Apeiron synthesis

Transforming your chemistry

New Olefin Metathesis Catalysts

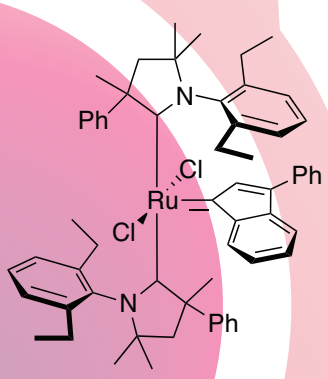
Bis-CAAC Catalyst Group

The Apeiron Synthesis' effort to explore new, versatile ruthenium-based catalysts for olefin metathesis resulted in a new class of complexes: bis(CAAC)ruthenium indenylidenes, which combine the benefits of both the NHC and the CAAC catalyst families. One of these catalysts, UltraCat, has proved to be extremely universal and highly efficient in virtually all metathesis transformations leading to terminal and internal olefins, such as ethenolysis via ring closing metathesis (including challenging macrocyclization), cross metathesis (involving electron deficient partners like acrylates), or ene-yne metathesis. These transformations are highly selective and take place at exceptionally low catalyst loadings. In one industrially relevant example, i.e. self metathesis of 1-decene, a turnover number of over 300000 was obtained. Importantly, these new catalysts were prepared using an efficient, low-cost and scalable synthetic route.

UltraCat

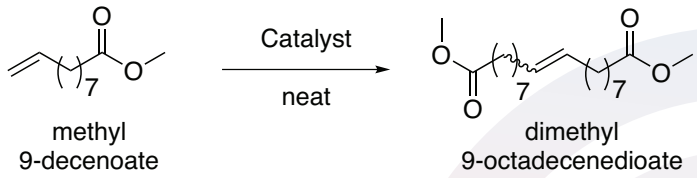
AS2086

CAS: 2055540-61-7



- Versatile catalyst, excellent for CM of terminal, type 1 olefins; excellent for ethenolysis, very good for mRCM and RCM leading to small/medium rings
- Compatible with toluene, ethyl acetate, dimethylcarbonate, CPME; neat substrate in the temperature range of 40 to 85°C
- High stability allows handling in air

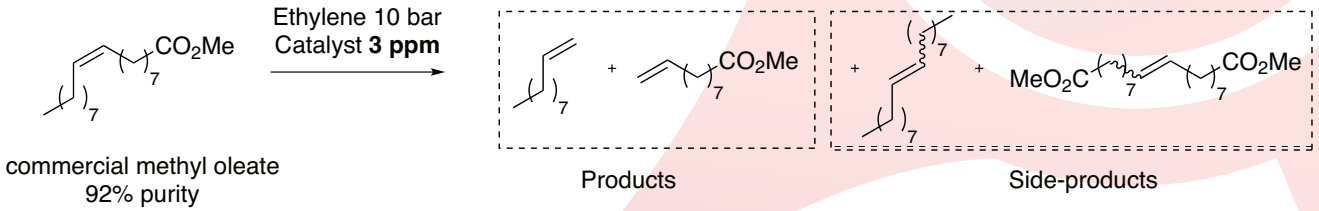
Case study: efficiency of UltraCat in cross metathesis



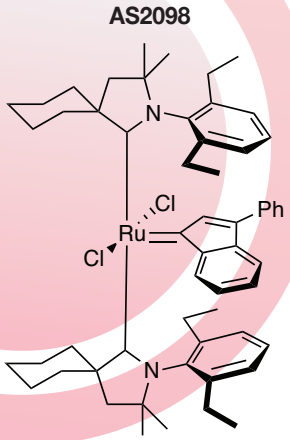
	Catalysts	Concentration [M]	Catalyst loading [ppm]	Isolated yield [%]	TON*
Elevance	C-827	neat	17.8 (80 ppm wt)	19	5 337
Apeiron	UltraCat	**neat**	**2 (11 ppm wt)**	**68**	**170 000**

* Catalyst turnover number calculated for productive dimethyl 9-octadecenedioate formation.

Estimated catalyst cost per 1 kg of product
with **UltraCat**: 0.85 EUR



Catalyst	Selectivity [%]	TON
UltraCat	**95**	**88 000**
Grubbs II	16	11 300



- Excellent for ROMP reaction of DCPD and NBE (catalyst loading as low as 3 ppm)
- Long pot life – several months – in DCPD with a simple additive
- High stability allows handling in air

References:

Gawin R., Kozakiewicz A., Guńka P. A., Dąbrowski P., Skowerski K. Angew. Chem. Int. Ed. Engl. 2017, 56, 981-986

Elevance Renewable Sciences INC: US 2013/0204022A1

Supporting patents: PCT/IB2016/054486, PCT/IB2017/056992

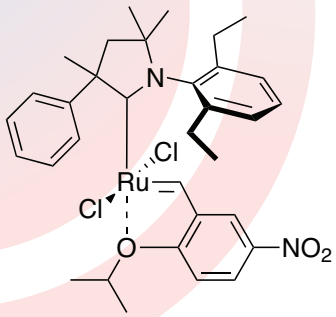
Mono-CAAC Catalyst Group

Apeiron's team found that substitution of the NHC group by carefully selected CAAC ligands significantly improves efficiency and selectivity of ruthenium benzylidene complexes in cross metathesis with acrylonitrile and in macrocyclization reactions. These two types of reactions were studied due to their importance in specialty chemical, pharmaceutical, and F&F industries. The newly designed class of catalysts allowed to accomplish both transformations with extraordinarily high turnover numbers.

UltraNitroCat

AS2091

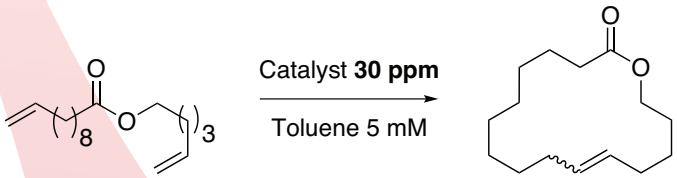
CAS: 2106819-64-9



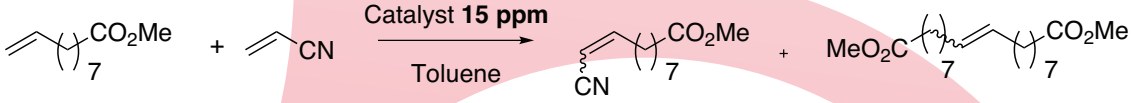
Group characteristics

- Exceptional efficiency in cross metathesis with electron deficient partners and in macrocyclizations
- Compatible with toluene, ethyl acetate, dimethylcarbonate, CPME in the temperature range of 25 to 85°C
- High stability allows handling in air

Case study: efficiency of UltraNitroCat in macrocyclization



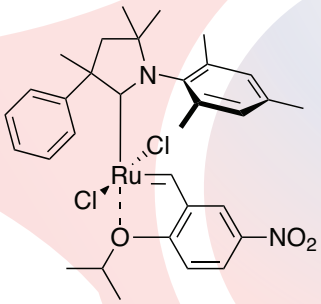
Catalysts	GC Yield [%]	TON
UltraNitroCat	**90**	**30 000**
nitro-Grela	**7**	**2 300**
Grubbs II	**12**	**4 000**



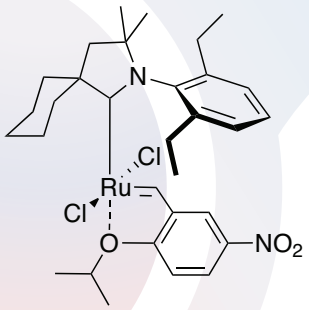
Catalyst	GC Yield [%]	Selectivity [%]*	TON
UltraNitroCat	75	75	38 000
nitro-Grela	34	81	18 400

* Numbers relate to cross metathesis selectivity over self metathesis.

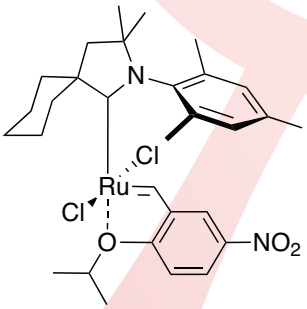
Other catalysts in this group:



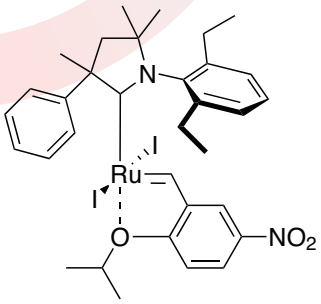
AS2101



AS2100



AS2099



AS2092

References:

Gawin R., Tracz A., Chwalba M., Kozakiewicz A., Trzaskowski B., Skowerski K. ACS Catal. 2017, 7, 5443-5449

Supporting patents: PCT/IB2016/054486, PCT/IB2017/056992, P.419421

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