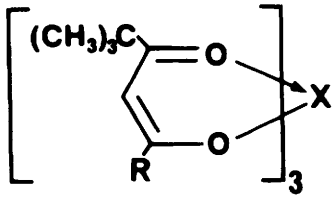
NMR Shift Reagents

Stretch Your NMR



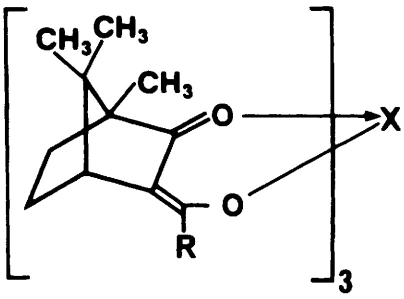
R = $C(CH_3)_3$;X = Eu(Resolve-Al™)
X = Pr(Resolve-Al Pr™)

R = n-C_3F_7;X = Eu(Resolve-Al EuFOD™)
X = Pr(Resolve-Al PrFOD™)

Since the initial report in 1969[1], the study of lanthanide shift reagents has been one of the most active areas of chemistry to the extent that a recent review[2a] cites 488 references! These rare-earth chelates of β-diketones have become important to all users of nmr[2a,c] because of their ability to simplify complex spectra by causing spectacular changes in the chemical shifts of nuclei adjacent to an electronegative substituent. The **Resolve-Al™** reagents produce, with little line broadening, large changes in the chemical shifts of protons adjacent to hydroxyl, amine, oxime, aldehyde, ketone, ester, amide, ether, thioamide, sulfoxide, sulfone, nitrile and phosphate groups. The addition of **Resolve-Al™** or **Resolve-Al EuFOD™** as either a solid or a solution generally results in a downfield change in resonances whereas the reverse is true with **Resolve-Al Pr™** or **Resolve-Al PrFOD™**. In addition, correlation of observed changes in chemical shift with the geometry of the substrate-shift reagent complex has been used to make assignments of structure[2], stereochemistry[2] and configuration[2,3]

Polarimetry by NMR

Furthermore, rare-earth chelates of chiral β-diketones provide a convenient spectroscopic means[2a,b] to determine enantiomeric or optical purity without relying on difficult or time-consuming classical methods. The nmr spectra of chiral alcohols, amines, esters, ketones, sulfoxides and epoxides observed in the presence of **TFMC-Eu**, **TFMC-Pr** or **THFC-Eu** generally show such large chemical shift differences for the enantiotopic nuclei that the proportions of enantiomers can be measured directly by integration[2a,b]



R = CF_3, X = Eu	**Tris[3-(trifluoromethylhydroxymethylene)-*d*-camphorato]-europium (TFMC-Eu)**
R = CF_3, X = Pr	**Tris[3-(trifluoromethylhydroxymethylene)-*d*-camphorato]-praseodymium (TFMC-Pr)**
R = n-C_3F_7, X=Eu	**Tris[3-(heptafluoropropylhydroxymethylene)-*d*-camphorato]-europium (THFC-Eu)**

References

1) C.C. Hinkley, *J. Amer. Chem. Soc.*, **91**, 5160 (1969).
2) (a) A.F. Cockerill, G.L.O. Davies, R.C. Harden, and D.M. Rackham, *Chem. Revs.*, **73**, 553 (1973). (b) R.E. Sievers, *Nuclear Magnetic Resonance Shift Reagents*, Academic Press, New York, N.Y., 1973. (c) J.R. Campbell, *Aldrichimica Acta*, **4**, 55 (1971); **5**, 29 (1972).
3) E.J. Warawa and J.R. Campbell, *J. Org. Chem.*, **39**, 0000 (1974).

17,649-4	**Tris[3-(trifluoromethylhydroxymethylene)-*d*-camphorato]europium (TFMC-Eu)**	**1g \$18.00; 5g \$60.00**
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