Subject: Re: Molecular models and contour maps
Posted by David Fanning on Mon, 29 Jul 2002 19:58:03 GMT
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Rick Matthews (matthews@wfu.edu) writes:

> Newbie question:

Oh, oh. :-(

> I want to use IDL for help with 3-D visualization of
> electron density calculations. I want like IDL to display a ball and
> stick model of a molecule, with interleaved contour maps of the density
> surrounding the atoms in planes of my choosing.
>
> 1. I have not found visualization routines to generate 3-d
> displays of the balls for atoms or sticks connecting them. Is
> there a straightforward way to do this?
> 2. If I succeed in 1, is there a way to display planar contour
> maps in the image?

Uh, Rick, our friend Rick Towler will get back to you ASAP. :-)

Do you mean you are a programming newbie, or an IDL
newbie? If the former, and you don't have any 3D
graphics or object experience, you may be looking
at quite a project here. If it's the latter, and
you are a proficient C++ programmer, then maybe
there is some hope ahead.

But what you want to do is in no way a trivial
programming exercise in IDL, I'm afraid. I'm hoping
Ronn Kling's latest book, due out soon, will shed
some light on this sort of thing. But you are going
to have to pretty much build this yourself, I think.
I'm reasonably sure it can be done with IDL, just not
as easily as you were probably hoping.

Cheers,

David
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