Compound Information

Tanase Group, Name Your name No 1

Compound Fill with the right formula including solvents of crystallization, which should be consistent with elemental analysis.

Preparation Experimental No. ex. #TT000919

Describe the detailed preparation procedures; mg and mmol of reagents, mL of solvents, mg and mmol of the product, temp, time, and procedures.
If necessary, describe in separate sheets.

Yield Max. 70 % (Exp No.) #TT000919 , Range 70 ~ 40 % #TT991212 #TT000213 #TT000716

Crystallization System

Describe the crystallization method to get analysis sample; solvents (mL), temp, time, mixing way etc.

Describe the crystallization mthod to get Xtals

Proposed Structure

Illustrate schematic view(s) of the proposed structure. When X-ray analysis done, please put it with ORTEP plots attached.

Analysis Sample No. @TT000919

Formura C12H30O2N3Ni Mol Weight Calcd. with Ryotaro

Calcd: C, H, N, Others, %

Found: C, H, N, Others, %

IR Method KBr Sample No. `@TT000826A

ν cm^{-1}

Summarize the wave number with s, m, w, br. Attach the original spectrum.

UV-Vis Solvent Sample No. @TT000826B

λ (ε), nm ($M^{-1}cm^{-1}Metal^{-1}$)

Summarize the max wave lengths with molar extinction coefficients. Attach the original spectrum.

^{1}H NMR Solvent Sample No. @TT000823A

Method Non Decouple Ref. TMS external (7.26ppm for CHCl3)

Machine Gemini2000 (300 MHz) Temp r.t.

δ

Summarize the chemical shifts with s, d, t and J. Attach the original spectrum.

Compound No 2

^{31}P NMR Solvent Sample No.
Method Ref.
Machine Temp
δ

Other NMR Solvent Sample No.
Method Ref.
Machine Temp
δ

Other Data and Comments <Please compile with raw data>

MS
CV
EXAFS
MO
Conductivity
Osmometry
Emission
etc

Summarize the other measurements and attach the full detailed data.

X-Ray Crystallography

When X-ray crystallography done, lists the crystal data, and attach the full detailed data (X-ray Report) and ORTEP drawings.

crystallization solvent system crystal shape
crystal size crystal color
crystal system space group
lattice const. a = α =
b = β =
c = γ=
V =
Z *D*(calcd) =
No of Obsd Data ($I > \sigma(I)$) 2θ max
R R_w
UNICS Dir Name Problem
Comments

Date prepared this datasheet: put the date when you prepared and revised data. When you want to revise the data, use red pen.