

Supporting Information: Crystal Structure Information for compound 2.

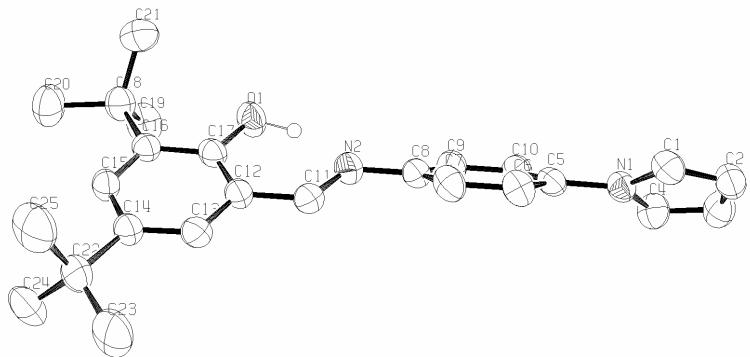


Figure 1: Crystal structure of monomer 2.

Table 1. Crystal data and structure refinement for 2.

| | | | |
|---------------------------------|--|------------------|--|
| Empirical formula | C ₂₅ H ₃₀ N ₂ O | | |
| Formula weight | 374.51 | | |
| Temperature | 193(2) K | | |
| Wavelength | 0.71073 Å | | |
| Crystal system | Triclinic | | |
| Space group | P-1 | | |
| Unit cell dimensions | a = 9.8773(6) Å | α = 100.878(2)°. | |
| | b = 12.1540(7) Å | β = 93.328(2)°. | |
| | c = 18.6430(11) Å | γ = 94.944(2)°. | |
| Volume | 2183.3(2) Å ³ | | |
| Z | 4 | | |
| Density (calculated) | 1.139 Mg/m ³ | | |
| Absorption coefficient | 0.069 mm ⁻¹ | | |
| F(000) | 808 | | |
| Crystal size | 0.24 x 0.16 x 0.07 mm ³ | | |
| Theta range for data collection | 1.71 to 25.00°. | | |
| Index ranges | -11 ≤ h ≤ 11, -14 ≤ k ≤ 14, -22 ≤ l ≤ 22 | | |
| Reflections collected | 16332 | | |
| Independent reflections | 7625 [R(int) = 0.0375] | | |

| | |
|-----------------------------------|---|
| Completeness to theta = 25.00° | 99.1 % |
| Absorption correction | Integration |
| Max. and min. transmission | 0.9952 and 0.9844 |
| Refinement method | Full-matrix least-squares on F ² |
| Data / restraints / parameters | 7625 / 0 / 581 |
| Goodness-of-fit on F ² | 1.021 |
| Final R indices [I>2sigma(I)] | R1 = 0.0552, wR2 = 0.1225 [4710] |
| R indices (all data) | R1 = 0.0987, wR2 = 0.1413 |
| Extinction coefficient | 0.0013(5) |
| Largest diff. peak and hole | 0.261 and -0.178 e.Å ⁻³ |

$$R1 = \sum(|F_O| - |F_C|) / \sum|F_O|$$

$$wR2 = [\sum(w(F_O^2 - F_C^2)^2) / \sum(w(F_O^2)^2)]^{1/2}$$

$$S = [\sum(w(F_O^2 - F_C^2)^2) / (n-p)]^{1/2}$$

$$w = 1/[\sigma^2(F_O^2) + (m*p)^2 + n*p], p = [\max(F_O^2, 0) + 2*F_C^2]/3, m \& n \text{ are constants.}$$