Locating Transition States

Gaussian 98 includes a new method for locating transition structures. The *Synchronous Transit-Guided Quasi-Newton* (STQN) Method, developed by H. B. Schlegel and coworkers, uses a linear synchronous transit or quadratic synchronous transit approach to get closer to the quadratic region around the transition state and then uses a quasi-Newton or eigenvector-following algorithm to complete the optimization. As for minimizations, it performs optimizations by default using redundant internal coordinates. This method will converge efficiently to the actual transition structure using an empirical estimate of the Hessian and suitable starting structures. Unlike other methods, STQN does not require a guess for the transition structure; instead, the reactant and product structures are input.

This method is requested with the **QST2** and **QST3** options to the **Opt** keyword. **QST2** requires two molecule specifications, for the reactant and product, as its input, while **QST3** requires three molecule specifications: the reactant, the product, and an initial structure for the transition state, in that order. The order of the atoms must be identical within all molecule specifications. Note that the **TS** option should not be specified with **QST2** or **QST3**.

For example, at the left is an input file which may be used to locate the transition structure for the reaction SiH4 -> SiH2 + H2. The title section and molecule specification for the product follows those of the reactant.

```
#T RHF/6-31G(d) Opt=(QST2,AddRedundant)
SiH2+H2>SiH4 Reactants  1st title section.
0,1  1st molecule spec.
Si
 X 1 1.0
 H 1 1.48 2 55.0
 H 1 1.48 2 55.0 3 180.0
 H 1 R 2 A1 3 90.0
 H 1 R 5 A2 2 180.0
 R=2.0
 A1=80.0
 A2=22.0
SiH2+H2>SiH4 Products  2nd title section.
0,1  2nd molecule spec.
Si
 X 1 1.0
 H 1 1.48 2 55.0
 ...
 R=1.48
 A1=125.2
 A2=109.5
4  5
```

In this case, because we happen to be interested in the H-H bond length, we specify the internal coordinate which bonds those two atoms to the **AddRedundant** option so that its...
value will be included in the printout of the optimized structure (the Si-H bond lengths will be included by default).

Input files for Opt=QST3 will similarly include three title and molecule specification sections: the reactants, the products, and an initial guess for the transition structure. The optimized structure found by QST2 or QST3 appears in the output in a format similar to that for other types of geometry optimizations:

```
---------------------------------
!     Optimized Parameters      !
!   (Angstroms and Degrees)     !
-----------------------------------------------------------------
! Name  Definition    Value    Reactant  Product  Deriv Info.    
-----------------------------------------------------------------
! R1    R(2,1)        1.0836    1.083     1.084   -DE/DX =  0.   
! R2    R(3,1)        1.4233    1.4047    1.4426  -DE/DX = -0.   
! R3    R(4,1)        1.4154    1.4347    1.3952  -DE/DX = -0.   
! ...                                                           
-----------------------------------------------------------------
```

In addition to listing the optimized values, the table includes those for the reactants and products.

**References**


**Setting up QST2 jobs in GaussView:**

**A Foolproof Technique for Achieving Identical Atom Ordering**

*Gaussian 03*’s Opt=QST2 and Opt=QST3 features are very useful for automating transition structure searches for a given set of reactants and products (and TS initial guess in the case of QST3). In order to use these features, you must provide *G03* with multiple molecular structures with the atoms specified in the same order in all of them. *GaussView* makes it easy to achieve this. The procedure is described below using an SN2 reaction as an example:
1. Draw the reactants in a new Molecule Group:

2. Choose **Edit ? Copy**.

3. Choose **Edit ? Paste ? Add to Molecule Group**. This will cause the reactant structure to be added to the Molecule Group as a second molecule. The window will now look like this:

At this point, you may view both structures in side-by-side panes by clicking the **View Both** button (a toggle) in the toolbar:
4. Modify the structure of molecule 2, using the normal GV tools (e.g. bond distance, bond angle, and dihedral angle), in order to transform the reactant structure into the product structure:

As long as you do not add or remove atoms, the atom ordering will remain the same.

5. Choose Calculate ? Gaussian to set up the job. In the Gaussian Calculation Setup dialog box, select the Job Type tab and choose Optimization from the drop-down list. In the Optimize to a drop-down list, choose TS (QST2). The window will now look like this:
Additional Notes:

- You can view the atom numbers by choosing View ? Labels to manually verify that the ordering is the same.
- To set up atom equivalencies manually, use the Connection Editor in the Edit menu (see GaussView manual for details).
- To optimize products and reactants separately before running a QST2 transition structure optimization, cut and paste each structure into its own new Molecule Group. Then optimize the individual molecules, open the Results file in GaussView, and copy & paste each optimized structure back into the original Molecule Group, replacing the original unoptimized structure you created. This technique works because atom order is maintained throughout the individual optimization.