# Thermally Curing Aryl-Ethynyl Endcapped Imide Oligomers: Study of New Aromatic End-Caps.

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## Supplementary Material

**Tables A-G.** Bond distances for **1**, bond angles for **1**, bond distances found in **2**, bond angles for **2**, Experimental details for the structures determinations, parameters and isotropic thermal parameters for **1** and **2** (14 pages total).

***Table A.*** Intramolecular Distances (Å) Involving the Nonhydrogen Atoms for N-phenyl-4-(1-naphthylethynyl)phthalimide (1). [a]

| *atom* | *atom* | *distance* | *atom* | *atom* | *distance* |
|---|---|---|---|---|---|
| O(1) | C(15) | 1.22(1) | C(9) | C(10) | 1.35(2) |
| O(2) | C(16) | 1.19(1) | C(9) | C(14) | 1.45(1) |
| O(101) | C(115) | 1.19(1) | C(10) | C(11) | 1.40(2) |
| O(102) | C(116) | 1.22(1) | C(11) | C(12) | 1.39(2) |
| O(201) | C(215) | 1.20(1) | C(12) | C(13) | 1.39(2) |
| O(202) | C(216) | 1.20(1) | C(13) | C(14) | 1.41(2) |
| N(1) | C(15) | 1.38(1) | C(13) | C(26) | 1.43(2) |
| N(1) | C(16) | 1.40(1) | C(14) | C(23) | 1.39(2) |
| N(1) | C(17) | 1.43(1) | C(17) | C(18) | 1.38(1) |
| N(101) | C(115) | 1.42(1) | C(17) | C(22) | 1.38(1) |
| N(101) | C(116) | 1.39(1) | C(18) | C(19) | 1.40(2) |
| N(101) | C(117) | 1.43(1) | C(19) | C(20) | 1.34(2) |
| N(201) | C(215) | 1.40(1) | C(20) | C(21) | 1.40(1) |
| N(201) | C(216) | 1.40(1) | C(21) | C(22) | 1.37(2) |
| N(201) | C(217) | 1.44(1) | C(23) | C(24) | 1.38(2) |
| C(1) | C(2) | 1.41(1) | C(24) | C(25) | 1.40(2) |
| C(1) | C(6) | 1.38(1) | C(25) | C(26) | 1.32(2) |
| C(1) | C(15) | 1.47(2) | C(101) | C(102) | 1.34(1) |
| C(2) | C(3) | 1.37(2) | C(101) | C(106) | 1.39(1) |
| C(2) | C(16) | 1.49(2) | C(101) | C(115) | 1.50(2) |
| C(3) | C(4) | 1.39(2) | C(102) | C(103) | 1.36(1) |
| C(4) | C(5) | 1.39(2) | C(102) | C(116) | 1.50(2) |
| C(4) | C(7) | 1.46(2) | C(103) | C(104) | 1.41(2) |
| C(5) | C(6) | 1.41(2) | C(104) | C(105) | 1.37(1) |
| C(7) | C(8) | 1.19(1) | C(104) | C(107) | 1.41(2) |
| C(8) | C(9) | 1.41(2) | C(105) | C(106) | 1.39(1) |

***Table A*** (continued). Intramolecular Distances (Å) Involving the Nonhydrogen Atoms for N-phenyl-4-(1-naphthylethynyl)phthalimide (1). [a]

| *atom* | *atom* | *distance* | *atom* | *atom* | *distance* |
|---|---|---|---|---|---|
| C(107) | C(108) | 1.19(2) | C(204) | C(207) | 1.42(1) |
| C(108) | C(109) | 1.47(2) | C(205) | C(206) | 1.39(1) |
| C(109) | C(110) | 1.39(2) | C(207) | C(208) | 1.19(1) |
| C(109) | C(114) | 1.45(1) | C(208) | C(209) | 1.47(2) |
| C(110) | C(111) | 1.41(2) | C(209) | C(210) | 1.34(1) |
| C(111) | C(112) | 1.33(1) | C(209) | C(214) | 1.42(1) |
| C(112) | C(113) | 1.41(2) | C(210) | C(211) | 1.41(2) |
| C(113) | C(114) | 1.44(2) | C(211) | C(212) | 1.33(2) |
| C(113) | C(126) | 1.40(1) | C(212) | C(213) | 1.40(1) |
| C(114) | C(123) | 1.39(2) | C(213) | C(214) | 1.43(1) |
| C(117) | C(118) | 1.40(1) | C(213) | C(226) | 1.41(2) |
| C(117) | C(122) | 1.35(1) | C(214) | C(223) | 1.42(1) |
| C(118) | C(119) | 1.38(2) | C(217) | C(218) | 1.36(1) |
| C(119) | C(120) | 1.38(2) | C(217) | C(222) | 1.39(1) |
| C(120) | C(121) | 1.37(2) | C(218) | C(219) | 1.41(2) |
| C(121) | C(122) | 1.40(2) | C(219) | C(220) | 1.35(2) |
| C(123) | C(124) | 1.36(2) | C(220) | C(221) | 1.39(2) |
| C(124) | C(125) | 1.37(2) | C(221) | C(222) | 1.39(2) |
| C(125) | C(126) | 1.39(2) | C(223) | C(224) | 1.38(2) |
| C(201) | C(202) | 1.39(1) | C(224) | C(225) | 1.41(2) |
| C(201) | C(206) | 1.41(1) | C(225) | C(226) | 1.35(1) |
| C(201) | C(215) | 1.47(1) | C(202) | C(203) | 1.37(1) |
| C(202) | C(216) | 1.49(1) | C(203) | C(204) | 1.38(1) |
| C(204) | C(205) | 1.36(1) | | | |

[a]Estimated standard deviations in the least significant figure are given in parentheses.

***Table B.*** Intramolecular Bond Angles (deg) Involving the Nonhydrogen Atoms for N-phenyl-4-(1-naphthylethynyl)phthalimide (1). [a]

| *atom* | *atom* | *atom* | *angle* | *atom* | *atom* | *atom* | *angle* |
|---|---|---|---|---|---|---|---|
| C(15) | N(1) | C(16) | 111.9(9) | C(9) | C(10) | C(11) | 121(1) |
| C(15) | N(1) | C(17) | 124.8(9) | C(10) | C(11) | C(12) | 120(1) |
| C(16) | N(1) | C(17) | 123.2(9) | C(11) | C(12) | C(13) | 120(1) |
| C(115) | N(101) | C(116) | 110.6(9) | C(12) | C(13) | C(14) | 122(1) |
| C(115) | N(101) | C(117) | 125.1(9) | C(12) | C(13) | C(26) | 119(1) |
| C(116) | N(101) | C(117) | 124.3(9) | C(14) | C(13) | C(26) | 119(1) |
| C(215) | N(201) | C(216) | 111.4(8) | C(9) | C(14) | C(13) | 117(1) |
| C(215) | N(201) | C(217) | 124.3(9) | C(9) | C(14) | C(23) | 124(1) |
| C(216) | N(201) | C(217) | 124.3(9) | C(13) | C(14) | C(23) | 120(1) |
| C(2) | C(1) | C(6) | 121(1) | O(1) | C(15) | N(1) | 125(1) |
| C(2) | C(1) | C(15) | 108(1) | O(1) | C(15) | C(1) | 128(1) |
| C(6) | C(1) | C(15) | 130(1) | N(1) | C(15) | C(1) | 107(1) |
| C(1) | C(2) | C(3) | 122(1) | O(2) | C(16) | N(1) | 125(1) |
| C(1) | C(2) | C(16) | 107(1) | O(2) | C(16) | C(2) | 129(1) |
| C(3) | C(2) | C(16) | 131(1) | N(1) | C(16) | C(2) | 105.7(9) |
| C(2) | C(3) | C(4) | 117(1) | N(1) | C(17) | C(18) | 120(1) |
| C(3) | C(4) | C(5) | 121(1) | N(1) | C(17) | C(22) | 119(1) |
| C(3) | C(4) | C(7) | 120(1) | C(18) | C(17) | C(22) | 120(1) |
| C(5) | C(4) | C(7) | 118(1) | C(17) | C(18) | C(19) | 119(1) |
| C(4) | C(5) | C(6) | 122(1) | C(18) | C(19) | C(20) | 120(1) |
| C(1) | C(6) | C(5) | 116(1) | C(19) | C(20) | C(21) | 121(1) |
| C(4) | C(7) | C(8) | 177(1) | C(20) | C(21) | C(22) | 119(1) |
| C(7) | C(8) | C(9) | 177(1) | C(17) | C(22) | C(21) | 120(1) |
| C(8) | C(9) | C(10) | 120(1) | C(14) | C(23) | C(24) | 119(1) |
| C(8) | C(9) | C(14) | 119(1) | C(23) | C(24) | C(25) | 120(1) |
| C(10) | C(9) | C(14) | 121(1) | C(24) | C(25) | C(26) | 122(1) |

***Table B*** **(continued). Intramolecular Bond Angles (deg) Involving the Nonhydrogen Atoms for N-phenyl-4-(1-naphthylethynyl)phthalimide (1).** [a]

| *atom* | *atom* | *atom* | *angle* | *atom* | *atom* | *atom* | *angle* |
|---|---|---|---|---|---|---|---|
| C(13) | C(26) | C(25) | 119(1) | C(113) | C(114) | C(123) | 119(1) |
| C(102) | C(101) | C(106) | 122(1) | O(101) | C(115) | N(101) | 124(1) |
| C(102) | C(101) | C(115) | 109(1) | O(101) | C(115) | C(101) | 131(1) |
| C(106) | C(101) | C(115) | 129(1) | N(101) | C(115) | C(101) | 105.0(9) |
| C(101) | C(102) | C(103) | 122(1) | O(102) | C(116) | N(101) | 127(1) |
| C(101) | C(102) | C(116) | 108(1) | O(102) | C(116) | C(102) | 127(1) |
| C(103) | C(102) | C(116) | 130(1) | N(101) | C(116) | C(102) | 106.5(9) |
| C(102) | C(103) | C(104) | 119(1) | N(101) | C(117) | C(118) | 117(1) |
| C(103) | C(104) | C(105) | 119(1) | N(101) | C(117) | C(122) | 121(1) |
| C(103) | C(104) | C(107) | 120(1) | C(118) | C(117) | C(122) | 122(1) |
| C(105) | C(104) | C(107) | 121(1) | C(117) | C(118) | C(119) | 117(1) |
| C(104) | C(105) | C(106) | 122(1) | C(118) | C(119) | C(120) | 120(1) |
| C(101) | C(106) | C(105) | 117(1) | C(119) | C(120) | C(121) | 122(1) |
| C(104) | C(107) | C(108) | 176(1) | C(120) | C(121) | C(122) | 118(1) |
| C(107) | C(108) | C(109) | 176(1) | C(117) | C(122) | C(121) | 120(1) |
| C(108) | C(109) | C(110) | 120(1) | C(114) | C(123) | C(124) | 121(1) |
| C(108) | C(109) | C(114) | 119(1) | C(123) | C(124) | C(125) | 121(1) |
| C(110) | C(109) | C(114) | 121(1) | C(124) | C(125) | C(126) | 120(1) |
| C(109) | C(110) | C(111) | 118(1) | C(113) | C(126) | C(125) | 121(1) |
| C(110) | C(111) | C(112) | 122(1) | C(202) | C(201) | C(206) | 122(1) |
| C(111) | C(112) | C(113) | 122(1) | C(202) | C(201) | C(215) | 109.5(9) |
| C(112) | C(113) | C(114) | 119(1) | C(206) | C(201) | C(215) | 129(1) |
| C(112) | C(113) | C(126) | 123(1) | C(201) | C(202) | C(203) | 120(1) |
| C(114) | C(113) | C(126) | 118(1) | C(201) | C(202) | C(216) | 107.1(9) |
| C(109) | C(114) | C(113) | 117(1) | C(203) | C(202) | C(216) | 132.9(9) |
| C(109) | C(114) | C(123) | 124(1) | C(202) | C(203) | C(204) | 119(1) |

***Table B*** (continued). Intramolecular Bond Angles (deg) Involving the Nonhydrogen Atoms for N-phenyl-4-(1-naphthylethynyl)phthalimide (1). [a]

| *atom* | *atom* | *atom* | *angle* | *atom* | *atom* | *atom* | *angle* |
|---|---|---|---|---|---|---|---|
| C(203) | C(204) | C(205) | 121(1) | N(201) | C(217) | C(222) | 117.6(9) |
| C(203) | C(204) | C(207) | 121(1) | C(218) | C(217) | C(222) | 123(1) |
| C(205) | C(204) | C(207) | 118(1) | C(217) | C(218) | C(219) | 117(1) |
| C(204) | C(205) | C(206) | 123(1) | C(218) | C(219) | C(220) | 121(1) |
| C(201) | C(206) | C(205) | 116(1) | C(219) | C(220) | C(221) | 121(1) |
| C(204) | C(207) | C(208) | 177(1) | C(220) | C(221) | C(222) | 119(1) |
| C(207) | C(208) | C(209) | 176(1) | C(217) | C(222) | C(221) | 118(1) |
| C(208) | C(209) | C(210) | 122(1) | C(214) | C(223) | C(224) | 122(1) |
| C(208) | C(209) | C(214) | 117.1(9) | C(223) | C(224) | C(225) | 118(1) |
| C(210) | C(209) | C(214) | 121(1) | C(224) | C(225) | C(226) | 121(1) |
| C(209) | C(210) | C(211) | 121(1) | C(213) | C(226) | C(225) | 122(1) |
| C(210) | C(211) | C(212) | 120(1) | C(211) | C(212) | C(213) | 122(1) |
| C(212) | C(213) | C(214) | 118(1) | C(212) | C(213) | C(226) | 124(1) |
| C(214) | C(213) | C(226) | 118.4(9) | C(209) | C(214) | C(213) | 118.4(9) |
| C(209) | C(214) | C(223) | 124(1) | C(213) | C(214) | C(223) | 117.6(9) |
| O(201) | C(215) | N(201) | 125(1) | O(201) | C(215) | C(201) | 129(1) |
| N(201) | C(215) | C(201) | 105.7(9) | O(202) | C(216) | N(201) | 126(1) |
| O(202) | C(216) | C(202) | 127(1) | N(201) | C(216) | C(202) | 106.3(8) |
| N(201) | C(217) | C(218) | 119(1) | | | | |

[a]Estimated standard deviations in the least significant figure are given in parentheses.

***Table C.*** Intramolecular Distances (Å) Involving the Nonhydrogen Atoms for N-phenyl-4-phenylethynylphthalimide (2). [a]

| *atom* | *atom* | *distance* | *atom* | *atom* | *distance* |
|---|---|---|---|---|---|
| O(1) | C(15) | 1.222(9) | C(7) | C(8) | 1.21(1) |
| O(2) | C(16) | 1.212(9) | C(8) | C(9) | 1.42(1) |
| N(1) | C(15) | 1.41(1) | C(9) | C(10) | 1.41(1) |
| N(1) | C(16) | 1.40(1) | C(9) | C(14) | 1.37(1) |
| N(1) | C(17) | 1.403(9) | C(10) | C(11) | 1.40(1) |
| C(1) | C(2) | 1.39(1) | C(11) | C(12) | 1.38(1) |
| C(1) | C(6) | 1.37(1) | C(12) | C(13) | 1.35(1) |
| C(1) | C(15) | 1.46(1) | C(13) | C(14) | 1.38(1) |
| C(2) | C(3) | 1.35(1) | C(17) | C(18) | 1.39(1) |
| C(2) | C(16) | 1.49(1) | C(17) | C(22) | 1.37(1) |
| C(3) | C(4) | 1.41(1) | C(18) | C(19) | 1.40(1) |
| C(4) | C(5) | 1.42(1) | C(19) | C(20) | 1.37(1) |
| C(4) | C(7) | 1.41(1) | C(20) | C(21) | 1.36(1) |
| C(5) | C(6) | 1.37(1) | C(21) | C(22) | 1.39(1) |

[a]Estimated standard deviations in the least significant figure are given in parentheses.

***Table D.*** Intramolecular Bond Angles (deg) Involving the Nonhydrogen Atoms for N-phenyl-4-phenylethynylphthalimide (2). [a]

| *atom* | *atom* | *atom* | *angle* | *atom* | *atom* | *atom* | *angle* |
|---|---|---|---|---|---|---|---|
| C(15) | N(1) | C(16) | 109.2(6) | C(9) | C(10) | C(11) | 118(1) |
| C(15) | N(1) | C(17) | 126.1(7) | C(10) | C(11) | C(12) | 121(1) |
| C(16) | N(1) | C(17) | 124.7(7) | C(11) | C(12) | C(13) | 121(1) |
| C(2) | C(1) | C(6) | 120.6(8) | C(12) | C(13) | C(14) | 120(1) |
| C(2) | C(1) | C(15) | 108.0(7) | C(9) | C(14) | C(13) | 121(1) |
| C(6) | C(1) | C(15) | 131.4(8) | O(1) | C(15) | N(1) | 123.2(7) |
| C(1) | C(2) | C(3) | 122.5(8) | O(1) | C(15) | C(1) | 128.7(8) |
| C(1) | C(2) | C(16) | 107.5(7) | N(1) | C(15) | C(1) | 108.0(7) |
| C(3) | C(2) | C(16) | 130.0(8) | O(2) | C(16) | N(1) | 125.1(7) |
| C(2) | C(3) | C(4) | 118.7(8) | O(2) | C(16) | C(2) | 127.7(8) |
| C(3) | C(4) | C(5) | 117.8(8) | N(1) | C(16) | C(2) | 107.2(7) |
| C(3) | C(4) | C(7) | 121.2(9) | N(1) | C(17) | C(18) | 118.7(8) |
| C(5) | C(4) | C(7) | 121.0(9) | N(1) | C(17) | C(22) | 119.7(8) |
| C(4) | C(5) | C(6) | 122.1(9) | C(18) | C(17) | C(22) | 121.6(8) |
| C(1) | C(6) | C(5) | 118.3(9) | C(17) | C(18) | C(19) | 118.3(9) |
| C(4) | C(7) | C(8) | 177(1) | C(18) | C(19) | C(20) | 119.4(9) |
| C(7) | C(8) | C(9) | 177(1) | C(19) | C(20) | C(21) | 121.6(9) |
| C(8) | C(9) | C(10) | 121.5(9) | C(20) | C(21) | C(22) | 119.9(9) |
| C(8) | C(9) | C(14) | 119.2(9) | C(17) | C(22) | C(21) | 119.2(9) |
| C(10) | C(9) | C(14) | 119.3(9) | | | | |

[a]Estimated standard deviations in the least significant figure are given in parentheses.

***Table E.*** Experimental Details of the X-ray Diffraction Studies[a]

| compound | *1* | *2* |
|---|---|---|
| formula | $C_{26}H_{15}NO_2$ | $C_{22}H_{13}NO_2$ |
| formula weight, g mol$^{-1}$ | 373.411 | 323.350 |
| crystal system | orthorhombic | monoclinic |
| space group | Pca21 (29) | Pa (7) |
| *a*, Å | 7.5065(8) | 7.983 (1) |
| *b*, Å | 20.119(3) | 5.6627 (6) |
| *c*, Å | 36.445(6) | 17.921 (4) |
| *β*, deg | | 99.37 (2) |
| *V*, Å$^3$ | 5504(1) | 799.3 (2) |
| *Z* | 12 15.8 | 2 16.0 |
| T, deg C | -75 | 22 |
| $\rho_{calcd}$, g cm$^{-1}$ | 1.352 | 1.343 |
| crystal dimensions, mm$^3$ | 0.41 x 0.38 x 0.20 | 0.28 x 0.30 x 0.33 |
| transmission factor range | 0.9303 - 1.0000 | 0.8612 - 1.0000 |
| crystal decay | 0.2% | - 0.5% |
| linear abs. coeff., cm$^{-1}$ | 0.856 | 0.864 |
| data collected | 3°<2θ < 44; +h, +k, ±l | 3°<2θ < 48; +h, +k, ±l |
| reflections collected | 8208 | 1897 |
| $R_{avg}$ for refl. averaging | 0.077 | 0.021 |
| no. of independent data | 3878 | 1401 |

***Table E*** (continued). Experimental Details of the X-ray Diffraction Studies[a]

| compound | *1* | 2 |
|---|---|---|
| no. of unique data with $I > 3\sigma(I)$ | 1888 | 819 |
| no. of variables | 348 | 99 |
| F(0,0,0) | 2328 | 336 |
| R[b] | 0.052 | 0.066 |
| $R_w$[c] | 0.054 | 0.067 |

[a]Data collected on an Enraf-Nonius CAD4-F kappa geometry diffractometer with graphite monochromatized Mo K$\bar{\alpha}$ radiation ($\bar{\lambda}$ = 0.71073 Å). [b]$R = \Sigma \, ||F_o| - |F_c|| / \Sigma |F_o|$. [c]$R_w = [\Sigma w(|F_o| - |F_c|)^2 / \Sigma w |F_o|^2]^{1/2}$, where $w = 4F^2/\sigma^2(F^2)$ and $\sigma^2(F^2) = [S^2(C+4B) + (pI)^2]/(Lp)^2$ with S = scan rate, C = peak counts, B = sum of left and right background counts, I = reflection intensity, Lp = Lorentz-polarization factor and p is a constant employed to avoid overweighting of intense reflections.

***Table F.*** **Atomic Positional Parameters and Isotropic Thermal Parameters for the Nonhydrogen Atoms of N-phenyl-4-(1-naphthylethynyl)phthalimide (1).** [a]

| *atom* | *x* | *y* | *z* | *B* |
|---|---|---|---|---|
| O(1) | -0.5330(9) | 1.1911(3) | 0.5984 | 3.1(1) |
| O(2) | -0.246(1) | 0.9936(3) | 0.5824(3) | 3.2(1) |
| O(101) | 0.1932(9) | 0.3143(3) | -0.0146(2) | 3.4(2) |
| O(102) | 0.4714(9) | 0.5135(3) | 0.0053(3) | 3.7(2) |
| O(201) | -0.2093(9) | 0.6529(3) | 0.2950(3) | 3.7(2) |
| O(202) | 0.1304(9) | 0.8413(3) | 0.2902(2) | 3.5(2) |
| N(1) | -0.389(1) | 1.0897(3) | 0.6000(3) | 2.1(2) |
| N(101) | 0.342(1) | 0.4145(3) | -0.0151(3) | 2.3(2) |
| N(201) | -0.053(1) | 0.7494(4) | 0.2828(2) | 2.4(2) |
| C(1) | -0.481(1) | 1.1258(5) | 0.5436(3) | 2.6(2) |
| C(2) | -0.399(1) | 1.0638(4) | 0.5384(3) | 2.1(2) |
| C(3) | -0.380(1) | 1.0360(5) | 0.5043(3) | 2.7(2) |
| C(4) | -0.458(1) | 1.0689(5) | 0.4750(3) | 3.0(2) |
| C(5) | -0.543(1) | 1.1296(5) | 0.4797(3) | 2.9(2) |
| C(6) | -0.557(1) | 1.1598(5) | 0.5146(3) | 2.7(2) |
| C(7) | -0.449(1) | 1.0410(5) | 0.4381(4) | 3.3(2) |
| C(8) | -0.449(1) | 1.0190(5) | 0.4078(3) | 3.0(2) |
| C(9) | -0.456(1) | 0.9913(5) | 0.3722(4) | 3.1(2) |
| C(10) | -0.487(1) | 1.0307(5) | 0.3429(4) | 3.3(2) |
| C(11) | -0.502(2) | 1.0039(5) | 0.3075(4) | 3.6(3) |
| C(12) | -0.480(1) | 0.9362(5) | 0.3021(4) | 3.5(2) |
| C(13) | -0.444(1) | 0.8954(5) | 0.3318(4) | 3.2(2) |
| C(14) | -0.427(1) | 0.9207(4) | 0.3677(3) | 2.6(2) |
| C(15) | -0.477(1) | 1.1415(5) | 0.5829(3) | 2.6(2) |
| C(16) | -0.333(1) | 1.0412(5) | 0.5748(3) | 2.3(2) |
| C(17) | -0.356(1) | 1.0853(5) | 0.6386(3) | 2.6(2) |
| C(18) | -0.407(1) | 1.0294(5) | 0.6579(3) | 2.7(2) |
| C(19) | -0.368(1) | 1.0257(5) | 0.6954(4) | 3.2(2) |
| C(20) | -0.277(2) | 1.0746(5) | 0.7119(4) | 3.8(2) |

**Table F** (continued). Atomic Positional Parameters and Isotropic Thermal Parameters for the Nonhydrogen Atoms of N-phenyl-4-(1-naphthylethynyl)phthalimide (1).

| *atom* | *x* | *y* | *z* | *B* |
|---|---|---|---|---|
| C(21) | -0.222(1) | 1.1308(5) | 0.6925(3) | 3.0(2) |
| C(22) | -0.261(1) | 1.1351(5) | 0.6558(3) | 3.1(2) |
| C(23) | -0.383(1) | 0.8781(5) | 0.3964(4) | 3.8(3) |
| C(24) | -0.366(1) | 0.8109(6) | 0.3897(4) | 4.0(3) |
| C(25) | -0.386(2) | 0.7863(6) | 0.3539(4) | 4.2(3) |
| C(26) | -0.422(2) | 0.8256(6) | 0.3258(4) | 4.1(3) |
| C(101) | 0.242(1) | 0.3787(4) | 0.0416(3) | 2.4(2) |
| C(102) | 0.325(1) | 0.4367(4) | 0.0471(3) | 1.9(2) |
| C(103) | 0.334(1) | 0.4652(5) | 0.0808(3) | 2.8(2) |
| C(104) | 0.255(1) | 0.4317(5) | 0.1108(3) | 2.5(2) |
| C(105) | 0.172(1) | 0.3719(5) | 0.1048(3) | 2.7(2) |
| C(106) | 0.163(1) | 0.3433(5) | 0.0702(3) | 3.3(2) |
| C(107) | 0.263(2) | 0.4596(5) | 0.1461(4) | 3.0(2) |
| C(108) | 0.260(1) | 0.4853(5) | 0.1755(4) | 3.1(2) |
| C(109) | 0.267(1) | 0.5136(4) | 0.2126(3) | 2.1(2) |
| C(110) | 0.232(1) | 0.4737(5) | 0.2429(4) | 3.1(2) |
| C(111) | 0.238(2) | 0.5032(5) | 0.2781(4) | 3.6(3) |
| C(112) | 0.270(2) | 0.5674(5) | 0.2829(4) | 3.7(2) |
| C(113) | 0.310(1) | 0.6098(5) | 0.2533(3) | 2.8(2) |
| C(114) | 0.304(1) | 0.5837(4) | 0.2167(3) | 2.7(2) |
| C(115) | 0.254(2) | 0.3602(5) | 0.0019(3) | 3.1(2) |
| C(116) | 0.391(1) | 0.4617(5) | 0.0109(3) | 2.6(2) |
| C(117) | 0.375(1) | 0.4207(5) | -0.0535(3) | 2.3(2) |
| C(118) | 0.315(1) | 0.4791(5) | -0.0704(3) | 2.8(2) |
| C(119) | 0.354(1) | 0.4871(5) | -0.1072(4) | 3.3(2) |
| C(120) | 0.444(1) | 0.4382(5) | -0.1260(3) | 3.4(2) |
| C(121) | 0.502(1) | 0.3809(5) | -0.1094(3) | 3.5(2) |
| C(122) | 0.465(1) | 0.3729(5) | -0.0721(3) | 3.3(2) |
| C(123) | 0.338(1) | 0.6260(5) | 0.1873(4) | 3.3(2) |
| C(124) | 0.380(2) | 0.6908(5) | 0.1929(4) | 4.1(3) |
| C(125) | 0.389(2) | 0.7170(5) | 0.2276(4) | 4.2(3) |

**Table F** (continued). Atomic Positional Parameters and Isotropic Thermal Parameters for the Nonhydrogen Atoms of N-phenyl-4-(1-naphthylethynyl)phthalimide (1).

| *atom* | *x* | *y* | *z* | *B* |
|---|---|---|---|---|
| C(126) | 0.353(1) | 0.6770(5) | 0.2578(3) | 3.6(2) |
| C(201) | -0.018(1) | 0.7048(4) | 0.3401(3) | 2.3(2) |
| C(202) | 0.082(1) | 0.7629(4) | 0.3393(3) | 2.0(2) |
| C(203) | 0.166(1) | 0.7845(5) | 0.3704(3) | 2.5(2) |
| C(204) | 0.151(1) | 0.7474(4) | 0.4021(3) | 2.3(2) |
| C(205) | 0.054(1) | 0.6904(5) | 0.4027(3) | 3.0(2) |
| C(206) | -0.030(1) | 0.6653(5) | 0.3718(3) | 3.5(2) |
| C(207) | 0.239(1) | 0.7668(4) | 0.4350(3) | 2.8(2) |
| C(208) | 0.307(1) | 0.7807(5) | 0.4634(3) | 3.2(2) |
| C(209) | 0.384(1) | 0.7947(4) | 0.4998(3) | 2.4(2) |
| C(210) | 0.464(1) | 0.8524(5) | 0.5076(3) | 2.8(2) |
| C(211) | 0.528(1) | 0.8655(5) | 0.5432(3) | 2.9(2) |
| C(212) | 0.510(1) | 0.8199(5) | 0.5695(3) | 2.9(2) |
| C(213) | 0.425(1) | 0.7592(5) | 0.5633(3) | 2.7(2) |
| C(214) | 0.362(1) | 0.7454(4) | 0.5271(3) | 2.2(2) |
| C(215) | -0.106(1) | 0.6953(5) | 0.3045(3) | 2.9(2) |
| C(216) | 0.061(1) | 0.7919(4) | 0.3020(3) | 2.3(2) |
| C(217) | -0.111(1) | 0.7604(4) | 0.2456(3) | 2.5(2) |
| C(218) | -0.188(1) | 0.8196(5) | 0.2366(3) | 3.3(2) |
| C(219) | -0.244(2) | 0.8281(5) | 0.2001(3) | 4.0(2) |
| C(220) | -0.226(2) | 0.7788(5) | 0.1754(4) | 4.2(3) |
| C(221) | -0.145(2) | 0.7192(5) | 0.1847(4) | 3.9(2) |
| C(222) | -0.088(1) | 0.7089(5) | 0.2207(3) | 3.0(2) |
| C(223) | 0.279(1) | 0.6828(5) | 0.5209(3) | 3.2(2) |
| C(224) | 0.260(2) | 0.6360(5) | 0.5482(4) | 3.6(2) |
| C(225) | 0.323(1) | 0.6516(5) | 0.5836(3) | 3.3(2) |
| C(226) | 0.400(1) | 0.7107(5) | 0.5906(3) | 3.6(2) |

[a]Numbers in parentheses are errors in the last significant digit

**Table G.** Atomic Positional Parameters and Isotropic Thermal Parameters for the Nonhydrogen Atoms of N-phenyl-4-(phenylethynyl)phthalimide (2). [a]

| *atom* | *x* | *y* | *z* | *B* |
|---|---|---|---|---|
| O(1) | 0.7374 | 0.4045(8) | 0.2469 | 3.4(1) |
| O(2) | 0.4410(7) | 1.0947(8) | 0.2476(3) | 3.31(9) |
| N(1) | 0.5805(8) | 0.750(1) | 0.2252(4) | 2.4(1) |
| C(1) | 0.671(1) | 0.642(1) | 0.3505(4) | 2.4(1) |
| C(2) | 0.585(1) | 0.855(1) | 0.3511(5) | 2.6(1) |
| C(3) | 0.565(1) | 0.965(1) | 0.4158(5) | 3.0(1) |
| C(4) | 0.636(1) | 0.862(1) | 0.4856(5) | 3.4(2) |
| C(5) | 0.723(1) | 0.644(1) | 0.4836(5) | 3.7(2) |
| C(6) | 0.741(1) | 0.535(1) | 0.4168(5) | 3.2(1) |
| C(7) | 0.624(1) | 0.973(1) | 0.5549(5) | 4.0(2) |
| C(8) | 0.617(1) | 1.061(1) | 0.6157(5) | 4.2(2) |
| C(9) | 0.608(1) | 1.153(1) | 0.6884(5) | 3.5(2) |
| C(10) | 0.528(1) | 1.372(2) | 0.6976(5) | 4.8(2) |
| C(11) | 0.521(1) | 1.450(2) | 0.7715(5) | 5.3(2) |
| C(12) | 0.590(1) | 1.316(2) | 0.8328(5) | 4.8(2) |
| C(13) | 0.669(1) | 1.109(2) | 0.8231(5) | 5.0(2) |
| C(14) | 0.679(1) | 1.029(1) | 0.7511(5) | 4.3(2) |
| C(15) | 0.6704(9) | 0.575(1) | 0.2718(4) | 2.6(1) |
| C(16) | 0.523(1) | 0.922(1) | 0.2707(4) | 2.5(1) |
| C(17) | 0.5532(9) | 0.754(1) | 0.1459(5) | 2.7(1) |
| C(18) | 0.470(1) | 0.564(1) | 0.1068(4) | 3.4(1) |
| C(19) | 0.443(1) | 0.569(1) | 0.0275(5) | 4.2(2) |
| C(20) | 0.504(1) | 0.757(1) | -0.0089(5) | 4.3(2) |
| C(21) | 0.585(1) | 0.941(1) | 0.0302(5) | 4.2(2) |
| C(22) | 0.612(1) | 0.940(1) | 0.1087(4) | 3.2(1) |

[a]Numbers in parentheses are errors in the last significant digit