

CHEM 455 - Homework 9 – Due Monday May 30 at 5pm

Note: Please work, and turn in, the questions in the following order

Q12.17 Justify the B.O. approximation. You must include numerical values for typical timescales of motion.

P12.2 Overlap integral for various effective orbital sizes

Q12.7 H_{aa} interpretation

Q12.15 magnitude of c_a and c_b in u and g MOs

Q12.23 delocalization and nodes

Q12.25 J and K values are positive

Q12.4 H_{11} and H_{22}

P12.5 bond orders

P12.6 sketch the homo

P12.8 MOs for NO –make sure to redraw the MOs in your homework so we know which one you are referring to

P12.10 Bond energy and bond length