***Supporting Information***

***Crystal data of N,N-dimethyl-2-benzoylbenzamide 3a***

GEOMETRY TABLES :***N,N*-dimethyl-2-benzoylbenzamide 3a**

FRACTIONAL ATOMIC COORDINATES & U(iso)

| Atom | x/a | y/b | z/c | U(iso) |
|---|---|---|---|---|
| O(1) | 1.06004(5) | 0.04895(4) | 0.33549(7) | 0.0663(3) |
| N(2) | 1.08876(5) | 0.07443(4) | 0.62752(7) | 0.0486(3) |
| O(3) | 0.99540(6) | 0.22831(3) | 0.40108(8) | 0.0651(3) |
| C(4) | 0.81742(5) | 0.14497(3) | 0.40176(8) | 0.0364(2) |
| C(5) | 0.90082(6) | 0.20656(3) | 0.32075(8) | 0.0405(3) |
| C(6) | 0.68413(5) | 0.15204(4) | 0.40143(9) | 0.0419(3) |
| C(7) | 0.87419(5) | 0.08361(3) | 0.49494(8) | 0.0379(2) |
| C(8) | 0.66454(7) | 0.03753(4) | 0.58051(9) | 0.0521(3) |
| C(9) | 0.86575(5) | 0.24113(3) | 0.14446(8) | 0.0411(2) |
| C(10) | 0.78462(6) | 0.20421(4) | 0.02455(9) | 0.0487(3) |
| C(11) | 0.60855(6) | 0.09829(4) | 0.48998(9) | 0.0481(3) |
| C(12) | 0.79782(6) | 0.03001(4) | 0.58378(9) | 0.0478(3) |
| C(13) | 0.91942(7) | 0.31311(4) | 0.1002(1) | 0.0516(3) |
| C(14) | 0.75630(8) | 0.23869(6) | -0.13744(9) | 0.0640(4) |
| C(15) | 1.01726(5) | 0.06928(4) | 0.47988(8) | 0.0426(3) |
| C(16) | 1.22557(7) | 0.05823(6) | 0.6137(1) | 0.0649(4) |
| C(17) | 1.04588(9) | 0.11260(7) | 0.7909(1) | 0.0654(4) |
| C(18) | 0.8082(1) | 0.30982(7) | -0.1798(1) | 0.0758(5) |
| C(19) | 0.8900(1) | 0.34748(5) | -0.0612(1) | 0.0711(5) |
| H(12) | 0.8408(8) | -0.0143(5) | 0.658(1) | 0.026(2) |
| H(13) | 0.9835(9) | 0.3350(5) | 0.194(1) | 0.032(2) |
| H(17A) | 0.959(1) | 0.1208(8) | 0.791(2) | 0.070(4) |
| H(19) | 0.933(1) | 0.3985(6) | -0.088(2) | 0.051(3) |
| H(16A) | 1.250(2) | 0.0272(8) | 0.718(2) | 0.081(4) |
| H(14) | 0.703(1) | 0.2117(6) | -0.222(2) | 0.053(3) |
| H(10) | 0.755(1) | 0.1519(6) | 0.057(1) | 0.040(2) |
| H(11) | 0.516(1) | 0.1032(6) | 0.485(2) | 0.048(3) |
| H(8) | 0.6104(9) | -0.0010(5) | 0.641(1) | 0.034(2) |
| H(16B) | 1.246(1) | 0.0334(7) | 0.502(2) | 0.057(3) |
| H(6) | 0.6452(8) | 0.1937(5) | 0.340(1) | 0.026(2) |
| H(16C) | 1.277(2) | 0.1095(9) | 0.610(2) | 0.106(6) |
| H(18) | 0.784(2) | 0.3441(9) | -0.297(2) | 0.106(6) |
| H(17B) | 1.067(2) | 0.079(1) | 0.876(3) | 0.121(7) |
| H(17C) | 1.104(2) | 0.1649(9) | 0.799(2) | 0.100(6) |

Temperature factor of the form: exp[-2pi^2U], U=U(iso)
or 1/3 SUM(i)SUM(j){U(ij)*astar(i).astar(j).a(i).a(j).cos(ij)}

INTRAMOLECULAR BOND LENGTHS: ***N,N*-dimethyl-2-benzoylbenzamide 3a**

Minimum bond length= 0.70A : Maximum bond length= 1.65A

| | | | |
|---|---|---|---|
| O(1) - C(15) | 1.225(1) | N(2) - C(15) | 1.340(1) |
| N(2) - C(16) | 1.456(1) | N(2) - C(17) | 1.463(2) |
| O(3) - C(5) | 1.215(1) | C(4) - C(5) | 1.500(1) |
| C(4) - C(6) | 1.394(1) | C(4) - C(7) | 1.398(1) |
| C(5) - C(9) | 1.498(1) | C(6) - C(11) | 1.385(1) |
| C(7) - C(12) | 1.389(1) | C(7) - C(15) | 1.515(1) |
| C(8) - C(11) | 1.377(1) | C(8) - C(12) | 1.395(1) |
| C(9) - C(10) | 1.390(1) | C(9) - C(13) | 1.399(1) |
| C(10) - C(14) | 1.387(2) | C(13) - C(19) | 1.384(2) |
| C(14) - C(18) | 1.376(2) | C(18) - C(19) | 1.394(2) |
| C(6) - H(6) | 0.943(9) | C(8) - H(8) | 0.98(1) |
| C(10) - H(10) | 0.98(1) | C(11) - H(11) | 0.97(2) |
| C(12) - H(12) | 1.045(9) | C(13) - H(13) | 1.04(1) |
| C(14) - H(14) | 0.96(2) | C(16) - H(16A) | 0.98(2) |
| C(16) - H(16B) | 0.96(2) | C(16) - H(16C) | 1.03(2) |
| C(17) - H(17A) | 0.92(2) | C(17) - H(17B) | 0.89(2) |
| C(17) - H(17C) | 1.09(2) | C(18) - H(18) | 1.09(2) |
| C(19) - H(19) | 1.01(2) | | |

INTRAMOLECULAR BOND ANGLES: ***N,N*-dimethyl-2-benzoylbenzamide 3a**

Minimum bond length= 0.70A : Maximum bond length= 1.65A

| | | | |
|---|---|---|---|
| C(15) - N(2) - C(16) | 118.2(1) | C(15) - N(2) - C(17) | 123.8(1) |
| C(16) - N(2) - C(17) | 116.4(1) | C(5) - C(4) - C(6) | 121.0(1) |
| C(5) - C(4) - C(7) | 119.5(1) | C(6) - C(4) - C(7) | 119.2(1) |
| O(3) - C(5) - C(4) | 119.1(1) | O(3) - C(5) - C(9) | 121.0(1) |
| C(4) - C(5) - C(9) | 119.9(1) | C(4) - C(6) - C(11) | 120.5(1) |
| C(4) - C(7) - C(12) | 120.0(1) | C(4) - C(7) - C(15) | 120.1(1) |
| C(12) - C(7) - C(15) | 119.4(1) | C(11) - C(8) - C(12) | 120.1(1) |
| C(5) - C(9) - C(10) | 122.7(1) | C(5) - C(9) - C(13) | 117.7(1) |
| C(10) - C(9) - C(13) | 119.6(1) | C(9) - C(10) - C(14) | 120.2(1) |
| C(6) - C(11) - C(8) | 120.2(1) | C(7) - C(12) - C(8) | 120.0(1) |
| C(9) - C(13) - C(19) | 119.9(1) | C(10) - C(14) - C(18) | 120.1(1) |
| O(1) - C(15) - N(2) | 123.4(1) | O(1) - C(15) - C(7) | 118.1(1) |
| N(2) - C(15) - C(7) | 118.3(1) | C(14) - C(18) - C(19) | 120.4(1) |
| C(13) - C(19) - C(18) | 119.9(1) | C(4) - C(6) - H(6) | 119.7(5) |
| C(11) - C(6) - H(6) | 119.8(5) | C(11) - C(8) - H(8) | 119.8(6) |
| C(12) - C(8) - H(8) | 120.1(6) | C(9) - C(10) - H(10) | 116.5(6) |
| C(14) - C(10) - H(10) | 123.1(6) | C(6) - C(11) - H(11) | 119.3(7) |
| C(8) - C(11) - H(11) | 120.4(7) | C(7) - C(12) - H(12) | 119.7(5) |
| C(8) - C(12) - H(12) | 120.2(5) | C(9) - C(13) - H(13) | 114.6(5) |
| C(19) - C(13) - H(13) | 125.5(5) | C(10) - C(14) - H(14) | 119.6(7) |
| C(18) - C(14) - H(14) | 120.3(7) | N(2) - C(16) - H(16A) | 107.3(11) |
| N(2) - C(16) - H(16B) | 111.3(8) | N(2) - C(16) - H(16C) | 110.3(10) |
| H(16A)- C(16) - H(16B) | 113.3(11) | H(16A)- C(16) - H(16C) | 110.7(13) |
| H(16B)- C(16) - H(16C) | 103.9(12) | N(2) - C(17) - H(17A) | 112.0(9) |
| N(2) - C(17) - H(17B) | 103.6(13) | N(2) - C(17) - H(17C) | 104.5(9) |
| H(17A)- C(17) - H(17B) | 109.9(16) | H(17A)- C(17) - H(17C) | 115.1(12) |
| H(17B)- C(17) - H(17C) | 111.1(15) | C(14) - C(18) - H(18) | 125.2(9) |
| C(19) - C(18) - H(18) | 114.1(9) | C(13) - C(19) - H(19) | 116.8(7) |
| C(18) - C(19) - H(19) | 123.3(7) | | |

INTRAMOLECULAR TORSION ANGLES: ***N,N*-dimethyl-2-benzoylbenzamide 3a**

Minimum bond length= 0.70A : Maximum bond length= 1.65A

| | | | |
|---|---|---|---|
| C(16)-N(2)-C(15)-O(1) | 2.7(1) | C(16)-N(2)-C(15)-C(7) | 178.1(1) |
| C(17)-N(2)-C(15)-O(1) | 167.6(2) | C(17)-N(2)-C(15)-C(7) | -17.0(1) |
| C(6)-C(4)-C(5)-O(3) | 135.2(1) | C(6)-C(4)-C(5)-C(9) | -43.9(1) |
| C(5)-C(4)-C(6)-C(11) | -174.4(1) | C(7)-C(4)-C(5)-O(3) | -38.1(1) |
| C(7)-C(4)-C(5)-C(9) | 142.8(1) | C(5)-C(4)-C(7)-C(12) | 174.3(1) |
| C(5)-C(4)-C(7)-C(15) | -13.6(1) | C(7)-C(4)-C(6)-C(11) | -1.0(1) |
| C(6)-C(4)-C(7)-C(12) | 0.9(1) | C(6)-C(4)-C(7)-C(15) | 172.9(1) |
| O(3)-C(5)-C(9)-C(10) | 160.2(1) | O(3)-C(5)-C(9)-C(13) | -18.9(1) |
| C(4)-C(5)-C(9)-C(10) | -20.8(1) | C(4)-C(5)-C(9)-C(13) | 160.2(1) |
| C(4)-C(6)-C(11)-C(8) | 0.5(1) | C(4)-C(7)-C(12)-C(8) | -0.2(1) |
| C(4)-C(7)-C(15)-O(1) | -66.0(1) | C(4)-C(7)-C(15)-N(2) | 118.4(1) |
| C(12)-C(7)-C(15)-O(1) | 106.1(1) | C(12)-C(7)-C(15)-N(2) | -69.5(1) |
| C(15)-C(7)-C(12)-C(8) | -172.3(1) | C(12)-C(8)-C(11)-C(6) | 0.2(1) |
| C(11)-C(8)-C(12)-C(7) | -0.3(1) | C(5)-C(9)-C(10)-C(14) | -179.5(1) |
| C(5)-C(9)-C(13)-C(19) | -180.0(1) | C(13)-C(9)-C(10)-C(14) | -0.4(1) |
| C(10)-C(9)-C(13)-C(19) | 0.9(1) | C(9)-C(10)-C(14)-C(18) | -0.2(1) |
| C(9)-C(13)-C(19)-C(18) | -0.8(1) | C(10)-C(14)-C(18)-C(19) | 0.4(1) |
| C(14)-C(18)-C(19)-C(13) | 0.1(1) | C(15)-N(2)-C(16)-H(16A) | -138.3(10) |
| C(15)-N(2)-C(16)-H(16B) | -13.7(8) | C(15)-N(2)-C(16)-H(16C) | 101.0(11) |
| C(15)-N(2)-C(17)-H(17A) | 15.2(10) | C(15)-N(2)-C(17)-H(17B) | 133.6(13) |
| C(15)-N(2)-C(17)-H(17C) | -110.0(9) | C(16)-N(2)-C(17)-H(17A) | -179.6(10) |
| C(17)-N(2)-C(16)-H(16A) | 55.7(10) | C(17)-N(2)-C(16)-H(16B) | -179.7(8) |
| C(17)-N(2)-C(16)-H(16C) | -65.0(10) | C(16)-N(2)-C(17)-H(17B) | -61.3(13) |
| C(16)-N(2)-C(17)-H(17C) | 55.1(9) | C(5)-C(4)-C(6)-H(6) | 5.8(6) |
| C(7)-C(4)-C(6)-H(6) | 179.2(7) | C(4)-C(6)-C(11)-H(11) | -177.9(8) |
| H(6)-C(6)-C(11)-C(8) | -179.7(7) | H(6)-C(6)-C(11)-H(11) | 1.9(10) |
| C(4)-C(7)-C(12)-H(12) | -177.4(6) | C(15)-C(7)-C(12)-H(12) | 10.5(6) |
| C(11)-C(8)-C(12)-H(12) | 176.9(6) | C(12)-C(8)-C(11)-H(11) | 178.6(8) |
| H(8)-C(8)-C(11)-C(6) | -178.6(7) | H(8)-C(8)-C(11)-H(11) | -0.2(10) |
| H(8)-C(8)-C(12)-C(7) | 178.5(7) | H(8)-C(8)-C(12)-H(12) | -4.4(9) |
| C(5)-C(9)-C(10)-H(10) | -4.0(7) | C(5)-C(9)-C(13)-H(13) | 2.8(6) |
| C(10)-C(9)-C(13)-H(13) | -176.3(6) | C(13)-C(9)-C(10)-H(10) | 175.0(7) |
| C(9)-C(10)-C(14)-H(14) | 177.5(8) | H(10)-C(10)-C(14)-C(18) | -175.3(8) |
| H(10)-C(10)-C(14)-H(14) | 2.3(11) | C(9)-C(13)-C(19)-H(19) | -178.2(8) |
| H(13)-C(13)-C(19)-C(18) | 176.1(7) | H(13)-C(13)-C(19)-H(19) | -1.3(10) |
| C(10)-C(14)-C(18)-H(18) | -173.3(11) | H(14)-C(14)-C(18)-C(19) | -177.3(8) |
| H(14)-C(14)-C(18)-H(18) | 9.1(13) | C(14)-C(18)-C(19)-H(19) | 177.4(8) |
| H(18)-C(18)-C(19)-C(13) | 174.4(10) | H(18)-C(18)-C(19)-H(19) | -8.3(13) |

***Crystal Data of N-Methyl-2-benzoylbenzanilide 3b***

GEOMETRY TABLES :***N*-Methyl-2-benzoylbenzanilide 3b**

FRACTIONAL ATOMIC COORDINATES & U(iso)

| Atom | x/a | y/b | z/c | U(iso) |
|---|---|---|---|---|
| O(1) | 0.0435(2) | 0.1342(1) | 0.8329(3) | 0.068(1) |
| O(2) | 0.1775(2) | 0.1767(1) | 1.1415(3) | 0.061(1) |
| N(3) | 0.2674(2) | 0.2405(1) | 0.9407(3) | 0.050(1) |
| C(4) | 0.2014(3) | 0.0560(2) | 0.8814(4) | 0.045(2) |
| C(5) | 0.2343(3) | 0.1782(2) | 1.0137(4) | 0.050(2) |
| C(6) | 0.3183(3) | 0.2452(2) | 0.7785(4) | 0.047(2) |
| C(7) | 0.3968(3) | 0.0948(2) | 0.9522(5) | 0.058(2) |
| C(8) | 0.2784(3) | 0.1096(2) | 0.9391(4) | 0.045(2) |
| C(9) | 0.4237(3) | 0.2802(2) | 0.7597(5) | 0.053(2) |
| C(10) | 0.0749(3) | 0.0728(2) | 0.8595(4) | 0.051(2) |
| C(11) | -0.0155(3) | 0.0155(2) | 0.8729(4) | 0.054(2) |
| C(12) | 0.2485(4) | -0.0112(2) | 0.8351(4) | 0.061(2) |
| C(13) | 0.2608(3) | 0.2163(2) | 0.6447(4) | 0.055(2) |
| C(14) | 0.3091(3) | 0.2234(2) | 0.4888(4) | 0.066(2) |
| C(15) | 0.4694(3) | 0.2875(2) | 0.6040(5) | 0.066(2) |
| C(16) | -0.1190(3) | 0.0249(2) | 0.7857(5) | 0.067(2) |
| C(17) | 0.4403(3) | 0.0279(2) | 0.9064(5) | 0.069(2) |
| C(18) | -0.0016(4) | -0.0448(2) | 0.9721(5) | 0.071(2) |
| C(19) | 0.4153(3) | 0.2593(2) | 0.4672(5) | 0.064(2) |
| C(20) | 0.3673(3) | -0.0235(2) | 0.8455(6) | 0.072(2) |
| C(21) | 0.2383(4) | 0.3083(2) | 1.0223(5) | 0.077(2) |
| C(22) | -0.1961(4) | -0.0841(3) | 0.8974(7) | 0.097(3) |
| C(23) | -0.0948(4) | -0.0943(2) | 0.9871(6) | 0.088(3) |
| C(24) | -0.2078(3) | -0.0249(2) | 0.7959(6) | 0.083(3) |
| H(7) | 0.449(4) | 0.131(2) | 0.994(5) | 0.05(5) |
| H(9) | 0.465(4) | 0.299(2) | 0.853(5) | 0.05(5) |
| H(12) | 0.19703 | -0.04842 | 0.79681 | 0.05000 |
| H(13) | 0.18787 | 0.19141 | 0.65803 | 0.05000 |
| H(14) | 0.26860 | 0.20334 | 0.39589 | 0.05000 |
| H(15) | 0.54170 | 0.31323 | 0.59317 | 0.05000 |
| H(16) | -0.12800 | 0.06663 | 0.71703 | 0.05000 |
| H(17) | 0.52235 | 0.01878 | 0.91727 | 0.05000 |
| H(18) | 0.06960 | -0.05426 | 1.03083 | 0.05000 |
| H(19) | 0.45093 | 0.26458 | 0.36068 | 0.05000 |
| H(20) | 0.39912 | -0.06880 | 0.81033 | 0.05000 |
| H(21A) | 0.20532 | 0.29848 | 1.12880 | 0.05000 |
| H(21B) | 0.18282 | 0.33438 | 0.95670 | 0.05000 |
| H(21C) | 0.30792 | 0.33658 | 1.03510 | 0.05000 |
| H(22) | -0.25854 | -0.11853 | 0.90348 | 0.05000 |
| H(23) | -0.08720 | -0.13426 | 1.06134 | 0.05000 |
| H(24) | -0.27799 | -0.01747 | 0.73340 | 0.05000 |

Temperature factor of the form: exp[-2pi^2U], U=U(iso)
or 1/3 SUM(i)SUM(j){U(ij)*astar(i).astar(j).a(i).a(j).cos(ij)}

INTRAMOLECULAR BOND LENGTHS :***N*-Methyl-2-benzoylbenzanilide 3b**

Minimum bond length= 0.70A : Maximum bond length= 1.70A

| | | | |
|---|---|---|---|
| O(1) - C(10) | 1.215(4) | O(2) - C(5) | 1.224(4) |
| N(3) - C(5) | 1.354(5) | N(3) - C(6) | 1.441(4) |
| N(3) - C(21) | 1.460(5) | C(4) - C(8) | 1.409(5) |
| C(4) - C(10) | 1.493(5) | C(4) - C(12) | 1.411(5) |
| C(5) - C(8) | 1.499(5) | C(6) - C(9) | 1.380(5) |
| C(6) - C(13) | 1.377(5) | C(7) - C(8) | 1.387(5) |
| C(7) - C(17) | 1.389(6) | C(9) - C(15) | 1.373(6) |
| C(10) - C(11) | 1.488(5) | C(11) - C(16) | 1.391(6) |
| C(11) - C(18) | 1.388(6) | C(12) - C(20) | 1.382(6) |
| C(13) - C(14) | 1.386(5) | C(14) - C(19) | 1.398(6) |
| C(15) - C(19) | 1.374(6) | C(16) - C(24) | 1.377(6) |
| C(17) - C(20) | 1.361(6) | C(18) - C(23) | 1.414(7) |
| C(22) - C(23) | 1.383(7) | C(22) - C(24) | 1.381(7) |
| C(7) - H(7) | 0.96(5) | C(9) - H(9) | 0.96(5) |
| C(12) - H(12) | 0.960(4) | C(13) - H(13) | 0.961(4) |
| C(14) - H(14) | 0.960(4) | C(15) - H(15) | 0.960(4) |
| C(16) - H(16) | 0.959(5) | C(17) - H(17) | 0.959(4) |
| C(18) - H(18) | 0.960(5) | C(19) - H(19) | 0.960(4) |
| C(20) - H(20) | 0.960(4) | C(21) - H(21A) | 0.960(5) |
| C(21) - H(21B) | 0.960(5) | C(21) - H(21C) | 0.960(5) |
| C(22) - H(22) | 0.960(5) | C(23) - H(23) | 0.960(5) |
| C(24) - H(24) | 0.960(5) | | |

INTRAMOLECULAR BOND ANGLES :***N*-Methyl-2-benzoylbenzanilide 3b**

Minimum bond length= 0.70A : Maximum bond length= 1.70A

| | | | |
|---|---|---|---|
| C(5) - N(3) - C(6) | 124.3(3) | C(5) - N(3) - C(21) | 118.3(3) |
| C(6) - N(3) - C(21) | 117.0(3) | C(8) - C(4) - C(10) | 120.0(3) |
| C(8) - C(4) - C(12) | 118.2(3) | C(10) - C(4) - C(12) | 121.6(3) |
| O(2) - C(5) - N(3) | 122.6(3) | O(2) - C(5) - C(8) | 120.1(3) |
| N(3) - C(5) - C(8) | 117.2(3) | N(3) - C(6) - C(9) | 118.9(3) |
| N(3) - C(6) - C(13) | 120.1(3) | C(9) - C(6) - C(13) | 121.0(3) |
| C(8) - C(7) - C(17) | 120.5(4) | C(4) - C(8) - C(5) | 121.6(3) |
| C(4) - C(8) - C(7) | 119.8(3) | C(5) - C(8) - C(7) | 117.8(3) |
| C(6) - C(9) - C(15) | 118.8(4) | O(1) - C(10) - C(4) | 120.3(3) |
| O(1) - C(10) - C(11) | 118.5(3) | C(4) - C(10) - C(11) | 121.1(3) |
| C(10) - C(11) - C(16) | 117.8(4) | C(10) - C(11) - C(18) | 122.6(4) |
| C(16) - C(11) - C(18) | 119.5(4) | C(4) - C(12) - C(20) | 120.4(4) |
| C(6) - C(13) - C(14) | 119.3(4) | C(13) - C(14) - C(19) | 120.5(4) |
| C(9) - C(15) - C(19) | 122.1(4) | C(11) - C(16) - C(24) | 121.0(4) |
| C(7) - C(17) - C(20) | 120.3(4) | C(11) - C(18) - C(23) | 119.2(4) |
| C(14) - C(19) - C(15) | 118.2(4) | C(12) - C(20) - C(17) | 120.7(4) |
| C(23) - C(22) - C(24) | 120.2(5) | C(18) - C(23) - C(22) | 120.0(5) |
| C(16) - C(24) - C(22) | 120.0(4) | C(8) - C(7) - H(7) | 119.7(28) |
| C(17) - C(7) - H(7) | 119.8(28) | C(6) - C(9) - H(9) | 121.1(28) |
| C(15) - C(9) - H(9) | 120.1(28) | C(4) - C(12) - H(12) | 119.2(4) |
| C(20) - C(12) - H(12) | 120.4(4) | C(6) - C(13) - H(13) | 121.0(4) |
| C(14) - C(13) - H(13) | 119.7(4) | C(13) - C(14) - H(14) | 119.0(4) |
| C(19) - C(14) - H(14) | 120.5(4) | C(9) - C(15) - H(15) | 117.5(4) |
| C(19) - C(15) - H(15) | 120.3(4) | C(11) - C(16) - H(16) | 119.2(4) |
| C(24) - C(16) - H(16) | 119.8(4) | C(7) - C(17) - H(17) | 119.0(4) |
| C(20) - C(17) - H(17) | 120.8(5) | C(11) - C(18) - H(18) | 122.2(4) |
| C(23) - C(18) - H(18) | 118.6(4) | C(14) - C(19) - H(19) | 122.1(4) |
| C(15) - C(19) - H(19) | 119.7(4) | C(12) - C(20) - H(20) | 120.0(4) |
| C(17) - C(20) - H(20) | 119.3(4) | N(3) - C(21) - H(21A) | 109.5(4) |
| N(3) - C(21) - H(21B) | 109.6(4) | N(3) - C(21) - H(21C) | 109.4(4) |
| H(21A)- C(21) - H(21B) | 109.5(5) | H(21A)- C(21) - H(21C) | 109.5(4) |
| H(21B)- C(21) - H(21C) | 109.5(4) | C(23) - C(22) - H(22) | 120.5(5) |
| C(24) - C(22) - H(22) | 119.3(5) | C(18) - C(23) - H(23) | 119.3(5) |
| C(22) - C(23) - H(23) | 120.7(5) | C(16) - C(24) - H(24) | 119.4(5) |
| C(22) - C(24) - H(24) | 120.6(5) | | |

INTRAMOLECULAR TORSION ANGLES :**N-Methyl-2-benzoylbenzanilide 3b**

Minimum bond length= 0.70A : Maximum bond length= 1.70A

| | | | |
|---|---|---|---|
| C(6)-N(3)-C(5)-O(2) | -170.0(5) | C(6)-N(3)-C(5)-C(8) | 14.8(3) |
| C(5)-N(3)-C(6)-C(9) | -125.8(5) | C(5)-N(3)-C(6)-C(13) | 55.5(4) |
| C(21)-N(3)-C(5)-O(2) | 2.9(4) | C(21)-N(3)-C(5)-C(8) | -172.3(5) |
| C(21)-N(3)-C(6)-C(9) | 61.2(4) | C(21)-N(3)-C(6)-C(13) | -117.4(4) |
| C(8)-C(4)-C(10)-O(1) | 26.4(4) | C(10)-C(4)-C(8)-C(5) | 13.3(3) |
| C(10)-C(4)-C(8)-C(7) | -177.1(5) | C(8)-C(4)-C(10)-C(11) | -152.4(5) |
| C(12)-C(4)-C(8)-C(5) | -170.9(5) | C(12)-C(4)-C(8)-C(7) | -1.3(4) |
| C(8)-C(4)-C(12)-C(20) | -0.4(4) | C(12)-C(4)-C(10)-O(1) | -149.3(5) |
| C(12)-C(4)-C(10)-C(11) | 31.9(4) | C(10)-C(4)-C(12)-C(20) | 175.3(6) |
| O(2)-C(5)-C(8)-C(4) | 63.4(4) | O(2)-C(5)-C(8)-C(7) | -106.4(4) |
| N(3)-C(5)-C(8)-C(4) | -121.3(4) | N(3)-C(5)-C(8)-C(7) | 68.9(4) |
| N(3)-C(6)-C(9)-C(15) | -177.0(5) | N(3)-C(6)-C(13)-C(14) | 177.8(5) |
| C(9)-C(6)-C(13)-C(14) | -0.8(4) | C(13)-C(6)-C(9)-C(15) | 1.6(4) |
| C(17)-C(7)-C(8)-C(4) | 1.1(4) | C(17)-C(7)-C(8)-C(5) | 171.0(5) |
| C(8)-C(7)-C(17)-C(20) | 1.0(4) | C(6)-C(9)-C(15)-C(19) | -2.0(4) |
| O(1)-C(10)-C(11)-C(16) | 28.5(4) | O(1)-C(10)-C(11)-C(18) | -149.3(6) |
| C(4)-C(10)-C(11)-C(16) | -152.7(5) | C(4)-C(10)-C(11)-C(18) | 29.5(4) |
| C(10)-C(11)-C(16)-C(24) | -178.2(6) | C(10)-C(11)-C(18)-C(23) | 175.6(6) |
| C(16)-C(11)-C(18)-C(23) | -2.2(4) | C(18)-C(11)-C(16)-C(24) | -0.3(4) |
| C(4)-C(12)-C(20)-C(17) | 2.5(4) | C(6)-C(13)-C(14)-C(19) | 0.2(4) |
| C(13)-C(14)-C(19)-C(15) | -0.6(4) | C(9)-C(15)-C(19)-C(14) | 1.5(4) |
| C(11)-C(16)-C(24)-C(22) | 1.9(5) | C(7)-C(17)-C(20)-C(12) | -2.9(4) |
| C(11)-C(18)-C(23)-C(22) | 3.1(5) | C(23)-C(22)-C(24)-C(16) | -1.0(5) |
| C(24)-C(22)-C(23)-C(18) | -1.5(5) | C(5)-N(3)-C(21)-H(21A) | 6.7(4) |
| C(5)-N(3)-C(21)-H(21B) | -113.4(5) | C(5)-N(3)-C(21)-H(21C) | 126.6(5) |
| C(6)-N(3)-C(21)-H(21A) | -179.9(5) | C(6)-N(3)-C(21)-H(21B) | 60.0(4) |
| C(6)-N(3)-C(21)-H(21C) | -60.0(4) | C(8)-C(4)-C(12)-H(12) | 179.3(6) |
| C(10)-C(4)-C(12)-H(12) | -5.0(4) | N(3)-C(6)-C(9)-H(9) | 3.1(32) |
| N(3)-C(6)-C(13)-H(13) | -2.2(3) | C(13)-C(6)-C(9)-H(9) | -178.3(32) |
| C(9)-C(6)-C(13)-H(13) | 179.2(6) | C(8)-C(7)-C(17)-H(17) | -179.6(6) |
| H(7)-C(7)-C(8)-C(4) | -178.7(31) | H(7)-C(7)-C(8)-C(5) | -8.8(31) |
| H(7)-C(7)-C(17)-C(20) | -179.2(32) | H(7)-C(7)-C(17)-H(17) | 0.2(31) |
| C(6)-C(9)-C(15)-H(15) | 178.3(6) | H(9)-C(9)-C(15)-C(19) | 178.0(32) |
| H(9)-C(9)-C(15)-H(15) | -1.7(31) | C(10)-C(11)-C(16)-H(16) | 2.3(4) |
| C(10)-C(11)-C(18)-H(18) | -4.8(4) | C(18)-C(11)-C(16)-H(16) | -179.8(6) |
| C(16)-C(11)-C(18)-H(18) | 177.5(7) | C(4)-C(12)-C(20)-H(20) | -177.9(7) |
| H(12)-C(12)-C(20)-C(17) | -177.2(7) | H(12)-C(12)-C(20)-H(20) | 2.4(4) |
| C(6)-C(13)-C(14)-H(14) | -179.9(6) | H(13)-C(13)-C(14)-C(19) | -179.8(6) |
| H(13)-C(13)-C(14)-H(14) | 0.1(4) | C(13)-C(14)-C(19)-H(19) | 179.5(7) |
| H(14)-C(14)-C(19)-C(15) | 179.5(6) | H(14)-C(14)-C(19)-H(19) | -0.4(4) |
| C(9)-C(15)-C(19)-H(19) | -178.6(7) | H(15)-C(15)-C(19)-C(14) | -178.8(6) |
| H(15)-C(15)-C(19)-H(19) | 1.1(4) | C(11)-C(16)-C(24)-H(24) | -179.2(7) |
| H(16)-C(16)-C(24)-C(22) | -178.6(7) | H(16)-C(16)-C(24)-H(24) | 0.3(5) |
| C(7)-C(17)-C(20)-H(20) | 177.6(7) | H(17)-C(17)-C(20)-C(12) | 177.8(7) |
| H(17)-C(17)-C(20)-H(20) | -1.8(4) | C(11)-C(18)-C(23)-H(23) | -175.9(7) |
| H(18)-C(18)-C(23)-C(22) | -176.6(7) | H(18)-C(18)-C(23)-H(23) | 4.4(5) |
| C(24)-C(22)-C(23)-H(23) | 177.5(8) | C(23)-C(22)-C(24)-H(24) | -179.9(8) |
| H(22)-C(22)-C(23)-C(18) | 177.5(8) | H(22)-C(22)-C(23)-H(23) | -3.5(5) |
| H(22)-C(22)-C(24)-C(16) | -180.0(8) | H(22)-C(22)-C(24)-H(24) | 1.1(5) |

***Crystal Data of 4,N-Dimethyl-2-benzoylbenzanilide 3c***

GEOMETRY TABLES :***4,N-Dimethyl-2-benzoylbenzanilide 3c***

FRACTIONAL ATOMIC COORDINATES & U(iso)

| Atom | x/a | y/b | z/c | U(iso) |
|---|---|---|---|---|
| O(1) | 0.1341(3) | 0.1790(7) | 0.0275(4) | 0.102(4) |
| O(2) | 0.1961(3) | -0.1295(7) | 0.1330(5) | 0.108(4) |
| N(3) | 0.2525(4) | 0.0743(6) | 0.2265(4) | 0.077(4) |
| C(4) | 0.1275(4) | 0.0417(8) | 0.2497(6) | 0.073(5) |
| C(5) | 0.1938(5) | -0.0068(9) | 0.1943(6) | 0.081(5) |
| C(6) | 0.2499(4) | 0.2324(8) | 0.2841(5) | 0.067(4) |
| C(7) | 0.0778(5) | 0.1273(9) | 0.0633(7) | 0.080(5) |
| C(8) | 0.0710(5) | 0.0929(8) | 0.1860(7) | 0.073(5) |
| C(9) | 0.2221(4) | 0.3692(8) | 0.2300(6) | 0.080(5) |
| C(10) | 0.2517(6) | 0.536(1) | 0.3884(7) | 0.101(6) |
| C(11) | 0.2776(4) | 0.246(1) | 0.3873(6) | 0.088(5) |
| C(12) | 0.0188(5) | 0.097(1) | -0.0179(7) | 0.082(5) |
| C(13) | -0.0335(5) | -0.010(1) | 0.0027(8) | 0.093(6) |
| C(14) | 0.0633(6) | 0.032(1) | 0.4143(8) | 0.100(7) |
| C(15) | 0.1221(6) | 0.017(1) | 0.3610(6) | 0.095(6) |
| C(16) | 0.0047(5) | 0.0918(9) | 0.3633(8) | 0.094(6) |
| C(17) | 0.0090(5) | 0.120(1) | 0.2433(9) | 0.101(6) |
| C(18) | 0.2783(5) | 0.399(1) | 0.4415(7) | 0.102(5) |
| C(19) | 0.0227(5) | 0.176(1) | -0.1206(9) | 0.098(6) |
| C(20) | 0.2232(5) | 0.5214(9) | 0.2811(7) | 0.094(5) |
| C(21) | -0.0623(6) | 0.111(2) | 0.423(1) | 0.126(8) |
| C(22) | -0.0872(7) | -0.034(2) | -0.076(2) | 0.137(9) |
| C(23) | -0.0826(8) | 0.051(2) | -0.177(1) | 0.14(1) |
| C(24) | 0.3211(7) | 0.014(1) | 0.190(1) | 0.128(8) |
| C(25) | -0.0269(7) | 0.157(2) | -0.197(1) | 0.123(9) |
| H(9) | 0.194(3) | 0.347(6) | 0.156(5) | 0.02(1) |
| H(10) | 0.246(5) | 0.66(1) | 0.424(6) | 0.07(2) |
| H(20) | 0.184(5) | 0.62(1) | 0.258(8) | 0.11(3) |
| H(11) | 0.297(6) | 0.15(1) | 0.42(1) | 0.08(3) |
| H(18) | 0.298(4) | 0.409(9) | 0.515(6) | 0.15(5) |
| H(24A) | 0.363(5) | 0.07(1) | 0.213(9) | 0.21(9) |
| H(24B) | 0.32028 | 0.01496 | 0.10974 | 0.25(9) |
| H(24C) | 0.32538 | -0.09954 | 0.21504 | 0.24(9) |
| H(21A) | -0.10300 | 0.15424 | 0.38546 | 0.24(9) |
| H(21B) | -0.05370 | 0.18244 | 0.48536 | 0.9(4) |
| H(21C) | -0.07490 | 0.00204 | 0.44926 | 1.0(9) |
| H(17) | -0.03192 | 0.15753 | 0.20344 | 0.050(9) |
| H(15) | 0.16394 | -0.01213 | 0.40136 | 0.12(4) |
| H(14) | 0.06061 | -0.00188 | 0.49107 | 0.11(4) |
| H(25) | -0.02509 | 0.21688 | -0.26663 | 0.10(4) |
| H(23) | -0.11890 | 0.03624 | -0.23143 | 0.10(3) |
| H(22) | -0.12593 | -0.10658 | -0.06037 | 0.05(2) |
| H(13) | -0.03434 | -0.06994 | 0.07195 | 0.05(2) |
| H(19) | 0.06211 | 0.24641 | -0.13635 | 0.04(2) |

Temperature factor of the form: exp[-2pi^2U], U=U(iso)
or 1/3 SUM(i)SUM(j){U(ij)*astar(i).astar(j).a(i).a(j).cos(ij)}

INTRAMOLECULAR BOND LENGTHS: ***4,N*-Dimethyl-2-benzoylbenzanilide 3c**

Minimum bond length= 0.70A : Maximum bond length= 1.70A

| | | | |
|---|---|---|---|
| O(1) - C(7) | 1.23(2) | O(2) - C(5) | 1.229(9) |
| N(3) - C(5) | 1.35(2) | N(3) - C(6) | 1.444(9) |
| N(3) - C(24) | 1.47(2) | C(4) - C(5) | 1.49(2) |
| C(4) - C(8) | 1.38(2) | C(4) - C(15) | 1.35(2) |
| C(6) - C(9) | 1.38(1) | C(6) - C(11) | 1.35(1) |
| C(7) - C(8) | 1.50(2) | C(7) - C(12) | 1.50(2) |
| C(8) - C(17) | 1.39(2) | C(9) - C(20) | 1.37(2) |
| C(10) - C(18) | 1.37(2) | C(10) - C(20) | 1.40(2) |
| C(11) - C(18) | 1.39(2) | C(12) - C(13) | 1.34(2) |
| C(12) - C(19) | 1.39(2) | C(13) - C(22) | 1.41(2) |
| C(14) - C(15) | 1.30(2) | C(14) - C(16) | 1.36(2) |
| C(16) - C(17) | 1.46(2) | C(16) - C(21) | 1.48(2) |
| C(19) - C(25) | 1.33(2) | C(22) - C(23) | 1.39(3) |
| C(23) - C(25) | 1.38(3) | C(9) - H(9) | 1.05(7) |
| C(10) - H(10) | 1.12(8) | C(11) - H(11) | 0.96(12) |
| C(13) - H(13) | 0.96(1) | C(14) - H(14) | 0.96(1) |
| C(15) - H(15) | 0.96(1) | C(17) - H(17) | 0.96(1) |
| C(18) - H(18) | 0.96(8) | C(19) - H(19) | 0.960(9) |
| C(20) - H(20) | 1.12(10) | C(21) - H(21A) | 0.96(2) |
| C(21) - H(21B) | 0.96(2) | C(21) - H(21C) | 0.96(2) |
| C(22) - H(22) | 0.96(2) | C(23) - H(23) | 0.96(2) |
| C(24) - H(24A) | 0.96(11) | C(24) - H(24B) | 0.96(2) |
| C(24) - H(24C) | 0.96(2) | C(25) - H(25) | 0.96(2) |

INTRAMOLECULAR BOND ANGLES: ***4,N*-Dimethyl-2-benzoylbenzanilide 3c**

Minimum bond length= 0.70A : Maximum bond length= 1.70A

| | | | |
|---|---|---|---|
| C(5) - N(3) - C(6) | 121.9(7) | C(5) - N(3) - C(24) | 119.7(7) |
| C(6) - N(3) - C(24) | 117.9(8) | C(5) - C(4) - C(8) | 119.8(7) |
| C(5) - C(4) - C(15) | 118.2(8) | C(8) - C(4) - C(15) | 121.6(9) |
| O(2) - C(5) - N(3) | 121.6(8) | O(2) - C(5) - C(4) | 120.7(8) |
| N(3) - C(5) - C(4) | 117.1(7) | N(3) - C(6) - C(9) | 119.2(6) |
| N(3) - C(6) - C(11) | 119.6(7) | C(9) - C(6) - C(11) | 121.1(7) |
| O(1) - C(7) - C(8) | 118.9(8) | O(1) - C(7) - C(12) | 118.7(8) |
| C(8) - C(7) - C(12) | 122.4(8) | C(4) - C(8) - C(7) | 121.6(8) |
| C(4) - C(8) - C(17) | 116.0(9) | C(7) - C(8) - C(17) | 122.3(9) |
| C(6) - C(9) - C(20) | 119.6(8) | C(18) - C(10) - C(20) | 120.3(8) |
| C(6) - C(11) - C(18) | 120.2(8) | C(7) - C(12) - C(13) | 122.6(8) |
| C(7) - C(12) - C(19) | 117.3(8) | C(13) - C(12) - C(19) | 120.0(9) |
| C(12) - C(13) - C(22) | 120.4(10) | C(15) - C(14) - C(16) | 121.5(10) |
| C(4) - C(15) - C(14) | 122.8(10) | C(14) - C(16) - C(17) | 116.6(9) |
| C(14) - C(16) - C(21) | 122.3(10) | C(17) - C(16) - C(21) | 120.8(10) |
| C(8) - C(17) - C(16) | 121.1(9) | C(10) - C(18) - C(11) | 119.3(8) |
| C(12) - C(19) - C(25) | 121.5(10) | C(9) - C(20) - C(10) | 119.4(8) |
| C(13) - C(22) - C(23) | 117.7(12) | C(22) - C(23) - C(25) | 120.8(14) |
| C(19) - C(25) - C(23) | 119.5(13) | C(6) - C(9) - H(9) | 117.1(29) |
| C(20) - C(9) - H(9) | 122.6(29) | C(18) - C(10) - H(10) | 126.5(41) |
| C(20) - C(10) - H(10) | 113.0(41) | C(6) - C(11) - H(11) | 119.9(72) |
| C(18) - C(11) - H(11) | 119.9(72) | C(12) - C(13) - H(13) | 119.8(9) |
| C(22) - C(13) - H(13) | 119.8(11) | C(15) - C(14) - H(14) | 119.8(11) |
| C(16) - C(14) - H(14) | 118.7(11) | C(4) - C(15) - H(15) | 117.7(10) |
| C(14) - C(15) - H(15) | 119.5(9) | C(8) - C(17) - H(17) | 119.7(11) |
| C(16) - C(17) - H(17) | 119.3(10) | C(10) - C(18) - H(18) | 120.3(45) |
| C(11) - C(18) - H(18) | 120.4(45) | C(12) - C(19) - H(19) | 119.2(10) |
| C(25) - C(19) - H(19) | 119.3(11) | C(9) - C(20) - H(20) | 119.9(50) |
| C(10) - C(20) - H(20) | 115.7(50) | C(16) - C(21) - H(21A) | 121.1(13) |
| C(16) - C(21) - H(21B) | 107.1(10) | C(16) - C(21) - H(21C) | 106.7(11) |
| H(21A)- C(21) - H(21B) | 106.3(12) | H(21A)- C(21) - H(21C) | 106.3(11) |
| H(21B)- C(21) - H(21C) | 109.0(13) | C(13) - C(22) - H(22) | 120.7(16) |
| C(23) - C(22) - H(22) | 121.6(16) | C(22) - C(23) - H(23) | 118.8(15) |
| C(25) - C(23) - H(23) | 120.4(16) | N(3) - C(24) - H(24A) | 120.1(65) |
| N(3) - C(24) - H(24B) | 106.7(11) | N(3) - C(24) - H(24C) | 107.1(11) |
| H(24A)- C(24) - H(24B) | 106.8(64) | H(24A)- C(24) - H(24C) | 106.8(65) |
| H(24B)- C(24) - H(24C) | 109.0(13) | C(19) - C(25) - H(25) | 120.9(13) |
| C(23) - C(25) - H(25) | 119.6(14) | | |

INTRAMOLECULAR TORSION ANGLES: ***4,N*-Dimethyl-2-benzoylbenzanilide 3c**

Minimum bond length= 0.70A : Maximum bond length= 1.70A

| | | | |
|---|---|---|---|
| C(6)-N(3)-C(5)-O(2) | 170.4(12) | C(6)-N(3)-C(5)-C(4) | -18.9(7) |
| C(5)-N(3)-C(6)-C(9) | -64.0(8) | C(5)-N(3)-C(6)-C(11) | 119.3(10) |
| C(24)-N(3)-C(5)-O(2) | -1.2(9) | C(24)-N(3)-C(5)-C(4) | 169.5(12) |
| C(24)-N(3)-C(6)-C(9) | 107.8(10) | C(24)-N(3)-C(6)-C(11) | -69.0(10) |
| C(8)-C(4)-C(5)-O(2) | -65.1(9) | C(8)-C(4)-C(5)-N(3) | 124.1(11) |
| C(5)-C(4)-C(8)-C(7) | -9.8(8) | C(5)-C(4)-C(8)-C(17) | 173.9(12) |
| C(15)-C(4)-C(5)-O(2) | 108.0(11) | C(15)-C(4)-C(5)-N(3) | -62.8(9) |
| C(5)-C(4)-C(15)-C(14) | -169.4(14) | C(15)-C(4)-C(8)-C(7) | 177.4(13) |
| C(8)-C(4)-C(15)-C(14) | 3.5(9) | C(15)-C(4)-C(8)-C(17) | 1.1(9) |
| N(3)-C(6)-C(9)-C(20) | -176.0(11) | N(3)-C(6)-C(11)-C(18) | 177.0(11) |
| C(9)-C(6)-C(11)-C(18) | 0.3(8) | C(11)-C(6)-C(9)-C(20) | 0.7(8) |
| O(1)-C(7)-C(8)-C(4) | -30.6(8) | O(1)-C(7)-C(8)-C(17) | 145.4(12) |
| O(1)-C(7)-C(12)-C(13) | 155.7(13) | O(1)-C(7)-C(12)-C(19) | -19.6(9) |
| C(12)-C(7)-C(8)-C(4) | 148.0(12) | C(8)-C(7)-C(12)-C(13) | -22.9(9) |
| C(12)-C(7)-C(8)-C(17) | -35.9(9) | C(8)-C(7)-C(12)-C(19) | 161.8(12) |
| C(4)-C(8)-C(17)-C(16) | -1.3(9) | C(7)-C(8)-C(17)-C(16) | -177.6(14) |
| C(6)-C(9)-C(20)-C(10) | -0.9(8) | C(18)-C(10)-C(20)-C(9) | 0.2(9) |
| C(20)-C(10)-C(18)-C(11) | 0.8(9) | C(6)-C(11)-C(18)-C(10) | -1.0(9) |
| C(7)-C(12)-C(13)-C(22) | -179.5(15) | C(7)-C(12)-C(19)-C(25) | 180.0(15) |
| C(19)-C(12)-C(13)-C(22) | -4.4(11) | C(13)-C(12)-C(19)-C(25) | 4.5(11) |
| C(12)-C(13)-C(22)-C(23) | 2.2(12) | C(16)-C(14)-C(15)-C(4) | -7.8(10) |
| C(15)-C(14)-C(16)-C(17) | 7.1(10) | C(15)-C(14)-C(16)-C(21) | -179.4(16) |
| C(14)-C(16)-C(17)-C(8) | -2.6(9) | C(21)-C(16)-C(17)-C(8) | -176.2(15) |
| C(12)-C(19)-C(25)-C(23) | -2.5(12) | C(13)-C(22)-C(23)-C(25) | -0.2(13) |
| C(22)-C(23)-C(25)-C(19) | 0.3(14) | C(5)-N(3)-C(24)-H(24A) | -179.7(75) |
| C(5)-N(3)-C(24)-H(24B) | 58.8(11) | C(5)-N(3)-C(24)-H(24C) | -57.8(11) |
| C(6)-N(3)-C(24)-H(24A) | 8.3(74) | C(6)-N(3)-C(24)-H(24B) | -113.2(13) |
| C(6)-N(3)-C(24)-H(24C) | 130.2(13) | C(5)-C(4)-C(15)-H(15) | 10.7(8) |
| C(8)-C(4)-C(15)-H(15) | -176.3(14) | N(3)-C(6)-C(9)-H(9) | 13.3(36) |
| N(3)-C(6)-C(11)-H(11) | -3.3(82) | C(11)-C(6)-C(9)-H(9) | -170.0(37) |
| C(9)-C(6)-C(11)-H(11) | -180.0(83) | C(4)-C(8)-C(17)-H(17) | 179.1(14) |
| C(7)-C(8)-C(17)-H(17) | 2.8(9) | C(6)-C(9)-C(20)-H(20) | -154.8(58) |
| H(9)-C(9)-C(20)-C(10) | 169.2(40) | H(9)-C(9)-C(20)-H(20) | 15.3(68) |
| C(18)-C(10)-C(20)-H(20) | 155.1(56) | C(20)-C(10)-C(18)-H(18) | 179.6(53) |
| H(10)-C(10)-C(18)-C(11) | 175.8(55) | H(10)-C(10)-C(18)-H(18) | -5.3(74) |
| H(10)-C(10)-C(20)-C(9) | -175.5(48) | H(10)-C(10)-C(20)-H(20) | -20.6(72) |
| C(6)-C(11)-C(18)-H(18) | -179.9(53) | H(11)-C(11)-C(18)-C(10) | 179.3(83) |
| H(11)-C(11)-C(18)-H(18) | 0.4(97) | C(7)-C(12)-C(13)-H(13) | 0.5(9) |
| C(7)-C(12)-C(19)-H(19) | -0.3(9) | C(19)-C(12)-C(13)-H(13) | 175.6(15) |
| C(13)-C(12)-C(19)-H(19) | -175.7(15) | C(12)-C(13)-C(22)-H(22) | -177.1(20) |
| H(13)-C(13)-C(22)-C(23) | -177.8(19) | H(13)-C(13)-C(22)-H(22) | 2.9(13) |
| C(16)-C(14)-C(15)-H(15) | 172.0(16) | H(14)-C(14)-C(15)-C(4) | 171.5(17) |
| H(14)-C(14)-C(15)-H(15) | -8.7(10) | H(14)-C(14)-C(16)-C(17) | -172.2(15) |
| H(14)-C(14)-C(16)-C(21) | 1.3(10) | C(14)-C(16)-C(17)-H(17) | 177.0(15) |
| C(14)-C(16)-C(21)-H(21A) | 179.6(18) | C(14)-C(16)-C(21)-H(21B) | 57.7(12) |
| C(14)-C(16)-C(21)-H(21C) | -59.0(12) | C(17)-C(16)-C(21)-H(21A) | -7.2(11) |
| C(17)-C(16)-C(21)-H(21B) | -129.1(15) | C(17)-C(16)-C(21)-H(21C) | 114.2(14) |
| C(21)-C(16)-C(17)-H(17) | 3.4(10) | C(12)-C(19)-C(25)-H(25) | 176.4(20) |
| H(19)-C(19)-C(25)-C(23) | 177.8(19) | H(19)-C(19)-C(25)-H(25) | -3.3(12) |
| C(13)-C(22)-C(23)-H(23) | -179.8(23) | H(22)-C(22)-C(23)-C(25) | 179.1(25) |
| H(22)-C(22)-C(23)-H(23) | -0.5(15) | C(22)-C(23)-C(25)-H(25) | -178.6(23) |
| H(23)-C(23)-C(25)-C(19) | 179.9(23) | H(23)-C(23)-C(25)-H(25) | 1.0(15) |