silica-alumina having a pore volume of 0.50 mL/g or more.

[0031]

Item 21. The production method according to Item 20, wherein the method satisfies the (E) and the metal oxide before fluorination has a pore volume of 0.45 mL/g or more.

[0032]

Item 22. The production method according to Item 20 or 21, wherein the method satisfies the (E) and the metal of the metal oxide before fluorination includes at least one element that belongs to Groups 3 to 14 of the periodic table.

[0032a]

In one aspect, the present disclosure refers to a method for producing a perfluoroalkyne compound,

the method comprising reacting a perfluoroalkadiene compound in the presence of a catalyst to obtain a perfluoroalkyne compound, and satisfying one of the following (A) to (G):

(A) the catalyst comprises at least one catalyst selected from the group consisting of catalysts containing a transition metal element, and catalysts containing at least two elements that belong to Groups 3 to 14 of the periodic table of elements;

(B) the catalyst comprises a catalyst containing at least one element that belongs to Groups 3 to 14 of the periodic table, and the contact time between the catalyst and the perfluoroalkadiene compound ~~represented by formula (2)~~ is 30 seconds or less;

(C) the catalyst comprises at least one catalyst selected from the group consisting of fluorinated chromium oxide having a pore volume of 0.08 mL/g or more, fluorinated alumina having a pore volume of 0.35 mL/g or more, and fluorinated silica alumina having a pore volume of 0.50 mL/g or more;

(D) the catalyst comprises a fluorinated metal oxide having a pore volume of 0.35 mL/g or more;

(E) the catalyst comprises a metal oxide fluorinated by reacting a metal oxide with at least one compound selected from the group consisting of hydrofluorocarbon, hydrochlorofluorocarbon, and chlorofluorocarbon, wherein a metal of the metal oxide is at

least one member selected from the group consisting of chromium, titanium, silicon, and zirconium;

(F) the catalyst comprises one or more catalysts obtained by fluorinating at least one metal oxide selected from the group consisting of chromium oxide having a pore volume of 0.10 mL/g or more, alumina having a pore volume of 0.45 mL/g or more, and silica alumina having a pore volume of 0.50 mL/g or more; and

(G) at least a part of the reaction of the perfluoroalkadiene compound from the start to the end of the reaction is performed under conditions in which the water content of the reaction system is 30 ppm by mass or less, based on the mass of the perfluoroalkadiene compound defined as 100 mass%.

[0032b]

In another aspect, the present disclosure refers to a method for producing a perfluoroalkyne compound, the method comprising obtaining the perfluoroalkadiene compound using as a substrate the perfluorocycloalkene compound obtained as a by-product by the production method as described herein.

~~[0032c]~~

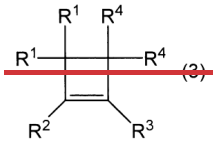
~~In another aspect, the present disclosure refers to a composition comprising a perfluoroalkyne compound and a perfluorocycloalkene compound,~~

~~the perfluoroalkyne compound being represented by formula (1):~~

~~$CR^1_2R^2-C\equiv C-CR^3R^4_2$ (1)~~

~~wherein R^1 to R^4 are the same or different and represent a fluorine atom or a perfluoroalkyl group,~~

~~the perfluorocycloalkene compound being represented by formula (3):~~



~~(3)~~

~~wherein R^1 to R^4 are as defined above, and~~

~~the composition containing the perfluoroalkyne compound represented by formula (1) in an amount of 40 to 99.999 mol%, based on the total amount of the composition defined as 100 mol%.~~

[~~0032d~~0032c]

In another aspect, the present disclosure refers to a catalyst for use in reacting a perfluoroalkadiene compound to obtain a perfluoroalkyne compound,

the catalyst satisfying the following (C) or (D):

(C) the catalyst contains at least one member selected from the group consisting of fluorinated chromium oxide having a pore volume of 0.08 mL/g or more, fluorinated alumina having a pore volume of 0.35 mL/g or more, and fluorinated silica alumina having a pore volume of 0.50 mL/g or more;

(D) the catalyst contains a fluorinated metal oxide having a pore volume of 0.35 mL/g or more.

[~~0032e~~0032d]

In another aspect, the present disclosure refers to a method for producing a catalyst for use in reacting a perfluoroalkadiene compound to obtain a perfluoroalkyne compound, the method comprising the following step (E) or (F):

(E) reacting a metal oxide with at least one compound selected from the group consisting of hydrofluorocarbon, hydrochlorofluorocarbon, and chlorofluorocarbon to thereby fluorinate the metal oxide, wherein a metal of the metal oxide is at least one member selected from the group consisting of chromium, titanium, silicon, and zirconium;

(F) fluorinating at least one metal oxide selected from the group consisting of chromium oxide having a pore volume of 0.10 mL/g or more, alumina having a pore volume of 0.45 mL/g or more, and silica-alumina having a pore volume of 0.50 mL/g or more.

Advantageous Effects of Invention

[0033]

According to the present disclosure, there can be provided a production method that can produce a perfluoroalkyne compound with a high selectivity at a high conversion rate of the reaction, and that is less likely to produce a fluoroalkene compound as a by-product. According to the present disclosure,

CLAIMS

[Claim 1]

A method for producing a perfluoroalkyne compound, the method comprising reacting a perfluoroalkadiene compound in the presence of a catalyst to obtain a perfluoroalkyne compound, and satisfying one of the following (A) to (G):

(A) the catalyst comprises at least one catalyst selected from the group consisting of catalysts containing a transition metal element, and catalysts containing at least two elements that belong to Groups 3 to 14 of the periodic table of elements;

(B) the catalyst comprises a catalyst containing at least one element that belongs to Groups 3 to 14 of the periodic table, and the contact time between the catalyst and the perfluoroalkadiene compound ~~represented by formula (2)~~ is 30 seconds or less;

(C) the catalyst comprises at least one catalyst selected from the group consisting of fluorinated chromium oxide having a pore volume of 0.08 mL/g or more, fluorinated alumina having a pore volume of 0.35 mL/g or more, and fluorinated silica alumina having a pore volume of 0.50 mL/g or more;

(D) the catalyst comprises a fluorinated metal oxide having a pore volume of 0.35 mL/g or more;

(E) the catalyst comprises a metal oxide fluorinated by reacting a metal oxide with at least one compound selected from the group consisting of hydrofluorocarbon, hydrochlorofluorocarbon, and chlorofluorocarbon, wherein a metal of the metal oxide is at least one member selected from the group consisting of chromium, titanium, silicon, and zirconium;

(F) the catalyst comprises one or more catalysts obtained by fluorinating at least one metal oxide selected from the group consisting of chromium oxide having a pore volume of 0.10 mL/g or more, alumina having a pore volume of 0.45 mL/g or more, and silica alumina having a pore volume of 0.50 mL/g or more; and

(G) at least a part of the reaction of the perfluoroalkadiene compound from the start to the end of the reaction is performed

under conditions in which the water content of the reaction system is 30 ppm by mass or less, based on the mass of the perfluoroalkadiene compound defined as 100 mass%.

[Claim 2]

The production method according to claim 1, wherein the perfluoroalkyne compound is represented by formula (1):

$CR^1_2R^2-C\equiv C-CR^3R^4_2$ (1)

wherein R^1 to R^4 are the same or different and represent a fluorine atom or a perfluoroalkyl group.

[Claim 3]

The production method according to claim 1 or 2, wherein the perfluoroalkadiene compound is represented by formula (2):

$CR^1_2=CR^2-CR^3=CR^4_2$ (2)

wherein R^1 to R^4 are the same or different and represent a fluorine atom or a perfluoroalkyl group.

[Claim 4]

The production method according to any one of claims 1 to 3, wherein the method satisfies the (A) or (B), and the catalyst is at least one catalyst selected from the group consisting of:

catalysts containing at least one transition metal element that belongs to Groups 4 to 6 of the periodic table; and

catalysts containing at least two elements that belong to Groups 4 to 6 and Groups 13 to 14 of the periodic table.

[Claim 5]

The production method according to any one of claims 1 to 4, wherein the method satisfies the (A) or (B), and the catalyst is at least one catalyst selected from the group consisting of optionally fluorinated chromium oxide catalysts, optionally fluorinated titanium oxide catalysts, optionally

fluorinated zirconia catalysts, and optionally fluorinated silica-alumina catalysts.

[Claim 6]

The production method according to any one of claims 1 to 3, wherein the method satisfies the (D) and the metal of the fluorinated metal oxide includes at least one element that belongs to Groups 3 to 14 of the periodic table.

[Claim 7]

The production method according to any one of claims 1 to 3, wherein the method satisfies the (E) and the metal oxide before fluorination has a pore volume of 0.45 mL/g or more.

[Claim 8]

The production method according to any one of claims 1 to 3, wherein the method satisfies the (G) and the catalyst contains at least one element that belongs to Groups 3 to 14 of the periodic table.

[Claim 9]

The production method according to any one of claims 1 to 8, wherein the reaction of the perfluoroalkadiene compound is performed in a gas phase.

[Claim 10]

The production method according to any one of claims 1 to 9, wherein the reaction of the perfluoroalkadiene compound is performed at 170°C or more.

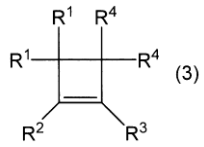
[Claim 11]

The production method according to any one of claims 1 to 10, wherein the reaction of the perfluoroalkadiene compound

produces a perfluorocycloalkene compound in addition to the perfluoroalkyne compound.

[Claim 12]

The production method according to claim 11, wherein the perfluorocycloalkene compound is represented by formula (3):



(3)

wherein R^1 to R^4 are as defined above.

[Claim 13]

A method for producing a perfluoroalkyne compound, the method comprising obtaining the perfluoroalkadiene compound using as a substrate the perfluorocycloalkene compound obtained as a by-product by the production method of claim 11 or 12.

[Claim 14]

The production method according to claim 13, wherein the perfluoroalkyne compound is represented by formula (1):

$CR^1_2R^2-C\equiv C-CR^3R^4_2$ (1)

wherein R^1 to R^4 are the same or different and represent a fluorine atom or a perfluoroalkyl group.

~~[Claim 15]~~

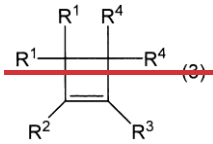
~~A composition comprising a perfluoroalkyne compound and a perfluorocycloalkene compound,~~

~~the perfluoroalkyne compound being represented by formula (1):~~

~~$CR^1_2R^2-C\equiv C-CR^3R^4_2$ (1)~~

~~wherein R^1 to R^4 are the same or different and represent a fluorine atom or a perfluoroalkyl group,~~

~~the perfluorocycloalkene compound being represented by formula (3):~~



(3)

~~wherein R^1 to R^4 are as defined above, and~~

~~the composition containing the perfluoroalkyne compound represented by formula (1) in an amount of 40 to 99.999 mol%, based on the total amount of the composition defined as 100 mol%.~~

~~[Claim 16]~~

~~The composition according to claim 15, which is for use as an etching gas or a building block for organic synthesis.~~

[Claim ~~17~~15]

A catalyst for use in reacting a perfluoroalkadiene compound to obtain a perfluoroalkyne compound,
the catalyst satisfying the following (C) or (D):
(C) the catalyst contains at least one member selected from the group consisting of fluorinated chromium oxide having a pore volume of 0.08 mL/g or more, fluorinated alumina having a pore volume of 0.35 mL/g or more, and fluorinated silica alumina having a pore volume of 0.50 mL/g or more;
(D) the catalyst contains a fluorinated metal oxide having a pore volume of 0.35 mL/g or more.

[Claim ~~18~~16]

The catalyst according to claim ~~17~~15, wherein the catalyst satisfies the (D) and the metal of the fluorinated metal oxide includes at least one element that belongs to Groups 3 to 14 of the periodic table.

[Claim 17~~19~~]

A method for producing a catalyst for use in reacting a perfluoroalkadiene compound to obtain a perfluoroalkyne compound, the method comprising the following step (E) or (F):
(E) reacting a metal oxide with at least one compound selected

from the group consisting of hydrofluorocarbon, hydrochlorofluorocarbon, and chlorofluorocarbon to thereby fluorinate the metal oxide, wherein a metal of the metal oxide is at least one member selected from the group consisting of chromium, titanium, silicon, and zirconium;

(F) fluorinating at least one metal oxide selected from the group consisting of chromium oxide having a pore volume of 0.10 mL/g or more, alumina having a pore volume of 0.45 mL/g or more, and silica-alumina having a pore volume of 0.50 mL/g or more.

[Claim ~~20~~18]

The production method according to claim ~~19~~17, wherein the method satisfies the (E) and the metal oxide before fluorination has a pore volume of 0.45 mL/g or more.