

Supplementary Information

N-(diisopropylphosphanyl)benzamide

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Table S1. Crystal data and structure refinement for compound **1**

| | | | |
|-----------------------------------|---------------------------------------------|-----------------|--|
| Empirical formula | C ₁₃ H ₂₀ NOP | | |
| Formula weight | 237.27 | | |
| Temperature | 193(2) K | | |
| Wavelength | 0.71073 Å | | |
| Crystal system | Monoclinic | | |
| Space group | P2 ₁ /c | | |
| Unit cell dimensions | a = 15.482(3) Å | α= 90°. | |
| | b = 8.741(2) Å | β= 98.382(10)°. | |
| | c = 10.260(2) Å | γ = 90°. | |
| Volume | 1373.7(5) Å ³ | | |
| Z | 4 | | |
| Density (calculated) | 1.147 Mg/m ³ | | |
| Absorption coefficient | 0.182 mm ⁻¹ | | |
| F(000) | 512 | | |
| Crystal size | 0.100 x 0.080 x 0.050 mm ³ | | |
| Theta range for data collection | 2.660 to 25.245°. | | |
| Index ranges | -18<=h<=18, -9<=k<=10, -12<=l<=11 | | |
| Reflections collected | 2489 | | |
| Independent reflections | 2489 [R(int) = 0.0843] | | |
| Completeness to theta = 25.242° | 99.9 % | | |
| Absorption correction | Semi-empirical from equivalents | | |
| Max. and min. transmission | 0.7460 and 0.6523 | | |
| Refinement method | Full-matrix least-squares on F ² | | |
| Data / restraints / parameters | 2489 / 291 / 183 | | |
| Goodness-of-fit on F ² | 1.113 | | |
| Final R indices [I>2sigma(I)] | R1 = 0.0864, wR2 = 0.1842 | | |
| R indices (all data) | R1 = 0.1289, wR2 = 0.2003 | | |
| Extinction coefficient | n/a | | |
| Largest diff. peak and hole | 0.380 and -0.322 e.Å ⁻³ | | |

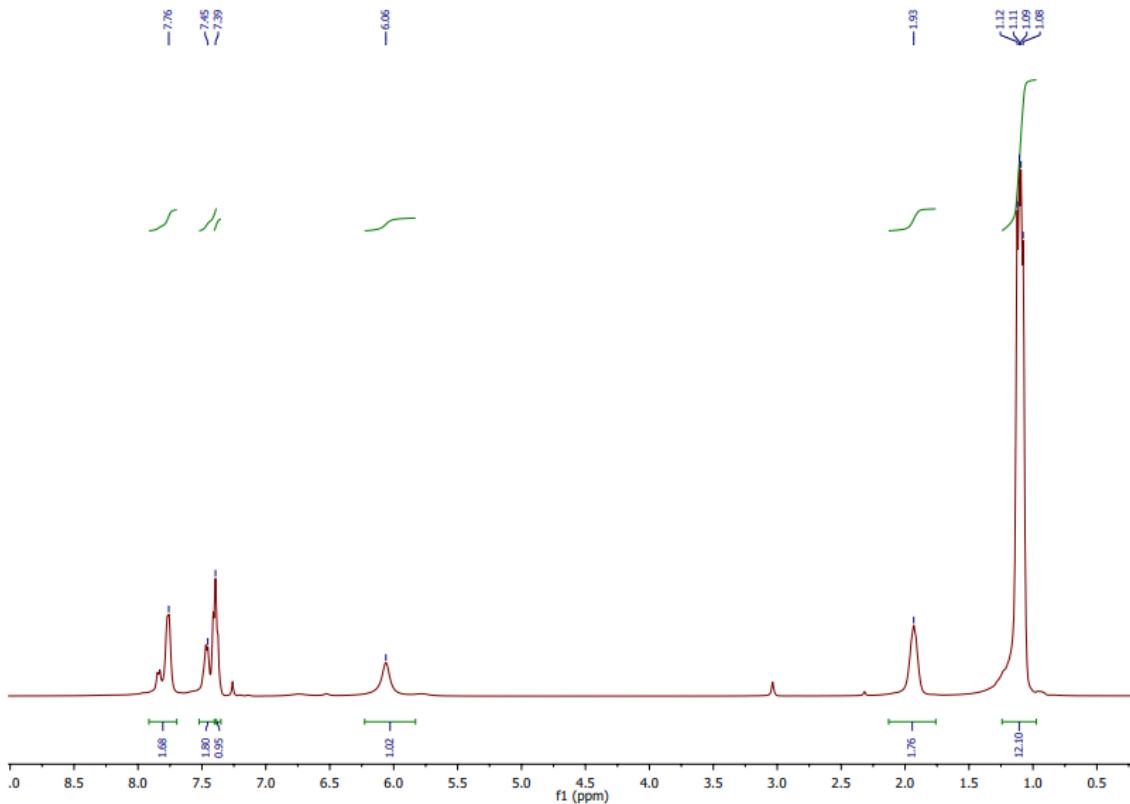


Figure S1. ^1H NMR spectrum of **1** (400 MHz, CDCl_3).

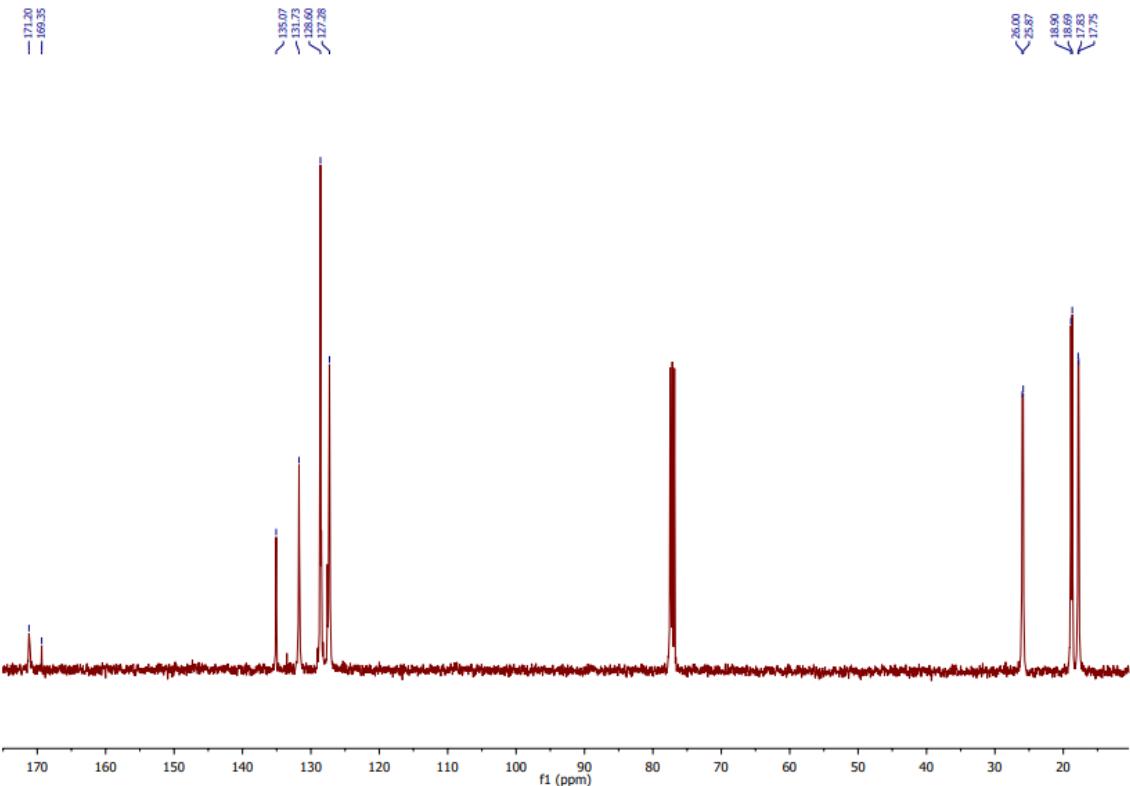


Figure S2. $^{13}\text{C}\{\text{H}\}$ NMR spectrum of **1** (100 MHz, CDCl_3).

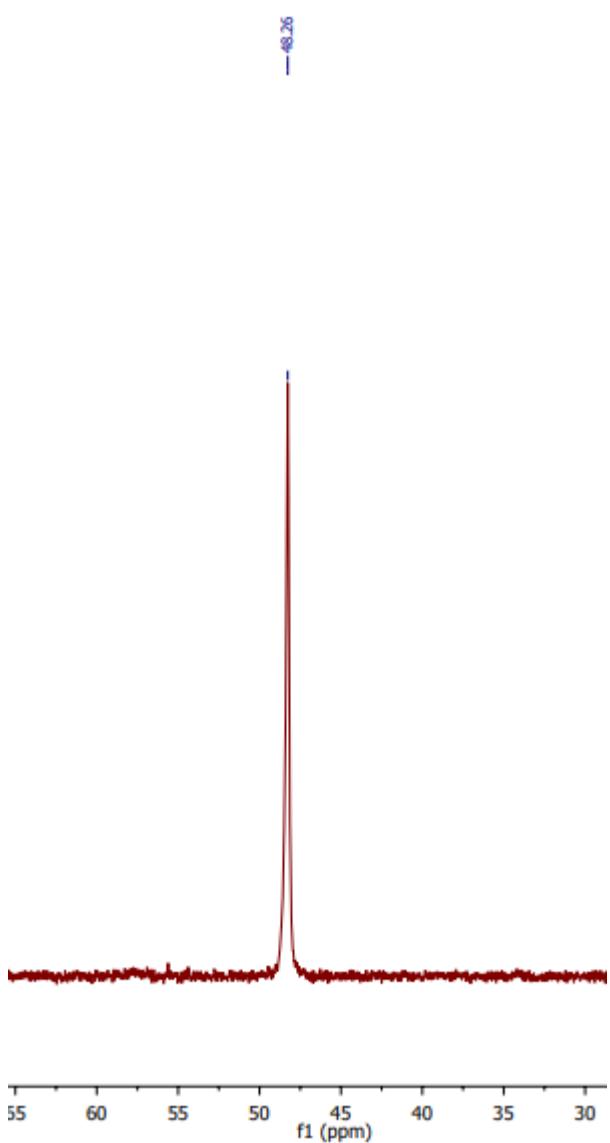


Figure S3. $^{31}\text{P}\{\text{H}\}$ NMR spectrum of **1** (162 MHz, CDCl_3).