Subject: Re: V3000 input
Posted by bruno.b on Mon, 27 Oct 2014 15:00:24 GMT

Hi Thomas,

according to the Symyx June 2010 documentation, the atom index can be any strictly positive number.

"Identifies atoms. The actual value of the index does not
matter as long as each index is unique to each atom. "

For the bonds:

"The actual value of the index does not matter as
long as all are unique."

I did not find comment about the order of the atom indices in the Symyx document.

Regards,

Bruno