**$[W(OC_6HPh_4\text{-}2,3,5,6)_2(bipy)_2]$ 3.**

CRYSTALLOGRAPHIC DATA FOR

$C_{80}H_{58}N_4O_2W, C_6H_6$

| | |
|---|---|
| $C_{86}H_{64}N_4O_2W$ | formula weight 1369.34 |
| a = 12.9675(2)Å | space group $P\bar{1}$ (No. 2) |
| b = 14.2048(2)Å | T = 150. K |
| c = 18.0995(3)Å | λ = 0.71073Å |
| α = 76.7830(10)° | $\rho_{calc}$ = 1.413g cm$^{-3}$ |
| β = 82.9220(10)° | μ = 1.884mm$^{-1}$ |
| γ = 86.6710(10)° | transmission coeff = 0.339-0.542 |
| V = 3219.35(13)Å$^3$ | $R(F_o)^a$ = 0.032 |
| Z = 2 | $R_w(F_o^2)^b$ = 0.077 |

---

[a] $R = \Sigma \; ||F_o| - |F_c|| / \Sigma \; |F_o|$ for $F_o^2 > 2\sigma(F_o^2)$

[b] $R_w = [\Sigma \; w \; (|F_o^2| - |F_c^2|)^2 / \Sigma \; w \; |F_o^2|^2]^{1/2}$

CRYSTAL DATA AND DATA COLLECTION PARAMETERS for

$C_{80}H_{58}N_4O_2W, C_6H_6$

| | |
|---|---|
| formula | $C_{86}H_{64}N_4O_2W$ |
| formula weight | 1369.34 |
| space group | P1 (No. 2) |
| a, Å | 12.9675(2) |
| b, Å | 14.2048(2) |
| c, Å | 18.0995(3) |
| α, deg | 76.7830(10) |
| β, deg | 82.9220(10) |
| γ, deg | 86.6710(10) |
| V, Å$^3$ | 3219.35(13) |
| Z | 2 |
| $d_{calc}$, g cm$^{-3}$ | 1.413 |
| crystal dimensions, mm | 0.40x0.35x0.33 |
| temperature, K | 150. |
| radiation (wavelength) | MO $K_\alpha$(0.71073Å) |
| monochromator | graphite |
| linear abs coef, mm$^{-1}$ | 1.884 |
| absorption correction applied | empirical[a] |
| transmission factors: min, max | 0.34, 0.54 |
| diffractometer | Nonius KappaCCD |
| h, k, l range | 0 to 17 -18 to 18 -23 to 23 |
| 2θ range, deg | 4.14-55.71 |
| mosaicity, deg | 0.55 |
| programs used | SHELXL-97 |
| $F_{000}$ | 1396.0 |
| weighting $1/[\sigma^2(Fo^2)+(0.0471P)^2+0.0000P]$ where $P=(Fo^2+2Fc^2)/3$ | |
| data collected | 33467 |
| unique data | 15086 |
| $R_{int}$ | 0.034 |
| data used in refinement | 15074 |
| cutoff used in R-factor calculations | $F_o^2>2.0\sigma(F_o^2)$ |
| data with $I>2.0\sigma(I)$ | 13181 |
| number of variables | 838 |
| largest shift/esd in final cycle | 0.00 |
| $R(F_o)$ | 0.032 |
| $R_w(F_o^2)$ | 0.077 |
| goodness of fit | 1.047 |

[a] Otwinowski Z. & Minor, W. Methods Enzymol.,**1996**, 276, 307.

Positional Parameters and Their Estimated Standard Deviations

for $C_{80}H_{58}N_4O_2W, C_6H_6$

| Atom | x | y | z | U(Å²) |
|---|---|---|---|---|
| W | 0.093706( 7) | 0.341943( 7) | 0.286081( 5) | 0.02171(3) |
| O(3) | 0.22251(14) | 0.37025(13) | 0.21293(10) | 0.0272(5) |
| O(4) | 0.09475(14) | 0.20229(13) | 0.34084(10) | 0.0242(5) |
| N(11) | 0.07768(18) | 0.49125(16) | 0.27806(13) | 0.0273(6) |
| N(12) | 0.13176(17) | 0.36464(16) | 0.38958(12) | 0.0236(6) |
| N(21) | -0.06826(16) | 0.35750(15) | 0.30713(12) | 0.0239(6) |
| N(22) | 0.03144(17) | 0.30510(16) | 0.19412(12) | 0.0253(6) |
| C(11) | 0.0419(2) | 0.5527(2) | 0.21614(18) | 0.0374(8) |
| C(12) | 0.0183(3) | 0.6482(2) | 0.2135(2) | 0.0529(10) |
| C(13) | 0.0314(3) | 0.6860(2) | 0.2772(2) | 0.0517(10) |
| C(14) | 0.0676(3) | 0.6267(2) | 0.3393(2) | 0.0402(9) |
| C(15) | 0.0900(2) | 0.5277(2) | 0.34094(16) | 0.0296(8) |
| C(16) | 0.1195(2) | 0.4566(2) | 0.40367(15) | 0.0269(7) |
| C(17) | 0.1304(2) | 0.4728(2) | 0.47647(17) | 0.0343(8) |
| C(18) | 0.1561(2) | 0.3986(2) | 0.53374(17) | 0.0382(9) |
| C(19) | 0.1743(2) | 0.3053(2) | 0.51851(16) | 0.0337(8) |
| C(1A) | 0.1626(2) | 0.2920(2) | 0.44820(15) | 0.0283(7) |
| C(21) | -0.1160(2) | 0.39748(19) | 0.36537(16) | 0.0287(7) |
| C(22) | -0.2207(2) | 0.4128(2) | 0.37690(18) | 0.0332(8) |
| C(23) | -0.2850(2) | 0.3866(2) | 0.32799(18) | 0.0359(9) |
| C(24) | -0.2394(2) | 0.3480(2) | 0.26956(18) | 0.0342(8) |
| C(25) | -0.1311(2) | 0.33354(19) | 0.25842(16) | 0.0274(7) |
| C(26) | -0.0750(2) | 0.3002(2) | 0.19714(16) | 0.0285(7) |
| C(27) | -0.1208(3) | 0.2657(3) | 0.14209(19) | 0.0417(10) |
| C(28) | -0.0596(3) | 0.2360(3) | 0.08443(19) | 0.0463(10) |
| C(29) | 0.0484(3) | 0.2414(2) | 0.08058(17) | 0.0397(9) |
| C(2A) | 0.0907(2) | 0.2755(2) | 0.13472(15) | 0.0297(8) |
| C(31) | 0.2854(2) | 0.44771(19) | 0.18937(15) | 0.0261(7) |
| C(32) | 0.2955(2) | 0.4933(2) | 0.11090(15) | 0.0271(7) |
| C(33) | 0.3534(2) | 0.5785(2) | 0.08448(15) | 0.0264(7) |
| C(34) | 0.3968(2) | 0.6161(2) | 0.13776(15) | 0.0289(8) |
| C(35) | 0.3935(2) | 0.5682(2) | 0.21382(15) | 0.0268(7) |
| C(36) | 0.3419(2) | 0.47983(19) | 0.24050(15) | 0.0255(7) |
| C(41) | 0.0448(2) | 0.12895(17) | 0.32526(14) | 0.0223(6) |
| C(42) | -0.05524(19) | 0.10330(18) | 0.36244(14) | 0.0231(6) |
| C(43) | -0.1087(2) | 0.03467(18) | 0.33716(15) | 0.0255(7) |
| C(44) | -0.0606(2) | -0.00568(19) | 0.27830(15) | 0.0273(7) |
| C(45) | 0.0422(2) | 0.01172(19) | 0.24749(15) | 0.0265(7) |
| C(46) | 0.0976(2) | 0.07727(18) | 0.27320(15) | 0.0250(7) |
| C(61) | 0.2120(2) | 0.08529(19) | 0.25377(16) | 0.0272(7) |
| C(321) | 0.2521(2) | 0.4512(2) | 0.05298(15) | 0.0316(8) |
| C(322) | 0.1733(3) | 0.4992(3) | 0.01244(17) | 0.0414(9) |
| C(323) | 0.1461(3) | 0.4674(3) | -0.0500(2) | 0.0596(13) |
| C(324) | 0.1969(4) | 0.3893(3) | -0.0717(2) | 0.0628(14) |

Positional Parameters and Their Estimated Standard Deviations (cont.)

for $C_{80}H_{58}N_4O_2W, C_6H_6$

| Atom | x | y | z | U(Å²) |
|---|---|---|---|---|
| C(325) | 0.2742(3) | 0.3395(3) | -0.0307(2) | 0.0539(11) |
| C(326) | 0.3007(3) | 0.3698(2) | 0.03198(17) | 0.0385(9) |
| C(331) | 0.3741(2) | 0.6284(2) | 0.00262(15) | 0.0280(7) |
| C(332) | 0.4110(2) | 0.5796(2) | -0.05474(15) | 0.0289(7) |
| C(333) | 0.4347(2) | 0.6297(2) | -0.12973(15) | 0.0316(8) |
| C(334) | 0.4217(2) | 0.7300(2) | -0.14968(17) | 0.0347(8) |
| C(335) | 0.3872(2) | 0.7791(2) | -0.09337(17) | 0.0350(8) |
| C(336) | 0.3647(2) | 0.7291(2) | -0.01825(16) | 0.0315(8) |
| C(351) | 0.4538(2) | 0.6128(2) | 0.26220(15) | 0.0293(8) |
| C(352) | 0.5574(2) | 0.5884(2) | 0.26799(18) | 0.0376(9) |
| C(353) | 0.6141(3) | 0.6309(2) | 0.3115(2) | 0.0447(10) |
| C(354) | 0.5670(3) | 0.6990(2) | 0.34924(18) | 0.0445(10) |
| C(355) | 0.4646(3) | 0.7263(3) | 0.34167(18) | 0.0451(10) |
| C(356) | 0.4073(2) | 0.6832(2) | 0.29865(18) | 0.0389(9) |
| C(361) | 0.3658(2) | 0.4159(2) | 0.31463(15) | 0.0276(7) |
| C(362) | 0.3682(2) | 0.4505(2) | 0.38054(15) | 0.0319(8) |
| C(363) | 0.4131(2) | 0.3943(2) | 0.44288(17) | 0.0399(9) |
| C(364) | 0.4546(2) | 0.3037(3) | 0.44044(18) | 0.0421(9) |
| C(365) | 0.4487(2) | 0.2663(2) | 0.37638(18) | 0.0380(9) |
| C(366) | 0.4033(2) | 0.3214(2) | 0.31451(16) | 0.0316(8) |
| C(421) | -0.0999(2) | 0.14264(18) | 0.42963(15) | 0.0239(7) |
| C(422) | -0.2011(2) | 0.17920(19) | 0.43685(16) | 0.0286(7) |
| C(423) | -0.2438(2) | 0.2063(2) | 0.50355(18) | 0.0370(9) |
| C(424) | -0.1857(3) | 0.1963(2) | 0.56417(17) | 0.0401(9) |
| C(425) | -0.0851(3) | 0.1604(2) | 0.55794(17) | 0.0393(9) |
| C(426) | -0.0419(2) | 0.1344(2) | 0.49081(16) | 0.0306(8) |
| C(431) | -0.2133(2) | -0.00093(18) | 0.37159(16) | 0.0267(7) |
| C(432) | -0.2392(2) | -0.03239(19) | 0.44996(16) | 0.0304(8) |
| C(433) | -0.3374(2) | -0.0678(2) | 0.47965(19) | 0.0381(9) |
| C(434) | -0.4097(2) | -0.0741(2) | 0.4313(2) | 0.0418(9) |
| C(435) | -0.3841(2) | -0.0464(2) | 0.35336(19) | 0.0399(9) |
| C(436) | -0.2871(2) | -0.0093(2) | 0.32354(18) | 0.0338(8) |
| C(451) | 0.0872(2) | -0.04581(19) | 0.19112(15) | 0.0280(7) |
| C(452) | 0.1758(2) | -0.1050(2) | 0.20089(17) | 0.0337(8) |
| C(453) | 0.2088(3) | -0.1643(2) | 0.15083(19) | 0.0427(10) |
| C(454) | 0.1532(3) | -0.1652(3) | 0.0907(2) | 0.0490(11) |
| C(455) | 0.0663(3) | -0.1056(3) | 0.0789(2) | 0.0453(10) |
| C(456) | 0.0331(2) | -0.0457(2) | 0.12904(17) | 0.0354(8) |
| C(462) | 0.2727(2) | 0.0645(2) | 0.31383(17) | 0.0343(8) |
| C(463) | 0.3800(2) | 0.0584(2) | 0.30088(19) | 0.0406(9) |
| C(464) | 0.4294(2) | 0.0740(2) | 0.2269(2) | 0.0408(10) |
| C(465) | 0.3696(2) | 0.0972(2) | 0.16631(19) | 0.0412(9) |
| C(466) | 0.2621(2) | 0.1020(2) | 0.17938(17) | 0.0338(8) |
| C(901) | 0.4203(5) | 0.0817(6) | 0.9253(6) | 0.133(4) |
| C(902) | 0.3294(6) | 0.0466(4) | 0.9734(3) | 0.094(2) |

Positional Parameters and Their Estimated Standard Deviations (cont.)

for $C_{80}H_{58}N_4O_2W, C_6H_6$

| Atom | x | y | z | U(Å²) |
|---|---|---|---|---|
| C(903) | 0.2374(5) | 0.0702(4) | 0.9470(3) | 0.085(2) |
| C(904) | 0.2310(6) | 0.1239(5) | 0.8776(4) | 0.126(3) |
| C(905) | 0.3113(8) | 0.1564(5) | 0.8322(3) | 0.124(3) |
| C(906) | 0.4082(6) | 0.1366(5) | 0.8521(5) | 0.118(3) |

$U_{eq} = (1/3)\Sigma_i\Sigma_j\ U_{ij}a^*_i a^*_j \mathbf{a}_i \cdot \mathbf{a}_j$

Positional Parameters and Their Estimated Standard Deviations

for $C_{80}H_{58}N_4O_2W, C_6H_6$

| Atom | x | y | z | U(Å²) |
|---|---|---|---|---|
| H(11) | 0.033 | 0.528 | 0.173 | 0.045 |
| H(12) | -0.007 | 0.689 | 0.169 | 0.064 |
| H(13) | 0.015 | 0.752 | 0.277 | 0.062 |
| H(14) | 0.078 | 0.652 | 0.382 | 0.048 |
| H(17) | 0.120 | 0.536 | 0.485 | 0.041 |
| H(18) | 0.162 | 0.409 | 0.583 | 0.046 |
| H(19) | 0.195 | 0.252 | 0.557 | 0.040 |
| H(1A) | 0.176 | 0.229 | 0.439 | 0.034 |
| H(21) | -0.074 | 0.415 | 0.399 | 0.034 |
| H(22) | -0.250 | 0.441 | 0.418 | 0.040 |
| H(23) | -0.358 | 0.396 | 0.336 | 0.043 |
| H(24) | -0.281 | 0.331 | 0.236 | 0.041 |
| H(27) | -0.194 | 0.263 | 0.145 | 0.050 |
| H(28) | -0.090 | 0.212 | 0.047 | 0.055 |
| H(29) | 0.092 | 0.221 | 0.041 | 0.048 |
| H(2A) | 0.164 | 0.279 | 0.131 | 0.036 |
| H(34) | 0.430 | 0.676 | 0.122 | 0.035 |
| H(44) | -0.099 | -0.047 | 0.258 | 0.033 |
| H(322) | 0.138 | 0.554 | 0.027 | 0.050 |
| H(323) | 0.092 | 0.500 | -0.078 | 0.071 |
| H(324) | 0.179 | 0.369 | -0.115 | 0.075 |
| H(325) | 0.309 | 0.285 | -0.045 | 0.065 |
| H(326) | 0.352 | 0.335 | 0.061 | 0.046 |
| H(332) | 0.420 | 0.511 | -0.042 | 0.035 |
| H(333) | 0.460 | 0.595 | -0.168 | 0.038 |
| H(334) | 0.436 | 0.764 | -0.201 | 0.042 |
| H(335) | 0.379 | 0.848 | -0.106 | 0.042 |
| H(336) | 0.343 | 0.764 | 0.020 | 0.038 |
| H(352) | 0.591 | 0.542 | 0.242 | 0.045 |
| H(353) | 0.685 | 0.613 | 0.315 | 0.054 |
| H(354) | 0.605 | 0.727 | 0.380 | 0.053 |
| H(355) | 0.433 | 0.775 | 0.366 | 0.054 |
| H(356) | 0.336 | 0.702 | 0.294 | 0.047 |
| H(362) | 0.339 | 0.513 | 0.383 | 0.038 |
| H(363) | 0.415 | 0.419 | 0.487 | 0.048 |
| H(364) | 0.487 | 0.267 | 0.482 | 0.050 |
| H(365) | 0.476 | 0.203 | 0.375 | 0.046 |
| H(366) | 0.398 | 0.295 | 0.272 | 0.038 |
| H(422) | -0.242 | 0.186 | 0.396 | 0.034 |
| H(423) | -0.313 | 0.232 | 0.507 | 0.044 |
| H(424) | -0.215 | 0.214 | 0.610 | 0.048 |
| H(425) | -0.045 | 0.153 | 0.600 | 0.047 |
| H(426) | 0.028 | 0.111 | 0.487 | 0.037 |
| H(432) | -0.189 | -0.030 | 0.484 | 0.037 |

Positional Parameters and Their Estimated Standard Deviations (cont.)

for $C_{80}H_{58}N_4O_2W, C_6H_6$

| Atom | x | y | z | U(Å²) |
|---|---|---|---|---|
| H(433) | -0.354 | -0.088 | 0.533 | 0.046 |
| H(434) | -0.477 | -0.097 | 0.452 | 0.050 |
| H(435) | -0.433 | -0.053 | 0.320 | 0.048 |
| H(436) | -0.271 | 0.011 | 0.270 | 0.041 |
| H(452) | 0.214 | -0.105 | 0.242 | 0.040 |
| H(453) | 0.270 | -0.204 | 0.158 | 0.051 |
| H(454) | 0.175 | -0.207 | 0.057 | 0.059 |
| H(455) | 0.029 | -0.105 | 0.037 | 0.054 |
| H(456) | -0.027 | -0.004 | 0.121 | 0.042 |
| H(462) | 0.240 | 0.054 | 0.365 | 0.041 |
| H(463) | 0.420 | 0.043 | 0.343 | 0.049 |
| H(464) | 0.503 | 0.069 | 0.218 | 0.049 |
| H(465) | 0.403 | 0.110 | 0.115 | 0.049 |
| H(466) | 0.222 | 0.117 | 0.137 | 0.041 |
| H(901) | 0.487 | 0.068 | 0.942 | 0.160 |
| H(902) | 0.334 | 0.007 | 1.023 | 0.113 |
| H(903) | 0.176 | 0.048 | 0.979 | 0.102 |
| H(904) | 0.164 | 0.139 | 0.861 | 0.150 |
| H(905) | 0.302 | 0.196 | 0.783 | 0.149 |
| H(906) | 0.467 | 0.160 | 0.817 | 0.141 |

Hydrogens included in calculation of structure factors but not refined

Anisotropic Temperature Factor Coefficients - U's

for $C_{80}H_{58}N_4O_2W, C_6H_6$

| Name | U(1,1) | U(2,2) | U(3,3) | U(1,2) | U(1,3) | U(2,3) |
|---|---|---|---|---|---|---|
| W | 0.02325(6) | 0.02489(6) | 0.01889(6) | -0.00440(4) | -0.00268(4) | -0.00772(4) |
| O(3) | 0.0258(9) | 0.0343(10) | 0.0233(9) | -0.0078(8) | -0.0006(7) | -0.0099(8) |
| O(4) | 0.0260(9) | 0.0257(9) | 0.0227(9) | -0.0029(7) | -0.0027(7) | -0.0088(7) |
| N(11) | 0.0319(12) | 0.0220(10) | 0.0292(12) | -0.0051(9) | -0.0033(9) | -0.0074(9) |
| N(12) | 0.0258(11) | 0.0267(11) | 0.0217(11) | -0.0038(9) | -0.0041(8) | -0.0110(9) |
| N(21) | 0.0207(10) | 0.0263(11) | 0.0257(11) | -0.0021(9) | -0.0027(8) | -0.0075(9) |
| N(22) | 0.0309(11) | 0.0297(11) | 0.0185(11) | -0.0061(9) | -0.0054(9) | -0.0091(9) |
| C(11) | 0.0462(17) | 0.0291(14) | 0.0358(16) | -0.0059(13) | -0.0088(13) | -0.0018(12) |
| C(12) | 0.070(2) | 0.0318(16) | 0.053(2) | -0.0042(16) | -0.0192(18) | 0.0054(15) |
| C(13) | 0.064(2) | 0.0256(15) | 0.065(2) | -0.0069(15) | -0.0075(19) | -0.0078(15) |
| C(14) | 0.0442(18) | 0.0318(15) | 0.0479(19) | -0.0074(14) | -0.0030(14) | -0.0151(14) |
| C(15) | 0.0300(14) | 0.0283(13) | 0.0341(15) | -0.0098(11) | -0.0006(11) | -0.0135(12) |
| C(16) | 0.0264(13) | 0.0321(14) | 0.0271(14) | -0.0077(11) | -0.0018(10) | -0.0157(11) |
| C(17) | 0.0353(15) | 0.0406(16) | 0.0331(16) | -0.0063(13) | -0.0014(12) | -0.0211(13) |
| C(18) | 0.0402(16) | 0.0529(19) | 0.0283(15) | -0.0087(14) | -0.0043(12) | -0.0209(14) |
| C(19) | 0.0362(15) | 0.0419(16) | 0.0250(14) | -0.0072(13) | -0.0070(11) | -0.0083(12) |
| C(1A) | 0.0289(13) | 0.0326(14) | 0.0254(14) | -0.0036(11) | -0.0062(10) | -0.0082(11) |
| C(21) | 0.0298(13) | 0.0289(13) | 0.0309(14) | -0.0030(11) | -0.0039(11) | -0.0131(11) |
| C(22) | 0.0307(14) | 0.0283(14) | 0.0418(17) | 0.0007(12) | 0.0001(12) | -0.0128(12) |
| C(23) | 0.0267(14) | 0.0347(15) | 0.0465(18) | 0.0008(12) | -0.0068(12) | -0.0088(13) |
| C(24) | 0.0303(14) | 0.0374(15) | 0.0381(17) | -0.0031(12) | -0.0127(12) | -0.0098(13) |
| C(25) | 0.0258(13) | 0.0290(13) | 0.0293(14) | -0.0027(11) | -0.0100(10) | -0.0063(11) |
| C(26) | 0.0280(13) | 0.0325(14) | 0.0280(14) | -0.0030(11) | -0.0097(11) | -0.0087(11) |
| C(27) | 0.0366(16) | 0.0560(19) | 0.0414(18) | -0.0014(15) | -0.0155(13) | -0.0234(15) |
| C(28) | 0.0480(19) | 0.062(2) | 0.0401(18) | -0.0036(17) | -0.0170(15) | -0.0279(16) |
| C(29) | 0.0513(19) | 0.0464(18) | 0.0267(15) | -0.0043(15) | -0.0052(13) | -0.0182(13) |
| C(2A) | 0.0360(15) | 0.0332(14) | 0.0222(13) | -0.0062(12) | -0.0024(11) | -0.0104(11) |
| C(31) | 0.0237(12) | 0.0329(13) | 0.0220(13) | -0.0054(11) | 0.0002(10) | -0.0072(11) |
| C(32) | 0.0254(13) | 0.0371(14) | 0.0203(13) | -0.0031(11) | -0.0020(10) | -0.0090(11) |
| C(33) | 0.0255(13) | 0.0336(14) | 0.0200(13) | -0.0024(11) | -0.0012(10) | -0.0061(11) |
| C(34) | 0.0305(14) | 0.0313(14) | 0.0253(14) | -0.0063(12) | -0.0015(11) | -0.0069(11) |
| C(35) | 0.0274(13) | 0.0328(14) | 0.0221(13) | -0.0030(11) | -0.0024(10) | -0.0100(11) |
| C(36) | 0.0234(12) | 0.0321(13) | 0.0213(13) | -0.0025(11) | -0.0015(10) | -0.0069(11) |
| C(41) | 0.0267(12) | 0.0199(11) | 0.0205(12) | -0.0014(10) | -0.0032(9) | -0.0047(9) |
| C(42) | 0.0242(12) | 0.0237(12) | 0.0209(12) | 0.0016(10) | -0.0012(10) | -0.0054(10) |
| C(43) | 0.0268(13) | 0.0241(12) | 0.0258(13) | -0.0007(10) | -0.0019(10) | -0.0064(10) |
| C(44) | 0.0276(13) | 0.0287(13) | 0.0280(14) | -0.0032(11) | -0.0016(10) | -0.0116(11) |
| C(45) | 0.0282(13) | 0.0281(13) | 0.0247(13) | 0.0001(11) | -0.0015(10) | -0.0098(11) |
| C(46) | 0.0276(13) | 0.0264(12) | 0.0216(13) | -0.0009(11) | -0.0010(10) | -0.0074(10) |
| C(61) | 0.0267(13) | 0.0258(12) | 0.0308(14) | -0.0033(11) | 0.0009(11) | -0.0117(11) |
| C(321) | 0.0313(14) | 0.0453(16) | 0.0184(13) | -0.0130(13) | 0.0002(10) | -0.0064(12) |
| C(322) | 0.0416(17) | 0.0529(19) | 0.0299(16) | -0.0161(15) | -0.0117(13) | -0.0023(14) |
| C(323) | 0.064(2) | 0.078(3) | 0.0366(19) | -0.031(2) | -0.0241(17) | 0.0044(19) |
| C(324) | 0.085(3) | 0.081(3) | 0.0300(18) | -0.037(3) | -0.0092(18) | -0.0181(19) |

Anisotropic Temperature Factor Coefficients - U's (Continued)

for $C_{80}H_{58}N_4O_2W, C_6H_6$

| Name | U(1,1) | U(2,2) | U(3,3) | U(1,2) | U(1,3) | U(2,3) |
|---|---|---|---|---|---|---|
| C(325) | 0.063(2) | 0.068(2) | 0.0382(19) | -0.027(2) | 0.0077(17) | -0.0281(18) |
| C(326) | 0.0421(17) | 0.0479(18) | 0.0293(15) | -0.0149(14) | 0.0012(13) | -0.0158(13) |
| C(331) | 0.0237(12) | 0.0397(15) | 0.0205(13) | -0.0046(11) | -0.0016(10) | -0.0061(11) |
| C(332) | 0.0256(13) | 0.0363(14) | 0.0256(14) | -0.0053(11) | -0.0025(10) | -0.0079(11) |
| C(333) | 0.0284(13) | 0.0464(16) | 0.0219(13) | -0.0076(12) | -0.0017(10) | -0.0103(12) |
| C(334) | 0.0299(14) | 0.0474(17) | 0.0249(14) | -0.0099(13) | -0.0023(11) | -0.0025(12) |
| C(335) | 0.0329(15) | 0.0370(15) | 0.0318(15) | -0.0052(13) | 0.0024(12) | -0.0031(12) |
| C(336) | 0.0304(14) | 0.0380(15) | 0.0255(14) | -0.0049(12) | 0.0024(11) | -0.0079(12) |
| C(351) | 0.0360(15) | 0.0321(14) | 0.0199(13) | -0.0082(12) | -0.0043(11) | -0.0039(11) |
| C(352) | 0.0416(17) | 0.0337(15) | 0.0415(17) | 0.0004(13) | -0.0151(13) | -0.0114(13) |
| C(353) | 0.0459(18) | 0.0399(17) | 0.052(2) | -0.0047(15) | -0.0257(16) | -0.0065(15) |
| C(354) | 0.063(2) | 0.0435(17) | 0.0315(16) | -0.0210(16) | -0.0145(15) | -0.0080(14) |
| C(355) | 0.059(2) | 0.0508(19) | 0.0315(16) | -0.0151(17) | 0.0034(15) | -0.0225(15) |
| C(356) | 0.0381(16) | 0.0479(18) | 0.0342(16) | -0.0074(14) | 0.0017(13) | -0.0182(14) |
| C(361) | 0.0235(12) | 0.0377(14) | 0.0214(13) | -0.0099(11) | -0.0018(10) | -0.0044(11) |
| C(362) | 0.0318(14) | 0.0416(15) | 0.0225(13) | -0.0135(13) | -0.0019(11) | -0.0049(12) |
| C(363) | 0.0408(17) | 0.057(2) | 0.0224(14) | -0.0193(15) | -0.0069(12) | -0.0038(13) |
| C(364) | 0.0355(16) | 0.056(2) | 0.0305(16) | -0.0121(15) | -0.0107(12) | 0.0053(14) |
| C(365) | 0.0324(15) | 0.0399(16) | 0.0374(17) | -0.0084(13) | -0.0013(12) | 0.0009(13) |
| C(366) | 0.0278(14) | 0.0386(15) | 0.0274(14) | -0.0071(12) | -0.0008(11) | -0.0049(12) |
| C(421) | 0.0283(13) | 0.0204(11) | 0.0234(13) | -0.0029(10) | 0.0008(10) | -0.0069(10) |
| C(422) | 0.0299(14) | 0.0272(13) | 0.0286(14) | 0.0018(11) | -0.0015(11) | -0.0075(11) |
| C(423) | 0.0369(16) | 0.0350(15) | 0.0372(17) | 0.0022(13) | 0.0079(13) | -0.0116(13) |
| C(424) | 0.0513(19) | 0.0420(16) | 0.0281(15) | -0.0041(15) | 0.0087(13) | -0.0166(13) |
| C(425) | 0.0479(18) | 0.0479(18) | 0.0244(15) | -0.0057(15) | -0.0024(13) | -0.0129(13) |
| C(426) | 0.0306(14) | 0.0352(14) | 0.0271(14) | -0.0013(12) | -0.0013(11) | -0.0102(12) |
| C(431) | 0.0260(13) | 0.0237(12) | 0.0316(14) | 0.0008(11) | -0.0013(11) | -0.0100(11) |
| C(432) | 0.0289(14) | 0.0284(13) | 0.0332(15) | -0.0014(11) | -0.0016(11) | -0.0062(11) |
| C(433) | 0.0345(15) | 0.0375(16) | 0.0386(17) | -0.0084(13) | 0.0065(13) | -0.0045(13) |
| C(434) | 0.0280(15) | 0.0422(17) | 0.054(2) | -0.0083(13) | 0.0057(14) | -0.0119(15) |
| C(435) | 0.0295(15) | 0.0441(17) | 0.0497(19) | -0.0024(13) | -0.0078(13) | -0.0160(15) |
| C(436) | 0.0278(14) | 0.0389(15) | 0.0372(16) | 0.0002(12) | -0.0037(12) | -0.0140(13) |
| C(451) | 0.0314(14) | 0.0285(13) | 0.0261(14) | -0.0032(11) | 0.0002(11) | -0.0112(11) |
| C(452) | 0.0342(15) | 0.0379(15) | 0.0326(15) | -0.0002(13) | -0.0023(12) | -0.0161(13) |
| C(453) | 0.0399(17) | 0.0492(18) | 0.0436(18) | 0.0098(15) | -0.0031(14) | -0.0235(15) |
| C(454) | 0.0478(19) | 0.063(2) | 0.046(2) | 0.0077(17) | -0.0018(15) | -0.0368(18) |
| C(455) | 0.0448(18) | 0.063(2) | 0.0371(18) | 0.0064(16) | -0.0071(14) | -0.0304(16) |
| C(456) | 0.0348(15) | 0.0413(16) | 0.0339(16) | 0.0039(13) | -0.0039(12) | -0.0174(13) |
| C(462) | 0.0315(14) | 0.0411(16) | 0.0334(16) | 0.0004(13) | -0.0007(12) | -0.0168(13) |
| C(463) | 0.0296(15) | 0.0512(18) | 0.0450(18) | 0.0013(14) | -0.0043(13) | -0.0195(15) |
| C(464) | 0.0239(14) | 0.0467(18) | 0.052(2) | -0.0024(13) | 0.0054(13) | -0.0160(15) |
| C(465) | 0.0373(16) | 0.0444(17) | 0.0384(17) | -0.0030(14) | 0.0109(13) | -0.0094(14) |
| C(466) | 0.0317(14) | 0.0366(15) | 0.0317(15) | -0.0025(12) | 0.0026(12) | -0.0074(12) |
| C(901) | 0.076(4) | 0.132(6) | 0.183(9) | 0.020(4) | -0.009(5) | -0.027(6) |
| C(902) | 0.121(5) | 0.095(4) | 0.059(3) | -0.003(4) | -0.006(3) | -0.003(3) |

Anisotropic Temperature Factor Coefficients - U's (Continued)

for $C_{80}H_{58}N_4O_2W, C_6H_6$

| Name | U(1,1) | U(2,2) | U(3,3) | U(1,2) | U(1,3) | U(2,3) |
|---|---|---|---|---|---|---|
| C(903) | 0.090(4) | 0.083(3) | 0.078(4) | -0.024(3) | 0.007(3) | -0.013(3) |
| C(904) | 0.156(7) | 0.114(5) | 0.107(5) | -0.071(5) | -0.052(5) | 0.011(4) |
| C(905) | 0.219(9) | 0.098(5) | 0.059(3) | -0.081(6) | 0.012(5) | -0.020(3) |
| C(906) | 0.124(6) | 0.098(5) | 0.121(6) | -0.042(5) | 0.074(5) | -0.039(4) |

The form of the anisotropic temperature factor is:

$\exp[-2\pi \{h^2a^{*2}U(1,1) + k^2b^{*2}U(2,2) + l^2c^{*2}U(3,3) + 2hka^*b^*U(1,2) + 2hla^*c^*U(1,3)$

$+ 2klb^*c^*U(2,3)\}]$ where $a^*$, $b^*$, and $c^*$ are reciprocal lattice constants.

Table of Bond Distances in Angstroms

for $C_{80}H_{58}N_4O_2W, C_6H_6$

| Atom 1 | Atom 2 | Distance | Atom 1 | Atom 2 | Distance |
|---|---|---|---|---|---|
| W | O(3) | 1.9985(17) | C(35) | C(351) | 1.502(4) |
| W | O(4) | 2.0048(18) | C(36) | C(361) | 1.494(4) |
| W | N(11) | 2.092(2) | C(41) | C(46) | 1.412(3) |
| W | N(12) | 2.093(2) | C(41) | C(42) | 1.412(3) |
| W | N(21) | 2.096(2) | C(42) | C(43) | 1.415(4) |
| W | N(22) | 2.115(2) | C(42) | C(421) | 1.492(3) |
| O(3) | C(31) | 1.365(3) | C(43) | C(44) | 1.388(4) |
| O(4) | C(41) | 1.357(3) | C(43) | C(431) | 1.487(3) |
| N(11) | C(11) | 1.366(4) | C(44) | C(45) | 1.393(4) |
| N(11) | C(15) | 1.383(3) | C(45) | C(46) | 1.399(4) |
| N(12) | C(1A) | 1.381(4) | C(45) | C(451) | 1.493(4) |
| N(12) | C(16) | 1.383(3) | C(46) | C(61) | 1.487(4) |
| N(21) | C(21) | 1.374(3) | C(61) | C(462) | 1.387(4) |
| N(21) | C(25) | 1.380(3) | C(61) | C(466) | 1.396(4) |
| N(22) | C(2A) | 1.374(3) | C(321) | C(322) | 1.387(4) |
| N(22) | C(26) | 1.380(3) | C(321) | C(326) | 1.391(4) |
| C(11) | C(12) | 1.365(4) | C(322) | C(323) | 1.399(5) |
| C(12) | C(13) | 1.411(5) | C(323) | C(324) | 1.367(6) |
| C(13) | C(14) | 1.358(5) | C(324) | C(325) | 1.383(6) |
| C(14) | C(15) | 1.414(4) | C(325) | C(326) | 1.389(4) |
| C(15) | C(16) | 1.412(4) | C(331) | C(336) | 1.395(4) |
| C(16) | C(17) | 1.414(4) | C(331) | C(332) | 1.398(4) |
| C(17) | C(18) | 1.357(5) | C(332) | C(333) | 1.387(4) |
| C(18) | C(19) | 1.415(4) | C(333) | C(334) | 1.393(4) |
| C(19) | C(1A) | 1.356(4) | C(334) | C(335) | 1.380(4) |
| C(21) | C(22) | 1.360(4) | C(335) | C(336) | 1.387(4) |
| C(22) | C(23) | 1.409(4) | C(351) | C(352) | 1.379(4) |
| C(23) | C(24) | 1.357(4) | C(351) | C(356) | 1.390(4) |
| C(24) | C(25) | 1.403(4) | C(352) | C(353) | 1.392(4) |
| C(25) | C(26) | 1.409(4) | C(353) | C(354) | 1.380(5) |
| C(26) | C(27) | 1.410(4) | C(354) | C(355) | 1.377(5) |
| C(27) | C(28) | 1.362(5) | C(355) | C(356) | 1.395(4) |
| C(28) | C(29) | 1.399(5) | C(361) | C(362) | 1.394(4) |
| C(29) | C(2A) | 1.370(4) | C(361) | C(366) | 1.402(4) |
| C(31) | C(32) | 1.413(4) | C(362) | C(363) | 1.395(4) |
| C(31) | C(36) | 1.414(3) | C(363) | C(364) | 1.373(5) |
| C(32) | C(33) | 1.417(4) | C(364) | C(365) | 1.393(5) |
| C(32) | C(321) | 1.498(4) | C(365) | C(366) | 1.386(4) |
| C(33) | C(34) | 1.392(4) | C(421) | C(422) | 1.385(4) |
| C(33) | C(331) | 1.488(4) | C(421) | C(426) | 1.394(4) |
| C(34) | C(35) | 1.386(4) | C(422) | C(423) | 1.391(4) |
| C(35) | C(36) | 1.414(4) | C(423) | C(424) | 1.383(5) |

Bond Distances (cont.)

| Atom 1 | Atom 2 | Distance | Atom 1 | Atom 2 | Distance |
|---|---|---|---|---|---|
| C(424) | C(425) | 1.374(5) | C(454) | C(455) | 1.377(5) |
| C(425) | C(426) | 1.393(4) | C(455) | C(456) | 1.397(4) |
| C(431) | C(432) | 1.391(4) | C(462) | C(463) | 1.384(4) |
| C(431) | C(436) | 1.397(4) | C(463) | C(464) | 1.387(4) |
| C(432) | C(433) | 1.395(4) | C(464) | C(465) | 1.387(5) |
| C(433) | C(434) | 1.378(5) | C(465) | C(466) | 1.386(4) |
| C(434) | C(435) | 1.379(5) | C(901) | C(906) | 1.397(11) |
| C(435) | C(436) | 1.389(4) | C(901) | C(902) | 1.419(9) |
| C(451) | C(452) | 1.388(4) | C(902) | C(903) | 1.336(8) |
| C(451) | C(456) | 1.396(4) | C(903) | C(904) | 1.322(8) |
| C(452) | C(453) | 1.388(4) | C(904) | C(905) | 1.283(9) |
| C(453) | C(454) | 1.379(5) | C(905) | C(906) | 1.345(11) |

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table of Bond Angles in Degrees

for $C_{80}H_{58}N_4O_2W, C_6H_6$

| Atom 1 | Atom 2 | Atom 3 | Angle | Atom 1 | Atom 2 | Atom 3 | Angle |
|---|---|---|---|---|---|---|---|
| O(3) | W | O(4) | 110.24(7) | C(19) | C(1A) | N(12) | 123.7(3) |
| O(3) | W | N(11) | 86.61(8) | C(22) | C(21) | N(21) | 123.0(3) |
| O(4) | W | N(11) | 155.19(8) | C(21) | C(22) | C(23) | 119.7(3) |
| O(3) | W | N(12) | 105.31(8) | C(24) | C(23) | C(22) | 118.3(3) |
| O(4) | W | N(12) | 83.79(8) | C(23) | C(24) | C(25) | 121.0(3) |
| N(11) | W | N(12) | 74.00(9) | N(21) | C(25) | C(24) | 120.7(3) |
| O(3) | W | N(21) | 148.25(8) | N(21) | C(25) | C(26) | 113.2(2) |
| O(4) | W | N(21) | 93.08(8) | C(24) | C(25) | C(26) | 125.9(2) |
| N(11) | W | N(21) | 79.57(8) | N(22) | C(26) | C(25) | 114.0(2) |
| N(12) | W | N(21) | 98.17(8) | N(22) | C(26) | C(27) | 121.5(3) |
| O(3) | W | N(22) | 84.98(8) | C(25) | C(26) | C(27) | 124.5(3) |
| O(4) | W | N(22) | 89.93(8) | C(28) | C(27) | C(26) | 120.0(3) |
| N(11) | W | N(22) | 110.17(9) | C(27) | C(28) | C(29) | 118.9(3) |
| N(12) | W | N(22) | 169.30(8) | C(2A) | C(29) | C(28) | 119.8(3) |
| N(21) | W | N(22) | 73.45(8) | C(29) | C(2A) | N(22) | 122.9(3) |
| C(31) | O(3) | W | 134.23(16) | O(3) | C(31) | C(32) | 117.6(2) |
| C(41) | O(4) | W | 127.70(16) | O(3) | C(31) | C(36) | 121.8(2) |
| C(11) | N(11) | C(15) | 118.4(2) | C(32) | C(31) | C(36) | 120.6(2) |
| C(11) | N(11) | W | 121.80(19) | C(31) | C(32) | C(33) | 119.8(2) |
| C(15) | N(11) | W | 119.27(18) | C(31) | C(32) | C(321) | 122.0(2) |
| C(1A) | N(12) | C(16) | 116.5(2) | C(33) | C(32) | C(321) | 118.1(2) |
| C(1A) | N(12) | W | 124.18(17) | C(34) | C(33) | C(32) | 118.3(2) |
| C(16) | N(12) | W | 119.20(18) | C(34) | C(33) | C(331) | 117.7(2) |
| C(21) | N(21) | C(25) | 117.2(2) | C(32) | C(33) | C(331) | 123.9(2) |
| C(21) | N(21) | W | 122.58(17) | C(35) | C(34) | C(33) | 122.1(2) |
| C(25) | N(21) | W | 120.05(17) | C(34) | C(35) | C(36) | 120.4(2) |
| C(2A) | N(22) | C(26) | 116.9(2) | C(34) | C(35) | C(351) | 115.6(2) |
| C(2A) | N(22) | W | 123.97(18) | C(36) | C(35) | C(351) | 123.9(2) |
| C(26) | N(22) | W | 118.72(17) | C(31) | C(36) | C(35) | 117.9(2) |
| C(12) | C(11) | N(11) | 123.0(3) | C(31) | C(36) | C(361) | 122.3(2) |
| C(11) | C(12) | C(13) | 119.0(3) | C(35) | C(36) | C(361) | 118.7(2) |
| C(14) | C(13) | C(12) | 119.2(3) | O(4) | C(41) | C(46) | 117.9(2) |
| C(13) | C(14) | C(15) | 120.6(3) | O(4) | C(41) | C(42) | 120.6(2) |
| N(11) | C(15) | C(16) | 113.6(2) | C(46) | C(41) | C(42) | 121.4(2) |
| N(11) | C(15) | C(14) | 119.9(3) | C(41) | C(42) | C(43) | 118.0(2) |
| C(16) | C(15) | C(14) | 126.5(3) | C(41) | C(42) | C(421) | 120.8(2) |
| N(12) | C(16) | C(15) | 113.6(2) | C(43) | C(42) | C(421) | 121.1(2) |
| N(12) | C(16) | C(17) | 121.1(3) | C(44) | C(43) | C(42) | 119.1(2) |
| C(15) | C(16) | C(17) | 125.2(3) | C(44) | C(43) | C(431) | 116.7(2) |
| C(18) | C(17) | C(16) | 120.5(3) | C(42) | C(43) | C(431) | 124.2(2) |
| C(17) | C(18) | C(19) | 118.7(3) | C(43) | C(44) | C(45) | 122.7(2) |
| C(1A) | C(19) | C(18) | 119.3(3) | C(44) | C(45) | C(46) | 119.0(2) |

Bond Angles (cont.)

| Atom 1 | Atom 2 | Atom 3 | Angle | Atom 1 | Atom 2 | Atom 3 | Angle |
|---|---|---|---|---|---|---|---|
| C(44) | C(45) | C(451) | 116.5(2) | C(366) | C(365) | C(364) | 120.0(3) |
| C(46) | C(45) | C(451) | 124.4(2) | C(365) | C(366) | C(361) | 120.6(3) |
| C(45) | C(46) | C(41) | 118.6(2) | C(422) | C(421) | C(426) | 118.2(2) |
| C(45) | C(46) | C(61) | 121.4(2) | C(422) | C(421) | C(42) | 122.3(2) |
| C(41) | C(46) | C(61) | 119.6(2) | C(426) | C(421) | C(42) | 119.2(2) |
| C(462) | C(61) | C(466) | 118.2(3) | C(421) | C(422) | C(423) | 120.9(3) |
| C(462) | C(61) | C(46) | 117.4(2) | C(424) | C(423) | C(422) | 120.3(3) |
| C(466) | C(61) | C(46) | 124.0(3) | C(425) | C(424) | C(423) | 119.7(3) |
| C(322) | C(321) | C(326) | 119.0(3) | C(424) | C(425) | C(426) | 120.1(3) |
| C(322) | C(321) | C(32) | 121.0(3) | C(425) | C(426) | C(421) | 120.9(3) |
| C(326) | C(321) | C(32) | 119.5(3) | C(432) | C(431) | C(436) | 118.0(3) |
| C(321) | C(322) | C(323) | 119.9(4) | C(432) | C(431) | C(43) | 122.8(2) |
| C(324) | C(323) | C(322) | 120.5(4) | C(436) | C(431) | C(43) | 119.1(3) |
| C(323) | C(324) | C(325) | 120.2(3) | C(431) | C(432) | C(433) | 120.8(3) |
| C(324) | C(325) | C(326) | 119.7(4) | C(434) | C(433) | C(432) | 120.2(3) |
| C(325) | C(326) | C(321) | 120.7(3) | C(433) | C(434) | C(435) | 119.7(3) |
| C(336) | C(331) | C(332) | 117.4(2) | C(434) | C(435) | C(436) | 120.3(3) |
| C(336) | C(331) | C(33) | 119.5(2) | C(435) | C(436) | C(431) | 120.9(3) |
| C(332) | C(331) | C(33) | 122.9(3) | C(452) | C(451) | C(456) | 118.7(3) |
| C(333) | C(332) | C(331) | 120.9(3) | C(452) | C(451) | C(45) | 122.9(3) |
| C(332) | C(333) | C(334) | 120.6(3) | C(456) | C(451) | C(45) | 118.2(3) |
| C(335) | C(334) | C(333) | 119.0(3) | C(453) | C(452) | C(451) | 120.7(3) |
| C(334) | C(335) | C(336) | 120.3(3) | C(454) | C(453) | C(452) | 120.0(3) |
| C(335) | C(336) | C(331) | 121.6(3) | C(455) | C(454) | C(453) | 120.4(3) |
| C(352) | C(351) | C(356) | 118.8(3) | C(454) | C(455) | C(456) | 119.7(3) |
| C(352) | C(351) | C(35) | 120.7(3) | C(451) | C(456) | C(455) | 120.4(3) |
| C(356) | C(351) | C(35) | 120.4(3) | C(463) | C(462) | C(61) | 121.3(3) |
| C(351) | C(352) | C(353) | 120.9(3) | C(462) | C(463) | C(464) | 120.2(3) |
| C(354) | C(353) | C(352) | 120.1(3) | C(463) | C(464) | C(465) | 119.0(3) |
| C(355) | C(354) | C(353) | 119.4(3) | C(466) | C(465) | C(464) | 120.7(3) |
| C(354) | C(355) | C(356) | 120.6(3) | C(465) | C(466) | C(61) | 120.5(3) |
| C(351) | C(356) | C(355) | 120.1(3) | C(906) | C(901) | C(902) | 117.8(7) |
| C(362) | C(361) | C(366) | 118.4(3) | C(903) | C(902) | C(901) | 118.2(6) |
| C(362) | C(361) | C(36) | 122.7(3) | C(904) | C(903) | C(902) | 121.1(6) |
| C(366) | C(361) | C(36) | 118.1(2) | C(905) | C(904) | C(903) | 122.6(8) |
| C(361) | C(362) | C(363) | 120.4(3) | C(904) | C(905) | C(906) | 121.8(7) |
| C(364) | C(363) | C(362) | 120.4(3) | C(905) | C(906) | C(901) | 118.5(6) |
| C(363) | C(364) | C(365) | 119.9(3) | | | | |

Numbers in parentheses are estimated standard deviations in the least significant digits.

**$[W(OC_6HPh_3\text{-}\eta^6\text{-}C_6H_5)(OC_6HPh_4\text{-}2,3,5,6)(py\text{-}Bu^t\text{-}4)]$ (4) and $[W(OC_6HPh_3\text{-}\eta^5\text{-}C_6H_6)(OC_6HPh_3\text{-}\eta^1\text{-}C_6H_4)(OC_6HPh_4\text{-}2,3,5,6)][Cl]$ (5).**

CRYSTALLOGRAPHIC DATA FOR

$C_{90}H_{63}O_3W, C_{69}H_{55}NO_2W, Cl$

| | |
|---|---|
| $C_{159}H_{118}ClNO_5W_2$ | formula weight 2525.87 |
| a = 11.72610(10)Å | space group $P\bar{1}$ (No. 2) |
| b = 19.1182(2)Å | T = 150. K |
| c = 29.6646(3)Å | λ = 0.71073Å |
| α = 87.8455(5)° | $\rho_{calc}$ = 1.342g $cm^{-3}$ |
| β = 79.6683(5)° | μ = 1.955$mm^{-1}$ |
| γ = 72.8854(5)° | transmission coeff = 0.306-0.644 |
| V = 6251.91(16)$Å^3$ | $R(F_o)^a$ = 0.052 |
| Z = 2 | $R_w(F_o^2)^b$ = 0.138 |

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[a] $R = \Sigma \, ||F_o| - |F_c|| / \Sigma \, |F_o|$ for $F_o^2 > 2\sigma(F_o^2)$

[b] $R_w = [\Sigma \, w \, (|F_o^2| - |F_c^2|)^2 / \Sigma \, w \, |F_o^2|^2]^{1/2}$

CRYSTAL DATA AND DATA COLLECTION PARAMETERS for

$C_{90}H_{63}O_3W, C_{69}H_{55}NO_2W, Cl$

| | |
|---|---|
| formula | $C_{159}H_{118}ClNO_5W_2$ |
| formula weight | 2525.87 |
| space group | P1 (No. 2) |
| a, Å | 11.72610(10) |
| b, Å | 19.1182(2) |
| c, Å | 29.6646(3) |
| α, deg | 87.8455(5) |
| β, deg | 79.6683(5) |
| γ, deg | 72.8854(5) |
| V, Å$^3$ | 6251.91(16) |
| Z | 2 |
| $d_{calc}$, g cm$^{-3}$ | 1.342 |
| crystal dimensions, mm | 0.30x0.28x0.22 |
| temperature, K | 150. |
| radiation (wavelength) | MO $K_\alpha$(0.71073Å) |
| monochromator | graphite |
| linear abs coef, mm$^{-1}$ | 1.955 |
| absorption correction applied | empirical[a] |
| transmission factors: min, max | 0.31, 0.64 |
| diffractometer | Nonius KappaCCD |
| h, k, l range | 0 to 15 -23 to 24 -37 to 38 |
| 2θ range, deg | 10.00-55.03 |
| mosaicity, deg | 0.53 |
| programs used | SHELXL-97 |
| $F_{000}$ | 2568.0 |
| weighting | |
| | |
| data collected | 79760 |
| unique data | 28211 |
| $R_{int}$ | 0.053 |
| data used in refinement | 28172 |
| cutoff used in R-factor calculations | $F_o^2>2.0\sigma(F_o^2)$ |
| data with $I>2.0\sigma(I)$ | 20678 |
| number of variables | 1516 |
| largest shift/esd in final cycle | 0.00 |
| $R(F_o)$ | 0.052 |
| $R_w(F_o^2)$ | 0.138 |
| goodness of fit | 1.037 |

[a] Otwinowski Z. & Minor, W. Methods Enzymol., **1996**, 276, 307.

Positional Parameters and Their Estimated Standard Deviations

for $C_{90}H_{63}O_3W, C_{69}H_{55}NO_2W, Cl$

| Atom | x | y | z | U(Å²) |
|---|---|---|---|---|
| W(1) | 0.178206(17) | 0.111332(11) | 0.337713( 6) | 0.01982(6) |
| W(2) | -0.29492(2) | -0.478325(12) | 0.139865( 7) | 0.02862(7) |
| Cl | 0.91289(19) | 0.06806(12) | 0.36573(7) | 0.0624(7) |
| O(1) | 0.0484(3) | 0.0811(2) | 0.30620(11) | 0.0228(10) |
| O(2) | 0.0484(3) | 0.1118(2) | 0.39315(11) | 0.0240(11) |
| O(3) | 0.2702(3) | 0.01282(19) | 0.31486(11) | 0.0230(10) |
| O(4) | -0.3230(4) | -0.5465(2) | 0.19108(13) | 0.0325(12) |
| O(5) | -0.4007(3) | -0.4687(2) | 0.09322(12) | 0.0301(11) |
| N(61) | -0.2059(4) | -0.5830(3) | 0.10264(16) | 0.0313(15) |
| C(11) | 0.0537(4) | 0.0948(3) | 0.26104(16) | 0.0214(14) |
| C(12) | 0.1134(4) | 0.1465(3) | 0.24269(17) | 0.0227(14) |
| C(13) | 0.1214(5) | 0.1630(3) | 0.19624(18) | 0.0258(15) |
| C(14) | 0.0819(5) | 0.1210(3) | 0.16835(18) | 0.0275(16) |
| C(15) | 0.0234(5) | 0.0697(3) | 0.18581(17) | 0.0262(16) |
| C(16) | 0.0009(5) | 0.0596(3) | 0.23320(17) | 0.0236(16) |
| C(21) | 0.0344(5) | 0.1486(3) | 0.43257(17) | 0.0249(16) |
| C(22) | 0.1344(5) | 0.1441(3) | 0.45369(17) | 0.0244(16) |
| C(23) | 0.1168(5) | 0.1922(3) | 0.49087(18) | 0.0287(16) |
| C(24) | 0.0035(6) | 0.2401(3) | 0.50579(18) | 0.0333(17) |
| C(25) | -0.0980(5) | 0.2407(3) | 0.48805(18) | 0.0315(17) |
| C(26) | -0.0830(5) | 0.1927(3) | 0.45042(18) | 0.0280(17) |
| C(31) | 0.2702(5) | -0.0463(3) | 0.29080(17) | 0.0229(16) |
| C(32) | 0.3412(5) | -0.0596(3) | 0.24649(18) | 0.0251(17) |
| C(33) | 0.3495(5) | -0.1230(3) | 0.22310(18) | 0.0276(17) |
| C(34) | 0.2858(5) | -0.1705(3) | 0.24261(19) | 0.0295(17) |
| C(35) | 0.2146(5) | -0.1585(3) | 0.28638(19) | 0.0273(17) |
| C(36) | 0.2058(5) | -0.0943(3) | 0.31098(17) | 0.0253(16) |
| C(41) | -0.3644(5) | -0.5195(3) | 0.23443(19) | 0.0311(17) |
| C(42) | -0.3667(5) | -0.4456(3) | 0.2419(2) | 0.0338(18) |
| C(43) | -0.4199(5) | -0.4116(3) | 0.28465(19) | 0.0323(17) |
| C(44) | -0.4655(6) | -0.4536(4) | 0.3188(2) | 0.039(2) |
| C(45) | -0.4570(6) | -0.5263(4) | 0.3130(2) | 0.0387(19) |
| C(46) | -0.4026(5) | -0.5618(3) | 0.2705(2) | 0.0345(18) |
| C(51) | -0.4957(5) | -0.4157(3) | 0.08127(19) | 0.0286(17) |
| C(52) | -0.4816(5) | -0.3881(3) | 0.03601(18) | 0.0272(17) |
| C(53) | -0.5786(5) | -0.3346(3) | 0.02229(19) | 0.0304(17) |
| C(54) | -0.6851(5) | -0.3082(3) | 0.05315(19) | 0.0301(17) |
| C(55) | -0.7024(5) | -0.3352(3) | 0.09782(19) | 0.0288(17) |
| C(56) | -0.6075(5) | -0.3909(3) | 0.11176(19) | 0.0294(17) |
| C(62) | -0.1544(6) | -0.6470(4) | 0.1216(2) | 0.040(2) |
| C(63) | -0.0861(6) | -0.7098(4) | 0.0969(2) | 0.042(2) |
| C(64) | -0.0655(5) | -0.7089(3) | 0.04892(19) | 0.0321(17) |
| C(65) | -0.1196(5) | -0.6434(3) | 0.0295(2) | 0.0345(17) |
| C(66) | -0.1871(5) | -0.5832(3) | 0.05723(19) | 0.0334(17) |

Positional Parameters and Their Estimated Standard Deviations (cont.)

for $C_{90}H_{63}O_3W, C_{69}H_{55}NO_2W, Cl$

| Atom | x | y | z | U(Å²) |
|---|---|---|---|---|
| C(121) | 0.1607(5) | 0.1798(3) | 0.27654(17) | 0.0231(16) |
| C(122) | 0.0707(5) | 0.2205(3) | 0.31446(18) | 0.0262(17) |
| C(123) | 0.1111(5) | 0.2413(3) | 0.35268(19) | 0.0301(17) |
| C(124) | 0.2335(5) | 0.2133(3) | 0.35522(19) | 0.0304(17) |
| C(125) | 0.3141(5) | 0.1723(3) | 0.31628(19) | 0.0292(17) |
| C(126) | 0.2835(5) | 0.1942(3) | 0.26909(18) | 0.0264(17) |
| C(131) | 0.1606(5) | 0.2278(3) | 0.17701(19) | 0.0313(17) |
| C(132) | 0.2368(6) | 0.2244(4) | 0.1349(2) | 0.0407(19) |
| C(133) | 0.2662(7) | 0.2870(5) | 0.1173(3) | 0.056(3) |
| C(134) | 0.2200(8) | 0.3517(5) | 0.1407(3) | 0.058(3) |
| C(135) | 0.1433(8) | 0.3558(4) | 0.1817(3) | 0.058(3) |
| C(136) | 0.1143(6) | 0.2944(4) | 0.2001(2) | 0.041(2) |
| C(151) | -0.1357(5) | 0.0310(4) | 0.1542(2) | 0.0366(19) |
| C(152) | -0.0167(5) | 0.0305(3) | 0.15145(18) | 0.0289(17) |
| C(153) | 0.0665(6) | -0.0049(4) | 0.1142(2) | 0.0398(19) |
| C(154) | 0.0313(7) | -0.0365(4) | 0.0794(2) | 0.049(2) |
| C(155) | -0.0875(7) | -0.0343(4) | 0.0825(2) | 0.047(2) |
| C(156) | -0.1722(6) | -0.0021(4) | 0.1201(2) | 0.044(2) |
| C(161) | -0.0753(5) | 0.0130(3) | 0.25610(17) | 0.0239(17) |
| C(162) | -0.1762(5) | 0.0465(3) | 0.28973(18) | 0.0266(17) |
| C(163) | -0.2517(5) | 0.0065(3) | 0.3120(2) | 0.0322(17) |
| C(164) | -0.2284(6) | -0.0661(4) | 0.3000(2) | 0.0375(19) |
| C(165) | -0.1309(5) | -0.0989(3) | 0.2662(2) | 0.0337(18) |
| C(166) | -0.0546(5) | -0.0600(3) | 0.24472(19) | 0.0305(17) |
| C(221) | 0.2519(5) | 0.0883(3) | 0.43684(17) | 0.0239(16) |
| C(222) | 0.2977(5) | 0.0753(3) | 0.38960(16) | 0.0224(16) |
| C(223) | 0.4137(5) | 0.0262(3) | 0.37760(18) | 0.0271(17) |
| C(224) | 0.4775(5) | -0.0145(3) | 0.4090(2) | 0.0314(17) |
| C(225) | 0.4255(5) | -0.0075(3) | 0.45534(19) | 0.0326(17) |
| C(226) | 0.3159(5) | 0.0440(3) | 0.46899(18) | 0.0287(17) |
| C(231) | 0.2169(5) | 0.1974(3) | 0.51506(18) | 0.0302(17) |
| C(232) | 0.1946(6) | 0.2031(3) | 0.56294(19) | 0.035(2) |
| C(233) | 0.2839(7) | 0.2094(4) | 0.5864(2) | 0.042(2) |
| C(234) | 0.3950(6) | 0.2102(4) | 0.5630(2) | 0.041(2) |
| C(235) | 0.4185(6) | 0.2065(4) | 0.5152(2) | 0.041(2) |
| C(236) | 0.3301(5) | 0.2001(3) | 0.49180(19) | 0.0325(17) |
| C(251) | -0.2152(6) | 0.2963(4) | 0.5063(2) | 0.0393(19) |
| C(252) | -0.3106(6) | 0.2791(4) | 0.5315(3) | 0.050(2) |
| C(253) | -0.4144(6) | 0.3327(4) | 0.5503(2) | 0.050(2) |
| C(254) | -0.4245(8) | 0.4045(5) | 0.5458(3) | 0.071(3) |
| C(255) | -0.3210(8) | 0.4256(5) | 0.5234(4) | 0.077(3) |
| C(256) | -0.2166(8) | 0.3708(5) | 0.5033(3) | 0.074(3) |
| C(261) | -0.1863(5) | 0.1873(3) | 0.42894(18) | 0.0292(17) |
| C(262) | -0.2182(6) | 0.2301(4) | 0.3917(2) | 0.0419(19) |
| C(263) | -0.3098(6) | 0.2223(4) | 0.3698(2) | 0.049(2) |

Positional Parameters and Their Estimated Standard Deviations (cont.)

for $C_{90}H_{63}O_3W, C_{69}H_{55}NO_2W, Cl$

| Atom | x | y | z | U(Å²) |
|---|---|---|---|---|
| C(264) | -0.3681(6) | 0.1717(4) | 0.3853(2) | 0.046(2) |
| C(265) | -0.3383(6) | 0.1284(4) | 0.4225(2) | 0.0404(19) |
| C(266) | -0.2477(5) | 0.1369(3) | 0.44391(19) | 0.0333(17) |
| C(321) | 0.4080(4) | -0.0072(3) | 0.22591(17) | 0.0240(14) |
| C(322) | 0.4994(5) | 0.0055(3) | 0.24568(18) | 0.0275(16) |
| C(323) | 0.5662(5) | 0.0499(3) | 0.2252(2) | 0.0330(17) |
| C(324) | 0.5447(5) | 0.0820(3) | 0.1839(2) | 0.0360(18) |
| C(325) | 0.4542(5) | 0.0704(3) | 0.1635(2) | 0.0336(17) |
| C(326) | 0.3861(5) | 0.0260(3) | 0.18443(19) | 0.0298(17) |
| C(331) | 0.4305(5) | -0.1445(3) | 0.17748(19) | 0.0308(17) |
| C(332) | 0.5521(6) | -0.1460(3) | 0.1701(2) | 0.0387(18) |
| C(333) | 0.6253(7) | -0.1645(4) | 0.1274(2) | 0.050(2) |
| C(334) | 0.5794(7) | -0.1835(4) | 0.0918(2) | 0.052(2) |
| C(335) | 0.4611(9) | -0.1845(4) | 0.0994(2) | 0.061(3) |
| C(336) | 0.3867(7) | -0.1646(4) | 0.1420(2) | 0.049(2) |
| C(351) | 0.1580(5) | -0.2161(3) | 0.3059(2) | 0.0316(17) |
| C(352) | 0.0992(5) | -0.2470(3) | 0.2780(2) | 0.0370(18) |
| C(353) | 0.0505(6) | -0.3022(4) | 0.2942(3) | 0.046(2) |
| C(354) | 0.0599(7) | -0.3297(4) | 0.3372(3) | 0.051(2) |
| C(355) | 0.1196(6) | -0.3004(4) | 0.3645(2) | 0.046(2) |
| C(356) | 0.1677(6) | -0.2440(3) | 0.3489(2) | 0.0353(18) |
| C(361) | 0.1320(5) | -0.0795(3) | 0.35821(17) | 0.0254(16) |
| C(362) | 0.0104(5) | -0.0781(3) | 0.36621(19) | 0.0288(17) |
| C(363) | -0.0580(6) | -0.0661(3) | 0.4099(2) | 0.0339(18) |
| C(364) | -0.0043(6) | -0.0562(3) | 0.4470(2) | 0.039(2) |
| C(365) | 0.1152(6) | -0.0568(3) | 0.43936(19) | 0.035(2) |
| C(366) | 0.1832(5) | -0.0681(3) | 0.39521(18) | 0.0292(17) |
| C(421) | -0.3051(6) | -0.4172(3) | 0.2010(2) | 0.0336(18) |
| C(422) | -0.1751(5) | -0.4558(3) | 0.1886(2) | 0.0340(18) |
| C(423) | -0.1165(6) | -0.4588(4) | 0.1434(2) | 0.0372(18) |
| C(424) | -0.1770(6) | -0.4109(4) | 0.1110(2) | 0.039(2) |
| C(425) | -0.2945(6) | -0.3619(3) | 0.1263(2) | 0.038(2) |
| C(426) | -0.3624(6) | -0.3649(3) | 0.1701(2) | 0.0366(18) |
| C(431) | -0.4233(6) | -0.3355(3) | 0.29438(19) | 0.035(2) |
| C(432) | -0.3302(7) | -0.3059(4) | 0.2773(2) | 0.048(2) |
| C(433) | -0.3394(7) | -0.2343(4) | 0.2867(2) | 0.050(3) |
| C(434) | -0.4410(7) | -0.1907(4) | 0.3141(2) | 0.045(2) |
| C(435) | -0.5314(7) | -0.2191(4) | 0.3322(3) | 0.048(2) |
| C(436) | -0.5255(6) | -0.2909(4) | 0.3229(2) | 0.042(2) |
| C(451) | -0.4986(8) | -0.5671(4) | 0.3542(2) | 0.055(3) |
| C(452) | -0.4292(9) | -0.5865(6) | 0.3884(3) | 0.091(4) |
| C(453) | -0.4669(13) | -0.6193(7) | 0.4288(4) | 0.106(5) |
| C(454) | -0.5728(17) | -0.6356(6) | 0.4340(4) | 0.113(7) |
| C(455) | -0.6392(19) | -0.6217(10) | 0.4022(5) | 0.167(10) |
| C(456) | -0.6084(17) | -0.5767(14) | 0.3615(4) | 0.215(15) |

Positional Parameters and Their Estimated Standard Deviations (cont.)

for $C_{90}H_{63}O_3W, C_{69}H_{55}NO_2W, Cl$

| Atom | x | y | z | U(Å²) |
|---|---|---|---|---|
| C(461) | -0.3747(5) | -0.6420(3) | 0.2611(2) | 0.0327(18) |
| C(462) | -0.4627(6) | -0.6778(4) | 0.2625(2) | 0.0432(19) |
| C(463) | -0.4287(6) | -0.7516(4) | 0.2499(3) | 0.047(2) |
| C(464) | -0.3092(6) | -0.7895(4) | 0.2368(2) | 0.043(2) |
| C(465) | -0.2215(6) | -0.7553(3) | 0.2362(2) | 0.0396(18) |
| C(466) | -0.2544(5) | -0.6822(3) | 0.2486(2) | 0.0348(18) |
| C(521) | -0.3626(5) | -0.4157(3) | 0.00486(19) | 0.0298(17) |
| C(522) | -0.3321(6) | -0.4784(3) | -0.0218(2) | 0.0380(18) |
| C(523) | -0.2167(6) | -0.5047(4) | -0.0484(2) | 0.047(2) |
| C(524) | -0.1616(6) | -0.4056(5) | -0.0215(2) | 0.051(3) |
| C(525) | -0.1327(6) | -0.4688(5) | -0.0469(2) | 0.054(3) |
| C(526) | -0.2754(6) | -0.3797(4) | 0.0038(2) | 0.0399(19) |
| C(531) | -0.5745(5) | -0.3059(3) | -0.02611(19) | 0.0308(17) |
| C(532) | -0.5660(5) | -0.3511(3) | -0.06223(19) | 0.0338(18) |
| C(533) | -0.5740(6) | -0.3238(4) | -0.1058(2) | 0.0398(19) |
| C(534) | -0.5913(7) | -0.2499(4) | -0.1132(2) | 0.051(2) |
| C(535) | -0.5987(7) | -0.2041(4) | -0.0773(2) | 0.052(3) |
| C(536) | -0.5897(7) | -0.2318(4) | -0.0337(2) | 0.043(2) |
| C(551) | -0.8251(5) | -0.3048(3) | 0.12678(19) | 0.0305(17) |
| C(552) | -0.8815(5) | -0.2299(3) | 0.12883(19) | 0.0326(17) |
| C(553) | -0.9980(5) | -0.1993(4) | 0.1517(2) | 0.0388(19) |
| C(554) | -1.0621(6) | -0.2448(4) | 0.1738(2) | 0.044(2) |
| C(555) | -1.0094(6) | -0.3197(4) | 0.1729(2) | 0.0411(19) |
| C(556) | -0.8908(5) | -0.3498(4) | 0.1496(2) | 0.0357(18) |
| C(561) | -0.6247(5) | -0.4260(3) | 0.15732(19) | 0.0307(17) |
| C(562) | -0.6545(5) | -0.3858(4) | 0.19828(19) | 0.0354(17) |
| C(563) | -0.6810(6) | -0.4191(4) | 0.2394(2) | 0.0429(19) |
| C(564) | -0.6787(6) | -0.4905(4) | 0.2408(2) | 0.048(2) |
| C(565) | -0.6472(6) | -0.5325(4) | 0.2002(2) | 0.048(2) |
| C(566) | -0.6181(6) | -0.5002(3) | 0.1590(2) | 0.038(2) |
| C(641) | 0.0106(6) | -0.7765(4) | 0.0208(2) | 0.039(2) |
| C(642) | -0.0525(8) | -0.8360(4) | 0.0289(3) | 0.057(3) |
| C(643) | 0.0344(7) | -0.7604(4) | -0.0311(2) | 0.050(2) |
| C(644) | 0.1365(6) | -0.8051(4) | 0.0346(2) | 0.050(2) |

$U_{eq} = (1/3)\Sigma_i\Sigma_j\ U_{ij}a^*_i a^*_j \mathbf{a}_i \cdot \mathbf{a}_j$

Positional Parameters and Their Estimated Standard Deviations

for $C_{90}H_{63}O_3W, C_{69}H_{55}NO_2W, Cl$

| Atom | x | y | z | U(Å²) |
|---|---|---|---|---|
| H(14) | 0.095 | 0.128 | 0.137 | 0.033 |
| H(24) | -0.005 | 0.274 | 0.529 | 0.040 |
| H(34) | 0.291 | -0.212 | 0.226 | 0.036 |
| H(44) | -0.504 | -0.431 | 0.347 | 0.047 |
| H(54) | -0.748 | -0.271 | 0.044 | 0.036 |
| H(62) | -0.166 | -0.649 | 0.153 | 0.048 |
| H(63) | -0.054 | -0.752 | 0.112 | 0.050 |
| H(65) | -0.111 | -0.640 | -0.002 | 0.041 |
| H(66) | -0.221 | -0.540 | 0.043 | 0.040 |
| H(122) | -0.012 | 0.233 | 0.313 | 0.031 |
| H(123) | 0.057 | 0.273 | 0.375 | 0.036 |
| H(124) | 0.263 | 0.221 | 0.381 | 0.037 |
| H(125) | 0.382 | 0.134 | 0.320 | 0.035 |
| H(12A) | 0.277 | 0.245 | 0.263 | 0.032 |
| H(12B) | 0.341 | 0.163 | 0.245 | 0.032 |
| H(132) | 0.268 | 0.181 | 0.118 | 0.049 |
| H(133) | 0.318 | 0.284 | 0.089 | 0.067 |
| H(134) | 0.240 | 0.393 | 0.129 | 0.069 |
| H(135) | 0.110 | 0.400 | 0.197 | 0.070 |
| H(136) | 0.063 | 0.298 | 0.228 | 0.049 |
| H(151) | -0.193 | 0.054 | 0.179 | 0.044 |
| H(153) | 0.148 | -0.008 | 0.112 | 0.048 |
| H(154) | 0.088 | -0.059 | 0.054 | 0.059 |
| H(155) | -0.111 | -0.055 | 0.059 | 0.056 |
| H(156) | -0.252 | -0.002 | 0.123 | 0.053 |
| H(162) | -0.193 | 0.096 | 0.297 | 0.032 |
| H(163) | -0.317 | 0.029 | 0.335 | 0.039 |
| H(164) | -0.278 | -0.093 | 0.315 | 0.045 |
| H(165) | -0.117 | -0.148 | 0.258 | 0.041 |
| H(166) | 0.011 | -0.083 | 0.222 | 0.036 |
| H(223) | 0.449 | 0.021 | 0.347 | 0.033 |
| H(224) | 0.554 | -0.046 | 0.399 | 0.038 |
| H(225) | 0.465 | -0.037 | 0.477 | 0.039 |
| H(226) | 0.283 | 0.050 | 0.500 | 0.034 |
| H(232) | 0.119 | 0.203 | 0.579 | 0.042 |
| H(233) | 0.268 | 0.213 | 0.618 | 0.051 |
| H(234) | 0.455 | 0.213 | 0.579 | 0.050 |
| H(235) | 0.493 | 0.208 | 0.499 | 0.049 |
| H(236) | 0.346 | 0.198 | 0.460 | 0.040 |
| H(252) | -0.306 | 0.230 | 0.536 | 0.061 |
| H(253) | -0.479 | 0.319 | 0.567 | 0.060 |
| H(254) | -0.497 | 0.440 | 0.557 | 0.085 |
| H(255) | -0.323 | 0.475 | 0.522 | 0.092 |
| H(256) | -0.149 | 0.383 | 0.488 | 0.088 |

Positional Parameters and Their Estimated Standard Deviations (cont.)

for $C_{90}H_{63}O_3W, C_{69}H_{55}NO_2W, Cl$

| Atom | x | y | z | U(Å²) |
|---|---|---|---|---|
| H(262) | -0.178 | 0.264 | 0.381 | 0.050 |
| H(263) | -0.331 | 0.251 | 0.345 | 0.059 |
| H(264) | -0.429 | 0.166 | 0.371 | 0.055 |
| H(265) | -0.379 | 0.094 | 0.433 | 0.049 |
| H(266) | -0.228 | 0.108 | 0.469 | 0.040 |
| H(322) | 0.516 | -0.016 | 0.273 | 0.033 |
| H(323) | 0.626 | 0.058 | 0.239 | 0.040 |
| H(324) | 0.591 | 0.111 | 0.170 | 0.043 |
| H(325) | 0.439 | 0.092 | 0.136 | 0.040 |
| H(326) | 0.325 | 0.018 | 0.171 | 0.036 |
| H(332) | 0.585 | -0.134 | 0.194 | 0.047 |
| H(333) | 0.706 | -0.164 | 0.123 | 0.059 |
| H(334) | 0.628 | -0.196 | 0.063 | 0.062 |
| H(335) | 0.430 | -0.199 | 0.076 | 0.073 |
| H(336) | 0.306 | -0.165 | 0.146 | 0.058 |
| H(352) | 0.093 | -0.230 | 0.248 | 0.044 |
| H(353) | 0.010 | -0.321 | 0.276 | 0.055 |
| H(354) | 0.027 | -0.367 | 0.348 | 0.061 |
| H(355) | 0.127 | -0.319 | 0.394 | 0.055 |
| H(356) | 0.207 | -0.225 | 0.368 | 0.043 |
| H(362) | -0.025 | -0.085 | 0.342 | 0.034 |
| H(363) | -0.139 | -0.065 | 0.415 | 0.041 |
| H(364) | -0.049 | -0.049 | 0.476 | 0.047 |
| H(365) | 0.151 | -0.050 | 0.464 | 0.042 |
| H(366) | 0.264 | -0.068 | 0.390 | 0.036 |
| H(422) | -0.132 | -0.478 | 0.211 | 0.041 |
| H(423) | -0.040 | -0.491 | 0.134 | 0.045 |
| H(424) | -0.140 | -0.412 | 0.080 | 0.046 |
| H(425) | -0.328 | -0.326 | 0.106 | 0.046 |
| H(426) | -0.441 | -0.334 | 0.179 | 0.044 |
| H(432) | -0.260 | -0.335 | 0.259 | 0.057 |
| H(433) | -0.276 | -0.215 | 0.274 | 0.060 |
| H(434) | -0.447 | -0.142 | 0.320 | 0.055 |
| H(435) | -0.599 | -0.190 | 0.351 | 0.057 |
| H(436) | -0.589 | -0.309 | 0.336 | 0.051 |
| H(452) | -0.354 | -0.577 | 0.384 | 0.109 |
| H(453) | -0.420 | -0.630 | 0.452 | 0.127 |
| H(454) | -0.599 | -0.657 | 0.461 | 0.136 |
| H(455) | -0.706 | -0.640 | 0.404 | 0.199 |
| H(456) | -0.664 | -0.556 | 0.342 | 0.258 |
| H(462) | -0.544 | -0.653 | 0.272 | 0.051 |
| H(463) | -0.488 | -0.775 | 0.250 | 0.057 |
| H(464) | -0.287 | -0.839 | 0.228 | 0.052 |
| H(465) | -0.140 | -0.781 | 0.227 | 0.048 |
| H(466) | -0.194 | -0.660 | 0.249 | 0.042 |

Positional Parameters and Their Estimated Standard Deviations (cont.)

for $C_{90}H_{63}O_3W, C_{69}H_{55}NO_2W, Cl$

| Atom | x | y | z | U(Å²) |
|---|---|---|---|---|
| H(522) | -0.389 | -0.503 | -0.022 | 0.045 |
| H(523) | -0.197 | -0.546 | -0.067 | 0.056 |
| H(524) | -0.104 | -0.381 | -0.022 | 0.061 |
| H(525) | -0.055 | -0.488 | -0.063 | 0.065 |
| H(526) | -0.295 | -0.337 | 0.021 | 0.048 |
| H(532) | -0.555 | -0.401 | -0.057 | 0.040 |
| H(533) | -0.568 | -0.355 | -0.130 | 0.048 |
| H(534) | -0.598 | -0.231 | -0.142 | 0.061 |
| H(535) | -0.610 | -0.154 | -0.082 | 0.063 |
| H(536) | -0.594 | -0.201 | -0.010 | 0.052 |
| H(552) | -0.839 | -0.199 | 0.114 | 0.039 |
| H(553) | -1.033 | -0.149 | 0.152 | 0.047 |
| H(554) | -1.141 | -0.225 | 0.189 | 0.053 |
| H(555) | -1.053 | -0.350 | 0.188 | 0.049 |
| H(556) | -0.855 | -0.400 | 0.149 | 0.043 |
| H(562) | -0.656 | -0.337 | 0.198 | 0.042 |
| H(563) | -0.701 | -0.392 | 0.267 | 0.052 |
| H(564) | -0.698 | -0.512 | 0.269 | 0.058 |
| H(565) | -0.646 | -0.581 | 0.201 | 0.057 |
| H(566) | -0.594 | -0.528 | 0.132 | 0.045 |
| H(64A) | -0.065 | -0.847 | 0.061 | 0.085 |
| H(64B) | -0.003 | -0.879 | 0.012 | 0.085 |
| H(64C) | -0.130 | -0.819 | 0.019 | 0.085 |
| H(64D) | -0.040 | -0.749 | -0.043 | 0.074 |
| H(64E) | 0.092 | -0.802 | -0.047 | 0.074 |
| H(64F) | 0.066 | -0.719 | -0.036 | 0.074 |
| H(64G) | 0.176 | -0.767 | 0.030 | 0.075 |
| H(64H) | 0.184 | -0.847 | 0.016 | 0.075 |
| H(64I) | 0.127 | -0.819 | 0.066 | 0.075 |

Hydrogens included in calculation of structure factors but not refined

## Anisotropic Temperature Factor Coefficients - U's

for $C_{90}H_{63}O_3W, C_{69}H_{55}NO_2W, Cl$

| Name | U(1,1) | U(2,2) | U(3,3) | U(1,2) | U(1,3) | U(2,3) |
|---|---|---|---|---|---|---|
| W(1) | 0.02103(11) | 0.02088(11) | 0.01889(10) | -0.00773(8) | -0.00440(8) | 0.00098(8) |
| W(2) | 0.03119(13) | 0.02569(13) | 0.02771(12) | -0.00759(10) | -0.00325(9) | 0.00088(9) |
| Cl | 0.0635(12) | 0.0700(14) | 0.0574(11) | -0.0266(11) | -0.0082(9) | 0.0018(10) |
| O(1) | 0.0224(17) | 0.027(2) | 0.0211(17) | -0.0099(15) | -0.0049(14) | 0.0020(15) |
| O(2) | 0.0258(18) | 0.027(2) | 0.0209(17) | -0.0108(16) | -0.0030(15) | -0.0011(15) |
| O(3) | 0.0252(18) | 0.0231(19) | 0.0224(17) | -0.0095(15) | -0.0039(14) | -0.0024(14) |
| O(4) | 0.037(2) | 0.030(2) | 0.028(2) | -0.0074(18) | -0.0030(17) | -0.0008(16) |
| O(5) | 0.032(2) | 0.029(2) | 0.0266(19) | -0.0049(17) | -0.0048(16) | 0.0006(16) |
| N(61) | 0.029(2) | 0.029(3) | 0.036(3) | -0.009(2) | -0.005(2) | 0.000(2) |
| C(11) | 0.020(2) | 0.025(3) | 0.019(2) | -0.005(2) | -0.0062(19) | 0.005(2) |
| C(12) | 0.021(2) | 0.028(3) | 0.020(2) | -0.007(2) | -0.007(2) | 0.003(2) |
| C(13) | 0.020(2) | 0.029(3) | 0.027(3) | -0.006(2) | -0.003(2) | 0.004(2) |
| C(14) | 0.025(3) | 0.036(3) | 0.022(2) | -0.009(2) | -0.006(2) | 0.004(2) |
| C(15) | 0.026(3) | 0.028(3) | 0.023(2) | -0.004(2) | -0.007(2) | 0.000(2) |
| C(16) | 0.024(3) | 0.023(3) | 0.023(2) | -0.005(2) | -0.005(2) | -0.002(2) |
| C(21) | 0.029(3) | 0.027(3) | 0.021(2) | -0.012(2) | -0.004(2) | 0.001(2) |
| C(22) | 0.027(3) | 0.027(3) | 0.020(2) | -0.010(2) | -0.003(2) | 0.003(2) |
| C(23) | 0.037(3) | 0.028(3) | 0.021(2) | -0.010(2) | -0.004(2) | 0.000(2) |
| C(24) | 0.044(3) | 0.035(3) | 0.021(3) | -0.012(3) | -0.004(2) | -0.005(2) |
| C(25) | 0.034(3) | 0.029(3) | 0.025(3) | -0.004(2) | 0.003(2) | -0.002(2) |
| C(26) | 0.029(3) | 0.028(3) | 0.027(3) | -0.009(2) | -0.005(2) | 0.005(2) |
| C(31) | 0.025(3) | 0.024(3) | 0.021(2) | -0.006(2) | -0.009(2) | -0.001(2) |
| C(32) | 0.023(3) | 0.027(3) | 0.026(3) | -0.008(2) | -0.005(2) | 0.001(2) |
| C(33) | 0.027(3) | 0.031(3) | 0.024(3) | -0.007(2) | -0.004(2) | -0.005(2) |
| C(34) | 0.033(3) | 0.024(3) | 0.033(3) | -0.011(2) | -0.004(2) | -0.007(2) |
| C(35) | 0.028(3) | 0.021(3) | 0.035(3) | -0.011(2) | -0.004(2) | -0.001(2) |
| C(36) | 0.023(3) | 0.029(3) | 0.024(2) | -0.008(2) | -0.004(2) | 0.001(2) |
| C(41) | 0.032(3) | 0.027(3) | 0.032(3) | -0.008(2) | -0.001(2) | 0.001(2) |
| C(42) | 0.037(3) | 0.031(3) | 0.032(3) | -0.008(3) | -0.006(3) | 0.000(2) |
| C(43) | 0.033(3) | 0.033(3) | 0.029(3) | -0.010(3) | 0.001(2) | -0.004(2) |
| C(44) | 0.046(4) | 0.038(4) | 0.033(3) | -0.015(3) | 0.001(3) | -0.004(3) |
| C(45) | 0.040(3) | 0.043(4) | 0.032(3) | -0.015(3) | 0.001(3) | 0.001(3) |
| C(46) | 0.036(3) | 0.030(3) | 0.036(3) | -0.009(3) | -0.004(3) | 0.002(2) |
| C(51) | 0.030(3) | 0.024(3) | 0.030(3) | -0.006(2) | -0.004(2) | 0.000(2) |
| C(52) | 0.031(3) | 0.023(3) | 0.027(3) | -0.009(2) | -0.002(2) | 0.001(2) |
| C(53) | 0.036(3) | 0.032(3) | 0.027(3) | -0.015(3) | -0.007(2) | 0.003(2) |
| C(54) | 0.027(3) | 0.031(3) | 0.031(3) | -0.006(2) | -0.007(2) | 0.006(2) |
| C(55) | 0.030(3) | 0.024(3) | 0.031(3) | -0.008(2) | -0.001(2) | -0.001(2) |
| C(56) | 0.035(3) | 0.025(3) | 0.027(3) | -0.008(2) | -0.003(2) | -0.002(2) |
| C(62) | 0.050(4) | 0.036(4) | 0.028(3) | -0.003(3) | -0.007(3) | 0.001(3) |
| C(63) | 0.047(4) | 0.034(3) | 0.034(3) | 0.003(3) | -0.006(3) | 0.002(3) |
| C(64) | 0.029(3) | 0.036(3) | 0.030(3) | -0.007(3) | -0.006(2) | 0.001(2) |
| C(65) | 0.039(3) | 0.035(3) | 0.028(3) | -0.007(3) | -0.008(2) | 0.000(2) |
| C(66) | 0.036(3) | 0.033(3) | 0.028(3) | -0.006(3) | -0.005(2) | 0.003(2) |

Anisotropic Temperature Factor Coefficients - U's (Continued)

for $C_{90}H_{63}O_3W, C_{69}H_{55}NO_2W, Cl$

| Name | U(1,1) | U(2,2) | U(3,3) | U(1,2) | U(1,3) | U(2,3) |
|---|---|---|---|---|---|---|
| C(121) | 0.028(3) | 0.020(3) | 0.024(2) | -0.011(2) | -0.006(2) | 0.007(2) |
| C(122) | 0.025(3) | 0.022(3) | 0.031(3) | -0.005(2) | -0.007(2) | 0.003(2) |
| C(123) | 0.039(3) | 0.022(3) | 0.029(3) | -0.010(2) | -0.003(2) | 0.000(2) |
| C(124) | 0.037(3) | 0.029(3) | 0.031(3) | -0.016(3) | -0.010(2) | 0.000(2) |
| C(125) | 0.033(3) | 0.025(3) | 0.031(3) | -0.008(2) | -0.010(2) | 0.002(2) |
| C(126) | 0.025(3) | 0.031(3) | 0.027(3) | -0.015(2) | -0.004(2) | 0.006(2) |
| C(131) | 0.030(3) | 0.038(3) | 0.029(3) | -0.011(3) | -0.014(2) | 0.013(2) |
| C(132) | 0.035(3) | 0.055(4) | 0.036(3) | -0.019(3) | -0.010(3) | 0.019(3) |
| C(133) | 0.049(4) | 0.085(6) | 0.047(4) | -0.039(4) | -0.018(3) | 0.036(4) |
| C(134) | 0.081(6) | 0.055(5) | 0.061(5) | -0.048(5) | -0.034(4) | 0.032(4) |
| C(135) | 0.087(6) | 0.043(4) | 0.061(5) | -0.031(4) | -0.041(4) | 0.024(4) |
| C(136) | 0.048(4) | 0.038(4) | 0.041(3) | -0.015(3) | -0.016(3) | 0.015(3) |
| C(151) | 0.033(3) | 0.042(4) | 0.033(3) | -0.004(3) | -0.011(3) | -0.010(3) |
| C(152) | 0.038(3) | 0.029(3) | 0.022(3) | -0.012(2) | -0.008(2) | 0.001(2) |
| C(153) | 0.041(3) | 0.048(4) | 0.030(3) | -0.015(3) | 0.000(3) | -0.009(3) |
| C(154) | 0.066(5) | 0.052(4) | 0.029(3) | -0.021(4) | 0.000(3) | -0.011(3) |
| C(155) | 0.066(5) | 0.043(4) | 0.035(3) | -0.016(4) | -0.016(3) | -0.010(3) |
| C(156) | 0.040(3) | 0.051(4) | 0.043(4) | -0.010(3) | -0.017(3) | -0.008(3) |
| C(161) | 0.025(3) | 0.025(3) | 0.025(3) | -0.011(2) | -0.007(2) | 0.003(2) |
| C(162) | 0.025(3) | 0.027(3) | 0.029(3) | -0.009(2) | -0.006(2) | 0.002(2) |
| C(163) | 0.026(3) | 0.040(3) | 0.033(3) | -0.013(3) | -0.006(2) | 0.003(3) |
| C(164) | 0.035(3) | 0.044(4) | 0.042(3) | -0.023(3) | -0.011(3) | 0.007(3) |
| C(165) | 0.036(3) | 0.030(3) | 0.042(3) | -0.017(3) | -0.012(3) | 0.001(3) |
| C(166) | 0.027(3) | 0.034(3) | 0.031(3) | -0.009(2) | -0.005(2) | -0.004(2) |
| C(221) | 0.029(3) | 0.026(3) | 0.021(2) | -0.013(2) | -0.007(2) | 0.001(2) |
| C(222) | 0.028(3) | 0.022(3) | 0.019(2) | -0.009(2) | -0.006(2) | -0.001(2) |
| C(223) | 0.026(3) | 0.031(3) | 0.025(3) | -0.008(2) | -0.006(2) | -0.002(2) |
| C(224) | 0.026(3) | 0.029(3) | 0.037(3) | -0.001(2) | -0.011(2) | -0.005(2) |
| C(225) | 0.037(3) | 0.034(3) | 0.028(3) | -0.007(3) | -0.015(2) | 0.003(2) |
| C(226) | 0.033(3) | 0.032(3) | 0.024(3) | -0.011(2) | -0.010(2) | 0.000(2) |
| C(231) | 0.042(3) | 0.025(3) | 0.025(3) | -0.010(2) | -0.009(2) | -0.001(2) |
| C(232) | 0.047(4) | 0.037(3) | 0.024(3) | -0.016(3) | -0.005(3) | 0.000(2) |
| C(233) | 0.068(5) | 0.039(4) | 0.025(3) | -0.019(3) | -0.016(3) | 0.000(3) |
| C(234) | 0.053(4) | 0.042(4) | 0.038(3) | -0.022(3) | -0.017(3) | -0.001(3) |
| C(235) | 0.045(4) | 0.044(4) | 0.040(3) | -0.020(3) | -0.011(3) | 0.003(3) |
| C(236) | 0.042(3) | 0.034(3) | 0.025(3) | -0.017(3) | -0.004(2) | -0.003(2) |
| C(251) | 0.040(3) | 0.037(4) | 0.031(3) | 0.000(3) | 0.002(3) | -0.008(3) |
| C(252) | 0.042(4) | 0.037(4) | 0.062(4) | -0.006(3) | 0.007(3) | -0.002(3) |
| C(253) | 0.041(4) | 0.048(4) | 0.053(4) | -0.010(3) | 0.012(3) | -0.009(3) |
| C(254) | 0.064(5) | 0.059(6) | 0.062(5) | 0.012(4) | 0.013(4) | -0.007(4) |
| C(255) | 0.060(5) | 0.039(5) | 0.114(8) | -0.001(4) | 0.010(5) | -0.014(5) |
| C(256) | 0.063(5) | 0.055(5) | 0.098(7) | -0.020(4) | 0.006(5) | -0.007(5) |
| C(261) | 0.025(3) | 0.031(3) | 0.026(3) | -0.002(2) | 0.000(2) | -0.002(2) |
| C(262) | 0.031(3) | 0.050(4) | 0.040(3) | -0.006(3) | -0.006(3) | 0.011(3) |
| C(263) | 0.037(4) | 0.061(5) | 0.044(4) | -0.003(3) | -0.017(3) | 0.011(3) |

Anisotropic Temperature Factor Coefficients - U's (Continued)

for $C_{90}H_{63}O_3W, C_{69}H_{55}NO_2W, Cl$

| Name | U(1,1) | U(2,2) | U(3,3) | U(1,2) | U(1,3) | U(2,3) |
|---|---|---|---|---|---|---|
| C(264) | 0.029(3) | 0.062(5) | 0.044(4) | -0.002(3) | -0.013(3) | -0.009(3) |
| C(265) | 0.039(3) | 0.048(4) | 0.037(3) | -0.018(3) | -0.003(3) | -0.008(3) |
| C(266) | 0.033(3) | 0.040(3) | 0.028(3) | -0.013(3) | -0.004(2) | 0.001(2) |
| C(321) | 0.020(2) | 0.025(3) | 0.025(2) | -0.005(2) | -0.001(2) | -0.001(2) |
| C(322) | 0.027(3) | 0.036(3) | 0.021(2) | -0.011(2) | -0.006(2) | 0.004(2) |
| C(323) | 0.026(3) | 0.040(3) | 0.036(3) | -0.014(3) | -0.006(2) | 0.003(3) |
| C(324) | 0.032(3) | 0.036(3) | 0.039(3) | -0.013(3) | 0.000(3) | 0.007(3) |
| C(325) | 0.035(3) | 0.034(3) | 0.028(3) | -0.006(3) | -0.004(2) | 0.008(2) |
| C(326) | 0.029(3) | 0.033(3) | 0.029(3) | -0.008(2) | -0.011(2) | 0.000(2) |
| C(331) | 0.040(3) | 0.024(3) | 0.030(3) | -0.014(3) | -0.002(2) | -0.001(2) |
| C(332) | 0.034(3) | 0.035(3) | 0.038(3) | -0.002(3) | 0.004(3) | -0.002(3) |
| C(333) | 0.044(4) | 0.044(4) | 0.045(4) | 0.002(3) | 0.008(3) | -0.001(3) |
| C(334) | 0.070(5) | 0.038(4) | 0.035(3) | -0.011(4) | 0.016(3) | -0.006(3) |
| C(335) | 0.097(7) | 0.050(5) | 0.040(4) | -0.029(5) | -0.006(4) | -0.021(3) |
| C(336) | 0.059(4) | 0.059(5) | 0.033(3) | -0.030(4) | 0.001(3) | -0.006(3) |
| C(351) | 0.031(3) | 0.022(3) | 0.039(3) | -0.006(2) | 0.000(2) | -0.007(2) |
| C(352) | 0.036(3) | 0.032(3) | 0.043(3) | -0.011(3) | -0.003(3) | -0.010(3) |
| C(353) | 0.041(4) | 0.041(4) | 0.061(4) | -0.023(3) | -0.001(3) | -0.014(3) |
| C(354) | 0.057(4) | 0.035(4) | 0.061(4) | -0.027(3) | 0.013(4) | -0.010(3) |
| C(355) | 0.054(4) | 0.037(4) | 0.042(4) | -0.018(3) | 0.009(3) | -0.001(3) |
| C(356) | 0.040(3) | 0.028(3) | 0.036(3) | -0.010(3) | -0.001(3) | -0.004(3) |
| C(361) | 0.031(3) | 0.024(3) | 0.021(2) | -0.008(2) | -0.004(2) | 0.001(2) |
| C(362) | 0.033(3) | 0.027(3) | 0.028(3) | -0.013(2) | -0.002(2) | 0.000(2) |
| C(363) | 0.037(3) | 0.027(3) | 0.034(3) | -0.010(3) | 0.005(3) | -0.002(2) |
| C(364) | 0.052(4) | 0.034(3) | 0.027(3) | -0.014(3) | 0.008(3) | -0.003(3) |
| C(365) | 0.056(4) | 0.029(3) | 0.025(3) | -0.018(3) | -0.011(3) | 0.006(2) |
| C(366) | 0.036(3) | 0.027(3) | 0.029(3) | -0.015(2) | -0.008(2) | 0.004(2) |
| C(421) | 0.039(3) | 0.026(3) | 0.036(3) | -0.013(3) | 0.000(3) | -0.005(2) |
| C(422) | 0.037(3) | 0.034(3) | 0.033(3) | -0.014(3) | -0.005(3) | 0.000(3) |
| C(423) | 0.037(3) | 0.036(3) | 0.039(3) | -0.011(3) | -0.006(3) | -0.004(3) |
| C(424) | 0.048(4) | 0.042(4) | 0.029(3) | -0.019(3) | -0.004(3) | 0.003(3) |
| C(425) | 0.049(4) | 0.031(3) | 0.037(3) | -0.017(3) | -0.004(3) | 0.004(3) |
| C(426) | 0.044(3) | 0.027(3) | 0.036(3) | -0.009(3) | -0.002(3) | -0.001(3) |
| C(431) | 0.046(4) | 0.033(3) | 0.026(3) | -0.009(3) | -0.009(3) | 0.000(2) |
| C(432) | 0.054(4) | 0.047(4) | 0.043(4) | -0.023(3) | 0.005(3) | -0.007(3) |
| C(433) | 0.068(5) | 0.055(5) | 0.038(3) | -0.040(4) | 0.004(3) | -0.012(3) |
| C(434) | 0.068(5) | 0.031(3) | 0.044(4) | -0.019(3) | -0.020(3) | 0.004(3) |
| C(435) | 0.048(4) | 0.037(4) | 0.055(4) | -0.005(3) | -0.012(3) | -0.013(3) |
| C(436) | 0.041(4) | 0.038(4) | 0.048(4) | -0.012(3) | -0.010(3) | 0.002(3) |
| C(451) | 0.081(6) | 0.048(4) | 0.034(3) | -0.029(4) | 0.010(4) | -0.007(3) |
| C(452) | 0.074(6) | 0.099(8) | 0.057(5) | 0.023(5) | 0.009(5) | 0.035(5) |
| C(453) | 0.132(11) | 0.081(8) | 0.064(6) | 0.014(7) | 0.010(7) | 0.026(6) |
| C(454) | 0.211(16) | 0.077(8) | 0.064(7) | -0.081(10) | 0.008(9) | 0.013(6) |
| C(455) | 0.28(2) | 0.23(2) | 0.076(8) | -0.205(19) | -0.040(11) | 0.054(10) |
| C(456) | 0.228(18) | 0.49(4) | 0.051(6) | -0.29(2) | -0.044(9) | 0.074(12) |

Anisotropic Temperature Factor Coefficients - U's (Continued)

for $C_{90}H_{63}O_3W, C_{69}H_{55}NO_2W, Cl$

| Name | U(1,1) | U(2,2) | U(3,3) | U(1,2) | U(1,3) | U(2,3) |
|---|---|---|---|---|---|---|
| C(461) | 0.039(3) | 0.026(3) | 0.034(3) | -0.010(3) | -0.009(3) | 0.004(2) |
| C(462) | 0.032(3) | 0.033(3) | 0.063(4) | -0.008(3) | -0.009(3) | 0.010(3) |
| C(463) | 0.046(4) | 0.035(4) | 0.070(5) | -0.020(3) | -0.022(4) | 0.011(3) |
| C(464) | 0.059(4) | 0.028(3) | 0.044(4) | -0.011(3) | -0.016(3) | -0.001(3) |
| C(465) | 0.041(3) | 0.033(3) | 0.040(3) | -0.005(3) | -0.004(3) | -0.002(3) |
| C(466) | 0.033(3) | 0.035(3) | 0.038(3) | -0.013(3) | -0.006(3) | 0.003(3) |
| C(521) | 0.029(3) | 0.029(3) | 0.027(3) | -0.004(2) | -0.002(2) | 0.006(2) |
| C(522) | 0.042(3) | 0.035(3) | 0.034(3) | -0.007(3) | -0.006(3) | -0.002(3) |
| C(523) | 0.049(4) | 0.044(4) | 0.034(3) | 0.004(3) | -0.003(3) | 0.001(3) |
| C(524) | 0.039(4) | 0.068(5) | 0.046(4) | -0.024(4) | 0.001(3) | 0.010(4) |
| C(525) | 0.031(3) | 0.074(6) | 0.040(4) | 0.002(4) | 0.007(3) | 0.011(4) |
| C(526) | 0.039(3) | 0.041(4) | 0.040(3) | -0.015(3) | -0.003(3) | 0.003(3) |
| C(531) | 0.027(3) | 0.030(3) | 0.033(3) | -0.007(2) | -0.003(2) | 0.009(2) |
| C(532) | 0.039(3) | 0.029(3) | 0.032(3) | -0.008(3) | -0.007(3) | 0.004(2) |
| C(533) | 0.042(3) | 0.042(4) | 0.032(3) | -0.009(3) | -0.004(3) | 0.003(3) |
| C(534) | 0.073(5) | 0.048(4) | 0.032(3) | -0.018(4) | -0.013(3) | 0.012(3) |
| C(535) | 0.081(5) | 0.034(4) | 0.040(4) | -0.017(4) | -0.009(4) | 0.014(3) |
| C(536) | 0.064(4) | 0.037(4) | 0.031(3) | -0.020(3) | -0.006(3) | 0.004(3) |
| C(551) | 0.028(3) | 0.036(3) | 0.029(3) | -0.011(2) | -0.006(2) | 0.000(2) |
| C(552) | 0.030(3) | 0.038(3) | 0.031(3) | -0.011(3) | -0.007(2) | 0.003(2) |
| C(553) | 0.032(3) | 0.043(4) | 0.034(3) | 0.002(3) | -0.007(3) | -0.008(3) |
| C(554) | 0.028(3) | 0.061(5) | 0.038(3) | -0.007(3) | 0.000(3) | -0.017(3) |
| C(555) | 0.034(3) | 0.057(4) | 0.038(3) | -0.027(3) | 0.004(3) | -0.010(3) |
| C(556) | 0.036(3) | 0.036(3) | 0.034(3) | -0.011(3) | -0.001(3) | -0.005(3) |
| C(561) | 0.030(3) | 0.028(3) | 0.029(3) | -0.004(2) | 0.000(2) | 0.001(2) |
| C(562) | 0.036(3) | 0.039(3) | 0.028(3) | -0.008(3) | -0.002(2) | -0.002(3) |
| C(563) | 0.036(3) | 0.056(4) | 0.028(3) | -0.001(3) | -0.003(3) | -0.004(3) |
| C(564) | 0.040(4) | 0.064(5) | 0.035(3) | -0.012(3) | -0.001(3) | 0.021(3) |
| C(565) | 0.046(4) | 0.045(4) | 0.054(4) | -0.018(3) | -0.010(3) | 0.016(3) |
| C(566) | 0.045(4) | 0.034(3) | 0.034(3) | -0.014(3) | -0.005(3) | 0.007(3) |
| C(641) | 0.045(4) | 0.035(3) | 0.035(3) | -0.008(3) | -0.005(3) | -0.005(3) |
| C(642) | 0.070(5) | 0.044(4) | 0.052(4) | -0.015(4) | 0.000(4) | -0.014(3) |
| C(643) | 0.054(4) | 0.047(4) | 0.036(3) | 0.005(3) | -0.007(3) | -0.010(3) |
| C(644) | 0.048(4) | 0.051(4) | 0.040(4) | 0.004(3) | -0.012(3) | -0.002(3) |

The form of the anisotropic temperature factor is:

$\exp[-2\pi \{h^2a^{*2}U(1,1) + k^2b^{*2}U(2,2) + l^2c^{*2}U(3,3) + 2hka^*b^*U(1,2) + 2hla^*c^*U(1,3) + 2klb^*c^*U(2,3)\}]$ where $a^*$, $b^*$, and $c^*$ are reciprocal lattice constants.

Table of Bond Distances in Angstroms

for $C_{90}H_{63}O_3W, C_{69}H_{55}NO_2W, Cl$

| Atom 1 | Atom 2 | Distance | Atom 1 | Atom 2 | Distance |
|---|---|---|---|---|---|
| W(1) | O(3) | 1.951(4) | C(25) | C(26) | 1.425(8) |
| W(1) | O(2) | 2.029(3) | C(25) | C(251) | 1.492(8) |
| W(1) | O(1) | 2.144(3) | C(26) | C(261) | 1.497(8) |
| W(1) | C(121) | 2.202(5) | C(31) | C(36) | 1.406(8) |
| W(1) | C(222) | 2.221(5) | C(31) | C(32) | 1.412(7) |
| W(1) | C(125) | 2.231(6) | C(32) | C(33) | 1.389(8) |
| W(1) | C(122) | 2.253(5) | C(32) | C(321) | 1.494(7) |
| W(1) | C(124) | 2.331(5) | C(33) | C(34) | 1.386(8) |
| W(1) | C(123) | 2.407(6) | C(33) | C(331) | 1.502(8) |
| W(2) | O(5) | 1.987(4) | C(34) | C(35) | 1.399(8) |
| W(2) | O(4) | 2.010(4) | C(35) | C(36) | 1.420(8) |
| W(2) | C(421) | 2.161(6) | C(35) | C(351) | 1.494(8) |
| W(2) | N(61) | 2.199(5) | C(36) | C(361) | 1.497(7) |
| W(2) | C(424) | 2.202(6) | C(41) | C(46) | 1.407(8) |
| W(2) | C(426) | 2.239(6) | C(41) | C(42) | 1.429(8) |
| W(2) | C(425) | 2.248(6) | C(42) | C(43) | 1.400(8) |
| W(2) | C(423) | 2.252(6) | C(42) | C(421) | 1.468(8) |
| W(2) | C(422) | 2.320(6) | C(43) | C(44) | 1.399(8) |
| O(1) | C(11) | 1.349(6) | C(43) | C(431) | 1.483(8) |
| O(2) | C(21) | 1.347(6) | C(44) | C(45) | 1.379(9) |
| O(3) | C(31) | 1.359(6) | C(45) | C(46) | 1.407(9) |
| O(4) | C(41) | 1.355(7) | C(45) | C(451) | 1.509(9) |
| O(5) | C(51) | 1.357(6) | C(46) | C(461) | 1.497(8) |
| N(61) | C(66) | 1.325(7) | C(51) | C(56) | 1.416(8) |
| N(61) | C(62) | 1.347(8) | C(51) | C(52) | 1.424(7) |
| C(11) | C(12) | 1.411(7) | C(52) | C(53) | 1.398(8) |
| C(11) | C(16) | 1.411(7) | C(52) | C(521) | 1.490(8) |
| C(12) | C(13) | 1.394(7) | C(53) | C(54) | 1.381(8) |
| C(12) | C(121) | 1.476(7) | C(53) | C(531) | 1.515(7) |
| C(13) | C(14) | 1.395(8) | C(54) | C(55) | 1.406(8) |
| C(13) | C(131) | 1.504(8) | C(55) | C(56) | 1.407(8) |
| C(14) | C(15) | 1.390(8) | C(55) | C(551) | 1.498(8) |
| C(15) | C(16) | 1.400(7) | C(56) | C(561) | 1.494(8) |
| C(15) | C(152) | 1.503(7) | C(62) | C(63) | 1.380(9) |
| C(16) | C(161) | 1.503(7) | C(63) | C(64) | 1.402(8) |
| C(21) | C(26) | 1.405(8) | C(64) | C(65) | 1.383(8) |
| C(21) | C(22) | 1.406(7) | C(64) | C(641) | 1.516(9) |
| C(22) | C(23) | 1.411(7) | C(65) | C(66) | 1.389(8) |
| C(22) | C(221) | 1.488(8) | C(121) | C(122) | 1.463(8) |
| C(23) | C(24) | 1.379(8) | C(121) | C(126) | 1.520(7) |
| C(23) | C(231) | 1.510(8) | C(122) | C(123) | 1.415(8) |
| C(24) | C(25) | 1.382(8) | C(123) | C(124) | 1.392(8) |

Bond Distances (cont.)

| Atom 1 | Atom 2 | Distance | Atom 1 | Atom 2 | Distance |
|---|---|---|---|---|---|
| C(124) | C(125) | 1.443(8) | C(264) | C(265) | 1.388(9) |
| C(125) | C(126) | 1.521(7) | C(265) | C(266) | 1.381(8) |
| C(131) | C(136) | 1.382(9) | C(321) | C(322) | 1.393(7) |
| C(131) | C(132) | 1.391(8) | C(321) | C(326) | 1.394(7) |
| C(132) | C(133) | 1.397(10) | C(322) | C(323) | 1.372(8) |
| C(133) | C(134) | 1.357(12) | C(323) | C(324) | 1.382(8) |
| C(134) | C(135) | 1.366(12) | C(324) | C(325) | 1.385(8) |
| C(135) | C(136) | 1.383(9) | C(325) | C(326) | 1.388(8) |
| C(151) | C(152) | 1.381(8) | C(331) | C(336) | 1.363(9) |
| C(151) | C(156) | 1.403(8) | C(331) | C(332) | 1.395(8) |
| C(152) | C(153) | 1.384(8) | C(332) | C(333) | 1.390(9) |
| C(153) | C(154) | 1.395(9) | C(333) | C(334) | 1.373(11) |
| C(154) | C(155) | 1.368(10) | C(334) | C(335) | 1.370(11) |
| C(155) | C(156) | 1.380(10) | C(335) | C(336) | 1.398(10) |
| C(161) | C(166) | 1.389(8) | C(351) | C(356) | 1.377(8) |
| C(161) | C(162) | 1.409(8) | C(351) | C(352) | 1.410(8) |
| C(162) | C(163) | 1.398(8) | C(352) | C(353) | 1.375(9) |
| C(163) | C(164) | 1.382(9) | C(353) | C(354) | 1.372(10) |
| C(164) | C(165) | 1.386(9) | C(354) | C(355) | 1.388(10) |
| C(165) | C(166) | 1.383(8) | C(355) | C(356) | 1.386(9) |
| C(221) | C(222) | 1.411(7) | C(361) | C(366) | 1.394(7) |
| C(221) | C(226) | 1.418(7) | C(361) | C(362) | 1.396(8) |
| C(222) | C(223) | 1.399(7) | C(362) | C(363) | 1.384(8) |
| C(223) | C(224) | 1.373(7) | C(363) | C(364) | 1.406(9) |
| C(224) | C(225) | 1.395(8) | C(364) | C(365) | 1.375(9) |
| C(225) | C(226) | 1.372(8) | C(365) | C(366) | 1.394(8) |
| C(231) | C(236) | 1.397(8) | C(421) | C(426) | 1.431(8) |
| C(231) | C(232) | 1.400(8) | C(421) | C(422) | 1.470(8) |
| C(232) | C(233) | 1.391(9) | C(422) | C(423) | 1.388(8) |
| C(233) | C(234) | 1.366(10) | C(423) | C(424) | 1.436(9) |
| C(234) | C(235) | 1.394(9) | C(424) | C(425) | 1.425(9) |
| C(235) | C(236) | 1.381(8) | C(425) | C(426) | 1.407(8) |
| C(251) | C(252) | 1.348(9) | C(431) | C(432) | 1.382(9) |
| C(251) | C(256) | 1.420(11) | C(431) | C(436) | 1.403(9) |
| C(252) | C(253) | 1.382(10) | C(432) | C(433) | 1.377(10) |
| C(253) | C(254) | 1.345(12) | C(433) | C(434) | 1.377(10) |
| C(254) | C(255) | 1.434(13) | C(434) | C(435) | 1.349(10) |
| C(255) | C(256) | 1.409(12) | C(435) | C(436) | 1.389(9) |
| C(261) | C(266) | 1.380(8) | C(451) | C(456) | 1.331(15) |
| C(261) | C(262) | 1.389(8) | C(451) | C(452) | 1.386(12) |
| C(262) | C(263) | 1.396(9) | C(452) | C(453) | 1.395(13) |
| C(263) | C(264) | 1.363(10) | C(453) | C(454) | 1.347(18) |

Bond Distances (cont.)

| Atom 1 | Atom 2 | Distance | Atom 1 | Atom 2 | Distance |
|---|---|---|---|---|---|
| C(454) | C(455) | 1.30(2) | C(534) | C(535) | 1.377(10) |
| C(455) | C(456) | 1.510(17) | C(535) | C(536) | 1.390(9) |
| C(461) | C(466) | 1.383(8) | C(551) | C(552) | 1.388(8) |
| C(461) | C(462) | 1.390(9) | C(551) | C(556) | 1.396(8) |
| C(462) | C(463) | 1.396(10) | C(552) | C(553) | 1.377(8) |
| C(463) | C(464) | 1.366(10) | C(553) | C(554) | 1.384(10) |
| C(464) | C(465) | 1.369(9) | C(554) | C(555) | 1.382(10) |
| C(465) | C(466) | 1.382(9) | C(555) | C(556) | 1.400(9) |
| C(521) | C(522) | 1.382(8) | C(561) | C(562) | 1.396(8) |
| C(521) | C(526) | 1.386(9) | C(561) | C(566) | 1.397(8) |
| C(522) | C(523) | 1.398(9) | C(562) | C(563) | 1.383(9) |
| C(523) | C(525) | 1.362(11) | C(563) | C(564) | 1.357(10) |
| C(524) | C(526) | 1.368(9) | C(564) | C(565) | 1.404(10) |
| C(524) | C(525) | 1.370(11) | C(565) | C(566) | 1.381(9) |
| C(531) | C(532) | 1.372(8) | C(641) | C(642) | 1.520(10) |
| C(531) | C(536) | 1.390(8) | C(641) | C(644) | 1.540(9) |
| C(532) | C(533) | 1.384(8) | C(641) | C(643) | 1.551(9) |
| C(533) | C(534) | 1.383(10) | | | |

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table of Bond Angles in Degrees

for $C_{90}H_{63}O_3W, C_{69}H_{55}NO_2W, Cl$

| Atom 1 | Atom 2 | Atom 3 | Angle | Atom 1 | Atom 2 | Atom 3 | Angle |
|---|---|---|---|---|---|---|---|
| O(3) | W(1) | O(2) | 112.87(15) | O(5) | W(2) | C(424) | 102.08(19) |
| O(3) | W(1) | O(1) | 78.60(14) | O(4) | W(2) | C(424) | 143.30(19) |
| O(2) | W(1) | O(1) | 79.38(13) | C(421) | W(2) | C(424) | 81.1(2) |
| O(3) | W(1) | C(121) | 105.66(17) | N(61) | W(2) | C(424) | 102.3(2) |
| O(2) | W(1) | C(121) | 127.71(17) | O(5) | W(2) | C(426) | 100.4(2) |
| O(1) | W(1) | C(121) | 74.98(16) | O(4) | W(2) | C(426) | 106.74(19) |
| O(3) | W(1) | C(222) | 79.28(16) | C(421) | W(2) | C(426) | 37.9(2) |
| O(2) | W(1) | C(222) | 81.65(16) | N(61) | W(2) | C(426) | 170.5(2) |
| O(1) | W(1) | C(222) | 142.31(16) | C(424) | W(2) | C(426) | 68.2(2) |
| C(121) | W(1) | C(222) | 140.83(19) | O(5) | W(2) | C(425) | 88.5(2) |
| O(3) | W(1) | C(125) | 101.39(18) | O(4) | W(2) | C(425) | 142.01(19) |
| O(2) | W(1) | C(125) | 136.17(17) | C(421) | W(2) | C(425) | 66.5(2) |
| O(1) | W(1) | C(125) | 135.66(16) | N(61) | W(2) | C(425) | 134.4(2) |
| C(121) | W(1) | C(125) | 62.20(19) | C(424) | W(2) | C(425) | 37.3(2) |
| C(222) | W(1) | C(125) | 78.67(19) | C(426) | W(2) | C(425) | 36.6(2) |
| O(3) | W(1) | C(122) | 141.62(17) | O(5) | W(2) | C(423) | 136.68(19) |
| O(2) | W(1) | C(122) | 92.40(17) | O(4) | W(2) | C(423) | 106.4(2) |
| O(1) | W(1) | C(122) | 78.34(17) | C(421) | W(2) | C(423) | 68.4(2) |
| C(121) | W(1) | C(122) | 38.3(2) | N(61) | W(2) | C(423) | 92.5(2) |
| C(222) | W(1) | C(122) | 134.89(19) | C(424) | W(2) | C(423) | 37.6(2) |
| C(125) | W(1) | C(122) | 75.3(2) | C(426) | W(2) | C(423) | 80.4(2) |
| O(3) | W(1) | C(124) | 133.48(18) | C(425) | W(2) | C(423) | 66.5(2) |
| O(2) | W(1) | C(124) | 99.98(17) | O(5) | W(2) | C(422) | 163.81(19) |
| O(1) | W(1) | C(124) | 141.58(17) | O(4) | W(2) | C(422) | 79.62(18) |
| C(121) | W(1) | C(124) | 75.64(19) | C(421) | W(2) | C(422) | 38.1(2) |
| C(222) | W(1) | C(124) | 73.78(19) | N(61) | W(2) | C(422) | 110.92(19) |
| C(125) | W(1) | C(124) | 36.8(2) | C(424) | W(2) | C(422) | 64.9(2) |
| C(122) | W(1) | C(124) | 63.26(19) | C(426) | W(2) | C(422) | 66.5(2) |
| O(3) | W(1) | C(123) | 164.07(17) | C(425) | W(2) | C(422) | 75.4(2) |
| O(2) | W(1) | C(123) | 82.54(17) | C(423) | W(2) | C(422) | 35.3(2) |
| O(1) | W(1) | C(123) | 109.46(17) | C(11) | O(1) | W(1) | 115.6(3) |
| C(121) | W(1) | C(123) | 64.90(19) | C(21) | O(2) | W(1) | 124.3(3) |
| C(222) | W(1) | C(123) | 99.91(19) | C(31) | O(3) | W(1) | 145.8(3) |
| C(125) | W(1) | C(123) | 63.1(2) | C(41) | O(4) | W(2) | 119.3(3) |
| C(122) | W(1) | C(123) | 35.16(19) | C(51) | O(5) | W(2) | 135.6(3) |
| C(124) | W(1) | C(123) | 34.11(19) | C(66) | N(61) | C(62) | 115.2(5) |
| O(5) | W(2) | O(4) | 114.45(16) | C(66) | N(61) | W(2) | 118.7(4) |
| O(5) | W(2) | C(421) | 134.4(2) | C(62) | N(61) | W(2) | 125.5(4) |
| O(4) | W(2) | C(421) | 76.10(19) | O(1) | C(11) | C(12) | 117.4(4) |
| O(5) | W(2) | N(61) | 80.32(16) | O(1) | C(11) | C(16) | 121.5(5) |
| O(4) | W(2) | N(61) | 81.28(17) | C(12) | C(11) | C(16) | 121.1(4) |
| C(421) | W(2) | N(61) | 144.3(2) | C(13) | C(12) | C(11) | 119.8(5) |

## Bond Angles (cont.)

| Atom 1 | Atom 2 | Atom 3 | Angle | Atom 1 | Atom 2 | Atom 3 | Angle |
|---|---|---|---|---|---|---|---|
| C(13) | C(12) | C(121) | 125.8(5) | C(31) | C(36) | C(361) | 120.8(5) |
| C(11) | C(12) | C(121) | 114.4(4) | C(35) | C(36) | C(361) | 120.3(5) |
| C(12) | C(13) | C(14) | 118.0(5) | O(4) | C(41) | C(46) | 122.0(5) |
| C(12) | C(13) | C(131) | 121.7(5) | O(4) | C(41) | C(42) | 116.7(5) |
| C(14) | C(13) | C(131) | 120.1(5) | C(46) | C(41) | C(42) | 121.3(5) |
| C(15) | C(14) | C(13) | 122.6(5) | C(43) | C(42) | C(41) | 119.8(5) |
| C(14) | C(15) | C(16) | 119.6(5) | C(43) | C(42) | C(421) | 129.2(6) |
| C(14) | C(15) | C(152) | 116.2(5) | C(41) | C(42) | C(421) | 110.9(5) |
| C(16) | C(15) | C(152) | 124.1(5) | C(44) | C(43) | C(42) | 117.2(6) |
| C(15) | C(16) | C(11) | 117.9(5) | C(44) | C(43) | C(431) | 120.8(5) |
| C(15) | C(16) | C(161) | 123.9(5) | C(42) | C(43) | C(431) | 122.0(5) |
| C(11) | C(16) | C(161) | 118.2(4) | C(45) | C(44) | C(43) | 123.7(6) |
| O(2) | C(21) | C(26) | 117.0(5) | C(44) | C(45) | C(46) | 120.1(6) |
| O(2) | C(21) | C(22) | 120.7(5) | C(44) | C(45) | C(451) | 118.1(6) |
| C(26) | C(21) | C(22) | 122.2(5) | C(46) | C(45) | C(451) | 121.6(6) |
| C(21) | C(22) | C(23) | 117.6(5) | C(45) | C(46) | C(41) | 117.5(6) |
| C(21) | C(22) | C(221) | 119.1(5) | C(45) | C(46) | C(461) | 125.5(5) |
| C(23) | C(22) | C(221) | 123.2(5) | C(41) | C(46) | C(461) | 116.9(5) |
| C(24) | C(23) | C(22) | 119.7(5) | O(5) | C(51) | C(56) | 121.5(5) |
| C(24) | C(23) | C(231) | 116.4(5) | O(5) | C(51) | C(52) | 117.9(5) |
| C(22) | C(23) | C(231) | 123.9(5) | C(56) | C(51) | C(52) | 120.5(5) |
| C(23) | C(24) | C(25) | 123.3(5) | C(53) | C(52) | C(51) | 119.3(5) |
| C(24) | C(25) | C(26) | 118.1(5) | C(53) | C(52) | C(521) | 121.7(5) |
| C(24) | C(25) | C(251) | 118.4(5) | C(51) | C(52) | C(521) | 119.0(5) |
| C(26) | C(25) | C(251) | 123.2(5) | C(54) | C(53) | C(52) | 119.5(5) |
| C(21) | C(26) | C(25) | 118.5(5) | C(54) | C(53) | C(531) | 117.6(5) |
| C(21) | C(26) | C(261) | 118.5(5) | C(52) | C(53) | C(531) | 122.8(5) |
| C(25) | C(26) | C(261) | 123.1(5) | C(53) | C(54) | C(55) | 122.5(5) |
| O(3) | C(31) | C(36) | 120.1(5) | C(54) | C(55) | C(56) | 118.9(5) |
| O(3) | C(31) | C(32) | 118.1(5) | C(54) | C(55) | C(551) | 116.9(5) |
| C(36) | C(31) | C(32) | 121.7(5) | C(56) | C(55) | C(551) | 124.2(5) |
| C(33) | C(32) | C(31) | 118.5(5) | C(55) | C(56) | C(51) | 119.2(5) |
| C(33) | C(32) | C(321) | 121.1(5) | C(55) | C(56) | C(561) | 121.0(5) |
| C(31) | C(32) | C(321) | 120.4(5) | C(51) | C(56) | C(561) | 119.8(5) |
| C(34) | C(33) | C(32) | 120.1(5) | N(61) | C(62) | C(63) | 124.3(6) |
| C(34) | C(33) | C(331) | 117.6(5) | C(62) | C(63) | C(64) | 119.8(6) |
| C(32) | C(33) | C(331) | 122.2(5) | C(65) | C(64) | C(63) | 115.8(6) |
| C(33) | C(34) | C(35) | 122.4(5) | C(65) | C(64) | C(641) | 123.0(5) |
| C(34) | C(35) | C(36) | 118.2(5) | C(63) | C(64) | C(641) | 121.2(5) |
| C(34) | C(35) | C(351) | 118.3(5) | C(64) | C(65) | C(66) | 120.2(5) |
| C(36) | C(35) | C(351) | 123.4(5) | N(61) | C(66) | C(65) | 124.7(5) |
| C(31) | C(36) | C(35) | 118.9(5) | C(122) | C(121) | C(12) | 116.0(4) |

## Bond Angles (cont.)

| Atom 1 | Atom 2 | Atom 3 | Angle | Atom 1 | Atom 2 | Atom 3 | Angle |
|---|---|---|---|---|---|---|---|
| C(122) | C(121) | C(126) | 115.9(5) | C(222) | C(221) | C(226) | 119.1(5) |
| C(12) | C(121) | C(126) | 125.7(5) | C(222) | C(221) | C(22) | 121.7(4) |
| C(122) | C(121) | W(1) | 72.7(3) | C(226) | C(221) | C(22) | 119.1(5) |
| C(12) | C(121) | W(1) | 110.5(3) | C(223) | C(222) | C(221) | 116.8(5) |
| C(126) | C(121) | W(1) | 98.8(3) | C(223) | C(222) | W(1) | 120.6(4) |
| C(123) | C(122) | C(121) | 118.9(5) | C(221) | C(222) | W(1) | 121.3(4) |
| C(123) | C(122) | W(1) | 78.4(3) | C(224) | C(223) | C(222) | 123.3(5) |
| C(121) | C(122) | W(1) | 68.9(3) | C(223) | C(224) | C(225) | 119.3(5) |
| C(124) | C(123) | C(122) | 117.9(5) | C(226) | C(225) | C(224) | 119.3(5) |
| C(124) | C(123) | W(1) | 70.0(3) | C(225) | C(226) | C(221) | 121.5(5) |
| C(122) | C(123) | W(1) | 66.5(3) | C(236) | C(231) | C(232) | 117.8(5) |
| C(123) | C(124) | C(125) | 118.1(5) | C(236) | C(231) | C(23) | 123.1(5) |
| C(123) | C(124) | W(1) | 75.9(3) | C(232) | C(231) | C(23) | 119.1(5) |
| C(125) | C(124) | W(1) | 67.8(3) | C(233) | C(232) | C(231) | 120.7(6) |
| C(124) | C(125) | C(126) | 117.3(5) | C(234) | C(233) | C(232) | 120.5(6) |
| C(124) | C(125) | W(1) | 75.4(3) | C(233) | C(234) | C(235) | 120.0(6) |
| C(126) | C(125) | W(1) | 97.6(3) | C(236) | C(235) | C(234) | 119.8(6) |
| C(121) | C(126) | C(125) | 97.7(4) | C(235) | C(236) | C(231) | 121.3(5) |
| C(136) | C(131) | C(132) | 118.2(6) | C(252) | C(251) | C(256) | 118.9(7) |
| C(136) | C(131) | C(13) | 119.7(5) | C(252) | C(251) | C(25) | 123.4(6) |
| C(132) | C(131) | C(13) | 122.0(6) | C(256) | C(251) | C(25) | 116.7(6) |
| C(131) | C(132) | C(133) | 120.1(7) | C(251) | C(252) | C(253) | 121.3(7) |
| C(134) | C(133) | C(132) | 120.7(7) | C(254) | C(253) | C(252) | 122.2(7) |
| C(133) | C(134) | C(135) | 119.6(7) | C(253) | C(254) | C(255) | 118.6(7) |
| C(134) | C(135) | C(136) | 120.8(8) | C(256) | C(255) | C(254) | 118.7(8) |
| C(131) | C(136) | C(135) | 120.7(7) | C(255) | C(256) | C(251) | 119.6(8) |
| C(152) | C(151) | C(156) | 121.5(6) | C(266) | C(261) | C(262) | 118.3(5) |
| C(151) | C(152) | C(153) | 117.7(5) | C(266) | C(261) | C(26) | 120.9(5) |
| C(151) | C(152) | C(15) | 122.6(5) | C(262) | C(261) | C(26) | 120.6(5) |
| C(153) | C(152) | C(15) | 119.5(5) | C(261) | C(262) | C(263) | 121.0(6) |
| C(152) | C(153) | C(154) | 121.5(6) | C(264) | C(263) | C(262) | 119.2(6) |
| C(155) | C(154) | C(153) | 119.7(6) | C(263) | C(264) | C(265) | 121.0(6) |
| C(154) | C(155) | C(156) | 120.4(6) | C(266) | C(265) | C(264) | 119.1(6) |
| C(155) | C(156) | C(151) | 119.1(6) | C(261) | C(266) | C(265) | 121.4(6) |
| C(166) | C(161) | C(162) | 118.5(5) | C(322) | C(321) | C(326) | 118.3(5) |
| C(166) | C(161) | C(16) | 123.8(5) | C(322) | C(321) | C(32) | 121.2(5) |
| C(162) | C(161) | C(16) | 117.7(5) | C(326) | C(321) | C(32) | 120.3(5) |
| C(163) | C(162) | C(161) | 120.7(5) | C(323) | C(322) | C(321) | 121.2(5) |
| C(164) | C(163) | C(162) | 119.5(6) | C(322) | C(323) | C(324) | 120.1(5) |
| C(163) | C(164) | C(165) | 120.1(6) | C(323) | C(324) | C(325) | 119.9(5) |
| C(166) | C(165) | C(164) | 120.7(6) | C(324) | C(325) | C(326) | 119.9(5) |
| C(165) | C(166) | C(161) | 120.6(5) | C(325) | C(326) | C(321) | 120.5(5) |

## Bond Angles (cont.)

| Atom 1 | Atom 2 | Atom 3 | Angle | Atom 1 | Atom 2 | Atom 3 | Angle |
|---|---|---|---|---|---|---|---|
| C(336) | C(331) | C(332) | 118.0(6) | C(425) | C(426) | C(421) | 117.0(6) |
| C(336) | C(331) | C(33) | 120.2(6) | C(425) | C(426) | W(2) | 72.1(4) |
| C(332) | C(331) | C(33) | 121.8(5) | C(421) | C(426) | W(2) | 68.1(3) |
| C(333) | C(332) | C(331) | 121.1(6) | C(432) | C(431) | C(436) | 117.8(6) |
| C(334) | C(333) | C(332) | 120.2(7) | C(432) | C(431) | C(43) | 123.5(6) |
| C(335) | C(334) | C(333) | 118.8(6) | C(436) | C(431) | C(43) | 118.7(6) |
| C(334) | C(335) | C(336) | 121.1(7) | C(433) | C(432) | C(431) | 121.0(7) |
| C(331) | C(336) | C(335) | 120.7(7) | C(432) | C(433) | C(434) | 120.7(7) |
| C(356) | C(351) | C(352) | 118.2(6) | C(435) | C(434) | C(433) | 119.2(6) |
| C(356) | C(351) | C(35) | 122.8(5) | C(434) | C(435) | C(436) | 121.5(7) |
| C(352) | C(351) | C(35) | 118.9(5) | C(435) | C(436) | C(431) | 119.8(6) |
| C(353) | C(352) | C(351) | 120.5(6) | C(456) | C(451) | C(452) | 118.3(9) |
| C(354) | C(353) | C(352) | 121.1(6) | C(456) | C(451) | C(45) | 121.3(9) |
| C(353) | C(354) | C(355) | 118.7(6) | C(452) | C(451) | C(45) | 119.8(8) |
| C(356) | C(355) | C(354) | 120.8(7) | C(451) | C(452) | C(453) | 122.6(12) |
| C(351) | C(356) | C(355) | 120.7(6) | C(454) | C(453) | C(452) | 118.7(12) |
| C(366) | C(361) | C(362) | 118.5(5) | C(455) | C(454) | C(453) | 121.5(11) |
| C(366) | C(361) | C(36) | 121.1(5) | C(454) | C(455) | C(456) | 119.9(13) |
| C(362) | C(361) | C(36) | 120.4(5) | C(451) | C(456) | C(455) | 117.4(15) |
| C(363) | C(362) | C(361) | 120.9(5) | C(466) | C(461) | C(462) | 118.3(6) |
| C(362) | C(363) | C(364) | 119.9(6) | C(466) | C(461) | C(46) | 117.9(5) |
| C(365) | C(364) | C(363) | 119.6(5) | C(462) | C(461) | C(46) | 123.8(6) |
| C(364) | C(365) | C(366) | 120.3(5) | C(461) | C(462) | C(463) | 119.9(6) |
| C(361) | C(366) | C(365) | 120.8(5) | C(464) | C(463) | C(462) | 120.5(6) |
| C(426) | C(421) | C(42) | 126.0(6) | C(463) | C(464) | C(465) | 120.2(6) |
| C(426) | C(421) | C(422) | 119.1(5) | C(464) | C(465) | C(466) | 119.7(6) |
| C(42) | C(421) | C(422) | 114.2(5) | C(465) | C(466) | C(461) | 121.5(6) |
| C(426) | C(421) | W(2) | 74.0(3) | C(522) | C(521) | C(526) | 117.7(6) |
| C(42) | C(421) | W(2) | 111.8(4) | C(522) | C(521) | C(52) | 122.8(5) |
| C(422) | C(421) | W(2) | 76.8(3) | C(526) | C(521) | C(52) | 119.5(5) |
| C(423) | C(422) | C(421) | 120.5(6) | C(521) | C(522) | C(523) | 120.8(6) |
| C(423) | C(422) | W(2) | 69.7(3) | C(525) | C(523) | C(522) | 119.2(7) |
| C(421) | C(422) | W(2) | 65.1(3) | C(526) | C(524) | C(525) | 119.2(7) |
| C(422) | C(423) | C(424) | 118.6(6) | C(523) | C(525) | C(524) | 121.1(6) |
| C(422) | C(423) | W(2) | 75.0(4) | C(524) | C(526) | C(521) | 122.0(7) |
| C(424) | C(423) | W(2) | 69.3(3) | C(532) | C(531) | C(536) | 119.2(5) |
| C(425) | C(424) | C(423) | 119.1(6) | C(532) | C(531) | C(53) | 120.8(5) |
| C(425) | C(424) | W(2) | 73.1(4) | C(536) | C(531) | C(53) | 119.8(5) |
| C(423) | C(424) | W(2) | 73.1(4) | C(531) | C(532) | C(533) | 121.1(6) |
| C(426) | C(425) | C(424) | 123.1(6) | C(534) | C(533) | C(532) | 119.6(6) |
| C(426) | C(425) | W(2) | 71.4(3) | C(535) | C(534) | C(533) | 119.8(6) |
| C(424) | C(425) | W(2) | 69.6(4) | C(534) | C(535) | C(536) | 120.4(6) |

Bond Angles (cont.)

| Atom 1 | Atom 2 | Atom 3 | Angle | Atom 1 | Atom 2 | Atom 3 | Angle |
|---|---|---|---|---|---|---|---|
| C(535) | C(536) | C(531) | 119.9(6) | C(563) | C(562) | C(561) | 119.8(6) |
| C(552) | C(551) | C(556) | 117.4(5) | C(564) | C(563) | C(562) | 121.1(6) |
| C(552) | C(551) | C(55) | 120.2(5) | C(563) | C(564) | C(565) | 120.3(6) |
| C(556) | C(551) | C(55) | 122.3(5) | C(566) | C(565) | C(564) | 119.0(7) |
| C(553) | C(552) | C(551) | 122.8(6) | C(565) | C(566) | C(561) | 120.9(6) |
| C(552) | C(553) | C(554) | 119.0(6) | C(64) | C(641) | C(642) | 109.3(5) |
| C(555) | C(554) | C(553) | 120.2(6) | C(64) | C(641) | C(644) | 110.6(5) |
| C(554) | C(555) | C(556) | 120.0(6) | C(642) | C(641) | C(644) | 108.9(6) |
| C(551) | C(556) | C(555) | 120.6(6) | C(64) | C(641) | C(643) | 112.2(5) |
| C(562) | C(561) | C(566) | 118.8(5) | C(642) | C(641) | C(643) | 110.0(6) |
| C(562) | C(561) | C(56) | 121.9(5) | C(644) | C(641) | C(643) | 105.8(6) |
| C(566) | C(561) | C(56) | 119.2(5) | | | | |

Numbers in parentheses are estimated standard deviations in the least significant digits.