b16 [#6X4:1]-[#8X2H0:2] Sage 2.1.0 (regroup) 10000 Sage 2.2.1 Sage 2.2.1-sdata 8000 6000 4000 2000 -0.20-0.15-0.10-0.050.05 0.10 0.00 Bond length error (A)