The Molecular Structure of $(C_{13}H_{21}N^{+})Br^{-}$

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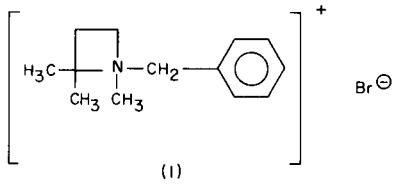
Sir:

The structure of the compound, 1-benzyl-1,2,2-trimethyl acetidinium bromide (I) has been determined by a single crystal X-ray diffraction study. This is the first reported structure determination in which an unfused azetidinium ring has been reported. The compound crystallizes in the space group Pnam with four formula weights in a unit cell of dimensions a = 14.36, b = 13.73, C = 6.90_6 Å.



(I)

Refinement of the structure, still in progress, has reached a value of R = 0.10. The azetedinium ring bears a close resemblance in bond distances (CN = 1.39_7, 1.60_2 ± .05 Å and CC = 1.53_4 ± .02 Å) and bond angles (clockwise, ∠*CNC* = 92°, ∠*NCC* = 86°, ∠*CCC* = 89.6°, ∠*CCN* = 92.1° ± 2.5°) to the β-lactam ring found in penicillin (1). Hydrogen atom positions in the azetidinium ring have not yet been included in the refinement. All bond distances and bond angles in the remainder of the structure agree within two standard deviations with other analogous compounds. The cation is partially disordered about the mirror plane with an orientational disorder involving alternating *d* and *l* conformations.

Acknowledgment.

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REFERENCES

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