SciFinder, Reaxys and Web of Knowledge

Organometallic chemistry information retrieval

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CHEM227

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Molecular formula search in SciFinder

Search for Ph₃PBH₃

To avoid ambiguity, enter molecular formula with spaces between elements. For salts and other multi-component systems, there is a special means of searching called “dot-connect” formula (e.g., NaBH₄ is searched as H₄B.Na). Help on constructing a complex formula search is available by clicking the ? icon or contacting the librarian.
Molecular formula search in SciFinder

Sort the results by the Number of References; well known substances appear often in the literature.

Click on the CAS registry number (CASRN) to view the substance record, including names, molecular formula, spectra and experimental properties.
Experimental data in SciFinder

The substance record links to references in the literature, commercial sources to purchase the substance, experimental properties and spectra and more. Click headings to see details and follow links for literature references.
References in SciFinder

Catalyst-free alcoholysis of phosphane-boranes: a simple procedure

By: Van Overschelde, Michel; Vervecken, Elias; Modha, Sachin G.; Cogen, Stijn

Catalyst-free alcoholytic deprotection of borane-protected phosphorus containing compounds is reported. The results on the general applicability of this new reaction are discussed. The reaction enables simple alcoholysis without the use of mol. sieves as a catalyst. Phosphane-boranes can be deprotected in high yields. Borane complexes of triarylphosphines or phosphines can be used as catalysts. The main merit of our method is its simplicity: apart from evapn. of the solvent, no organic modification is required. Ph₃P·BH₃ (prepn. given) in EtOH for 24 h gave 95% Ph₃P.

Indexing

Organometallic and Organometalloidal Compounds (Section29-7)

Concepts

Alcoholysis

catalyst-free alcoholysis of phosphane-boranes as smooth, cheap, and efficient deprotection procedure

Substances

121-45-0P Trimethyl phosphite
122-52-1P Triethyl phosphite
2622-14-2P Tricyclohexylphosphine
13716-12-6P Tris-tert-butylphosphine

Click “Link to Other Sources” for full text of articles. Depending on the source, you may be referred to the University of Chicago FindIt! menu.

Reference details are shown to the right in the display.
Look for the part of the article with the experimental details. Compounds are often identified with only internal reference numbers (e.g., 1a) so you may need to refer back to the earlier parts of the article to find the correct compound in the experimental section.
Drawing inorganics and organometallics can be tricky. You may need to draw generic substructures and scan the results for appropriate hits. Bond orders can also be tricky; there is help available online, or contact the librarian if you are not retrieving structures you expect. HINT: sometimes you can search a similar structure by name (e.g., ferrocene) and copy the structure to the editor to modify without drawing the entire structure.)
Click on the Show Details to see a larger structure and a listing of available information. You may have to scroll through a couple of screens to find spectral data.
Basic identification and physical data

Links to the original literature references are provided.

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>Coupling Nuclei</th>
<th>Solvents</th>
<th>Temperature</th>
<th>Comment</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>21P</td>
<td></td>
<td>tetrahydrofuran</td>
<td>Signals</td>
<td>Kriter, Richard J.; Madison, Matthew J.</td>
<td>Title/Abstract Full Text View citing articles Show Details</td>
</tr>
</tbody>
</table>
Molybdenum carbonyl complexes of di- and triphosphines: hydrophosphinination reactions of \((\text{HC}=\text{CCH}_2\text{PPh}_2)\text{Mo}(\text{CO})_5\)

Kalyani Maitra, Vincent J. Catalano, John H. Nelson

Department of Chemistry, University of Nevada, Reno, NV 89557-0020, USA

Received 24 April 1996; revised 17 June 1996

\[\begin{align*}
\text{C}_{26} \text{H}_{32} \text{Mo}_{6} \text{P}_{12} \text{O}_{34}, \text{M.p.} 175^\circ \text{C} \text{ (decomp.), IR} \\
2042 \text{ (m), } 2012 \text{ (sh), } 1924 \text{ (sh), } 1908 \text{ (s), } 1890 \text{ (sh).} \]

\[^{31} \text{P} \{^{1} \text{H}\} \text{ NMR (CDCl}_3, 121.66 \text{ MHz) \delta 52.1 (d, } {^2} \text{J}_{\text{PP}} = 6.3 \text{ Hz, P}_\text{A}, 70.1 \text{ (d, } {^2} \text{J}_{\text{PP}} = 6.3 \text{ Hz, P}_\text{B}, 1 \text{H NMR (CDCl}_3, 500 \text{ MHz) \delta 2.17 (dd, } {^3} \text{J}_{\text{PH}} = 6 \text{ Hz, } {^4} \text{J}_{\text{HH}} = 1 \text{ Hz, 3H, CH_3}, 7.35-7.60 \text{ (m, 21H, H_\gamma \text{ and aromatic H's).}^{13} \text{C} \{^{1} \text{H}\} \text{ NMR (CDCl}_3, 125.71 \text{ MHz) \delta 20.40 \text{ (dd, } {^2} \text{J}_{\text{PC}} = 1.07 \text{ Hz, } {^3} \text{J}_{\text{PC}} = 15.78 \text{ Hz, C}_\alpha, 128.54 \text{ (d, } {^3} \text{J}_{\text{PC}} = 8.79 \text{ Hz, C}_\beta, 128.59 \text{ (d, } {^3} \text{J}_{\text{PC}} = 9.18 \text{ Hz, C}_\gamma, 129.75 \text{ (s, C}_\delta, 129.76 \text{ (s, C}_\varepsilon, 131.59 \text{ (d, } {^2} \text{J}_{\text{PC}} = 12.82 \text{ Hz, C}_\zeta, 131.98 \text{ (d, } {^2} \text{J}_{\text{PC}} = 15.15 \text{ Hz, C}_\eta, 134.91 \text{ (dd, } {^1} \text{J}_{\text{PC}} = 33.69 \text{ Hz, } {^4} \text{J}_{\text{PC}} = 2.26 \text{ Hz, C}_1, 137.18 \text{ (dd, } {^1} \text{J}_{\text{PC}} = 33.65 \text{ Hz, } {^4} \text{J}_{\text{PC}} = 1.70 \text{ Hz, C}_2, \text{ apparent t, } {^1} \text{J}_{\text{PC}} = 2 \text{J}_{\text{PC}} = 38.3 \text{ Hz, C}_3, 157.16 \text{ (dd, } {^1} \text{J}_{\text{PC}} = 30.17 \text{ Hz, } {^2} \text{J}_{\text{PC}} = 23.88 \text{ Hz, C}_4, 208.98 \text{ (apparent t, } {^2} \text{J}_{\text{PC}} = 8.55 \text{ Hz, CO}_a, {^2} \text{J}_{\text{PC}} = 20.08 \text{ Hz, } {^2} \text{J}_{\text{PC}} = 8.24 \text{ Hz, CO}_b \text{ or b'}, 216.78 \text{ (dd, } {^2} \text{J}_{\text{PC}} = 26.09 \text{ Hz, } {^2} \text{J}_{\text{PC}} = 8.61 \text{ Hz, CO}_b \text{ or b').} \text{ Anal. Found: C, 60.06; H, 4.12. C}_{31} \text{H}_{24} \text{MoO}_4 \text{P}_2 \text{ Calc.: C, 60.21; H, 3.91%.)}
\end{align*}\]
Using cited references to find related research articles

Search for a known article as a starting point for your cited reference search.
Select the original article reference

After identifying the article of interest, click on the number labeled “Times Cited” to see related articles.
Sometimes you can successfully use search terms or various filters to narrow your results. Other times you will need to browse results to locate articles on specific aspects, such as reaction mechanism.
Chemistry 22700 Advanced synthetic chemistry laboratory

Course-specific guide to introduce resources for inorganic and organometallic synthesis and compound characterization laboratory projects.

Starting points

- CHEM 227 Library Orientation
- ChemDraw
- Finding Journal Titles
- Find It!

Writing & presentation resources

- Tutorials/Guides for Databases

CHEM 227 Library Orientation

- CHEM 227 Organometallic Chemistry Information Retrieval
  Slides from class presentation

ChemDraw

- ChemDraw instructions

Finding Journal Titles

Subject Specialist

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Contact:
Director of Research and...
Questions?

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