Table 9.3 Chemical Markup Representation of Acetic Acid

```
(molecule convention="MDLMol" id="acetate" title="ACETATE")
(date day="23" month="11" year="1995" /)
⟨atomArray⟩
(atom id="a1")
(string builtin="elementType")C⟨/string⟩
(float builtin="x2")0.27⟨/float⟩
(float builtin="y2")0.1217⟨/float⟩
⟨/atom⟩
(atom id="a2")
(string builtin="elementType")C⟨/string⟩
(float builtin="x2")−1.27⟨/float⟩
(float builtin="y2")0.1246⟨/float⟩
⟨/atom⟩
(atom id="a3")
(string builtin="elementType")O⟨/string⟩
(float builtin="x2")1.0623⟨/float⟩
(float builtin="y2")−1.2937⟨/float⟩
⟨/atom⟩
(atom id="a4")
(string builtin="elementType")O⟨/string⟩
(float builtin="x2")1.1008⟨/float⟩
(float builtin="y2")1.4332⟨/float⟩
⟨/atom⟩
⟨/atomArray⟩
⟨bondArray⟩
(bond id="b1")
(string builtin="atomRef")a1⟨/string⟩
(string builtin="atomRef")a2⟨/string⟩
(string builtin="order")1⟨/string⟩
⟨/bond⟩
(bond id="b2")
(string builtin="atomRef")a1⟨/string⟩
(string builtin="atomRef")a3⟨/string⟩
(string builtin="order")1⟨/string⟩
(/bond)
(bond id="b3")
(string builtin="atomRef")a1⟨/string⟩
(string builtin="atomRef")a4⟨/string⟩
(string builtin="order")2⟨/string⟩
(/bond)
⟨/bondArray⟩
(Imolecule)
```

files, and they are difficult for chemists to read (although they are not usually meant for chemist interpretation). This is evident in Table **9.3,** which shows the CML for acetic acid. By comparison, the SMILES for acetic acid is simply "CC(=O)O".

2.3 Chemical Structure File Conversion

Many chemical information management systems, especially modeling programs, permit a chemist to import and export structures using a variety of file formats. Commercial programs designed specifically for file conversion are available (57). **A** widely used public domain program, Babel, is available in source code and in a Windows version (58). It is being extended by the "OpenBabel" programming project (59). It is possible, with a fair amount of accuracy, to convert a chemical structure from a connection table format to an acceptable