

Table 1. Crystal and Structure Refinement parameters for compounds **1**, **3**, and **4**.

Parameters	1	3	4
Empirical formula	C ₂₇ H ₃₃ N ₂ P Si	C ₂₇ H ₄₅ N ₃ Si	C ₂₁ H ₃₇ N ₃ Si
Formula Weight	444.61	439.75	359.63
Crystal system	triclinic	monoclinic	monoclinic
Space group	<i>P</i> $\bar{1}$	<i>P</i> 2 ₁ / <i>c</i>	<i>C</i> 2/ <i>c</i>
Unit cell dimensions	<i>a</i> = 8.384 (3) Å <i>b</i> = 9.073 (3) Å <i>c</i> = 17.254 (4) Å α = 89.190 (10)° β = 86.06 (2)° γ = 72.48 (1)°	<i>a</i> = 15.040 (4) Å <i>b</i> = 11.542 (4) Å <i>c</i> = 16.516 (6) Å α = 90° β = 111.70 (2)° γ = 90°	<i>a</i> = 27.820 (2) Å <i>b</i> = 8.447 (3) Å <i>c</i> = 19.099 (2) Å α = 90° β = 99.35(2)° γ = 90°
Volume, <i>Z</i>	1248.5 (7) Å ³ , 2	2663.9 (15) Å ³ , 4	4428.6 (17) Å ³ , 8
Density (Calcd)	1.183 g/cm ³	1.096 mg/m ³	1.079 mg/m ³
Absorption coefficient	0.175 mm ⁻¹	0.106 mm ⁻¹	0.114 mm ⁻¹
<i>F</i> (000)	476	968	1584
Crystal size [mm ³]	0.10 x 0.10 x 0.10	0.20 x 0.10 x 0.02	0.15 x 0.10 x 0.02
θ range for data collection	1.18 to 28.30°	1.46 to 26.35°	1.48 to 27.58°
Limiting indices	-11 ≤ <i>h</i> ≤ 11, -12 ≤ <i>k</i> ≤ 12, -22 ≤ <i>l</i> ≤ 22	-18 ≤ <i>h</i> ≤ 18, -14 ≤ <i>k</i> ≤ 14, -20 ≤ <i>l</i> ≤ 20	-36 ≤ <i>h</i> ≤ 36, -10 ≤ <i>k</i> ≤ 10, -24 ≤ <i>l</i> ≤ 24
Reflections collected	42389	60239	39498
Independent reflections	6185 (<i>R</i> _{int} = 0.0192)	5422 (<i>R</i> _{int} = 0.0398)	5111 (<i>R</i> _{int} = 0.0492)

Completeness to θ	99.7% ($\theta = 28.30$)	99.5% ($\theta = 26.35$)	99.9% ($\theta = 27.58$)
Refinement method	Full - matrix least - squares on F^2	Full - matrix least - squares on F^2	Full - matrix least - squares on F^2
Data/ restraints/ parameters	6185 / 0 / 286	5422 / 0 / 286	5111 / 0 / 236
Goodness - of - fit on F^2	1.061	1.043	1.047
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0311, wR2 = 0.0828$	$R1 = 0.0379, wR2 = 0.0876$	$R1 = 0.0416, wR2 = 0.0936$
R indices (all data)	$R1 = 0.0333, wR2 = 0.0841$	$R1 = 0.0493, wR2 = 0.0921$	$R1 = 0.0621, wR2 = 0.1002$
Largest diff. peak and hole	0.355 and -0.259 eÅ ⁻³	0.219 and -0.264 eÅ ⁻³	0.299 and -0.263 eÅ ⁻³
