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## Supplementary Material

## Calcium-Mediated Hydrophosphorylation of Organic Isocyanates with Diphenylphosphane Oxide

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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.

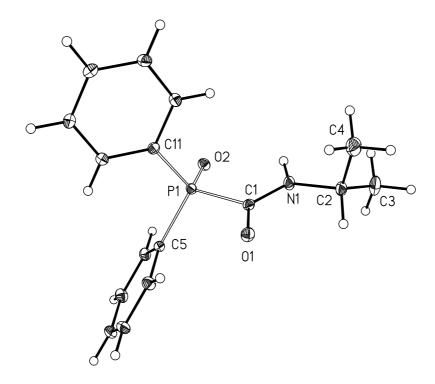


Figure S2: Molecular structure and numbering scheme of *N*-tert-butyl-(diphenylphosphoryl)-formamide (2). The ellipsoids represent a probability of 40 %, H atoms are shown with arbitrary radii. Selected structural parameters are listed in Table 2.

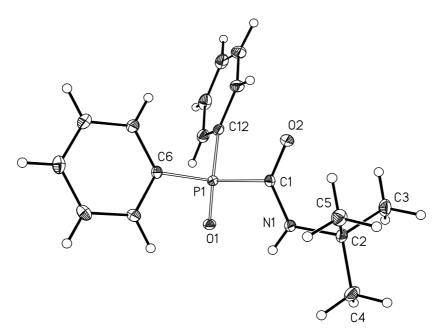


Figure S3: Molecular structure and numbering scheme of *N*-cyclohexyl-(diphenyl-phosphoryl)formamide (3). The ellipsoids represent a probability of 40 %, H atoms are shown with arbitrary radii. Selected structural parameters are listed in Table 2.

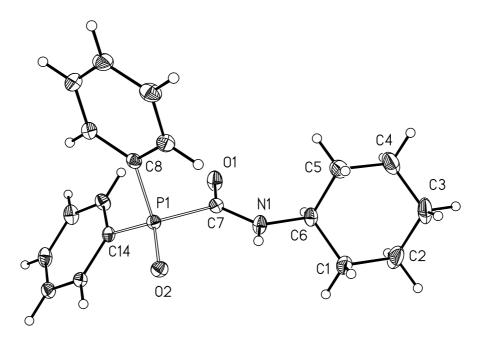


Figure S4: Molecular structure and numbering scheme of *N*-phenyl-(diphenylphosphoryl)-formamide (4). The ellipsoids represent a probability of 40 %, H atoms are shown with arbitrary radii. Selected structural parameters are listed in Table 2.

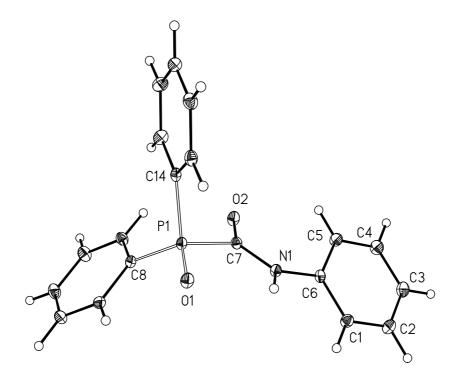


Figure S5: Molecular structure and numbering scheme of *N*-2,4,6-trimethylphenyl-(diphenylphosphoryl)formamide (6). The ellipsoids represent a probability of 40 %, H atoms are shown with arbitrary radii. Selected structural parameters are listed in Table 2.

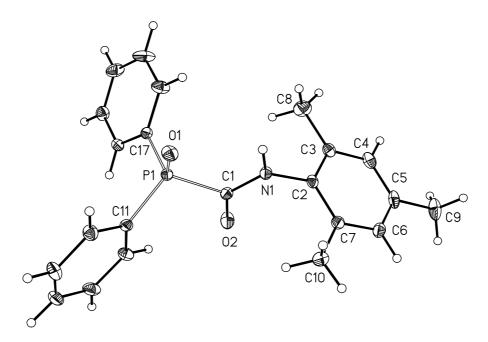


Figure S6: Molecular structure and numbering scheme of *N*-naphthyl-(diphenylphosphoryl)-formamide (7). The ellipsoids represent a probability of 40 %, H atoms are shown with arbitrary radii. The asymmetric unit contains two crystallographically independent molecules "A" and "B"; only molecule A is displayed.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

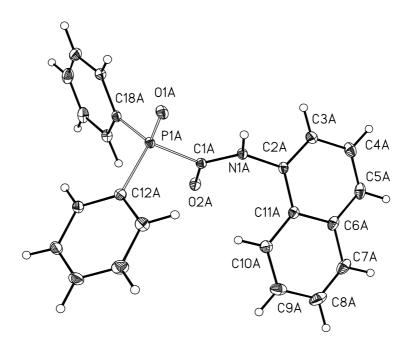


Figure S7: Molecular structure and numbering scheme of *N*-cyclohexyl-(diphenyl-phosphoryl)thioformamide (9). The ellipsoids represent a probability of 40 %, H atoms are shown with arbitrary radii. The asymmetric unit contains two crystallographically independent molecules "A" and "B"; only molecule A is displayed. Selected structural parameters are listed in Table 2.

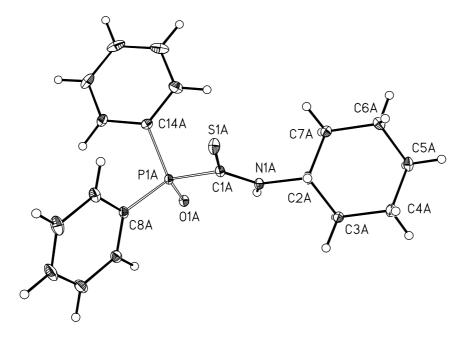


Figure S8: Molecular structure and numbering scheme of *N*-phenyl-(diphenylphosphoryl)-thioformamide (**10**). The ellipsoids represent a probability of 40 %, H atoms are shown with arbitrary radii. Selected structural parameters are listed in Table 2.

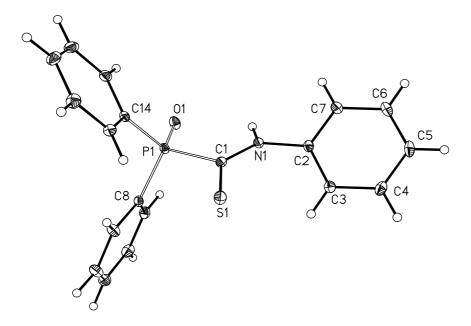


Figure S9: Molecular structure and numbering scheme of *N*-4-methylphenyl-(diphenyl-phosphoryl)thioformamide (**11**). The ellipsoids represent a probability of 40 %, H atoms are shown with arbitrary radii. Selected structural parameters are listed in Table 2.

