陕西师范大学
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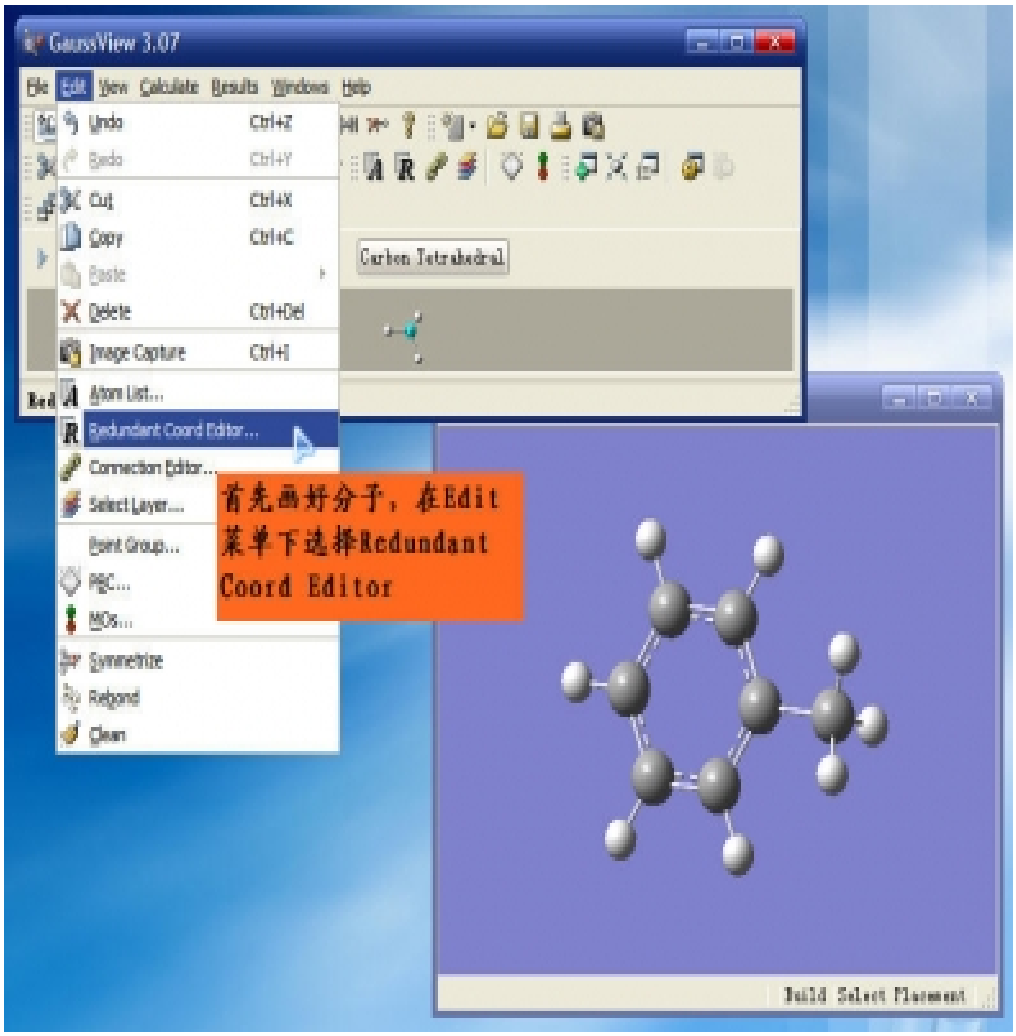
计算中利用 GaussView 固定原子坐标、键角、二面角的方法

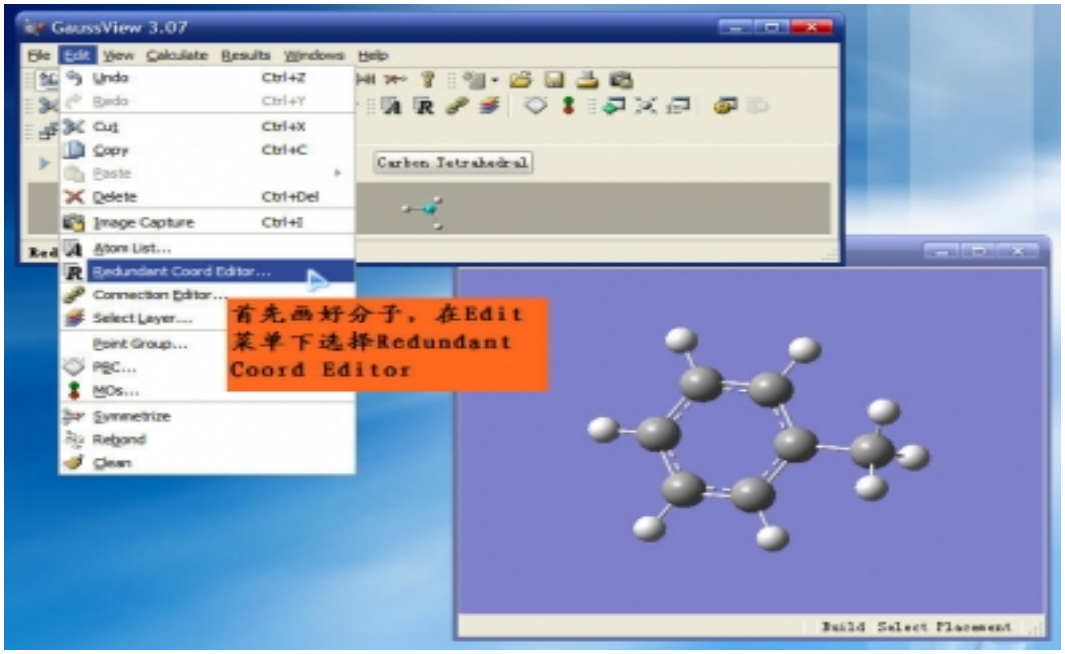
理论与计算化学实验室

最近做一个分子结构优化，想看看不同扭曲状态下得分子能量，所以需要冻结二面角，发现在 GaussView 可以用比较直观的办法实现，这里我简单介绍一下。

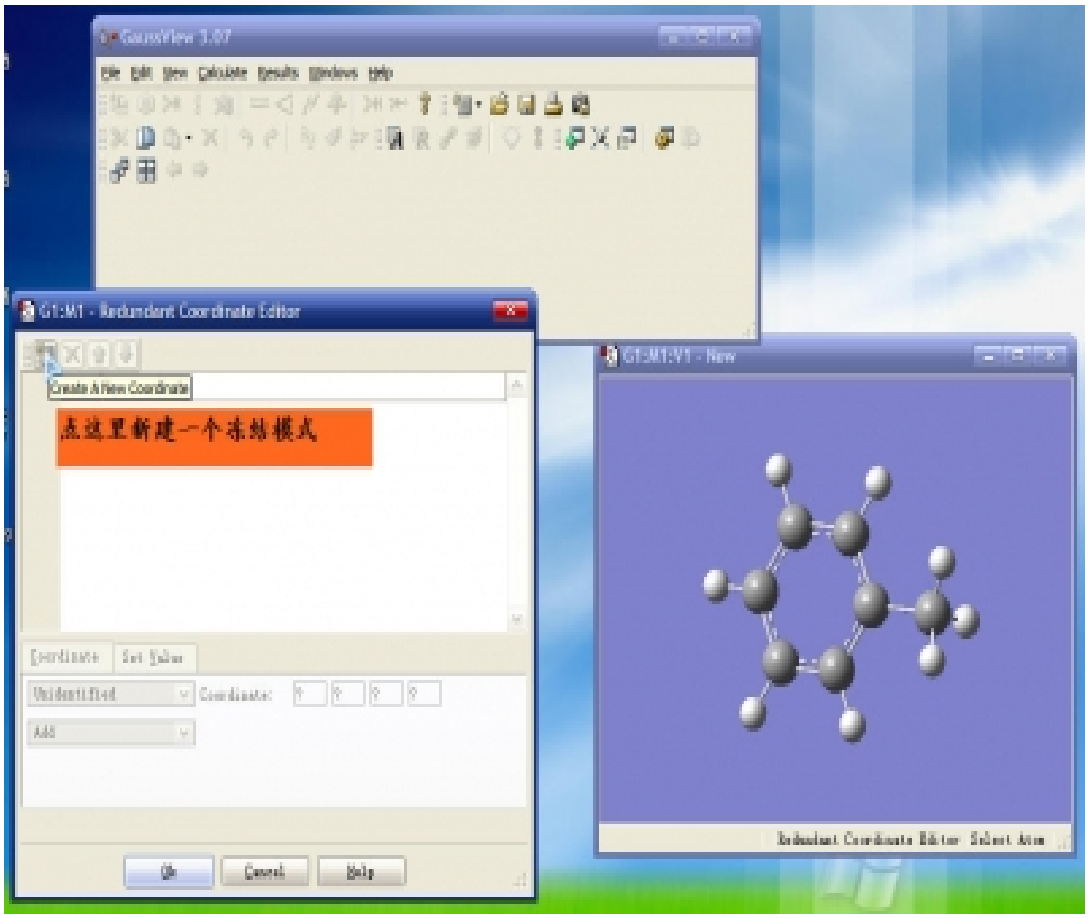
附件 1: 1.jpg (2008-11-27 10:48, 80.06 K)



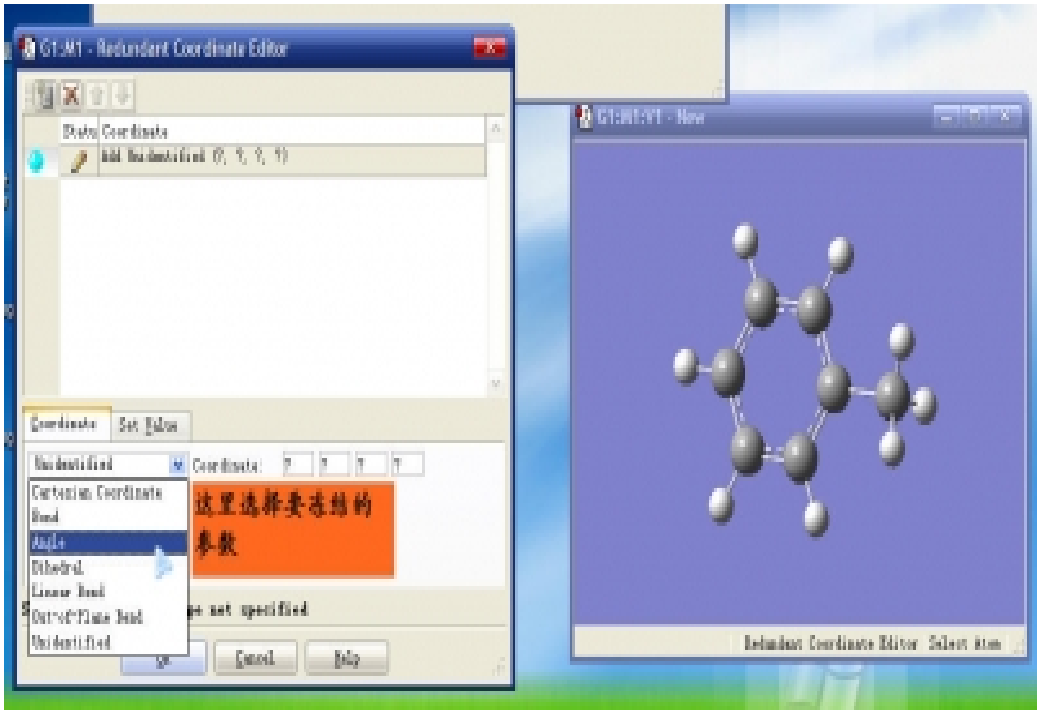
附件 2: 2.jpg (2008-1-27 10:48, 80.06 K)



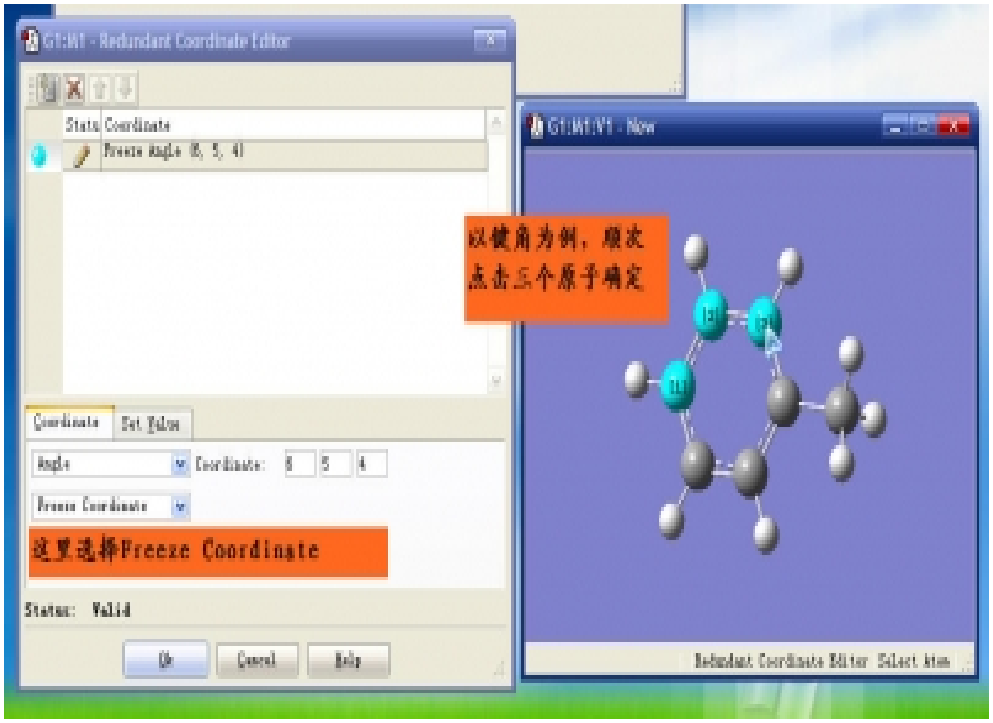
附件 3: 3.jpg (2008-11-27 10:48, 64.26 K)



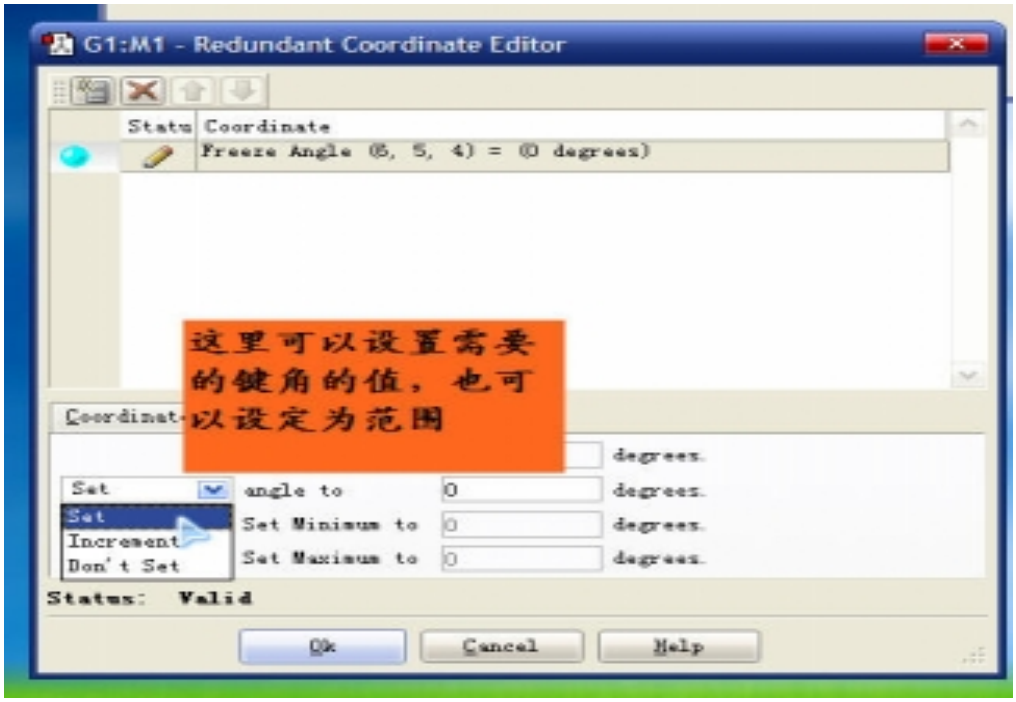
附件 4: 4.jpg (2008-11-27 10:53, 51.13 K)



附件 5: 5.jpg (2008-11-27 10:53, 53.94 K)



附件 6: 6.jpg (2008-11-27 10:53, 65.55 K)



附件 7: 7.jpg (2008-11-27 10:58, 76.21 K)