

Benzannulated Cycloheptanones from Binaphthyl Platforms

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Description

Preparations of benzannulated cycloheptanones starting from unique binaphthyl molecular platforms are described. Binaphthyl acetic acids proved suitable precursors for fused cycloheptanone architectures. Seven-membered rings embedded in binaphthyl units were selectively generated by use of Eaton's reagent. Isomeric helical architectures arising from electrophilic cyclisation processes at second reaction sites in the precursors could also be obtained under different acidic conditions. Unambiguous discrimination between isomeric geometries was provided by multiple quantum NMR sequences. DFT calculations were performed and gave evidence of different behaviour of the substrates towards intramolecular electrophilic substitution. The theoretical approach confirmed the experimental results, agreeing completely with X-ray data.