



Figure 3. The XSophe (v 1.1.4) main Window. The interface allows creation and execution of multiple input files on local or remote hosts. There are macro task buttons to guide the novice through the various menus and two button bars to allow easy access to the menus. For example, the bottom bar (left to right), Experimental Parameters, Spin System, Spin Hamiltonian, Instrumental Parameters, Single Crystal Settings, Lineshape Parameters, Transition Labels/Probabilities, File Parameters, Sophe Grid Parameters, Optimisation Parameters, Execution Parameters and Batch Parameters.