Subject: Re: Molecular models and contour maps
Posted by Rick Matthews on Thu, 01 Aug 2002 20:49:54 GMT
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Thanks for the reply. This helps.

Rick

Mark Hadfield wrote:
> From: "Rick Matthews" <matthews@wfu.edu>
>
>> 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.
>
>
> IDL can certainly do this.
>
> The IDL Object Graphics system is (for the most part) a collection of
> building blocks with which you can build visualisations. You have to
> assemble the building blocks yourself. This is simple in principle but
> there are a lot of details to learn and you will encounter a few
> surprises.
>
>
>> 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?
>
>
> Routine MESH_OBJ generates data describing a simple shape like a ball
> or a cylinder. You pass the data to an IDLgrPolygon object to display the
> shape. You then mount the IDLgrPolygons in IDLgrModel objects to
> translate, scale & rotate them. You can use XOBJVIEW to display the
> collection of IDLgrModels.
>
> I suggest you search the group archives at http://groups.google.co/m
> for a thread earlier this month entitled "Plotting on a sphere". While
> you're at it, try a search for "mesh_obj".
>
>
>> If I succeed in 1, is there a way to display planar contour maps in
>> the image?
>
>
> The IDLgrContour object implements planar (or non-planar) contour-map
> objects.

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