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A High Level Computational Study of the Stereoelectronic Effects of Substituents on Alkene Epoxidations with Peroxyformic Acid

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Supporting Information

Table 1S. G2 Energies (in hartrees) of Ethylene, 1,3-Butadiene, and Acrylonitrile, Their Epoxides, Peroxyformic and Formic Acids

Molecule	G2 0 K	G2 298 K
Ethylene	-78.41593	-78.41193
Propene	-117.64509	-117.63998
Isobutene	-156.87634	-156.86996
1,3-Butadiene	-155.66427	-155.65855
Acrylonitrile	-170.53398	-170.52885
Ethylene Epoxide	-153.53290	-153.52879
Propene Epoxide	-192.76604	-192.76061
Isobutene Epoxide	-232.00024	-231.99342
1,3-Butadiene Epoxide	-230.78001	-230.77385
Acrylonitrile Epoxide	-245.64579	-245.64026
Peroxyformic Acid	-264.55747	-264.55229
Formic Acid	-189.51648	-189.51234