Functionalized Sila-Adamantane

Tech ID: 32903 / UC Case 2022-883-0

**FULL DESCRIPTION**

**Background:**

The carbon based adamantane has enabled a myriad of valuable applications in medicine, imaging probes, catalysts, etc. because chemists have been able to install site selective functional groups. The silicon version of adamantane, sila-adamantane shares similar fundamental properties that make it useful. Despite its promise, the development of silicon diamondoids has remained in its infancy because of the difficulty in its synthesis.

**Technology:**

Prof. Timothy Su and his research team have developed a novel, patent pending method for the gram-scale synthesis and its regioselective functionalization at five discrete silicon centers within its core. These syntheses are guided by mechanistic insights that implicate an aluminate-stabilized silylium ion at the 2-position as the final intermediate in the isomerization synthesis.

#### a) Synthesis of sila-adamantane

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  2-azaadamantane
  + SiCl₄ → 2
  1

  R = Cl, Br
```

#### b) Site-selective functionalization

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  2-functionalization
  1-functionalization
  1,2,3,7-functionalization
```

#### c) Site-selective sila-adamantane functionalization

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  R = Cl, Br
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Synthetic strategies for functionalizing sila-adamantane at five discrete locations within the cluster core, paving the way for functional silicon diamondoid materials.

**ADVANTAGES**

The significant aspects of this invention are:

- Significantly more efficient as evidenced by the ability to access sila-adamantane on gram scales and in higher purity compared to prior art.
- No chlorinated by-products.

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**OTHER INFORMATION**

**KEYWORDS**

Silanes, Oligosilanes, Sila-Adamantane, Sila-diamondoids, Nano Electronics, Diamondoids, Silicon nanocrystals, Catalysts

**CATEGORIZED AS**

- Optics and Photonics
- All Optics and Photonics
- Computer
- Hardware
- Energy
- Storage/Battery
- Medical
- New Chemical Entities, Drug Leads
- Nanotechnology
- Materials
- Semiconductors
- Materials

**RELATED CASES**

2022-883-0
Provides for derivatizing the sila-adamantane cluster in site selective fashion with either the same or unique functional groups.

Atomically precise structure of sila-adamantane is an advantage over existing silicon nanocrystals that are heterogeneous in core size and surface chemistry.

SUGGESTED USES

Applications that could be enabled by this invention include:

- Use as a ligand for improved chemical catalysis
- Nanoscale silicon electronics
- Battery anode materials
- Pharmacology and medicine
- UV/blue-emitting materials
- Atomically precise versions of silicon donor qubits

STATE OF DEVELOPMENT

Experimental, lab-level demonstration of the process. 20 derivatives of sila-adamantane have been successfully synthesized and are ready for testing.

RELATED MATERIALS

- Site-Selective Functionalization of Sila-Adamantane and Its Ensuing Optical Effects