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# *Supporting Information For:*

## Carbene•Pnictinidene Adducts

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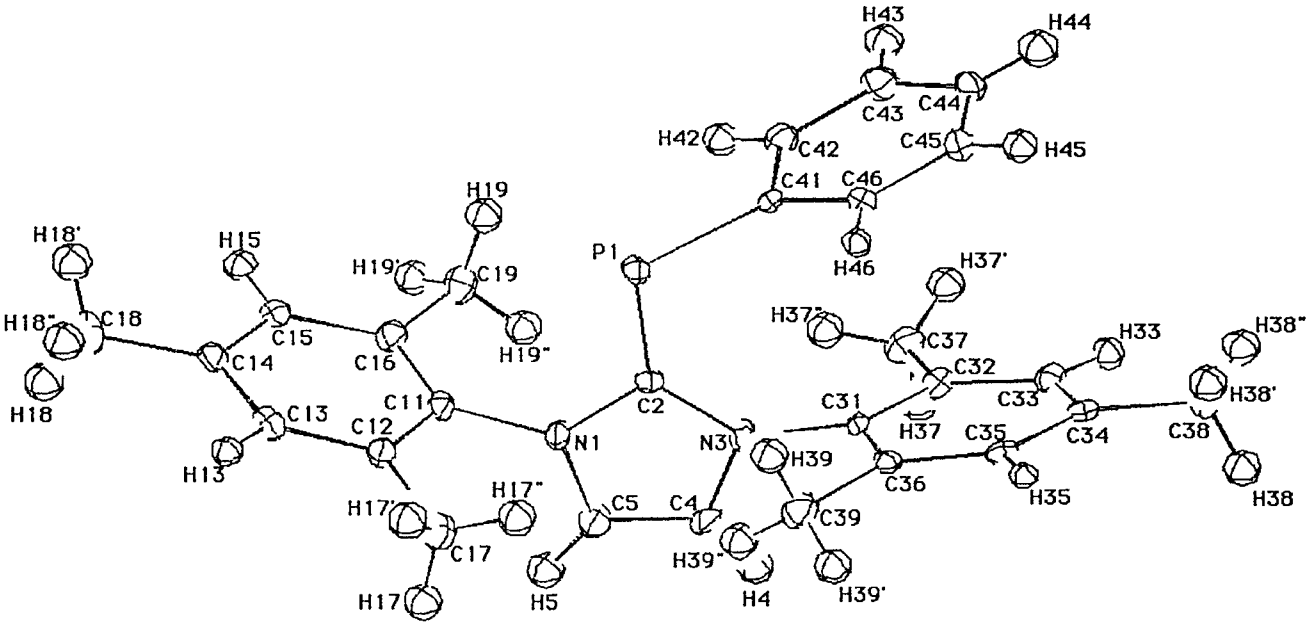
**Table I.** Summary of X-ray Diffraction Data for 2-(phenylphosphinidene)-1,3-dimesitylimidazole (**1•PPh**).

| | |
|---|---|
| formula | $C_{27}H_{29}N_2P$ |
| crystallization method | from toluene/hexane on cooling (-25 °C) |
| color | yellow |
| shape | parallelopiped |
| size, mm | 0.35 x 0.10 x 0.46 |
| symmetry | monoclinic |
| space group | $P2_1/c$ (No. 14) |
| a, Å | 16.981 (5) |
| b, Å | 7.678 (1) |
| c, Å | 18.441 (6) |
| β, deg | 107.05 (1) |
| temperature, °C | -68 |
| volume, $Å^3$ | 2298.7 |
| Z | 4 |
| Fw | 412.52 |
| calculated density, g/cc | 1.192 |
| μ(Mo), $cm^{-1}$ | 1.30 |
| diffractometer | Enraf-Nonius CAD4 |
| radiation (graphite monochromator) | MoKα |
| scan method | ω |
| data octants | +++, -++ |
| 2θ | ≥2.3°, ≤ 50.0° |
| maximum h k l | 20 9 21 |
| scan width | 1.20-2.50 ω |
| scan speed | 1.70-4.00°/min |
| typical peak-with @ half height | 0.15° |
| data collected | 4515 |
| 2 standards collected 41x | no correction for 2% intensity fluctuation |
| variation in azimuthal scan | 12.0% |
| duplicates | 146 (1.9% R-merge) |
| no. of unique data (I≥ 3.0σ(I)) | 1462 |

**Table I** (cont'd).

| | |
|---|---|
| absorption correction | none |
| solution method | direct methods (MULTAN) |
| refinement method | full-matrix least squares on F |
| anomalous dispersion | P |
| weighting scheme | weights $\propto [\sigma^2(I)+0.0009I^2]^{-1/2}$ |
| atoms refined | aniso: all non-hydrogen atoms<br>isotropic $H_{4,5}$<br>fixed all other H (near refined positions) |
| parameters varied | 279 |
| data/parameter ratio | 5.22 |
| R, Rw | 0.059. 0.047 |
| error of fit | 1.23 |
| max shift $\Delta/\sigma$ | 0.05 |
| max residual density, e/Å$^3$ | 0.26 (background) |




ORTEP drawing of 2-(phenylphosphinidene)-1,3-dimesitylimidazole (**1•PPh**).

**Table II.** Fractional Coordinates ($x10^4$) and Isotropic Thermal Parameters

| Atom | X | Y | Z | $B_{ISO}$ |
|---|---|---|---|---|
| P(1) | 3035 (1) | 618 (2) | 2866 (1) | 2.5 (1)' |
| N(1) | 3654 (3) | 3875 (7) | 3359 (3) | 2.7 (2)' |
| N(3) | 2397 (3) | 4120 (7) | 2642 (3) | 2.5 (2)' |
| C(2) | 3003 (4) | 2905 (7) | 2940 (3) | 2.2 (2)' |
| C(4) | 2687 (4) | 5785(11) | 2872 (4) | 3.8 (3)' |
| C(5) | 3447 (4) | 5634(11) | 3321 (4) | 3.8 (3)' |
| C(11) | 4456 (3) | 3198 (8) | 3754 (3) | 2.4 (2)' |
| C(12) | 4615 (3) | 2721 (8) | 4513 (4) | 2.7 (2)' |
| C(13) | 5400 (4) | 2118 (8) | 4879 (3) | 2.6 (2)' |
| C(14) | 6019 (3) | 2071 (8) | 4525 (3) | 2.8 (2)' |
| C(15) | 5830 (4) | 2531 (8) | 3776 (4) | 3.1 (2)' |
| C(16) | 5049 (4) | 3105 (9) | 3370 (3) | 2.8 (2)' |
| C(17) | 3974 (4) | 2895 (9) | 4918 (4) | 4.0 (2)' |
| C(18) | 6883 (4) | 1484 (9) | 4966 (4) | 4.5 (2)' |
| C(19) | 4845 (4) | 3571 (9) | 2539 (4) | 3.9 (2)' |
| C(31) | 1531 (3) | 3787 (7) | 2285 (3) | 2.1 (2)' |
| C(32) | 1194 (3) | 4186 (9) | 1519 (3) | 2.6 (2)' |
| C(33) | 357 (4) | 3883 (8) | 1206 (3) | 3.0 (2)' |
| C(34) | -136 (3) | 3198 (8) | 1613 (3) | 2.4 (2)' |
| C(35) | 222 (3) | 2840 (8) | 2372 (3) | 2.4 (2)' |
| C(36) | 1061 (3) | 3132 (8) | 2728 (3) | 2.2 (2)' |
| C(37) | 1704 (4) | 4901 (8) | 1057 (4) | 3.6 (2)' |
| C(38) | -1041 (3) | 2869 (9) | 1240 (3) | 3.8 (2)' |
| C(39) | 1428 (4) | 2773 (9) | 3560 (3) | 3.6 (2)' |
| C(41) | 2258 (3) | 303 (8) | 1943 (3) | 2.1 (2)' |
| C(42) | 2463 (3) | 624(10) | 1275 (3) | 3.4 (2)' |
| C(43) | 1908 (4) | 329 (9) | 574 (3) | 3.8 (2)' |
| C(44) | 1127 (4) | -306(10) | 516 (3) | 4.2 (2)' |
| C(45) | 920 (4) | -641 (9) | 1163 (4) | 3.1 (2)' |
| C(46) | 1478 (3) | -345 (8) | 1857 (3) | 2.4 (2)' |
| H(4) | 2362(36) | 6702(85) | 2713(34) | 5.0(20) |
| H(5) | 3858(30) | 6411(68) | 3545(27) | 2.6(14) |
| H(13) | 5520 | 1730 | 5383 | 2.7 |
| H(15) | 6244 | 2446 | 3526 | 3.0 |

**Table II.** Fractional Coordinates ($x10^4$) and Isotropic Thermal Parameters (cont'd.)

| | | | | |
|---|---|---|---|---|
| H(17) | 4103 | 2120 | 5341 | 4.0 |
| H(17') | 3450 | 2600 | 4584 | 4.0 |
| H(17") | 3967 | 4053 | 5091 | 4.0 |
| H(18) | 6928 | 1430 | 5485 | 4.5 |
| H(18') | 7270 | 2297 | 4880 | 4.5 |
| H(18") | 6985 | 367 | 4787 | 4.5 |
| H(19) | 5335 | 3789 | 2411 | 3.6 |
| H(19') | 4508 | 4596 | 2444 | 3.6 |
| H(19") | 4549 | 2643 | 2241 | 3.6 |
| H(33) | 108 | 4178 | 691 | 3.0 |
| H(35) | -112 | 2364 | 2659 | 2.2 |
| H(37) | 2042 | 5847 | 1332 | 3.8 |
| H(37') | 1370 | 5343 | 590 | 3.8 |
| H(37") | 2066 | 4034 | 967 | 3.8 |
| H(38) | -1184 | 1764 | 1393 | 3.9 |
| H(38') | -1147 | 2882 | 703 | 3.9 |
| H(38") | -1355 | 3749 | 1385 | 3.9 |
| H(39) | 1643 | 3827 | 3810 | 3.8 |
| H(39') | 1862 | 1949 | 3626 | 3.8 |
| H(39") | 1018 | 2327 | 3761 | 3.8 |
| H(42) | 3002 | 1056 | 1308 | 3.3 |
| H(43) | 2060 | 557 | 129 | 4.0 |
| H(44) | 43 | -506 | 29 | 4.2 |
| H(45) | 88 | -1052 | 1133 | 3.2 |
| H(46) | 1317 | -584 | 2304 | 2.4 |

**Table III.** Anisotropic Thermal Parameters (Å x $10^3$)
exp[-19.739($U_{11}$hha*a*...+2($U_{12}$hka*b*...))]

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|
| P(1) | 32 (1) | 21 (1) | 35 (1) | 1 (1) | -1 (1) | -1 (1) |
| N(1) | 22 (3) | 27 (4) | 49 (4) | 0 (3) | 3 (3) | -3 (3) |
| N(3) | 26 (3) | 18 (4) | 45 (3) | 4 (3) | -1 (2) | 3 (3) |
| C(2) | 27 (3) | 19 (4) | 36 (4) | -2 (4) | 4 (3) | -1 (4) |
| C(4) | 35 (4) | 28 (5) | 77 (6) | 8 (5) | 9 (4) | -6 (5) |

**Table III.** Anisotropic Thermal Parameters (Å x $10^3$) (cont'd.)

| | | | | | | |
|---|---|---|---|---|---|---|
| C(5) | 29 (4) | 27 (5) | 81 (6) | -8 (4) | 6 (4) | -12 (5) |
| C(11) | 25 (4) | 20 (4) | 39 (4) | -5 (3) | -2 (3) | -3 (4) |
| C(12) | 25 (4) | 33 (5) | 43 (4) | 2 (3) | 6 (3) | 0 (4) |
| C(13) | 47 (4) | 18 (4) | 31 (4) | -5 (4) | 4 (3) | 5 (3) |
| C(14) | 31 (4) | 29 (4) | 39 (4) | -5 (3) | -1 (3) | -7 (4) |
| C(15) | 33 (4) | 41 (5) | 44 (4) | -1 (4) | 13 (3) | -15 (4) |
| C(16) | 33 (4) | 28 (4) | 43 (4) | 1 (4) | 7 (3) | 1 (4) |
| C(17) | 49 (4) | 48 (5) | 58 (5) | -11 (4) | 19 (4) | -5 (4) |
| C(18) | 45 (4) | 59 (5) | 60 (5) | 0 (4) | 2 (4) | 4 (4) |
| C(19) | 41 (4) | 50 (5) | 52 (4) | 2 (4) | 8 (3) | 6 (4) |
| C(31) | 22 (3) | 15 (4) | 36 (4) | 5 (3) | -1 (3) | -5 (3) |
| C(32) | 29 (4) | 30 (4) | 43 (4) | 3 (4) | 14 (3) | 7 (4) |
| C(33) | 45 (4) | 32 (5) | 35 (4) | 12 (4) | 9 (3) | 2 (3) |
| C(34) | 32 (4) | 25 (4) | 35 (4) | 5 (4) | 10 (3) | -6 (4) |
| C(35) | 35 (4) | 28 (4) | 35 (4) | 1 (4) | 20 (3) | -5 (3) |
| C(36) | 34 (4) | 20 (4) | 28 (3) | 7 (3) | 7 (3) | -1 (3) |
| C(37) | 47 (4) | 36 (5) | 56 (4) | 11 (4) | 17 (4) | 14 (4) |
| C(38) | 31 (4) | 58 (5) | 51 (4) | 1 (4) | 5 (3) | -11 (4) |
| C(39) | 43 (4) | 49 (5) | 44 (4) | 6 (4) | 14 (3) | 0 (4) |
| C(41) | 25 (3) | 21 (4) | 31 (4) | 8 (3) | 3 (3) | -2 (3) |
| C(42) | 36 (4) | 54 (5) | 43 (4) | 0 (4) | 18 (3) | 4 (5) |
| C(43) | 65 (5) | 57 (6) | 26 (4) | 12 (5) | 16 (4) | 5 (4) |
| C(44) | 53 (5) | 56 (6) | 33 (4) | 16 (4) | -15 (4) | -16 (4) |
| C(45) | 37 (4) | 38 (4) | 39 (4) | 4 (4) | 4 (3) | -5 (4) |
| C(46) | 29 (4) | 31 (4) | 30 (4) | 0 (4) | 5 (3) | -5 (3) |

**Table IV.** Interatomic Distances (Å)

| | | | | | |
|---|---|---|---|---|---|
| P(1)-C(2) | 1.763 (6) | C(11)-C(16) | 1.393 (7) | C(32)-C(33) | 1.388 (7) |
| P(1)-C(41) | 1.839 (5) | C(12)-C(13) | 1.384 (7) | C(32)-C(37) | 1.486 (8) |
| N(1)-C(2) | 1.369 (7) | C(12)-C(17) | 1.496 (8) | C(33)-C(34) | 1.382 (7) |
| N(1)-C(5) | 1.393 (8) | C(13)-C(14) | 1.392 (8) | C(34)-C(35) | 1.380 (7) |
| N(1)-C(11) | 1.440 (7) | C(14)-C(15) | 1.370 (7) | C(34)-C(38) | 1.510 (7) |
| N(3)-C(2) | 1.378 (7) | C(14)-C(18) | 1.522 (7) | C(35)-C(36) | 1.401 (7) |
| N(3)-C(4) | 1.391 (8) | C(15)-C(16) | 1.390 (8) | C(36)-C(39) | 1.503 (7) |
| N(3)-C(31) | 1.447 (7) | C(16)-C(19) | 1.512 (8) | C(41)-C(42) | 1.396 (7) |
| C(4)-C(5) | 1.318 (9) | C(31)-C(32) | 1.394 (7) | C(41)-C(46) | 1.380 (7) |
| C(11)-C(12) | 1.394 (7) | C(31)-C(36) | 1.392 (7) | C(42)-C(43) | 1.377 (7) |

**Table IV.** Interatomic Distances (Å) (cont'd.)

| | | | | | |
|---|---|---|---|---|---|
| C(43)-C(44) | 1.387 (8) | C(18)-H(18') | 0.953 (0) | C(38)-H(38') | 0.953 (0) |
| C(44)-C(45) | 1.363 (8) | C(18)-H(18") | 0.953 (0) | C(38)-H(38") | 0.947 (0) |
| C(45)-C(46) | 1.370 (7) | C(19)-H(19) | 0.944 (0) | C(39)-H(39) | 0.949 (0) |
| C(4)-H(4) | 0.889 (59) | C(19)-H(19') | 0.958 (0) | C(39)-H(39') | 0.951 (0) |
| C(5)-H(5) | 0.919 (48) | C(19)-H(19") | 0.949 (0) | C(39)-H(39") | 0.944 (0) |
| C(13)-H(13) | 0.939 (0) | C(33)-H(33) | 0.947 (0) | C(42)-H(42) | 0.959 (0) |
| C(15)-H(15) | 0.948 (0) | C(35)-H(35) | 0.954 (0) | C(43)-H(43) | 0.946 (0) |
| C(17)-H(17) | 0.954 (0) | C(37)-H(37) | 0.971 (0) | C(44)-H(44) | 0.955 (0) |
| C(17)-H(17') | 0.949 (0) | C(37)-H(37') | 0.944 (0) | C(45)-H(45) | 0.942 (0) |
| C(17)-H(17") | 0.946 (0) | C(37)-H(37") | 0.954 (0) | C(46)-H(46) | 0.958 (0) |
| C(18)-H(18) | 0.938 (0) | C(38)-H(38) | 0.948 (0) | | |

**Table V.** Intramolecular Angles (°)

| | | | |
|---|---|---|---|
| C(2)-P(1)-C(41) | 99.9 (3) | C(11)-C(16)-C(15) | 117.5 (6) |
| C(2)-N(1)-C(5) | 110.4 (5) | C(11)-C(16)-C(19) | 121.2 (5) |
| C(2)-N(1)-C(11) | 125.2 (5) | C(15)-C(16)-C(19) | 121.3 (6) |
| C(5)-N(1)-C(11) | 124.3 (5) | C(32)-C(31)-C(36) | 122.6 (5) |
| C(2)-N(3)-C(4) | 110.2 (5) | C(31)-C(32)-C(33) | 116.8 (6) |
| C(2)-N(3)-C(31) | 127.0 (5) | C(31)-C(32)-C(37) | 121.8 (5) |
| C(4)-N(3)-C(31) | 121.5 (5) | C(33)-C(32)-C(37) | 121.4 (6) |
| P(1)-C(2)-N(1) | 123.2 (5) | C(32)-C(33)-C(34) | 123.2 (6) |
| P(1)-C(2)-N(3) | 132.8 (5) | C(33)-C(34)-C(35) | 118.0 (5) |
| P(1)-C(41)-C(42) | 119.7 (4) | C(33)-C(34)-C(38) | 121.0 (6) |
| P(1)-C(41)-C(46) | 123.9 (5) | C(35)-C(34)-C(38) | 121.0 (6) |
| N(1)-C(2)-N(3) | 104.0 (5) | C(34)-C(35)-C(36) | 121.9 (5) |
| N(3)-C(4)-C(5) | 107.7 (7) | C(31)-C(36)-C(35) | 117.5 (5) |
| N(1)-C(5)-C(4) | 107.7 (7) | C(31)-C(36)-C(39) | 121.9 (5) |
| N(1)-C(11)-C(12) | 118.7 (5) | C(35)-C(36)-C(39) | 120.6 (6) |
| N(1)-C(11)-C(16) | 118.6 (6) | C(42)-C(41)-C(46) | 116.3 (5) |
| N(3)-C(31)-C(32) | 118.8 (5) | C(41)-C(42)-C(43) | 121.3 (6) |
| N(3)-C(31)-C(36) | 118.6 (5) | C(42)-C(43)-C(44) | 120.4 (6) |
| N(3)-C(4)-H(4) | 120 (4) | C(43)-C(44)-C(45) | 119.0 (6) |
| N(1)-C(5)-H(5) | 117 (3) | C(44)-C(45)-C(46) | 120.1 (6) |
| C(12)-C(11)-C(16) | 122.7 (5) | C(41)-C(46)-C(45) | 122.9 (6) |
| C(11)-C(12)-C(13) | 116.9 (6) | C(5)-C(4)-H(4) | 132 (4) |
| C(11)-C(12)-C(17) | 121.4 (5) | C(4)-C(5)-H(5) | 134 (3) |
| C(13)-C(12)-C(17) | 121.6 (6) | C(12)-C(13)-H(13) | 119 (0) |
| C(12)-C(13)-C(14) | 122.1 (6) | C(14)-C(13)-H(13) | 119 (0) |
| C(13)-C(14)-C(15) | 118.7 (5) | C(14)-C(15)-H(15) | 119 (0) |
| C(13)-C(14)-C(18) | 120.0 (6) | C(16)-C(15)-H(15) | 119 (0) |
| C(15)-C(14)-C(18) | 121.3 (6) | C(12)-C(17)-H(17) | 109 (0) |
| C(14)-C(15)-C(16) | 121.9 (6) | C(12)-C(17)-H(17') | 110 (0) |

**Table V.** Intramolecular Angles (°) (cont'd.)

| | | | |
|---|---|---|---|
| C(12)-C(17)-H(17") | 110 (0) | C(43)-C(44)-H(44) | 120 (0) |
| C(14)-C(18)-H(18) | 110 (0) | C(45)-C(44)-H(44) | 121 (0) |
| C(14)-C(18)-H(18') | 109 (0) | C(44)-C(45)-H(45) | 120 (0) |
| C(14)-C(18)-H(18") | 109 (0) | C(46)-C(45)-H(45) | 120 (0) |
| C(16)-C(19)-H(19) | 110 (0) | C(41)-C(46)-H(46) | 119 (0) |
| C(16)-C(19)-H(19') | 109 (0) | C(45)-C(46)-H(46) | 119 (0) |
| C(16)-C(19)-H(19") | 110 (0) | H(17)-C(17)-H(17') | 109 (0) |
| C(32)-C(33)-H(33) | 119 (0) | H(17)-C(17)-H(17") | 109 (0) |
| C(34)-C(33)-H(33) | 118 (0) | H(17')-C(17)-H(17") | 110 (0) |
| C(34)-C(35)-H(35) | 119 (0) | H(18)-C(18)-H(18') | 110 (0) |
| C(36)-C(35)-H(35) | 119 (0) | H(18)-C(18)-H(18") | 110 (0) |
| C(32)-C(37)-H(37) | 109 (0) | H(18')-C(18)-H(18") | 109 (0) |
| C(32)-C(37)-H(37') | 111 (0) | H(19)-C(19)-H(19') | 109 (0) |
| C(32)-C(37)-H(37") | 111 (0) | H(19)-C(19)-H(19") | 110 (0) |
| C(34)-C(38)-H(38) | 109 (0) | H(19')-C(19)-H(19") | 109 (0) |
| C(34)-C(38)-H(38') | 109 (0) | H(37)-C(37)-H(37') | 108 (0) |
| C(34)-C(38)-H(38") | 110 (0) | H(37)-C(37)-H(37") | 107 (0) |
| C(36)-C(39)-H(39) | 109 (0) | H(37')-C(37)-H(37") | 110 (0) |
| C(36)-C(39)-H(39') | 109 (0) | H(38)-C(38)-H(38') | 109 (0) |
| C(36)-C(39)-H(39") | 110 (0) | H(38)-C(38)-H(38") | 110 (0) |
| C(41)-C(42)-H(42) | 119 (0) | H(38')-C(38)-H(38") | 110 (0) |
| C(43)-C(42)-H(42) | 120 (0) | H(39)-C(39)-H(39') | 109 (0) |
| C(42)-C(43)-H(43) | 120 (0) | H(39)-C(39)-H(39") | 110 (0) |
| C(44)-C(43)-H(43) | 120 (0) | H(39')-C(39)-H(39") | 110 (0) |

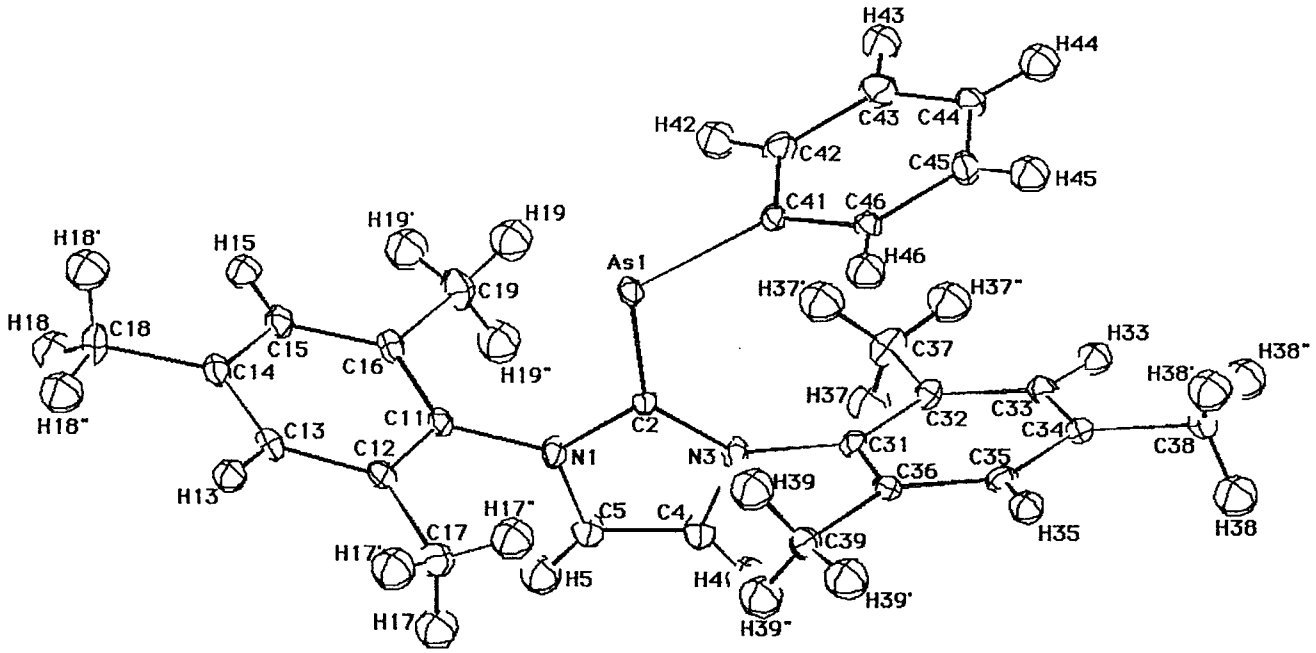
**Table VI.** Intramolecular Non-Bonding Distances (Å)

| | | | | | |
|---|---|---|---|---|---|
| P(1)···C(12) | 3.776 (6) | C(2)···C(39) | 3.204 (8) | C(32)···C(42) | 3.591 (9) |
| P(1)···C(16) | 3.787 (6) | C(4)···C(37) | 3.342 (10) | C(32)···C(46) | 3.542 (9) |
| P(1)···C(17) | 4.047 (6) | C(4)···C(39) | 3.622 (10) | C(33)···C(45) | 3.610 (9) |
| P(1)···C(19) | 4.004 (7) | C(5)···C(17) | 3.515 (10) | C(34)···C(45) | 3.669 (9) |
| P(1)···C(36) | 3.811 (6) | C(5)···C(19) | 3.497 (10) | C(35)···C(46) | 3.551 (8) |
| P(1)···C(39) | 3.725 (6) | C(31)···C(41) | 3.088 (8) | C(36)···C(41) | 3.559 (8) |
| N(3)···C(42) | 3.706 (8) | C(31)···C(42) | 3.688 (9) | C(36)···C(46) | 3.297 (8) |
| C(2)···C(17) | 3.535 (8) | C(31)···C(46) | 3.264 (8) | C(37)···C(42) | 3.507 (9) |
| C(2)···C(19) | 3.456 (9) | C(32)···C(41) | 3.454 (8) | C(37)···C(43) | 3.662 (9) |

**Table I.** Summary of X-ray Diffraction Data for 2-(phenylarsenidene)-1,3-dimesitylimidazole (**1•AsPh**).

| | | |
|---|---|---|
| Empirical formula | $C_{27}H_{29}AsN_2$ | |
| Formula weight | 456.44 | |
| Temperature | 183(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | P2(1)/c | |
| Unit cell dimensions | a = 17.086(3) Å | α = 90° |
| | b = 7.694(2) Å | β = 107.49(2)° |
| | c = 18.574(5) Å | γ = 90° |
| Volume, Z | 2328.9(8) $Å^3$, 4 | |
| Density (calculated) | 1.302 $g/cm^3$ | |
| Absorption coefficient | 14.75 $cm^{-1}$ | |
| F(000) | 952 | |
| Crystal size | .5 x .5 x .14 mm | |
| Theta range for data collection | 2.26 to 32.50° | |
| Limiting indices | $-25 \le h \le 25$, $-1 \le k \le 11$, $-28 \le l \le 28$ | |
| Reflections collected | 16839 | |
| Independent reflections | 8433 [R(int) = 0.0868] | |
| Absorption correction | None | |
| Refinement method | Full-matrix least-squares on $F^2$ (SHELXL-93) | |
| Data / restraints / parameters | 8431 / 0 / 282 | |
| Goodness-of-fit on $F^2$ | 0.987 | |
| Final R indices [$I>2\sigma(I)$] | R1 = 0.0570, wR2 = 0.0906 | |
| R indices (all data) | R1 = 0.1374, wR2 = 0.1155 | |
| Extinction coefficient, $\chi^a$ | 0.0009(2) | |
| Largest diff. peak and hole | 0.402 and -0.460 $eÅ^{-3}$ | |

a) $F^* = F[1 + 0.001\chi F^2\lambda^3/\sin(2\theta)]^{-1/4}$




ORTEP drawing of 2-(phenylarsenidene)-1,3-dimesitylimidazole (**1•AsPh**).

**Table II.** Fractional Coordinates ($x10^4$) and Isotropic Thermal Parameters

| Atom | X | Y | Z | $U_{eq}$ ($Å^2 \times 10^3$) |
|---|---|---|---|---|
| As(1) | 3071 (1) | 443 (1) | 2914 (1) | 29 (1) |
| N(1) | 3660 (1) | 3885 (3) | 3399 (2) | 32 (1) |
| N(3) | 2391 (1) | 4079 (3) | 2712 (1) | 31 (1) |
| C(2) | 3010 (2) | 2899 (3) | 2985 (2) | 26 (1) |
| C(4) | 2667 (2) | 5760 (4) | 2932 (2) | 42 (1) |
| C(5) | 3451 (2) | 5623 (4) | 3356 (2) | 43 (1) |
| C(11) | 4467 (2) | 3217 (4) | 3770 (2) | 30 (1) |
| C(12) | 5034 (2) | 3134 (4) | 3374 (2) | 32 (1) |
| C(13) | 5816 (2) | 2569 (4) | 3752 (2) | 35 (1) |
| C(14) | 6033 (2) | 2034 (4) | 4502 (2) | 36 (1) |
| C(15) | 5440 (2) | 2081 (4) | 4872 (2) | 33 (1) |
| C(16) | 4650 (2) | 2706 (4) | 4525 (2) | 32 (1) |
| C(17) | 4804 (2) | 3635 (5) | 2550 (2) | 47 (1) |
| C(18) | 6895 (2) | 1442 (5) | 4905 (2) | 49 (1) |
| C(19) | 4034 (2) | 2849 (5) | 4954 (2) | 45 (1) |
| C(31) | 1534 (2) | 3724 (4) | 2338 (2) | 27 (1) |
| C(32) | 1060 (2) | 3062 (4) | 2758 (2) | 29 (1) |
| C(33) | 231 (2) | 2750 (4) | 2393 (2) | 31 (1) |
| C(34) | -117 (2) | 3144 (4) | 1631 (2) | 31 (1) |
| C(35) | 377 (2) | 3838 (4) | 1240 (2) | 32 (1) |
| C(36) | 1211 (2) | 4139 (4) | 1574 (2) | 30 (1) |
| C(37) | 1420 (2) | 2663 (5) | 3589 (2) | 41 (1) |
| C(38) | -1020 (2) | 2813 (5) | 1246 (2) | 44 (1) |
| C(39) | 1741 (2) | 4855 (4) | 1130 (2) | 45 (1) |
| C(41) | 2231 (2) | 180 (4) | 1922 (2) | 26 (1) |
| C(42) | 1448 (2) | -439 (4) | 1845 (2) | 31 (1) |
| C(43) | 889 (2) | -710 (4) | 1142 (2) | 43 (1) |
| C(44) | 1102 (2) | -352 (5) | 502 (2) | 52 (1) |
| C(45) | 1882 (2) | 242 (5) | 567 (2) | 54 (1) |
| C(46) | 2443 (2) | 497 (5) | 1272 (2) | 40 (1) |
| H(4) | 2358 (2) | 6802 (4) | 2805 (2) | 60 (8) |
| H(5) | 3801 (2) | 6556 (4) | 3586 (2) | 60 (8) |
| H(13) | 6218 (2) | 2544 (4) | 3493 (2) | 35 (5) |
| H(15) | 5575 (2) | 1675 (4) | 5378 (2) | 35 (5) |

**Table II.** Fractional Coordinates ($x10^4$) and Isotropic Thermal Parameters (cont'd.)

| | | | | |
|---|---|---|---|---|
| H(17) | 5302 (3) | 3718 (33) | 2393 (4) | 77 (3) |
| H(17') | 4524 (14) | 4761 (16) | 2477 (3) | 77 (3) |
| H(17") | 4439 (13) | 2751 (17) | 2246 (2) | 77 (3) |
| H(18) | 6957 (5) | 1285 (32) | 5443 (3) | 77 (3) |
| H(18') | 7286 (2) | 2319 (16) | 4845 (12) | 77 (3) |
| H(18") | 7002 (6) | 337 (17) | 4690 (10) | 77 (3) |
| H(19) | 3492 (4) | 2496 (30) | 4628 (5) | 77 (3) |
| H(19') | 4010 (11) | 4055 (8) | 5116 (12) | 77 (3) |
| H(19") | 4198 (8) | 2090 (24) | 5398 (8) | 77 (3) |
| H(33) | -102 (2) | 2260 (4) | 2669 (2) | 35 (5) |
| H(35) | 140 (2) | 4122 (4) | 722 (2) | 35 (5) |
| H(37) | 1794 (12) | 1669 (21) | 3653 (2) | 77 (3) |
| H(37') | 977 (2) | 2383 (32) | 3804 (4) | 77 (3) |
| H(37") | 1723 (13) | 3678 (12) | 3849 (3) | 77 (3) |
| H(38) | -1349 (2) | 3604 (22) | 1451 (10) | 77 (3) |
| H(38') | -1152 (4) | 1608 (10) | 1335 (12) | 77 (3) |
| H(38") | -1143 (4) | 3013 (31) | 702 (3) | 77 (3) |
| H(39) | 1889 (12) | 6060 (11) | 1282 (10) | 77 (3) |
| H(39') | 1440 (6) | 4819 (29) | 590 (2) | 77 (3) |
| H(39") | 2241 (7) | 4154 (19) | 1226 (11) | 77 (3) |
| H(42) | 1293 (2) | -681 (4) | 2285 (2) | 50 (5) |
| H(43) | 357 (2) | -1145 (4) | 1102 (2) | 50 (5) |
| H(44) | 716 (2) | -512 (5) | 18 (2) | 50 (5) |
| H(45) | 2035 (2) | 477 (5) | 125 (2) | 50 (5) |
| H(46) | 2980 (2) | 894 (5) | 1309 (2) | 50 (5) |

**Table III.** Anisotropic Thermal Parameters (Å x $10^3$)
$\exp[-19.739(U_{11}hha^*a^*...+2(U_{12}hka^*b^*...))]$

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| As(1) | 27 (1) | 21 (1) | 31 (1) | -1 (1) | -3 (1) | 2 (1) |
| N(1) | 23 (1) | 22 (1) | 45 (2) | -3 (1) | 0 (1) | -1 (1) |
| N(3) | 24 (1) | 20 (1) | 44 (2) | 1 (1) | 2 (1) | 3 (1) |
| C(2) | 22 (1) | 24 (1) | 30 (2) | -1 (1) | 3 (1) | 0 (1) |
| C(4) | 35 (2) | 17 (2) | 65 (2) | -4 (1) | 0 (2) | -2 (1) |

**Table III.** Anisotropic Thermal Parameters (Å x $10^3$) (cont'd.)

| | | | | | | |
|---|---|---|---|---|---|---|
| C(5) | 36 (2) | 20 (2) | 64 (2) | -6 (2) | 0 (2) | -4 (2) |
| C(11) | 22 (1) | 24 (2) | 37 (2) | -4 (1) | -1 (1) | -4 (1) |
| C(12) | 29 (2) | 31 (2) | 31 (2) | 1 (1) | 2 (1) | -6 (1) |
| C(13) | 26 (2) | 42 (2) | 37 (2) | -3 (2) | 7 (1) | -5 (1) |
| C(14) | 26 (2) | 33 (2) | 39 (2) | -3 (1) | -4 (1) | -3 (1) |
| C(15) | 31 (2) | 34 (2) | 29 (2) | -3 (1) | 1 (1) | -7 (1) |
| C(16) | 29 (2) | 27 (2) | 35 (2) | -8 (1) | 4 (1) | -8 (1) |
| C(17) | 42 (2) | 58 (2) | 35 (2) | 10 (2) | 3 (2) | -5 (2) |
| C(18) | 25 (2) | 63 (3) | 51 (2) | 10 (2) | -1 (2) | 3 (2) |
| C(19) | 44 (2) | 43 (2) | 49 (2) | -4 (2) | 16 (2) | -5 (2) |
| C(31) | 23 (1) | 19 (1) | 35 (2) | -1 (1) | 4 (1) | 5 (1) |
| C(32) | 31 (2) | 28 (2) | 25 (1) | -3 (1) | 5 (1) | 5 (1) |
| C(33) | 28 (1) | 32 (2) | 36 (2) | -4 (1) | 14 (1) | 0 (1) |
| C(34) | 26 (1) | 29 (2) | 35 (2) | -8 (1) | 4 (1) | 5 (1) |
| C(35) | 36 (2) | 34 (2) | 23 (2) | 3 (1) | 3 (1) | 7 (1) |
| C(36) | 27 (2) | 27 (2) | 37 (2) | 5 (1) | 9 (1) | 6 (1) |
| C(37) | 41 (2) | 50 (2) | 27 (2) | 1 (2) | 5 (1) | 8 (2) |
| C(38) | 30 (2) | 54 (2) | 45 (2) | -16 (2) | 5 (2) | -1 (2) |
| C(39) | 44 (2) | 43 (2) | 52 (2) | 15 (2) | 21 (2) | 6 (2) |
| C(41) | 25 (1) | 23 (2) | 28 (1) | 0 (1) | 2 (1) | 5 (1) |
| C(42) | 30 (1) | 27 (1) | 32 (2) | -2 (2) | 3 (1) | 2 (2) |
| C(43) | 32 (2) | 40 (2) | 46 (2) | -7 (2) | -6 (1) | 2 (2) |
| C(44) | 50 (2) | 62 (2) | 30 (2) | -14 (2) | -10 (2) | 25 (2) |
| C(45) | 62 (2) | 77 (3) | 25 (2) | 7 (2) | 15 (2) | 24 (2) |
| C(46) | 39 (2) | 46 (2) | 36 (2) | 5 (2) | 12 (1) | 9 (2) |

**Table IV.** Interatomic Distances (Å)

| | | | | | |
|---|---|---|---|---|---|
| As(1)-C(2) | 1.899 (3) | C(41)-C(42) | 1.386 (4) | C(14)-C(15) | 1.385 (4) |
| As(1)-C(41) | 1.977 (3) | C(42)-C(43) | 1.383 (4) | C(14)-C(18) | 1.508 (4) |
| N(1)-C(2) | 1.373 (3) | C(43)-C(44) | 1.371 (5) | C(15)-C(16) | 1.395 (4) |
| N(1)-C(5) | 1.380 (4) | C(44)-C(45) | 1.380 (5) | C(16)-C(19) | 1.502 (4) |
| N(1)-C(11) | 1.439 (3) | C(45)-C(46) | 1.384 (4) | C(31)-C(32) | 1.379 (4) |
| N(3)-C(2) | 1.370 (3) | C(11)-C(12) | 1.383 (4) | C(31)-C(36) | 1.397 (4) |
| N(3)-C(4) | 1.395 (4) | C(11)-C(16) | 1.398 (4) | C(32)-C(33) | 1.395 (4) |
| N(3)-C(31) | 1.446 (3) | C(12)-C(13) | 1.380 (4) | C(32)-C(37) | 1.512 (4) |
| C(5)-C(4) | 1.338 (4) | C(12)-C(17) | 1.511 (4) | C(33)-C(34) | 1.394 (4) |
| C(41)-C(46) | 1.383 (4) | C(13)-C(14) | 1.393 (4) | C(34)-C(35) | 1.377 (4) |

**Table IV.** Interatomic Distances (Å) (cont'd.)

| | | | | | |
|---|---|---|---|---|---|
| C(34)-C(38) | 1.514 (4) | C(35)-C(36) | 1.392 (4) | C(36)-C(39) | 1.501 (4) |

**Table V.** Intramolecular Angles (°)

| | | | |
|---|---|---|---|
| C(2)-As(1)-C(41) | 97.31 (12) | C(13)-C(12)-C(17) | 120.9 (3) |
| C(2)-N(1)-C(5) | 110.6 (2) | C(11)-C(12)-C(17) | 121.1 (3) |
| C(2)-N(1)-C(11) | 124.6 (2) | C(12)-C(13)-C(14) | 121.8 (3) |
| C(5)-N(1)-C(11) | 124.6 (2) | C(15)-C(14)-C(13) | 118.4 (3) |
| C(2)-N(3)-C(4) | 110.5 (2) | C(15)-C(14)-C(18) | 120.9 (3) |
| C(2)-N(3)-C(31) | 127.6 (2) | C(13)-C(14)-C(18) | 120.8 (3) |
| C(4)-N(3)-C(31) | 121.4 (2) | C(14)-C(15)-C(16) | 122.0 (3) |
| N(3)-C(2)-N(1) | 104.2 (2) | C(15)-C(16)-C(11) | 117.0 (3) |
| N(3)-C(2)-As(1) | 133.3 (2) | C(15)-C(16)-C(19) | 121.0 (3) |
| N(1)-C(2)-As(1) | 122.5 (2) | C(11)-C(16)-C(19) | 122.0 (3) |
| C(4)-C(5)-N(1) | 107.8 (3) | C(32)-C(31)-C(36) | 122.6 (3) |
| C(5)-C(4)-N(3) | 106.9 (3) | C(32)-C(31)-N(3) | 118.7 (3) |
| C(46)-C(41)-C(42) | 118.0 (3) | C(36)-C(31)-N(3) | 118.5 (3) |
| C(46)-C(41)-As(1) | 119.3 (2) | C(31)-C(32)-C(33) | 118.2 (3) |
| C(42)-C(41)-As(1) | 122.6 (2) | C(31)-C(32)-C(37) | 121.6 (3) |
| C(43)-C(42)-C(41) | 121.4 (3) | C(33)-C(32)-C(37) | 120.2 (3) |
| C(44)-C(43)-C(42) | 120.0 (3) | C(34)-C(33)-C(32) | 121.1 (3) |
| C(43)-C(44)-C(45) | 119.5 (3) | C(35)-C(34)-C(33) | 118.5 (3) |
| C(44)-C(45)-C(46) | 120.4 (3) | C(35)-C(34)-C(38) | 121.0 (3) |
| C(41)-C(46)-C(45) | 120.8 (3) | C(33)-C(34)-C(38) | 120.4 (3) |
| C(12)-C(11)-C(16) | 122.7 (3) | C(34)-C(35)-C(36) | 122.6 (3) |
| C(12)-C(11)-N(1) | 119.0 (3) | C(35)-C(36)-C(31) | 116.9 (3) |
| C(16)-C(11)-N(1) | 118.3 (3) | C(35)-C(36)-C(39) | 121.5 (3) |
| C(13)-C(12)-C(11) | 118.0 (3) | C(31)-C(36)-C(39) | 121.6 (3) |

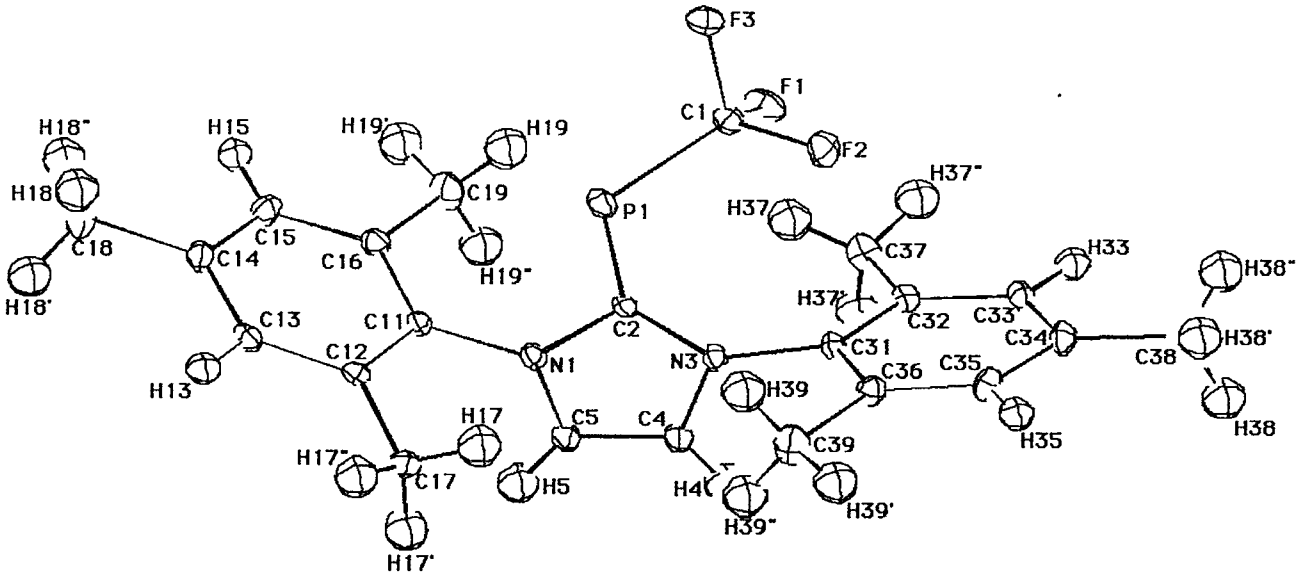
 



**Table I.** Summary of X-ray Diffraction Data for 2 - (trifluoromethylphosphinidene)-1,3-dimesitylimidazole (**1•PCF$_3$**).

| | | |
|---|---|---|
| Empirical formula | $C_{22}H_{24}F_3N_2P$ | |
| Formula weight | 404.40 | |
| Temperature | 178(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | P2(1)/n | |
| Unit cell dimensions | a = 8.1365(6) Å | $\alpha = 90°$ |
| | b = 7.6265(4) Å | $\beta = 91.243(6)°$ |
| | c = 34.251(3) Å | $\gamma = 90°$ |
| Volume, Z | 2124.9(3) Å$^3$, 4 | |
| Density (calculated) | 1.264 g/cm$^3$ | |
| Absorption coefficient | 1.64 cm$^{-1}$ | |
| F(000) | 848 | |
| Crystal size | .84 x .21 x .21 mm | |
| Theta range for data collection | 2.38 to 32.50° | |
| Limiting indices | $-12 \le h \le 12, -1 \le k \le 11, -51 \le l \le 51$ | |
| Reflections collected | 16799 | |
| Independent reflections | 7582 [R(int) = 0.0415] | |
| Absorption correction | None | |
| Refinement method | Full-matrix least-squares on F$^2$ (SHELXL-93) | |
| Data / restraints / parameters | 7576 / 0 / 263 | |
| Goodness-of-fit on F$^2$ | 1.098 | |
| Final R indices [I>2σ(I)] | R1 = 0.0545, wR2 = 0.1347 | |
| R indices (all data) | R1 = 0.1056, wR2 = 0.1629 | |
| Extinction coefficient, $\chi^a$ | 0.0016(2) | |
| Largest diff. peak and hole | 0.410 and -0.322 eÅ$^{-3}$ | |

a) $F^* = F[1 + 0.001\chi F^2\lambda^3/\sin(2\theta)]^{-1/4}$




ORTEP drawing of 2-(trifluoromethylphosphinidene)-1,3-dimesitylimidazole (**1•PCF$_3$**).

**Table II.** Fractional Coordinates ($x10^4$) and Isotropic Thermal Parameters

| Atom | X | Y | Z | $U_{eq}$ ($Å^2 \times 10^3$) |
|---|---|---|---|---|
| P(1) | 3478 (1) | 165 (1) | 1047 (1) | 33 (1) |
| F(11) | 1899 (1) | 677 (2) | 1733 (1) | 46 (1) |
| F(12) | 4005 (2) | -973 (2) | 1804 (1) | 48 (1) |
| F(13) | 1879 (2) | -1945 (2) | 1496 (1) | 46 (1) |
| N(1) | 3848 (2) | 3539 (2) | 807 (1) | 27 (1) |
| N(3) | 4558 (2) | 3442 (2) | 1419 (1) | 26 (1) |
| C(1) | 2826 (2) | -489 (3) | 1539 (1) | 32 (1) |
| C(2) | 3966 (2) | 2423 (2) | 1120 (1) | 23 (1) |
| C(4) | 4778 (2) | 5154 (3) | 1291 (1) | 35 (1) |
| C(5) | 4349 (2) | 5204 (3) | 910 (1) | 34 (1) |
| C(11) | 3167 (2) | 3057 (2) | 431 (1) | 25 (1) |
| C(12) | 4223 (2) | 2532 (2) | 137 (1) | 25 (1) |
| C(13) | 3510 (2) | 2022 (2) | -218 (1) | 29 (1) |
| C(14) | 1824 (2) | 2060 (3) | -286 (1) | 35 (1) |
| C(15) | 826 (2) | 2628 (3) | 14 (1) | 37 (1) |
| C(16) | 1471 (2) | 3135 (3) | 375 (1) | 31 (1) |
| C(17) | 6057 (2) | 2542 (3) | 199 (1) | 36 (1) |
| C(18) | 1091 (3) | 1475 (4) | -672 (1) | 54 (1) |
| C(19) | 377 (2) | 3695 (4) | 704 (1) | 47 (1) |
| C(31) | 5100 (2) | 2908 (2) | 1805 (1) | 24 (1) |
| C(32) | 4160 (2) | 3386 (2) | 2125 (1) | 27 (1) |
| C(33) | 4787 (2) | 2964 (3) | 2496 (1) | 32 (1) |
| C(34) | 6277 (2) | 2115 (3) | 2548 (1) | 34 (1) |
| C(35) | 7175 (2) | 1676 (3) | 2223 (1) | 35 (1) |
| C(36) | 6621 (2) | 2074 (3) | 1847 (1) | 31 (1) |
| C(37) | 2540 (2) | 4343 (3) | 2080 (1) | 41 (1) |
| C(38) | 6936 (3) | 1713 (4) | 2955 (1) | 54 (1) |
| C(39) | 7635 (3) | 1645 (4) | 1497 (1) | 50 (1) |
| H(4) | 5161 (2) | 6114 (3) | 1444 (1) | 49 (5) |
| H(5) | 4384 (2) | 6199 (3) | 744 (1) | 49 (5) |
| H(13) | 4202 (2) | 1634 (2) | -421 (1) | 44 (3) |
| H(15) | -330 (2) | 2671 (3) | -30 (1) | 44 (3) |
| H(17) | 6336 (3) | 2014 (23) | 452 (3) | 88 (2) |
| H(17') | 6460 (3) | 3753 (3) | 193 (5) | 88 (2) |

**Table II.** Fractional Coordinates (x$10^4$) and Isotropic Thermal Parameters (cont'd.)

| | | | | |
|---|---|---|---|---|
| H(17") | 6572 (3) | 1867 (21) | -9 (3) | 88 (2) |
| H(18) | 1391 (21) | 250 (9) | -720 (3) | 88 (2) |
| H(18') | 1514 (19) | 2213 (17) | -882 (1) | 88 (2) |
| H(18") | -109 (3) | 1580 (25) | -666 (2) | 88 (2) |
| H(19) | 397 (20) | 2795 (12) | 908 (3) | 88 (2) |
| H(19') | -751 (6) | 3845 (26) | 604 (1) | 88 (2) |
| H(19") | 777 (15) | 4807 (14) | 813 (4) | 88 (2) |
| H(33) | 4172 (2) | 3268 (3) | 2718 (1) | 44 (3) |
| H(35) | 8196 (2) | 1087 (3) | 2258 (1) | 44 (3) |
| H(37) | 1952 (11) | 3918 (18) | 1846 (3) | 88 (2) |
| H(37') | 2745 (3) | 5604 (4) | 2055 (6) | 88 (2) |
| H(37") | 1874 (10) | 4128 (20) | 2310 (3) | 88 (2) |
| H(38) | 7543 (21) | 2731 (10) | 3057 (2) | 88 (2) |
| H(38') | 7673 (19) | 699 (16) | 2945 (1) | 88 (2) |
| H(38") | 6019 (4) | 1450 (25) | 3126 (2) | 88 (2) |
| H(39) | 7102 (13) | 700 (18) | 1347 (3) | 88 (2) |
| H(39') | 8733 (8) | 1266 (26) | 1585 (1) | 88 (2) |
| H(39") | 7728 (21) | 2688 (8) | 1332 (3) | 88 (2) |

**Table III.** Anisotropic Thermal Parameters (Å x $10^3$)
exp[-19.739($U_{11}$hha*a*...+2($U_{12}$hka*b*...))]

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| P(1) | 50 (1) | 24 (1) | 27 (1) | 0 (1) | 5 (1) | -8 (1) |
| F(11) | 48 (1) | 42 (1) | 50 (1) | -1 (1) | 20 (1) | 0 (1) |
| F(12) | 60 (1) | 39 (1) | 43 (1) | 15 (1) | -14 (1) | -1 (1) |
| F(13) | 58 (1) | 34 (1) | 48 (1) | 9 (1) | 2 (1) | -18 (1) |
| N(1) | 34 (1) | 24 (1) | 22 (1) | 4 (1) | -1 (1) | -4 (1) |
| N(3) | 33 (1) | 23 (1) | 22 (1) | 2 (1) | -2 (1) | 1 (1) |
| C(1) | 37 (1) | 24 (1) | 34 (1) | 6 (1) | 1 (1) | -2 (1) |
| C(2) | 27 (1) | 22 (1) | 21 (1) | 3 (1) | 2 (1) | 0 (1) |
| C(4) | 50 (1) | 24 (1) | 30 (1) | 2 (1) | -5 (1) | -6 (1) |
| C(5) | 49 (1) | 23 (1) | 29 (1) | 6 (1) | -4 (1) | -6 (1) |
| C(11) | 29 (1) | 25 (1) | 21 (1) | 3 (1) | 1 (1) | -2 (1) |
| C(12) | 27 (1) | 22 (1) | 26 (1) | 5 (1) | 3 (1) | -1 (1) |

**Table III.** Anisotropic Thermal Parameters (Å x $10^3$) (cont'd.)

| | | | | | | |
|---|---|---|---|---|---|---|
| C(13) | 37 (1) | 24 (1) | 25 (1) | 0 (1) | 8 (1) | 0 (1) |
| C(14) | 41 (1) | 35 (1) | 27 (1) | -1 (1) | -5 (1) | -2 (1) |
| C(15) | 26 (1) | 50 (1) | 35 (1) | -2 (1) | -5 (1) | 0 (1) |
| C(16) | 29 (1) | 37 (1) | 28 (1) | 2 (1) | 4 (1) | 2 (1) |
| C(17) | 27 (1) | 36 (1) | 45 (1) | 3 (1) | 4 (1) | 0 (1) |
| C(18) | 63 (1) | 62 (2) | 36 (1) | -12 (1) | -13 (1) | 2 (1) |
| C(19) | 36 (1) | 68 (2) | 38 (1) | -3 (1) | 10 (1) | 8 (1) |
| C(31) | 31 (1) | 22 (1) | 21 (1) | 1 (1) | -1 (1) | 1 (1) |
| C(32) | 34 (1) | 23 (1) | 24 (1) | -1 (1) | 2 (1) | 3 (1) |
| C(33) | 46 (1) | 27 (1) | 22 (1) | 0 (1) | 4 (1) | 0 (1) |
| C(34) | 48 (1) | 27 (1) | 27 (1) | 2 (1) | -9 (1) | 1 (1) |
| C(35) | 35 (1) | 34 (1) | 35 (1) | 0 (1) | -9 (1) | 7 (1) |
| C(36) | 29 (1) | 33 (1) | 30 (1) | -1 (1) | 0 (1) | 2 (1) |
| C(37) | 44 (1) | 38 (1) | 42 (1) | 0 (1) | 6 (1) | 16 (1) |
| C(38) | 77 (2) | 50 (1) | 33 (1) | 5 (1) | -21 (1) | 10 (1) |
| C(39) | 36 (1) | 74 (2) | 41 (1) | -6 (1) | 7 (1) | 15 (1) |

**Table IV.** Interatomic Distances (Å)

| | | | | | |
|---|---|---|---|---|---|
| P(1)-C(1) | 1.845 (2) | N(3)-C(31) | 1.446 (2) | C(16)-C(19) | 1.512 (2) |
| P(1)-C(2) | 1.784 (2) | C(4)-C(5) | 1.343 (2) | C(31)-C(36) | 1.396 (2) |
| F(11)-C(1) | 1.351 (2) | C(11)-C(16) | 1.390 (2) | C(31)-C(32) | 1.397 (2) |
| F(12)-C(1) | 1.359 (2) | C(11)-C(12) | 1.396 (2) | C(32)-C(33) | 1.395 (2) |
| F(13)-C(1) | 1.358 (2) | C(12)-C(13) | 1.391 (2) | C(32)-C(37) | 1.511 (2) |
| N(1)-C(2) | 1.370 (2) | C(12)-C(17) | 1.503 (2) | C(33)-C(34) | 1.382 (3) |
| N(1)-C(5) | 1.378 (2) | C(13)-C(14) | 1.387 (3) | C(34)-C(35) | 1.387 (3) |
| N(1)-C(11) | 1.439 (2) | C(14)-C(15) | 1.393 (3) | C(34)-C(38) | 1.513 (2) |
| N(3)-C(2) | 1.365 (2) | C(14)-C(18) | 1.507 (3) | C(35)-C(36) | 1.388 (2) |
| N(3)-C(4) | 1.390 (2) | C(15)-C(16) | 1.389 (2) | C(36)-C(39) | 1.505 (2) |

**Table V.** Intramolecular Angles (°)

| | | | |
|---|---|---|---|
| C(2)-P(1)-C(1) | 101.66 (8) | F(13)-C(1)-F(12) | 103.93 (14) |
| C(2)-N(1)-C(5) | 110.87 (13) | F(11)-C(1)-P(1) | 116.55 (13) |
| C(2)-N(1)-C(11) | 124.1 (2) | F(13)-C(1)-P(1) | 107.25 (12) |
| C(5)-N(1)-C(11) | 124.87 (14) | F(12)-C(1)-P(1) | 118.14 (13) |
| C(2)-N(3)-C(4) | 110.10 (13) | N(3)-C(2)-N(1) | 104.54 (14) |
| C(2)-N(3)-C(31) | 128.6 (2) | N(3)-C(2)-P(1) | 136.69 (12) |
| C(4)-N(3)-C(31) | 120.97 (14) | N(1)-C(2)-P(1) | 118.66 (12) |
| F(11)-C(1)-F(13) | 105.66 (14) | C(5)-C(4)-N(3) | 107.5 (2) |
| F(11)-C(1)-F(12) | 104.0 (2) | C(4)-C(5)-N(1) | 107.0 (2) |

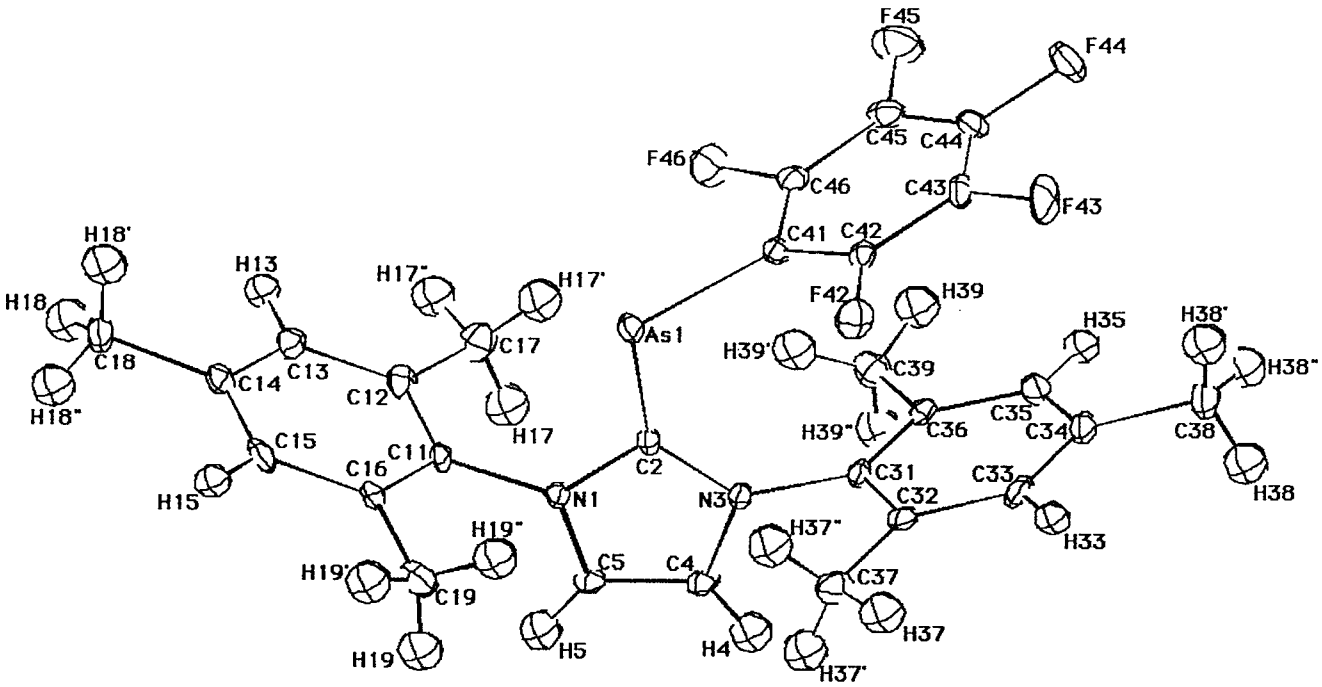
**Table V.** Intramolecular Angles (°) (cont'd.)

| | | | |
|---|---|---|---|
| C(16)-C(11)-C(12) | 122.58 (14) | C(36)-C(31)-C(32) | 122.61 (14) |
| C(16)-C(11)-N(1) | 118.23 (14) | C(36)-C(31)-N(3) | 118.24 (14) |
| C(12)-C(11)-N(1) | 119.20 (14) | C(32)-C(31)-N(3) | 118.89 (14) |
| C(13)-C(12)-C(11) | 117.35 (14) | C(33)-C(32)-C(31) | 117.2 (2) |
| C(13)-C(12)-C(17) | 121.2 (2) | C(33)-C(32)-C(37) | 120.4 (2) |
| C(11)-C(12)-C(17) | 121.4 (2) | C(31)-C(32)-C(37) | 122.5 (2) |
| C(14)-C(13)-C(12) | 122.2 (2) | C(34)-C(33)-C(32) | 121.9 (2) |
| C(13)-C(14)-C(15) | 118.3 (2) | C(33)-C(34)-C(35) | 119.0 (2) |
| C(13)-C(14)-C(18) | 120.8 (2) | C(33)-C(34)-C(38) | 120.4 (2) |
| C(15)-C(14)-C(18) | 120.9 (2) | C(35)-C(34)-C(38) | 120.6 (2) |
| C(16)-C(15)-C(14) | 121.9 (2) | C(34)-C(35)-C(36) | 121.8 (2) |
| C(15)-C(16)-C(11) | 117.7 (2) | C(35)-C(36)-C(31) | 117.6 (2) |
| C(15)-C(16)-C(19) | 121.7 (2) | C(35)-C(36)-C(39) | 121.2 (2) |
| C(11)-C(16)-C(19) | 120.6 (2) | C(31)-C(36)-C(39) | 121.2 (2) |

**Table I.** Summary of X-ray Diffraction Data for 2-(pentafluorophenyl-arsenidene)-1,3-dimesitylimidazole (**1•AsC$_6$F$_5$**).

| | | |
|---|---|---|
| Empirical formula | $C_{27}H_{24}AsF_5N_2$ | |
| Formula weight | 546.40 | |
| Temperature | 183(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Triclinic | |
| Space group | P-1 | |
| Unit cell dimensions | a = 7.146(2) Å | α = 83.158(7)° |
| | b = 12.306(2) Å | β = 76.370(10)° |
| | c = 14.646(2) Å | γ = 84.310(10)° |
| Volume, Z | 1239.4(4) Å$^3$, 2 | |
| Density (calculated) | 1.464 g/cm$^3$ | |
| Absorption coefficient | 14.27 cm$^{-1}$ | |
| F(000) | 556 | |
| Crystal size | .59 x .74 x .35 mm | |
| Theta range for data collection | 2.09 to 27.50° | |
| Limiting indices | $-1 \le h \le 9$, $-15 \le k \le 15$, $-18 \le l \le 19$ | |
| Reflections collected | 6836 | |
| Independent reflections | 5477 [R(int) = 0.0599] | |
| Absorption correction | None | |
| Refinement method | Full-matrix least-squares on F$^2$ (SHELXL-93) | |
| Data / restraints / parameters | 5477 / 0 / 327 | |
| Goodness-of-fit on F$^2$ | 1.024 | |
| Final R indices [I>2σ(I)] | R1 = 0.0868, wR2 = 0.1834 | |
| R indices (all data) | R1 = 0.1772, wR2 = 0.2322 | |
| Extinction coefficient, $\chi$[a] | 0.005(2) | |
| Largest diff. peak and hole | 1.415 and -1.017eÅ$^{-3}$ | |

a) $F^* = F[1 + 0.001\chi F^2\lambda^3/\sin(2\theta)]^{-1/4}$




ORTEP drawing of 2-(pentafluorophenyl-arsenidene)-1,3-dimesitylimidazole (**1•AsC$_6$F$_5$**).

**Table II.** Fractional Coordinates ($x10^4$) and Isotropic Thermal Parameters

| Atom | X | Y | Z | $U_{eq}$ ($Å^2 \times 10^3$) |
|---|---|---|---|---|
| As(1) | 6899 (1) | 8215 (1) | 8144 (1) | 36 (1) |
| F(42) | 8423 (7) | 9341 (3) | 6077 (3) | 51 (1) |
| F(43) | 9191 (8) | 8525 (5) | 4409 (3) | 69 (2) |
| F(44) | 8764 (8) | 6383 (5) | 4308 (3) | 71 (2) |
| F(45) | 7580 (9) | 5049 (4) | 5912 (4) | 75 (2) |
| F(46) | 6875 (8) | 5826 (4) | 7597 (3) | 59 (1) |
| N(1) | 8953 (8) | 7596 (5) | 9597 (4) | 28 (1) |
| N(3) | 10990 (8) | 7474 (4) | 8263 (4) | 26 (1) |
| C(2) | 9078 (10) | 7692 (5) | 8649 (4) | 24 (2) |
| C(4) | 12013 (11) | 7249 (6) | 8973 (5) | 32 (2) |
| C(5) | 10736 (10) | 7328 (6) | 9802 (5) | 32 (2) |
| C(11) | 7144 (10) | 7625 (6) | 10300 (4) | 27 (2) |
| C(12) | 6237 (12) | 6649 (6) | 10580 (5) | 35 (2) |
| C(13) | 4485 (11) | 6690 (6) | 11229 (5) | 36 (2) |
| C(14) | 3672 (12) | 7643 (7) | 11612 (5) | 38 (2) |
| C(15) | 4621 (13) | 8578 (7) | 11336 (5) | 43 (2) |
| C(16) | 6375 (11) | 8595 (6) | 10670 (4) | 29 (2) |
| C(17) | 7126 (13) | 5607 (6) | 10168 (6) | 50 (2) |
| C(18) | 1719 (13) | 7658 (9) | 12308 (6) | 63 (3) |
| C(19) | 7420 (13) | 9637 (7) | 10364 (6) | 49 (2) |
| C(31) | 11893 (10) | 7531 (6) | 7258 (4) | 29 (2) |
| C(32) | 12359 (11) | 8558 (6) | 6802 (5) | 34 (2) |
| C(33) | 13153 (11) | 8595 (7) | 5818 (5) | 41 (2) |
| C(34) | 13483 (12) | 7678 (8) | 5351 (5) | 47 (2) |
| C(35) | 13060 (12) | 6679 (7) | 5849 (5) | 45 (2) |
| C(36) | 12267 (10) | 6573 (6) | 6825 (5) | 32 (2) |
| C(37) | 12017 (13) | 9564 (6) | 7300 (6) | 46 (2) |
| C(38) | 14286 (14) | 7760 (9) | 4288 (6) | 70 (3) |
| C(39) | 11840 (13) | 5469 (6) | 7352 (6) | 50 (2) |
| C(41) | 7681 (10) | 7616 (6) | 6906 (5) | 26 (2) |
| C(42) | 8254 (10) | 8264 (6) | 6071 (5) | 31 (2) |
| C(43) | 8613 (12) | 7862 (7) | 5202 (5) | 42 (2) |
| C(44) | 8438 (12) | 6782 (8) | 5154 (5) | 45 (2) |
| C(45) | 7819 (12) | 6103 (6) | 5962 (6) | 43 (2) |

**Table II.** Fractional Coordinates (x$10^4$) and Isotropic Thermal Parameters (cont'd.)

| | | | | |
|---|---|---|---|---|
| C(46) | 7491 (11) | 6541 (6) | 6814 (5) | 36 (2) |
| H(4) | 13364 (11) | 7073 (6) | 8887 (5) | 42 (16) |
| H(5) | 11009 (10) | 7220 (6) | 10412 (5) | 42 (16) |
| H(13) | 3821 (11) | 6040 (6) | 11418 (5) | 36 (10) |
| H(15) | 4073 (13) | 9235 (7) | 11605 (5) | 36 (10) |
| H(17) | 8454 (32) | 5471 (27) | 10249 (39) | 83 (10) |
| H(17') | 7131 (82) | 5676 (20) | 9493 (12) | 83 (10) |
| H(17") | 6372 (53) | 4993 (10) | 10491 (30) | 83 (10) |
| H(18) | 1614 (41) | 6963 (23) | 12714 (32) | 105 (16) |
| H(18') | 689 (13) | 7753 (57) | 11960 (6) | 105 (16) |
| H(18") | 1596 (42) | 8267 (34) | 12697 (33) | 105 (16) |
| H(19) | 8515 (54) | 9604 (23) | 10666 (35) | 83 (10) |
| H(19') | 6530 (27) | 10272 (8) | 10553 (39) | 83 (10) |
| H(19") | 7892 (80) | 9710 (27) | 9677 (7) | 83 (10) |
| H(33) | 13466 (11) | 9281 (7) | 5473 (5) | 36 (10) |
| H(35) | 13312 (12) | 6039 (7) | 5522 (5) | 36 (10) |
| H(37) | 12500 (83) | 10189 (12) | 6856 (12) | 83 (10) |
| H(37') | 12696 (73) | 9464 (20) | 7816 (28) | 83 (10) |
| H(37") | 10630 (14) | 9705 (29) | 7557 (37) | 83 (10) |
| H(38) | 15381 (66) | 8223 (49) | 4122 (8) | 105 (16) |
| H(38') | 13277 (32) | 8086 (56) | 3966 (6) | 105 (16) |
| H(38") | 14717 (99) | 7026 (11) | 4091 (9) | 105 (16) |
| H(39) | 11692 (90) | 4961 (15) | 6912 (10) | 83 (10) |
| H(39') | 10642 (48) | 5541 (11) | 7839 (30) | 83 (10) |
| H(39") | 12905 (42) | 5186 (23) | 7651 (36) | 83 (10) |

**Table III.** Anisotropic Thermal Parameters (Å x $10^3$)
exp[-19.739($U_{11}$hha*a*...+2($U_{12}$hka*b*...))]

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| As(1) | 24 (1) | 62 (1) | 23 (1) | -10 (1) | -6 (1) | 3 (1) |
| F(42) | 57 (3) | 39 (3) | 50 (3) | 4 (2) | -5 (2) | -7 (2) |
| F(43) | 67 (4) | 105 (4) | 22 (2) | 15 (3) | 2 (2) | -5 (3) |
| F(44) | 59 (4) | 116 (5) | 43 (3) | -42 (3) | -15 (3) | 9 (3) |
| F(45) | 81 (5) | 60 (4) | 94 (5) | -35 (3) | -26 (4) | -7 (3) |
| F(46) | 73 (4) | 50 (3) | 48 (3) | 10 (2) | -8 (3) | -16 (3) |

**Table III.** Anisotropic Thermal Parameters (Å x $10^3$) (cont'd.)

| | | | | | | |
|---|---|---|---|---|---|---|
| N(1) | 22 (3) | 39 (3) | 21 (3) | -4 (2) | -6 (2) | -1 (3) |
| N(3) | 19 (3) | 39 (3) | 18 (3) | -1 (2) | -1 (2) | -5 (2) |
| C(2) | 24 (4) | 30 (4) | 18 (3) | -1 (3) | -2 (3) | -3 (3) |
| C(4) | 22 (4) | 41 (4) | 33 (4) | 3 (3) | -10 (3) | -1 (3) |
| C(5) | 24 (4) | 45 (4) | 29 (4) | 0 (3) | -13 (3) | -1 (3) |
| C(11) | 27 (4) | 41 (4) | 13 (3) | 1 (3) | -3 (3) | -4 (3) |
| C(12) | 39 (5) | 39 (4) | 23 (4) | 6 (3) | -7 (3) | 0 (4) |
| C(13) | 33 (5) | 46 (5) | 27 (4) | 6 (3) | -8 (3) | -6 (4) |
| C(14) | 34 (5) | 63 (5) | 18 (3) | -2 (3) | -8 (3) | -5 (4) |
| C(15) | 48 (5) | 62 (6) | 21 (4) | -18 (4) | -9 (4) | 8 (4) |
| C(16) | 35 (4) | 39 (4) | 15 (3) | -3 (3) | -6 (3) | -5 (3) |
| C(17) | 46 (6) | 44 (5) | 54 (5) | 0 (4) | -3 (4) | -4 (4) |
| C(18) | 36 (6) | 126 (9) | 26 (4) | -18 (5) | 0 (4) | 0 (5) |
| C(19) | 56 (6) | 53 (5) | 44 (5) | -16 (4) | -17 (4) | 0 (4) |
| C(31) | 16 (4) | 49 (5) | 19 (3) | 0 (3) | 0 (3) | -4 (3) |
| C(32) | 21 (4) | 55 (5) | 30 (4) | 0 (3) | -11 (3) | -10 (3) |
| C(33) | 20 (4) | 73 (6) | 27 (4) | 7 (4) | -1 (3) | -11 (4) |
| C(34) | 29 (5) | 89 (7) | 22 (4) | -5 (4) | -3 (3) | -8 (4) |
| C(35) | 32 (5) | 71 (6) | 33 (4) | -21 (4) | -6 (4) | 2 (4) |
| C(36) | 14 (4) | 49 (5) | 33 (4) | -10 (3) | -3 (3) | -1 (3) |
| C(37) | 48 (6) | 45 (5) | 44 (5) | 6 (4) | -12 (4) | -14 (4) |
| C(38) | 40 (6) | 137 (10) | 28 (4) | -8 (5) | -1 (4) | -6 (6) |
| C(39) | 58 (6) | 45 (5) | 50 (5) | -13 (4) | -17 (5) | 7 (4) |
| C(41) | 23 (4) | 32 (4) | 24 (3) | 1 (3) | -8 (3) | -3 (3) |
| C(42) | 18 (4) | 49 (5) | 25 (4) | -2 (3) | -5 (3) | 2 (3) |
| C(43) | 28 (5) | 71 (6) | 20 (4) | 0 (4) | -2 (3) | 3 (4) |
| C(44) | 33 (5) | 75 (6) | 31 (4) | -20 (4) | -12 (4) | -1 (4) |
| C(45) | 36 (5) | 38 (5) | 58 (6) | -17 (4) | -12 (4) | -4 (4) |
| C(46) | 29 (4) | 50 (5) | 29 (4) | 6 (3) | -12 (3) | -9 (3) |

**Table IV.** Interatomic Distances (Å)

| | | | | | |
|---|---|---|---|---|---|
| C(2)-As(1) | 1.902 (7) | C(4)-N(3) | 1.393 (9) | C(42)-C(43) | 1.378 (10) |
| C(41)-As(1) | 1.976 (7) | C(5)-C(4) | 1.344 (10) | C(43)-F(43) | 1.342 (9) |
| C(2)-N(1) | 1.361 (8) | C(41)-C(46) | 1.368 (10) | C(43)-C(44) | 1.359 (12) |
| C(2)-N(3) | 1.363 (8) | C(41)-C(42) | 1.376 (9) | C(44)-F(44) | 1.347 (8) |
| C(5)-N(1) | 1.377 (9) | C(42)-F(42) | 1.344 (8) | C(44)-C(45) | 1.373 (12) |

**Table IV.** Interatomic Distances (Å) (cont'd.)

| | | |
|---|---|---|
| C(45)-F(45) 1.338 (9) | C(13)-C(14) 1.377 (10) | C(32)-C(33) 1.416 (10) |
| C(45)-C(46) 1.379 (10) | C(14)-C(15) 1.365 (11) | C(32)-C(37) 1.482 (11) |
| C(46)-F(46) 1.372 (8) | C(14)-C(18) 1.521 (11) | C(33)-C(34) 1.361 (11) |
| C(11)-C(16) 1.380 (9) | C(15)-C(16) 1.395 (11) | C(34)-C(35) 1.375 (12) |
| C(11)-C(12) 1.394 (10) | C(16)-C(19) 1.517 (11) | C(34)-C(38) 1.522 (10) |
| C(11)-N(1) 1.450 (8) | C(31)-C(36) 1.379 (10) | C(35)-C(36) 1.403 (10) |
| C(12)-C(13) 1.383 (10) | C(31)-C(32) 1.391 (10) | C(36)-C(39) 1.502 (11) |
| C(12)-C(17) 1.502 (10) | C(31)-N(3) 1.457 (8) | |

**Table V.** Intramolecular Angles (°)

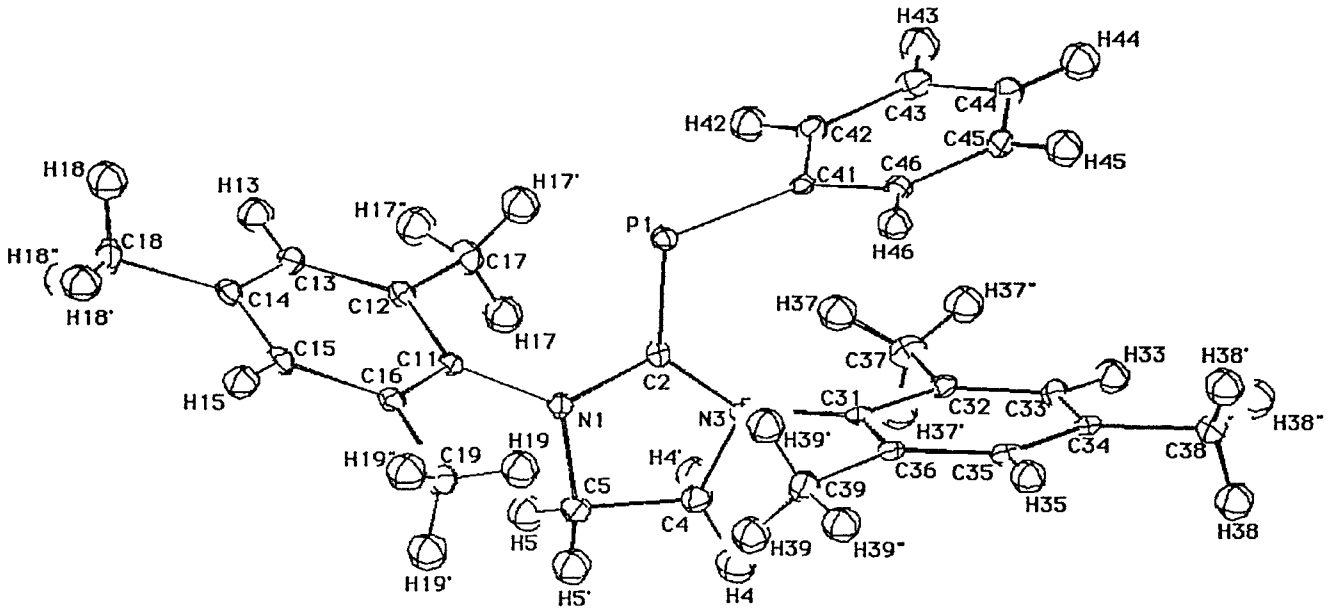
| | | | |
|---|---|---|---|
| C(2)-As(1)-C(41) | 99.8 (3) | F(46)-C(46)-C(45) | 115.2 (7) |
| N(1)-C(2)-N(3) | 104.6 (6) | C(16)-C(11)-C(12) | 122.0 (7) |
| N(1)-C(2)-As(1) | 120.9 (5) | C(16)-C(11)-N(1) | 120.2 (6) |
| N(3)-C(2)-As(1) | 134.1 (5) | C(12)-C(11)-N(1) | 117.8 (6) |
| C(2)-N(1)-C(5) | 111.3 (6) | C(13)-C(12)-C(11) | 117.4 (7) |
| C(2)-N(1)-C(11) | 123.9 (6) | C(13)-C(12)-C(17) | 122.0 (7) |
| C(5)-N(1)-C(11) | 124.2 (6) | C(11)-C(12)-C(17) | 120.6 (7) |
| C(2)-N(3)-C(4) | 110.0 (5) | C(14)-C(13)-C(12) | 122.1 (7) |
| C(2)-N(3)-C(31) | 126.1 (6) | C(15)-C(14)-C(13) | 118.9 (7) |
| C(4)-N(3)-C(31) | 123.8 (6) | C(15)-C(14)-C(18) | 120.7 (8) |
| C(4)-C(5)-N(1) | 106.7 (6) | C(13)-C(14)-C(18) | 120.4 (8) |
| C(5)-C(4)-N(3) | 107.4 (6) | C(14)-C(15)-C(16) | 121.8 (7) |
| C(46)-C(41)-C(42) | 115.3 (6) | C(11)-C(16)-C(15) | 117.8 (7) |
| C(46)-C(41)-As(1) | 121.6 (5) | C(11)-C(16)-C(19) | 120.7 (7) |
| C(42)-C(41)-As(1) | 122.8 (5) | C(15)-C(16)-C(19) | 121.5 (7) |
| F(42)-C(42)-C(41) | 120.2 (6) | C(36)-C(31)-C(32) | 124.1 (6) |
| F(42)-C(42)-C(43) | 117.1 (7) | C(36)-C(31)-N(3) | 118.7 (6) |
| C(41)-C(42)-C(43) | 122.6 (7) | C(32)-C(31)-N(3) | 117.2 (6) |
| F(43)-C(43)-C(44) | 120.1 (7) | C(31)-C(32)-C(33) | 115.9 (7) |
| F(43)-C(43)-C(42) | 120.3 (8) | C(31)-C(32)-C(37) | 122.7 (7) |
| C(44)-C(43)-C(42) | 119.6 (7) | C(33)-C(32)-C(37) | 121.4 (7) |
| F(44)-C(44)-C(43) | 120.1 (8) | C(34)-C(33)-C(32) | 122.1 (8) |
| F(44)-C(44)-C(45) | 119.4 (8) | C(33)-C(34)-C(35) | 119.2 (7) |
| C(43)-C(44)-C(45) | 120.4 (7) | C(33)-C(34)-C(38) | 120.3 (8) |
| F(45)-C(45)-C(44) | 120.4 (8) | C(35)-C(34)-C(38) | 120.5 (8) |
| F(45)-C(45)-C(46) | 121.8 (8) | C(34)-C(35)-C(36) | 122.2 (7) |
| C(44)-C(45)-C(46) | 117.8 (7) | C(31)-C(36)-C(35) | 116.4 (7) |
| C(41)-C(46)-F(46) | 120.5 (7) | C(31)-C(36)-C(39) | 122.6 (6) |
| C(41)-C(46)-C(45) | 124.3 (7) | C(35)-C(36)-C(39) | 121.0 (7) |

**Table I.** Summary of X-ray Diffraction Data for 2-(phenylphosphinidene)-1,3-dimesitylimidazoline (**3•PPh**).

| | |
|---|---|
| formula | $C_{27}H_{31}N_2P$ |
| crystallization method | from hexane on cooling (-25 °C) |
| color | yellow |
| shape | irregular block |
| size, mm | 0.28 x 0.24 x 0.30 |
| symmetry | monoclinic |
| space group | $P2_1/c$ (No. 14) |
| a, Å | 17.044 (5) |
| b, Å | 7.626 (2) |
| c, Å | 18.525 (4) |
| β, deg | 107.76 (2) |
| temperature, °C | -100 |
| volume, $Å^3$ | 2293.1.0 |
| Z | 4 |
| Fw | 414.53 |
| calculated density, g/cc | 1.201 |
| μ(Mo), $cm^{-1}$ | 1.31 |
| diffractometer | Syntex R3 |
| radiation (graphite monochromator) | MoKα |
| scan method | ω |
| data octants | +++, ++- |
| 2θ | ≥4.5°, ≤ 48.0° |
| maximum h k l | 19 8 21 |
| scan width | 1.00 ω |
| scan speed | 2.00-8.40°/min |
| typical peak-with @ half height | 0.28° |
| data collected | 4054 |
| 2 standards collected 43x | no correction for 2% intensity fluctuation |
| variation in azimuthal scan | 2.5% |
| duplicates | 143 (1.6% R-merge) |
| no. of unique data (I≥ 3.0σ(I)) | 1652 |
| absorption correction | none |
| solution method | direct methods (MULTAN) |
| refinement method | full-matrix least squares on F |
| anomalous dispersion | P |
| weighting scheme | weights ∝ $[\sigma^2(I)+0.0009I^2]^{-1/2}$ |
| atoms refined | aniso: all non-hydrogen atoms<br>isotropic H (near refined positions) |
| parameters varied | 271 |
| data/parameter ratio | 6.09 |

**Table I** (cont'd).

| | |
|---|---|
| R, Rw | 0.044. 0.036 |
| error of fit | 1.03 |
| max shift $\Delta/\sigma$ | 0.02 |
| max residual density, e/Å$^3$ | 0.25 (near C21) |




ORTEP drawing of 2-(phenylphosphinidene)-1,3-dimesitylimidazoline (**3•PPh**).

**Table II.** Fractional Coordinates (x$10^4$) and Isotropic Thermal Parameters

| Atom | X | Y | Z | $B_{ISO}$ |
|---|---|---|---|---|
| P(1) | 3053.0 (7) | 572.5 (14) | 2828.2 (6) | 2.0 (0)' |
| N(1) | 3648 (2) | 3760 (4) | 3392 (2) | 2.1 (1)' |
| N(3) | 2424 (2) | 4040 (4) | 2551 (2) | 2.0 (1)' |
| C(2) | 3024 (3) | 2850 (5) | 2910 (2) | 1.8 (1)' |
| C(4) | 2712 (3) | 5850 (6) | 2734 (2) | 3.0 (1)' |
| C(5) | 3462 (2) | 5628 (6) | 3429 (2) | 2.9 (1)' |
| C(11) | 4449 (2) | 3084 (5) | 3779 (2) | 1.9 (1)' |
| C(12) | 5038 (2) | 2972 (5) | 3390 (2) | 2.1 (1)' |
| C(13) | 5828 (2) | 2408 (6) | 3792 (2) | 2.4 (1)' |
| C(14) | 6032 (2) | 1927 (5) | 4551 (2) | 2.1 (1)' |
| C(15) | 5434 (2) | 2040 (5) | 4914 (2) | 2.1 (1)' |
| C(16) | 4640 (2) | 2640 (5) | 4545 (2) | 2.1 (1)' |
| C(17) | 4827 (3) | 3448 (6) | 2567 (2) | 3.1 (1)' |
| C(18) | 6898 (2) | 1356 (6) | 4979 (2) | 3.2 (1)' |
| C(19) | 4028 (3) | 2852 (6) | 4971 (2) | 3.0 (1)' |
| C(31) | 1559 (2) | 3715 (5) | 2242 (2) | 1.8 (1)' |
| C(32) | 1177 (2) | 4103 (5) | 1471 (2) | 2.0 (1)' |
| C(33) | 332 (2) | 3823 (5) | 1185 (2) | 2.2 (1)' |
| C(34) | -125 (2) | 3162 (6) | 1622 (2) | 2.2 (1)' |
| C(35) | 267 (2) | 2817 (5) | 2384 (2) | 2.1 (1)' |
| C(36) | 1108 (2) | 3109 (5) | 2703 (2) | 1.9 (1)' |
| C(37) | 1662 (3) | 4777 (6) | 982 (2) | 3.0 (1)' |
| C(38) | -1038 (3) | 2835 (6) | 1282 (2) | 3.0 (1)' |
| C(39) | 1504 (2) | 2772 (6) | 3540 (2) | 2.7 (1)' |
| C(41) | 2259 (2) | 247 (5) | 1907 (2) | 1.7 (1)' |
| C(42) | 2459 (2) | 541 (6) | 1238 (2) | 2.6 (1)' |
| C(43) | 1889 (3) | 219 (6) | 532 (2) | 3.1 (1)' |
| C(44) | 1112 (3) | -392 (6) | 481 (2) | 3.1 (1)' |
| C(45) | 916 (2) | -724 (6) | 1132 (2) | 2.8 (1)' |
| C(46) | 1482 (2) | -413 (5) | 1830 (2) | 2.0 (1)' |
| H(4) | 2302 | 6510 | 2864 | 4.0 |
| H(4') | 2884 | 6318 | 2330 | 4.0 |
| H(5) | 3905 | 6313 | 3376 | 3.8 |
| H(5') | 3305 | 5842 | 3876 | 3.8 |

**Table II.** Fractional Coordinates (x$10^4$) and Isotropic Thermal Parameters (cont'd.)

| | | | | |
|---|---|---|---|---|
| H(13) | 6237 | 2348 | 3542 | 3.5 |
| H(15) | 5565 | 1705 | 5429 | 3.2 |
| H(17) | 4523 | 4509 | 2474 | 4.1 |
| H(17') | 4506 | 2535 | 2266 | 4.1 |
| H(17") | 5321 | 3591 | 2433 | 4.1 |
| H(18) | 7042 | 364 | 4732 | 4.2 |
| H(18') | 6929 | 1052 | 5482 | 4.2 |
| H(18") | 7272 | 2287 | 4983 | 4.2 |
| H(19) | 3492 | 2599 | 4651 | 4.0 |
| H(19') | 4048 | 4026 | 5152 | 4.0 |
| H(19") | 4164 | 2069 | 5393 | 4.0 |
| H(33) | 64 | 4098 | 668 | 3.3 |
| H(35) | -43 | 2382 | 2689 | 3.2 |
| H(37) | 2204 | 4284 | 1151 | 4.0 |
| H(37') | 1702 | 6016 | 1024 | 4.0 |
| H(37") | 1405 | 4447 | 473 | 4.0 |
| H(38) | -1337 | 3613 | 1496 | 4.0 |
| H(38') | -1159 | 1657 | 1372 | 4.0 |
| H(38") | -1189 | 3030 | 745 | 4.0 |
| H(39) | 1845 | 3739 | 3761 | 3.7 |
| H(39') | 1823 | 1735 | 3609 | 3.7 |
| H(39") | 1083 | 2646 | 3779 | 3.7 |
| H(42) | 2989 | 959 | 1262 | 3.6 |
| H(43) | 2032 | 424 | 83 | 4.2 |
| H(44) | 716 | -592 | 0 | 4.1 |
| H(45) | 387 | -1179 | 1106 | 3.8 |
| H(46) | 1332 | -653 | 2274 | 3.0 |

**Table III.** Anisotropic Thermal Parameters (Å x $10^3$)
exp[-19.739($U_{11}$hha*a*...+2($U_{12}$hka*b*...))]

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|
| P(1) | 26.9 (6) | 18.5 (6) | 25.4 (6) | 1.5 (7) | 1.2 (5) | -1.1 (6) |
| N(1) | 23 (2) | 17 (2) | 35 (2) | 1 (2) | 0 (2) | -5 (2) |
| N(3) | 24 (2) | 15 (2) | 33 (2) | 1 (2) | 3 (2) | -1 (2) |
| C(2) | 22 (2) | 24 (2) | 23 (2) | -1 (2) | 6 (2) | 0 (2) |

**Table III.** Anisotropic Thermal Parameters (Å x $10^3$) (cont'd.)

| | | | | | | |
|---|---|---|---|---|---|---|
| C(4) | 32 (3) | 24 (3) | 56 (3) | 3 (2) | 11 (2) | -4 (2) |
| C(5) | 29 (3) | 23 (3) | 54 (3) | -5 (2) | 8 (2) | -6 (3) |
| C(11) | 20 (2) | 18 (2) | 30 (2) | -2 (2) | 1 (2) | -5 (2) |
| C(12) | 28 (3) | 24 (2) | 26 (2) | -5 (2) | 7 (2) | -2 (2) |
| C(13) | 23 (2) | 34 (3) | 36 (3) | -4 (2) | 12 (2) | -7 (2) |
| C(14) | 29 (2) | 20 (2) | 27 (2) | -5 (2) | 2 (2) | -3 (2) |
| C(15) | 31 (3) | 21 (3) | 24 (2) | -4 (2) | 2 (2) | -1 (2) |
| C(16) | 25 (2) | 23 (2) | 31 (3) | -5 (2) | 7 (2) | -7 (2) |
| C(17) | 43 (3) | 40 (3) | 30 (2) | -2 (3) | 7 (2) | 4 (2) |
| C(18) | 27 (3) | 40 (3) | 46 (3) | 0 (2) | -2 (2) | 1 (2) |
| C(19) | 36 (3) | 38 (3) | 42 (3) | -1 (2) | 14 (2) | -5 (2) |
| C(31) | 25 (2) | 14 (2) | 30 (2) | 4 (2) | 7 (2) | -4 (2) |
| C(32) | 31 (3) | 21 (3) | 25 (2) | 8 (2) | 10 (2) | 4 (2) |
| C(33) | 30 (3) | 31 (3) | 20 (2) | 8 (2) | 2 (2) | 3 (2) |
| C(34) | 25 (2) | 24 (2) | 34 (3) | 6 (2) | 5 (2) | -10 (2) |
| C(35) | 31 (3) | 25 (3) | 28 (3) | 4 (2) | 15 (2) | -5 (2) |
| C(36) | 26 (2) | 21 (2) | 24 (2) | 7 (2) | 8 (2) | -5 (2) |
| C(37) | 44 (3) | 34 (3) | 37 (3) | 6 (2) | 15 (2) | 10 (2) |
| C(38) | 29 (3) | 43 (3) | 41 (3) | 1 (2) | 10 (2) | -9 (2) |
| C(39) | 32 (3) | 44 (3) | 29 (2) | 4 (2) | 9 (2) | 1 (2) |
| C(41) | 23 (2) | 17 (2) | 23 (2) | 7 (2) | 6 (2) | 0 (2) |
| C(42) | 31 (2) | 34 (3) | 33 (3) | 7 (2) | 10 (2) | 2 (2) |
| C(43) | 51 (3) | 44 (3) | 25 (3) | 16 (3) | 13 (2) | 4 (2) |
| C(44) | 42 (3) | 46 (3) | 20 (2) | 18 (3) | -5 (2) | -6 (2) |
| C(45) | 27 (2) | 28 (3) | 41 (3) | 6 (2) | -1 (2) | -3 (3) |
| C(46) | 28 (2) | 22 (2) | 24 (2) | 4 (2) | 5 (2) | 1 (2) |

**Table IV.** Interatomic Distances (Å)

| | | | | | |
|---|---|---|---|---|---|
| P(1)-C(2) | 1.746 (4) | C(11)-C(12) | 1.406 (5) | C(31)-C(32) | 1.408 (5) |
| P(1)-C(41) | 1.843 (4) | C(11)-C(16) | 1.397 (5) | C(31)-C(36) | 1.391 (5) |
| N(1)-C(2) | 1.352 (5) | C(12)-C(13) | 1.393 (5) | C(32)-C(33) | 1.391 (5) |
| N(1)-C(5) | 1.465 (5) | C(12)-C(17) | 1.500 (5) | C(32)-C(37) | 1.493 (5) |
| N(1)-C(11) | 1.431 (5) | C(13)-C(14) | 1.391 (5) | C(33)-C(34) | 1.379 (5) |
| N(3)-C(2) | 1.378 (5) | C(14)-C(15) | 1.384 (5) | C(34)-C(35) | 1.391 (5) |
| N(3)-C(4) | 1.469 (5) | C(14)-C(18) | 1.511 (5) | C(34)-C(38) | 1.510 (5) |
| N(3)-C(31) | 1.432 (5) | C(15)-C(16) | 1.395 (5) | C(35)-C(36) | 1.392 (5) |
| C(4)-C(5) | 1.522 (6) | C(16)-C(19) | 1.497 (5) | C(36)-C(39) | 1.512 (5) |

**Table IV.** Interatomic Distances (Å) (cont'd.)

| | | | | | |
|---|---|---|---|---|---|
| C(41)-C(42) | 1.400 (5) | C(17)-H(17') | 0.953 (0) | C(38)-H(38) | 0.944 (0) |
| C(41)-C(46) | 1.383 (5) | C(17)-H(17") | 0.953 (0) | C(38)-H(38') | 0.948 (0) |
| C(42)-C(43) | 1.392 (5) | C(18)-H(18) | 0.955 (0) | C(38)-H(38") | 0.959 (0) |
| C(43)-C(44) | 1.380 (6) | C(18)-H(18') | 0.945 (0) | C(39)-H(39) | 0.951 (0) |
| C(44)-C(45) | 1.371 (6) | C(18)-H(18") | 0.953 (0) | C(39)-H(39') | 0.946 (0) |
| C(45)-C(46) | 1.378 (5) | C(19)-H(19) | 0.945 (0) | C(39)-H(39") | 0.956 (0) |
| C(4)-H(4) | 0.950 (0) | C(19)-H(19') | 0.953 (0) | C(42)-H(42) | 0.947 (0) |
| C(4)-H(4') | 0.952 (0) | C(19)-H(19") | 0.954 (0) | C(43)-H(43) | 0.949 (0) |
| C(5)-H(5) | 0.948 (0) | C(33)-H(33) | 0.950 (0) | C(44)-H(44) | 0.952 (0) |
| C(5)-H(5') | 0.958 (0) | C(35)-H(35) | 0.942 (0) | C(45)-H(45) | 0.953 (0) |
| C(13)-H(13) | 0.948 (0) | C(37)-H(37) | 0.958 (0) | C(46)-H(46) | 0.951 (0) |
| C(15)-H(15) | 0.947 (0) | C(37)-H(37') | 0.948 (0) | | |
| C(17)-H(17) | 0.948 (0) | C(37)-H(37") | 0.944 (0) | | |

**Table V.** Intramolecular Angles (°)

| | | | |
|---|---|---|---|
| C(2)-P(1)-C(41) | 100.5 (2) | C(13)-C(14)-C(15) | 118.7 (4) |
| C(2)-N(1)-C(5) | 113.1 (3) | C(13)-C(14)-C(18) | 120.7 (4) |
| C(2)-N(1)-C(11) | 125.7 (3) | C(15)-C(14)-C(18) | 120.6 (4) |
| C(5)-N(1)-C(11) | 120.9 (3) | C(14)-C(15)-C(16) | 122.1 (4) |
| C(2)-N(3)-C(4) | 111.2 (3) | C(11)-C(16)-C(15) | 117.8 (4) |
| C(2)-N(3)-C(31) | 127.0 (3) | C(11)-C(16)-C(19) | 121.7 (4) |
| C(4)-N(3)-C(31) | 119.0 (3) | C(15)-C(16)-C(19) | 120.4 (4) |
| P(1)-C(2)-N(1) | 122.1 (3) | C(32)-C(31)-C(36) | 121.4 (4) |
| P(1)-C(2)-N(3) | 130.5 (3) | C(31)-C(32)-C(33) | 117.3 (4) |
| P(1)-C(41)-C(42) | 119.4 (3) | C(31)-C(32)-C(37) | 121.2 (4) |
| P(1)-C(41)-C(46) | 123.6 (3) | C(33)-C(32)-C(37) | 121.5 (4) |
| N(1)-C(2)-N(3) | 107.4 (3) | C(32)-C(33)-C(34) | 122.5 (4) |
| N(3)-C(4)-C(5) | 103.0 (3) | C(33)-C(34)-C(35) | 118.8 (4) |
| N(1)-C(5)-C(4) | 101.9 (3) | C(33)-C(34)-C(38) | 120.7 (4) |
| N(1)-C(11)-C(12) | 119.1 (4) | C(35)-C(34)-C(38) | 120.5 (4) |
| N(1)-C(11)-C(16) | 119.1 (4) | C(34)-C(35)-C(36) | 121.0 (4) |
| N(3)-C(31)-C(32) | 118.0 (4) | C(31)-C(36)-C(35) | 118.9 (4) |
| N(3)-C(31)-C(36) | 120.5 (4) | C(31)-C(36)-C(39) | 121.9 (4) |
| N(3)-C(4)-H(4) | 110 (0) | C(35)-C(36)-C(39) | 119.2 (4) |
| N(3)-C(4)-H(4') | 109 (0) | C(42)-C(41)-C(46) | 116.9 (3) |
| N(1)-C(5)-H(5) | 110 (0) | C(41)-C(42)-C(43) | 121.0 (4) |
| N(1)-C(5)-H(5') | 109 (0) | C(42)-C(43)-C(44) | 120.3 (4) |
| C(12)-C(11)-C(16) | 121.7 (4) | C(43)-C(44)-C(45) | 119.3 (4) |
| C(11)-C(12)-C(13) | 118.0 (4) | C(44)-C(45)-C(46) | 120.3 (4) |
| C(11)-C(12)-C(17) | 121.3 (4) | C(41)-C(46)-C(45) | 122.3 (4) |
| C(13)-C(12)-C(17) | 120.7 (4) | C(5)-C(4)-H(4) | 110 (0) |
| C(12)-C(13)-C(14) | 121.7 (4) | C(5)-C(4)-H(4') | 109 (0) |

**Table V.** Intramolecular Angles (°) (cont'd.)

| | | | |
|---|---|---|---|
| C(4)-C(5)-H(5) | 110 (0) | C(43)-C(42)-H(42) | 119 (0) |
| C(4)-C(5)-H(5') | 109 (0) | C(42)-C(43)-H(43) | 120 (0) |
| C(12)-C(13)-H(13) | 119 (0) | C(44)-C(43)-H(43) | 120 (0) |
| C(14)-C(13)-H(13) | 119 (0) | C(43)-C(44)-H(44) | 121 (0) |
| C(14)-C(15)-H(15) | 119 (0) | C(45)-C(44)-H(44) | 120 (0) |
| C(16)-C(15)-H(15) | 118 (0) | C(44)-C(45)-H(45) | 120 (0) |
| C(12)-C(17)-H(17) | 110 (0) | C(46)-C(45)-H(45) | 119 (0) |
| C(12)-C(17)-H(17') | 110 (0) | C(41)-C(46)-H(46) | 119 (0) |
| C(12)-C(17)-H(17") | 110 (0) | C(45)-C(46)-H(46) | 119 (0) |
| C(14)-C(18)-H(18) | 109 (0) | H(4)-C(4)-H(4') | 115 (0) |
| C(14)-C(18)-H(18') | 110 (0) | H(5)-C(5)-H(5') | 116 (0) |
| C(14)-C(18)-H(18") | 109 (0) | H(17)-C(17)-H(17') | 109 (0) |
| C(16)-C(19)-H(19) | 110 (0) | H(17)-C(17)-H(17") | 109 (0) |
| C(16)-C(19)-H(19') | 109 (0) | H(17')-C(17)-H(17") | 109 (0) |
| C(16)-C(19)-H(19") | 109 (0) | H(18)-C(18)-H(18') | 109 (0) |
| C(32)-C(33)-H(33) | 118 (0) | H(18)-C(18)-H(18") | 109 (0) |
| C(34)-C(33)-H(33) | 119 (0) | H(18')-C(18)-H(18") | 110 (0) |
| C(34)-C(35)-H(35) | 119 (0) | H(19)-C(19)-H(19') | 110 (0) |
| C(36)-C(35)-H(35) | 120 (0) | H(19)-C(19)-H(19") | 109 (0) |
| C(32)-C(37)-H(37) | 109 (0) | H(19')-C(19)-H(19") | 109 (0) |
| C(32)-C(37)-H(37') | 109 (0) | H(37)-C(37)-H(37') | 109 (0) |
| C(32)-C(37)-H(37") | 110 (0) | H(37)-C(37)-H(37") | 109 (0) |
| C(34)-C(38)-H(38) | 110 (0) | H(37')-C(37)-H(37") | 110 (0) |
| C(34)-C(38)-H(38') | 110 (0) | H(38)-C(38)-H(38') | 110 (0) |
| C(34)-C(38)-H(38") | 109 (0) | H(38)-C(38)-H(38") | 109 (0) |
| C(36)-C(39)-H(39) | 109 (0) | H(38')-C(38)-H(38") | 109 (0) |
| C(36)-C(39)-H(39') | 110 (0) | H(39)-C(39)-H(39') | 110 (0) |
| C(36)-C(39)-H(39") | 109 (0) | H(39)-C(39)-H(39") | 109 (0) |
| C(41)-C(42)-H(42) | 120 (0) | H(39')-C(39)-H(39") | 110 (0) |

**Table VI.** Intramolecular Non-Bonding Distances (Å)

| | | | | | |
|---|---|---|---|---|---|
| P(1)···C(12) | 3.705 (4) | C(2)···C(39) | 3.151 (6) | C(32)···C(45) | 3.738 (6) |
| P(1)···C(16) | 3.830 (4) | C(4)···C(37) | 3.296 (6) | C(32)···C(46) | 3.516 (6) |
| P(1)···C(17) | 3.884 (5) | C(4)···C(39) | 3.722 (6) | C(33)···C(45) | 3.617 (6) |
| P(1)···C(36) | 3.784 (4) | C(5)···C(17) | 3.606 (6) | C(34)···C(45) | 3.706 (6) |
| P(1)···C(39) | 3.694 (4) | C(5)···C(19) | 3.448 (6) | C(35)···C(46) | 3.565 (5) |
| N(1)···C(39) | 3.822 (5) | C(31)···C(41) | 3.042 (5) | C(36)···C(41) | 3.544 (5) |
| N(3)···C(42) | 3.623 (5) | C(31)···C(42) | 3.662 (6) | C(36)···C(46) | 3.296 (5) |
| N(3)···C(46) | 3.819 (5) | C(31)···C(46) | 3.232 (6) | C(37)···C(42) | 3.480 (6) |
| C(2)···C(17) | 3.354 (6) | C(32)···C(41) | 3.433 (5) | C(37)···C(43) | 3.623 (6) |
| C(2)···C(19) | 3.677 (6) | C(32)···C(42) | 3.593 (6) | | |