

# ChemFiles

 **ALDRICH**<sup>®</sup>

## *Encapsulated Catalysts and Metal Scavengers*

DIHYDROXYLATION  
CATALYST

COUPLING CATALYSTS

HYDROGENATION  
CATALYSTS

METAL SCAVENGERS

*Sigma-Aldrich and Reaxa partner to bring you...  
...easier, faster, cleaner processes.*

# Easier, Faster, Cleaner Processes with Encapsulated Catalysts and Metal Scavengers

Sigma-Aldrich is pleased to partner with Reaxa Ltd to offer an array of new technologies for precious metal catalysis to achieve easier, faster and cleaner processes. The technology integrates smoothly with existing methods, reduces purification steps, cuts contamination, and allows for efficient recovery of precious metals. Encapsulated catalysts (EnCat™) and metal scavengers (QuadraPure™ and QuadraSil™) are available exclusively through Sigma-Aldrich at research scale.

# Easier Faster



# Cleaner

## Dihydroxylation Catalyst

### Os EnCat™ 40

Osmium tetroxide is known to be one of the most reliable and effective catalysts for oxidative cleavage and dihydroxylation of olefins. However, it is very toxic, volatile and expensive, limiting its use at large-scale. Os EnCat™ 40 effectively immobilizes and stabilizes osmium tetroxide to produce a safer and easier to use catalyst for use in oxidation chemistry. In the picture on the right, a sample of Os EnCat™ 40 placed in corn oil is unchanged after several months, whereas an equivalent sample of volatile osmium tetroxide quickly reacts to produce black decomposition products.



#### Cleaner products

typically less than 100 ppm Os in crude product

#### Easier storage, transport & use

low residual OsO<sub>4</sub> vapor over Os EnCat™ 40 product

#### Faster, efficient processes

resin beads filter easily

#### High selectivity

can be used for asymmetric dihydroxylation

#### Reduced plant contamination

OsO<sub>4</sub> is trapped in the beads

#### Improved cost effectiveness

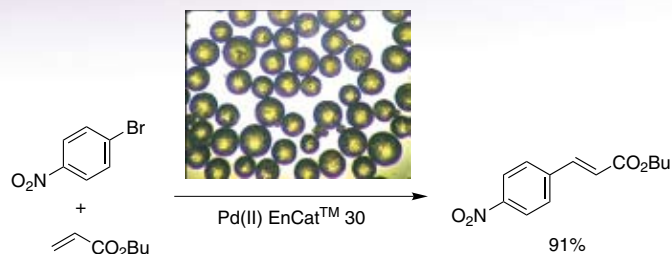
Os EnCat™ 40 may be reused in repeat reaction cycles

Product No.	Name	Metal content (w/w%)	Loading (mmol/g)	Particle size range in µm (average)
658685	Os EnCat™ 40	4.8 – 5.7	0.25 – 0.30	40 – 300 (165)

# Coupling Catalysts

## Pd(II) EnCat™

Pd(II) EnCat™ covers a versatile range of immobilized palladium acetate catalysts with or without activating ligands contained in a robust, porous polyurea matrix which allow easier, faster and cleaner C–C coupling processes to be developed.

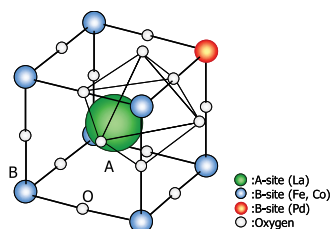


<b>Cleaner products</b>	typically less than 10 ppm Pd in crude product
<b>Cleaner waste streams</b>	reduced metal losses in Pd(II) EnCat™ processes
<b>Fast, efficient processes</b>	EnCat™ beads filter easily
<b>No plant contamination</b>	metal & ligands are trapped within the beads
<b>Improved processes</b>	high activity in many types of coupling reactions
<b>Process intensification</b>	can be used in batch & flow processes

Product No.	Name	Metal content (w/w%)	Co-encapsulated ligand
644714	Pd(II) EnCat™ 30	4.3	none
644722	Pd(II) EnCat™ 40	4.6	none
644706	Pd(II) EnCat™ TPP30	4.7	
644692	Pd(II) EnCat™ TOTP30	4.7	
658693	Pd(II) EnCat™ BINAP30	4.7	
666335	Pd(II) EnCat™ Kit I (five component kit of 1 gram units of each Pd(II) EnCat™)		

## LaPCat™

An exclusive collection of palladium and copper containing perovskite heterogeneous catalysts for use in a range of organic reactions. The LaPCat™ perovskite catalysts have shown very high catalytic activity in many coupling reactions with a wide variety of substrates.



<b>Cleaner products</b>	typically 10 ppm or less of metal contamination in crude product
<b>Cleaner waste streams</b>	reduced metal losses in LaPCat™ processes
<b>Fast, efficient processes</b>	equivalent or better than homogeneous catalysts
<b>Improved processes</b>	very low catalyst loadings achieved
<b>Improved cost effectiveness</b>	LaPCat™ catalysts may be reused in repeat reaction cycles

### 674052 LaPCat™ Perovskite Catalyst Kit I (100 mg units of each LaPCat™)

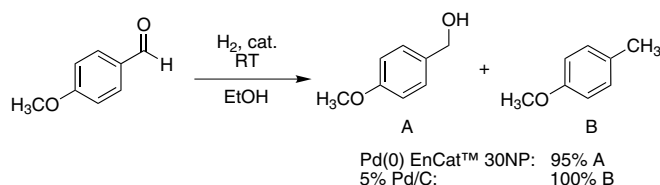
Catalyst	Formulation	Surface area (m <sup>2</sup> /g)	Particle size (μm)	Reactions
FP2	LaFe <sub>0.95</sub> Pd <sub>0.05</sub> O <sub>3</sub>	5.5	41.1	Suzuki
FP8	LaFe <sub>0.80</sub> Pd <sub>0.20</sub> O <sub>3</sub>	5.7	3.3	Suzuki
CoP	LaFe <sub>0.57</sub> Co <sub>0.38</sub> Pd <sub>0.05</sub> O <sub>3</sub>	3.4	4.0	Suzuki, Heck, Sonogashira
CuP	LaFe <sub>0.57</sub> Cu <sub>0.38</sub> Pd <sub>0.05</sub> O <sub>3</sub>	12	3.7	Suzuki, Sonogashira, Ullmann
CoCu	La <sub>0.9</sub> Ce <sub>0.1</sub> Co <sub>0.60</sub> Cu <sub>0.40</sub> O <sub>3</sub>	7.9	5.4	Ullmann
YBCu	YBa <sub>2</sub> Cu <sub>3</sub> O <sub>7</sub>	0.3	10.6	Ullmann

# Hydrogenation Catalysts

## Pd(0) EnCat™ 30NP

Pd(0) EnCat™ 30NP is a versatile polymer encapsulated nano-particulate Pd(0) hydrogenation and transfer hydrogenation catalyst with high chemoselectivity and improved safety profile allowing easier, faster and cleaner processes to be developed. Reaxa's controlled manufacturing process produces regular palladium(0) nano-particles stabilized by the polymer matrix within the EnCat™ beads, ensuring that the catalyst performance is extremely reproducible from batch to batch (c.f. palladium on carbon).

<b>Cleaner products</b>	typically less than 1 ppm Pd in crude product
<b>Cleaner waste streams</b>	reduced metal losses in EnCat™ processes
<b>Fast, efficient processes</b>	EnCat™ beads filter easily and can be recycled
<b>No plant contamination</b>	palladium metal is trapped within the beads
<b>High selectivity</b>	in hydrogenation & transfer hydrogenation reactions
<b>Improved safety profile</b>	non-pyrophoric compared with Pd/C catalysts
<b>Process intensification</b>	can be used in batch & flow processes



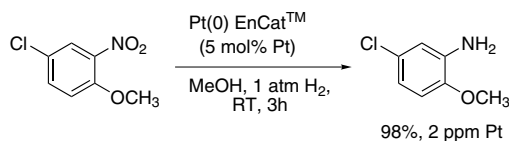
Product No.	Name	Metal content* (w/w%)	Loading* (mmol/g)	Particle size range in μm (average)
653667	Pd(0) EnCat™ 30NP	4.3	0.40	100 – 350 (200)

\* based on dry material; product supplied water wet

## Pt(0) EnCat™ 40

Pt(0) EnCat™ 40 is a versatile hydrogenation catalyst demonstrating high chemoselectivity and improved safety profile over platinum on carbon allowing easier, faster and cleaner processes to be developed. Isolating the active platinum within the polymer matrix has produced an easily handled and safer alternative to Pt/C.

<b>Cleaner products</b>	very low levels of Pt in crude product
<b>Cleaner waste streams</b>	reduced metal losses in EnCat™ process (typically <0.005% Pt loss)
<b>Fast, efficient processes</b>	EnCat™ beads filter easily
<b>No plant contamination</b>	platinum metal remains entrapped within the beads
<b>High selectivity</b>	in hydrogenation reactions
<b>Process intensification</b>	can be used in batch & flow processes
<b>Improved safety profile</b>	initial tests show no tendency for activated catalyst to ignite upon exposure to air



Product No.	Name	Metal content* (w/w%)	Loading* (mmol/g)	Particle size range in μm (average)
681504	Pt(0) EnCat™ 40	2.3	0.12	100 – 350 (200)

\* based on dry material; product supplied water wet

**For detailed technical information on these encapsulated catalysts or metal scavengers, including application guides and references, please visit [sigma-aldrich.com/reaxa](http://sigma-aldrich.com/reaxa).**

# Metal Scavengers

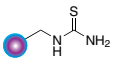
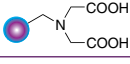
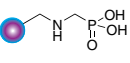
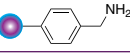
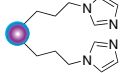
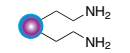
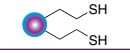
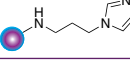
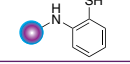
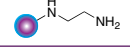
**QuadraPure™** and **QuadraSil™** metal scavengers offer a variety of complementary solutions for efficient removal and economic recovery of precious metal contamination from products and process streams (aqueous or organic). The picture shows a typical 'before-and-after' scavenger treatment of a metal catalyst solution (initial metal content 1000 ppm) at room temperature.



## QuadraPure™

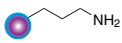
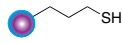
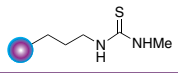
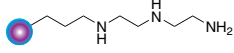
The QuadraPure™ collection consists of two ranges of functionalized polystyrene beads:

- Macroporous, low-swell, robust beads for use in manufacturing either in batch or flow processes.
- Microporous, solvent swellable beads with high capacity intended largely for R&D application.

	Product No.	Name	Functional group	Examples of metals removed
Macroporous	655422	QuadraPure™ TU		thiourea Pd, Pt, Ru, Rh, Au, Ag, Cu, Hg, Pb, Cd, Ni, Co, Fe, V, Zn
	657026	QuadraPure™ IDA		iminodiacetate Cu, Al, Ga, In, V, Pb, Ni, Zn, Cd, Be, Mn, Sr, Ba, Co, Fe
	657611	QuadraPure™ AMPA		aminomethylphosphonic acid Fe, Cu, Ni, Al, Co, V
	668591	QuadraPure™ BZA		benzylamine Rh, Pd, Cu, Co, Ni
	668605	QuadraPure™ BDZ		imidazole Rh, Co, Pd, Ni
	668583	QuadraPure™ EDA		amine Pd in basic media and with phosphines, Co, Ni, Rh
	668575	QuadraPure™ DET		thiol Pd in acidic media and with phosphines, Co, Fe, Ni, Rh
Microporous	657654	QuadraPure™ IMDAZ		imidazolylpropyl-amino Pd, Ru, Os, Co, Ni, V, Rh, Cu, Fe, Sn
	657662	QuadraPure™ MPA		mercaptophenyl-amino Pd, Pt, Rh, Ni, Ru, Cu, Sn, Ag, Au, Cd, Hg, Pb
	657646	QuadraPure™ AEA		aminoethylamino Pd, Rh, V, Cu, Fe
	659428	QuadraPure™ Metal Scavengers Kit I (six component kit of 5 g units of QuadraPure™ TU, IDA, AMPA, IMDAZ, MPA, and AEA)		
681547	QuadraPure™ Metal Scavengers Kit II (ten component kit of 5 g units of each QuadraPure™)			

## QuadraSil™

The QuadraSil™ scavengers offer extremely rapid removal of metal catalyst residues. QuadraSil™ products are based on high-quality spherical silica beads with well defined porosity that can be used in aqueous or organic solution and in batch or flow processes.

Product No.	Name	Functional group	Examples of metals removed
679534	QuadraSil™ AP		aminopropyl Pd, Ru, Rh, Cu, Fe, Co, Ni
679526	QuadraSil™ MP		mercaptopropyl Pd, Rh, Cu, Ru, Pt, Pb, Ag, Hg
679518	QuadraSil™ MTU		methylthiourea Pd, Rh, Cu, Ru, Pb, Fe, Co
679496	QuadraSil™ TA		triamine Pd, Rh, Co, Cu, Fe, Ru, Cd, Au, V, Zn, Pt
680427	QuadraSil™ Metal Scavengers Kit I (four component kit of 5 g units of each QuadraSil™)		

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