r$ = 885.62 | $D_x$ = 1.728 Mg m$^{-3}$ |
| Orthorhombic, *Pnma* | Mo- *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ac 2n | Cell parameters from 7019 reflections |
| *a* = 12.2127 (6) Å | θ = 2.5–28.2º |
| *b* = 16.4205 (8) Å | μ = 2.28 mm$^{-1}$ |
| *c* = 16.9790 (8) Å | *T* = 173 K |
| *V* = 3404.9 (3) Å$^3$ | Block, yellow |
| *Z* = 4 | 0.22 × 0.20 × 0.16 mm |

*Data collection*

| | |
|---|---|
| Bruker SMART APEX CCD area-detector diffractometer | 4250 independent reflections |
| Radiation source: fine-focus sealed tube | 3911 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.018 |
| *T* = 173 K | $\theta_{max}$ = 28.3º |
| 0.30° ω scans | $\theta_{min}$ = 2.1º |
| Absorption correction: multi-scan (SADABS; Bruker, 2003) | *h* = −15→16 |

| | |
|---|---|
| $T_{min}$ = 0.613, $T_{max}$ = 0.697 | $k$ = −21→21 |
| 28535 measured reflections | $l$ = −22→22 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.025 | H-atom parameters not refined |
| $wR(F^2)$ = 0.063 | $w = 1/[\sigma^2(F_o^2) + (0.0304P)^2 + 3.1621P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 1.05 | $(\Delta/\sigma)_{max} < 0.001$ |
| 4250 reflections | $\Delta\rho_{max}$ = 0.89 e Å$^{-3}$ |
| 189 parameters | $\Delta\rho_{min}$ = −0.98 e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| La1 | 0.106393 (12) | 0.2500 | 0.425620 (9) | 0.02758 (6) | |
| Al1 | 0.09537 (6) | 0.04272 (4) | 0.32343 (5) | 0.04146 (16) | |
| Al2 | −0.20200 (8) | 0.2500 | 0.41914 (6) | 0.0403 (2) | |
| Cl1 | −0.02765 (6) | 0.03298 (4) | 0.23836 (5) | 0.06224 (19) | |
| Cl2 | 0.18966 (7) | −0.06204 (4) | 0.34109 (6) | 0.0684 (2) | |
| Cl3 | 0.19872 (5) | 0.14875 (3) | 0.30139 (3) | 0.04206 (13) | |
| Cl4 | 0.02586 (5) | 0.08226 (4) | 0.43571 (3) | 0.04489 (14) | |
| Cl5 | −0.09121 (6) | 0.2500 | 0.52121 (4) | 0.04250 (18) | |
| Cl6 | −0.08346 (6) | 0.2500 | 0.32208 (4) | 0.03682 (16) | |
| Cl7 | −0.29273 (6) | 0.14181 (5) | 0.41927 (4) | 0.05841 (18) | |
| C1 | 0.3384 (3) | 0.2500 | 0.4729 (2) | 0.0515 (10) | |
| C2 | 0.3003 (3) | 0.17691 (17) | 0.50333 (19) | 0.0609 (8) | |
| C3 | 0.2212 (3) | 0.1777 (3) | 0.5621 (2) | 0.0823 (13) | |
| C4 | 0.1820 (3) | 0.2500 | 0.5901 (2) | 0.096 (3) | |
| C5 | 0.4271 (4) | 0.2500 | 0.4107 (3) | 0.194 (5) | |
| H5A | 0.4789 | 0.2943 | 0.4214 | 0.291* | 0.50 |

| | | | | | |
|---|---|---|---|---|---|
| H5B | 0.3940 | 0.2580 | 0.3587 | 0.291* | 0.50 |
| H5C | 0.4659 | 0.1978 | 0.4118 | 0.291* | 0.50 |
| C6 | 0.3258 (8) | 0.0879 (6) | 0.4928 (7) | 0.087 (3) | 0.50 |
| H6A | 0.3781 | 0.0706 | 0.5332 | 0.130* | 0.50 |
| H6B | 0.3577 | 0.0791 | 0.4405 | 0.130* | 0.50 |
| H6C | 0.2583 | 0.0561 | 0.4977 | 0.130* | 0.50 |
| C7 | 0.1582 (8) | 0.1206 (6) | 0.6166 (5) | 0.093 (3) | 0.50 |
| H7A | 0.1812 | 0.1299 | 0.6711 | 0.139* | 0.50 |
| H7B | 0.1735 | 0.0640 | 0.6019 | 0.139* | 0.50 |
| H7C | 0.0796 | 0.1312 | 0.6117 | 0.139* | 0.50 |
| C6X | 0.3773 (8) | 0.1077 (7) | 0.4617 (6) | 0.084 (4) | 0.50 |
| H6X1 | 0.4398 | 0.0956 | 0.4959 | 0.126* | 0.50 |
| H6X2 | 0.4039 | 0.1281 | 0.4109 | 0.126* | 0.50 |
| H6X3 | 0.3344 | 0.0581 | 0.4533 | 0.126* | 0.50 |
| C7X | 0.2146 (9) | 0.0787 (5) | 0.5824 (6) | 0.092 (3) | 0.50 |
| H7X1 | 0.1425 | 0.0659 | 0.6045 | 0.137* | 0.50 |
| H7X2 | 0.2716 | 0.0646 | 0.6206 | 0.137* | 0.50 |
| H7X3 | 0.2257 | 0.0473 | 0.5339 | 0.137* | 0.50 |
| C8 | 0.1026 (4) | 0.2500 | 0.6586 (3) | 0.194 (5) | |
| H8A | 0.0691 | 0.1960 | 0.6636 | 0.291* | 0.50 |
| H8B | 0.0454 | 0.2907 | 0.6494 | 0.291* | 0.50 |
| H8C | 0.1420 | 0.2633 | 0.7072 | 0.291* | 0.50 |
| C9 | 0.5948 (4) | 0.2500 | 0.6119 (3) | 0.088 (2) | |
| H9 | 0.6600 | 0.2500 | 0.5814 | 0.106* | |
| C10 | 0.5464 (3) | 0.1771 (2) | 0.6345 (2) | 0.0750 (10) | |
| H10 | 0.5779 | 0.1265 | 0.6193 | 0.090* | |
| C11 | 0.4547 (3) | 0.1790 (2) | 0.6780 (2) | 0.0679 (9) | |
| H11 | 0.4212 | 0.1293 | 0.6936 | 0.082* | |
| C12 | 0.4094 (3) | 0.2500 | 0.7000 (3) | 0.0646 (12) | |
| H12 | 0.3449 | 0.2500 | 0.7312 | 0.077* | |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| La1 | 0.02175 (8) | 0.03570 (10) | 0.02528 (9) | 0.000 | 0.00028 (5) | 0.000 |
| Al1 | 0.0428 (4) | 0.0342 (3) | 0.0475 (4) | −0.0003 (3) | −0.0093 (3) | −0.0026 (3) |
| Al2 | 0.0247 (4) | 0.0577 (6) | 0.0384 (5) | 0.000 | 0.0008 (4) | 0.000 |
| Cl1 | 0.0664 (4) | 0.0525 (4) | 0.0678 (4) | 0.0015 (3) | −0.0311 (3) | −0.0082 (3) |
| Cl2 | 0.0666 (4) | 0.0438 (3) | 0.0947 (6) | 0.0136 (3) | −0.0232 (4) | −0.0036 (4) |
| Cl3 | 0.0434 (3) | 0.0424 (3) | 0.0404 (3) | −0.0030 (2) | 0.0099 (2) | −0.0068 (2) |
| Cl4 | 0.0460 (3) | 0.0431 (3) | 0.0456 (3) | −0.0101 (2) | 0.0013 (2) | 0.0080 (2) |
| Cl5 | 0.0288 (3) | 0.0687 (5) | 0.0300 (3) | 0.000 | 0.0031 (3) | 0.000 |
| Cl6 | 0.0277 (3) | 0.0530 (4) | 0.0298 (3) | 0.000 | −0.0025 (3) | 0.000 |
| Cl7 | 0.0418 (3) | 0.0720 (5) | 0.0615 (4) | −0.0171 (3) | 0.0028 (3) | −0.0021 (3) |
| C1 | 0.0227 (14) | 0.099 (3) | 0.0325 (16) | 0.000 | −0.0035 (12) | 0.000 |
| C2 | 0.0654 (17) | 0.0486 (14) | 0.0688 (18) | 0.0173 (13) | −0.0438 (16) | −0.0151 (13) |
| C3 | 0.071 (2) | 0.114 (3) | 0.0617 (19) | −0.055 (2) | −0.0416 (18) | 0.055 (2) |
| C4 | 0.0269 (19) | 0.237 (9) | 0.0259 (18) | 0.000 | −0.0009 (14) | 0.000 |

| | | | | | | |
|---|---|---|---|---|---|---|
| C5 | 0.0328 (17) | 0.507 (15) | 0.0414 (19) | 0.000 | 0.0080 (14) | 0.000 |
| C6 | 0.082 (7) | 0.060 (5) | 0.118 (9) | 0.034 (5) | −0.054 (6) | −0.025 (5) |
| C7 | 0.099 (7) | 0.110 (7) | 0.070 (5) | −0.061 (6) | −0.042 (5) | 0.058 (5) |
| C6X | 0.075 (6) | 0.089 (8) | 0.087 (7) | 0.044 (6) | −0.037 (5) | −0.040 (6) |
| C7X | 0.111 (8) | 0.067 (5) | 0.097 (7) | −0.032 (5) | −0.053 (6) | 0.048 (5) |
| C8 | 0.0328 (17) | 0.507 (15) | 0.0414 (19) | 0.000 | 0.0080 (14) | 0.000 |
| C9 | 0.052 (3) | 0.172 (7) | 0.041 (2) | 0.000 | 0.0042 (19) | 0.000 |
| C10 | 0.081 (2) | 0.080 (2) | 0.0634 (19) | 0.029 (2) | −0.0217 (18) | −0.0169 (17) |
| C11 | 0.070 (2) | 0.069 (2) | 0.0653 (19) | −0.0142 (17) | −0.0277 (16) | 0.0189 (16) |
| C12 | 0.039 (2) | 0.105 (4) | 0.049 (2) | 0.000 | −0.0136 (17) | 0.000 |

*Geometric parameters (Å, °)*

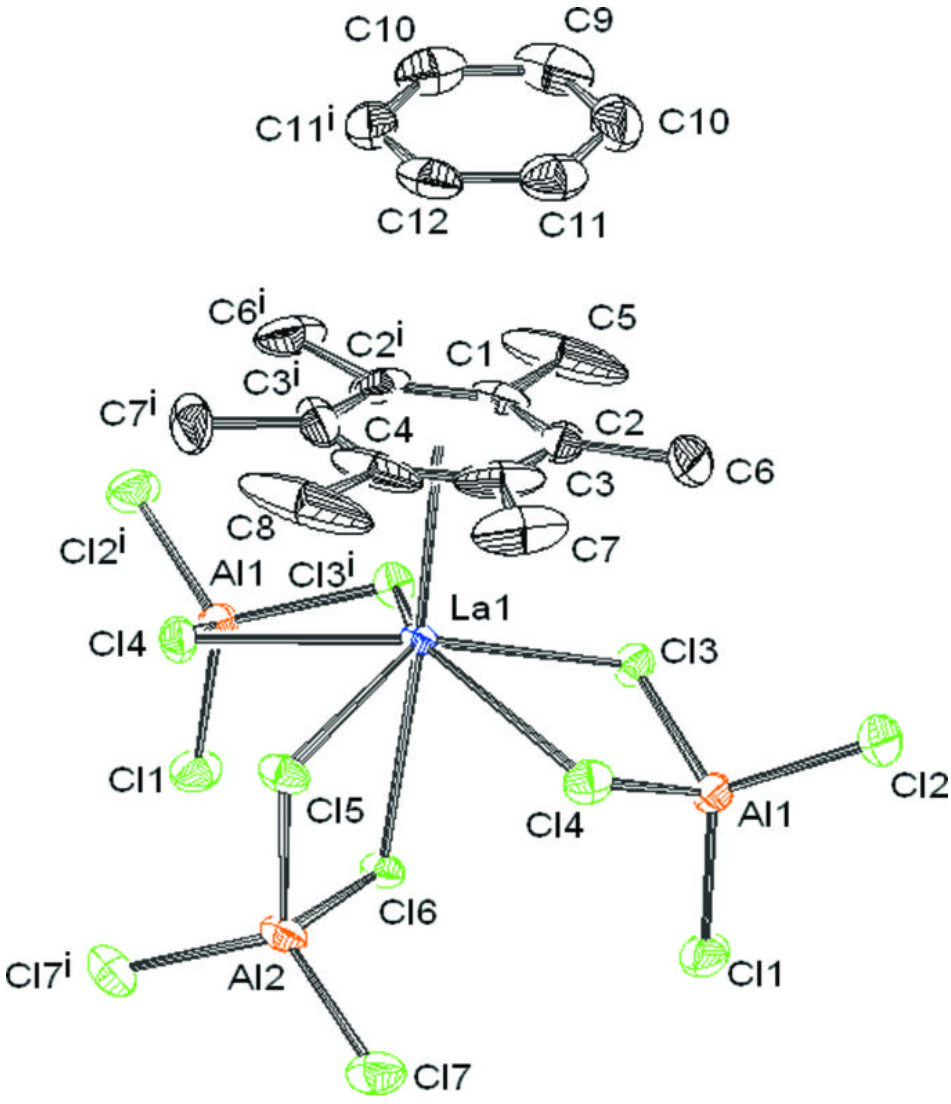
| | | | |
|---|---|---|---|
| La1—C1 | 2.945 (3) | C3—C7X | 1.663 (8) |
| La1—C2 | 2.965 (2) | C4—C3$^{i}$ | 1.366 (5) |
| La1—C3 | 2.957 (3) | C4—C8 | 1.514 (6) |
| La1—C4 | 2.941 (4) | C5—H5A | 0.9800 |
| La1—Cl3 | 2.9128 (5) | C5—H5B | 0.9800 |
| La1—Cl4 | 2.9298 (6) | C5—H5C | 0.9800 |
| La1—Cl5 | 2.9083 (7) | C8—H8A | 0.9800 |
| La1—Cl6 | 2.9097 (7) | C8—H8B | 0.9800 |
| La1—Cg1 | 2.613 (3) | C8—H8C | 0.9800 |
| Cg1—Cg2 | 3.612 (4) | C6—H6A | 0.9800 |
| La1—Cl3$^{i}$ | 2.9128 (5) | C6—H6B | 0.9800 |
| La1—Cl4$^{i}$ | 2.9298 (6) | C6—H6C | 0.9800 |
| La1—C3$^{i}$ | 2.957 (3) | C7—H7A | 0.9800 |
| La1—C2$^{i}$ | 2.965 (2) | C7—H7B | 0.9800 |
| Al1—Cl1 | 2.0902 (10) | C7—H7C | 0.9800 |
| Al1—Cl2 | 2.0918 (10) | C6X—H6X1 | 0.9800 |
| Al1—Cl3 | 2.1828 (9) | C6X—H6X2 | 0.9800 |
| Al1—Cl4 | 2.1855 (10) | C6X—H6X3 | 0.9800 |
| Al2—Cl7 | 2.0937 (9) | C7X—H7X1 | 0.9800 |
| Al2—Cl7$^{i}$ | 2.0937 (9) | C7X—H7X2 | 0.9800 |
| Al2—Cl6 | 2.1936 (12) | C7X—H7X3 | 0.9800 |
| Al2—Cl5 | 2.1987 (12) | C9—C10 | 1.389 (5) |
| C1—C2$^{i}$ | 1.387 (4) | C9—C10$^{i}$ | 1.389 (5) |
| C1—C2 | 1.387 (4) | C9—H9 | 0.9500 |
| C1—C5 | 1.513 (6) | C10—C11 | 1.343 (5) |
| C2—C3 | 1.389 (5) | C10—H10 | 0.9500 |
| C2—C6 | 1.505 (10) | C11—C12 | 1.344 (4) |
| C2—C6X | 1.635 (10) | C11—H11 | 0.9500 |
| C3—C4 | 1.366 (5) | C12—C11$^{i}$ | 1.344 (4) |
| C3—C7 | 1.525 (7) | C12—H12 | 0.9500 |
| Cl5—La1—Cl6 | 71.09 (2) | Cl7—Al2—Cl5 | 108.96 (4) |
| Cl5—La1—Cl3 | 136.497 (15) | Cl7$^{i}$—Al2—Cl5 | 108.96 (4) |
| Cl6—La1—Cl3 | 82.586 (17) | Cl6—Al2—Cl5 | 100.72 (5) |
| Cl5—La1—Cl3$^{i}$ | 136.497 (14) | Al1—Cl3—La1 | 96.16 (3) |

| | | | |
|---|---|---|---|
| Cl6—La1—Cl3$^{i}$ | 82.586 (17) | Al1—Cl4—La1 | 95.61 (3) |
| Cl3—La1—Cl3$^{i}$ | 69.61 (2) | Al2—Cl5—La1 | 94.06 (4) |
| Cl5—La1—Cl4 | 71.868 (13) | Al2—Cl6—La1 | 94.13 (4) |
| Cl6—La1—Cl4 | 76.576 (13) | C2$^{i}$—C1—C2 | 119.9 (4) |
| Cl3—La1—Cl4 | 68.636 (17) | C2$^{i}$—C1—C5 | 119.99 (18) |
| Cl3$^{i}$—La1—Cl4 | 135.147 (17) | C2—C1—C5 | 119.99 (18) |
| Cl5—La1—Cl4$^{i}$ | 71.868 (13) | C2$^{i}$—C1—La1 | 77.23 (17) |
| Cl6—La1—Cl4$^{i}$ | 76.576 (13) | C2—C1—La1 | 77.23 (17) |
| Cl3—La1—Cl4$^{i}$ | 135.147 (17) | C5—C1—La1 | 119.9 (3) |
| Cl3$^{i}$—La1—Cl4$^{i}$ | 68.636 (17) | C1—C2—C3 | 119.5 (3) |
| Cl4—La1—Cl4$^{i}$ | 140.15 (3) | C1—C2—C6 | 136.6 (6) |
| Cl5—La1—C4 | 74.37 (8) | C3—C2—C6 | 103.8 (6) |
| Cl6—La1—C4 | 145.46 (8) | C1—C2—La1 | 75.63 (16) |
| Cl3—La1—C4 | 124.47 (6) | C3—C2—La1 | 76.11 (16) |
| Cl3$^{i}$—La1—C4 | 124.47 (6) | C6—C2—La1 | 120.4 (4) |
| Cl4—La1—C4 | 92.86 (3) | C6X—C2—La1 | 123.2 (4) |
| Cl4$^{i}$—La1—C4 | 92.86 (3) | C4—C3—C2 | 120.1 (3) |
| Cl5—La1—C1 | 130.25 (7) | C4—C3—C7 | 98.4 (6) |
| Cl6—La1—C1 | 158.66 (7) | C2—C3—C7 | 141.3 (6) |
| Cl3—La1—C1 | 79.93 (6) | C4—C3—La1 | 76.0 (2) |
| Cl3$^{i}$—La1—C1 | 79.93 (6) | C2—C3—La1 | 76.76 (15) |
| Cl4—La1—C1 | 107.879 (16) | C7—C3—La1 | 118.9 (3) |
| Cl4$^{i}$—La1—C1 | 107.879 (17) | C3$^{i}$—C4—C3 | 120.8 (4) |
| C4—La1—C1 | 55.88 (10) | C3$^{i}$—C4—C8 | 119.5 (2) |
| Cl5—La1—C3$^{i}$ | 87.49 (8) | C3—C4—C8 | 119.5 (2) |
| Cl6—La1—C3$^{i}$ | 148.34 (6) | C3$^{i}$—C4—La1 | 77.2 (2) |
| Cl3—La1—C3$^{i}$ | 127.81 (6) | C3—C4—La1 | 77.2 (2) |
| Cl3$^{i}$—La1—C3$^{i}$ | 98.90 (10) | C8—C4—La1 | 121.9 (3) |
| Cl4—La1—C3$^{i}$ | 119.39 (10) | C1—C5—H5A | 109.5 |
| Cl4$^{i}$—La1—C3$^{i}$ | 74.68 (7) | C1—C5—H5B | 109.5 |
| C4—La1—C3$^{i}$ | 26.77 (10) | H5A—C5—H5B | 109.5 |
| C1—La1—C3$^{i}$ | 47.94 (8) | C1—C5—H5C | 109.5 |
| Cl5—La1—C3 | 87.49 (8) | H5A—C5—H5C | 109.5 |
| Cl6—La1—C3 | 148.34 (6) | H5B—C5—H5C | 109.5 |
| Cl3—La1—C3 | 98.90 (10) | C4—C8—H8A | 109.5 |
| Cl3$^{i}$—La1—C3 | 127.81 (6) | C4—C8—H8B | 109.5 |
| Cl4—La1—C3 | 74.68 (7) | H8A—C8—H8B | 109.5 |
| Cl4$^{i}$—La1—C3 | 119.39 (10) | C4—C8—H8C | 109.5 |
| C4—La1—C3 | 26.77 (10) | H8A—C8—H8C | 109.5 |
| C1—La1—C3 | 47.94 (8) | H8B—C8—H8C | 109.5 |
| C3$^{i}$—La1—C3 | 47.35 (17) | C2—C6—H6A | 109.5 |
| Cl5—La1—C2$^{i}$ | 114.49 (8) | C2—C6—H6B | 109.5 |
| Cl6—La1—C2$^{i}$ | 154.88 (5) | C2—C6—H6C | 109.5 |

| | | | |
|---|---|---|---|
| Cl3—La1—C2$^{i}$ | 104.12 (8) | C3—C7—H7A | 109.5 |
| Cl3$^{i}$—La1—C2$^{i}$ | 77.41 (6) | C3—C7—H7B | 109.5 |
| Cl4—La1—C2$^{i}$ | 128.51 (5) | C3—C7—H7C | 109.5 |
| Cl4$^{i}$—La1—C2$^{i}$ | 82.04 (6) | C2—C6X—H6X1 | 109.5 |
| C4—La1—C2$^{i}$ | 47.68 (9) | C2—C6X—H6X2 | 109.5 |
| C1—La1—C2$^{i}$ | 27.14 (7) | H6X1—C6X—H6X2 | 109.5 |
| C3$^{i}$—La1—C2$^{i}$ | 27.13 (10) | C2—C6X—H6X3 | 109.5 |
| C3—La1—C2$^{i}$ | 55.61 (8) | H6X1—C6X—H6X3 | 109.5 |
| Cl5—La1—C2 | 114.49 (8) | H6X2—C6X—H6X3 | 109.5 |
| Cl6—La1—C2 | 154.88 (5) | C3—C7X—H7X1 | 109.5 |
| Cl3—La1—C2 | 77.41 (6) | C3—C7X—H7X2 | 109.5 |
| Cl3$^{i}$—La1—C2 | 104.12 (8) | H7X1—C7X—H7X2 | 109.5 |
| Cl4—La1—C2 | 82.04 (6) | C3—C7X—H7X3 | 109.5 |
| Cl4$^{i}$—La1—C2 | 128.51 (5) | H7X1—C7X—H7X3 | 109.5 |
| C4—La1—C2 | 47.68 (9) | H7X2—C7X—H7X3 | 109.5 |
| C1—La1—C2 | 27.14 (7) | C10—C9—C10$^{i}$ | 119.1 (5) |
| C3$^{i}$—La1—C2 | 55.61 (8) | C10—C9—H9 | 120.5 |
| C3—La1—C2 | 27.13 (10) | C10$^{i}$—C9—H9 | 120.5 |
| C2$^{i}$—La1—C2 | 47.76 (11) | C11—C10—C9 | 119.2 (4) |
| Cl1—Al1—Cl2 | 115.58 (4) | C11—C10—H10 | 120.4 |
| Cl1—Al1—Cl3 | 110.99 (4) | C9—C10—H10 | 120.4 |
| Cl2—Al1—Cl3 | 111.24 (4) | C10—C11—C12 | 121.1 (4) |
| Cl1—Al1—Cl4 | 110.26 (4) | C10—C11—H11 | 119.5 |
| Cl2—Al1—Cl4 | 109.45 (5) | C12—C11—H11 | 119.5 |
| Cl3—Al1—Cl4 | 97.89 (3) | C11$^{i}$—C12—C11 | 120.5 (5) |
| Cl7—Al2—Cl7$^{i}$ | 116.10 (6) | C11$^{i}$—C12—H12 | 119.8 |
| Cl7—Al2—Cl6 | 110.49 (4) | C11—C12—H12 | 119.8 |
| Cl7$^{i}$—Al2—Cl6 | 110.49 (4) | | |

Symmetry codes: (i) *x*, −*y*+1/2, *z*.

**Fig. 1**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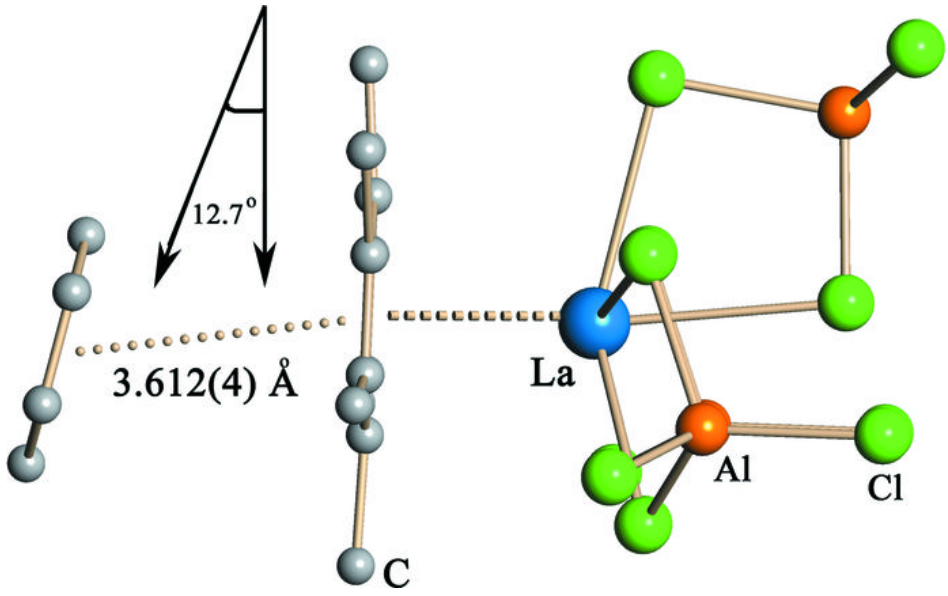
**Fig. 2**