

## Additions and Corrections

**Extreme Conformational Flexibility of the Furanose 2607 in DNA and RNA** [*J. Am. Chem. Soc.* 1978, 100, 2607]. M. LEVITT\* and ARIEH WARSHEL, Laboratory of Molecular Biology, Cambridge CB2 2QH, England.

The coordinate values in Table II, p 2611, were distorted by a nonorthogonal transformation used to rotate them into a common orientation. The correct coordinate values are given in the table below. The errors in the coordinates were introduced in preparing the original table and have no effect on the other published results.

Table II. Cartesian Coordinates and some Torsion Angles of Ten Relaxed Conformations

| Atom and coordinate |   | Nominal pseudorotation phase $\Psi$ (in degrees) |       |       |       |       |       |       |       |       |       |
|---------------------|---|--|-------|-------|-------|-------|-------|-------|-------|-------|-------|
|                     |   | 0  | 20    | 40    | 60    | 80    | 100   | 120   | 140   | 160   | 180   |
| C5'                 | x | -1.93  | -1.97 | -1.99 | -1.98 | -1.96 | -1.94 | -1.87 | -1.74 | -1.59 | -1.43 |
|                     | y | -1.66  | -1.68 | -1.71 | -1.71 | -1.72 | -1.67 | -1.54 | -1.35 | -1.18 | -1.06 |
|                     | z | -0.67  | -0.53 | -0.42 | -0.48 | -0.51 | -0.66 | -0.92 | -1.22 | -1.44 | -1.60 |
| H51                 | x | -1.69  | -1.80 | -1.91 | -1.87 | -1.89 | -1.84 | -1.66 | -1.36 | -1.07 | -0.81 |
|                     | y | -1.57  | -1.64 | -1.67 | -1.64 | -1.60 | -1.45 | -1.19 | -0.88 | -0.63 | -0.48 |
|                     | z | -1.75  | -1.61 | -1.52 | -1.57 | -1.60 | -1.73 | -1.94 | -2.14 | -2.25 | -2.31 |
| H52                 | x | -1.82  | -1.85 | -1.82 | -1.81 | -1.77 | -1.75 | -1.69 | -1.58 | -1.45 | -1.30 |
|                     | y | -2.71  | -2.72 | -2.75 | -2.75 | -2.78 | -2.74 | -2.63 | -2.44 | -2.26 | -2.13 |
|                     | z | -0.37  | -0.19 | -0.09 | -0.17 | -0.26 | -0.50 | -0.88 | -1.30 | -1.61 | -1.83 |
| H53                 | x | -2.98  | -3.01 | -3.01 | -3.01 | -2.99 | -2.97 | -2.93 | -2.82 | -2.66 | -2.49 |
|                     | y | -1.36  | -1.37 | -1.42 | -1.42 | -1.47 | -1.45 | -1.35 | -1.16 | -0.94 | -0.79 |
|                     | z | -0.52  | -0.32 | -0.13 | -0.20 | -0.19 | -0.35 | -0.70 | -1.13 | -1.49 | -1.76 |
| C4'                 | x | -0.99  | -0.98 | -0.96 | -0.97 | -0.95 | -0.95 | -0.97 | -1.00 | -1.02 | -1.01 |
|                     | y | -0.77  | -0.76 | -0.78 | -0.79 | -0.82 | -0.83 | -0.82 | -0.81 | -0.78 | -0.77 |
|                     | z | 0.16   | 0.21  | 0.24  | 0.22  | 0.21  | 0.16  | 0.10  | 0.01  | -0.07 | -0.15 |
| H4'                 | x | -1.23  | -1.15 | -1.05 | -1.08 | -1.02 | -1.05 | -1.18 | -1.36 | -1.52 | -1.62 |
|                     | y | -0.88  | -0.83 | -0.84 | -0.87 | -0.97 | -1.08 | -1.19 | -1.28 | -1.34 | -1.37 |
|                     | z | 1.23   | 1.30  | 1.34  | 1.32  | 1.30  | 1.24  | 1.12  | 0.94  | 0.74  | 0.55  |
| O1'                 | x | 0.38   | 0.37  | 0.37  | 0.38  | 0.39  | 0.40  | 0.40  | 0.39  | 0.38  | 0.37  |
|                     | y | -1.11  | -1.11 | -1.09 | -1.09 | -1.06 | -1.06 | -1.05 | -1.07 | -1.10 | -1.11 |
|                     | z | -0.03  | -0.08 | -0.15 | -0.14 | -0.21 | -0.23 | -0.21 | -0.16 | -0.08 | 0.01  |
| C3'                 | x | -1.02  | -1.02 | -1.04 | -1.04 | -1.07 | -1.08 | -1.06 | -1.03 | -1.01 | -1.00 |
|                     | y | 0.70   | 0.69  | 0.66  | 0.67  | 0.66  | 0.68  | 0.70  | 0.72  | 0.72  | 0.70  |
|                     | z | -0.23  | -0.25 | -0.23 | -0.22 | -0.13 | -0.04 | 0.05  | 0.14  | 0.20  | 0.23  |
| H3'                 | x | -1.13  | -1.11 | -1.17 | -1.21 | -1.47 | -1.58 | -1.71 | -1.78 | -1.81 | -1.82 |
|                     | y | 0.84   | 0.77  | 0.73  | 0.76  | 0.81  | 0.91  | 1.05  | 1.17  | 1.24  | 1.26  |
|                     | z | -1.32  | -1.35 | -1.33 | -1.30 | -1.17 | -0.99 | -0.77 | -0.53 | -0.35 | -0.25 |
| O3'                 | x | -2.06  | -2.07 | -2.08 | -2.06 | -1.98 | -1.80 | -1.57 | -1.35 | -1.22 | -1.17 |
|                     | y | 1.40   | 1.40  | 1.37  | 1.37  | 1.31  | 1.27  | 1.20  | 1.09  | 0.96  | 0.85  |
|                     | z | 0.47   | 0.39  | 0.44  | 0.51  | 0.77  | 1.05  | 1.30  | 1.48  | 1.59  | 1.65  |
| H03                 | x | -2.19  | -2.20 | -2.23 | -2.22 | -2.17 | -1.98 | -1.69 | -1.40 | -1.24 | -1.17 |
|                     | y | 2.38   | 2.38  | 2.35  | 2.34  | 2.29  | 2.25  | 2.18  | 2.05  | 1.90  | 1.75  |
|                     | z | 0.34   | 0.22  | 0.27  | 0.35  | 0.69  | 1.07  | 1.45  | 1.75  | 1.95  | 2.08  |
| C2'                 | x | 0.36   | 0.35  | 0.35  | 0.35  | 0.36  | 0.37  | 0.39  | 0.39  | 0.39  | 0.38  |
|                     | y | 1.18   | 1.19  | 1.20  | 1.21  | 1.22  | 1.20  | 1.17  | 1.16  | 1.16  | 1.18  |
|                     | z | 0.21   | 0.20  | 0.14  | 0.13  | 0.00  | -0.10 | -0.18 | -0.23 | -0.24 | -0.23 |
| H21                 | x | 0.38   | 0.35  | 0.35  | 0.37  | 0.44  | 0.53  | 0.60  | 0.65  | 0.67  | 0.67  |
|                     | y | 1.37   | 1.40  | 1.54  | 1.56  | 1.83  | 2.01  | 2.09  | 2.11  | 2.12  | 2.11  |
|                     | z | 1.30   | 1.29  | 1.20  | 1.18  | 0.92  | 0.63  | 0.39  | 0.26  | 0.23  | 0.29  |
| H22                 | x | 0.66   | 0.65  | 0.64  | 0.64  | 0.61  | 0.58  | 0.53  | 0.47  | 0.42  | 0.37  |
|                     | y | 2.10   | 2.09  | 2.04  | 2.03  | 1.84  | 1.60  | 1.40  | 1.30  | 1.30  | 1.38  |
|                     | z | -0.32  | -0.35 | -0.51 | -0.54 | -0.87 | -1.11 | -1.26 | -1.33 | -1.34 | -1.31 |
| C1'                 | x | 1.28   | 1.28  | 1.28  | 1.28  | 1.27  | 1.25  | 1.24  | 1.24  | 1.25  | 1.27  |
|                     | y | 0.0  | 0.0   | 0.0   | 0.00  | 0.00  | -0.00 | 0.00  | -0.00 | 0.00  | 0.0   |
|                     | z | -0.11  | -0.07 | 0.00  | 0.00  | 0.13  | 0.21  | 0.24  | 0.24  | 0.20  | 0.13  |
| H1'                 | x | 2.06   | 1.99  | 1.85  | 1.86  | 1.61  | 1.43  | 1.35  | 1.36  | 1.45  | 1.60  |
|                     | y | -0.12  | -0.14 | -0.15 | -0.14 | -0.12 | -0.09 | -0.04 | 0.00  | 0.05  | 0.07  |
|                     | z | 0.67   | 0.76  | 0.94  | 0.94  | 1.18  | 1.30  | 1.35  | 1.34  | 1.29  | 1.19  |
| N1                  | x | 1.84   | 1.94  | 2.14  | 2.14  | 2.38  | 2.49  | 2.52  | 2.52  | 2.47  | 2.38  |
|                     | y | 0.09   | 0.10  | 0.10  | 0.08  | 0.04  | -0.01 | -0.04 | -0.08 | -0.12 | -0.16 |
|                     | z | -1.45  | -1.36 | -1.16 | -1.17 | -0.81 | -0.57 | -0.45 | -0.46 | -0.58 | -0.79 |
| HN1                 | x | 2.72   | 2.82  | 3.03  | 3.06  | 3.24  | 3.33  | 3.37  | 3.40  | 3.40  | 3.37  |
|                     | y | 0.70   | 0.72  | 0.71  | 0.65  | 0.65  | 0.57  | 0.47  | 0.35  | 0.25  | 0.14  |
|                     | z | -1.62  | -1.47 | -1.13 | -1.12 | -0.60 | -0.23 | -0.03 | -0.01 | -0.18 | -0.49 |
| HN2                 | x | 1.40   | 1.56  | 1.91  | 1.87  | 2.35  | 2.55  | 2.62  | 2.58  | 2.45  | 2.21  |
|                     | y | -0.47  | -0.44 | -0.47 | -0.43 | -0.57 | -0.59 | -0.60 | -0.59 | -0.59 | -0.59 |
|                     | z | -2.26  | -2.21 | -2.06 | -2.07 | -1.71 | -1.47 | -1.37 | -1.41 | -1.56 | -1.77 |
| Actual $\Psi$       |   | 7.8  | 21.0  | 39.4  | 39.6  | 73.1  | 98.2  | 118.8 | 138.6 | 159.7 | 182.5 |
| u'                  |   | 86.9   | 82.6  | 89.2  | 89.4  | 89.6  | 100.6 | 116.8 | 134.3 | 146.9 | 155.6 |