Carbon-13 NMR lanthanide induced shifts and T1 studies of the conformation of friedelin.

Abstract

By measuring the shifts of the 13C NMR signals of 29 C's of friedelin, induced by the lanthanide shift reagent Pr(fod)3, and using a computer program, it is shown that friedelin exists in a chair-chair-chair-twist boat-boat conformation in soln.  Lanthanide metal binds exclusively to one site on the carbonyl group of friedelin, away from the nearest Me group.  13C T1 data are consistent with the suggested conformation of friedelin.