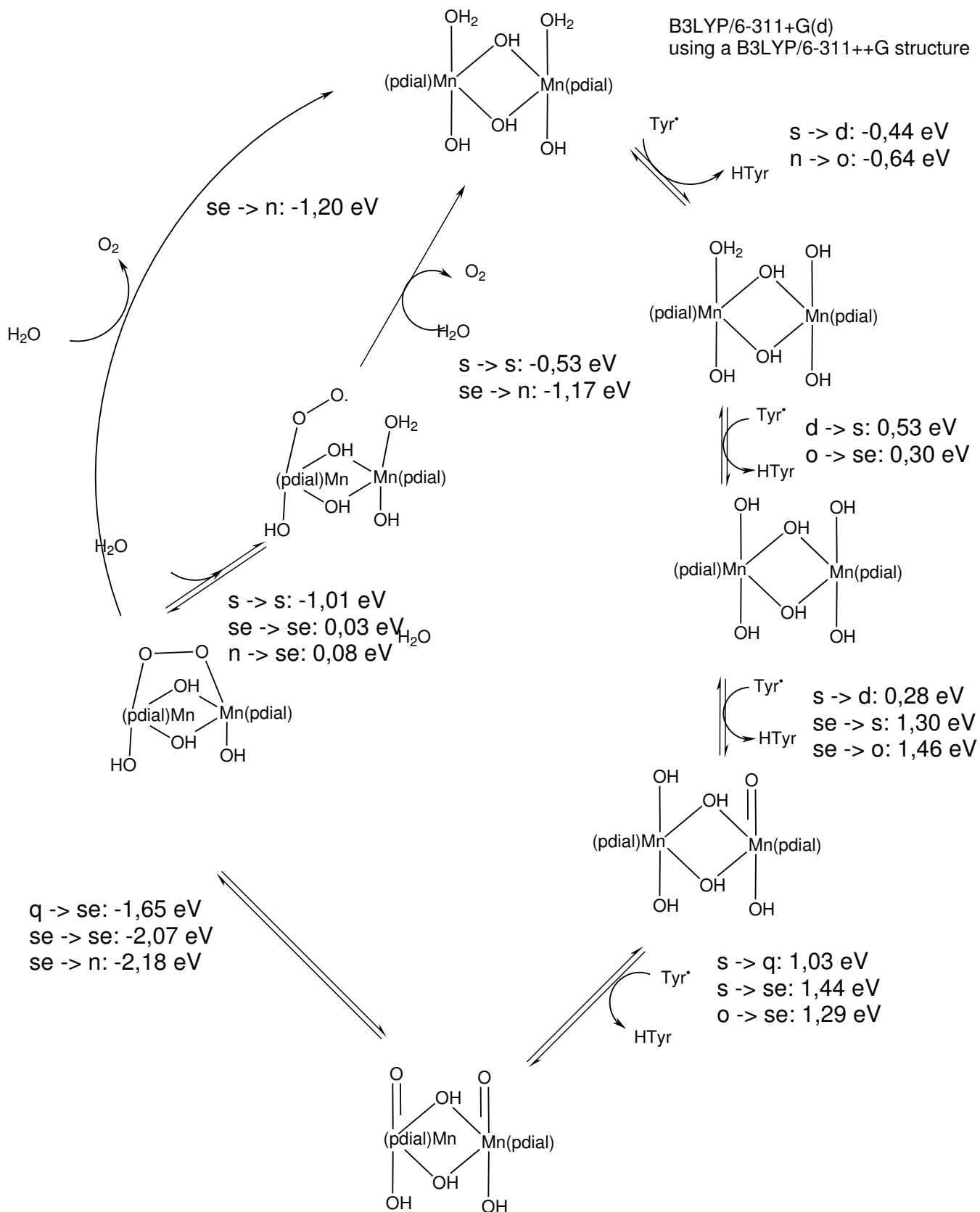


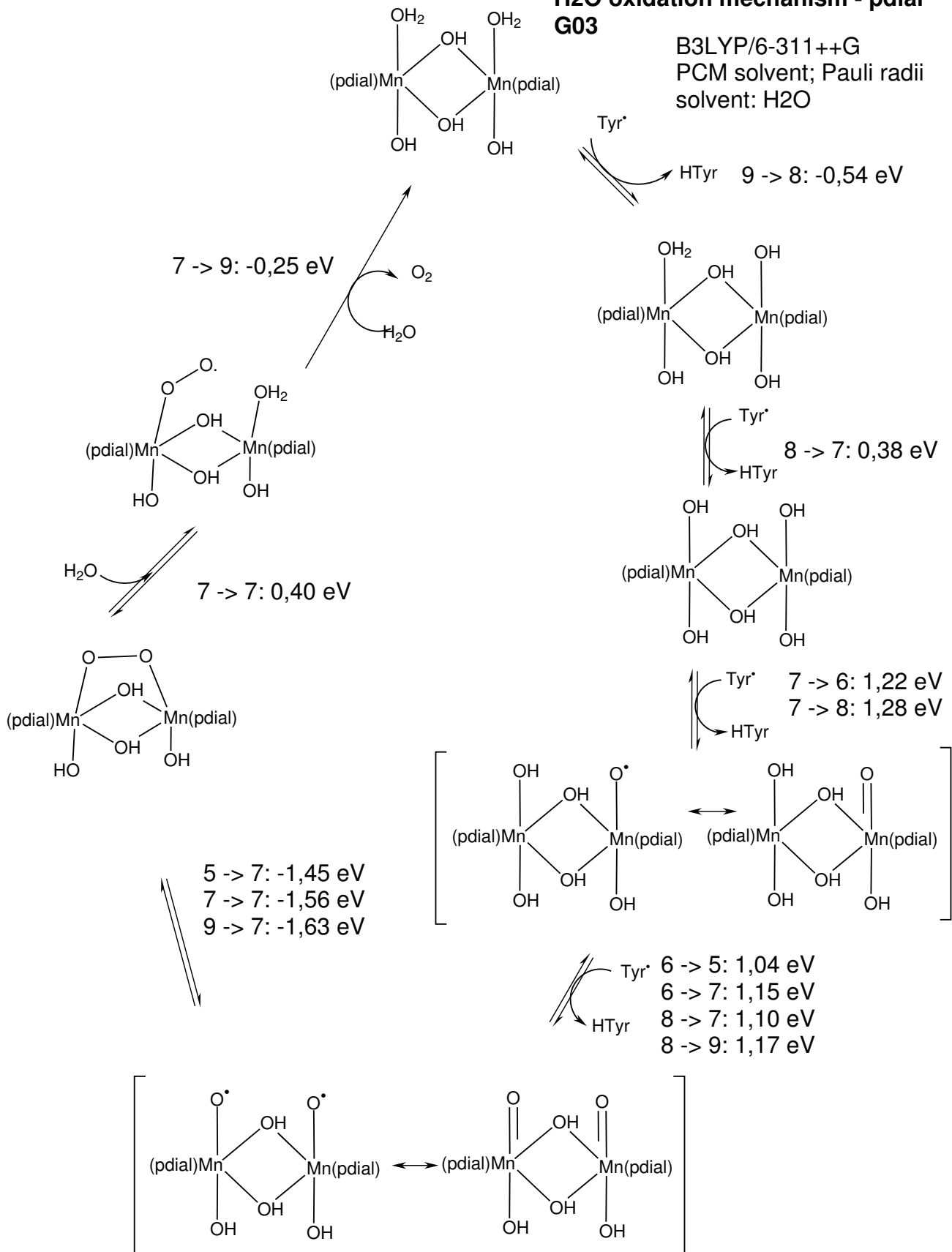
H₂O oxidation mechanism - pdial G03

B3LYP/6-311+G(d)
 using a B3LYP/6-311++G structure



H₂O oxidation mechanism - pdial G03

B3LYP/6-311++G
 PCM solvent; Pauli radii
 solvent: H₂O



H₂O oxidation mechanism - pdial G03

B3LYP/6-311++G
 PCM solvent; Pauli radii
 solvent: Acetonitrile

