

# Determining Factors of the Regioisomeric Ratios of

## $M_3N@I_h-C_{80}$ Fulleropyrrolidines

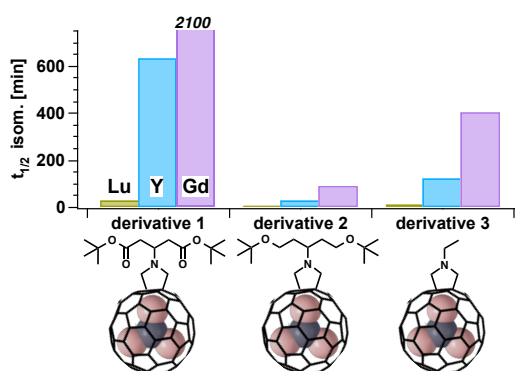
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The use of fullerenes for biologically relevant applications such as magnetic resonance imaging (MRI) contrast enhancement has been considered promising for decades. Obstacles to such bio-applications of fullerenes include their poor solubility in water necessitating the preparation of water-soluble materials by suitable modifications. The 1,3-dipolar cycloaddition (i.e. Prato reaction) of fullerenes is known as a useful method to functionalize fullerenes with reasonable yields. In contrast to the  $C_{60}$  case, which always yield only [6,6]-adduct (addition at the junction of two hexagons), the cycloadducts from  $M_3N@C_{80}$  varied in the individual Prato reaction and seemed random; the rules and factors governing the regioisomers of the final Prato adducts ([6,6]- and [5,6]-adducts) still remained unclear.

Effects of exohedral moieties and endohedral metal clusters on the regioisomeric ratios of Prato products of  $M_3N@I_h-C_{80}$  ( $M = Sc, Lu, Y, Gd$ ) were investigated using three fulleropyrrolidines with different exohedral functional groups from both experimental and computational point of view.



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Aroua, S.\*; Garcia-Borràs, M.\*; Osuna, S.\*; Yamahoshi, Y.\*; **2014**, *submitted for publication*. (\*These authors contributed equally.)