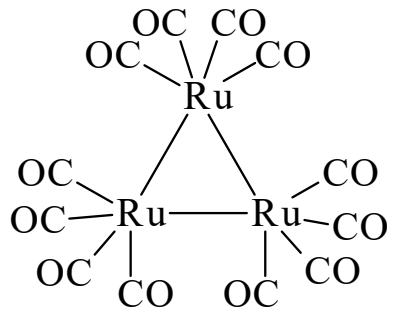
>>**Entry Name: Dodecacarbonyltriruthenium,** 9CI
Synonym(s): Triruthenium dodecacarbonyl. Ruthenium carbonyl ($Ru_3(CO)_{12}$)



CAS Registry Number: 15243-33-1
Type of Compound Code(s): BA0650 BA0180 BA0610 BA0300 BA0490 BA0040 BA0270 BA0070 BA0095 BA0275 BA0482 BA0495 BA0290 BA0440 BA0407 BA0080 BA0345 BA0230 BA0060 BA0430 BA0130 BA0235 BA0170 BA0320 BA0030 BA0360 BA0460 BA0330

Molecular Formula: $C_{12}O_{12}Ru_3$
Molecular Weight: 639.335
Accurate Mass: 641.652024
Percentage Composition: C 22.54%; O 30.03%; Ru 47.43%
Source/Synthesis: Synth. either by high pressure carbonylation of a wide range of ruthenium compds. (e.g. $RuCl_3$, $Ru(acac)_3$ and Ru^{III} carboxylates) or by treating a 2-ethoxyethanol soln. of $RuCl_3$ with CO, followed by Zn redn.
Use/Importance: A vastly important reagent. Active catalyst for many processes including: water-gas shift reaction; addn. of carboxylic acids to alkynes → vinyl esters; hydrogenation of alkynes, dienes, polyenes; Fischer-Tropsch reaction; decarbonylation of formates → alcohols; allylation of RCHO with allyl acetates in presence of CO/Et_3N → homoallyl alcohols; *N*-alkylation of amines by alcohols, diols in presence of PBu_3; carbonylation of cyclic amines → formamides; transfer hydrogenolysis of CX_4 (X = Cl, Br); hydroformylation and hydroacylation of alkenes; carbonylation/homologation of alcohols; homologation of HOAc with CO; carbonylation of $ArNO_2$ → isocyanates; precursor to catalysts for rearrangement of azobenzenes → 1-phenyl-2-alkylbenzimidazoles; isom. of alkenes, dienes; transfer hydrogenation of ketones with MeOH; dehydrogenation of alcohols → esters; oxidn. of alkynyl ethers, amines by PhIO → α-keto esters, α-keto amides; redn. of $ArNO_2$ to $ArNH_2$ using CO/H_2O or CO/H_2; reaction of alkenes with CO in presence of base → ketones; hydrosilylation of fluorinated alkenes; with $Fe_3(CO)_{12}$, reductive amination of ketones; amidocarboxylation of alkynes → enol carbamates; reductive *N*-heterocyclisation; reductive carbonylation of $ArNO_2$ with CO/MeOH → ArNHCOOMe; H/D exchange in tertiary amines; alcohol oxidn. with Bu^tOOH; dehydrogenative hydrosilylation of alkenesr vinyl silanes; reductive decarboxylation of acids; hydrocarbonylation of ethyne → hydroquinone; *ortho*-acylation of pyridines with $RCH{=}CH_2/CO$; silylcarbonylation of alkenes → silyl enol ethers; amines/CO_2 → ureas; RCHO + $R'CH_2OH$ → $RC(O)OCH_2R'$; Pauson-Khand cocyclisation of alkynes, alkenes and CO; undergoes subst. reactions; can be converted to other Ru cluster complexes
Physical Description: Air-stable orange cryst. (hexane or C_6H_6)
Melting Point: Mp 154-155 dec.°
Boiling Point: Subl. 80-100° *in vacuo*
Solubility: Sol. most org. solvs. (e.g. hexane, C_6H_6, $CHCl_3$, EtOH); insol. MeOH, H_2O
Other Data: ΔH_f° –1903 kJ mol^{-1}; ΔH_{fusion} 43.5 kJ mol^{-1}

Aldrich: 24501-1
Fluka: 84055

References: