



APPLICATION NOTE

Catalyst quench & removal with an isonitrile scavenger

Developed in the laboratories of Prof. Steven Diver at the University of Buffalo, potassium isocynoacetate (**1**) irreversibly binds a variety of homogeneous catalysts to aid in product purification.

In Pd-catalyzed cross couplings and aminations using 2-5 mol % Pd(PPh₃)₄, Pd(OAc)₂, or Pd₂(dba)₃ precatalysts, Prof. Diver's team reports reduction in product metals content to 0.02 - 11 wt ppm Pd after a single treatment and silica gel chromatography. In Ru-catalyzed olefin metathesis reactions using a variety of Grubbs-type catalysts at 5 mol % loading, Prof. Diver reports that products contain only 0.8 - 11 wt ppm Ru after one treatment. Removal of additional spent metal catalysts may also be possible, but data are not publically available.

The product is weakly hygroscopic, and storage in a benchtop desiccator is recommended.

Representative procedure:

On completion of the catalytic reaction, prepare a solution of **1** in MeOH (4 - 8 equiv relative to the catalyst) with a concentration of approx. 40 mg / mL. Note: turbidity may indicate product hydrolysis, requiring the use of additional **1**.

Introduce the solution to the reaction mixture. For colored complexes, decolorization typically occurs within minutes to indicate isonitrile coordination. Spent catalysts with bulky ligands may require heating to 60 °C to affect complete binding. The quenched catalyst is then removable by aqueous wash during workup, or by concentration of the crude reaction mixture and filtration through silica gel.

Before quench:

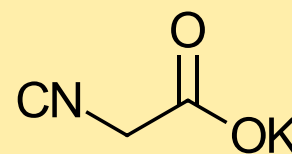
1st. gen. Grubbs catalyst #02-01-1001 at 0.05 mM in a reaction mixture



After quench:

the same mixture 5 min after addition of 4 equiv **1** (relative to catalyst) in MeOH shows a large chromatic shift

Product Highlight



Name: Potassium 2-isocynoacetate

CAS: 58948-98-4

Formula: C₃H₂KNO₂

MW: 123.15 g/mol

Catalog: 01-09-1001

Further reading:

Org. Lett. **2007**, 9, 1203-1206. DOI: 10.1021/ol0631399

Adv. Synth. Catal. **2015**, 357, 361-365. DOI: 10.1002/adsc.201400754