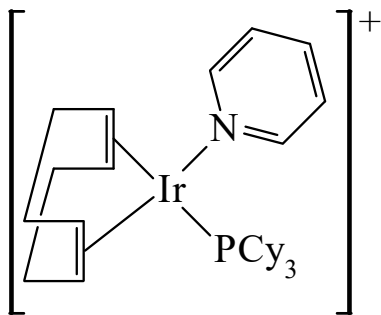




>>Entry Name: [(1,2,5,6-η)-1,5-Cyclooctadiene](pyridine)(tricyclohexylphosphine)iridium(1+), 12Cl, 11Cl, 10Cl



Molecular Formula: C₃₁H₅₀IrNP⁽⁺⁾

Molecular Weight: 659.936

Accurate Mass: 660.331003

Percentage Composition: C 56.42%; H 7.64%; Ir 29.13%; N 2.12%; P 4.69%

>>Derivative: Hexafluorophosphate

Synonym(s): Crabtree's catalyst

CAS Registry Number: 64536-78-3

Molecular Formula: C₃₁H₅₀F₆IrNP₂

Molecular Weight: 804.901

Percentage Composition: C 46.26%; H 6.26%; F 14.16%; Ir 23.88%; N 1.74%; P 7.70%

Source/Synthesis: Synth. from [Ir(cod)(Py)₂](PF₆) + PCy₃ in MeOH for 15 min.

Use/Importance: Catalyst for hydrogenation of simple alkenes and diastereoselective hydrogenation of functionalised alkenes, e.g. allylic, homoallylic alcohols

Physical Description: Air-stable orange cryst. (CH₂Cl₂/Et₂O)

Solubility: Sol. CHCl₃, CH₂Cl₂, Me₂CO; insol. alcohols

Aldrich: 33749-8

Fluka: 29590

Sigma: T4156

>>Derivative: Tetrafluoroborate

CAS Registry Number: 80409-82-1

>>Derivative: Perchlorate

CAS Registry Number: 118229-26-8

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Stork, G. *et al.*, *J.A.C.S.*, 1983, **105**, 1072, (*use, diastereoselective hydrogenation*)

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Brown, J.M. *et al.*, *Tetrahedron*, 1985, **41**, 4639; 4647, (*use, diastereoselective hydrogenation*)

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Cabeza, J.A. *et al.*, *J.C.S. Perkin I*, 1988, 1881, (*use*)

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