We have calculated the optimized structure of the isolated cations of salts (E)- and (Z)-10a using Hartree-Fock theory and the standard 6-31+G(d,p) basis set with the Gaussian 03 program suite\(^1\) (Figure 1).

Figure 1 also suggests that free rotation around the N–C bonds, which leads to magnetic equivalence of the methyl groups in the NMR spectra, may be hampered by the opposite phenyl ring in (E)-10a. In fact, the presence of two broadened NCH\(_3\) signals in the \(^1\)H NMR spectrum indicates a hindered rotation, while the sterically less encumbered (Z)-10a is already in the stage of fast exchange under the same conditions.

References

(1) a) Frisch, M. J. et al. Gaussian 03, Revision E.01, 2004, Gaussian, Inc., Wallingford CT.
   b) Frisch A.; Frisch, M. J.; Trucks, G. W. Gaussian 03 User’s Reference, 2003, Gaussian, Inc.