



Preparation of aromatic compound e.g. 1-chloronaphthalene involves exposing pre-formed benzenoid to an energy source in the presence of a catalyst system

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2006.06.20 2006-012219(+2006GB-012219) (2007.12.27) C07C
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Preparation of aromatic compound e.g. 1-chloronaphthalene involves exposing pre-formed benzenoid to an energy source in the presence of a catalyst system (Eng)

C2008-351838 N(AE AG AL AM AT AU AZ BA BB BG BH BR BW
BY BZ CA CH CN CO CR CU CZ DE DK DM DO DZ
EC EE EG ES FI GB GD GE GH GM GT HN HR HU
ID IL IN IS JP KE KG KM KN KP KR KZ LA LC LK
LR LS LT LU LY MA MD ME MG MK MN MW MX
MY MZ NA NG NI NO NZ OM PG PH PL PT RO RS
RU SC SD SE SG SK SL SM SV SY TJ TM TN TR TT
TZ UA UG US UZ VC VN ZA ZM ZW) R(AT BE BG
BW CH CY CZ DE DK EA EE ES FI FR GB GH GM
GR HU IE IS IT KE LS LT LU LV MC MT MW MZ
NA NL OA PL PT RO SD SE SI SK SL SZ TR TZ UG
ZM ZW)

AzM

HUTCHINGS M G, QUAYLE P, BULL J A, BARROSO C

A(1-EE) B(5-A3, 6-H, 10-A15, 10-D1, 10-G3, 10-H2A,
10-H2C, 10-H2E, 14-R1) C(5-A3, 6-H, 10-A15, 10-D1, 10-G3, 10-
H2A, 10-H2C, 10-H2E) D(8-B12) E(6-H, 8-H, 10-A15E, 10-B4A1,
10-D1C, 10-F2A1, 10-F2A2, 10-G2A1, 10-G3A, 10-H1C, 10-H3B1,
10-H3C1, 11-A1, 11-P) J(4-E4) N(1-D1, 5-B, 7-F7) .9

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2007.06.14 2007WO-EP055923

NOVELTY

An aromatic compound is prepared by exposing pre-formed benzenoid or other organic compound to an energy source in the presence of a catalyst system.

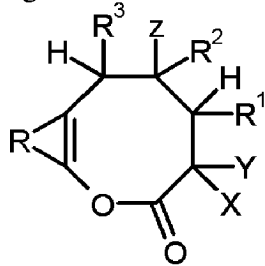
DETAILED DESCRIPTION

Preparation of an aromatic compound of formula (I) comprises exposing pre-formed benzenoid or other organic compound of formula (II) or (VI) to an energy source in the presence of a catalyst system.

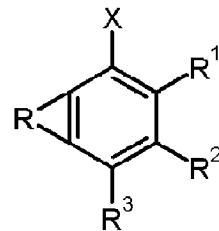
R = organic radical which, together with two carbon atoms to which it is bonded, forms a carbocyclic or heterocyclic ring;
R¹, R², R³ and X = H, halo, N, CN, or organic radical;

WO 2007147775-A+

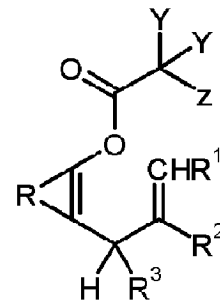
$C-R^1R^2-C$ or $C-R^2R^3-C = \text{ring}$; and
 Y and Z = have the meanings of X.



(VI)



(I)



(II)

USE

For preparing an aromatic compound (e.g. 1-chloronaphthalene) useful for pharmaceuticals, agrochemicals, dyes and pigments, cosmetics, oil chemicals, electronic chemicals, auxiliaries, flavors and fragrances and as components or intermediates of polymers and catalysts.

ADVANTAGE

The process allows conversion of readily available organic

chemical starting materials to aromatic species of potential use in many organic chemistry-based industries.

SPECIFIC COMPOUNDS

The aromatic compound is one or more of 41 compounds e.g. 1-chloronaphthalene; 1-chloro,7-fluoronaphthalene; 1-chloro,9-phenylnaphthalene; 1,3-dichloronaphthalene; or 4,10-dichlorochrysene of formula (22b) (disclosed).

EXAMPLE

Trichloroacetate ester of o-allylphenol (640 parts) dissolved in 1,2-dichloroethane (10000 parts) was added with cuprous chloride (11 parts) and the dipyridinium ligand in a glass vessel, designed for use in microwave apparatus. The vessel and contents were flushed with nitrogen. The mixture was irradiated by microwave energy to give a reaction mixture temperature of 200°C which was maintained for 2 hours. The reaction vessel was cooled, and 1-chloronaphthalene was found to be the sole product. It was isolated in 81% yield and was found to be identical to authentic material by chromatographic and spectroscopic comparison.

DEFINITIONS

Preferred Definition:

C-R-C = benzene ring optionally substituted by up to 4 substituents; R¹, R², R³ = H; F; Cl; Br; 1-4C alkyl optionally substituted by methoxy, phenoxy or halo such as F or Cl; Ph optionally substituted with methoxy, phenoxy or halo such as F, Cl or Br, nitro, CN, -CO₂H or CO₂CH₃; 1-4C alkoxy optionally substituted by methoxy, phenoxy, halo such as F or Cl; phenoxy optionally substituted by methoxy, phenoxy or halo such as F, Cl or Br, nitro, CN, -CO₂H or -CO₂CH₃;

Y and Z = Cl or Br; and

X = Cl, Br or I.

TECHNOLOGY FOCUS

Inorganic Chemistry - Preferred Components: The catalyst system comprises a transition metal, optionally ligands for that metal and optional Lewis acid. The transition metal is copper, iron, nickel,

palladium, platinum or ruthenium.

Organic Chemistry - Preferred Process: The energy source is conventional external heating or microwave irradiation.

(27ppDwgNo.0/0)