b13 [#6X3:1]=[#7X2,#7X3+1:2] 3500 Sage 2.1.0 (regroup) Sage 2.2.1 Sage 2.2.1-sdata 3000 2500 2000 -Count 1500 1000 500 0 -0.06-0.04-0.020.02 0.04 0.06 0.00

Bond length error (A)