b44 [#16:1]-[#6:2] 1.0 Sage 2.1.0 (regroup) Sage 2.2.1 Sage 2.2.1-sdata Sage 2.2.1-tm-sdata 8.0 0.6 0.4 0.2 0.0 -0.4-0.20.0 0.2 0.4 0.6 Bond length error (A)