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**(S)-4-Benzyl-3-[(R)-4,4,4-trifluoro-3-(4-methoxyphenyl)butanoyl]-1,3-oxazolidin-2-one**

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## (S)-4-Benzyl-3-[(R)-4,4,4-trifluoro-3-(4-methoxyphenyl)butanoyl]-1,3-oxazolidin-2-one

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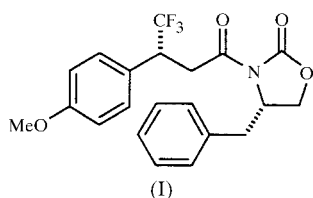
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The C atom at the chiral centre of the title compound, C<sub>21</sub>H<sub>20</sub>F<sub>3</sub>NO<sub>4</sub>, takes an *R* configuration. From this assignment, useful information on the intermediate process of the reaction was deduced.

### Comment

The title compound, (I), was prepared by way of Michael addition of an organocopper species to 3-[(*E*)-4,4,4-trifluorobut-2-enoyl]oxazolidin-2-ones in order to obtain optically active molecules with a CF<sub>3</sub> moiety at the chiral centre. The structure determination was made so as to clarify how the molecule is built up through the synthetic reaction. The C atom at the chiral centre takes an *R* configuration. From this assignment, a useful information on the intermediate process of the reaction was deduced: the construction of the molecule possibly proceeded *via* intramolecular bidentate chelation between Cu atom and carbonyl groups, rather than a conformation which without such chelation reduces the dipolar repulsion between the carbonyl groups and results in *S* configuration of the chiral atom owing to stereoselectivity (Yamazaki *et al.*, 1999). The configuration of the asymmetric C atom in the five-membered ring is *S*. The C—F bond lengths are 1.330 (6) Å on average. The CF<sub>3</sub> and CH<sub>3</sub> groups as well as the benzene-ring part show large atomic displacement parameters.



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### Experimental

The preparation of the title compound was presented in a report by Yamazaki *et al.* (1999). Single crystals were grown by slow evaporation from a mixture of hexane and ethyl acetate.

#### Crystal data

C<sub>21</sub>H<sub>20</sub>F<sub>3</sub>NO<sub>4</sub>  
M<sub>r</sub> = 407.39  
Orthorhombic, *P*2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>  
a = 13.115 (3) Å  
b = 24.305 (3) Å  
c = 6.388 (3) Å  
V = 2036.2 (11) Å<sup>3</sup>  
Z = 4  
D<sub>x</sub> = 1.329 Mg m<sup>-3</sup>

Mo Kα radiation  
Cell parameters from 25 reflections  
θ = 14.6–17.2°  
μ = 0.110 mm<sup>-1</sup>  
T = 298.2 K  
Plate, colourless  
0.70 × 0.50 × 0.30 mm

#### Data collection

Rigaku AFC-5R diffractometer  
ω-2θ scans  
Absorption correction: ψ scan  
(North *et al.*, 1968)  
T<sub>min</sub> = 0.865, T<sub>max</sub> = 0.999  
2716 measured reflections  
2641 independent reflections  
1619 reflections with *F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)

R<sub>int</sub> = 0.017  
θ<sub>max</sub> = 27.51°  
h = 0 → 17  
k = 0 → 31  
l = 0 → 8  
4 standard reflections  
every 150 reflections  
intensity decay: 0.27%

#### Refinement

Refinement on *F*<sup>2</sup>  
R(*F*) = 0.0483  
wR(*F*<sup>2</sup>) = 0.1371  
S = 1.998  
2689 reflections  
275 parameters  
Only some H-atom *U*'s refined  
w = 1/[σ<sup>2</sup>(*F*<sub>o</sub><sup>2</sup>) + 0.0016(*F*<sub>o</sub><sup>2</sup>)<sup>2</sup>]  
(Δ/σ)<sub>max</sub> = 0.0002

Δρ<sub>max</sub> = 0.15 e Å<sup>-3</sup>  
Δρ<sub>min</sub> = -0.12 e Å<sup>-3</sup>  
Extinction correction: Zachariasen (1967), type 2, Gaussian isotropic  
Extinction coefficient: 0.007 (2)  
Absolute configuration: from the configuration of C14 in the starting material.

**Table 1**

Selected geometric parameters (Å, °).

F1—C9	1.310 (6)	O3—C12	1.190 (4)
F2—C9	1.340 (5)	O4—C12	1.334 (4)
F3—C9	1.339 (6)	O4—C13	1.441 (5)
O1—C1	1.392 (7)	N1—C11	1.397 (4)
O1—C2	1.372 (5)	N1—C12	1.380 (4)
O2—C11	1.213 (4)	N1—C14	1.460 (4)
C1—O1—C2	117.6 (4)	F2—C9—C8	111.5 (4)
C12—O4—C13	111.6 (3)	F3—C9—C8	110.5 (5)
C11—N1—C12	127.0 (3)	O2—C11—N1	117.7 (3)
C11—N1—C14	120.3 (3)	O2—C11—C10	123.2 (3)
C12—N1—C14	112.6 (3)	N1—C11—C10	119.0 (3)
O1—C2—C3	116.8 (4)	O3—C12—O4	123.0 (3)
O1—C2—C7	124.0 (4)	O3—C12—N1	128.6 (3)
F1—C9—F2	106.6 (5)	O4—C12—N1	108.4 (3)
F1—C9—F3	105.8 (5)	O4—C13—C14	105.7 (3)
F1—C9—C8	115.5 (4)	N1—C14—C13	100.8 (3)
F2—C9—F3	106.4 (4)	N1—C14—C15	113.5 (3)

No Friedel pairs were measured. All H atoms were located in difference maps. Only their *U*<sub>iso</sub> were refined [0.064 (9)–0.11 (1) Å<sup>2</sup>], but some of these were fixed.

Data collection: *MSC/AFC Diffractometer Control System* (Rigaku, 1991); cell refinement: *MSC/AFC Diffractometer Control System*; data reduction: *teXsan* (Molecular Structure Corporation, 1998); program(s) used to solve structure: *MULTAN88* (Debaedemaeker *et al.*, 1985); program(s) used to refine structure: *teXsan*; software used to prepare material for publication: *teXsan*.

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