Supplementary Material

Calcium-Mediated Hydrophosphorylation
of Organic Isocyanates with Diphenylphosphane Oxide

Stephan Härling, Julia Greiser, Tareq M. A. Al-Shboul,
Helmar Görls, Sven Krieck, Matthias Westerhausen*

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Figure S1: Molecular structure and numbering scheme of $N$-isopropyl-(diphenylphosphoryl)-formamide (1). The ellipsoids represent a probability of 40 %, H atoms are shown with arbitrary radii. Selected structural parameters are listed in Table 2.

Figure S2: Molecular structure and numbering scheme of $N$-tert-butyl-(diphenylphosphoryl)-formamide (2). The ellipsoids represent a probability of 40 %, H atoms are shown with arbitrary radii. Selected structural parameters are listed in Table 2.
Figure S3: Molecular structure and numbering scheme of \( N \)-cyclohexyl-(diphenylphosphoryl)formamide (3). The ellipsoids represent a probability of 40 \%, H atoms are shown with arbitrary radii. Selected structural parameters are listed in Table 2.

Figure S4: Molecular structure and numbering scheme of \( N \)-phenyl-(diphenylphosphoryl)formamide (4). The ellipsoids represent a probability of 40 \%, H atoms are shown with arbitrary radii. Selected structural parameters are listed in Table 2.
Figure S5: Molecular structure and numbering scheme of $N$-2,4,6-trimethylphenyl-(diphenylphosphoryl)formamide (6). The ellipsoids represent a probability of 40%, H atoms are shown with arbitrary radii. Selected structural parameters are listed in Table 2.

Figure S6: Molecular structure and numbering scheme of $N$-naphthyl-(diphenylphosphoryl)-formamide (7). The ellipsoids represent a probability of 40%, H atoms are shown with arbitrary radii. The asymmetric unit contains two crystallographically independent molecules “A” and “B”; only molecule A is displayed. Selected structural parameters are listed in Table 2.
Figure S7: Molecular structure and numbering scheme of \( N\text{-cyclohexyl-(diphenylphosphoryl)} \text{thioformamide (9)}. \) The ellipsoids represent a probability of 40 %, H atoms are shown with arbitrary radii. The asymmetric unit contains two crystallographically independent molecules “A” and “B”; only molecule A is displayed. Selected structural parameters are listed in Table 2.

Figure S8: Molecular structure and numbering scheme of \( N\text{-phenyl-(diphenylphosphoryl)} \text{thioformamide (10)}. \) The ellipsoids represent a probability of 40 %, H atoms are shown with arbitrary radii. Selected structural parameters are listed in Table 2.
Figure S9: Molecular structure and numbering scheme of N-4-methylphenyl-(diphenyl-phosphoryl)thioformamide (11). The ellipsoids represent a probability of 40 %, H atoms are shown with arbitrary radii. Selected structural parameters are listed in Table 2.