

Methods, IAAC, Crossing

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| <p>Krossing Group Compute Cluster</p> <p><i>Quantum Chemistry</i></p> | <p>Model: Unit and Room: Responsible: Further information:</p> | <p><i>Dalco Computing Opteron Nodes Deltacomputer Xeon Nodes Rechenzentrum der Albert-Ludwigs- Universität Freiburg, Maschinenraum Dr. Anke Schaub</i></p> |
| <p>Short Description:</p> <p>Linux-based compute cluster with 7 Opteron nodes (2 cpu cores & 8 GB memory each) and 3 Xeon nodes (8 cpu cores & 16 GB memory each).. Runs with Rocks/Centos Linux..</p> | <p>Picture of the Equipment</p> | |
| <p>Available Experiments/Techniques:</p> <p>DFT, perturbation methods, coupled cluster and other highly correlated methods. Visualization, rendering, structure refinement and mathematical analysis software.</p> | | |
| <p>Special Equipment:</p> <p>Commercial licenses: Turbomole, Gaussian 03, Cosmotherm, Crystal 06</p> | | |
| <p>Measurements on the equipment are currently done by:</p> | <p><input type="checkbox"/> Students <input checked="" type="checkbox"/> Students after Introduction <input checked="" type="checkbox"/> Students after extensive training <input checked="" type="checkbox"/> Trained scientific service personal</p> | |
| <p>Recent Publications, where this instrument was important (optional): Give citation</p> | <p>Chem. Eur. J. 2009, 15, 3426-3434. Angew. Chem. 120, 7914-7917.</p> | |
| <p>Typical problems that may be solved with this instrument:</p> | <p><i>Quantum chemical calculations:</i></p> <ul style="list-style-type: none"> - <i>Geometry optimization</i> - <i>Reaction enthalpies</i> - <i>Prediction of properties</i> - <i>Thermodynamics</i> - <i>Transition state search</i> - <i>Understanding of bonding situations</i> | |