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# Structure of $\mu_3$-(1–6-$\eta$-Bitropyl)-carbido-$\mu$-carbonyl-tridecacarbonyl-*octahedro*-hexaruthenium

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**Abstract.** $[Ru_6C(C_{14}H_{14})(CO)_{14}]$, monoclinic, $P2_1/c$, $a = 10{\cdot}393\,(1)$, $b = 16{\cdot}568\,(2)$, $c = 19{\cdot}646\,(2)$ Å, $\beta = 101{\cdot}24\,(8)^\circ$, $Z = 4$, $D_c = 2{\cdot}37$ Mg m$^{-3}$. 3672 independent reflections have been used to refine the structure, giving an $R$ value of 0·031. The central C atom lies close to the center of a slightly distorted octahedron of Ru atoms. The mean Ru—C distance is 2·055 Å. The $Ru_6$ cluster has one bridging and thirteen terminal carbonyl groupings. A bitropyl molecule resides on one triangular face of the cluster.

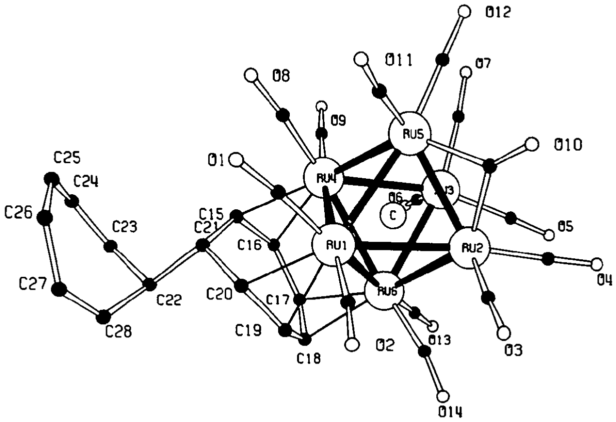

Fig. 1. The molecular configuration and numbering scheme.

**Introduction.** The high-yield synthesis of $[Ru_6C(CO)_{14}(\text{bitropyl})]$ from $[NMe_4]_2[Ru_6C(CO)_{16}]$ has been discussed by Bradley & Ansell (1979). Intensity data for $0 < 2\theta < 45^\circ$ (Mo $K\alpha$) were collected using a crystal of dimensions 0·22 × 0·22 × 0·20 mm encapsulated in a thin glass tube on an Enraf–Nonius CAD-4 diffractometer.* A variable scan rate (4–20° min$^{-1}$) was used for data collection with fast scans for intense reflections and slower scans for weaker ones. 4278 independent reflections were measured. Of these, 3672 had $F > 3\sigma(I)$ and were utilized for the subsequent structure solution and refinement. $\{\sigma(I) = [S^2(C + R^2B) + (pI)^2]^{1/2}$ where $S$ = scan rate, $C$ is the total integrated peak count, $R$ is the ratio of scan time to background counting time, $B$ is the background count and parameter $p$ is the factor introduced to down-weight intense reflections and was set to 0·05.$\}$ The crystal remained stable throughout the collection period. An absorption correction was not made since $\psi$ scans indicated that the correction to $I$ was small. The structure was solved using a combination of direct methods (*MULTAN*), Fourier maps and least-squares techniques. During the final stages of least-squares refinement, all atoms were assigned anisotropic temperature factors. Ru scattering factors were corrected for anomalous dispersion ($f' = -1{\cdot}2$, $f'' = 1{\cdot}1$ e). A weighting scheme was chosen such that for $F > 85$ $\sqrt{w} = 85/F_o$, for $41 < F < 85$ $\sqrt{w} = 1$ and for $F \le 41$ $\sqrt{w} = F_o/41$. This gave similar average $w\Delta^2$ values for ranges of increasing $F_o$ and $R = 0{\cdot}031$ and $wR = 0{\cdot}036$.* All parameter changes were less than their e.s.d.'s. Final atomic coordinates are listed in Table 1, bond lengths and angles in Table 2. Fig. 1 illustrates the molecular configuration and the atomic numbering scheme.

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* Data were collected by Molecular Structures Corporation, College Station, Texas.

* Lists of structure factors, anisotropic thermal parameters and r.m.s. radii have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35200 (25 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 1. *Fractional atomic coordinates* ($\times 10^4$) *with e.s.d.'s in parentheses*

| | *x* | *y* | *z* |
|---|---|---|---|
| Ru(1) | 3909 (<1) | 1638 (<1) | 2122 (<1) |
| Ru(2) | 1901 (<1) | 1338 (<1) | 847 (<1) |
| Ru(3) | −96 (<1) | 1531 (<1) | 1725 (<1) |
| Ru(4) | 1900 (<1) | 1962 (<1) | 2873 (<1) |
| Ru(5) | 1847 (<1) | 2796 (<1) | 1540 (<1) |
| Ru(6) | 1976 (<1) | 406 (<1) | 2129 (<1) |
| O(1) | 5637 (6) | 3079 (3) | 2617 (3) |
| O(2) | 5955 (5) | 1076 (4) | 1316 (3) |
| O(3) | 3910 (6) | 933 (5) | −20 (3) |
| O(4) | −11 (5) | 855 (4) | −445 (3) |
| O(5) | −1863 (5) | 608 (3) | 563 (3) |
| O(6) | −1530 (6) | 744 (5) | 2756 (4) |
| O(7) | −1931 (6) | 2954 (4) | 1688 (4) |
| O(8) | 3130 (6) | 3582 (3) | 3273 (3) |
| O(9) | −349 (6) | 2474 (4) | 3571 (3) |
| O(10) | 1683 (6) | 2867 (3) | −1 (3) |
| O(11) | 3805 (6) | 4110 (4) | 1475 (3) |
| O(12) | −87 (7) | 4162 (4) | 1178 (4) |
| O(13) | −172 (6) | −837 (4) | 2084 (3) |
| O(14) | 3007 (6) | −646 (3) | 1100 (3) |
| C(1) | 4944 (7) | 2559 (4) | 2410 (4) |
| C(2) | 5140 (7) | 1295 (5) | 1588 (4) |
| C(3) | 3177 (7) | 1083 (5) | 322 (4) |
| C(4) | 682 (7) | 1022 (4) | 61 (4) |
| C(5) | −1184 (7) | 967 (4) | 970 (4) |
| C(6) | −968 (8) | 1042 (5) | 2376 (4) |
| C(7) | −1224 (7) | 2435 (5) | 1670 (4) |
| C(8) | 2663 (7) | 2987 (5) | 3088 (4) |
| C(9) | 496 (8) | 2263 (5) | 3328 (4) |
| C(10) | 1768 (7) | 2509 (4) | 517 (3) |
| C(11) | 3078 (7) | 3601 (4) | 1522 (3) |
| C(12) | 617 (8) | 3624 (5) | 1334 (4) |
| C(13) | 634 (7) | −370 (4) | 2114 (4) |
| C(14) | 2578 (7) | −199 (5) | 1428 (4) |
| C | 1927 (6) | 1606 (4) | 1882 (3) |
| C(15) | 3300 (7) | 1544 (4) | 3797 (3) |
| C(16) | 2399 (6) | 901 (4) | 3647 (3) |
| C(17) | 2556 (7) | 144 (4) | 3302 (3) |
| C(18) | 3554 (7) | −76 (4) | 2922 (4) |
| C(19) | 4586 (7) | 433 (4) | 2775 (3) |
| C(20) | 5105 (6) | 1163 (4) | 3102 (3) |
| C(21) | 4747 (6) | 1498 (4) | 3762 (3) |
| C(22) | 5465 (7) | 971 (4) | 4400 (3) |
| C(23) | 5228 (7) | 1318 (5) | 5074 (3) |
| C(24) | 5644 (8) | 2052 (5) | 5311 (4) |
| C(25) | 6476 (9) | 2603 (5) | 5029 (4) |
| C(26) | 7437 (9) | 2377 (6) | 4694 (4) |
| C(27) | 7766 (8) | 1540 (6) | 4552 (4) |
| C(28) | 6926 (8) | 919 (5) | 4450 (4) |

**Discussion.** The octahedral Ru framework of the cluster is very nearly regular. The 12 Ru—Ru bonds may be grouped as follows: (*a*) eight unbridged distances averaging 2·925 Å, (*b*) three distances bridged by C atoms in one of the seven-membered rings of the bitropyl molecule averaging 2·890 Å, and (*c*) one distance of 2·778 Å which is symmetrically bridged by a carbonyl group. The bridging by bitropyl carbons is the first to be noted. The Ru—Ru distances in groups *A* and *B* are essentially the same. Ru—Ru shortenings due to bridging carbonyls have been observed in $[Ru_6C(CO)_{17}]$ [2·907 (unbridged), 2·855 Å)] (Sirigu, Bianchi & Benedetti, 1969), the cluster $[H_2Ru_6(CO)_{18}]$ (2·954, 2·867 Å) (Churchill & Wormald, 1971) and $[Me_4N_2][Ru_6C(CO)_{16}]$ (2·903, 2·852 Å) (Ansell & Bradley, 1980). The encapsulated C lies close to the geometric center of the cluster and is six coordinate. Ru—C distances range from 2·022–2·080 Å (average 2·055 Å) and are almost identical to similar values of 2·05 Å in $[Ru_6C(CO)_{17}]$ (Sirigu *et al.*, 1969), 2·04 Å in $[Ru_6C(CO)_{14}(arene)]$ (Mason & Robinson, 1968) and 2·042 Å in $[NMe_4]_2[Ru_6C(CO)_{16}]$ (Ansell & Bradley, 1980). Ru—C—Ru angles range from 174·8 to 175·3°. Ru(1), Ru(4) and Ru(6) have two terminal carbonyl ligands, Ru(3) has three, and Ru(2) and Ru(5) have two terminal carbonyls and each shares a bridging carbonyl. The near linearity of the terminal carbonyls is clearly demonstrated with Ru—C—O angles ranging from 168·4–178·0°. Ru—C distances range from 1·853–1·924 Å and C—O from 1·127–1·156 Å. The bridging carbonyl has C(10) symmetrically placed between Ru(2) and Ru(5) [Ru(2)—C(10), Ru(5)—C(10), 2·042, 2·051 Å] and Ru—C—O angles of 138·5 and 136·0° respectively. The geometry of the carbonyls, the Ru—C values of bridged, semi-bridged, and non-bridged carbonyls and the corresponding angles are comparable with those in the compounds mentioned above. The stereochemistry around the triangular Ru(1), Ru(4), Ru(6) face is unique, however. The equation of the mean plane through Ru(1), Ru(4), Ru(6) is $-0{\cdot}4103\,X' + 0{\cdot}3981\,Y' - 0{\cdot}8206\,Z' + 3{\cdot}6072 = 0$ and carbonyl-group deviations from this plane are: C(1), O(1) (−0·24, −0·49 Å); C(2), O(2) (0·01, −0·10 Å); C(8), O(8) (0·40, −0·03 Å); C(9), O(9) (0·15, 0·30 Å); C(13), O(13) (0·08, 0·16 Å); and C(14), O(14) (−0·34, 0·33 Å). These three rutheniums and the six carbonyls linked to them are clearly almost coplanar. The angles between the pairs of carbonyls are 90·1, 89·2, and 88·6°. The three rutheniums also make close contact with the three short C=C bonds in one of the bitropyl rings. The six resulting close Ru···[C(15)...C(20)] contacts range from 2·174–2·399 Å. They clearly indicate an interaction between the triangular face of the cluster and the alternating double- and single-bond system over six of the seven atoms in this ring. This interaction results in near equalization of the five corresponding C—C bonds in the bitropyl ring (1·411–1·450 Å). The equation

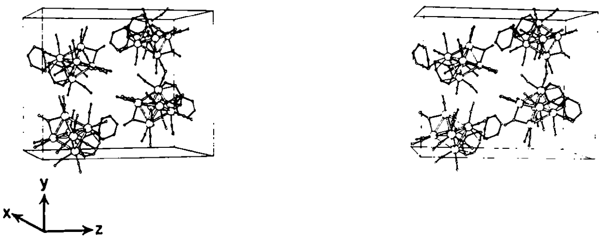

Fig. 2. A stereoscopic view of the molecular packing within the unit cell.

Table 2. *Bond lengths* (Å) *and angles* (°)

Ru-Ru

| | | |
|---|---|---|
| RU1 | RU2 | 2.972(<1) |
| RU1 | RU4 | 2.832(<1) |
| RU1 | RU5 | 2.936(<1) |
| RU1 | RU6 | 2.867(<1) |
| RU2 | RU3 | 2.964(<1) |
| RU2 | RU5 | 2.778(<1) |
| RU2 | RU6 | 2.943(<1) |
| RU3 | RU4 | 2.841(<1) |
| RU3 | RU5 | 2.982(<1) |
| RU3 | RU6 | 2.842(<1) |
| RU4 | RU5 | 2.952(<1) |
| RU4 | RU6 | 2.971(<1) |

Ru-C Bridged Carbonyl

| | | |
|---|---|---|
| RU2 | C10 | 2.042( 6) |
| RU5 | C10 | 2.051( 6) |

Ru-C Terminal Carbonyl

| | | |
|---|---|---|
| RU1 | C1 | 1.889( 7) |
| RU1 | C2 | 1.894( 7) |
| RU2 | C3 | 1.879( 7) |
| RU2 | C4 | 1.872( 7) |
| RU3 | C5 | 1.924( 7) |
| RU3 | C6 | 1.887( 8) |
| RU3 | C7 | 1.891( 7) |
| RU4 | C8 | 1.887( 7) |
| RU4 | C9 | 1.921( 7) |
| RU5 | C11 | 1.853( 7) |
| RU5 | C12 | 1.866( 8) |
| RU6 | C13 | 1.892( 7) |
| RU6 | C14 | 1.905( 7) |

C-O Bridged Carbonyl

| | | |
|---|---|---|
| C10 | 010 | 1.166( 8) |

C-O Terminal Carbonyl

| | | |
|---|---|---|
| C1 | 01 | 1.144( 9) |
| C2 | 02 | 1.144( 9) |
| C3 | 03 | 1.137(10) |
| C4 | 04 | 1.142( 9) |
| C5 | 05 | 1.127( 9) |
| C6 | 06 | 1.147(11) |
| C7 | 07 | 1.137(10) |
| C8 | 08 | 1.127( 9) |
| C9 | 09 | 1.133( 9) |
| C11 | 011 | 1.149( 9) |
| C12 | 012 | 1.156(10) |
| C13 | 013 | 1.133( 9) |
| C14 | 014 | 1.129( 9) |

Ru-C Carbido

| | | |
|---|---|---|
| RU1 | C | 2.022( 5) |
| RU2 | C | 2.076( 5) |
| RU3 | C | 2.069( 5) |
| RU4 | C | 2.039( 5) |
| RU5 | C | 2.080( 5) |
| RU6 | C | 2.045( 5) |

Ru-C Bitropyl

| | | |
|---|---|---|
| RU1 | C19 | 2.403( 6) |
| RU1 | C20 | 2.224( 6) |
| RU4 | C15 | 2.205( 6) |
| RU4 | C16 | 2.316( 6) |
| RU6 | C17 | 2.305( 7) |
| RU6 | C18 | 2.181( 6) |

C-C Bitropyl

| | | |
|---|---|---|
| C15 | C16 | 1.411( 9) |
| C16 | C17 | 1.450( 9) |
| C17 | C18 | 1.437( 9) |
| C18 | C19 | 1.438( 9) |
| C19 | C20 | 1.426( 9) |
| C20 | C21 | 1.522( 9) |
| C21 | C15 | 1.520( 9) |
| C21 | C22 | 1.590( 9) |
| C22 | C23 | 1.506(10) |
| C23 | C24 | 1.343(11) |
| C24 | C25 | 1.442(11) |
| C25 | C26 | 1.351(12) |
| C26 | C27 | 1.468(12) |
| C27 | C28 | 1.339(11) |
| C28 | C22 | 1.504(10) |

Triangular Faces of $Ru_6$ Clusters

| | | | |
|---|---|---|---|
| RU1 | RU2 | RU5 | 61.3(<0.1) |
| RU1 | RU5 | RU2 | 62.6(<0.1) |
| RU5 | RU1 | RU2 | 56.1(<0.1) |
| RU1 | RU2 | RU6 | 58.0(<0.1) |
| RU2 | RU1 | RU6 | 60.5(<0.1) |
| RU1 | RU6 | RU2 | 61.5(<0.1) |
| RU1 | RU4 | RU5 | 61.0(<0.1) |
| RU4 | RU1 | RU5 | 61.5(<0.1) |
| RU4 | RU5 | RU1 | 57.5(<0.1) |
| RU1 | RU4 | RU6 | 59.2(<0.1) |
| RU4 | RU1 | RU6 | 62.8(<0.1) |
| RU4 | RU6 | RU1 | 58.0(<0.1) |
| RU4 | RU3 | RU5 | 60.9(<0.1) |
| RU3 | RU4 | RU5 | 61.9(<0.1) |
| RU3 | RU5 | RU4 | 57.2(<0.1) |
| RU4 | RU3 | RU6 | 63.1(<0.1) |
| RU6 | RU4 | RU3 | 58.5(<0.1) |
| RU4 | RU6 | RU3 | 58.5(<0.1) |
| RU2 | RU3 | RU5 | 55.7(<0.1) |
| RU5 | RU2 | RU3 | 62.5(<0.1) |
| RU2 | RU5 | RU3 | 61.8(<0.1) |
| RU2 | RU3 | RU6 | 60.9(<0.1) |
| RU3 | RU2 | RU6 | 57.5(<0.1) |
| RU3 | RU6 | RU2 | 61.6(<0.1) |

Between the Cluster & CO

| | | | |
|---|---|---|---|
| RU2 | RU1 | C1 | 130.8(0.2) |
| RU2 | RU1 | C2 | 85.5(0.2) |
| RU4 | RU1 | C1 | 97.2(0.2) |
| RU4 | RU1 | C2 | 172.6(0.2) |
| RU5 | RU1 | C1 | 85.4(0.2) |
| RU5 | RU1 | C2 | 120.1(0.2) |
| RU6 | RU1 | C1 | 158.8(0.2) |
| RU6 | RU1 | C2 | 109.8(0.2) |
| RU1 | RU2 | C3 | 92.6(0.2) |
| RU1 | RU2 | C4 | 173.4(0.2) |
| RU1 | RU2 | C10 | 95.8(0.2) |
| RU3 | RU2 | C3 | 173.0(0.2) |
| RU3 | RU2 | C4 | 94.1(0.2) |
| RU3 | RU2 | C10 | 94.1(0.2) |
| RU5 | RU2 | C3 | 123.2(0.2) |
| RU5 | RU2 | C4 | 124.9(0.2) |
| RU5 | RU2 | C10 | 47.4(0.2) |
| RU6 | RU2 | C3 | 116.6(0.2) |
| RU6 | RU2 | C4 | 117.4(0.2) |
| RU6 | RU2 | C10 | 139.4(0.2) |
| RU2 | RU3 | C5 | 82.6(0.2) |
| RU2 | RU3 | C6 | 146.2(0.3) |
| RU2 | RU3 | C7 | 123.2(0.2) |
| RU4 | RU3 | C5 | 164.3(0.2) |
| RU4 | RU3 | C6 | 86.8(0.3) |
| RU4 | RU3 | C7 | 101.3(0.2) |
| RU5 | RU3 | C5 | 123.9(0.2) |
| RU5 | RU3 | C6 | 144.1(0.3) |
| RU5 | RU3 | C7 | 82.1(0.2) |
| RU6 | RU3 | C5 | 101.3(0.2) |
| RU6 | RU3 | C6 | 88.1(0.3) |
| RU6 | RU3 | C7 | 164.3(0.2) |
| RU1 | RU4 | C8 | 88.1(0.2) |
| RU1 | RU4 | C9 | 174.9(0.2) |
| RU3 | RU4 | C8 | 127.9(0.2) |
| RU3 | RU4 | C9 | 86.0(0.2) |
| RU5 | RU4 | C8 | 73.2(0.2) |
| RU5 | RU4 | C9 | 114.0(0.2) |
| RU6 | RU4 | C8 | 147.2(0.2) |
| RU6 | RU4 | C9 | 123.3(0.2) |
| RU1 | RU5 | C10 | 96.7(0.2) |
| RU1 | RU5 | C11 | 91.3(0.2) |
| RU1 | RU5 | C12 | 169.1(0.3) |
| RU2 | RU5 | C10 | 47.1(0.2) |
| RU2 | RU5 | C11 | 122.5(0.2) |
| RU2 | RU5 | C12 | 127.7(0.3) |
| RU3 | RU5 | C10 | 93.3(0.2) |
| RU3 | RU5 | C11 | 174.1(0.2) |
| RU3 | RU5 | C12 | 95.3(0.3) |
| RU4 | RU5 | C10 | 138.7(0.2) |
| RU4 | RU5 | C11 | 117.4(0.2) |
| RU4 | RU5 | C12 | 115.5(0.3) |
| RU1 | RU6 | C13 | 177.1(0.2) |
| RU1 | RU6 | C14 | 92.4(0.2) |
| RU2 | RU6 | C13 | 116.5(0.2) |
| RU2 | RU6 | C14 | 67.3(0.2) |
| RU3 | RU6 | C13 | 85.7(0.2) |
| RU3 | RU6 | C14 | 118.7(0.2) |
| RU4 | RU6 | C13 | 120.5(0.2) |
| RU4 | RU6 | C14 | 148.8(0.2) |

Equatorial Belts of $Ru_6$ Clusters

| | | | |
|---|---|---|---|
| RU4 | RU1 | RU2 | 90.2(<0.1) |
| RU6 | RU1 | RU5 | 90.5(<0.1) |
| RU1 | RU2 | RU3 | 87.0(<0.1) |
| RU5 | RU2 | RU6 | 92.1(<0.1) |
| RU4 | RU3 | RU2 | 90.2(<0.1) |
| RU5 | RU3 | RU6 | 90.0(<0.1) |
| RU1 | RU4 | RU3 | 92.2(<0.1) |
| RU6 | RU4 | RU5 | 88.2(<0.1) |
| RU2 | RU5 | RU4 | 91.7(<0.1) |
| RU1 | RU5 | RU3 | 87.3(<0.1) |
| RU1 | RU6 | RU3 | 91.4(<0.1) |
| RU4 | RU6 | RU2 | 88.1(<0.1) |

Angles Involving Carbido C

| | | | |
|---|---|---|---|
| RU1 | C | RU3 | 174.8(0.3) |
| RU4 | C | RU2 | 175.3(0.3) |
| RU5 | C | RU6 | 175.0(0.3) |

Interligand Angles

| | | | |
|---|---|---|---|
| C1 | RU1 | C2 | 90.1(0.3) |
| C3 | RU2 | C4 | 85.4(0.3) |
| C3 | RU2 | C10 | 92.9(0.3) |
| C4 | RU2 | C10 | 90.6(0.3) |
| C5 | RU3 | C6 | 91.5(0.3) |
| C5 | RU3 | C7 | 94.3(0.3) |
| C6 | RU3 | C7 | 90.3(0.3) |
| C8 | RU4 | C9 | 89.2(0.3) |
| C10 | RU5 | C11 | 92.6(0.3) |
| C10 | RU5 | C12 | 93.6(0.3) |
| C11 | RU5 | C12 | 85.0(0.3) |
| C14 | RU6 | C13 | 88.6(0.3) |

Angles in Bridging Carbonyl

| | | | |
|---|---|---|---|
| RU2 | C10 | 010 | 138.5(0.6) |
| RU5 | C10 | 010 | 136.0(0.6) |

Angles in Terminal Carbonyl

| | | | |
|---|---|---|---|
| RU1 | C1 | 01 | 174.7(0.7) |
| RU1 | C2 | 02 | 174.3(0.7) |
| RU2 | C3 | 03 | 177.2(0.7) |
| RU2 | C4 | 04 | 175.4(0.6) |
| RU3 | C5 | 05 | 174.9(0.6) |
| RU3 | C6 | 06 | 178.0(0.8) |
| RU3 | C7 | 07 | 174.0(0.7) |
| RU4 | C8 | 08 | 174.2(0.7) |
| RU4 | C9 | 09 | 176.2(0.7) |
| RU5 | C11 | 011 | 176.2(0.7) |
| RU5 | C12 | 012 | 175.1(0.7) |
| RU6 | C13 | 013 | 177.9(0.7) |
| RU6 | C14 | 014 | 168.4(0.7) |

Between Cluster and Bitropyl

| | | | |
|---|---|---|---|
| RU4 | RU1 | C19 | 92.8(0.2) |
| RU6 | RU1 | C19 | 62.5(0.2) |
| RU4 | RU1 | C20 | 87.7(0.2) |
| RU6 | RU1 | C20 | 91.0(0.2) |
| RU6 | RU4 | C15 | 93.2(0.2) |
| RU1 | RU4 | C16 | 96.0(0.2) |
| RU6 | RU4 | C15 | 93.2(0.2) |
| RU1 | RU4 | C16 | 96.0(0.2) |
| RU4 | RU6 | C17 | 72.5(0.2) |
| RU1 | RU6 | C18 | 80.5(0.2) |
| RU4 | RU6 | C18 | 93.2(0.2) |
| RU1 | RU6 | C17 | 95.3(0.2) |

Bitropyl Angles

| | | | |
|---|---|---|---|
| C21 | C15 | C16 | 125.1(0.6) |
| C15 | C16 | C17 | 128.3(0.6) |
| C16 | C17 | C18 | 128.4(0.6) |
| C17 | C18 | C19 | 126.7(0.6) |
| C18 | C19 | C20 | 129.7(0.6) |
| C19 | C20 | C21 | 124.1(0.6) |
| C20 | C21 | C15 | 117.7(0.5) |
| C20 | C21 | C22 | 108.4(0.5) |
| C15 | C21 | C22 | 108.0(0.5) |
| C21 | C22 | C23 | 110.6(0.6) |
| C21 | C22 | C28 | 113.3(0.6) |
| C23 | C22 | C28 | 107.5(0.6) |
| C22 | C23 | C24 | 123.6(0.7) |
| C23 | C24 | C25 | 128.1(0.8) |
| C24 | C25 | C26 | 124.5(0.8) |
| C25 | C26 | C27 | 125.3(0.8) |
| C26 | C27 | C28 | 125.8(0.8) |
| C27 | C28 | C22 | 125.9(0.7) |

of the mean plane through these six C atoms is $-0{\cdot}3873X' + 0{\cdot}4319Y' - 0{\cdot}8145Z' + 5{\cdot}5823 = 0$ and they deviate −0·04, 0·08, −0·04, −0·05, 0·10, and −0·050 Å from it. The seventh non-bonded C atom, C(21), deviates −0·60 Å from this plane. This plane makes an angle of 2·36° with that through the three rutheniums. The arrangement of the six corresponding atoms in the second bitropyl ring results in more clearly defined alternating long and short bonds (1·343, 1·442, 1·351, 1·468, 1·339 Å). The bond values of 1·522, 1·520, 1·590, 1·506, and 1·504 Å associated with C(21) and C(22) and the corresponding angles are consistent with these atoms having normal tetrahedral bonding. Inspection of Fig. 1 shows that the two bitropyl rings are twisted away from each other so as to minimize intramolecular ring–ring interaction. Molecular packing is shown in Fig. 2. All closest intermolecular distances are consistent with van der Waals packing radii.

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