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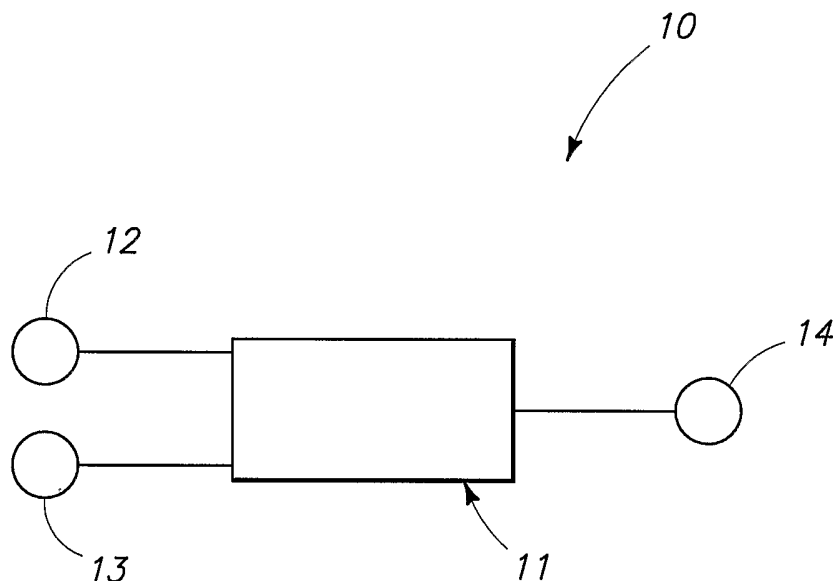
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(54) Title: CHEMICAL PRODUCTION PROCESSES AND SYSTEMS



(57) Abstract: Chemical Production Processes and Systems. Chemical production processes are provided that include replacing a halogen of an unsaturated halocarbon to produce an unsaturated hydrohalocarbon. Chemical production systems are provided that include a reaction zone coupled to first and second reservoirs, the first reservoir containing an unsaturated halocarbon and the second reservoir containing a hydrogenating reagent with the system being configured to expose the unsaturated halocarbon of the first reservoir to the hydrogenating agent of the second reservoir within the reaction zone.



For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

CHEMICAL PRODUCTION PROCESSES AND SYSTEMS

CLAIM FOR PRIORITY

5 This application claims priority to U.S. Provisional Patent Application, Serial No. 60/605,232, entitled "Chemical Preparation Processes", filed August 26, 2004; as well as International Patent Application No. _____, entitled "Chemical Preparation Processes", filed August 26, 2005; the entirety of both of which are incorporated by reference herein.

TECHNICAL FIELD

10 The present invention relates to the field of chemical production processes and systems and more specifically to the production of hydrogenated olefins.

BACKGROUND

15 Hydrogenated olefins can be produced in numerous ways, including via elimination reactions for example. Hydrogenating an olefin, particularly halogenated olefins, can prove to be difficult for at least the reason that the drawback of hydrogenating an olefin is that the hydrogens typically add across the double bond
20 saturating the compound. It can be beneficial to be able to add a hydrogen to an olefin without saturating the compound. The present invention provides chemical production processes and systems for hydrogenating olefins.

SUMMARY

25 Chemical production processes are provided that include replacing a halogen of an unsaturated halocarbon to produce an unsaturated hydrohalocarbon.

 Chemical production systems are provided that include a reaction zone coupled to first and second reservoirs, the first reservoir containing an unsaturated halocarbon and the second reservoir containing a hydrogenating reagent with the system being
30 configured to expose the unsaturated halocarbon of the first reservoir to the hydrogenating agent of the second reservoir within the reaction zone.

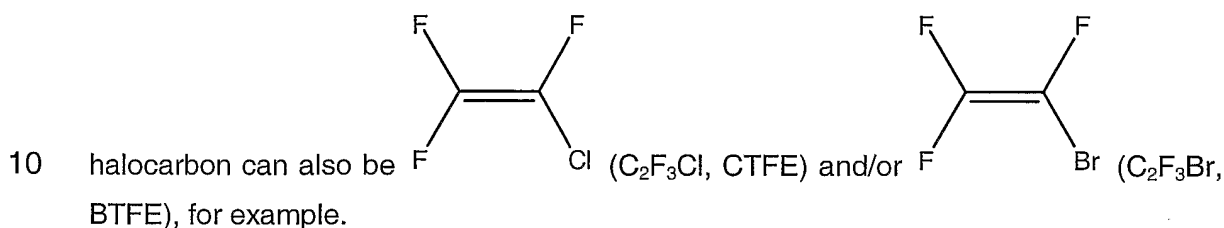
BRIEF DESCRIPTION OF THE FIGURE

35 The figure is an exemplary system for preparing compositions according to an embodiment.

DETAILED DESCRIPTION OF THE PREFERRED EMBODIMENTS

Chemical production processes and systems as described with reference to the Figure depicting a system 10 that includes a reaction zone 11 coupled to a halocarbon reservoir 12 and a hydrogenating reagent reservoir 13. System 10 further includes a product recovery reservoir 14.

The halocarbon of reservoir 12 can be a C-2 halocarbon, and in exemplary embodiments, the halocarbon can be a heterohalocarbon. For example, and by way of example only, the halocarbon can comprise both F and Cl, and, as another example, the halocarbon can comprise both F and Br. In exemplary embodiments, the



According to exemplary embodiments, the hydrogenating reagent from hydrogenating reagent reservoir 13 can be provided to reaction zone 11. According to exemplary embodiments, the hydrogenating reagent may include H, such as H₂.

15 Reaction zone 11 can be coupled to reservoirs 13 and 14 via separate conduits with each conduit configured to control the flow of the contents of the reservoirs to reaction zone 11. The conduits may be equipped with flow meters, for example. Both the halocarbon and the hydrogenating reagent may be provided to the reaction zone at a mole ratio of hydrogenating reagent to halocarbon utilizing the flow meters. For

20 example, the mole ratio of hydrogenating reagent to halocarbon may be from about 0.66 to about 11. By way of another example, the mole ratio may be at least about 0.66 and/or the mole ratio may be less than 11. In another exemplary embodiment, the mole ratio may be at least about 1.8.

Reaction zone 11 can include a single and/or multiple reactors. A reactor within reaction zone 11 can be constructed of a nickel-alloy such as an Inconel[®] (Tevco Industries 9337 Ravenna Rd. Twinsburg, OH 44087) tube having a volume of 34cc (OD = 0.5", length = 14.125", wall thickness = 0.035") equipped with a pressure gauge, pressure relief valve, Matheson Gas rotometers for gas feeds, and/or a vaporizer, for example.

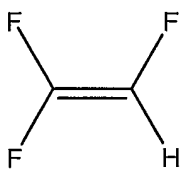
30 Reaction zone 11 may include a catalyst composition within a reactor. The catalyst composition may comprise a catalyst support and/or the catalyst composition may comprise activated carbon. The catalyst composition provided within reaction zone 11 may comprise one or more Pd, Cu, and/or Ni and/or the catalyst composition may

comprise both Pd and Cu. Where the catalyst composition comprises both Pd and Cu, the composition may include at least about 0.6% (wt./wt.) Pd and/or the composition may be at least about 5.5% (wt./wt.) Cu. In accordance with other embodiments, the catalyst composition may comprise nickel and nickel may be at least about 5% (wt./wt.) of the composition. Additional catalyst compositions can include; Pricat CZ 29/4, Al₂O₃, ZnO, CuO, (Syntex (PO Box 1, Billingham, Cleveland, TS23 1LB, UK); 7% FeCl₃ on Takeda Carbon (Life-Environment Company, 12-10, Nihonbashi 2-chamo Chuo-ku, Tokyo 103-8868, Japan); FeCl₃ (in-house, and/or ZnCl₂ (in-house); and those obtained from Engelhard (Chemical Catalysts Group, 554 Engelhard Drive, Seneca, SC 29678), such as, 0.6%Pd/5.5%Cu and/or Ni (Engelhard, 5% Ni on 1.5mm carbon).

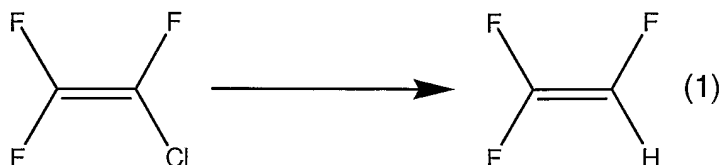
Prior to providing the halocarbon and/or the hydrogenating agent from reservoirs 12 and 13, respectively, a reactor of reaction zone 11 may be packed with the catalyst composition and heated to a temperature and/or exposed to a reducing agent for a sufficient time to activate the catalyst composition. Activation of the catalyst composition may be performed over a period of from about an hour to about 24 hours, for example. Typically, the catalyst composition within the reactor may be heated to from about 150°C to about 300°C during the activation. The catalyst composition may also be re-activated intermittently during the process at temperatures of from about 150°C to 400°C.

The halocarbon and hydrogenating reagent may be formed into a mixture within the reactor and a portion of the mixture may be heated to at least 300°C. According to an exemplary embodiment, the portion may be heated to from about 300°C and to about 400°C. The portion may also be heated to greater than about 400°C, for example. The temperature within the reaction zone can also be from 150°C to 475°C when providing mole ratios of reducing-reagent to halocarbon of 0.1 to 10.0. The reactants can reside within reaction zone 11 to provide contact times of from about 2 to about 20 seconds and reducing-reagent flow rates can be from 25-100cc/min while the halocarbon flow rates can be from 8-410cc/min.

Products leaving the reactor can be captured and/or further processed within product recovery reservoir 14. Reservoir 14 can include an apparatus such as a 10% KOH scrubber, a Drierite tube, and/or a dry ice/ acetone trap, for example. Exemplary products include, but are not limited to, unsaturated hydrohalocarbons including C-2 hydrohalocarbons. For example, and by way of example only, the hydrohalocarbon can comprise both F and H. In exemplary embodiments, the hydrohalocarbon can be

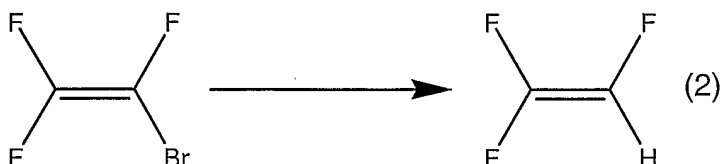
trifluoroethylene (C_2F_3H , TriFE), and/or , for example. As such system 10 can be used to replace a halogen of an unsaturated halocarbon to produce an unsaturated hydrohalocarbon.

Exemplary schemes 1 and 2 demonstrate exemplary reactions that can be performed utilizing system 10 of the Figure.



According to scheme (1) above, an Inconel tube can be packed with 0.6%Pd/5.5%Cu catalyst on activated carbon and maintained at 400°C. The reactants can be provided to the tube at a 4.5 mole ratio of H_2 to CTFE and exposed to the catalyst for a 9.6 second contact time. The conversion of CTFE to TriFE can be about 30.3% and selectivity can be 83.5% as determined by gas chromatography.

According to another embodiment, the Inconel tube can be packed with a Ni (Engelhard, 5% Ni on 1.5mm carbon) catalyst and maintained at 350°C. The reactants can be provided to the tube at a 0.66 mole ratio of H_2 to CTFE and exposed to the catalyst for an 11.2 second contact time. The conversion of CTFE to TriFE can be about 50.1% and the selectivity can be 61.1% as determined by gas chromatography.



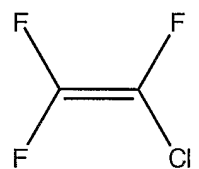
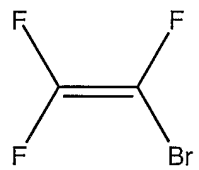
According to scheme (2) above, an Inconel tube can be packed with the 0.6%Pd/5.5%Cu catalyst on activated carbon and maintained at 300°C. The reactants can be provided to the tube at a 4.5 mole ratio of H_2 to BTFE and can be exposed to the catalyst for a 19.6 second contact time. The conversion of BTFE to TriFE can be 72.3% and selectivity can be 87.0% as determined by gas chromatography.

According to still another embodiment, an Inconel tube can be packed with the Ni (Engelhard, 5% Ni on 1.5mm carbon) catalyst and maintained at 400°C. The reactants can be provided to the tube at a 1.8 mole ratio of H_2 to BTFE and can be exposed to the catalyst for a 12.9 second contact time. The conversion of BTFE to

TriFE can be 96.8% and selectivity can be 90.7% as determined by gas chromatography.

CLAIMS

What is claimed is:

1. A chemical production process comprising replacing a halogen of an unsaturated halocarbon to produce an unsaturated hydrohalocarbon.
- 5 2. The chemical production process of claim 1 wherein the halocarbon comprises one or more of F, Cl, Br, and I.
3. The chemical production process of claim 1 wherein the halocarbon is a C-2 halocarbon.
4. The chemical production process of claim 1 wherein the halocarbon is a
10 heterohalocarbon.
5. The chemical production process of claim 1 wherein the halocarbon comprises both F and Cl.
6. The chemical production process of claim 1 wherein the halocarbon comprises both F and Br.
- 15 7. The chemical production process of claim 1 wherein the halocarbon is C₂F₃Cl.
8. The chemical production process of claim 1 wherein the halocarbon is C₂F₃Br.
9. The chemical production process of claim 1 wherein the halocarbon is

ClC(F)(F)=C(F)F
10. The chemical production process of claim 1 wherein the halocarbon is

BrC(F)(F)=C(F)F
- 20 11. The chemical production process of claim 1 wherein the replacing comprises:
 providing the halocarbon to within a reactor;
 providing a hydrogenating reagent to within the reactor; and
 recovering the hydrohalocarbon from the reactor.

12. The chemical production process of claim 11 wherein the halocarbon and the hydrogenating reagent are provided to within the reactor at a mole ratio of hydrogenating reagent to halocarbon, the mole ratio being from about 0.1 to about 11.
13. The chemical production process of claim 11 wherein the halocarbon and the hydrogenating reagent are provided to within the reactor at a mole ratio is at least 0.1.
14. The chemical production process of claim 11 wherein the halocarbon and the hydrogenating reagent are provided to within the reactor at a mole ratio is less than 11.
15. The chemical production process of claim 11 wherein the halocarbon and the hydrogenating reagent are provided to within the reactor at a mole ratio is at least 1.8.
16. The chemical production process of claim 11 wherein the hydrogenating reagent comprises H.
17. The chemical production process of claim 11 wherein the hydrogenating reagent is H₂.
18. The chemical production process of claim 11 further comprising providing a catalyst composition to within the reactor.
19. The chemical production process of claim 18 wherein the catalyst composition comprises a catalyst support.
20. The chemical production process of claim 18 wherein the catalyst composition comprises activated carbon.
21. The chemical production process of claim 18 wherein the catalyst composition comprises one or more of Pd, Cu, and/or Ni.
22. The chemical production process of claim 18 wherein the catalyst composition comprises Pd and Cu.
23. The chemical production process of claim 22 wherein the Pd is at least about 0.6% (wt./wt.) of the composition.
24. The chemical production process of claim 22 wherein the Cu is at least about 5.5% (wt./wt.) of the composition.
25. The chemical production process of claim 18 wherein the catalyst composition comprises Ni.
26. The chemical production process of claim 25 wherein the Ni is at least about 5% (wt./wt.) of the composition.

27. The chemical production process of claim 11 wherein the reactor is constructed of a nickel alloy.
28. The chemical production process of claim 11 further comprising:
forming a mixture comprising the halocarbon and the hydrogenating reagent
5 within the reactor; and
heating a portion of the mixture to at least about 300°C.
29. The chemical production process of claim 28 wherein the portion is heated to from about 150°C to about 400°C.
30. The chemical production process of claim 28 wherein the portion is heated to at
10 least about 400°C.
31. A chemical production system comprising a reaction zone coupled to first and second reservoirs, the first reservoir containing an unsaturated halocarbon and the second reservoir containing a hydrogenating reagent, the system being configured to expose the unsaturated halocarbon of the first reservoir to the hydrogenating agent of
15 the second reservoir within the reaction zone.
32. The system of claim 31 wherein the reaction zone houses a catalyst composition, the catalyst composition comprising one or more of Cu, Pd, and Ni.
33. The system of claim 32 wherein the catalyst composition comprises at least 0.6 %(wt./wt.) Pd.
- 20 34. The system of claim 32 wherein the catalyst composition comprises at least 5.5 %(wt./wt.) Cu.
35. The system of claim 32 wherein the catalyst composition comprises at least 5.0 %(wt./wt.) Ni.

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