Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information: High Throughput Screening of Norbornadiene/Quadricyclane Derivates for Molecular Solar Thermal Energy Storage

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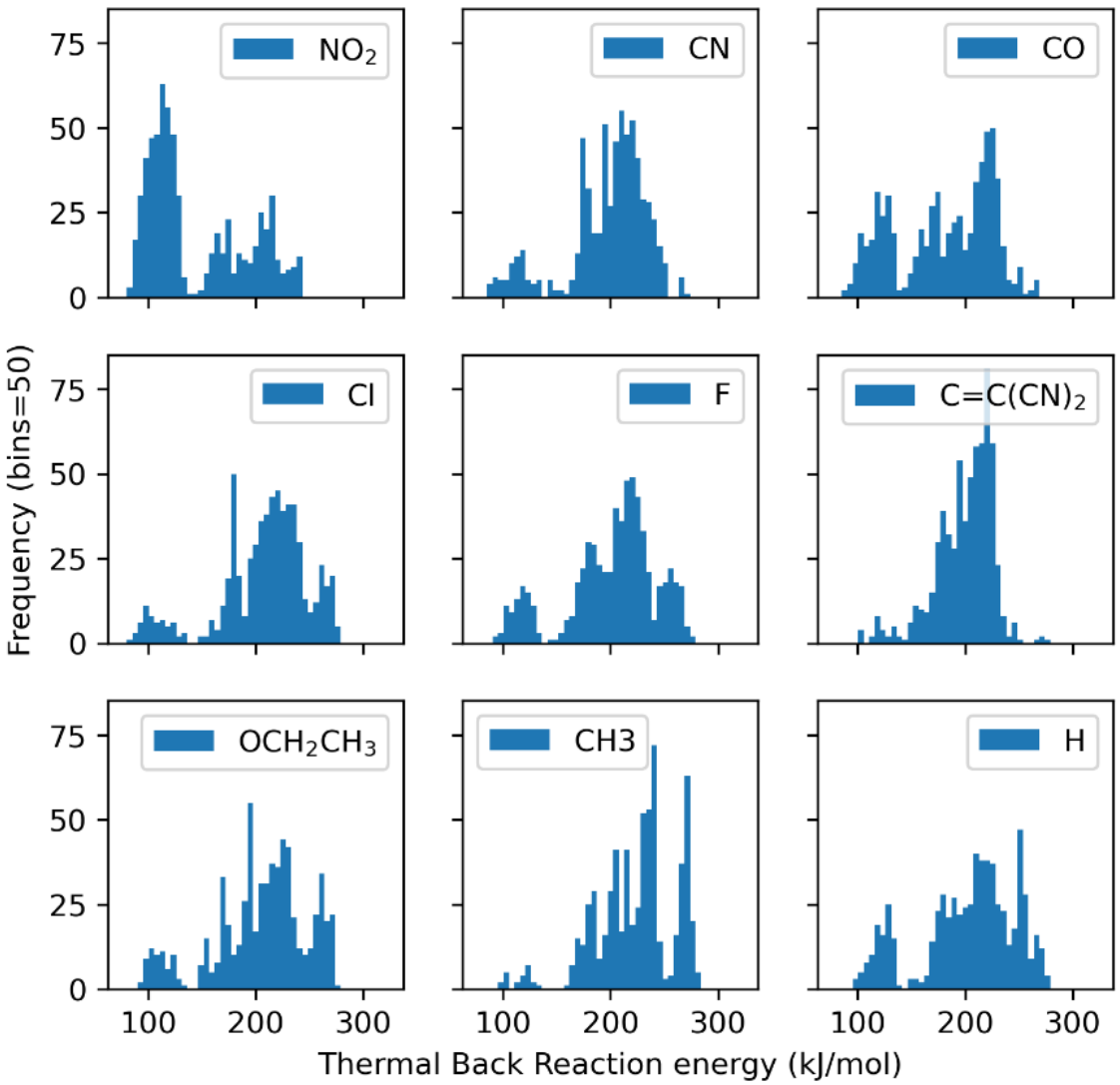

Figure 1: In each plot is a histogram of the structures with at least one of the specified substituents on the ortho-position on the phenyl ring coupled to the NBD core structure. We see a tendency, that if the substituent NO_2 is on the ortho position, then TBR energy is generally lower. This can be due to the overestimation of the product energy or underestimation of the transition state energy. This was not investigated further.