

**Table 1. Crystal data and structure refinement for (C<sub>5</sub>Me<sub>5</sub>)U(CH<sub>2</sub>C<sub>5</sub>H<sub>6</sub>)<sub>3</sub> (3).**

|                                   |                                             |                  |
|-----------------------------------|---------------------------------------------|------------------|
| Identification code               | ccd478d                                     |                  |
| Empirical formula                 | C <sub>31</sub> H <sub>36</sub> U           |                  |
| Formula weight                    | 646.63                                      |                  |
| Temperature                       | 203(2) K                                    |                  |
| Wavelength                        | 0.71073 Å                                   |                  |
| Crystal system                    | monoclinic                                  |                  |
| Space group                       | P 2 <sub>1</sub> /n                         |                  |
| Unit cell dimensions              | a = 9.556(2) Å                              |                  |
|                                   | b = 30.725(8) Å                             | β = 100.351(5)°. |
|                                   | c = 17.877(5) Å                             |                  |
| Volume                            | 5163(2) Å <sup>3</sup>                      |                  |
| Z                                 | 8                                           |                  |
| Density (calculated)              | 1.664 Mg/m <sup>3</sup>                     |                  |
| Absorption coefficient            | 6.303 mm <sup>-1</sup>                      |                  |
| F(000)                            | 2512                                        |                  |
| Crystal size                      | 0.25 x 0.12 x 0.12 mm <sup>3</sup>          |                  |
| Theta range for data collection   | 1.33 to 22.46°.                             |                  |
| Index ranges                      | -9 ≤ h ≤ 9, 0 ≤ k ≤ 32, 0 ≤ l ≤ 19          |                  |
| Reflections collected             | 37913                                       |                  |
| Independent reflections           | 6380 [R(int) = 0.071]                       |                  |
| Max. and min. transmission        | 0.5184 and 0.3017                           |                  |
| Refinement method                 | Full-matrix least-squares on F <sup>2</sup> |                  |
| Data / restraints / parameters    | 6380 / 396 / 529                            |                  |
| Goodness-of-fit on F <sup>2</sup> | 3.331                                       |                  |
| Final R indices [I > 2σ(I)]       | R1 = 0.1180, wR2 = 0.1767                   |                  |
| R indices (all data)              | R1 = 0.1220, wR2 = 0.1770                   |                  |
| Largest diff. peak and hole       | 2.851 and -4.214 e.Å <sup>-3</sup>          |                  |

**Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for  $(\text{C}_5\text{Me}_5)\text{U}(\text{CH}_2\text{C}_5\text{H}_6)_3$  (3). U(eq) is defined as one third of the trace of the orthogonalized  $U^{\text{ij}}$  tensor.**

|       | x        | y        | z        | U(eq) |
|-------|----------|----------|----------|-------|
| U(1)  | 4807(1)  | 89(1)    | 7642(1)  | 18(1) |
| U(2)  | 4187(1)  | 2445(1)  | 4653(1)  | 17(1) |
| C(1)  | 3730(20) | 792(6)   | 7168(11) | 21(5) |
| C(2)  | 2970(20) | 784(6)   | 7804(11) | 22(5) |
| C(3)  | 3570(20) | 934(7)   | 8538(12) | 35(6) |
| C(4)  | 2870(20) | 902(7)   | 9157(12) | 36(6) |
| C(5)  | 1560(30) | 721(7)   | 9070(14) | 45(7) |
| C(6)  | 920(30)  | 547(7)   | 8382(13) | 41(6) |
| C(7)  | 1630(20) | 569(6)   | 7765(12) | 29(5) |
| C(8)  | 4580(20) | -481(6)  | 6618(12) | 31(6) |
| C(9)  | 3620(20) | -171(6)  | 6157(11) | 22(5) |
| C(10) | 4040(30) | 139(7)   | 5673(12) | 43(6) |
| C(11) | 3120(20) | 431(7)   | 5265(12) | 33(6) |
| C(12) | 1700(30) | 441(7)   | 5309(13) | 44(6) |
| C(13) | 1210(30) | 139(7)   | 5783(12) | 41(6) |
| C(14) | 2120(20) | -162(7)  | 6190(12) | 35(6) |
| C(15) | 4240(20) | -185(6)  | 8889(12) | 34(6) |
| C(16) | 3720(20) | -577(7)  | 8489(12) | 33(6) |
| C(17) | 2310(20) | -626(7)  | 8058(12) | 34(6) |
| C(18) | 1860(30) | -981(7)  | 7618(12) | 36(6) |
| C(19) | 2720(30) | -1330(7) | 7579(12) | 39(6) |
| C(20) | 4110(30) | -1307(7) | 8005(12) | 40(6) |
| C(21) | 4600(30) | -945(7)  | 8436(12) | 37(6) |
| C(22) | 7344(11) | 396(3)   | 8559(4)  | 31(6) |
| C(23) | 7630(12) | -44(2)   | 8391(5)  | 34(6) |
| C(24) | 7704(12) | -70(2)   | 7606(5)  | 40(6) |
| C(25) | 7463(11) | 353(3)   | 7289(4)  | 26(5) |
| C(26) | 7241(11) | 641(2)   | 7877(5)  | 23(5) |
| C(27) | 7179(18) | 571(4)   | 9326(5)  | 48(7) |
| C(28) | 7822(18) | -417(3)  | 8949(6)  | 68(8) |
| C(29) | 7988(19) | -477(3)  | 7183(7)  | 72(9) |

|       |          |         |          |       |
|-------|----------|---------|----------|-------|
| C(30) | 7447(17) | 474(4)  | 6469(5)  | 50(7) |
| C(31) | 6947(18) | 1122(2) | 7794(7)  | 55(7) |
| C(32) | 5460(20) | 2241(6) | 5941(11) | 23(5) |
| C(33) | 6280(20) | 1942(6) | 5571(10) | 24(5) |
| C(34) | 7590(20) | 2074(6) | 5303(11) | 21(5) |
| C(35) | 8330(20) | 1797(6) | 4893(12) | 30(6) |
| C(36) | 7800(30) | 1384(7) | 4706(12) | 39(6) |
| C(37) | 6610(20) | 1242(7) | 4941(12) | 37(6) |
| C(38) | 5860(20) | 1505(6) | 5379(11) | 31(5) |
| C(39) | 4190(20) | 3240(6) | 4364(10) | 19(5) |
| C(40) | 5210(20) | 3304(6) | 5088(11) | 24(5) |
| C(41) | 4660(20) | 3388(6) | 5765(11) | 22(5) |
| C(42) | 5610(20) | 3392(6) | 6461(12) | 32(6) |
| C(43) | 7020(20) | 3323(6) | 6503(12) | 27(5) |
| C(44) | 7540(20) | 3238(6) | 5850(11) | 25(5) |
| C(45) | 6650(20) | 3217(6) | 5160(12) | 23(5) |
| C(46) | 4700(20) | 1981(6) | 3566(11) | 22(5) |
| C(47) | 5150(20) | 2385(6) | 3194(11) | 25(5) |
| C(48) | 4130(20) | 2614(6) | 2645(11) | 32(6) |
| C(49) | 4500(20) | 3006(6) | 2349(11) | 29(5) |
| C(50) | 5850(30) | 3189(7) | 2592(12) | 35(6) |
| C(51) | 6790(30) | 2975(7) | 3105(12) | 37(6) |
| C(52) | 6510(20) | 2588(6) | 3401(11) | 26(5) |
| C(53) | 1699(10) | 1937(2) | 4383(4)  | 24(5) |
| C(54) | 1989(10) | 1985(2) | 5186(4)  | 29(5) |
| C(55) | 1752(10) | 2428(2) | 5357(4)  | 17(4) |
| C(56) | 1316(10) | 2652(2) | 4660(4)  | 13(4) |
| C(57) | 1283(10) | 2349(2) | 4058(4)  | 18(5) |
| C(58) | 1814(16) | 1520(3) | 3951(6)  | 38(6) |
| C(59) | 2465(16) | 1630(3) | 5757(5)  | 40(6) |
| C(60) | 1932(15) | 2624(3) | 6143(4)  | 36(6) |
| C(61) | 951(16)  | 3130(2) | 4575(6)  | 45(7) |
| C(62) | 878(15)  | 2447(3) | 3220(4)  | 42(6) |

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**Table 3. Bond lengths [Å] and angles [°] for (C<sub>5</sub>Me<sub>5</sub>)U(CH<sub>2</sub>C<sub>5</sub>H<sub>6</sub>)<sub>3</sub> (3).**


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|             |           |
|-------------|-----------|
| U(1)-C(1)   | 2.477(18) |
| U(1)-C(8)   | 2.51(2)   |
| U(1)-C(15)  | 2.53(2)   |
| U(1)-C(9)   | 2.809(19) |
| U(1)-C(2)   | 2.814(19) |
| U(1)-C(23)  | 2.817(10) |
| U(1)-C(24)  | 2.823(11) |
| U(1)-C(22)  | 2.833(10) |
| U(1)-C(25)  | 2.841(10) |
| U(1)-C(26)  | 2.847(10) |
| U(1)-C(16)  | 2.85(2)   |
| U(2)-C(32)  | 2.483(19) |
| U(2)-C(39)  | 2.496(17) |
| U(2)-C(46)  | 2.526(19) |
| U(2)-C(57)  | 2.803(9)  |
| U(2)-C(53)  | 2.813(9)  |
| U(2)-C(33)  | 2.81(2)   |
| U(2)-C(56)  | 2.820(9)  |
| U(2)-C(54)  | 2.835(9)  |
| U(2)-C(55)  | 2.839(9)  |
| U(2)-C(40)  | 2.876(19) |
| U(2)-C(47)  | 2.923(19) |
| C(1)-C(2)   | 1.46(3)   |
| C(2)-C(3)   | 1.41(3)   |
| C(2)-C(7)   | 1.43(3)   |
| C(3)-C(4)   | 1.40(3)   |
| C(4)-C(5)   | 1.35(3)   |
| C(5)-C(6)   | 1.38(3)   |
| C(6)-C(7)   | 1.40(3)   |
| C(8)-C(9)   | 1.47(3)   |
| C(9)-C(10)  | 1.39(3)   |
| C(9)-C(14)  | 1.44(3)   |
| C(10)-C(11) | 1.38(3)   |
| C(11)-C(12) | 1.37(3)   |

|             |         |
|-------------|---------|
| C(12)-C(13) | 1.40(3) |
| C(13)-C(14) | 1.38(3) |
| C(15)-C(16) | 1.44(3) |
| C(16)-C(21) | 1.42(3) |
| C(16)-C(17) | 1.44(3) |
| C(17)-C(18) | 1.37(3) |
| C(18)-C(19) | 1.36(3) |
| C(19)-C(20) | 1.40(3) |
| C(20)-C(21) | 1.39(3) |
| C(22)-C(23) | 1.4200  |
| C(22)-C(26) | 1.4200  |
| C(22)-C(27) | 1.5095  |
| C(23)-C(24) | 1.4200  |
| C(23)-C(28) | 1.5095  |
| C(24)-C(25) | 1.4200  |
| C(24)-C(29) | 1.5095  |
| C(25)-C(26) | 1.4200  |
| C(25)-C(30) | 1.5095  |
| C(26)-C(31) | 1.5095  |
| C(32)-C(33) | 1.45(3) |
| C(33)-C(38) | 1.42(3) |
| C(33)-C(34) | 1.47(3) |
| C(34)-C(35) | 1.40(3) |
| C(35)-C(36) | 1.39(3) |
| C(36)-C(37) | 1.36(3) |
| C(37)-C(38) | 1.41(3) |
| C(39)-C(40) | 1.49(3) |
| C(40)-C(45) | 1.38(3) |
| C(40)-C(41) | 1.43(3) |
| C(41)-C(42) | 1.40(3) |
| C(42)-C(43) | 1.35(3) |
| C(43)-C(44) | 1.38(3) |
| C(44)-C(45) | 1.37(3) |
| C(46)-C(47) | 1.51(3) |
| C(47)-C(52) | 1.42(3) |
| C(47)-C(48) | 1.44(3) |

|             |         |
|-------------|---------|
| C(48)-C(49) | 1.39(3) |
| C(49)-C(50) | 1.40(3) |
| C(50)-C(51) | 1.33(3) |
| C(51)-C(52) | 1.35(3) |
| C(53)-C(54) | 1.4200  |
| C(53)-C(57) | 1.4200  |
| C(53)-C(58) | 1.5095  |
| C(54)-C(55) | 1.4200  |
| C(54)-C(59) | 1.5095  |
| C(55)-C(56) | 1.4200  |
| C(55)-C(60) | 1.5095  |
| C(56)-C(57) | 1.4200  |
| C(56)-C(61) | 1.5095  |
| C(57)-C(62) | 1.5095  |

|                  |           |
|------------------|-----------|
| C(1)-U(1)-C(8)   | 112.4(6)  |
| C(1)-U(1)-C(15)  | 116.6(6)  |
| C(8)-U(1)-C(15)  | 114.0(7)  |
| C(1)-U(1)-C(9)   | 81.5(6)   |
| C(8)-U(1)-C(9)   | 31.4(6)   |
| C(15)-U(1)-C(9)  | 128.5(6)  |
| C(1)-U(1)-C(2)   | 31.1(6)   |
| C(8)-U(1)-C(2)   | 129.0(6)  |
| C(15)-U(1)-C(2)  | 85.6(6)   |
| C(9)-U(1)-C(2)   | 99.2(5)   |
| C(1)-U(1)-C(23)  | 126.4(5)  |
| C(8)-U(1)-C(23)  | 101.3(5)  |
| C(15)-U(1)-C(23) | 82.7(6)   |
| C(9)-U(1)-C(23)  | 126.8(4)  |
| C(2)-U(1)-C(23)  | 128.5(4)  |
| C(1)-U(1)-C(24)  | 119.6(5)  |
| C(8)-U(1)-C(24)  | 79.6(5)   |
| C(15)-U(1)-C(24) | 109.3(6)  |
| C(9)-U(1)-C(24)  | 99.3(5)   |
| C(2)-U(1)-C(24)  | 140.1(4)  |
| C(23)-U(1)-C(24) | 29.16(10) |

|                  |           |
|------------------|-----------|
| C(1)-U(1)-C(22)  | 99.7(5)   |
| C(8)-U(1)-C(22)  | 127.3(5)  |
| C(15)-U(1)-C(22) | 84.2(5)   |
| C(9)-U(1)-C(22)  | 143.2(5)  |
| C(2)-U(1)-C(22)  | 99.9(4)   |
| C(23)-U(1)-C(22) | 29.11(10) |
| C(24)-U(1)-C(22) | 47.94(14) |
| C(1)-U(1)-C(25)  | 90.5(5)   |
| C(8)-U(1)-C(25)  | 90.1(5)   |
| C(15)-U(1)-C(25) | 129.3(6)  |
| C(9)-U(1)-C(25)  | 95.6(5)   |
| C(2)-U(1)-C(25)  | 113.9(4)  |
| C(23)-U(1)-C(25) | 47.91(14) |
| C(24)-U(1)-C(25) | 29.04(10) |
| C(22)-U(1)-C(25) | 47.77(14) |
| C(1)-U(1)-C(26)  | 79.1(5)   |
| C(8)-U(1)-C(26)  | 119.0(5)  |
| C(15)-U(1)-C(26) | 111.5(5)  |
| C(9)-U(1)-C(26)  | 119.4(5)  |
| C(2)-U(1)-C(26)  | 92.4(4)   |
| C(23)-U(1)-C(26) | 47.85(14) |
| C(24)-U(1)-C(26) | 47.81(14) |
| C(22)-U(1)-C(26) | 28.95(9)  |
| C(25)-U(1)-C(26) | 28.91(9)  |
| C(1)-U(1)-C(16)  | 129.7(6)  |
| C(8)-U(1)-C(16)  | 84.0(7)   |
| C(15)-U(1)-C(16) | 30.4(6)   |
| C(9)-U(1)-C(16)  | 100.0(6)  |
| C(2)-U(1)-C(16)  | 101.3(6)  |
| C(23)-U(1)-C(16) | 93.0(5)   |
| C(24)-U(1)-C(16) | 109.9(5)  |
| C(22)-U(1)-C(16) | 106.7(5)  |
| C(25)-U(1)-C(16) | 138.4(5)  |
| C(26)-U(1)-C(16) | 135.6(5)  |
| C(32)-U(2)-C(39) | 114.8(6)  |
| C(32)-U(2)-C(46) | 116.1(6)  |

|                  |           |
|------------------|-----------|
| C(39)-U(2)-C(46) | 112.6(6)  |
| C(32)-U(2)-C(57) | 127.7(5)  |
| C(39)-U(2)-C(57) | 93.6(5)   |
| C(46)-U(2)-C(57) | 88.0(5)   |
| C(32)-U(2)-C(53) | 106.0(5)  |
| C(39)-U(2)-C(53) | 122.7(5)  |
| C(46)-U(2)-C(53) | 80.2(5)   |
| C(57)-U(2)-C(53) | 29.29(9)  |
| C(32)-U(2)-C(33) | 30.9(6)   |
| C(39)-U(2)-C(33) | 129.1(6)  |
| C(46)-U(2)-C(33) | 85.6(6)   |
| C(57)-U(2)-C(33) | 135.7(4)  |
| C(53)-U(2)-C(33) | 106.6(4)  |
| C(32)-U(2)-C(56) | 111.5(5)  |
| C(39)-U(2)-C(56) | 79.5(5)   |
| C(46)-U(2)-C(56) | 117.0(5)  |
| C(57)-U(2)-C(56) | 29.25(9)  |
| C(53)-U(2)-C(56) | 48.15(13) |
| C(33)-U(2)-C(56) | 135.4(4)  |
| C(32)-U(2)-C(54) | 80.3(5)   |
| C(39)-U(2)-C(54) | 125.8(5)  |
| C(46)-U(2)-C(54) | 103.6(5)  |
| C(57)-U(2)-C(54) | 48.09(12) |
| C(53)-U(2)-C(54) | 29.12(9)  |
| C(33)-U(2)-C(54) | 91.3(4)   |
| C(56)-U(2)-C(54) | 47.95(12) |
| C(32)-U(2)-C(55) | 83.5(5)   |
| C(39)-U(2)-C(55) | 98.2(5)   |
| C(46)-U(2)-C(55) | 128.2(5)  |
| C(57)-U(2)-C(55) | 48.05(12) |
| C(53)-U(2)-C(55) | 47.97(12) |
| C(33)-U(2)-C(55) | 106.6(4)  |
| C(56)-U(2)-C(55) | 29.06(8)  |
| C(54)-U(2)-C(55) | 28.98(8)  |
| C(32)-U(2)-C(40) | 83.9(6)   |
| C(39)-U(2)-C(40) | 31.2(6)   |

|                  |           |
|------------------|-----------|
| C(46)-U(2)-C(40) | 128.5(6)  |
| C(57)-U(2)-C(40) | 117.8(4)  |
| C(53)-U(2)-C(40) | 142.5(4)  |
| C(33)-U(2)-C(40) | 100.0(6)  |
| C(56)-U(2)-C(40) | 94.4(4)   |
| C(54)-U(2)-C(40) | 127.1(4)  |
| C(55)-U(2)-C(40) | 99.5(4)   |
| C(32)-U(2)-C(47) | 129.2(6)  |
| C(39)-U(2)-C(47) | 82.2(6)   |
| C(46)-U(2)-C(47) | 31.0(5)   |
| C(57)-U(2)-C(47) | 96.0(5)   |
| C(53)-U(2)-C(47) | 101.8(4)  |
| C(33)-U(2)-C(47) | 100.4(6)  |
| C(56)-U(2)-C(47) | 118.8(4)  |
| C(54)-U(2)-C(47) | 129.8(4)  |
| C(55)-U(2)-C(47) | 144.1(5)  |
| C(40)-U(2)-C(47) | 98.8(6)   |
| C(2)-C(1)-U(1)   | 87.3(11)  |
| C(3)-C(2)-C(7)   | 114.1(19) |
| C(3)-C(2)-C(1)   | 122.9(19) |
| C(7)-C(2)-C(1)   | 122.4(18) |
| C(3)-C(2)-U(1)   | 100.6(13) |
| C(7)-C(2)-U(1)   | 102.3(12) |
| C(1)-C(2)-U(1)   | 61.6(10)  |
| C(4)-C(3)-C(2)   | 122(2)    |
| C(5)-C(4)-C(3)   | 120(2)    |
| C(4)-C(5)-C(6)   | 121(2)    |
| C(5)-C(6)-C(7)   | 119(2)    |
| C(6)-C(7)-C(2)   | 123(2)    |
| C(9)-C(8)-U(1)   | 85.5(12)  |
| C(10)-C(9)-C(14) | 114(2)    |
| C(10)-C(9)-C(8)  | 125(2)    |
| C(14)-C(9)-C(8)  | 121.0(19) |
| C(10)-C(9)-U(1)  | 106.2(14) |
| C(14)-C(9)-U(1)  | 101.1(13) |
| C(8)-C(9)-U(1)   | 63.1(11)  |

|                   |           |
|-------------------|-----------|
| C(11)-C(10)-C(9)  | 123(2)    |
| C(12)-C(11)-C(10) | 122(2)    |
| C(11)-C(12)-C(13) | 118(2)    |
| C(14)-C(13)-C(12) | 121(2)    |
| C(13)-C(14)-C(9)  | 122(2)    |
| C(16)-C(15)-U(1)  | 87.0(13)  |
| C(21)-C(16)-C(17) | 113(2)    |
| C(21)-C(16)-C(15) | 123(2)    |
| C(17)-C(16)-C(15) | 124(2)    |
| C(21)-C(16)-U(1)  | 105.0(14) |
| C(17)-C(16)-U(1)  | 100.8(13) |
| C(15)-C(16)-U(1)  | 62.6(11)  |
| C(18)-C(17)-C(16) | 124(2)    |
| C(19)-C(18)-C(17) | 122(2)    |
| C(18)-C(19)-C(20) | 117(2)    |
| C(21)-C(20)-C(19) | 122(2)    |
| C(20)-C(21)-C(16) | 122(2)    |
| C(23)-C(22)-C(26) | 108.0     |
| C(23)-C(22)-C(27) | 126.0     |
| C(26)-C(22)-C(27) | 126.0     |
| C(23)-C(22)-U(1)  | 74.8(3)   |
| C(26)-C(22)-U(1)  | 76.1(3)   |
| C(27)-C(22)-U(1)  | 115.3(3)  |
| C(24)-C(23)-C(22) | 108.0     |
| C(24)-C(23)-C(28) | 126.0     |
| C(22)-C(23)-C(28) | 126.0     |
| C(24)-C(23)-U(1)  | 75.6(3)   |
| C(22)-C(23)-U(1)  | 76.0(3)   |
| C(28)-C(23)-U(1)  | 114.6(3)  |
| C(23)-C(24)-C(25) | 108.0     |
| C(23)-C(24)-C(29) | 126.0     |
| C(25)-C(24)-C(29) | 126.0     |
| C(23)-C(24)-U(1)  | 75.2(3)   |
| C(25)-C(24)-U(1)  | 76.2(3)   |
| C(29)-C(24)-U(1)  | 114.8(3)  |
| C(26)-C(25)-C(24) | 108.0     |

|                   |           |
|-------------------|-----------|
| C(26)-C(25)-C(30) | 126.0     |
| C(24)-C(25)-C(30) | 126.0     |
| C(26)-C(25)-U(1)  | 75.8(3)   |
| C(24)-C(25)-U(1)  | 74.8(3)   |
| C(30)-C(25)-U(1)  | 115.6(3)  |
| C(25)-C(26)-C(22) | 108.0     |
| C(25)-C(26)-C(31) | 126.0     |
| C(22)-C(26)-C(31) | 126.0     |
| C(25)-C(26)-U(1)  | 75.3(3)   |
| C(22)-C(26)-U(1)  | 75.0(3)   |
| C(31)-C(26)-U(1)  | 115.9(3)  |
| C(33)-C(32)-U(2)  | 87.2(11)  |
| C(38)-C(33)-C(32) | 123.6(19) |
| C(38)-C(33)-C(34) | 113.8(18) |
| C(32)-C(33)-C(34) | 122.4(17) |
| C(38)-C(33)-U(2)  | 103.6(13) |
| C(32)-C(33)-U(2)  | 61.9(10)  |
| C(34)-C(33)-U(2)  | 102.4(12) |
| C(35)-C(34)-C(33) | 122.9(19) |
| C(36)-C(35)-C(34) | 119(2)    |
| C(37)-C(36)-C(35) | 121(2)    |
| C(36)-C(37)-C(38) | 122(2)    |
| C(37)-C(38)-C(33) | 122(2)    |
| C(40)-C(39)-U(2)  | 88.6(11)  |
| C(45)-C(40)-C(41) | 118(2)    |
| C(45)-C(40)-C(39) | 122.8(19) |
| C(41)-C(40)-C(39) | 118.5(19) |
| C(45)-C(40)-U(2)  | 97.6(12)  |
| C(41)-C(40)-U(2)  | 103.6(12) |
| C(39)-C(40)-U(2)  | 60.2(9)   |
| C(42)-C(41)-C(40) | 119(2)    |
| C(43)-C(42)-C(41) | 122(2)    |
| C(42)-C(43)-C(44) | 120(2)    |
| C(45)-C(44)-C(43) | 121(2)    |
| C(44)-C(45)-C(40) | 121(2)    |
| C(47)-C(46)-U(2)  | 89.2(11)  |

|                   |           |
|-------------------|-----------|
| C(52)-C(47)-C(48) | 115.9(18) |
| C(52)-C(47)-C(46) | 124.4(19) |
| C(48)-C(47)-C(46) | 119(2)    |
| C(52)-C(47)-U(2)  | 99.1(12)  |
| C(48)-C(47)-U(2)  | 107.1(13) |
| C(46)-C(47)-U(2)  | 59.8(10)  |
| C(49)-C(48)-C(47) | 120(2)    |
| C(48)-C(49)-C(50) | 121(2)    |
| C(51)-C(50)-C(49) | 119(2)    |
| C(50)-C(51)-C(52) | 123(2)    |
| C(51)-C(52)-C(47) | 121(2)    |
| C(54)-C(53)-C(57) | 108.0     |
| C(54)-C(53)-C(58) | 126.0     |
| C(57)-C(53)-C(58) | 126.0     |
| C(54)-C(53)-U(2)  | 76.3(3)   |
| C(57)-C(53)-U(2)  | 75.0(3)   |
| C(58)-C(53)-U(2)  | 114.9(3)  |
| C(53)-C(54)-C(55) | 108.0     |
| C(53)-C(54)-C(59) | 126.0     |
| C(55)-C(54)-C(59) | 126.0     |
| C(53)-C(54)-U(2)  | 74.6(3)   |
| C(55)-C(54)-U(2)  | 75.7(3)   |
| C(59)-C(54)-U(2)  | 115.9(3)  |
| C(56)-C(55)-C(54) | 108.0     |
| C(56)-C(55)-C(60) | 126.0     |
| C(54)-C(55)-C(60) | 126.0     |
| C(56)-C(55)-U(2)  | 74.7(3)   |
| C(54)-C(55)-U(2)  | 75.3(3)   |
| C(60)-C(55)-U(2)  | 116.1(3)  |
| C(57)-C(56)-C(55) | 108.0     |
| C(57)-C(56)-C(61) | 126.0     |
| C(55)-C(56)-C(61) | 126.0     |
| C(57)-C(56)-U(2)  | 74.7(3)   |
| C(55)-C(56)-U(2)  | 76.2(3)   |
| C(61)-C(56)-U(2)  | 115.2(3)  |
| C(56)-C(57)-C(53) | 108.0     |

|                   |          |
|-------------------|----------|
| C(56)-C(57)-C(62) | 126.0    |
| C(53)-C(57)-C(62) | 126.0    |
| C(56)-C(57)-U(2)  | 76.0(3)  |
| C(53)-C(57)-U(2)  | 75.7(3)  |
| C(62)-C(57)-U(2)  | 114.5(3) |

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Symmetry transformations used to generate equivalent atoms:

**Table 4.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for  $(\text{C}_5\text{Me}_5)\text{U}(\text{CH}_2\text{C}_5\text{H}_6)_3$  (3). The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

|       | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|-------|----------|----------|----------|----------|----------|----------|
| U(1)  | 17(1)    | 19(1)    | 18(1)    | -1(1)    | 3(1)     | 0(1)     |
| U(2)  | 18(1)    | 15(1)    | 17(1)    | 1(1)     | 3(1)     | 2(1)     |
| C(1)  | 17(9)    | 24(8)    | 22(8)    | 0(7)     | 6(7)     | 5(7)     |
| C(2)  | 18(9)    | 19(8)    | 25(8)    | -1(7)    | -3(7)    | -1(7)    |
| C(3)  | 31(9)    | 39(9)    | 35(9)    | -2(7)    | 5(8)     | -5(7)    |
| C(4)  | 36(10)   | 39(9)    | 32(9)    | -4(7)    | 5(8)     | 5(8)     |
| C(5)  | 46(10)   | 49(10)   | 42(10)   | -3(8)    | 12(8)    | 3(8)     |
| C(6)  | 38(10)   | 41(9)    | 44(10)   | 2(8)     | 7(8)     | -3(8)    |
| C(7)  | 29(9)    | 31(8)    | 28(9)    | -2(7)    | 7(7)     | 1(7)     |
| C(8)  | 25(9)    | 34(9)    | 32(9)    | -2(7)    | -4(7)    | 4(7)     |
| C(9)  | 31(9)    | 14(8)    | 22(8)    | 1(7)     | 8(7)     | 9(7)     |
| C(10) | 45(10)   | 50(9)    | 34(9)    | -11(8)   | 12(8)    | -3(8)    |
| C(11) | 35(10)   | 38(9)    | 27(9)    | -8(7)    | 7(8)     | -5(8)    |
| C(12) | 45(10)   | 41(9)    | 42(10)   | -1(8)    | -1(8)    | -1(8)    |
| C(13) | 35(10)   | 49(9)    | 36(9)    | -7(8)    | 4(8)     | 0(8)     |
| C(14) | 36(10)   | 32(9)    | 35(9)    | 3(7)     | 5(8)     | -15(8)   |
| C(15) | 41(10)   | 33(9)    | 29(9)    | 2(7)     | 8(8)     | -4(8)    |
| C(16) | 31(9)    | 37(9)    | 33(9)    | 7(7)     | 11(8)    | 1(7)     |
| C(17) | 31(9)    | 35(9)    | 37(9)    | 9(7)     | 11(8)    | 1(7)     |
| C(18) | 29(9)    | 37(9)    | 43(10)   | 1(8)     | 6(8)     | 3(8)     |
| C(19) | 40(10)   | 35(9)    | 39(9)    | 1(7)     | 4(8)     | -5(8)    |
| C(20) | 41(10)   | 35(9)    | 44(10)   | 2(8)     | 7(8)     | 4(8)     |
| C(21) | 34(10)   | 40(9)    | 37(9)    | 3(8)     | 2(8)     | -2(8)    |
| C(22) | 34(9)    | 30(8)    | 30(9)    | 5(7)     | 6(7)     | -1(7)    |
| C(23) | 32(9)    | 33(9)    | 38(9)    | 10(7)    | 5(8)     | -10(7)   |
| C(24) | 35(10)   | 34(9)    | 49(10)   | -14(8)   | 5(8)     | 2(8)     |
| C(25) | 21(9)    | 31(8)    | 22(8)    | 2(7)     | -1(7)    | 0(7)     |
| C(26) | 23(9)    | 21(8)    | 24(9)    | 1(7)     | -1(7)    | 1(7)     |
| C(27) | 48(10)   | 50(10)   | 43(10)   | -4(8)    | 3(8)     | -8(8)    |
| C(28) | 69(12)   | 62(11)   | 70(11)   | 6(8)     | 7(9)     | 1(9)     |
| C(29) | 66(12)   | 75(11)   | 75(12)   | -11(9)   | 8(9)     | 6(9)     |

|       |        |        |        |       |       |       |
|-------|--------|--------|--------|-------|-------|-------|
| C(30) | 43(10) | 63(10) | 46(10) | -2(8) | 15(8) | -6(8) |
| C(31) | 59(11) | 51(10) | 53(10) | 1(8)  | 7(8)  | -7(8) |
| C(32) | 23(9)  | 29(8)  | 19(8)  | 9(7)  | 6(7)  | 5(7)  |
| C(33) | 23(9)  | 34(8)  | 12(8)  | 3(7)  | -3(7) | -2(7) |
| C(34) | 22(9)  | 20(8)  | 23(8)  | -3(7) | 6(7)  | 5(7)  |
| C(35) | 23(9)  | 35(9)  | 34(9)  | 6(7)  | 11(7) | 2(7)  |
| C(36) | 39(10) | 40(9)  | 37(9)  | 0(8)  | 4(8)  | 9(8)  |
| C(37) | 43(10) | 31(9)  | 34(9)  | 1(7)  | 3(8)  | 1(8)  |
| C(38) | 24(9)  | 35(9)  | 32(9)  | 1(7)  | 3(7)  | 1(7)  |
| C(39) | 18(8)  | 20(8)  | 16(8)  | 3(6)  | 0(7)  | -2(7) |
| C(40) | 25(9)  | 24(8)  | 25(9)  | -1(7) | 7(7)  | -1(7) |
| C(41) | 20(9)  | 23(8)  | 25(9)  | -5(7) | 10(7) | 1(7)  |
| C(42) | 34(10) | 36(9)  | 29(9)  | -4(7) | 12(8) | 2(7)  |
| C(43) | 29(9)  | 26(8)  | 25(9)  | 0(7)  | 0(7)  | -2(7) |
| C(44) | 17(9)  | 31(8)  | 28(9)  | -2(7) | 8(7)  | -2(7) |
| C(45) | 22(9)  | 25(8)  | 26(9)  | 0(7)  | 13(7) | -6(7) |
| C(46) | 27(9)  | 24(8)  | 18(8)  | 3(7)  | 9(7)  | 0(7)  |
| C(47) | 29(9)  | 25(8)  | 22(8)  | -8(7) | 7(7)  | 9(7)  |
| C(48) | 30(9)  | 38(9)  | 29(9)  | -9(7) | 7(7)  | -2(7) |
| C(49) | 34(9)  | 35(9)  | 20(8)  | -5(7) | 8(7)  | 7(7)  |
| C(50) | 39(10) | 37(9)  | 34(9)  | 2(7)  | 19(8) | 1(8)  |
| C(51) | 36(10) | 37(9)  | 38(9)  | -3(8) | 5(8)  | 0(8)  |
| C(52) | 24(9)  | 30(8)  | 23(8)  | -5(7) | 5(7)  | 1(7)  |
| C(53) | 17(9)  | 31(8)  | 25(9)  | 2(7)  | 9(7)  | -1(7) |
| C(54) | 29(9)  | 29(8)  | 27(9)  | 0(7)  | 3(7)  | 15(7) |
| C(55) | 18(6)  | 13(5)  | 19(6)  | 4(4)  | 1(4)  | 8(4)  |
| C(56) | 15(6)  | 18(6)  | 10(6)  | 4(4)  | 7(4)  | 0(4)  |
| C(57) | 14(8)  | 24(8)  | 17(8)  | 6(7)  | 3(7)  | -7(7) |
| C(58) | 42(10) | 34(9)  | 38(9)  | -4(7) | 9(8)  | -9(8) |
| C(59) | 49(10) | 32(9)  | 40(9)  | 2(7)  | 14(8) | 1(8)  |
| C(60) | 38(10) | 45(9)  | 27(9)  | -9(7) | 12(8) | -1(8) |
| C(61) | 42(10) | 45(9)  | 51(10) | 6(8)  | 13(8) | 10(8) |
| C(62) | 37(10) | 51(10) | 39(9)  | 3(8)  | 9(8)  | -2(8) |

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**Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^{-3}$ ) for  $(\text{C}_5\text{Me}_5)\text{U}(\text{CH}_2\text{C}_5\text{H}_6)_3$  (3).**

|        | x    | y     | z    | U(eq) |
|--------|------|-------|------|-------|
| H(3)   | 4475 | 1058  | 8613 | 42    |
| H(4)   | 3299 | 1005  | 9631 | 43    |
| H(5)   | 1086 | 713   | 9480 | 54    |
| H(6)   | 27   | 417   | 8330 | 50    |
| H(7)   | 1213 | 438   | 7310 | 35    |
| H(10)  | 4994 | 148   | 5625 | 51    |
| H(11)  | 3462 | 628   | 4948 | 40    |
| H(12)  | 1088 | 643   | 5033 | 52    |
| H(13)  | 251  | 139   | 5826 | 49    |
| H(14)  | 1756 | -364  | 6492 | 42    |
| H(17)  | 1664 | -402  | 8080 | 40    |
| H(18)  | 936  | -984  | 7339 | 44    |
| H(19)  | 2412 | -1572 | 7283 | 46    |
| H(20)  | 4713 | -1543 | 7999 | 48    |
| H(21)  | 5536 | -942  | 8697 | 45    |
| H(27A) | 6991 | 878   | 9287 | 72    |
| H(27B) | 8039 | 521   | 9685 | 72    |
| H(27C) | 6402 | 427   | 9495 | 72    |
| H(28A) | 8004 | -680  | 8692 | 102   |
| H(28B) | 6973 | -452  | 9160 | 102   |
| H(28C) | 8611 | -357  | 9350 | 102   |
| H(29A) | 8113 | -719  | 7528 | 109   |
| H(29B) | 8834 | -438  | 6971 | 109   |
| H(29C) | 7196 | -532  | 6782 | 109   |
| H(30A) | 7625 | 220   | 6188 | 74    |
| H(30B) | 8171 | 688   | 6444 | 74    |
| H(30C) | 6533 | 593   | 6254 | 74    |
| H(31A) | 6838 | 1242  | 8276 | 82    |
| H(31B) | 6089 | 1169  | 7431 | 82    |
| H(31C) | 7727 | 1264  | 7621 | 82    |

|        |      |      |      |    |
|--------|------|------|------|----|
| H(34)  | 7932 | 2355 | 5412 | 26 |
| H(35)  | 9175 | 1888 | 4748 | 36 |
| H(36)  | 8263 | 1202 | 4415 | 47 |
| H(37)  | 6272 | 963  | 4810 | 44 |
| H(38)  | 5068 | 1392 | 5548 | 37 |
| H(41)  | 3699 | 3438 | 5745 | 26 |
| H(42)  | 5259 | 3444 | 6905 | 39 |
| H(43)  | 7629 | 3333 | 6970 | 33 |
| H(44)  | 8513 | 3193 | 5877 | 30 |
| H(45)  | 7020 | 3143 | 4730 | 28 |
| H(48)  | 3223 | 2500 | 2489 | 38 |
| H(49)  | 3849 | 3150 | 1984 | 35 |
| H(50)  | 6093 | 3455 | 2400 | 43 |
| H(51)  | 7682 | 3098 | 3265 | 45 |
| H(52)  | 7209 | 2451 | 3749 | 31 |
| H(58A) | 1560 | 1575 | 3415 | 57 |
| H(58B) | 1181 | 1307 | 4097 | 57 |
| H(58C) | 2773 | 1414 | 4066 | 57 |
| H(59A) | 2587 | 1747 | 6262 | 60 |
| H(59B) | 3352 | 1511 | 5671 | 60 |
| H(59C) | 1759 | 1404 | 5702 | 60 |
| H(60A) | 1705 | 2929 | 6102 | 54 |
| H(60B) | 2898 | 2588 | 6397 | 54 |
| H(60C) | 1306 | 2481 | 6428 | 54 |
| H(61A) | 1058 | 3262 | 5068 | 68 |
| H(61B) | -15  | 3162 | 4316 | 68 |
| H(61C) | 1577 | 3269 | 4285 | 68 |
| H(62A) | 943  | 2186 | 2933 | 63 |
| H(62B) | 1512 | 2663 | 3081 | 63 |
| H(62C) | -80  | 2556 | 3113 | 63 |

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**Table 1. Crystal data and structure refinement for (C<sub>5</sub>Me<sub>5</sub>)(C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>U(CH<sub>2</sub>C<sub>6</sub>H<sub>5</sub>) (4).**

|                                   |                                                                          |
|-----------------------------------|--------------------------------------------------------------------------|
| Identification code               | ccd580d                                                                  |
| Empirical formula                 | C <sub>27</sub> H <sub>32</sub> U                                        |
| Formula weight                    | 594.56                                                                   |
| Temperature                       | 203(2) K                                                                 |
| Wavelength                        | 0.71073 Å                                                                |
| Crystal system                    | monoclinic                                                               |
| Space group                       | P 2 <sub>1</sub> /n                                                      |
| Unit cell dimensions              | a = 8.099(3) Å<br>b = 19.261(6) Å      β = 92.016(5)°<br>c = 14.495(5) Å |
| Volume                            | 2259.7(12) Å <sup>3</sup>                                                |
| Z                                 | 4                                                                        |
| Density (calculated)              | 1.748 Mg/m <sup>3</sup>                                                  |
| Absorption coefficient            | 7.192 mm <sup>-1</sup>                                                   |
| F(000)                            | 1144                                                                     |
| Crystal size                      | 0.25 x 0.21 x 0.21 mm <sup>3</sup>                                       |
| Theta range for data collection   | 1.76 to 23.28°                                                           |
| Index ranges                      | -8 ≤ h ≤ 8, 0 ≤ k ≤ 21, 0 ≤ l ≤ 16                                       |
| Reflections collected             | 7046                                                                     |
| Independent reflections           | 3237 [R(int) = 0.0683]                                                   |
| Max. and min. transmission        | 0.3135 and 0.2665                                                        |
| Refinement method                 | Full-matrix least-squares on F <sup>2</sup>                              |
| Data / restraints / parameters    | 3237 / 0 / 244                                                           |
| Goodness-of-fit on F <sup>2</sup> | 1.027                                                                    |
| Final R indices [I > 2σ(I)]       | R1 = 0.0540, wR2 = 0.1356                                                |
| R indices (all data)              | R1 = 0.0760, wR2 = 0.1479                                                |
| Largest diff. peak and hole       | 1.788 and -1.315 e.Å <sup>-3</sup>                                       |

**Table 2.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for  $(\text{C}_5\text{Me}_5)(\text{C}_5\text{H}_5)_2\text{U}(\text{CH}_2\text{C}_6\text{H}_5)$  (**4**).  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

|       | x         | y        | z        | $U(\text{eq})$ |
|-------|-----------|----------|----------|----------------|
| U(1)  | 1936(1)   | 2766(1)  | 999(1)   | 31(1)          |
| C(1)  | 2290(20)  | 2651(7)  | -864(9)  | 46(4)          |
| C(2)  | 3830(20)  | 2866(9)  | -533(10) | 63(5)          |
| C(3)  | 4390(30)  | 2288(11) | -30(12)  | 80(7)          |
| C(4)  | 3370(30)  | 1744(10) | -71(12)  | 98(8)          |
| C(5)  | 2030(20)  | 1964(9)  | -585(11) | 62(5)          |
| C(6)  | 3230(30)  | 1715(7)  | 2095(10) | 155(16)        |
| C(7)  | 4430(17)  | 2254(11) | 2122(9)  | 151(16)        |
| C(8)  | 3779(18)  | 2819(8)  | 2624(9)  | 78(6)          |
| C(9)  | 2180(17)  | 2628(8)  | 2907(8)  | 78(6)          |
| C(10) | 1840(20)  | 1946(9)  | 2580(11) | 94(7)          |
| C(11) | 2239(16)  | 4202(7)  | 1062(12) | 52(4)          |
| C(12) | 1270(20)  | 4070(7)  | 247(10)  | 56(4)          |
| C(13) | -220(18)  | 3829(6)  | 506(10)  | 46(4)          |
| C(14) | -201(18)  | 3822(6)  | 1468(11) | 47(4)          |
| C(15) | 1240(20)  | 4045(7)  | 1813(9)  | 51(4)          |
| C(16) | 3930(20)  | 4524(10) | 1170(20) | 148(12)        |
| C(17) | 1730(40)  | 4327(10) | -726(14) | 178(16)        |
| C(18) | -1710(20) | 3706(9)  | -151(17) | 124(10)        |
| C(19) | -1800(30) | 3681(10) | 1969(18) | 134(11)        |
| C(20) | 1660(40)  | 4279(11) | 2781(12) | 142(11)        |
| C(21) | -802(19)  | 2183(9)  | 904(17)  | 82(6)          |
| C(22) | -1360(20) | 1436(7)  | 958(13)  | 63(5)          |
| C(23) | -1460(30) | 1007(12) | 180(13)  | 139(12)        |
| C(24) | -1970(40) | 337(12)  | 252(14)  | 179(16)        |
| C(25) | -2410(30) | 54(8)    | 1044(11) | 90(7)          |
| C(26) | -2180(20) | 437(8)   | 1799(12) | 81(6)          |
| C(27) | -1700(20) | 1123(8)  | 1777(12) | 84(6)          |

**Table 3. Bond lengths [Å] and angles [°] for (C<sub>5</sub>Me<sub>5</sub>)(C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>U(CH<sub>2</sub>C<sub>6</sub>H<sub>5</sub>) (4).**


---

|             |           |
|-------------|-----------|
| U(1)-C(21)  | 2.485(16) |
| U(1)-C(3)   | 2.687(17) |
| U(1)-C(7)   | 2.734(11) |
| U(1)-C(1)   | 2.734(14) |
| U(1)-C(8)   | 2.746(11) |
| U(1)-C(2)   | 2.748(15) |
| U(1)-C(6)   | 2.759(12) |
| U(1)-C(13)  | 2.769(11) |
| U(1)-C(5)   | 2.771(15) |
| U(1)-C(14)  | 2.771(13) |
| U(1)-C(11)  | 2.777(13) |
| U(1)-C(9)   | 2.778(12) |
| C(1)-C(2)   | 1.38(2)   |
| C(1)-C(5)   | 1.40(2)   |
| C(2)-C(3)   | 1.40(2)   |
| C(3)-C(4)   | 1.33(3)   |
| C(4)-C(5)   | 1.36(3)   |
| C(6)-C(7)   | 1.4200    |
| C(6)-C(10)  | 1.4200    |
| C(7)-C(8)   | 1.4200    |
| C(8)-C(9)   | 1.4200    |
| C(9)-C(10)  | 1.4200    |
| C(11)-C(15) | 1.41(2)   |
| C(11)-C(12) | 1.42(2)   |
| C(11)-C(16) | 1.50(2)   |
| C(12)-C(13) | 1.36(2)   |
| C(12)-C(17) | 1.55(2)   |
| C(13)-C(14) | 1.394(19) |
| C(13)-C(18) | 1.53(2)   |
| C(14)-C(15) | 1.324(19) |
| C(14)-C(19) | 1.53(2)   |
| C(15)-C(20) | 1.503(19) |
| C(21)-C(22) | 1.51(2)   |
| C(22)-C(27) | 1.37(2)   |

|             |         |
|-------------|---------|
| C(22)-C(23) | 1.40(3) |
| C(23)-C(24) | 1.36(3) |
| C(24)-C(25) | 1.33(2) |
| C(25)-C(26) | 1.33(2) |
| C(26)-C(27) | 1.38(2) |

|                  |           |
|------------------|-----------|
| C(21)-U(1)-C(3)  | 119.3(7)  |
| C(21)-U(1)-C(7)  | 120.6(6)  |
| C(3)-U(1)-C(7)   | 70.3(5)   |
| C(21)-U(1)-C(1)  | 91.8(7)   |
| C(3)-U(1)-C(1)   | 47.1(5)   |
| C(7)-U(1)-C(1)   | 117.3(4)  |
| C(21)-U(1)-C(8)  | 121.4(6)  |
| C(3)-U(1)-C(8)   | 95.7(6)   |
| C(7)-U(1)-C(8)   | 30.04(11) |
| C(1)-U(1)-C(8)   | 141.1(5)  |
| C(21)-U(1)-C(2)  | 120.6(7)  |
| C(3)-U(1)-C(2)   | 29.8(5)   |
| C(7)-U(1)-C(2)   | 94.9(5)   |
| C(1)-U(1)-C(2)   | 29.3(5)   |
| C(8)-U(1)-C(2)   | 112.9(5)  |
| C(21)-U(1)-C(6)  | 91.2(7)   |
| C(3)-U(1)-C(6)   | 78.1(6)   |
| C(7)-U(1)-C(6)   | 29.96(12) |
| C(1)-U(1)-C(6)   | 117.3(4)  |
| C(8)-U(1)-C(6)   | 49.34(13) |
| C(2)-U(1)-C(6)   | 107.8(6)  |
| C(21)-U(1)-C(13) | 76.5(5)   |
| C(3)-U(1)-C(13)  | 125.6(5)  |
| C(7)-U(1)-C(13)  | 150.1(5)  |
| C(1)-U(1)-C(13)  | 83.8(4)   |
| C(8)-U(1)-C(13)  | 120.9(4)  |
| C(2)-U(1)-C(13)  | 96.0(5)   |
| C(6)-U(1)-C(13)  | 156.2(6)  |
| C(21)-U(1)-C(5)  | 75.6(7)   |
| C(3)-U(1)-C(5)   | 46.2(6)   |

|                  |           |
|------------------|-----------|
| C(7)-U(1)-C(5)   | 104.6(5)  |
| C(1)-U(1)-C(5)   | 29.5(5)   |
| C(8)-U(1)-C(5)   | 134.6(5)  |
| C(2)-U(1)-C(5)   | 48.5(5)   |
| C(6)-U(1)-C(5)   | 92.7(4)   |
| C(13)-U(1)-C(5)  | 103.5(5)  |
| C(21)-U(1)-C(14) | 77.4(5)   |
| C(3)-U(1)-C(14)  | 150.2(5)  |
| C(7)-U(1)-C(14)  | 125.0(5)  |
| C(1)-U(1)-C(14)  | 112.9(4)  |
| C(8)-U(1)-C(14)  | 95.0(5)   |
| C(2)-U(1)-C(14)  | 121.2(5)  |
| C(6)-U(1)-C(14)  | 128.7(5)  |
| C(13)-U(1)-C(14) | 29.1(4)   |
| C(5)-U(1)-C(14)  | 130.4(5)  |
| C(21)-U(1)-C(11) | 121.9(5)  |
| C(3)-U(1)-C(11)  | 107.1(6)  |
| C(7)-U(1)-C(11)  | 106.1(6)  |
| C(1)-U(1)-C(11)  | 95.8(5)   |
| C(8)-U(1)-C(11)  | 83.7(4)   |
| C(2)-U(1)-C(11)  | 84.6(5)   |
| C(6)-U(1)-C(11)  | 132.9(5)  |
| C(13)-U(1)-C(11) | 47.6(4)   |
| C(5)-U(1)-C(11)  | 125.3(5)  |
| C(14)-U(1)-C(11) | 46.8(4)   |
| C(21)-U(1)-C(9)  | 92.5(7)   |
| C(3)-U(1)-C(9)   | 119.4(5)  |
| C(7)-U(1)-C(9)   | 49.26(12) |
| C(1)-U(1)-C(9)   | 165.7(4)  |
| C(8)-U(1)-C(9)   | 29.78(11) |
| C(2)-U(1)-C(9)   | 142.1(5)  |
| C(6)-U(1)-C(9)   | 49.03(13) |
| C(13)-U(1)-C(9)  | 110.4(4)  |
| C(5)-U(1)-C(9)   | 140.2(5)  |
| C(14)-U(1)-C(9)  | 81.3(4)   |
| C(11)-U(1)-C(9)  | 93.4(5)   |

|                   |           |
|-------------------|-----------|
| C(2)-C(1)-C(5)    | 109.0(14) |
| C(2)-C(1)-U(1)    | 75.9(8)   |
| C(5)-C(1)-U(1)    | 76.7(9)   |
| C(1)-C(2)-C(3)    | 102.4(17) |
| C(1)-C(2)-U(1)    | 74.8(9)   |
| C(3)-C(2)-U(1)    | 72.7(10)  |
| C(4)-C(3)-C(2)    | 114(2)    |
| C(4)-C(3)-U(1)    | 80.0(12)  |
| C(2)-C(3)-U(1)    | 77.5(9)   |
| C(3)-C(4)-C(5)    | 105.2(17) |
| C(3)-C(4)-U(1)    | 71.9(10)  |
| C(5)-C(4)-U(1)    | 75.2(10)  |
| C(4)-C(5)-C(1)    | 109.0(16) |
| C(4)-C(5)-U(1)    | 76.3(9)   |
| C(1)-C(5)-U(1)    | 73.8(8)   |
| C(7)-C(6)-C(10)   | 108.0     |
| C(7)-C(6)-U(1)    | 74.0(5)   |
| C(10)-C(6)-U(1)   | 76.2(5)   |
| C(8)-C(7)-C(6)    | 108.0     |
| C(8)-C(7)-U(1)    | 75.4(5)   |
| C(6)-C(7)-U(1)    | 76.0(5)   |
| C(7)-C(8)-C(9)    | 108.0     |
| C(7)-C(8)-U(1)    | 74.5(5)   |
| C(9)-C(8)-U(1)    | 76.4(5)   |
| C(8)-C(9)-C(10)   | 108.0     |
| C(8)-C(9)-U(1)    | 73.8(5)   |
| C(10)-C(9)-U(1)   | 75.5(5)   |
| C(9)-C(10)-C(6)   | 108.0     |
| C(9)-C(10)-U(1)   | 74.9(5)   |
| C(6)-C(10)-U(1)   | 74.1(5)   |
| C(15)-C(11)-C(12) | 106.7(12) |
| C(15)-C(11)-C(16) | 123.6(18) |
| C(12)-C(11)-C(16) | 129.3(19) |
| C(15)-C(11)-U(1)  | 76.1(8)   |
| C(12)-C(11)-U(1)  | 75.4(7)   |
| C(16)-C(11)-U(1)  | 119.5(11) |

|                   |           |
|-------------------|-----------|
| C(13)-C(12)-C(11) | 107.6(12) |
| C(13)-C(12)-C(17) | 127(2)    |
| C(11)-C(12)-C(17) | 124(2)    |
| C(13)-C(12)-U(1)  | 75.3(7)   |
| C(11)-C(12)-U(1)  | 75.0(7)   |
| C(17)-C(12)-U(1)  | 126.5(10) |
| C(12)-C(13)-C(14) | 107.5(13) |
| C(12)-C(13)-C(18) | 124.7(17) |
| C(14)-C(13)-C(18) | 127.1(17) |
| C(12)-C(13)-U(1)  | 76.4(8)   |
| C(14)-C(13)-U(1)  | 75.5(7)   |
| C(18)-C(13)-U(1)  | 121.5(9)  |
| C(15)-C(14)-C(13) | 110.7(13) |
| C(15)-C(14)-C(19) | 128.9(17) |
| C(13)-C(14)-C(19) | 119.7(17) |
| C(15)-C(14)-U(1)  | 77.3(9)   |
| C(13)-C(14)-U(1)  | 75.3(7)   |
| C(19)-C(14)-U(1)  | 122.1(10) |
| C(14)-C(15)-C(11) | 107.4(12) |
| C(14)-C(15)-C(20) | 128.2(18) |
| C(11)-C(15)-C(20) | 122.5(17) |
| C(14)-C(15)-U(1)  | 75.2(8)   |
| C(11)-C(15)-U(1)  | 74.5(8)   |
| C(20)-C(15)-U(1)  | 128.0(11) |
| C(22)-C(21)-U(1)  | 134.0(11) |
| C(27)-C(22)-C(23) | 115.5(14) |
| C(27)-C(22)-C(21) | 122.3(18) |
| C(23)-C(22)-C(21) | 122.1(18) |
| C(24)-C(23)-C(22) | 120.6(17) |
| C(25)-C(24)-C(23) | 123(2)    |
| C(26)-C(25)-C(24) | 116.7(16) |
| C(25)-C(26)-C(27) | 123.0(16) |
| C(22)-C(27)-C(26) | 120.6(16) |

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Symmetry transformations used to generate equivalent atoms:

**Table 4.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for  $(\text{C}_5\text{Me}_5)(\text{C}_5\text{H}_5)_2\text{U}(\text{CH}_2\text{C}_6\text{H}_5)$  (4). The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$ .

|       | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|-------|----------|----------|----------|----------|----------|----------|
| U(1)  | 32(1)    | 31(1)    | 30(1)    | 4(1)     | 1(1)     | 0(1)     |
| C(1)  | 54(10)   | 49(9)    | 34(7)    | -12(6)   | -7(7)    | 21(7)    |
| C(2)  | 71(12)   | 87(13)   | 33(8)    | -11(8)   | 9(8)     | 7(10)    |
| C(3)  | 90(15)   | 96(16)   | 53(10)   | -4(11)   | -2(10)   | 67(13)   |
| C(4)  | 200(30)  | 44(10)   | 50(10)   | -18(9)   | 15(14)   | 28(15)   |
| C(5)  | 72(12)   | 58(10)   | 56(10)   | -8(8)    | -23(9)   | -7(9)    |
| C(6)  | 330(50)  | 89(17)   | 44(13)   | 18(13)   | -40(20)  | 70(20)   |
| C(7)  | 81(18)   | 320(40)  | 51(13)   | 60(20)   | 2(12)    | 130(20)  |
| C(8)  | 53(12)   | 145(19)  | 35(9)    | 33(10)   | -10(8)   | -1(12)   |
| C(9)  | 103(18)  | 89(15)   | 41(9)    | 10(9)    | -12(10)  | 13(12)   |
| C(10) | 104(18)  | 113(18)  | 63(13)   | 52(12)   | -1(12)   | -39(14)  |
| C(11) | 34(9)    | 22(7)    | 99(13)   | -4(7)    | 3(9)     | -13(6)   |
| C(12) | 100(14)  | 31(8)    | 39(8)    | 16(6)    | 34(9)    | 24(8)    |
| C(13) | 57(10)   | 17(6)    | 61(9)    | -7(6)    | -28(8)   | 22(6)    |
| C(14) | 56(10)   | 15(6)    | 70(10)   | 2(6)     | 13(8)    | 10(6)    |
| C(15) | 74(11)   | 53(9)    | 24(7)    | -6(6)    | -15(7)   | 10(8)    |
| C(16) | 48(12)   | 61(13)   | 330(40)  | -16(18)  | 25(18)   | -21(10)  |
| C(17) | 400(50)  | 42(11)   | 96(16)   | 39(11)   | 120(20)  | 80(20)   |
| C(18) | 122(18)  | 48(11)   | 190(20)  | -35(13)  | -111(17) | 41(12)   |
| C(19) | 140(20)  | 49(12)   | 220(30)  | -10(14)  | 140(20)  | 11(13)   |
| C(20) | 300(30)  | 62(12)   | 56(12)   | -29(10)  | -82(16)  | 16(17)   |
| C(21) | 24(9)    | 76(13)   | 140(20)  | 21(12)   | 1(10)    | 6(8)     |
| C(22) | 61(11)   | 22(7)    | 106(14)  | 21(8)    | -11(10)  | -2(7)    |
| C(23) | 250(30)  | 115(18)  | 49(11)   | 27(12)   | -37(15)  | -130(20) |
| C(24) | 370(40)  | 120(20)  | 50(12)   | -6(12)   | 23(19)   | -160(30) |
| C(25) | 170(20)  | 32(9)    | 67(12)   | -9(9)    | 44(12)   | -42(11)  |
| C(26) | 139(18)  | 38(9)    | 67(11)   | 5(8)     | 30(11)   | -36(10)  |
| C(27) | 123(16)  | 50(10)   | 82(13)   | -23(9)   | 59(12)   | -47(11)  |

**Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^{-3}$ ) for  $(\text{C}_5\text{Me}_5)(\text{C}_5\text{H}_5)_2\text{U}(\text{CH}_2\text{C}_6\text{H}_5)$  (4).**

|        | x     | y    | z     | U(eq) |
|--------|-------|------|-------|-------|
| H(1)   | 1544  | 2919 | -1215 | 55    |
| H(2)   | 4356  | 3288 | -623  | 76    |
| H(3)   | 5387  | 2283 | 306   | 96    |
| H(4)   | 3538  | 1309 | 193   | 117   |
| H(5)   | 1089  | 1700 | -728  | 75    |
| H(6)   | 3342  | 1285 | 1810  | 186   |
| H(7)   | 5459  | 2240 | 1858  | 181   |
| H(8)   | 4307  | 3239 | 2746  | 94    |
| H(9)   | 1477  | 2903 | 3246  | 94    |
| H(10)  | 880   | 1695 | 2668  | 112   |
| H(16A) | 4375  | 4589 | 568   | 222   |
| H(16B) | 4640  | 4223 | 1528  | 222   |
| H(16C) | 3845  | 4965 | 1471  | 222   |
| H(17A) | 2866  | 4467 | -714  | 266   |
| H(17B) | 1041  | 4715 | -901  | 266   |
| H(17C) | 1559  | 3958 | -1165 | 266   |
| H(18A) | -2620 | 3537 | 191   | 187   |
| H(18B) | -1428 | 3369 | -608  | 187   |
| H(18C) | -2016 | 4134 | -450  | 187   |
| H(19A) | -2635 | 3520 | 1532  | 201   |
| H(19B) | -2168 | 4101 | 2253  | 201   |
| H(19C) | -1604 | 3333 | 2434  | 201   |
| H(20A) | 2804  | 4414 | 2827  | 214   |
| H(20B) | 1474  | 3906 | 3203  | 214   |
| H(20C) | 982   | 4668 | 2933  | 214   |
| H(21A) | -1421 | 2414 | 1376  | 98    |
| H(21B) | -1287 | 2344 | 321   | 98    |
| H(23)  | -1183 | 1182 | -392  | 167   |
| H(24)  | -2011 | 64   | -277  | 215   |
| H(25)  | -2854 | -391 | 1067  | 108   |

|       |       |      |      |     |
|-------|-------|------|------|-----|
| H(26) | -2347 | 232  | 2370 | 97  |
| H(27) | -1612 | 1376 | 2323 | 101 |

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