

CORRECTIONS

Anil M. Dwivedi and S. Krimm*: Vibrational Analysis of Peptides, Polypeptides, and Proteins. XI. β -Poly(L-alanine) and Its N-Deuterated Derivative. Volume 15, Number 1, January-February 1982, page 186.

Due to an inadvertent choice of origin, the axial shift, Δb , which can be defined as negative¹ or positive,² was given the wrong sign in the calculation. (The magnitude of this shift, 0.27 Å, should be such that the distance between nearest carbonyl oxygen atoms on adjacent chains increases with respect to its value for $\Delta b = 0$.) After this correction is made, a refinement of the force field gives the following revised values of some of the force constants: 12. $f(\text{C}^\alpha\text{CN}) = 0.933$; 14. $f(\text{NCO}) = 1.306$; 17. $f(\text{C}^\alpha\text{NH}) = 0.566$; 18. $f(\text{C}^\alpha\text{CO}) = 1.306$; 21. $f(\text{CNH}) = 0.566$; 26. $f(\text{NH}\cdots\text{O ib}) = 0.036$; 27. $f(\text{CO ob}) = 0.621$; 28. $f(\text{NH ob}) = 0.157$; 32. $f(\text{NH t}) = 0.0005$; 75. $f(\text{NC}^\alpha\text{C,CO ob}) = -0.1725$; 97. $f(\text{CO ob,NH ob}) = 0.000$; 98. $f(\text{NH}\cdots\text{O ib,NH ob}) = 0.007$; and a (nonzero) value for $f(\text{CO,C}^\alpha\text{CN}) = 0.050$. The revised force field gives the same assignments and slightly better frequency agreement than did the earlier one. A detailed table of frequencies and potential energy distributions will be given in a forthcoming publication³ on approximate force fields for α -helix and β -sheet polypeptides.

(1) Moore, W. H.; Krimm, S. *Biopolymers* **1976**, *15*, 2439.

(2) Arnott, S.; Dover, S. D.; Elliott, A. *J. Mol. Biol.* **1967**, *30*, 201.

(3) Dwivedi, A. M.; Krimm, S. *Biopolymers*, in press.