## Methods, IPC, Koslowski

Quantum chemistry  Gaussian 03 and Gaussview	Mod Unit and Rod Responsib Furth informatio	m: ole: ner	Gaussian 03 and Gaussview Physical Chemistry, various Prof. Thorsten Koslowski www.theochem.uni-freiburg.de	
	imormati	J11.		
Short Description:  Ready-to-use quantum chemistry p	rogram		Picture of the Equipment	
package and user interface			1 3 4 50	
Available Experiments/Techniques:				
HF, DFT, various post-SCF method	ds			
Special Equipment:				
Measurements on the equipment are currently done by:			☐ Students ☐ Students after Introduction ☐ Students after extensive training ☐ Trained scientific service personal	
Recent Publications, where this instrument was important (optional): Give citation			CS 131, 8134 (2009); Phys. Rev. Lett. 2, 183401 (2009)	
Typical problems that may be solved with this instrument:		ge	Electronic structure computations, geometry optimizations, vibrational and UV-VIS spectra calculations	