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Electronic Supporting Information

Applications of noisy quantum computing and quantum error mitigation to "adamantaneland": A benchmarking study for quantum chemistry

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Data set details

The optimization of geometries employed a default self-consistent field convergence criterion of 10^{-8} Hartree, *ultrafine* integration grid (pruned 99×590 grid), and *tight* optimization convergence criteria (maximum force = 1.5×10^{-5} Hartree/Bohr, RMS force = 1×10^{-5} Hartree/Bohr, maximum displacement = 6×10^{-5} Bohr, RMS displacement = 4×10^{-5} Bohr). For transition state structures, the *CalcFC* and *NoEigenTest* options were used to compute force constants in the first step of the optimization and suppress the curvature test during optimization, respectively. Each optimized structure was subjected to an additional vibrational frequency calculation to verify the nature of the stationary point, i.e., all positive frequencies for minima and one negative frequency corresponding to the reaction coordinate for the transition state structure. For the isomer set, all geometry optimizations were started from identical looking structures reported in the work of Engler *et al.*[5] with the exception that we modeled two additional missing isomer structures resulting in overall 21 isomers of $C_{10}H_{16}$. All geometry optimizations successfully converged to the correct energy-relaxed stationary point and are included in the set. For the reaction set, we modeled the proposed route mapped out in the work of Kirchen *et al.*[10] (see Figure S1 below) which included performing geometry optimizations for obtaining the energy-relaxed structures of the reactant, transition state, and product of various steps. Tabulated below is also the information associated with the outcome of modeling each chemical reaction for the reaction set.

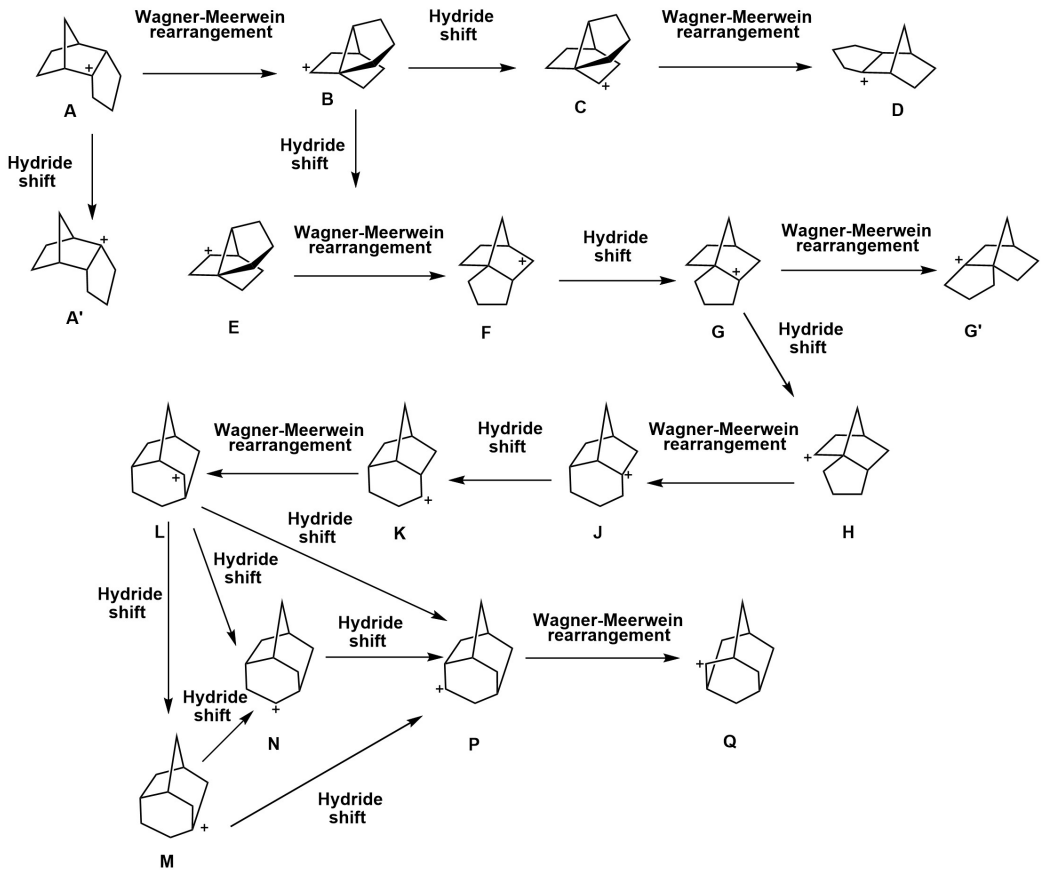

Figure S1: Chemical reaction scheme modeled in our work for the reaction set corresponding to the proposed route mapped out in figure 2 of the work of Kirchen *et al.*[10].

Reaction	**Remarks**
A $\rightarrow$ A'	Transition state structure successfully located (negative frequency of the normal mode corresponding to the reaction coordinate is $-641.45\ cm^{-1}$). No issues with geometry optimizations of reactant A and product A'.
A $\rightarrow$ B	Transition state structure not located (geometry optimization converges to a local minimum instead). Geometry optimization of product B converges to that of more stable structure A. No issues with geometry optimization of reactant A.
B $\rightarrow$ C	Transition state structure successfully located (negative frequency of the normal mode corresponding to the reaction coordinate is $-457.05\ cm^{-1}$). Geometry optimization of reactant B converges to that of more stable structure A. Geometry optimization of product C converges to that of more stable structure D.
C $\rightarrow$ D	Transition state structure not located (geometry optimization converges to a local minimum instead). Geometry optimization of reactant C converges to that of more stable structure D. No issues with geometry optimization of product D.
B $\rightarrow$ E	Transition state structure successfully located (negative frequency of the normal mode corresponding to the reaction coordinate is $-598.77\ cm^{-1}$). Geometry optimization of reactant B converges to that of more stable structure A. Geometry optimization of product E converges to that of more stable structure F.

E $\rightarrow$ F	Transition state structure not located (geometry optimization converges to a local minimum instead). Geometry optimization of reactant E converges to that of more stable structure F. No issues with geometry optimization of product F.
F $\rightarrow$ G	Transition state structure successfully located (negative frequency of the normal mode corresponding to the reaction coordinate is $-538.36\ cm^{-1}$). No issues with geometry optimizations of reactant F and product G.
G $\rightarrow$ G'	Transition state structure successfully located (negative frequency of the normal mode corresponding to the reaction coordinate is $-171.20\ cm^{-1}$). No issues with geometry optimizations of reactant G and product G'.
G $\rightarrow$ H	Transition state structure successfully located (negative frequency of the normal mode corresponding to the reaction coordinate is $-460.80\ cm^{-1}$). Geometry optimization of product H converges to that of more stable structure J. No issues with geometry optimization of reactant G.
H $\rightarrow$ J	Transition state structure not located (geometry optimization converges to a local minimum instead). Geometry optimization of reactant H converges to that of more stable structure J. No issues with geometry optimization of product J.
J $\rightarrow$ K	Transition state structure successfully located (negative frequency of the normal mode corresponding to the reaction coordinate is $-750.29\ cm^{-1}$). No issues with geometry optimizations of reactant J and product K.

K $\rightarrow$ L	Transition state structure successfully located (negative frequency of the normal mode corresponding to the reaction coordinate is $-166.92\ cm^{-1}$). No issues with geometry optimizations of reactant K and product L.
L $\rightarrow$ M	Transition state structure successfully located (negative frequency of the normal mode corresponding to the reaction coordinate is $-1359.35\ cm^{-1}$). No issues with geometry optimizations of reactant L and product M.
L $\rightarrow$ N	Transition state structure successfully located (negative frequency of the normal mode corresponding to the reaction coordinate is $-394.35\ cm^{-1}$). No issues with geometry optimizations of reactant L and product N.
M $\rightarrow$ N	Transition state structure successfully located (negative frequency of the normal mode corresponding to the reaction coordinate is $-1062.67\ cm^{-1}$). No issues with geometry optimizations of reactant M and product N.
L $\rightarrow$ P	Transition state structure successfully located (negative frequency of the normal mode corresponding to the reaction coordinate is $-467.59\ cm^{-1}$). Geometry optimization of product P converges to that of more stable structure Q. No issues with geometry optimization of reactant L.
M $\rightarrow$ P	Transition state structure not located (geometry optimization converges to structure of a wrong mechanism). Geometry optimization of product P converges to that of more stable structure Q. No issues with geometry optimization of reactant M.

$N \rightarrow P$	Transition state structure successfully located (negative frequency of the normal mode corresponding to the reaction coordinate is $-492.65\ cm^{-1}$). Geometry optimization of product P converges to that of more stable structure Q. No issues with geometry optimization of reactant N.
$P \rightarrow Q$	Transition state structure not located (geometry optimization converges to a local minimum instead). Geometry optimization of reactant P converges to that of more stable structure Q. No issues with geometry optimization of product Q.

Quantum state tomography

Given a prepared n-qubit quantum state $|\psi\rangle$ in the Hilbert space $\mathscr{H} = \mathbb{C}^{2^n}$, quantum state tomography is a procedure to reconstruct ρ in $B(\mathscr{H})$, the space of bounded operators on $\mathscr{H}$. We do this by subjecting identical copies of $|\psi\rangle$ to a sequence of measurements (here, 3^n times).[1] Now, let us denote $|\psi_i^+\rangle$ and $|\psi_i^-\rangle$ as the eigenvectors of σ_i with corresponding eigenvalues of 1 and -1 for $i = 1, 2, 3$ and take $|\psi_0^+\rangle = |0\rangle, |\psi_0^-\rangle = |1\rangle$. Also, equip $B(\mathscr{H})$ with the Hilbert–Schmidt inner product given by $\langle S,\ T\rangle_{\mathrm{Tr}} = \mathrm{Tr}(S^\dagger T)$, where Tr is the trace, and let $\Pr\left(|\psi_{i_j}^{\pm}\rangle \mid \rho\right)$ be the probability of measuring $|\psi_{i_j}^{\pm}\rangle$ in the j-th qubit. As $\left\{\frac{\sigma_0}{\sqrt{2}}, \frac{\sigma_1}{\sqrt{2}}, \frac{\sigma_2}{\sqrt{2}}, \frac{\sigma_3}{\sqrt{2}}\right\}$ forms an orthonormal basis for $B(\mathbb{C}^2)$, it follows from Tr being multiplicative with respect to the Kronecker tensor product that $\left\{\frac{\sigma_0}{\sqrt{2}}, \frac{\sigma_1}{\sqrt{2}}, \frac{\sigma_2}{\sqrt{2}}, \frac{\sigma_3}{\sqrt{2}}\right\}^{\otimes_{i=1}^n}$ forms an orthonormal basis for $B(\mathscr{H})$.[11] Therefore, ρ can be decomposed as,

$$\rho = \frac{1}{2^n} \sum_{i \in \{0,\ldots,3\}^n} \left\langle \otimes_{j=1}^n \sigma_{i_j},\ \rho \right\rangle \otimes_{j=1}^n \sigma_{i_j} \tag{1}$$

$$= \frac{1}{2^n} \sum_{i \in \{0,\ldots,3\}^n} \mathrm{Tr}\left[\left(\otimes_{j=1}^n \sigma_{i_j}\right) \rho\right] \otimes_{j=1}^n \sigma_{i_j} \tag{2}$$

$$= \frac{1}{2^n} \sum_{i \in \{0,\ldots,3\}^n} \left\langle \otimes_{j=1}^n \sigma_{i_j} \right\rangle \otimes_{j=1}^n \sigma_{i_j} \tag{3}$$

where,

$$\left\langle \otimes_{j=1}^n \sigma_{i_j} \right\rangle = \otimes_{j=1}^n \left(\Pr\left(|\psi_{i_j}^+\rangle \mid \rho\right) - (-1)^{\delta(i_j,0)} \Pr\left(|\psi_{i_j}^-\rangle \mid \rho\right)\right) \tag{4}$$

Under a noisy system, we reconstruct ${\rho'}_{\text{noisy}} \approx \rho$ (normalized to trace 1) by measuring in the appropriate basis $\left\langle \otimes_{j=1}^{n} \sigma_{i_j} \right\rangle$. As σ_0 and σ_3 share eigenvectors, measuring $\left\langle \otimes_{j=1}^{n} \sigma_{i_j} \right\rangle$ for $i \in \{1, ..., 3\}^n$ is sufficient. Since it's possible that ${\rho'}_{\text{noisy}}$ is not positive, maximum likelihood estimation is used to extract $\rho' \approx \rho$ satisfying $\text{Tr}(\rho') = 1$ and $\rho' \geq 0$. Assuming Gaussian noise with variance s^2, the probability of measuring m for $\left\langle \otimes_{j=1}^{n} \sigma_{i_j} \right\rangle$ is,

$$\Pr\left(m \mid \rho\right) = \frac{1}{\sqrt{2\pi s^2}} \exp\left(-\frac{\left(m - \left\langle \otimes_{j=1}^{n} \sigma_{i_j} \right\rangle\right)^2}{2s^2} \right) \tag{5}$$

Maximum likelihood estimation under this assumption is equivalent to the constrained least-squares optimization problem (see below),

$$\begin{aligned} \min_{\rho'} \quad & ||\rho' - {\rho'}_{\text{noisy}}||_{\text{Tr}}^2 \\ \text{subject to} \quad & \rho' \geq 0, \text{Tr}(\rho') = 1 \end{aligned} \tag{6}$$

for which the method developed by Smolin *et al.*[12] is used to obtain ρ' in $O(2^{3n})$.

Maximum likelihood estimation for $\hat{\rho}$ in quantum state tomography

Let $m = \{m_i \mid i \in \{0, 1, 2, 3\}^n\}$.
We have,

$$\log\left[\Pr(m_i \mid \rho)\right] = \log\left[\frac{1}{\sqrt{2\pi s^2}}\exp\left(-\frac{\left(m - \left\langle \bigotimes_{j=1}^{n}\sigma_{i_j}\right\rangle\right)^2}{2s^2}\right)\right]$$
$$= \log\left[\frac{1}{\sqrt{2\pi s^2}}\right] + \log\left[2s^2\right]$$
$$- \left(m - \left\langle \bigotimes_{j=1}^{n}\sigma_{i_j}\right\rangle\right)^2.$$

Then,

$$\arg\max_{\rho}\Pr\left(m \mid \rho\right) = \arg\max_{\rho}\log\left[\Pr\left(m \mid \rho\right)\right]$$
$$= \arg\max_{\rho}\log\left[\prod_{i\in\{0,1,2,3\}^n}\Pr\left(m_i \mid \rho\right)\right]$$
$$= \arg\min_{\rho}\sum_{i\in\{0,1,2,3\}^n}\left(m - \left\langle \bigotimes_{j=1}^{n}\sigma_{i_j}\right\rangle\right)^2$$
$$= \arg\min_{\rho}||\hat{\rho}_{\text{noisy}} - \hat{\rho}||_{\text{Tr}}^2.$$

Noisy simulation

Our noise model (excluding readout error) is a combination of ε^{DP} (a depolarizing channel), ε^{AD} (a Clifford and measurement channel approximation of an amplitude damping channel[8]), and ε^{PD} (a phase damping channel). Specifically, our noise

model is described by applying the quantum channel,

$$\varepsilon_{q_i}^{\text{one}} = \underbrace{\varepsilon_{q_i}^{\text{PD}} \circ \varepsilon_{q_i}^{\text{AD}}}_{\varepsilon_{q_i}^{\text{TR}}} \circ \varepsilon_{q_i}^{\text{DP}} \tag{7}$$

after a one-qubit gate g on qubit q_i and

$$\varepsilon_{q_i,q_j}^{\text{two}} = \underbrace{[(\varepsilon_{q_i}^{\text{PD}} \circ \varepsilon_{q_i}^{\text{AD}}) \otimes (\varepsilon_{q_j}^{\text{PD}} \circ \varepsilon_{q_j}^{\text{AD}})]}_{\varepsilon_{q_i,q_j}^{\text{TR}}} \circ \varepsilon_{q_i,q_j}^{\text{DP}} \tag{8}$$

after a two-qubit gate g on qubit q_i and q_j.[6, 3] The channels take in as parameters g_e (average gate error), g_t (gate time), T_1 (relaxation time), and T_2 (dephasing time). Readout error is simulated by assuming the independence of each qubit's readout error. This is valid for $T_1[q] \leq T_2[q]$ for all qubits q (see Reference [6] for more details). The Gottesman–Knill theorem allows our noise model to be efficiently simulated with a stabilizer circuit simulator such as Stim[7]. This allows our benchmarking framework to be extended to use stabilizer-circuit-based bootstrapping methods like Clifford Data Regression (CDR).[4]

Additional VQE details

Solving the electronic structure problem via the VQE algorithm requires some key steps. At first, the molecular Hamiltonian $\hat{H}$ is expressed in the second quantization formalism,

$$\hat{H} = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s \tag{9}$$

where p, q, r, s are the indices corresponding to the spin orbitals whereas a_p, $a_p^\dagger$, h_{pq}, and h_{pqrs} represent an annihilation op-

erator acting on the p-th spin-orbital, a creation operator acting on the p-th spin-orbital, one-electron molecular orbital integrals, and two-electron molecular orbital integrals, respectively.

Another step in the execution of VQE includes transforming the second quantized Hamiltonian to an equivalent spin-based Hamiltonian. Such transformation is performed to map the electronic structure problem from fermionic to qubit representation (where each qubit directly maps to one spin-orbital) via well-known schemes. The Hamiltonian yielded via the fermion–qubit transformation can then be described by a linear combination of Pauli spin operators,

$$\hat{H} = \sum_i w_i \hat{P}_i \tag{10}$$

where each $\hat{P}_i$ term is multiplied by the corresponding Hamiltonian coefficient w_i and comprises a tensor product belonging to $\{\sigma_0, \sigma_1, \sigma_2, \sigma_3\}$ operators or $\{I, X, Y, Z\}$ quantum gates acting on the i-th qubit,

$$\hat{P}_i = \sigma_N \otimes \sigma_{N-1} \otimes \cdots \otimes \sigma_1 \tag{11}$$

The variational energy (Equation 1) is produced by grouping the individual Pauli term expectation values. These expectations are obtained by performing repetitive measurements. More details about measurement techniques can be found in References [2, 16].

For comparison with traditional quantum chemistry methods, the energetic reference data from Tables 1 and 2 in the main manuscript were used, i.e., ΔE_{ref}^{iso} and $\Delta E_{ref}^{\ddagger}$. The experiments conducted on *FakeQuito* backend and *ibmq_quito* device using error mitigation were aimed at reproducing the exact di-

agonalization results of the frozen-orbitals system as obtained from the noiseless statevector simulations. The initial HF calculation was performed internally in *qiskit* with an interface to the $PySCF$[15] computational chemistry program. Calculations for each molecule on the statevector and *FakeQuito* backend used 8912 shots per VQE iteration and were repeated 10 times for (2,2) active space and 5 times for (4,4) and (6,6) active spaces. Therefore, the error statistics for these simulations were obtained on the average value of the ten runs for (2,2) active space and five runs for (4,4) and (6,6) active spaces. For molecules in our data set, chosen (2,2) active space corresponds to the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), whereas the (4,4) and (6,6) active spaces correspond to up to two molecular orbitals below the HOMO and up to two molecular orbitals above the LUMO. To minimize the energy in each VQE iteration, we utilized the Simultaneous Perturbation Stochastic Approximation (SPSA) optimizer, which is particularly recommended for noisy simulations.[13, 14, 9] For a (2,2) active space calculation, we use 100 iterations of the SPSA algorithm, which comprises 251 energy evaluations: the first 50 evaluations to tune the learning rate and perturbation coefficients as required by the optimization algorithm, followed by the next 200 for gradient calculations, and the final evaluation to obtain the energy expectation value. To attain energy convergence with larger (4,4) and (6,6) active spaces, we use 500 iterations of the SPSA algorithm, which comprises overall 1051 energy evaluations.

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Optimized geometry of 1 from the isomer set

26
0 1
C -0.891558 0.927572 -1.210071
C -0.039234 1.530094 -0.090254
C 1.405086 1.044009 -0.235073
C 1.447748 -0.483579 -0.145304
C 0.891617 -0.927569 1.210012
C -0.553954 -0.446206 1.358173
C -1.405198 -1.043958 0.235039
C -0.854469 -0.600276 -1.122599
C 0.591792 -1.081361 -1.264875
C -0.591801 1.081292 1.264953
H -1.920977 1.281703 -1.127880
H -0.517513 1.255361 -2.181945
H -0.067078 2.618702 -0.154514
H 1.816298 1.373707 -1.191158
H 2.026964 1.481817 0.548195
H 2.477725 -0.827698 -0.248705
H 1.505139 -0.521816 2.016755
H 0.933442 -2.015347 1.292905
H -0.948099 -0.763629 2.324541
H -2.442896 -0.721610 0.340798
H -1.400691 -2.133612 0.302153
H -1.462399 -1.027332 -1.921361
H 0.628777 -2.171636 -1.221943
H 0.989802 -0.786254 -2.237695
H -1.616373 1.437895 1.387295
H -0.002295 1.519643 2.072558

Optimized geometry of exo-2 from the isomer set

26
0 1
C 2.123458 -0.776830 -0.503963
C 0.878758 -1.126834 0.324289
C 2.123458 0.776830 -0.503963
H 2.074591 -1.197126 -1.506921
H 3.023783 -1.166526 -0.032072
C 0.878758 1.126834 0.324289
H 2.074591 1.197126 -1.506921
H 3.023783 1.166526 -0.032072
C 0.887598 0.000000 1.365108
H 0.018394 0.000000 2.018679
H 1.783960 0.000000 1.984075
C -0.361315 -0.783011 -0.511774
H 0.877909 -2.142434 0.714225
C -0.361315 0.783011 -0.511774
H 0.877909 2.142434 0.714225
C -1.714242 -1.197582 0.080763
C -1.714242 1.197582 0.080763
C -2.628543 0.000000 -0.170512
H -2.091473 2.121961 -0.352699
H -1.618871 1.364611 1.155012
H -2.960900 0.000000 -1.210346
H -3.519803 0.000000 0.454853
H -1.618871 -1.364611 1.155012
H -2.091473 -2.121961 -0.352699
H -0.263885 1.181758 -1.520862
H -0.263885 -1.181758 -1.520862

Optimized geometry of endo-2 from the isomer set

26
0 1
C -1.362112 -0.775742 1.135935
C -1.050595 -1.129386 -0.323861
C -1.362112 0.775742 1.135935
H -0.650834 -1.197193 1.840576
H -2.341395 -1.164880 1.409375
C -1.050595 1.129386 -0.323861
H -0.650834 1.197193 1.840576
H -2.341395 1.164880 1.409375
C -1.793176 -0.000000 -1.057009
H -1.618258 -0.000000 -2.132237
H -2.867388 -0.000000 -0.873505
C 0.404365 -0.782913 -0.690204
H -1.340372 -2.141874 -0.595747
C 0.404365 0.782913 -0.690204
H -1.340372 2.141874 -0.595747
C 1.570215 -1.202675 0.209169
H 0.591415 -1.148449 -1.699914
C 1.570215 1.202675 0.209169
H 0.591415 1.148449 -1.699914
C 2.516101 0.000000 0.171268
H 1.240042 1.366126 1.234080
H 2.044503 2.124512 -0.122306
H 3.243320 0.000000 0.981813
H 3.075575 0.000000 -0.766230
H 2.044503 -2.124512 -0.122306
H 1.240042 -1.366126 1.234080

Optimized geometry of 3 from the isomer set

26
0 1
C -0.482594 -1.347440 -0.971677
C 0.761967 -1.301148 -0.065209
C 0.362730 -0.901734 1.355484
C -0.477438 0.377691 1.273662
H 1.256152 -0.754265 1.963299
H -0.217911 -1.688055 1.838911
C -1.413352 -0.138075 -0.824359
H -1.053806 -2.247343 -0.732813
H -0.165173 -1.447973 -2.011157
C -1.822437 0.014633 0.639620
H -2.260870 -0.886245 1.068194
H -2.544934 0.824518 0.748551
C 1.837425 -0.312950 -0.553082
H 1.196708 -2.300851 -0.061658
C 1.627484 1.094828 0.021400
H 1.840878 -0.284990 -1.642603
H 2.820789 -0.677652 -0.256413
C 0.147516 1.378805 0.250351
H 2.053746 1.843573 -0.646250
H 2.160263 1.193397 0.967985
H -0.585045 0.827041 2.259308
C -0.676754 1.182736 -1.045721
H -2.265417 -0.251637 -1.494011
H -1.401660 1.987495 -1.162847
H -0.052692 1.181575 -1.938313
H 0.031695 2.397342 0.617003

Optimized geometry of 4 from the isomer set

26
0 1
C 0.000000 0.000005 -1.560367
C 0.468383 -1.119740 -0.621205
C -0.468383 1.119745 -0.621198
H -0.815944 -0.312528 -2.210555
H 0.815944 0.312544 -2.210553
C 0.468383 1.119740 0.621205
C -0.000000 -0.000005 1.560367
C -0.468383 -1.119745 0.621198
H -0.815944 0.312528 2.210555
H 0.815944 -0.312544 2.210553
C 1.894702 -0.745559 -0.204380
H 0.445557 -2.092244 -1.110873
C 1.894702 0.745559 0.204381
H 2.583402 -0.918666 -1.030547
H 2.229388 -1.374851 0.620146
H 2.229388 1.374851 -0.620145
H 2.583402 0.918666 1.030548
H 0.445557 2.092244 1.110873
C -1.894702 0.745561 -0.204375
H -0.445557 2.092251 -1.110858
C -1.894702 -0.745561 0.204375
H -2.583402 0.918673 -1.030541
H -2.229388 1.374847 0.620155
H -0.445557 -2.092251 1.110858
H -2.229388 -1.374847 -0.620155
H -2.583402 -0.918673 1.030541

Optimized geometry of syn-5 from the isomer set

26
0 1
C -0.828596 -1.569685 -0.659810
C -2.012346 -0.870890 0.002601
C -1.423341 0.401495 0.622958
H -2.412766 -1.503926 0.796455
H -2.831036 -0.665576 -0.686387
C 0.016095 0.009733 1.022365
C 0.352409 -1.319570 0.290420
H -0.625099 -1.116624 -1.630766
H -1.007802 -2.628751 -0.838397
C 1.722250 -1.114403 -0.388577
H 0.403361 -2.134195 1.011392
C 0.976012 1.045898 0.425190
C 2.235042 0.253536 0.091284
H 2.835096 0.129922 0.993654
H 2.866810 0.747926 -0.646338
H 1.604324 -1.118271 -1.471625
H 2.426025 -1.910137 -0.153736
C -1.256561 1.592659 -0.347062
H -2.019004 0.709096 1.479878
C 0.210205 1.595251 -0.783547
H -1.478160 2.519604 0.182100
H -1.945669 1.539509 -1.189328
H 1.180271 1.857171 1.124761
H 0.351643 0.938737 -1.642180
H 0.559355 2.582335 -1.082253
H 0.145639 -0.090977 2.097845

Optimized geometry of anti-5 from the isomer set

26
0 1
C -1.739886 -1.406032 0.183334
C -0.349187 -2.209511 0.183430
C 0.713438 -1.236653 -0.413680
H -0.434972 -3.135394 -0.379884
H -0.087536 -2.481517 1.205112
C -0.000007 0.000019 -0.105684
C -1.427708 0.000475 -0.413715
H -2.106389 -1.315251 1.204958
H -2.499046 -1.942815 -0.380120
C -1.738936 1.407181 0.183320
H -1.610925 0.000539 -1.490516
C 0.714247 1.236190 -0.413680
H -0.000015 0.000017 1.001360
C -0.347703 2.209773 0.183421
H -0.432877 3.135719 -0.379874
H -0.085897 2.481591 1.205114
H -2.105466 1.316674 1.204956
H -2.497774 1.944446 -0.380109
C 2.087580 -0.803767 0.183314
H 0.804893 -1.395379 -1.490475
C 2.088163 0.802344 0.183309
H 2.932037 -1.192933 -0.380058
H 2.192165 -1.166453 1.204982
H 0.805867 1.394783 -1.490485
H 2.932848 1.190895 -0.380137
H 2.193077 1.164969 1.204967

Optimized geometry of syn-6 from the isomer set

26
0 1
C -0.067902 -1.461487 -0.898087
C 1.006700 -1.127925 0.168689
C 0.239447 -0.272799 1.190842
C -1.387487 -0.829345 -0.406624
H -0.185918 -2.540642 -0.980856
H 0.209344 -1.099286 -1.887760
C 0.358376 1.180446 0.634324
C -1.589114 0.615599 -0.905226
C -0.967635 1.652143 0.039373
H -2.654248 0.826049 -1.001861
H -1.172227 0.711923 -1.908060
H -1.665340 1.857732 0.851069
H -0.825979 2.599562 -0.481651
C 2.137649 -0.229879 -0.311168
H 1.387229 -2.045206 0.615016
C 1.489724 1.149752 -0.420451
H 2.583689 -0.565391 -1.246751
H 2.930640 -0.217797 0.438225
H 0.631200 1.855092 1.444372
H 1.067065 1.283814 -1.416221
H 2.204140 1.957988 -0.278212
C -1.184853 -0.812307 1.110390
H 0.668482 -0.339231 2.188964
H -2.238468 -1.436035 -0.710603
H -1.921944 -0.212014 1.640978
H -1.227105 -1.821749 1.520970

Optimized geometry of anti-6 from the isomer set

26
0 1
C -0.198632 -1.472828 -0.884481
C 0.997104 -1.161263 0.103691
C 0.270225 -0.205472 1.027704
C -1.494594 -0.793670 -0.284479
H -0.372891 -2.548182 -0.912911
H 0.003350 -1.166549 -1.910464
C 0.347118 0.990010 0.049513
C -1.865364 0.680787 -0.668774
C -0.961330 1.755094 0.024197
H -2.915230 0.834661 -0.417769
H -1.775963 0.807804 -1.749322
H -1.330868 2.032606 1.010948
H -0.928642 2.659887 -0.580271
C 2.214287 -0.289070 -0.363884
H 1.342443 -2.082585 0.569931
C 1.855261 1.199253 0.001489
H 2.387008 -0.379621 -1.435902
H 3.123140 -0.620848 0.133878
H 0.269123 0.574604 -0.947932
H 2.180520 1.893886 -0.769864
H 2.299856 1.504954 0.948205
C -1.130991 -0.748093 1.190877
H 0.782355 0.025868 1.962152
H -2.356386 -1.418989 -0.508155
H -1.792697 -0.111749 1.776163
H -1.113622 -1.734236 1.656201

Optimized geometry of 7 from the isomer set

26
0 1
C 0.148668 0.674121 0.255387
C -0.256140 -0.178916 1.479065
C -1.206553 -1.250900 0.891370
H -0.732894 0.437587 2.239047
H 0.614360 -0.636532 1.944680
C -1.273969 -0.862046 -0.589003
H -2.191711 -1.244325 1.353949
H -0.800049 -2.252295 1.020093
C -2.047851 0.472744 -0.689137
C -1.053696 1.536128 -0.118230
H -2.984759 0.434258 -0.136174
H -2.294925 0.696486 -1.725447
H -1.467500 2.082728 0.727415
H -0.784520 2.266061 -0.880988
C 0.142488 -0.361426 -0.873039
H -1.670308 -1.639802 -1.237638
C 1.433762 -1.138772 -0.658815
H 0.182822 0.143342 -1.841642
C 2.420596 -0.072643 -0.098466
H 1.804290 -1.594408 -1.574228
H 1.297828 -1.944416 0.059961
C 1.577805 1.176700 0.288649
H 3.172296 0.191321 -0.839373
H 2.962405 -0.464730 0.759645
H 1.871235 1.587000 1.253844
H 1.710771 1.967784 -0.449834

Optimized geometry of exo-8 from the isomer set

26
0 1
C -0.975684 -1.346480 -0.704005
details C -2.227461 -0.462606 -0.446958
C -1.719016 0.609675 0.536094
H -3.031917 -1.043874 -0.000176
H -2.620244 -0.017533 -1.359764
C 0.118631 -0.615436 0.073909
H -0.729347 -1.436470 -1.761246
H -1.120001 -2.354360 -0.315172
C 0.386172 0.743961 -0.613513
C -0.833327 1.607515 -0.226357
H -0.538739 2.433238 0.422036
H -1.341512 2.035581 -1.088704
C -0.666720 -0.174110 1.320516
H -2.510158 1.077863 1.116891
H -0.086185 0.444513 2.003147
H -1.073124 -1.019766 1.875636
C 1.484498 -1.272579 0.274438
C 2.529005 -0.193927 -0.094977
H 1.598264 -2.156889 -0.350901
H 1.603805 -1.603467 1.305653
C 1.765136 1.134275 -0.095267
H 1.683679 1.526816 0.919596
H 2.251202 1.900755 -0.697072
H 2.916026 -0.386172 -1.095810
H 3.384581 -0.187978 0.577390
H 0.446268 0.606018 -1.694784

Optimized geometry of endo-8 from the isomer set

26
0 1
C 0.428191 -0.970003 1.053794
C 1.889787 -0.466117 1.003919
C 1.921046 0.293733 -0.324585
H 2.591625 -1.298740 0.990758
H 2.150528 0.169424 1.848139
C -0.152332 -0.568918 -0.320257
H -0.132525 -0.544386 1.882611
H 0.382628 -2.052477 1.166013
C -0.389193 0.943618 -0.367816
C 1.010587 1.539000 -0.152549
H 1.233998 2.315132 -0.881721
H 1.141239 1.978472 0.836342
C 1.086655 -0.662531 -1.211336
H 2.922851 0.521856 -0.679668
H 0.910374 -0.289748 -2.219495
H 1.532551 -1.654880 -1.271722
C -1.543888 -1.108050 -0.577971
C -2.453826 -0.136088 0.229858
H -1.676193 -2.144323 -0.271659
H -1.778919 -1.048746 -1.640925
C -1.619705 1.152397 0.499186
H -0.689351 1.162312 -1.396231
H -2.168985 2.056155 0.244369
H -1.354607 1.230539 1.552642
H -2.764601 -0.591484 1.167892
H -3.364547 0.088643 -0.320809

Optimized geometry of 9 from the isomer set

26
0 1
C -0.439125 0.746633 -1.358613
C -0.107302 1.362809 0.022451
C -1.107879 -0.557878 -0.942488
H 0.443985 0.623109 -1.978931
H -1.139696 1.364519 -1.918497
C -1.011957 0.552938 1.002483
C -0.326916 -0.763422 1.354890
C -0.110276 -1.369439 -0.054055
H -0.994397 -1.378285 1.956920
H 0.594105 -0.649207 1.917576
C -2.106722 0.004751 0.077170
H -1.525851 -1.137126 -1.762454
H -1.347615 1.131552 1.859863
H -2.724540 -0.746679 0.566261
H -2.754639 0.765734 -0.355023
C 1.398616 1.311739 0.288676
H -0.407549 2.409639 0.054545
C 2.123001 -0.051271 0.107307
H 1.597133 1.680254 1.296347
H 1.855239 2.038709 -0.383106
C 1.353868 -1.245366 -0.495466
H 2.496195 -0.363508 1.080553
H 3.015893 0.106121 -0.496911
H -0.393321 -2.420382 -0.071127
H 1.889727 -2.146627 -0.196329
H 1.403483 -1.226794 -1.583815

Optimized geometry of 10 from the isomer set

26
0 1
C -1.152947 1.348378 -0.384327
C -0.000000 0.784258 -1.217512
C -0.789559 0.728641 0.974694
C 0.789560 0.728641 0.974693
C 1.425426 -0.665221 0.974262
C -0.000000 -0.789450 -1.129403
C 1.152947 1.348378 -0.384328
H 2.147245 1.063811 -0.720574
H 1.110304 2.436087 -0.374221
H -0.000001 1.118497 -2.253133
C 1.253095 -1.311188 -0.412717
C -1.425425 -0.665221 0.974263
C -1.253095 -1.311188 -0.412716
H -2.147245 1.063811 -0.720573
H -1.110304 2.436087 -0.374221
H 1.162848 1.305327 1.818314
H -1.162847 1.305327 1.818315
H -1.006947 -1.292591 1.757530
H -2.487020 -0.566236 1.201800
H -2.128026 -1.101643 -1.026302
H -1.198486 -2.396218 -0.329723
H 2.487020 -0.566236 1.201798
H 1.006948 -1.292591 1.757530
H 1.198486 -2.396218 -0.329724
H 2.128025 -1.101643 -1.026304
H -0.000001 -1.191745 -2.141974

Optimized geometry of syn-11 from the isomer set

26
0 1
C -1.449671 -0.955706 -0.776645
C -0.787760 0.381892 -1.161491
C -1.449676 -0.955703 0.776643
H -0.966818 -1.828077 -1.202552
H -2.472000 -0.957328 -1.151063
C -0.787766 0.381896 1.161487
H -0.966828 -1.828072 1.202558
H -2.472008 -0.957321 1.151054
C 0.787760 0.381895 1.161490
C 1.449671 -0.955704 0.776647
C 1.449676 -0.955705 -0.776640
H 0.966818 -1.828074 1.202557
H 2.472000 -0.957325 1.151066
C -1.295626 1.243916 -0.000005
H -1.141696 0.726393 2.130877
H -0.954863 2.272510 -0.000006
H -2.385666 1.267735 -0.000008
C 1.295626 1.243916 0.000002
H 1.141686 0.726390 2.130882
C 0.787766 0.381893 -1.161488
H -1.141686 0.726384 -2.130884
H 2.385666 1.267735 0.000005
H 0.954863 2.272510 0.000000
H 1.141696 0.726388 -2.130879
H 0.966828 -1.828075 -1.202553
H 2.472008 -0.957324 -1.151052

Optimized geometry of anti-11 from the isomer set

26
0 1
C -1.899765 -0.779535 0.344867
C -0.634913 -1.166342 -0.445726
C -1.899766 0.779535 0.344867
H -1.913523 -1.200924 1.347775
H -2.781946 -1.157512 -0.168821
C -0.634913 1.166342 -0.445726
H -1.913523 1.200925 1.347774
H -2.781946 1.157512 -0.168822
C 0.634913 1.166342 0.445726
C 0.634913 -1.166342 0.445726
C -0.570568 -0.000000 -1.433247
H -0.737413 2.132097 -0.938686
H 0.298252 -0.000000 -2.081567
H -1.452179 -0.000000 -2.075890
H -0.737413 -2.132097 -0.938686
C 1.899766 0.779535 -0.344867
C 1.899765 -0.779535 -0.344867
H 2.781946 1.157512 0.168822
H 1.913523 1.200925 -1.347774
H 2.781946 -1.157512 0.168821
H 1.913523 -1.200924 -1.347775
C 0.570568 -0.000000 1.433247
H 0.737413 2.132097 0.938686
H 0.737413 -2.132097 0.938686
H -0.298251 -0.000000 2.081567
H 1.452180 -0.000000 2.075890

Optimized geometry of 12 from the isomer set

26
0 1
C 1.580630 -0.760652 -0.998959
C 0.084335 -0.973271 -0.761918
C 2.097405 -0.089211 0.297315
H 1.774134 -0.156819 -1.883901
H 2.076003 -1.716101 -1.160538
C 0.843693 0.199704 1.137769
H 2.670215 0.816172 0.101169
H 2.755899 -0.770010 0.834799
C -0.843693 0.199704 -1.137769
C 0.204467 1.530295 0.737834
C -0.204467 1.530295 -0.737834
H 0.896837 2.348612 0.937084
H -0.670215 1.713805 1.362476
H 0.670215 1.713805 -1.362476
H -0.896837 2.348612 -0.937084
C -0.084335 -0.973271 0.761918
H 1.070704 0.212534 2.203759
H -0.283490 -1.889381 -1.224506
C -1.580630 -0.760652 0.998959
H 0.283490 -1.889381 1.224506
C -2.097405 -0.089211 -0.297315
H -1.774134 -0.156819 1.883901
H -2.076003 -1.716101 1.160538
H -2.670215 0.816172 -0.101169
H -2.755899 -0.770010 -0.834799
H -1.070704 0.212534 -2.203759

Optimized geometry of 13 from the isomer set

26
0 1
C -0.302606 -1.203741 0.107513
C 0.292120 -0.315663 -0.996069
C 0.327567 -0.584690 1.388691
C 1.021910 0.686180 0.874004
H 1.035373 -1.257797 1.869465
H -0.441591 -0.354692 2.124013
C 2.322343 0.271185 0.185662
C 1.812318 -0.493089 -1.063534
H 2.213704 -0.062924 -1.979382
H 2.092388 -1.545536 -1.053813
H 2.952216 -0.340290 0.829084
H 2.902877 1.146304 -0.103128
C 0.129953 1.061362 -0.322087
H 1.143999 1.461421 1.627438
H -0.198094 -0.437666 -1.959308
C -1.833251 -1.090786 0.103244
H -0.009570 -2.245870 -0.010278
C -2.296489 0.296180 -0.358094
H -2.208970 -1.306364 1.104410
H -2.261739 -1.847154 -0.555124
C -1.324647 1.406107 0.042905
H -3.295025 0.510145 0.021266
H -2.381607 0.297097 -1.445021
H -1.399319 1.594838 1.115352
H -1.622650 2.333204 -0.444332
H 0.582701 1.857012 -0.914060

Optimized geometry of 14 from the isomer set

26
0 1
C -0.103393 1.250340 0.266089
C 1.002676 1.242344 -0.831983
C 1.837708 -0.000008 -0.500162
C 0.256406 -0.000009 1.093180
C -0.103412 -1.250342 0.266073
C 1.002644 -1.242331 -0.832013
C 1.782938 -0.000023 1.030492
H 2.230500 -0.886998 1.478069
H 2.230518 0.886935 1.478086
H 2.828855 -0.000016 -0.947181
C -1.555773 1.253972 -0.251745
C -2.318220 0.000016 0.156073
C -1.555800 -1.253961 -0.251735
H -3.309914 0.000024 -0.296433
H -2.473782 0.000022 1.236527
H 0.582842 1.192299 -1.835840
H 1.610668 2.144426 -0.780930
H -2.082311 2.137213 0.107801
H -1.557445 1.324491 -1.341001
H 0.043391 2.125610 0.897011
H -0.174922 -0.000012 2.091303
H -1.557492 -1.324501 -1.340990
H -2.082346 -2.137185 0.107838
H 0.043380 -2.125623 0.896978
H 1.610615 -2.144429 -0.781001
H 0.582796 -1.192241 -1.835862

Optimized geometry of 18 from the isomer set

26
0 1
C 1.669409 0.333662 0.389992
C 1.291907 -0.904216 -0.426814
C 0.423876 0.657126 1.244960
H 1.979842 1.177905 -0.224428
H 2.509367 0.086899 1.039107
C -0.423876 -0.657126 1.244960
C -1.669409 -0.333662 0.389992
C -1.291907 0.904216 -0.426814
H -2.509367 -0.086899 1.039107
H -1.979842 -1.177905 -0.224428
C -0.485485 1.700009 0.598471
H 0.719331 0.959406 2.247120
H 0.065713 2.531387 0.160122
H -1.163991 2.115284 1.345637
C 0.485485 -1.700009 0.598471
H -0.719331 -0.959406 2.247120
H -0.065713 -2.531387 0.160122
H 1.163991 -2.115284 1.345637
C 0.485485 -0.598032 -1.699251
H 2.180280 -1.459840 -0.727232
C -0.485485 0.598032 -1.699251
H -0.063989 -1.502456 -1.964778
H 1.184844 -0.432564 -2.519690
H -1.184844 0.432564 -2.519690
H 0.063989 1.502456 -1.964778
H -2.180280 1.459840 -0.727232

Optimized geometry of 19 from the isomer set

26
0 1
C 0.293529 1.250962 -0.983530
C -0.585447 1.176074 0.288854
C -0.093698 -0.000005 1.147506
C 1.165592 0.000004 -1.096531
H 0.935238 2.131974 -0.953077
H -0.335992 1.355971 -1.867954
C 0.293527 -1.250953 -0.983542
C -0.585447 -1.176076 0.288845
H 0.935234 -2.131967 -0.953098
H -0.335995 -1.355952 -1.867966
C -2.034335 0.774366 -0.020125
H -0.544181 2.121032 0.828336
C -2.034336 -0.774366 -0.020129
H -2.377395 1.194710 -0.963649
H -2.701125 1.151058 0.754049
H -0.544180 -2.121039 0.828318
H -2.377399 -1.194705 -0.963654
H -2.701124 -1.151061 0.754044
C 1.408550 -0.000006 1.394635
H -0.626390 -0.000008 2.100166
C 2.170685 -0.000002 0.053674
H 1.676420 -0.871581 1.991821
H 1.676420 0.871566 1.991826
H 2.816304 -0.874534 -0.024249
H 2.816307 0.874528 -0.024242
H 1.696130 0.000008 -2.048600

Optimized geometry of A from the reaction set

25
1 1
C -1.338535 0.706937 1.158939
C -1.511044 -0.812689 1.036605
C -0.980175 1.201718 -0.348403
H -0.611685 1.022564 1.900285
H -2.266730 1.230963 1.368637
C 0.364901 0.717834 -0.334491
C 1.678714 1.210965 0.081748
C 2.573448 -0.047774 0.070859
H 1.575521 1.644593 1.081952
H 2.013006 2.040952 -0.544234
C -1.121457 -1.081420 -0.422029
H -2.544010 -1.101723 1.207061
H -0.897449 -1.360308 1.745235
C 0.372377 -0.719927 -0.575364
C 1.589899 -1.226368 0.203169
H 0.599088 -0.782787 -1.656305
H 1.987359 -2.155852 -0.189970
H 1.326353 -1.393578 1.246816
H 3.318981 -0.029472 0.858620
H 3.105080 -0.109497 -0.876820
C -1.745222 0.123491 -1.143730
H -1.172199 2.257421 -0.487923
H -1.523534 0.157174 -2.208402
H -2.819459 0.202379 -1.004350
H -1.387754 -2.059424 -0.804412

Optimized geometry of TS-AA' from the reaction set

25
1 1
C -1.598249 0.772552 1.020485
C -1.598249 -0.772552 1.020485
C -1.038881 1.140944 -0.391450
H -1.009580 1.201640 1.826598
H -2.603226 1.174352 1.105574
C 0.386484 0.697959 -0.296827
C 1.700365 1.231461 0.167117
C 2.626610 0.000000 0.049923
H 1.563384 1.533290 1.208497
H 2.045715 2.105490 -0.376467
C -1.038881 -1.140944 -0.391449
H -2.603226 -1.174352 1.105574
H -1.009580 -1.201640 1.826598
C 0.386484 -0.697959 -0.296827
C 1.700365 -1.231461 0.167117
H 0.644039 0.000000 -1.390413
H 2.045715 -2.105490 -0.376467
H 1.563384 -1.533290 1.208497
H 3.413160 0.000000 0.796080
H 3.108223 0.000000 -0.926956
C -1.641383 -0.000000 -1.232304
H -1.217268 2.159483 -0.711167
H -1.304929 -0.000000 -2.268685
H -2.726543 -0.000000 -1.213720
H -1.217268 -2.159483 -0.711167

Optimized geometry of A' from the reaction set

25
1 1
C 1.511039 -0.812695 1.036603
C 1.338533 0.706932 1.158942
C 1.121458 -1.081418 -0.422033
H 0.897441 -1.360316 1.745228
H 2.544003 -1.101732 1.207062
C -0.372377 -0.719925 -0.575370
C -1.589896 -1.226369 0.203164
C -2.573447 -0.047775 0.070865
H -1.326345 -1.393587 1.246808
H -1.987358 -2.155851 -0.189978
C 0.980176 1.201719 -0.348395
H 2.266730 1.230953 1.368643
H 0.611686 1.022558 1.900292
C -0.364901 0.717835 -0.334493
C -1.678715 1.210966 0.081745
H -0.599085 -0.782785 -1.656312
H -2.013009 2.040944 -0.544247
H -1.575523 1.644607 1.081943
H -3.318969 -0.029475 0.858637
H -3.105093 -0.109498 -0.876805
C 1.745224 0.123498 -1.143727
H 1.387755 -2.059420 -0.804422
H 1.523539 0.157186 -2.208399
H 2.819461 0.202384 -1.004344
H 1.172198 2.257423 -0.487911

Optimized geometry of F from the reaction set

25
1 1
C 1.960363 0.007929 -0.589094
C 1.610613 0.378724 1.105373
C 0.387849 -0.473322 1.359351
H 1.537044 1.411104 1.447214
C -0.149780 -0.698384 -0.065234
H -0.323257 0.028430 2.006885
C -0.256888 0.712220 -0.667856
C 1.158415 1.148224 -0.579883
H 1.539872 2.157567 -0.632168
C 1.092602 -1.226882 -0.782452
H 3.024347 0.037118 -0.768092
H 1.533254 -2.124506 -0.358921
H 0.653435 -1.422132 1.817398
H 2.580756 0.032349 1.450505
H 0.927807 -1.383982 -1.848988
C -1.572749 -1.202122 -0.146766
C -2.422917 0.073331 0.136483
H -1.783406 -2.001566 0.558332
H -1.779298 -1.587079 -1.143596
C -1.499876 1.318452 -0.041532
H -2.834948 0.051504 1.141123
H -3.269417 0.120299 -0.541579
H -0.418672 0.587070 -1.747274
H -1.280500 1.784524 0.916717
H -1.952803 2.080275 -0.667900

Optimized geometry of TS-FG from the reaction set

25
1 1
C 1.910296 0.390359 -0.413090
C 1.899468 -0.288199 1.021793
C 0.525693 -0.975814 1.074456
H 2.067919 0.421108 1.827928
C -0.122475 -0.596479 -0.287601
H -0.071889 -0.658994 1.924752
C -0.332109 0.901387 -0.169733
C 0.944174 1.472972 -0.162063
C 1.093171 -0.652324 -1.210759
H 2.890642 0.679839 -0.768246
H 1.592256 -1.615879 -1.237320
H 0.622266 -2.056946 1.125608
H 2.726939 -0.991381 1.035123
H 0.881260 -0.329188 -2.230115
C -1.519081 -1.116503 -0.560429
C -2.420615 -0.181065 0.275737
H -1.650554 -2.160586 -0.290953
H -1.749139 -1.021007 -1.621756
C -1.725193 1.209403 0.319467
H -2.519154 -0.567254 1.286995
H -3.423188 -0.111567 -0.133514
H -0.138838 1.346144 -1.264909
H -1.710085 1.638114 1.318250
H -2.218015 1.931469 -0.326581
H 1.179596 2.513702 0.028064

Optimized geometry of G from the reaction set

25
1 1
C 1.930752 0.269252 -0.373962
C 1.915118 -0.403185 1.003573
C 0.446974 -0.808380 1.144326
H 2.240360 0.261830 1.798446
C -0.188657 -0.557996 -0.364960
H -0.081542 -0.307417 1.951475
C -0.306576 0.827207 -0.077295
C 0.989816 1.490339 -0.254297
H 1.236111 2.240264 0.494333
C 1.077642 -0.699841 -1.208742
H 2.913597 0.505050 -0.763704
H 1.471995 -1.711560 -1.224475
H 0.272623 -1.874597 1.263626
H 2.562803 -1.275025 1.012512
H 0.914584 -0.367244 -2.232440
C -1.589319 -1.106934 -0.545250
C -2.447352 -0.130336 0.287797
H -1.694103 -2.140042 -0.227519
H -1.858356 -1.059635 -1.600118
C -1.683982 1.210968 0.232983
H -2.515735 -0.467215 1.319851
H -3.461291 -0.038848 -0.086234
H -1.795348 1.874344 1.088533
H -1.995403 1.804523 -0.639068
H 0.923208 2.008998 -1.220263

Optimized geometry of TS-GG' from the reaction set

25
1 1
C -0.330798 -1.967109 -0.000000
C -1.728087 -1.339492 0.000000
C -1.390867 0.139320 0.000000
H -2.299484 -1.617942 0.880539
C 0.355214 0.119508 -0.693451
H -1.694370 0.708979 0.872186
C 0.355214 0.119508 0.693451
C 0.355214 -1.289952 1.201354
H -0.156155 -1.433106 2.148960
C 0.355214 -1.289952 -1.201354
H -0.308564 -3.049987 -0.000000
H -0.156155 -1.433106 -2.148960
H -1.694370 0.708979 -0.872186
H -2.299484 -1.617942 -0.880539
H 1.392232 -1.609875 -1.317650
C 0.763519 1.452232 -1.229718
C 0.633307 2.378559 0.000000
H 0.197972 1.781449 -2.097239
H 1.803703 1.356136 -1.548061
C 0.763519 1.452232 1.229718
H -0.342635 2.859439 0.000000
H 1.374695 3.170136 -0.000000
H 0.197972 1.781449 2.097239
H 1.803703 1.356136 1.548061
H 1.392232 -1.609875 1.317650

Optimized geometry of G' from the reaction set

25
1 1
C -1.930752 0.269252 -0.373962
C -0.989816 1.490339 -0.254296
C 0.306576 0.827207 -0.077295
H -1.236111 2.240264 0.494334
C 0.188657 -0.557996 -0.364960
C -0.446974 -0.808380 1.144326
C -1.915118 -0.403185 1.003573
H -2.240360 0.261829 1.798446
C -1.077642 -0.699840 -1.208742
H -2.913597 0.505050 -0.763704
H -0.914584 -0.367243 -2.232440
H -0.923208 2.008999 -1.220262
H -1.471995 -1.711559 -1.224476
H -2.562803 -1.275025 1.012511
H 0.081542 -0.307417 1.951475
H -0.272623 -1.874598 1.263626
C 1.683983 1.210968 0.232983
C 2.447352 -0.130337 0.287798
H 1.795349 1.874345 1.088532
H 1.995403 1.804522 -0.639069
C 1.589319 -1.106933 -0.545250
H 2.515734 -0.467216 1.319852
H 3.461291 -0.038849 -0.086232
H 1.694103 -2.140042 -0.227520
H 1.858357 -1.059634 -1.600118

Optimized geometry of J from the reaction set

25
1 1
C 1.865536 -0.015113 -0.489552
C 1.118851 1.321597 -0.611151
C -0.086320 1.135908 0.310960
H 0.812372 1.527371 -1.633330
C 0.318038 -0.346990 1.143637
C -0.196191 -0.989581 0.008426
C 0.877097 -1.078457 -1.005648
H 0.526402 -0.960225 -2.027811
C 1.828575 -0.292076 1.015207
H 2.841870 -0.045758 -0.958373
H 2.277261 0.493763 1.615943
H 1.745166 2.144584 -0.277719
H 2.282598 -1.243664 1.287406
H 1.321454 -2.077590 -0.916103
H -0.195461 -0.375588 2.093293
C -1.499140 1.233888 -0.263751
H -0.008226 1.736045 1.213473
C -2.360494 0.064420 0.203604
H -1.451886 1.232169 -1.352428
H -1.944236 2.181416 0.031188
C -1.629120 -1.238203 -0.199080
H -3.351870 0.089124 -0.238839
H -2.491978 0.095389 1.283592
H -1.827952 -1.506444 -1.233252
H -1.956511 -2.062955 0.437047

Optimized geometry of TS-JK from the reaction set

25
1 1
C -1.826432 -0.080200 -0.470828
C -0.797928 -1.093743 -1.024778
C 0.270100 -1.238645 0.111573
H -0.358886 -0.756356 -1.963360
C -0.219854 -0.138810 1.094149
C 0.017475 1.074608 0.218684
C -1.236132 1.353758 -0.564856
H -1.031525 1.699239 -1.574267
C -1.735137 -0.310229 1.040102
H -2.812340 -0.146465 -0.917216
H -2.040971 -1.305631 1.349800
H -1.273157 -2.048760 -1.227520
H -2.285311 0.424164 1.623325
H -1.902314 2.055890 -0.069516
H 0.266962 -0.138872 2.063274
C 1.748303 -1.071563 -0.271766
H 0.139723 -2.198464 0.603760
C 2.331942 0.310058 0.181966
H 1.883645 -1.175730 -1.345913
H 2.358212 -1.839731 0.195380
C 1.309459 1.288374 -0.233654
H 3.300577 0.517094 -0.259386
H 2.453963 0.296623 1.263106
H 1.490464 2.034825 -0.999585
H 0.640179 2.020514 0.774564

Optimized geometry of K from the reaction set

25
1 1
C 1.515334 0.039313 0.802042
C 0.575364 -1.137809 1.066693
C -0.181321 -1.304009 -0.283035
H -0.089309 -0.966154 1.911624
C 0.494064 -0.252942 -1.185204
C -0.009133 1.127057 -0.816979
C 0.708904 1.333469 0.761049
H 0.061238 1.448881 1.627890
C 1.929258 -0.207443 -0.648702
H 2.321813 0.144796 1.524448
H 2.456210 -1.148522 -0.780759
H 1.154096 -2.027427 1.297108
H 2.528798 0.592860 -1.078234
H 1.265994 2.253638 0.630446
H 0.389380 -0.440503 -2.250179
C -1.689696 -1.121559 -0.188288
H 0.019207 -2.288388 -0.697135
C -2.073039 0.255796 0.346324
H -2.124569 -1.889315 0.446917
H -2.128239 -1.254490 -1.176770
C -1.187846 1.337435 -0.116212
H -2.145339 0.290425 1.435760
H -3.074501 0.553624 0.018308
H -1.500526 2.360264 0.063709
H 0.374404 1.954453 -1.399264

Optimized geometry of TS-KL from the reaction set

25
1 1
C -1.385648 0.077454 -0.861832
C -0.500265 -1.145990 -1.101255
C 0.231562 -1.351845 0.253034
H 0.184956 -1.024822 -1.936256
C -0.503873 -0.393129 1.215239
C 0.025816 0.973681 1.131033
C -0.581589 1.364277 -0.828706
H -0.039381 1.565877 -1.748242
C -1.901354 -0.191681 0.547384
H -2.176060 0.196487 -1.601468
H -2.482519 -1.107471 0.616151
H -1.130876 -2.000584 -1.330072
H -2.482159 0.620602 0.978573
H -1.165477 2.238884 -0.562959
H -0.582219 -0.723133 2.249402
C 1.718267 -1.028656 0.174679
H 0.099452 -2.370870 0.604362
C 1.942065 0.373611 -0.383577
H 2.230492 -1.759714 -0.445714
H 2.158016 -1.102865 1.169769
C 0.914160 1.355271 0.135801
H 1.951407 0.381866 -1.471022
H 2.914954 0.754667 -0.077447
H 1.207561 2.397708 0.119556
H -0.442996 1.735401 1.744571

Optimized geometry of L from the reaction set

25
1 1
C -1.370027 0.017853 -0.839035
C -0.497278 -1.197955 -1.133991
C 0.426073 -1.391449 0.090374
H 0.072703 -1.084897 -2.052780
C -0.239943 -0.694452 1.268089
C -0.082545 0.685607 1.353293
C -0.624950 1.339114 -0.941080
C -1.745105 -0.131274 0.615659
H -2.266139 0.039522 -1.457167
H -2.319698 -1.008960 0.901339
H -1.129426 -2.075223 -1.255596
H -2.243803 0.729618 1.057936
H -0.441376 -1.246444 2.175463
C 1.823637 -0.784383 -0.081243
H 0.526473 -2.448977 0.315492
C 1.795505 0.738129 -0.264041
H 2.313734 -1.259900 -0.927087
H 2.414855 -1.040347 0.796822
C 0.463522 1.403377 0.177028
H 1.956886 1.010395 -1.303880
H 2.610306 1.187847 0.296929
H -0.349837 1.205777 2.264250
H 0.639612 2.445526 0.424900
H -1.323993 2.161345 -0.796819
H -0.153635 1.477308 -1.910118

Optimized geometry of TS-LM from the reaction set

25
1 1
C -1.414997 0.370624 -0.789797
C -0.780765 -0.960643 -1.176176
C 0.100828 -1.346667 0.030814
H -0.195442 -0.908033 -2.091944
C -0.642701 -0.506191 1.272915
C 0.469343 0.447245 1.381723
C -0.354331 1.484930 -0.738910
C -1.893889 0.064798 0.624461
H -2.216054 0.664928 -1.461264
H -2.679581 -0.686275 0.605108
H -1.560835 -1.701691 -1.333757
H -2.276222 0.926292 1.167968
H -0.806925 -1.091391 2.169255
C 1.603381 -1.043879 -0.256436
H 0.030209 -2.401306 0.278708
C 2.026781 0.501015 -0.346839
H 1.855402 -1.533204 -1.192730
H 2.221413 -1.496216 0.515954
C 0.770210 1.092790 0.194750
H 2.251418 0.847307 -1.349747
H 2.901231 0.652843 0.279791
H -0.807473 2.415508 -0.400999
H 0.059866 1.678986 -1.724490
H 0.610619 1.815761 1.342292
H 1.309213 0.192364 2.016811

Optimized geometry of TS-LN from the reaction set

25
1 1
C 1.524710 -0.358879 -0.536944
C 1.273752 1.135428 -0.670582
C 0.085865 1.381432 0.274510
H 1.069411 1.456018 -1.688868
C 0.174178 0.207327 1.322712
C -0.896059 -0.798104 1.011287
C 0.399699 -1.186862 -1.178548
C 1.492767 -0.519927 0.980435
H 2.473042 -0.662463 -0.971840
H 2.331038 -0.007421 1.444765
H 2.147604 1.685413 -0.327976
H 1.509266 -1.553664 1.323713
H 0.107687 0.544187 2.351520
C -1.271264 1.334703 -0.457480
H 0.181593 2.334742 0.783249
C -1.856632 -0.039462 -0.265472
H -1.148289 1.526674 -1.520387
H -1.965311 2.080114 -0.076960
C -0.907743 -1.236253 -0.391623
H -2.883231 -0.270901 -0.531419
H -1.465440 -2.146523 -0.566678
H 0.730645 -2.220910 -1.257531
H 0.206587 -0.853260 -2.196795
H -1.358091 -1.411225 1.776880
H -2.052147 -0.017200 0.928564

Optimized geometry of TS-MN from the reaction set

25
1 1
C -1.399180 0.063591 -0.759697
C -0.326922 -0.885651 -1.333509
C 0.581383 -1.283531 -0.116021
H 0.223537 -0.480173 -2.181151
C -0.263119 -0.839409 1.109578
C 0.215880 0.573230 1.547731
C -0.879869 1.539502 -0.527280
C -1.680980 -0.642495 0.566238
H -2.270901 0.132475 -1.404415
H -2.168172 -1.596222 0.374867
H -0.833689 -1.770836 -1.707666
H -2.315630 -0.079870 1.246803
H -0.192312 -1.527760 1.946384
C 1.968166 -0.538307 -0.143646
H 0.775975 -2.351152 -0.104040
C 1.458131 0.806015 -0.516352
H 2.646215 -0.922659 -0.898464
H 2.461581 -0.603308 0.821135
C 0.376511 1.251946 0.230632
H 1.443663 1.989573 0.241536
H -0.528425 1.057944 2.170541
H -1.602491 2.118821 0.038411
H -0.695821 2.019937 -1.485151
H 1.148328 0.528373 2.101885
H 1.608138 1.215509 -1.506733

Optimized geometry of M from the reaction set

25
1 1
C 1.415375 0.075739 -0.802649
C 0.507041 1.296517 -0.953816
C -0.345625 1.304313 0.347071
H -0.100290 1.280203 -1.855874
C 0.395386 0.307916 1.285817
C -0.293641 -1.167834 1.250846
C 0.628633 -1.297496 -1.050404
C 1.775141 0.154874 0.670859
H 2.255771 0.065160 -1.489420
H 2.362003 1.055970 0.848054
H 1.128399 2.186162 -1.010879
H 2.340561 -0.690276 1.054142
H 0.367512 0.595006 2.332317
C -1.780732 0.859517 0.085269
H -0.351674 2.290022 0.803267
C -1.756064 -0.539607 -0.625930
H -2.308056 1.562753 -0.552866
H -2.337266 0.785416 1.015985
C -0.516602 -1.166671 -0.165322
H -1.790871 -0.452287 -1.705908
H -2.615588 -1.121510 -0.290452
H 0.433410 -1.880653 1.619106
H 1.293746 -2.109696 -0.770932
H 0.346228 -1.365289 -2.096098
H -1.197357 -1.164581 1.849106

Optimized geometry of N from the reaction set

25
1 1
C 1.298399 -0.132144 -0.908099
C 0.916031 1.331535 -0.703807
C 0.066487 1.282215 0.583564
H 0.387754 1.778368 -1.545277
C 0.528554 -0.024200 1.314403
C -0.531977 -1.124404 1.207319
C 0.110674 -0.988865 -1.343089
C 1.743282 -0.491843 0.504594
H 2.077803 -0.264897 -1.656610
H 2.638994 0.069186 0.760303
H 1.817880 1.916844 -0.546417
H 1.961753 -1.547178 0.652307
H 0.761244 0.161363 2.357866
C -1.422781 1.262325 0.174312
H 0.218760 2.158633 1.203902
C -1.729279 0.053644 -0.567436
H -1.729224 2.168452 -0.339337
H -2.059337 1.171169 1.072593
C -1.092577 -1.148769 -0.202841
H -2.408962 0.068641 -1.413784
H -0.097332 -2.087988 1.457499
H 0.385685 -2.034995 -1.458085
H -0.287710 -0.667678 -2.304648
H -1.357038 -0.962755 1.901509
H -1.631148 -2.044131 -0.495337

Table S1: Total energies (in Hartee) of various molecules in the isomer set obtained with CBS-QB3 and L-W1X composite methods

Molecule	**CBS-QB3**	**L-W1X**
1	-390.14386	-390.76306
exo-2	-390.11972	-390.73909
endo-2	-390.11318	-390.73256
3	-390.12687	-390.74625
4	-390.12067	-390.73971
syn-5	-390.12223	-390.74225
anti-5	-390.05023	-390.66950
syn-6	-390.12096	-390.74066
anti-6	-390.06243	-390.68081
7	-390.10856	-390.72731
exo-8	-390.11639	-390.73537
endo-8	-390.10605	-390.72471
9	-390.10324	-390.72243
10	-390.11069	-390.72976
syn-11	-390.09825	-390.71742
anti-11	-390.11339	-390.73237
12	-390.12466	-390.74402
13	-390.11586	-390.73513
14	-390.11343	-390.73280
18	-390.12121	-390.74084
19	-390.12268	-390.74212

Table S2: Total energies (in Hartee) of various molecules in the reaction set obtained with CBS-QB3 and L-W1X composite methods

Molecule	**CBS-QB3**	**L-W1X**
A	-389.21701	-389.83715
TS-AA'	-389.20412	-389.82468
A'	-389.21701	-389.83715
F	-389.19984	-389.81933
TS-FG	-389.18939	-389.80906
G	-389.22250	-389.84220
TS-GG'	-389.22356	-389.84321
G'	-389.22250	-389.84219
J	-389.22610	-389.84589
TS-JK	-389.18723	-389.80747
K	-389.21242	-389.83239
TS-KL	-389.21071	-389.83067
L	-389.21556	-389.83563
TS-LM	-389.13873	-389.75909
TS-LN	-389.20098	-389.82168
TS-MN	-389.17492	-389.79490
M	-389.22482	-389.84484
N	-389.20585	-389.82570

Table S3: Total energies (in Hartee) of various molecules in the isomer set for HWE-1(2,2)/STO-3G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
1	-383.51257	-383.51209	-383.51288	-383.51214	-383.51289	-383.51297	-383.51278	-383.51273	-383.51204	-383.51261	-383.51262
exo-2	-383.48266	-383.48272	-383.48274	-383.48280	-383.48286	-383.48277	-383.48247	-383.48210	-383.48263	-383.48276	-383.48276
endo-2	-383.47542	-383.47583	-383.47562	-383.47521	-383.47454	-383.47548	-383.47472	-383.47529	-383.47598	-383.47558	-383.47594
3	-383.49189	-383.49210	-383.49259	-383.49256	-383.49231	-383.49271	-383.49260	-383.49248	-383.49224	-383.49234	-383.48696
4	-383.48302	-383.47774	-383.48274	-383.48377	-383.48360	-383.48364	-383.48363	-383.48422	-383.48359	-383.48360	-383.48370
syn-5	-383.49291	-383.49343	-383.49336	-383.49308	-383.49298	-383.49333	-383.49304	-383.49052	-383.49264	-383.49343	-383.49328
anti-5	-383.39367	-383.39321	-383.39371	-383.39340	-383.39396	-383.39369	-383.39381	-383.39371	-383.39398	-383.39358	-383.39365
syn-6	-383.48658	-383.48761	-383.48755	-383.48698	-383.48788	-383.47885	-383.48721	-383.48705	-383.48779	-383.48704	-383.48780
anti-6	-383.40168	-383.40164	-383.40194	-383.40137	-383.40160	-383.40124	-383.40209	-383.40137	-383.40171	-383.40182	-383.40201
7	-383.46812	-383.46837	-383.46855	-383.46797	-383.46705	-383.46608	-383.46870	-383.46864	-383.46857	-383.46832	-383.46898
exo-8	-383.47957	-383.47941	-383.47938	-383.47901	-383.47953	-383.47986	-383.47990	-383.47966	-383.47955	-383.47961	-383.47976
endo-8	-383.46392	-383.46416	-383.46397	-383.46426	-383.46393	-383.46292	-383.46411	-383.46386	-383.46453	-383.46331	-383.46418
9	-383.46068	-383.45957	-383.46074	-383.46148	-383.46053	-383.46025	-383.46114	-383.46114	-383.46080	-383.46066	-383.46046
10	-383.47052	-383.47051	-383.47043	-383.47081	-383.47060	-383.47044	-383.47068	-383.46949	-383.47108	-383.47066	-383.47052
syn-11	-383.45422	-383.45368	-383.45450	-383.45433	-383.45437	-383.45413	-383.45429	-383.45446	-383.45388	-383.45420	-383.45435
anti-11	-383.47029	-383.47090	-383.46493	-383.47082	-383.47095	-383.47114	-383.47084	-383.47060	-383.47120	-383.47073	-383.47074
12	-383.48978	-383.49045	-383.48998	-383.48949	-383.49032	-383.48823	-383.48989	-383.49029	-383.48899	-383.48948	-383.49068
13	-383.47910	-383.47904	-383.47888	-383.47901	-383.47917	-383.47907	-383.47922	-383.47931	-383.47930	-383.47900	-383.47895
14	-383.47795	-383.47839	-383.47803	-383.47782	-383.47567	-383.47839	-383.47829	-383.47853	-383.47807	-383.47838	-383.47798
18	-383.48741	-383.48720	-383.48788	-383.48697	-383.48737	-383.48732	-383.48730	-383.48775	-383.48728	-383.48762	-383.48738
19	-383.49121	-383.49130	-383.49123	-383.49120	-383.49124	-383.49049	-383.49103	-383.49135	-383.49147	-383.49135	-383.49145

Table S4: Total energies (in Hartee) of various molecules in the isomer set for HWE-2(2,2)/STO-3G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
1	-383.51248	-383.51305	-383.51034	-383.51299	-383.51197	-383.51291	-383.51306	-383.51290	-383.51343	-383.51170	-383.51245
exo-2	-383.48186	-383.48125	-383.48251	-383.48240	-383.48162	-383.48263	-383.48245	-383.48256	-383.48206	-383.48218	-383.47893
endo-2	-383.47460	-383.47249	-383.47580	-383.47468	-383.47502	-383.47474	-383.47550	-383.47453	-383.47448	-383.47528	-383.47343
3	-383.49205	-383.49242	-383.49252	-383.49185	-383.49250	-383.49247	-383.49264	-383.49277	-383.49260	-383.49248	-383.48824
4	-383.48335	-383.48305	-383.48370	-383.48386	-383.48398	-383.48408	-383.48386	-383.47959	-383.48410	-383.48389	-383.48336
syn-5	-383.49268	-383.49125	-383.49343	-383.49258	-383.49332	-383.49080	-383.49303	-383.49315	-383.49317	-383.49261	-383.49346
anti-5	-383.39277	-383.39395	-383.38929	-383.39258	-383.39383	-383.39359	-383.39208	-383.39093	-383.39399	-383.39388	-383.39358
syn-6	-383.48680	-383.48205	-383.48741	-383.48694	-383.48746	-383.48771	-383.48729	-383.48741	-383.48750	-383.48668	-383.48756
anti-6	-383.40107	-383.40111	-383.40231	-383.40147	-383.39978	-383.40203	-383.40130	-383.40124	-383.40084	-383.40206	-383.39855
7	-383.46810	-383.46834	-383.46818	-383.46825	-383.46853	-383.46693	-383.46788	-383.46766	-383.46725	-383.46905	-383.46895
exo-8	-383.47958	-383.47949	-383.47959	-383.47965	-383.47926	-383.47978	-383.47973	-383.47975	-383.47923	-383.47964	-383.47969
endo-8	-383.46356	-383.46403	-383.46397	-383.46237	-383.46132	-383.46284	-383.46397	-383.46492	-383.46429	-383.46392	-383.46401
9	-383.46018	-383.46102	-383.45850	-383.46006	-383.45982	-383.45984	-383.46038	-383.46030	-383.46078	-383.46084	-383.46025
10	-383.47018	-383.47081	-383.47085	-383.46736	-383.46982	-383.47082	-383.47087	-383.47027	-383.47021	-383.47003	-383.47075
syn-11	-383.45259	-383.44682	-383.45398	-383.45436	-383.45343	-383.45179	-383.45161	-383.45446	-383.45341	-383.45427	-383.45175
anti-11	-383.47048	-383.47078	-383.47100	-383.47080	-383.47085	-383.47069	-383.47130	-383.46853	-383.47009	-383.47095	-383.46981
12	-383.48972	-383.49016	-383.48958	-383.48962	-383.48695	-383.49017	-383.49097	-383.49047	-383.48939	-383.49061	-383.48930
13	-383.47825	-383.47854	-383.47963	-383.47769	-383.47588	-383.47893	-383.47940	-383.47528	-383.47874	-383.47913	-383.47930
14	-383.47758	-383.47811	-383.47704	-383.47791	-383.47734	-383.47828	-383.47809	-383.47498	-383.47798	-383.47813	-383.47796
18	-383.48669	-383.48668	-383.48732	-383.48528	-383.48762	-383.48707	-383.48508	-383.48601	-383.48808	-383.48693	-383.48681
19	-383.48998	-383.49140	-383.49135	-383.49081	-383.49102	-383.48334	-383.48861	-383.49089	-383.49015	-383.49105	-383.49122

Table S5: Total energies (in Hartee) of various molecules in the isomer set for ESU2-RY(2,2)/STO-3G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
1	-383.51271	-383.51226	-383.51282	-383.51241	-383.51305	-383.51270	-383.51160	-383.51251	-383.51261	-383.51391	-383.51322
exo-2	-383.48254	-383.48257	-383.48050	-383.48279	-383.48283	-383.48271	-383.48285	-383.48285	-383.48282	-383.48264	-383.48282
endo-2	-383.47530	-383.47547	-383.47474	-383.47588	-383.47606	-383.47552	-383.47526	-383.47518	-383.47561	-383.47480	-383.47445
3	-383.49251	-383.49180	-383.49189	-383.49278	-383.49271	-383.49277	-383.49275	-383.49252	-383.49274	-383.49266	-383.49246
4	-383.48379	-383.48418	-383.48378	-383.48403	-383.48395	-383.48387	-383.48329	-383.48343	-383.48412	-383.48275	-383.48450
syn-5	-383.49199	-383.49343	-383.49358	-383.49351	-383.49331	-383.49009	-383.49327	-383.49349	-383.49131	-383.48449	-383.49338
anti-5	-383.39366	-383.39400	-383.39346	-383.39346	-383.39356	-383.39351	-383.39307	-383.39396	-383.39370	-383.39397	-383.39391
syn-6	-383.48743	-383.48778	-383.48774	-383.48787	-383.48473	-383.48764	-383.48767	-383.48764	-383.48786	-383.48774	-383.48759
anti-6	-383.40179	-383.40149	-383.40238	-383.40186	-383.40154	-383.40166	-383.40216	-383.40149	-383.40164	-383.40210	-383.40159
7	-383.46815	-383.46867	-383.46909	-383.46811	-383.46709	-383.46855	-383.46792	-383.46726	-383.46807	-383.46870	-383.46799
exo-8	-383.47968	-383.48001	-383.47994	-383.47844	-383.47970	-383.47972	-383.47982	-383.47976	-383.47983	-383.47977	-383.47983
endo-8	-383.46364	-383.46359	-383.46056	-383.46464	-383.46415	-383.46432	-383.46357	-383.46337	-383.46422	-383.46432	-383.46370
9	-383.46094	-383.46040	-383.46034	-383.46122	-383.46096	-383.46102	-383.46109	-383.46109	-383.46109	-383.46121	-383.46097
10	-383.47069	-383.47029	-383.47065	-383.47050	-383.47093	-383.47087	-383.47082	-383.47098	-383.47055	-383.47078	-383.47051
syn-11	-383.45399	-383.45456	-383.45389	-383.45418	-383.45411	-383.45404	-383.45430	-383.45447	-383.45473	-383.45433	-383.45128
anti-11	-383.46984	-383.47083	-383.46506	-383.47114	-383.46698	-383.47099	-383.47002	-383.47101	-383.47068	-383.47096	-383.47075
12	-383.49068	-383.49023	-383.49049	-383.49108	-383.49046	-383.49083	-383.49120	-383.49030	-383.49050	-383.49101	-383.49068
13	-383.47835	-383.47935	-383.47865	-383.47822	-383.47933	-383.47826	-383.47925	-383.47601	-383.47626	-383.47869	-383.47947
14	-383.47838	-383.47855	-383.47834	-383.47833	-383.47823	-383.47841	-383.47831	-383.47842	-383.47846	-383.47850	-383.47821
18	-383.48768	-383.48773	-383.48806	-383.48736	-383.48779	-383.48753	-383.48802	-383.48763	-383.48798	-383.48688	-383.48779
19	-383.49102	-383.49026	-383.49129	-383.49081	-383.49129	-383.49106	-383.49105	-383.49146	-383.49133	-383.49035	-383.49132

Table S6: Total energies (in Hartee) of various molecules in the isomer set for ESU2-RYRZ(2,2)/STO-3G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
1	-383.51272	-383.51307	-383.51325	-383.51236	-383.51266	-383.51268	-383.51277	-383.51225	-383.51315	-383.51249	-383.51254
exo-2	-383.48252	-383.48290	-383.48229	-383.48276	-383.48256	-383.48277	-383.48232	-383.48288	-383.48156	-383.48276	-383.48242
endo-2	-383.47518	-383.47547	-383.47567	-383.47570	-383.47514	-383.47604	-383.47521	-383.47611	-383.47615	-383.47274	-383.47361
3	-383.49210	-383.49237	-383.49229	-383.49242	-383.49205	-383.49230	-383.49254	-383.49198	-383.49218	-383.49037	-383.49250
4	-383.48319	-383.48359	-383.48406	-383.48078	-383.48391	-383.48367	-383.48248	-383.48352	-383.48364	-383.48254	-383.48370
syn-5	-383.49292	-383.49326	-383.49344	-383.48930	-383.49355	-383.49337	-383.49357	-383.49352	-383.49306	-383.49322	-383.49294
anti-5	-383.39358	-383.39367	-383.39265	-383.39376	-383.39358	-383.39346	-383.39409	-383.39350	-383.39407	-383.39394	-383.39305
syn-6	-383.48730	-383.48788	-383.48759	-383.48539	-383.48791	-383.48800	-383.48731	-383.48786	-383.48546	-383.48772	-383.48787
anti-6	-383.40167	-383.40105	-383.40138	-383.40175	-383.40208	-383.40142	-383.40105	-383.40177	-383.40226	-383.40212	-383.40185
7	-383.46767	-383.46721	-383.46785	-383.46742	-383.46828	-383.46791	-383.46835	-383.46685	-383.46866	-383.46680	-383.46736
exo-8	-383.47931	-383.47859	-383.47888	-383.47952	-383.47931	-383.47946	-383.47907	-383.47971	-383.47928	-383.47967	-383.47960
endo-8	-383.46358	-383.46434	-383.46293	-383.46369	-383.46405	-383.46423	-383.46460	-383.46387	-383.46324	-383.46320	-383.46171
9	-383.46089	-383.46053	-383.46100	-383.46121	-383.46089	-383.46126	-383.46132	-383.46022	-383.46081	-383.46090	-383.46075
10	-383.47053	-383.47002	-383.47075	-383.47098	-383.47000	-383.47073	-383.46975	-383.47053	-383.47086	-383.47099	-383.47072
syn-11	-383.45419	-383.45441	-383.45417	-383.45398	-383.45409	-383.45450	-383.45450	-383.45435	-383.45438	-383.45356	-383.45393
anti-11	-383.47037	-383.47081	-383.47099	-383.47050	-383.47095	-383.47070	-383.46687	-383.47079	-383.47078	-383.47063	-383.47073
12	-383.48983	-383.48999	-383.49116	-383.48723	-383.49045	-383.49047	-383.49098	-383.48995	-383.48875	-383.49078	-383.48849
13	-383.47905	-383.47904	-383.47923	-383.47926	-383.47933	-383.47897	-383.47921	-383.47901	-383.47910	-383.47916	-383.47818
14	-383.47815	-383.47796	-383.47847	-383.47678	-383.47840	-383.47830	-383.47846	-383.47821	-383.47796	-383.47846	-383.47846
18	-383.48706	-383.48572	-383.48778	-383.48736	-383.48530	-383.48786	-383.48751	-383.48695	-383.48705	-383.48710	-383.48799
19	-383.48987	-383.49130	-383.48577	-383.49145	-383.49067	-383.49120	-383.48797	-383.49126	-383.49043	-383.48791	-383.49071

Table S7: Total energies (in Hartee) of various molecules in the isomer set for EXCT. PRESERV.(2,2)/STO-3G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
1	-383.51279	-383.51247	-383.51252	-383.51183	-383.51320	-383.51315	-383.51326	-383.51293	-383.51298	-383.51239	-383.51321
exo-2	-383.48273	-383.48269	-383.48271	-383.48272	-383.48283	-383.48278	-383.48271	-383.48278	-383.48266	-383.48268	-383.48270
endo-2	-383.47575	-383.47577	-383.47536	-383.47582	-383.47636	-383.47584	-383.47570	-383.47613	-383.47556	-383.47499	-383.47594
3	-383.49253	-383.49263	-383.49241	-383.49233	-383.49253	-383.49268	-383.49247	-383.49249	-383.49252	-383.49270	-383.49258
4	-383.48392	-383.48440	-383.48398	-383.48358	-383.48410	-383.48366	-383.48362	-383.48381	-383.48443	-383.48418	-383.48341
syn-5	-383.49351	-383.49353	-383.49361	-383.49350	-383.49351	-383.49347	-383.49350	-383.49347	-383.49344	-383.49351	-383.49356
anti-5	-383.39376	-383.39311	-383.39399	-383.39401	-383.39371	-383.39378	-383.39355	-383.39383	-383.39380	-383.39377	-383.39406
syn-6	-383.48779	-383.48769	-383.48778	-383.48797	-383.48756	-383.48811	-383.48749	-383.48775	-383.48803	-383.48774	-383.48778
anti-6	-383.40164	-383.40212	-383.40094	-383.40187	-383.40207	-383.40109	-383.40176	-383.40193	-383.40123	-383.40169	-383.40167
7	-383.46813	-383.46791	-383.46859	-383.46771	-383.46773	-383.46807	-383.46812	-383.46933	-383.46779	-383.46834	-383.46765
exo-8	-383.47964	-383.47965	-383.47966	-383.47980	-383.47960	-383.47959	-383.47948	-383.47950	-383.47962	-383.47971	-383.47976
endo-8	-383.46422	-383.46387	-383.46491	-383.46438	-383.46404	-383.46405	-383.46368	-383.46360	-383.46462	-383.46437	-383.46467
9	-383.46075	-383.46105	-383.46031	-383.46097	-383.46052	-383.46063	-383.46126	-383.46067	-383.46010	-383.46090	-383.46106
10	-383.47071	-383.47064	-383.47068	-383.47077	-383.47043	-383.47076	-383.47038	-383.47090	-383.47081	-383.47064	-383.47107
syn-11	-383.45443	-383.45435	-383.45466	-383.45424	-383.45423	-383.45444	-383.45442	-383.45440	-383.45453	-383.45449	-383.45451
anti-11	-383.47093	-383.47080	-383.47097	-383.47112	-383.47094	-383.47088	-383.47086	-383.47110	-383.47102	-383.47069	-383.47091
12	-383.49041	-383.49034	-383.49099	-383.49001	-383.49003	-383.49060	-383.49048	-383.49065	-383.49049	-383.49053	-383.49002
13	-383.47913	-383.47918	-383.47907	-383.47903	-383.47910	-383.47908	-383.47910	-383.47877	-383.47933	-383.47922	-383.47937
14	-383.47845	-383.47855	-383.47848	-383.47835	-383.47840	-383.47845	-383.47842	-383.47830	-383.47853	-383.47852	-383.47847
18	-383.48745	-383.48753	-383.48769	-383.48756	-383.48787	-383.48758	-383.48688	-383.48723	-383.48717	-383.48758	-383.48743
19	-383.49132	-383.49103	-383.49149	-383.49134	-383.49122	-383.49145	-383.49115	-383.49142	-383.49137	-383.49133	-383.49144

Table S8: Total energies (in Hartee) of various molecules in the reaction set for HWE-1(2,2)/STO-3G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
A	-382.65879	-382.65928	-382.65925	-382.65908	-382.65914	-382.65888	-382.65915	-382.65920	-382.65842	-382.65903	-382.65641
TS-AA'	-382.62634	-382.62719	-382.62650	-382.62586	-382.62576	-382.62685	-382.62618	-382.62594	-382.62641	-382.62657	-382.62614
A'	-382.65870	-382.65845	-382.65912	-382.65933	-382.65918	-382.65923	-382.65919	-382.65889	-382.65510	-382.65921	-382.65924
F	-382.61873	-382.61394	-382.62001	-382.61924	-382.61982	-382.61999	-382.61712	-382.61970	-382.61759	-382.61999	-382.61985
TS-FG	-382.61259	-382.61291	-382.61160	-382.61290	-382.61232	-382.61292	-382.61292	-382.61290	-382.61177	-382.61290	-382.61272
G	-382.66135	-382.66279	-382.66289	-382.66181	-382.66090	-382.66131	-382.66059	-382.65792	-382.66069	-382.66245	-382.66217
TS-GG'	-382.65120	-382.65360	-382.64963	-382.65263	-382.65096	-382.65194	-382.65167	-382.64954	-382.65029	-382.65130	-382.65042
G'	-382.66028	-382.66071	-382.66135	-382.66265	-382.66117	-382.65948	-382.65153	-382.66138	-382.66091	-382.66219	-382.66142
J	-382.66161	-382.66070	-382.66259	-382.66145	-382.65909	-382.66359	-382.66192	-382.66167	-382.66342	-382.66138	-382.66030
TS-JK	-382.60643	-382.60703	-382.60597	-382.60706	-382.60607	-382.60566	-382.60722	-382.60713	-382.60419	-382.60690	-382.60709
K	-382.63987	-382.63760	-382.64049	-382.63880	-382.64043	-382.64066	-382.63851	-382.64063	-382.64024	-382.64068	-382.64068
TS-KL	-382.63812	-382.63807	-382.63816	-382.63850	-382.63807	-382.63787	-382.63833	-382.63805	-382.63792	-382.63818	-382.63809
L	-382.64958	-382.65000	-382.64998	-382.65000	-382.65000	-382.64997	-382.64999	-382.64987	-382.64990	-382.64795	-382.64814
TS-LM	-382.54199	-382.54235	-382.54195	-382.54217	-382.54209	-382.54136	-382.54140	-382.54200	-382.54233	-382.54208	-382.54214
TS-LN	-382.62252	-382.62224	-382.62224	-382.62318	-382.61912	-382.62301	-382.62284	-382.62279	-382.62322	-382.62330	-382.62328
TS-MN	-382.58595	-382.58598	-382.58597	-382.58402	-382.58643	-382.58659	-382.58652	-382.58627	-382.58632	-382.58614	-382.58524
M	-382.66688	-382.66747	-382.66717	-382.66392	-382.66729	-382.66701	-382.66690	-382.66723	-382.66736	-382.66745	-382.66702
N	-382.64426	-382.64470	-382.64484	-382.64445	-382.64533	-382.64491	-382.64491	-382.64063	-382.64353	-382.64399	-382.64535

Table S9: Total energies (in Hartee) of various molecules in the reaction set for HWE-2(2,2)/STO-3G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
A	-382.65855	-382.65910	-382.65889	-382.65840	-382.65854	-382.65824	-382.65731	-382.65875	-382.65882	-382.65914	-382.65833
TS-AA'	-382.62594	-382.62547	-382.62648	-382.62575	-382.62661	-382.62641	-382.62563	-382.62537	-382.62639	-382.62584	-382.62548
A'	-382.65823	-382.65561	-382.65888	-382.65911	-382.65913	-382.65735	-382.65871	-382.65874	-382.65884	-382.65775	-382.65819
F	-382.61812	-382.61987	-382.61188	-382.61911	-382.61994	-382.61928	-382.61890	-382.61988	-382.61433	-382.61922	-382.61880
TS-FG	-382.61149	-382.61236	-382.61229	-382.61238	-382.61171	-382.61266	-382.61227	-382.61278	-382.61217	-382.61260	-382.60370
G	-382.66169	-382.66111	-382.66333	-382.66139	-382.66224	-382.66178	-382.66222	-382.66277	-382.65923	-382.66162	-382.66125
TS-GG'	-382.65175	-382.65214	-382.65100	-382.65146	-382.65293	-382.65143	-382.65236	-382.65229	-382.64745	-382.65295	-382.65353
G'	-382.66150	-382.66143	-382.66224	-382.66067	-382.66108	-382.66223	-382.66254	-382.66044	-382.66172	-382.66172	-382.66094
J	-382.66089	-382.66283	-382.66016	-382.66306	-382.66168	-382.65939	-382.66058	-382.66225	-382.65437	-382.66216	-382.66239
TS-JK	-382.60547	-382.60566	-382.60569	-382.60690	-382.60680	-382.60660	-382.60663	-382.60618	-382.60397	-382.59914	-382.60714
K	-382.64000	-382.63801	-382.64030	-382.64015	-382.64056	-382.64016	-382.64030	-382.63943	-382.64039	-382.64051	-382.64020
TS-KL	-382.63783	-382.63826	-382.63793	-382.63798	-382.63794	-382.63819	-382.63791	-382.63820	-382.63715	-382.63778	-382.63698
L	-382.64918	-382.64996	-382.64986	-382.64964	-382.64958	-382.64971	-382.64906	-382.64830	-382.64609	-382.64986	-382.64977
TS-LM	-382.54144	-382.54188	-382.54181	-382.54042	-382.54237	-382.54176	-382.53861	-382.54218	-382.54126	-382.54249	-382.54158
TS-LN	-382.62199	-382.62319	-382.62272	-382.62286	-382.62330	-382.62278	-382.62286	-382.62301	-382.62115	-382.61791	-382.62015
TS-MN	-382.58424	-382.57949	-382.58103	-382.58406	-382.58568	-382.58610	-382.58624	-382.58658	-382.58446	-382.58322	-382.58554
M	-382.66712	-382.66686	-382.66699	-382.66738	-382.66728	-382.66705	-382.66643	-382.66710	-382.66742	-382.66730	-382.66740
N	-382.64461	-382.64334	-382.64518	-382.64476	-382.64528	-382.64420	-382.64432	-382.64486	-382.64418	-382.64497	-382.64505

Table S10: Total energies (in Hartee) of various molecules in the reaction set for ESU2-RY(2,2)/STO-3G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
A	-382.65908	-382.65923	-382.65922	-382.65889	-382.65832	-382.65943	-382.65918	-382.65918	-382.65919	-382.65917	-382.65903
TS-AA'	-382.62633	-382.62623	-382.62655	-382.62669	-382.62649	-382.62671	-382.62668	-382.62515	-382.62686	-382.62747	-382.62444
A'	-382.65798	-382.65907	-382.65143	-382.65906	-382.65577	-382.65929	-382.65926	-382.65873	-382.65895	-382.65909	-382.65918
F	-382.61975	-382.61956	-382.61950	-382.61991	-382.61996	-382.61998	-382.61987	-382.62000	-382.61873	-382.62014	-382.61980
TS-FG	-382.61282	-382.61292	-382.61298	-382.61268	-382.61266	-382.61270	-382.61283	-382.61288	-382.61270	-382.61293	-382.61294
G	-382.66049	-382.66019	-382.66146	-382.66292	-382.66161	-382.66228	-382.65438	-382.66307	-382.66261	-382.65483	-382.66156
TS-GG'	-382.65245	-382.65250	-382.65139	-382.65402	-382.65187	-382.65395	-382.65305	-382.65329	-382.65102	-382.65179	-382.65158
G'	-382.66213	-382.66257	-382.66194	-382.66163	-382.66249	-382.66203	-382.66130	-382.66187	-382.66153	-382.66275	-382.66319
J	-382.66185	-382.66320	-382.66305	-382.66271	-382.65906	-382.66252	-382.66130	-382.66335	-382.66362	-382.66213	-382.65761
TS-JK	-382.60594	-382.60735	-382.60700	-382.60679	-382.60708	-382.59715	-382.60604	-382.60725	-382.60710	-382.60733	-382.60636
K	-382.63941	-382.64063	-382.64068	-382.63059	-382.64060	-382.64065	-382.63831	-382.64064	-382.64072	-382.64058	-382.64066
TS-KL	-382.63760	-382.63847	-382.63806	-382.63828	-382.63705	-382.63826	-382.63809	-382.63810	-382.63810	-382.63354	-382.63806
L	-382.64974	-382.64990	-382.65004	-382.65003	-382.64998	-382.65007	-382.64923	-382.64985	-382.64996	-382.64988	-382.64842
TS-LM	-382.54224	-382.54211	-382.54257	-382.54165	-382.54298	-382.54248	-382.54254	-382.54172	-382.54230	-382.54175	-382.54227
TS-LN	-382.62279	-382.62317	-382.62332	-382.62311	-382.62328	-382.62333	-382.62309	-382.62335	-382.62326	-382.61919	-382.62284
TS-MN	-382.58624	-382.58640	-382.58631	-382.58650	-382.58638	-382.58672	-382.58587	-382.58633	-382.58660	-382.58435	-382.58695
M	-382.66705	-382.66742	-382.66565	-382.66712	-382.66682	-382.66747	-382.66697	-382.66724	-382.66720	-382.66731	-382.66726
N	-382.64427	-382.64530	-382.64517	-382.64497	-382.64463	-382.64504	-382.64511	-382.64529	-382.64249	-382.63959	-382.64507

Table S11: Total energies (in Hartee) of various molecules in the reaction set for ESU2-RYRZ(2,2)/STO-3G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
A	-382.65856	-382.65889	-382.65764	-382.65920	-382.65879	-382.65922	-382.65900	-382.65639	-382.65846	-382.65870	-382.65926
TS-AA'	-382.62542	-382.62576	-382.62600	-382.62603	-382.62549	-382.62498	-382.62650	-382.62526	-382.62587	-382.62572	-382.62257
A'	-382.65891	-382.65909	-382.65930	-382.65894	-382.65873	-382.65921	-382.65925	-382.65910	-382.65910	-382.65890	-382.65744
F	-382.61885	-382.61963	-382.61995	-382.61598	-382.61659	-382.61997	-382.61993	-382.61907	-382.61990	-382.61762	-382.61982
TS-FG	-382.61260	-382.61296	-382.61284	-382.61243	-382.61275	-382.61199	-382.61273	-382.61275	-382.61289	-382.61183	-382.61282
G	-382.66050	-382.66054	-382.66207	-382.65904	-382.66088	-382.66079	-382.66048	-382.66188	-382.65755	-382.66142	-382.66033
TS-GG'	-382.65005	-382.65015	-382.65051	-382.65011	-382.65088	-382.64961	-382.64860	-382.65014	-382.65110	-382.65067	-382.64876
G'	-382.66058	-382.65794	-382.66045	-382.66134	-382.66137	-382.66120	-382.66147	-382.66089	-382.65791	-382.66088	-382.66235
J	-382.66044	-382.65922	-382.66217	-382.65130	-382.66134	-382.66091	-382.65880	-382.66212	-382.66365	-382.66098	-382.66389
TS-JK	-382.60687	-382.60717	-382.60716	-382.60740	-382.60718	-382.60688	-382.60606	-382.60710	-382.60578	-382.60687	-382.60713
K	-382.64023	-382.64066	-382.64060	-382.63995	-382.63880	-382.64066	-382.64030	-382.64047	-382.64067	-382.64066	-382.63949
TS-KL	-382.63761	-382.63828	-382.63838	-382.63832	-382.63780	-382.63562	-382.63761	-382.63724	-382.63663	-382.63808	-382.63814
L	-382.64972	-382.64964	-382.64996	-382.64971	-382.65000	-382.64952	-382.64995	-382.65000	-382.65001	-382.64983	-382.64861
TS-LM	-382.54055	-382.54158	-382.54111	-382.54203	-382.54141	-382.54170	-382.54202	-382.53948	-382.53237	-382.54206	-382.54173
TS-LN	-382.62208	-382.61485	-382.62312	-382.62121	-382.62325	-382.62290	-382.62253	-382.62314	-382.62319	-382.62324	-382.62333
TS-MN	-382.58549	-382.58640	-382.58656	-382.58531	-382.58475	-382.58549	-382.58331	-382.58601	-382.58625	-382.58498	-382.58584
M	-382.66581	-382.66642	-382.66703	-382.66714	-382.65797	-382.66592	-382.66704	-382.66678	-382.66588	-382.66736	-382.66652
N	-382.64379	-382.64255	-382.64450	-382.64312	-382.64360	-382.64533	-382.64501	-382.64523	-382.64504	-382.63861	-382.64493

Table S12: Total energies (in Hartee) of various molecules in the reaction set for EXCT. PRESERV.(2,2)/STO-3G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
A	-382.65921	-382.65923	-382.65929	-382.65917	-382.65915	-382.65917	-382.65920	-382.65919	-382.65930	-382.65937	-382.65905
TS-AA'	-382.62629	-382.62709	-382.62577	-382.62671	-382.62641	-382.62652	-382.62671	-382.62571	-382.62591	-382.62643	-382.62565
A'	-382.65915	-382.65928	-382.65908	-382.65919	-382.65929	-382.65894	-382.65902	-382.65928	-382.65910	-382.65901	-382.65927
F	-382.61999	-382.61999	-382.62005	-382.61996	-382.62006	-382.61997	-382.61992	-382.61990	-382.62004	-382.62005	-382.62000
TS-FG	-382.61290	-382.61288	-382.61291	-382.61288	-382.61291	-382.61293	-382.61284	-382.61291	-382.61288	-382.61287	-382.61296
G	-382.66174	-382.66209	-382.66082	-382.66331	-382.66232	-382.66091	-382.66209	-382.66076	-382.66178	-382.66142	-382.66192
TS-GG'	-382.65037	-382.65232	-382.65150	-382.65017	-382.64786	-382.64869	-382.65032	-382.65066	-382.64821	-382.65071	-382.65322
G'	-382.66121	-382.66115	-382.66098	-382.66182	-382.66208	-382.66173	-382.66095	-382.66095	-382.66081	-382.66101	-382.66059
J	-382.66163	-382.66204	-382.66239	-382.66240	-382.66267	-382.65918	-382.65889	-382.66294	-382.66237	-382.66218	-382.66123
TS-JK	-382.60710	-382.60706	-382.60708	-382.60703	-382.60711	-382.60700	-382.60744	-382.60702	-382.60702	-382.60706	-382.60718
K	-382.64066	-382.64066	-382.64066	-382.64066	-382.64067	-382.64068	-382.64067	-382.64064	-382.64066	-382.64065	-382.64068
TS-KL	-382.63820	-382.63816	-382.63822	-382.63819	-382.63853	-382.63811	-382.63834	-382.63808	-382.63807	-382.63811	-382.63822
L	-382.65000	-382.64999	-382.65002	-382.64998	-382.65005	-382.65002	-382.64995	-382.65000	-382.65001	-382.64998	-382.64999
TS-LM	-382.54203	-382.54216	-382.54187	-382.54222	-382.54209	-382.54164	-382.54185	-382.54253	-382.54153	-382.54213	-382.54228
TS-LN	-382.62330	-382.62328	-382.62332	-382.62328	-382.62333	-382.62327	-382.62327	-382.62326	-382.62332	-382.62336	-382.62326
TS-MN	-382.58636	-382.58634	-382.58667	-382.58665	-382.58596	-382.58602	-382.58642	-382.58608	-382.58649	-382.58684	-382.58617
M	-382.66722	-382.66725	-382.66702	-382.66741	-382.66731	-382.66694	-382.66731	-382.66732	-382.66729	-382.66713	-382.66718
N	-382.64514	-382.64562	-382.64521	-382.64515	-382.64483	-382.64517	-382.64491	-382.64517	-382.64550	-382.64473	-382.64511

Table S13: Total energies (in Hartee) of various molecules in the isomer set for HWE-1(4,4)/STO-3G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**
1	-383.51238	-383.51287	-383.51202	-383.51238	-383.51233	-383.51229
exo-2	-383.48167	-383.48364	-383.48271	-383.47566	-383.48252	-383.48381
endo-2	-383.47580	-383.47480	-383.47551	-383.47615	-383.47682	-383.47574
3	-383.49251	-383.49229	-383.49244	-383.49261	-383.49263	-383.49258
4	-383.48340	-383.48376	-383.48261	-383.48315	-383.48394	-383.48352
syn-5	-383.49275	-383.49185	-383.49358	-383.49176	-383.49308	-383.49348
anti-5	-383.39274	-383.39326	-383.39365	-383.39387	-383.39216	-383.39077
syn-6	-383.48737	-383.48786	-383.48753	-383.48676	-383.48728	-383.48743
anti-6	-383.40157	-383.40254	-383.40217	-383.40142	-383.40032	-383.40139
7	-383.46777	-383.46810	-383.46770	-383.46783	-383.46786	-383.46738
exo-8	-383.47956	-383.47961	-383.47963	-383.47927	-383.47988	-383.47941
endo-8	-383.46387	-383.46415	-383.46369	-383.46336	-383.46360	-383.46455
9	-383.46079	-383.46040	-383.46090	-383.46093	-383.46081	-383.46090
10	-383.47019	-383.46927	-383.46948	-383.47081	-383.47061	-383.47079
syn-11	-383.45473	-383.45448	-383.45549	-383.45433	-383.45437	-383.45497
anti-11	-383.47089	-383.47083	-383.47134	-383.47062	-383.47086	-383.47079
12	-383.49020	-383.49106	-383.49005	-383.49027	-383.48908	-383.49055
13	-383.47893	-383.47925	-383.47876	-383.47879	-383.47794	-383.47991
14	-383.47802	-383.47830	-383.47812	-383.47677	-383.47839	-383.47851
18	-383.48538	-383.48747	-383.48761	-383.48737	-383.47682	-383.48764
19	-383.49141	-383.49170	-383.49159	-383.49125	-383.49126	-383.49125

Table S14: Total energies (in Hartee) of various molecules in the isomer set for HWE-2(4,4)/STO-3G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**
1	-383.51027	-383.51213	-383.51134	-383.50550	-383.50942	-383.51296
exo-2	-383.48069	-383.48204	-383.48122	-383.47927	-383.48005	-383.48086
endo-2	-383.47365	-383.47549	-383.47113	-383.47359	-383.47490	-383.47316
3	-383.49062	-383.49100	-383.48969	-383.49254	-383.48903	-383.49085
4	-383.48203	-383.48342	-383.47958	-383.48276	-383.48196	-383.48243
syn-5	-383.49042	-383.48443	-383.49069	-383.49315	-383.49085	-383.49299
anti-5	-383.39318	-383.39206	-383.39253	-383.39399	-383.39419	-383.39313
syn-6	-383.48524	-383.48574	-383.48429	-383.48686	-383.48229	-383.48703
anti-6	-383.40103	-383.40174	-383.40035	-383.40074	-383.40155	-383.40076
7	-383.46617	-383.46619	-383.46715	-383.46453	-383.46607	-383.46691
exo-8	-383.47876	-383.47903	-383.47781	-383.47937	-383.47917	-383.47843
endo-8	-383.46197	-383.45927	-383.46260	-383.46200	-383.46381	-383.46216
9	-383.45804	-383.46028	-383.45855	-383.45043	-383.46071	-383.46022
10	-383.46924	-383.47018	-383.46907	-383.46944	-383.46952	-383.46798
syn-11	-383.45178	-383.45273	-383.44962	-383.45264	-383.45249	-383.45141
anti-11	-383.46927	-383.47111	-383.47029	-383.47073	-383.46577	-383.46844
12	-383.48598	-383.48833	-383.48536	-383.49038	-383.48649	-383.47936
13	-383.47739	-383.47531	-383.47660	-383.47828	-383.47781	-383.47896
14	-383.47476	-383.47793	-383.47753	-383.47715	-383.46313	-383.47804
18	-383.48595	-383.48696	-383.48609	-383.48490	-383.48602	-383.48580
19	-383.49042	-383.49123	-383.48847	-383.49134	-383.49089	-383.49016

Table S15: Total energies (in Hartee) of various molecules in the isomer set for ESU2-RY(4,4)/STO-3G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**
1	-383.5121	-383.51169	-383.51242	-383.51230	-383.51197	-383.51212
exo-2	-383.48256	-383.48253	-383.48238	-383.48256	-383.48282	-383.48252
endo-2	-383.47545	-383.47562	-383.47576	-383.47517	-383.47534	-383.47536
3	-383.49237	-383.49231	-383.49226	-383.49241	-383.49220	-383.49265
4	-383.48301	-383.48305	-383.48043	-383.48409	-383.48377	-383.48371
syn-5	-383.49338	-383.49343	-383.49248	-383.49414	-383.49316	-383.49367
anti-5	-383.39338	-383.39216	-383.39378	-383.39441	-383.39377	-383.39278
syn-6	-383.48692	-383.48719	-383.48828	-383.48793	-383.48452	-383.48670
anti-6	-383.40128	-383.40177	-383.40079	-383.40047	-383.40187	-383.40152
7	-383.46745	-383.46740	-383.46757	-383.46708	-383.46792	-383.46730
exo-8	-383.47953	-383.47910	-383.48035	-383.47952	-383.47936	-383.47930
endo-8	-383.46367	-383.46446	-383.46411	-383.46380	-383.46204	-383.46394
9	-383.46035	-383.45993	-383.46020	-383.46053	-383.46059	-383.46052
10	-383.47004	-383.47031	-383.46996	-383.46923	-383.47024	-383.47046
syn-11	-383.45446	-383.45446	-383.45465	-383.45388	-383.45434	-383.45497
anti-11	-383.47066	-383.47134	-383.46969	-383.47017	-383.47094	-383.47117
12	-383.48853	-383.49019	-383.49070	-383.49007	-383.49078	-383.48089
13	-383.47907	-383.47906	-383.47868	-383.47959	-383.47875	-383.47929
14	-383.47834	-383.47815	-383.47827	-383.47806	-383.47849	-383.47875
18	-383.48742	-383.48748	-383.48764	-383.48749	-383.48719	-383.48732
19	-383.49082	-383.48983	-383.49037	-383.49106	-383.49154	-383.49129

Table S16: Total energies (in Hartee) of various molecules in the isomer set for ESU2-RYRZ(4,4)/STO-3G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**
1	-383.51245	-383.51224	-383.51210	-383.51318	-383.51251	-383.51221
exo-2	-383.48348	-383.48370	-383.48287	-383.48397	-383.48285	-383.48403
endo-2	-383.47524	-383.47582	-383.47522	-383.47427	-383.47505	-383.47582
3	-383.49221	-383.49269	-383.49255	-383.49120	-383.49231	-383.49230
4	-383.48351	-383.48360	-383.48327	-383.48368	-383.48345	-383.48357
syn-5	-383.49401	-383.49425	-383.49386	-383.49402	-383.49403	-383.49388
anti-5	-383.39400	-383.39401	-383.39414	-383.39373	-383.39453	-383.39357
syn-6	-383.48775	-383.48743	-383.48763	-383.48757	-383.48788	-383.48825
anti-6	-383.40120	-383.40125	-383.40062	-383.40030	-383.40164	-383.40220
7	-383.46646	-383.46167	-383.46702	-383.46780	-383.46788	-383.46794
exo-8	-383.47914	-383.47922	-383.47925	-383.47893	-383.47908	-383.47921
endo-8	-383.46371	-383.46420	-383.46300	-383.46411	-383.46431	-383.46293
9	-383.46063	-383.46070	-383.46016	-383.46079	-383.46054	-383.46094
10	-383.4707	-383.47078	-383.47068	-383.47083	-383.47007	-383.47114
syn-11	-383.45410	-383.45396	-383.45448	-383.45326	-383.45443	-383.45439
anti-11	-383.47088	-383.47057	-383.47049	-383.47109	-383.47097	-383.47127
12	-383.49013	-383.49031	-383.48990	-383.49017	-383.49032	-383.48997
13	-383.47932	-383.47906	-383.47962	-383.47913	-383.48021	-383.47859
14	-383.47748	-383.47324	-383.47875	-383.47818	-383.47871	-383.47851
18	-383.48703	-383.48564	-383.48731	-383.48714	-383.48769	-383.48739
19	-383.49137	-383.49104	-383.49136	-383.49141	-383.49151	-383.49153

Table S17: Total energies (in Hartee) of various molecules in the isomer set for EXCT. PRESERV.(4,4)/STO-3G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**
1	-383.51275	-383.51278	-383.51290	-383.51257	-383.51289	-383.51263
exo-2	-383.48278	-383.48278	-383.48302	-383.48300	-383.48271	-383.48237
endo-2	-383.47535	-383.47538	-383.47551	-383.47537	-383.47564	-383.47483
3	-383.49235	-383.49262	-383.49190	-383.49242	-383.49225	-383.49255
4	-383.48368	-383.48379	-383.48375	-383.48330	-383.48384	-383.48374
syn-5	-383.49308	-383.49332	-383.49327	-383.49318	-383.49281	-383.49284
anti-5	-383.39337	-383.39308	-383.39397	-383.39350	-383.39324	-383.39305
syn-6	-383.48776	-383.48770	-383.48744	-383.48802	-383.48746	-383.48816
anti-6	-383.40115	-383.40123	-383.40101	-383.40129	-383.40163	-383.40057
7	-383.46767	-383.46751	-383.46732	-383.46764	-383.46798	-383.46789
exo-8	-383.47934	-383.47927	-383.47960	-383.47897	-383.47950	-383.47934
endo-8	-383.46399	-383.46407	-383.46441	-383.46449	-383.46350	-383.46347
9	-383.46080	-383.46084	-383.46097	-383.46068	-383.46063	-383.46087
10	-383.47041	-383.47081	-383.47024	-383.47024	-383.47046	-383.47030
syn-11	-383.45431	-383.45441	-383.45406	-383.45457	-383.45387	-383.45465
anti-11	-383.47101	-383.47154	-383.47085	-383.47093	-383.47074	-383.47098
12	-383.49065	-383.49030	-383.49082	-383.49111	-383.49064	-383.49036
13	-383.47924	-383.47917	-383.47895	-383.47932	-383.47948	-383.47927
14	-383.47828	-383.47833	-383.47839	-383.47817	-383.47828	-383.47823
18	-383.48738	-383.48748	-383.48728	-383.48722	-383.48772	-383.48718
19	-383.49135	-383.49121	-383.49138	-383.49105	-383.49184	-383.49128

Table S18: Total energies (in Hartee) of various molecules in the reaction set for HWE-1(4,4)/STO-3G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**
A	-382.65709	-382.65926	-382.65817	-382.65937	-382.65531	-382.65332
TS-AA'	-382.62379	-382.62558	-382.62601	-382.61561	-382.62647	-382.62526
A'	-382.65684	-382.66007	-382.65927	-382.65822	-382.64798	-382.65864
F	-382.61939	-382.62036	-382.61950	-382.61895	-382.61858	-382.61956
TS-FG	-382.61271	-382.61317	-382.61224	-382.61171	-382.61411	-382.61230
G	-382.65930	-382.66019	-382.65998	-382.66100	-382.66014	-382.65519
TS-GG'	-382.64912	-382.64938	-382.65028	-382.64907	-382.64791	-382.64898
G'	-382.66113	-382.66230	-382.66148	-382.66126	-382.65978	-382.66081
J	-382.65829	-382.65613	-382.65931	-382.66069	-382.66089	-382.65442
TS-JK	-382.60663	-382.60576	-382.60558	-382.60769	-382.60747	-382.60663
K	-382.63991	-382.63839	-382.64081	-382.64075	-382.63866	-382.64093
TS-KL	-382.63676	-382.63622	-382.63771	-382.63714	-382.63690	-382.63582
L	-382.64808	-382.64909	-382.64882	-382.64985	-382.64225	-382.65039
TS-LM	-382.54175	-382.54209	-382.54043	-382.54267	-382.54133	-382.54223
TS-LN	-382.62279	-382.62318	-382.62279	-382.62204	-382.62317	-382.62279
TS-MN	-382.58705	-382.58632	-382.58626	-382.58886	-382.58670	-382.58712
M	-382.66377	-382.66825	-382.66687	-382.65203	-382.66588	-382.66584
N	-382.64438	-382.64490	-382.64411	-382.64421	-382.64359	-382.64509

Table S19: Total energies (in Hartee) of various molecules in the reaction set for HWE-2(4,4)/STO-3G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**
A	-382.65586	-382.65867	-382.65794	-382.65738	-382.65126	-382.65406
TS-AA'	-382.62463	-382.62687	-382.62496	-382.62257	-382.62414	-382.62462
A'	-382.65749	-382.65703	-382.65678	-382.65763	-382.65792	-382.65809
F	-382.61912	-382.61857	-382.61782	-382.61974	-382.62013	-382.61932
TS-FG	-382.61109	-382.60902	-382.61313	-382.60855	-382.61205	-382.61271
G	-382.65646	-382.65778	-382.66078	-382.65047	-382.65893	-382.65434
TS-GG'	-382.64887	-382.64755	-382.64525	-382.65288	-382.65020	-382.64849
G'	-382.65994	-382.65814	-382.66035	-382.65952	-382.66126	-382.66042
J	-382.65779	-382.66092	-382.65242	-382.65797	-382.65908	-382.65855
TS-JK	-382.60282	-382.60616	-382.60411	-382.60340	-382.60508	-382.59537
K	-382.63894	-382.64098	-382.63803	-382.63771	-382.63677	-382.64122
TS-KL	-382.63763	-382.63614	-382.63847	-382.63796	-382.63711	-382.63846
L	-382.64525	-382.64555	-382.63934	-382.64653	-382.64690	-382.64793
TS-LM	-382.53893	-382.53925	-382.54088	-382.54043	-382.54156	-382.53254
TS-LN	-382.61780	-382.61124	-382.61693	-382.62011	-382.62106	-382.61966
TS-MN	-382.58460	-382.58465	-382.58417	-382.58677	-382.58312	-382.58427
M	-382.66440	-382.66718	-382.66496	-382.66344	-382.66581	-382.66063
N	-382.64384	-382.64430	-382.64444	-382.64256	-382.64356	-382.64436

Table S20: Total energies (in Hartee) of various molecules in the reaction set for ESU2-RY(4,4)/STO-3G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**
A	-382.65744	-382.65628	-382.65838	-382.65958	-382.65741	-382.65557
TS-AA'	-382.62500	-382.62572	-382.62594	-382.62616	-382.62517	-382.62202
A'	-382.65868	-382.65665	-382.65933	-382.65882	-382.65921	-382.65938
F	-382.61881	-382.61953	-382.62039	-382.61706	-382.61947	-382.61762
TS-FG	-382.61126	-382.61229	-382.61373	-382.60814	-382.60986	-382.61230
G	-382.66092	-382.66090	-382.66109	-382.66087	-382.66138	-382.66034
TS-GG'	-382.64803	-382.64977	-382.64835	-382.64960	-382.64530	-382.64714
G'	-382.65991	-382.65962	-382.66091	-382.65540	-382.66264	-382.66097
J	-382.65926	-382.65817	-382.65848	-382.66010	-382.66064	-382.65891
TS-JK	-382.60585	-382.60752	-382.60498	-382.60737	-382.60375	-382.60564
K	-382.64017	-382.64062	-382.64046	-382.64049	-382.63886	-382.64040
TS-KL	-382.63811	-382.63938	-382.63654	-382.63778	-382.63897	-382.63787
L	-382.64850	-382.65053	-382.65116	-382.64516	-382.64548	-382.65015
TS-LM	-382.54154	-382.54223	-382.54136	-382.54159	-382.54183	-382.54067
TS-LN	-382.62224	-382.62297	-382.62334	-382.62240	-382.61917	-382.62333
TS-MN	-382.58511	-382.58691	-382.58238	-382.58810	-382.58593	-382.58222
M	-382.66490	-382.66718	-382.65980	-382.66607	-382.66476	-382.66671
N	-382.64509	-382.64494	-382.64709	-382.64344	-382.64475	-382.64521

Table S21: Total energies (in Hartee) of various molecules in the reaction set for ESU2-RYRZ(4,4)/STO-3G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**
A	-382.65857	-382.65913	-382.65687	-382.65911	-382.65782	-382.65992
TS-AA'	-382.62536	-382.62498	-382.62623	-382.62543	-382.62486	-382.62530
A'	-382.65889	-382.65874	-382.65849	-382.65852	-382.65956	-382.65916
F	-382.61998	-382.61968	-382.62012	-382.61989	-382.61955	-382.62067
TS-FG	-382.61268	-382.61312	-382.61138	-382.61285	-382.61244	-382.61362
G	-382.65952	-382.66082	-382.65902	-382.66069	-382.66048	-382.65658
TS-GG'	-382.64871	-382.64853	-382.64983	-382.64958	-382.64946	-382.64617
G'	-382.66028	-382.66087	-382.65920	-382.66043	-382.66061	-382.66028
J	-382.65883	-382.65898	-382.65904	-382.65845	-382.66059	-382.65711
TS-JK	-382.60667	-382.60640	-382.60643	-382.60789	-382.60580	-382.60684
K	-382.63938	-382.64054	-382.64071	-382.64080	-382.63800	-382.63684
TS-KL	-382.63825	-382.63970	-382.63786	-382.63667	-382.64019	-382.63681
L	-382.64685	-382.65025	-382.63646	-382.64833	-382.64929	-382.64990
TS-LM	-382.53992	-382.54166	-382.54167	-382.53952	-382.54092	-382.53582
TS-LN	-382.62278	-382.62297	-382.62217	-382.62341	-382.62312	-382.62224
TS-MN	-382.58706	-382.58730	-382.58732	-382.58787	-382.58729	-382.58553
M	-382.66740	-382.66737	-382.66775	-382.66701	-382.66747	-382.66740
N	-382.64399	-382.64368	-382.64555	-382.64308	-382.64396	-382.64368

Table S22: Total energies (in Hartee) of various molecules in the reaction set for EXCT. PRESERV.(4,4)/STO-3G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**
A	-382.65902	-382.65807	-382.65889	-382.65998	-382.65806	-382.66011
TS-AA'	-382.62554	-382.62550	-382.62574	-382.62564	-382.62527	-382.62556
A'	-382.65935	-382.65984	-382.65855	-382.65887	-382.65969	-382.65978
F	-382.61952	-382.61875	-382.61983	-382.61968	-382.61954	-382.61978
TS-FG	-382.61330	-382.61260	-382.61290	-382.61302	-382.61379	-382.61420
G	-382.66102	-382.66114	-382.66085	-382.66054	-382.66192	-382.66065
TS-GG'	-382.64806	-382.64875	-382.64771	-382.64723	-382.64905	-382.64755
G'	-382.66088	-382.66160	-382.66051	-382.66102	-382.66117	-382.66011
J	-382.65875	-382.65813	-382.65842	-382.65928	-382.65815	-382.65976
TS-JK	-382.60756	-382.60725	-382.60673	-382.60799	-382.60769	-382.60816
K	-382.64101	-382.64028	-382.64073	-382.64170	-382.64080	-382.64155
TS-KL	-382.63775	-382.63672	-382.63776	-382.63960	-382.63689	-382.63776
L	-382.64965	-382.64915	-382.64958	-382.64979	-382.65015	-382.64959
TS-LM	-382.54197	-382.54122	-382.54211	-382.54276	-382.54027	-382.54350
TS-LN	-382.62280	-382.62357	-382.62306	-382.62252	-382.62228	-382.62258
TS-MN	-382.58662	-382.58723	-382.58654	-382.58611	-382.58698	-382.58625
M	-382.66707	-382.66740	-382.66677	-382.66780	-382.66732	-382.66607
N	-382.64571	-382.64554	-382.64449	-382.64717	-382.64605	-382.64531

Table S23: Total energies (in Hartee) of various molecules in the isomer set for EXCT. PRESERV.(4,4)/6-31G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**
1	-387.86396	-387.86397	-387.86405	-387.86411	-387.86373	-387.86395
exo-2	-387.83921	-387.83912	-387.83919	-387.83935	-387.83919	-387.83919
endo-2	-387.83141	-387.83169	-387.83122	-387.83152	-387.83123	-387.83137
3	-387.84547	-387.84526	-387.84547	-387.84572	-387.84553	-387.84536
4	-387.83573	-387.83566	-387.83563	-387.83586	-387.83572	-387.83578
syn-5	-387.84689	-387.84690	-387.84696	-387.84671	-387.84704	-387.84685
anti-5	-387.76034	-387.76047	-387.76041	-387.76044	-387.76023	-387.76013
syn-6	-387.84161	-387.84156	-387.84168	-387.84167	-387.84152	-387.84162
anti-6	-387.76508	-387.76520	-387.76503	-387.76482	-387.76515	-387.76521
7	-387.82524	-387.82478	-387.82562	-387.82506	-387.82548	-387.82526
exo-8	-387.83564	-387.83590	-387.83561	-387.83573	-387.83557	-387.83540
endo-8	-387.82194	-387.82197	-387.82189	-387.82153	-387.82208	-387.82221
9	-387.81674	-387.81682	-387.81747	-387.81729	-387.81644	-387.81570
10	-387.82476	-387.82460	-387.82506	-387.82462	-387.82491	-387.82463
syn-11	-387.81025	-387.81014	-387.81023	-387.81031	-387.81043	-387.81012
anti-11	-387.82662	-387.82676	-387.82638	-387.82674	-387.82643	-387.82681
12	-387.84452	-387.84431	-387.84449	-387.84487	-387.84446	-387.84447
13	-387.83406	-387.83414	-387.83399	-387.83420	-387.83391	-387.83404
14	-387.83248	-387.83248	-387.83260	-387.83281	-387.83204	-387.83247
18	-387.84135	-387.84136	-387.84134	-387.84148	-387.84135	-387.84121
19	-387.84392	-387.84379	-387.84399	-387.84390	-387.84379	-387.84413

Table S24: Total energies (in Hartee) of various molecules in the reaction set for EXCT. PRESERV.(4,4)/6-31G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**
A	-386.99392	-386.99405	-386.99349	-386.99345	-386.99338	-386.99522
TS-AA'	-386.96349	-386.96339	-386.96363	-386.96329	-386.96306	-386.96406
A'	-386.99394	-386.99440	-386.99291	-386.99468	-386.99313	-386.99458
F	-386.96137	-386.96190	-386.96125	-386.96193	-386.96113	-386.96063
TS-FG	-386.95374	-386.95441	-386.95348	-386.95310	-386.95423	-386.95346
G	-386.99689	-386.99750	-386.99614	-386.99702	-386.99652	-386.99728
TS-GG'	-386.98952	-386.98967	-386.98988	-386.98907	-386.98939	-386.98961
G'	-386.99700	-386.99659	-386.99761	-386.99670	-386.99728	-386.99682
J	-386.99753	-386.99736	-386.99805	-386.99756	-386.99826	-386.99641
TS-JK	-386.94900	-386.94809	-386.94933	-386.94923	-386.94885	-386.94950
K	-386.98313	-386.98304	-386.98314	-386.98319	-386.98306	-386.98322
TS-KL	-386.98004	-386.98026	-386.97994	-386.98047	-386.97960	-386.97993
L	-386.98559	-386.98536	-386.98509	-386.98566	-386.98638	-386.98549
TS-LM	-386.89149	-386.89195	-386.89210	-386.89058	-386.89139	-386.89144
TS-LN	-386.95591	-386.95588	-386.95613	-386.95576	-386.95582	-386.95594
TS-MN	-386.93058	-386.93020	-386.93147	-386.92959	-386.93130	-386.93034
M	-387.00079	-387.00092	-387.00082	-387.00076	-387.00059	-387.00083
N	-386.98233	-386.98208	-386.98200	-386.98241	-386.98234	-386.98284

Table S25: Total energies (in Hartee) of various molecules in the isomer set for EXCT. PRESERV.(6,6)/STO-3G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**
1	-383.51273	-383.51274	-383.51320	-383.51290	-383.51256	-383.51227
exo-2	-383.48265	-383.48225	-383.48315	-383.48301	-383.48210	-383.48274
endo-2	-383.47582	-383.47562	-383.47594	-383.47664	-383.47514	-383.47574
3	-383.49312	-383.49186	-383.49441	-383.49310	-383.49324	-383.49297
4	-383.48364	-383.48343	-383.48385	-383.48336	-383.48342	-383.48412
syn-5	-383.49329	-383.49269	-383.49456	-383.49385	-383.49335	-383.49198
anti-5	-383.39417	-383.39347	-383.39383	-383.39371	-383.39486	-383.39500
syn-6	-383.48785	-383.48891	-383.48735	-383.48807	-383.48714	-383.48779
anti-6	-383.40172	-383.40219	-383.40294	-383.40050	-383.40115	-383.40180
7	-383.46767	-383.46678	-383.46785	-383.46839	-383.46699	-383.46834
exo-8	-383.47957	-383.47802	-383.48063	-383.48077	-383.48014	-383.47828
endo-8	-383.46372	-383.46252	-383.46311	-383.46482	-383.46366	-383.46447
9	-383.46093	-383.46067	-383.46095	-383.46133	-383.46076	-383.46096
10	-383.47068	-383.47096	-383.46988	-383.47105	-383.47055	-383.47099
syn-11	-383.45423	-383.45480	-383.45393	-383.45361	-383.45468	-383.45410
anti-11	-383.47066	-383.47019	-383.47102	-383.47065	-383.47055	-383.47091
12	-383.49009	-383.49037	-383.49032	-383.48974	-383.49044	-383.48959
13	-383.47879	-383.47930	-383.47868	-383.47865	-383.47881	-383.47851
14	-383.47825	-383.47824	-383.47850	-383.47840	-383.47805	-383.47807
18	-383.48726	-383.48794	-383.48688	-383.48717	-383.48713	-383.48720
19	-383.49137	-383.49161	-383.49112	-383.49208	-383.49059	-383.49148

Table S26: Total energies (in Hartee) of various molecules in the reaction set for EXCT. PRESERV.(6,6)/STO-3G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**
A	-382.65863	-382.65916	-382.65956	-382.65858	-382.65745	-382.65841
TS-AA'	-382.62522	-382.62441	-382.62441	-382.62687	-382.62557	-382.62486
A'	-382.65882	-382.65993	-382.65956	-382.65784	-382.65861	-382.65818
F	-382.62080	-382.61993	-382.62184	-382.62117	-382.62018	-382.62090
TS-FG	-382.61094	-382.61285	-382.61261	-382.60717	-382.61035	-382.61170
G	-382.66182	-382.66298	-382.66134	-382.66116	-382.66127	-382.66234
TS-GG'	-382.64804	-382.64711	-382.64735	-382.64928	-382.64912	-382.64736
G'	-382.66144	-382.65932	-382.66209	-382.66417	-382.66069	-382.66093
J	-382.65947	-382.66053	-382.65927	-382.65690	-382.65813	-382.66252
TS-JK	-382.60657	-382.60543	-382.60542	-382.60738	-382.60766	-382.60697
K	-382.64005	-382.64022	-382.63905	-382.64001	-382.64024	-382.64075
TS-KL	-382.63849	-382.64069	-382.63704	-382.63776	-382.63793	-382.63901
L	-382.64996	-382.64860	-382.65034	-382.65020	-382.64947	-382.65118
TS-LM	-382.54112	-382.54262	-382.53973	-382.54243	-382.54147	-382.53934
TS-LN	-382.62341	-382.62537	-382.62315	-382.62138	-382.62317	-382.62398
TS-MN	-382.58728	-382.58460	-382.58842	-382.58726	-382.58625	-382.58988
M	-382.66670	-382.66479	-382.66700	-382.66709	-382.66600	-382.66861
N	-382.64489	-382.64598	-382.64341	-382.64388	-382.64538	-382.64579

Table S27: Total energies (in Hartee) of various molecules in the isomer set for EXCT. PRESERV.(6,6)/6-31G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**
1	-387.86380	-387.86387	-387.86356	-387.86445	-387.86393	-387.86320
exo-2	-387.83927	-387.83872	-387.83882	-387.83997	-387.83951	-387.83936
endo-2	-387.83153	-387.83075	-387.83122	-387.83199	-387.83181	-387.83187
3	-387.84532	-387.84622	-387.84476	-387.84507	-387.84549	-387.84504
4	-387.83596	-387.83561	-387.83645	-387.83635	-387.83598	-387.83540
syn-5	-387.84698	-387.84726	-387.84777	-387.84643	-387.84706	-387.84637
anti-5	-387.76026	-387.76049	-387.76048	-387.76068	-387.75972	-387.75995
syn-6	-387.84120	-387.84241	-387.84083	-387.84112	-387.84075	-387.84090
anti-6	-387.76476	-387.76396	-387.76471	-387.76487	-387.76528	-387.76499
7	-387.82542	-387.82470	-387.82578	-387.82584	-387.82530	-387.82551
exo-8	-387.83586	-387.83616	-387.83581	-387.83580	-387.83597	-387.83553
endo-8	-387.82216	-387.82197	-387.82116	-387.82213	-387.82265	-387.82291
9	-387.81704	-387.81738	-387.81723	-387.81808	-387.81629	-387.81624
10	-387.82463	-387.82485	-387.82407	-387.82474	-387.82436	-387.82515
syn-11	-387.81030	-387.81020	-387.80995	-387.81026	-387.81088	-387.81020
anti-11	-387.82710	-387.82739	-387.82754	-387.82642	-387.82694	-387.82719
12	-387.84419	-387.84437	-387.84402	-387.84396	-387.84427	-387.84434
13	-387.83402	-387.83424	-387.83344	-387.83476	-387.83381	-387.83385
14	-387.83304	-387.83319	-387.83291	-387.83345	-387.83276	-387.83290
18	-387.84142	-387.84071	-387.84125	-387.84173	-387.84202	-387.84137
19	-387.84380	-387.84319	-387.84332	-387.84539	-387.84345	-387.84366

Table S28: Total energies (in Hartee) of various molecules in the reaction set for EXCT. PRESERV.(6,6)/6-31G calculations on statevector simulator

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**
A	-386.99365	-386.99355	-386.99336	-386.99471	-386.99307	-386.99355
TS-AA'	-386.96380	-386.96421	-386.96266	-386.96422	-386.96510	-386.96283
A'	-386.99407	-386.99405	-386.99412	-386.99363	-386.99405	-386.99449
F	-386.96146	-386.96223	-386.96094	-386.96131	-386.96095	-386.96187
TS-FG	-386.95312	-386.95227	-386.95306	-386.95400	-386.95271	-386.95355
G	-386.99709	-386.99817	-386.99726	-386.99563	-386.99757	-386.99684
TS-GG'	-386.98868	-386.98861	-386.98947	-386.98812	-386.98809	-386.98911
G'	-386.99621	-386.99786	-386.99558	-386.99453	-386.99638	-386.99671
J	-386.99734	-386.99752	-386.99723	-386.99784	-386.99783	-386.99628
TS-JK	-386.94932	-386.94847	-386.94976	-386.95096	-386.94788	-386.94954
K	-386.98377	-386.98468	-386.98363	-386.98312	-386.98426	-386.98315
TS-KL	-386.97942	-386.97941	-386.97999	-386.97904	-386.97891	-386.97975
L	-386.98627	-386.98604	-386.98745	-386.98609	-386.98599	-386.98579
TS-LM	-386.89094	-386.89216	-386.89228	-386.88878	-386.89000	-386.89148
TS-LN	-386.95514	-386.95456	-386.95678	-386.95551	-386.95393	-386.95494
TS-MN	-386.93074	-386.93134	-386.93054	-386.93062	-386.93005	-386.93115
M	-387.00049	-386.99960	-387.00083	-387.00067	-387.00042	-387.00095
N	-386.98247	-386.98211	-386.98340	-386.98172	-386.98365	-386.98145

Table S29: Total energies (in Hartee) of various molecules in the isomer set for Hartree–Fock (HF) and CASSCI methods

Molecule	**HF/ STO-3G**	**CASCI(2,2)/ STO-3G**	**CASCI(4,4)/ STO-3G**	**CASCI(6,6)/ STO-3G**	**HF/ 6-31G**	**CASCI(2,2)/ 6-31G**	**CASCI(4,4)/ 6-31G**	**CASCI(6,6)/ 6-31G**
1	-383.51261	-383.51308	-383.51355	-383.51473	-387.86394	-387.86396	-387.86400	-387.86416
exo-2	-383.48273	-383.48278	-383.48415	-383.48543	-387.83917	-387.83917	-387.83924	-387.83930
endo-2	-383.47549	-383.47583	-383.47658	-383.47775	-387.83136	-387.83140	-387.83145	-387.83150
3	-383.49254	-383.49261	-383.49308	-383.49420	-387.84545	-387.84547	-387.84552	-387.84558
4	-383.48359	-383.48396	-383.48460	-383.48532	-387.83579	-387.83580	-387.83586	-387.83590
syn-5	-383.49347	-383.49351	-383.49443	-383.49617	-387.84690	-387.84691	-387.84696	-387.84703
anti-5	-383.39370	-383.39386	-383.39496	-383.39622	-387.76035	-387.76037	-387.76041	-387.76069
syn-6	-383.48775	-383.48781	-383.48818	-383.48928	-387.84156	-387.84158	-387.84163	-387.84168
anti-6	-383.40164	-383.40189	-383.40267	-383.40365	-387.76514	-387.76516	-387.76522	-387.76529
7	-383.46785	-383.46861	-383.46947	-383.47047	-387.82529	-387.82530	-387.82535	-387.82541
exo-8	-383.47965	-383.47972	-383.48093	-383.48233	-387.83561	-387.83562	-387.83566	-387.83575
endo-8	-383.46395	-383.46434	-383.46541	-383.46687	-387.82192	-387.82193	-387.82199	-387.82206
9	-383.46075	-383.46099	-383.46148	-383.46240	-387.81648	-387.81650	-387.81655	-387.81660
10	-383.47065	-383.47080	-383.47107	-383.47216	-387.82474	-387.82474	-387.82478	-387.82488
syn-11	-383.45433	-383.45442	-383.45521	-383.45671	-387.81024	-387.81025	-387.81029	-387.81035
anti-11	-383.47090	-383.47099	-383.47173	-383.47265	-387.82680	-387.82681	-387.82685	-387.82694
12	-383.49028	-383.49066	-383.49155	-383.49250	-387.84450	-387.84452	-387.84455	-387.84463
13	-383.47917	-383.47927	-383.48021	-383.48127	-387.83410	-387.83412	-387.83418	-387.83423
14	-383.47840	-383.47843	-383.47902	-383.48016	-387.83237	-387.83240	-387.83243	-387.83254
18	-383.48741	-383.48767	-383.48783	-383.48825	-387.84139	-387.84140	-387.84145	-387.84154
19	-383.49133	-383.49139	-383.49212	-383.49292	-387.84386	-387.84388	-387.84392	-387.84398

Table S30: Total energies (in Hartee) of various molecules in the reaction set for Hartree–Fock (HF) and CASCI methods

Molecule	**HF/ STO-3G**	**CASCI(2,2)/ STO-3G**	**CASCI(4,4)/ STO-3G**	**CASCI(6,6)/ STO-3G**	**HF/ 6-31G**	**CASCI(2,2)/ 6-31G**	**CASCI(4,4)/ 6-31G**	**CASCI(6,6)/ 6-31G**
A	-382.65919	-382.65923	-382.65945	-382.66306	-386.99379	-386.99385	-386.99403	-386.99506
TS-AA'	-382.62591	-382.62661	-382.62757	-382.62859	-386.96381	-386.96465	-386.96512	-386.96566
A'	-382.65919	-382.65923	-382.65945	-382.66306	-386.99379	-386.99385	-386.99403	-386.99506
F	-382.62000	-382.62001	-382.62004	-382.62123	-386.96160	-386.96162	-386.96168	-386.96215
TS-FG	-382.61290	-382.61291	-382.61301	-382.61398	-386.95329	-386.95329	-386.95347	-386.95380
G	-382.66094	-382.66218	-382.66417	-382.66543	-386.99696	-386.99790	-386.99805	-386.99822
TS-GG'	-382.64868	-382.65254	-382.65672	-382.65790	-386.98903	-386.99145	-386.99383	-386.99460
G'	-382.66094	-382.66218	-382.66417	-382.66543	-386.99696	-386.99790	-386.99805	-386.99822
J	-382.65929	-382.66271	-382.66705	-382.66816	-386.99781	-387.00041	-387.00110	-387.00172
TS-JK	-382.60705	-382.60714	-382.60722	-382.60773	-386.94955	-386.94971	-386.94981	-386.94997
K	-382.64066	-382.64066	-382.64082	-382.64116	-386.98326	-386.98326	-386.98330	-386.98375
TS-KL	-382.63815	-382.63828	-382.63904	-382.63945	-386.97994	-386.98027	-386.98067	-386.98105
L	-382.64999	-382.65000	-382.65009	-382.65039	-386.98571	-386.98573	-386.98580	-386.98604
TS-LM	-382.54171	-382.54245	-382.54347	-382.54603	-386.89178	-386.89263	-386.89314	-386.89403
TS-LN	-382.62329	-382.62330	-382.62332	-382.62356	-386.95596	-386.95598	-386.95600	-386.95606
TS-MN	-382.58622	-382.58657	-382.58708	-382.58762	-386.93034	-386.93102	-386.93127	-386.93148
M	-382.66722	-382.66735	-382.66774	-382.66870	-387.00049	-387.00067	-387.00079	-387.00109
N	-382.64500	-382.64521	-382.64563	-382.64578	-386.98233	-386.98256	-386.98261	-386.98267

Table S31: Total energies (in Hartee) of various molecules in the isomer set for density functional theory based methods with STO-3G basis set

Molecule	**BLYP-D3BJ**	**B3LYP-D3BJ**	**CAM-B3LYP-D3BJ**	**LCωPBE-D3BJ**	**ωB97xD**	**M06-2X**
1	-385.85214	-386.14840	-385.88301	-385.94900	-386.07447	-386.11216
exo-2	-385.82193	-386.11717	-385.85237	-385.91942	-386.04462	-386.08018
endo-2	-385.81727	-386.11206	-385.84705	-385.91355	-386.03897	-386.07413
3	-385.83423	-386.12975	-385.86447	-385.93063	-386.05602	-386.09328
4	-385.82642	-386.12208	-385.85717	-385.92438	-386.04790	-386.08698
syn-5	-385.83199	-386.12717	-385.86220	-385.92828	-386.05489	-386.08887
anti-5	-385.74743	-386.03882	-385.77266	-385.83814	-385.96503	-385.99962
syn-6	-385.82890	-386.12409	-385.85896	-385.92507	-386.05099	-386.08671
anti-6	-385.75742	-386.04977	-385.78384	-385.85075	-385.97490	-386.01284
7	-385.81038	-386.10502	-385.83990	-385.90712	-386.03197	-386.06777
exo-8	-385.81930	-386.11436	-385.84947	-385.91661	-386.04172	-386.07689
endo-8	-385.80674	-386.10129	-385.83617	-385.90335	-386.02815	-386.06391
9	-385.80672	-386.10123	-385.83592	-385.90235	-386.02725	-386.06497
10	-385.81686	-386.11167	-385.84635	-385.91260	-386.03705	-386.07548
syn-11	-385.80332	-386.09738	-385.83196	-385.89787	-386.02266	-386.06031
anti-11	-385.81597	-386.11100	-385.84594	-385.91294	-386.03693	-386.07577
12	-385.83122	-386.12662	-385.86146	-385.92802	-386.05336	-386.08986
13	-385.82019	-386.11538	-385.85045	-385.91730	-386.04221	-386.07873
14	-385.81968	-386.11470	-385.84974	-385.91610	-386.04153	-386.07736
18	-385.82918	-386.12421	-385.85880	-385.92433	-386.05101	-386.08663
19	-385.83161	-386.12702	-385.86198	-385.92813	-386.05339	-386.08958

Table S32: Total energies (in Hartee) of various molecules in the reaction set for density functional theory based methods with STO-3G basis set

Molecule	**BLYP-D3BJ**	**B3LYP-D3BJ**	**CAM-B3LYP-D3BJ**	**LCωPBE-D3BJ**	**ωB97xD**	**M06-2X**
A	-384.97418	-385.24871	-384.98365	-385.03453	-385.17094	-385.20956
TS-AA'	-384.94096	-385.21669	-384.95342	-385.00747	-385.14132	-385.18308
A'	-384.97418	-385.24871	-384.98365	-385.03453	-385.17094	-385.20956
F	-384.94296	-385.21744	-384.95285	-385.00560	-385.14098	-385.18302
TS-FG	-384.93245	-385.20660	-384.94180	-384.99435	-385.12925	-385.16998
G	-384.97688	-385.25159	-384.98663	-385.03803	-385.17399	-385.21312
TS-GG'	-384.97036	-385.24501	-384.98028	-385.03230	-385.16841	-385.20991
G'	-384.97688	-385.25159	-384.98663	-385.03803	-385.17399	-385.21312
J	-384.98174	-385.25553	-384.98955	-385.03948	-385.17689	-385.21754
TS-JK	-384.92750	-385.20213	-384.93793	-384.99069	-385.12537	-385.16770
K	-384.96425	-385.23823	-384.97224	-385.02208	-385.15939	-385.20080
TS-KL	-384.96444	-385.23792	-384.97156	-385.02055	-385.15853	-385.20085
L	-384.97251	-385.24696	-384.98154	-385.03156	-385.16868	-385.21099
TS-LM	-384.88303	-385.15335	-384.88643	-384.93617	-385.07370	-385.11676
TS-LN	-384.94120	-385.21856	-384.95620	-385.01348	-385.14418	-385.18823
TS-MN	-384.91754	-385.19059	-384.92513	-384.97711	-385.11182	-385.15632
M	-384.98907	-385.26295	-384.99635	-385.04583	-385.18281	-385.22406
N	-384.96674	-385.24045	-384.97409	-385.02311	-385.16014	-385.20125

Table S33: Total energies (in Hartee) of various molecules in the isomer set for HWE-1(2,2)/STO-3G calculations on noisy *FakeQuito* backend without any error mitigation

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
1	-383.44570	-383.44636	-383.44464	-383.45137	-383.44424	-383.44233	-383.44225	-383.44792	-383.44119	-383.44987	-383.44683
exo-2	-383.41742	-383.41985	-383.41608	-383.40939	-383.41813	-383.41483	-383.41725	-383.41782	-383.42187	-383.42414	-383.41485
endo-2	-383.41038	-383.40848	-383.41266	-383.41291	-383.40649	-383.41025	-383.41337	-383.40752	-383.40755	-383.41138	-383.41320
3	-383.42713	-383.43118	-383.43323	-383.42785	-383.42779	-383.42411	-383.42450	-383.42654	-383.42333	-383.42329	-383.42949
4	-383.42059	-383.42072	-383.42162	-383.42590	-383.41701	-383.41934	-383.41610	-383.42288	-383.42367	-383.41620	-383.42243
syn-5	-383.42977	-383.42964	-383.43344	-383.42951	-383.42737	-383.42804	-383.42864	-383.43276	-383.42940	-383.42996	-383.42899
anti-5	-383.33654	-383.34171	-383.33067	-383.34135	-383.33663	-383.33806	-383.33435	-383.33614	-383.33638	-383.33694	-383.33313
syn-6	-383.42224	-383.42201	-383.42211	-383.42566	-383.42036	-383.42178	-383.41972	-383.42159	-383.41919	-383.43063	-383.41933
anti-6	-383.34209	-383.34152	-383.34012	-383.34947	-383.34150	-383.34839	-383.33999	-383.33754	-383.34228	-383.33799	-383.34212
7	-383.40782	-383.41154	-383.40738	-383.40190	-383.40294	-383.40923	-383.40713	-383.41027	-383.40925	-383.40879	-383.40979
exo-8	-383.41936	-383.41733	-383.41930	-383.42128	-383.42179	-383.41316	-383.41878	-383.41739	-383.42478	-383.42088	-383.41890
endo-8	-383.40566	-383.40490	-383.40134	-383.41096	-383.40142	-383.41018	-383.40340	-383.41115	-383.40165	-383.40384	-383.40773
9	-383.39584	-383.39437	-383.40207	-383.38928	-383.39494	-383.39515	-383.39846	-383.39876	-383.39513	-383.39360	-383.39668
10	-383.40729	-383.40278	-383.40719	-383.40880	-383.40918	-383.40679	-383.40487	-383.41021	-383.40595	-383.40694	-383.41015
syn-11	-383.39041	-383.39418	-383.39321	-383.38608	-383.38906	-383.39519	-383.39369	-383.38452	-383.38873	-383.38596	-383.39348
anti-11	-383.40841	-383.40521	-383.41486	-383.40697	-383.40832	-383.40441	-383.40304	-383.41182	-383.41267	-383.40902	-383.40774
12	-383.42659	-383.42372	-383.42846	-383.42851	-383.42630	-383.42984	-383.42323	-383.42203	-383.43112	-383.42543	-383.42725
13	-383.41522	-383.41698	-383.42228	-383.41592	-383.41008	-383.41445	-383.42085	-383.40842	-383.41177	-383.41649	-383.41495
14	-383.41689	-383.42049	-383.42054	-383.41884	-383.41546	-383.41466	-383.41532	-383.41793	-383.41585	-383.41337	-383.41646
18	-383.42207	-383.41878	-383.42057	-383.41800	-383.42196	-383.42466	-383.42767	-383.42108	-383.42541	-383.42028	-383.42225
19	-383.42662	-383.41942	-383.42619	-383.42941	-383.43076	-383.42775	-383.43019	-383.42486	-383.42857	-383.42391	-383.42514

Table S34: Total energies (in Hartee) of various molecules in the isomer set for HWE-2(2,2)/STO-3G calculations on noisy *FakeQuito* backend without any error mitigation

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
1	-383.42512	-383.42082	-383.42429	-383.43347	-383.42677	-383.42167	-383.42287	-383.42349	-383.42730	-383.42693	-383.42354
exo-2	-383.40445	-383.40114	-383.40131	-383.40183	-383.40168	-383.40841	-383.40134	-383.41227	-383.40304	-383.40424	-383.40926
endo-2	-383.39758	-383.39233	-383.40220	-383.39412	-383.39586	-383.40106	-383.39919	-383.40139	-383.40333	-383.39753	-383.38879
3	-383.40956	-383.41260	-383.40790	-383.40771	-383.41002	-383.40735	-383.41112	-383.40403	-383.41755	-383.40744	-383.40991
4	-383.40386	-383.41296	-383.40103	-383.39694	-383.40648	-383.40102	-383.40530	-383.40754	-383.40203	-383.39734	-383.40801
syn-5	-383.41328	-383.40932	-383.41070	-383.42287	-383.41539	-383.40654	-383.41706	-383.40659	-383.41844	-383.41591	-383.40991
anti-5	-383.32249	-383.32854	-383.31777	-383.32429	-383.31717	-383.31612	-383.32409	-383.32303	-383.32094	-383.32656	-383.32635
syn-6	-383.40752	-383.41148	-383.40337	-383.40887	-383.41128	-383.41468	-383.40462	-383.40492	-383.40936	-383.40537	-383.40121
anti-6	-383.32743	-383.32440	-383.32857	-383.33133	-383.33018	-383.32907	-383.32458	-383.32993	-383.32203	-383.32293	-383.33131
7	-383.39472	-383.39370	-383.39445	-383.39431	-383.39279	-383.39845	-383.39685	-383.38899	-383.39127	-383.40462	-383.39180
exo-8	-383.40226	-383.40922	-383.39802	-383.40634	-383.40329	-383.40633	-383.40171	-383.40220	-383.40359	-383.39699	-383.39489
endo-8	-383.39071	-383.39714	-383.38636	-383.38621	-383.39565	-383.38409	-383.38976	-383.39065	-383.39040	-383.39904	-383.38777
9	-383.38061	-383.38378	-383.38423	-383.38419	-383.37426	-383.38052	-383.38152	-383.37958	-383.37745	-383.38270	-383.37782
10	-383.39202	-383.39091	-383.39158	-383.39198	-383.38777	-383.39512	-383.39646	-383.39608	-383.38941	-383.38945	-383.39146
syn-11	-383.37566	-383.37583	-383.37714	-383.37886	-383.37598	-383.37680	-383.37553	-383.37269	-383.37671	-383.37144	-383.37564
anti-11	-383.39448	-383.39247	-383.39755	-383.39452	-383.38516	-383.39242	-383.39652	-383.39264	-383.39690	-383.39515	-383.40147
12	-383.40946	-383.40761	-383.40369	-383.40903	-383.41166	-383.40502	-383.41242	-383.41766	-383.40798	-383.41279	-383.40674
13	-383.39783	-383.39725	-383.39727	-383.39044	-383.39163	-383.39726	-383.40054	-383.40009	-383.40441	-383.40206	-383.39734
14	-383.40003	-383.39475	-383.40067	-383.40749	-383.39938	-383.39536	-383.39992	-383.40132	-383.39460	-383.39945	-383.40732
18	-383.40386	-383.40418	-383.41149	-383.40112	-383.40077	-383.40703	-383.40436	-383.41258	-383.39788	-383.40325	-383.39593
19	-383.40845	-383.40196	-383.41305	-383.40772	-383.40888	-383.41159	-383.40696	-383.40098	-383.41242	-383.41449	-383.40643

Table S35: Total energies (in Hartee) of various molecules in the isomer set for ESU2-RY(2,2)/STO-3G calculations on noisy *FakeQuito* backend without any error mitigation

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
1	-383.44503	-383.44669	-383.44495	-383.44145	-383.44247	-383.44307	-383.44777	-383.44448	-383.44831	-383.44422	-383.44686
exo-2	-383.42012	-383.41554	-383.41777	-383.41597	-383.41795	-383.42373	-383.42308	-383.42232	-383.42015	-383.42731	-383.41736
endo-2	-383.40871	-383.41103	-383.40736	-383.40953	-383.40718	-383.40652	-383.41377	-383.40765	-383.40394	-383.41202	-383.40809
3	-383.42624	-383.42313	-383.42414	-383.42640	-383.42582	-383.42515	-383.42815	-383.42980	-383.42799	-383.42559	-383.42618
4	-383.41982	-383.41846	-383.42291	-383.41992	-383.42720	-383.41551	-383.41720	-383.41635	-383.41828	-383.42075	-383.42165
syn-5	-383.42840	-383.42425	-383.42656	-383.43212	-383.43123	-383.42892	-383.42984	-383.42645	-383.42898	-383.42989	-383.42573
anti-5	-383.33284	-383.33492	-383.33301	-383.33115	-383.33101	-383.33606	-383.33337	-383.33261	-383.33320	-383.33228	-383.33074
syn-6	-383.42139	-383.42694	-383.42188	-383.41906	-383.42746	-383.41589	-383.41623	-383.42638	-383.42311	-383.41676	-383.42016
anti-6	-383.34263	-383.34791	-383.34478	-383.34570	-383.33982	-383.34561	-383.34483	-383.33937	-383.33565	-383.33755	-383.34510
7	-383.40915	-383.40593	-383.40680	-383.40992	-383.41325	-383.40390	-383.41058	-383.41178	-383.41095	-383.41401	-383.40441
exo-8	-383.41602	-383.41558	-383.41955	-383.42063	-383.41426	-383.41288	-383.41533	-383.41698	-383.41172	-383.41648	-383.41677
endo-8	-383.40362	-383.40069	-383.40780	-383.40595	-383.40506	-383.40423	-383.40396	-383.40143	-383.40260	-383.40526	-383.39919
9	-383.39648	-383.39611	-383.39632	-383.39578	-383.39254	-383.39928	-383.39244	-383.39931	-383.39723	-383.39575	-383.40006
10	-383.40737	-383.40547	-383.40329	-383.40326	-383.41083	-383.40872	-383.40818	-383.40792	-383.40570	-383.41070	-383.40962
syn-11	-383.39185	-383.39180	-383.39291	-383.39376	-383.38887	-383.39426	-383.38613	-383.39362	-383.38695	-383.39340	-383.39681
anti-11	-383.40697	-383.41096	-383.40550	-383.40767	-383.40510	-383.40804	-383.39995	-383.41162	-383.40729	-383.40566	-383.40793
12	-383.42441	-383.42455	-383.42173	-383.42115	-383.42546	-383.42959	-383.42672	-383.42209	-383.41889	-383.42858	-383.42529
13	-383.41645	-383.41524	-383.41628	-383.41781	-383.41807	-383.41191	-383.41816	-383.42021	-383.41380	-383.41612	-383.41688
14	-383.41627	-383.41498	-383.41588	-383.42076	-383.41993	-383.41248	-383.41494	-383.41460	-383.41678	-383.41372	-383.41865
18	-383.42014	-383.41937	-383.42183	-383.41910	-383.41783	-383.42355	-383.41817	-383.41764	-383.42275	-383.41793	-383.42321
19	-383.42625	-383.42886	-383.42371	-383.42998	-383.42873	-383.43367	-383.42360	-383.42127	-383.42217	-383.42634	-383.42414

Table S36: Total energies (in Hartee) of various molecules in the isomer set for ESU2-RYRZ(2,2)/STO-3G calculations on noisy *FakeQuito* backend without any error mitigation

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
1	-383.44416	-383.44199	-383.44942	-383.44646	-383.44548	-383.44028	-383.44199	-383.44733	-383.44020	-383.44046	-383.44802
exo-2	-383.41820	-383.41574	-383.42036	-383.42109	-383.41614	-383.41844	-383.41388	-383.41553	-383.42221	-383.41821	-383.42034
endo-2	-383.41073	-383.41454	-383.41015	-383.40785	-383.41236	-383.41073	-383.41057	-383.40402	-383.41165	-383.41893	-383.40648
3	-383.42852	-383.42985	-383.42818	-383.42492	-383.42708	-383.42509	-383.42700	-383.43627	-383.42666	-383.42491	-383.43526
4	-383.42129	-383.42247	-383.42333	-383.42894	-383.41675	-383.41992	-383.41986	-383.41741	-383.42447	-383.42134	-383.41839
syn-5	-383.43081	-383.43412	-383.43227	-383.42306	-383.42816	-383.42936	-383.42459	-383.43563	-383.43348	-383.43345	-383.43394
anti-5	-383.33450	-383.33698	-383.33519	-383.33584	-383.33364	-383.33943	-383.33475	-383.33150	-383.32981	-383.33535	-383.33249
syn-6	-383.42173	-383.41976	-383.42366	-383.41982	-383.42242	-383.42100	-383.42352	-383.42174	-383.42417	-383.41919	-383.42201
anti-6	-383.34132	-383.34343	-383.34379	-383.33803	-383.33945	-383.33976	-383.34274	-383.33852	-383.34430	-383.34194	-383.34120
7	-383.41046	-383.40847	-383.41138	-383.40696	-383.40585	-383.41103	-383.41326	-383.41183	-383.41587	-383.41071	-383.40920
exo-8	-383.41940	-383.41724	-383.41813	-383.41423	-383.41860	-383.42162	-383.42474	-383.42254	-383.42221	-383.41351	-383.42114
endo-8	-383.40363	-383.39825	-383.40279	-383.40697	-383.39979	-383.39940	-383.40002	-383.40565	-383.41005	-383.40481	-383.40855
9	-383.39770	-383.39774	-383.39798	-383.39406	-383.39931	-383.39675	-383.39530	-383.39635	-383.39909	-383.39795	-383.40246
10	-383.40631	-383.40337	-383.40845	-383.40527	-383.40649	-383.40341	-383.40950	-383.40946	-383.40299	-383.40604	-383.40810
syn-11	-383.38948	-383.38631	-383.39161	-383.39299	-383.38865	-383.39127	-383.38904	-383.38588	-383.38644	-383.38866	-383.39391
anti-11	-383.40907	-383.40891	-383.41153	-383.40642	-383.41213	-383.41080	-383.40926	-383.40532	-383.40888	-383.40749	-383.40991
12	-383.42309	-383.41918	-383.42652	-383.42803	-383.41930	-383.42794	-383.42249	-383.41998	-383.42233	-383.42139	-383.42376
13	-383.41632	-383.40812	-383.41804	-383.41916	-383.41654	-383.41508	-383.41167	-383.42396	-383.41814	-383.41672	-383.41576
14	-383.41523	-383.41213	-383.41552	-383.41659	-383.41292	-383.42032	-383.41845	-383.41386	-383.41274	-383.41639	-383.41335
18	-383.42260	-383.42489	-383.42139	-383.42075	-383.42365	-383.42285	-383.41796	-383.42358	-383.42535	-383.42501	-383.42060
19	-383.42577	-383.42945	-383.42511	-383.43268	-383.42232	-383.42855	-383.42524	-383.42222	-383.42435	-383.42498	-383.42274

Table S37: Total energies (in Hartee) of various molecules in the isomer set for EXCT. PRESERV.(2,2)/STO-3G calculations on noisy *FakeQuito* backend without any error mitigation

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
1	-383.41276	-383.41929	-383.41240	-383.40761	-383.41372	-383.41775	-383.40981	-383.41057	-383.41410	-383.41216	-383.41017
exo-2	-383.39006	-383.39296	-383.38872	-383.38868	-383.39310	-383.38846	-383.38874	-383.39306	-383.38813	-383.38912	-383.38961
endo-2	-383.38115	-383.38445	-383.38097	-383.38477	-383.37882	-383.38143	-383.37909	-383.38002	-383.37965	-383.37913	-383.38314
3	-383.39654	-383.40096	-383.39709	-383.39631	-383.39584	-383.40199	-383.39786	-383.39599	-383.39591	-383.39472	-383.38870
4	-383.39553	-383.39545	-383.38830	-383.39883	-383.39508	-383.39689	-383.39860	-383.39238	-383.39327	-383.39907	-383.39746
syn-5	-383.40165	-383.40161	-383.40240	-383.40111	-383.40161	-383.39601	-383.40176	-383.40248	-383.40136	-383.40197	-383.40619
anti-5	-383.30694	-383.31085	-383.30412	-383.30575	-383.30766	-383.30721	-383.30833	-383.30341	-383.30535	-383.30651	-383.31023
syn-6	-383.39170	-383.39607	-383.38948	-383.39633	-383.39207	-383.38834	-383.38537	-383.39515	-383.39318	-383.39291	-383.38812
anti-6	-383.31651	-383.31915	-383.31983	-383.31277	-383.31600	-383.31643	-383.31100	-383.31907	-383.31704	-383.31754	-383.31624
7	-383.38249	-383.38228	-383.37912	-383.38535	-383.38365	-383.38550	-383.38182	-383.38269	-383.37977	-383.38316	-383.38154
exo-8	-383.39031	-383.38516	-383.38745	-383.38691	-383.39088	-383.38855	-383.39286	-383.39704	-383.39238	-383.39130	-383.39052
endo-8	-383.37852	-383.38033	-383.37170	-383.38075	-383.37665	-383.38061	-383.37863	-383.37780	-383.38062	-383.38216	-383.37595
9	-383.36759	-383.36544	-383.36705	-383.37182	-383.36809	-383.36951	-383.36312	-383.36676	-383.36812	-383.36766	-383.36833
10	-383.37757	-383.38093	-383.37105	-383.37984	-383.37914	-383.37871	-383.37970	-383.37452	-383.37541	-383.38197	-383.37447
syn-11	-383.36523	-383.36523	-383.36818	-383.36418	-383.36639	-383.36111	-383.36600	-383.36268	-383.36671	-383.36404	-383.36781
anti-11	-383.37972	-383.37705	-383.37806	-383.37972	-383.37968	-383.37845	-383.38311	-383.37804	-383.38351	-383.37749	-383.38209
12	-383.39598	-383.39797	-383.39131	-383.39832	-383.39571	-383.39533	-383.39842	-383.39808	-383.39627	-383.39288	-383.39554
13	-383.38832	-383.38665	-383.38705	-383.38928	-383.39189	-383.39104	-383.38907	-383.38738	-383.38766	-383.38930	-383.38387
14	-383.38842	-383.39064	-383.38964	-383.38898	-383.38267	-383.38480	-383.39455	-383.38863	-383.38746	-383.38869	-383.38817
18	-383.39171	-383.39241	-383.39205	-383.39467	-383.39194	-383.39185	-383.38996	-383.38774	-383.39449	-383.39097	-383.39099
19	-383.39594	-383.39441	-383.39498	-383.39860	-383.39643	-383.39697	-383.39624	-383.39471	-383.39731	-383.39411	-383.39565

Table S38: Total energies (in Hartee) of various molecules in the reaction set for HWE-1(2,2)/STO-3G calculations on noisy *FakeQuito* backend without any error mitigation

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
A	-382.62805	-382.62656	-382.62767	-382.63096	-382.62991	-382.63018	-382.62642	-382.62744	-382.62515	-382.62942	-382.62677
TS-AA'	-382.59112	-382.59020	-382.59046	-382.59233	-382.58857	-382.59267	-382.58991	-382.59403	-382.59178	-382.58974	-382.59152
A'	-382.62661	-382.62783	-382.63019	-382.62803	-382.62398	-382.62724	-382.62600	-382.62720	-382.62777	-382.62056	-382.62730
F	-382.57766	-382.57477	-382.57545	-382.58295	-382.58229	-382.57495	-382.57688	-382.57697	-382.57819	-382.57671	-382.57737
TS-FG	-382.57498	-382.57551	-382.57562	-382.57720	-382.57736	-382.57493	-382.56966	-382.57852	-382.57573	-382.57401	-382.57127
G	-382.63205	-382.63277	-382.63365	-382.63093	-382.62979	-382.63398	-382.63271	-382.63199	-382.62964	-382.63180	-382.63320
TS-GG'	-382.61738	-382.61849	-382.61743	-382.61421	-382.61744	-382.61503	-382.61828	-382.61673	-382.61628	-382.62136	-382.61856
G'	-382.63169	-382.63295	-382.63137	-382.63137	-382.62928	-382.63164	-382.63309	-382.63097	-382.63516	-382.62782	-382.63326
J	-382.63232	-382.63096	-382.63426	-382.63070	-382.63476	-382.63245	-382.63233	-382.63303	-382.63282	-382.62901	-382.63291
TS-JK	-382.57200	-382.57133	-382.57164	-382.57298	-382.57345	-382.57382	-382.56780	-382.56983	-382.57462	-382.57296	-382.57157
K	-382.60567	-382.60371	-382.60683	-382.60545	-382.60393	-382.60601	-382.60649	-382.60603	-382.60471	-382.60853	-382.60503
TS-KL	-382.60590	-382.60619	-382.60955	-382.60640	-382.60572	-382.60297	-382.60298	-382.60928	-382.60598	-382.60740	-382.60249
L	-382.61354	-382.61267	-382.61492	-382.61514	-382.61185	-382.61333	-382.61178	-382.61320	-382.61304	-382.61597	-382.61349
TS-LM	-382.51657	-382.51804	-382.51671	-382.51650	-382.51513	-382.51609	-382.51680	-382.51807	-382.51626	-382.51741	-382.51470
TS-LN	-382.58043	-382.58099	-382.58086	-382.58181	-382.57883	-382.57660	-382.58335	-382.58031	-382.58367	-382.57757	-382.58025
TS-MN	-382.55373	-382.55523	-382.54742	-382.55509	-382.55360	-382.55774	-382.55464	-382.55413	-382.55177	-382.55555	-382.55212
M	-382.63735	-382.63773	-382.63413	-382.63429	-382.63842	-382.64026	-382.63832	-382.63735	-382.63715	-382.64058	-382.63526
N	-382.61522	-382.61319	-382.61559	-382.60902	-382.61768	-382.61589	-382.61663	-382.61567	-382.61686	-382.61606	-382.61557

Table S39: Total energies (in Hartee) of various molecules in the reaction set for HWE-2(2,2)/STO-3G calculations on noisy *FakeQuito* backend without any error mitigation

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
A	-382.61892	-382.61754	-382.61684	-382.62005	-382.62163	-382.61634	-382.62077	-382.62165	-382.61793	-382.62076	-382.61564
TS-AA'	-382.58247	-382.57796	-382.58734	-382.58899	-382.58211	-382.58449	-382.58477	-382.57854	-382.58160	-382.57929	-382.57961
A'	-382.61691	-382.61264	-382.61492	-382.62065	-382.62174	-382.61798	-382.61724	-382.61552	-382.61211	-382.61805	-382.61824
F	-382.56435	-382.56363	-382.56959	-382.56506	-382.56844	-382.56511	-382.56059	-382.56154	-382.56078	-382.56219	-382.56661
TS-FG	-382.56510	-382.56907	-382.56783	-382.56987	-382.56188	-382.56165	-382.56140	-382.56388	-382.56275	-382.56220	-382.57043
G	-382.62352	-382.61758	-382.62356	-382.62671	-382.62039	-382.62425	-382.62362	-382.62036	-382.62283	-382.62861	-382.62729
TS-GG'	-382.60802	-382.61188	-382.61077	-382.60716	-382.60806	-382.60667	-382.61064	-382.60904	-382.60738	-382.60156	-382.60703
G'	-382.62322	-382.62670	-382.62407	-382.62100	-382.62173	-382.61898	-382.62430	-382.62354	-382.62258	-382.62372	-382.62560
J	-382.62522	-382.62175	-382.62899	-382.62513	-382.62190	-382.62462	-382.62580	-382.62391	-382.62520	-382.62723	-382.62770
TS-JK	-382.56355	-382.55820	-382.56394	-382.56277	-382.56996	-382.56352	-382.55481	-382.56583	-382.56039	-382.56935	-382.56676
K	-382.59403	-382.59344	-382.59497	-382.59500	-382.59755	-382.59914	-382.59043	-382.59332	-382.59011	-382.59457	-382.59181
TS-KL	-382.59760	-382.59983	-382.59323	-382.60068	-382.60465	-382.59433	-382.59875	-382.59239	-382.59679	-382.59615	-382.59917
L	-382.60308	-382.60948	-382.60384	-382.60097	-382.60189	-382.61057	-382.60028	-382.59764	-382.60330	-382.60304	-382.59976
TS-LM	-382.50904	-382.51176	-382.50977	-382.51113	-382.50716	-382.51214	-382.51125	-382.50491	-382.50611	-382.50731	-382.50889
TS-LN	-382.56572	-382.56863	-382.56791	-382.56127	-382.56761	-382.56974	-382.57543	-382.56380	-382.56251	-382.56159	-382.55873
TS-MN	-382.54363	-382.54466	-382.54061	-382.53722	-382.54477	-382.54079	-382.53922	-382.54745	-382.54733	-382.54693	-382.54735
M	-382.62888	-382.62739	-382.62677	-382.63134	-382.63320	-382.62913	-382.62653	-382.62780	-382.63405	-382.62638	-382.62625
N	-382.60563	-382.60491	-382.60554	-382.60644	-382.60690	-382.61013	-382.60385	-382.59791	-382.61135	-382.60612	-382.60315

Table S40: Total energies (in Hartee) of various molecules in the reaction set for ESU2-RY(2,2)/STO-3G calculations on noisy *FakeQuito* backend without any error mitigation

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
A	-382.62774	-382.62828	-382.62553	-382.62842	-382.62748	-382.62596	-382.62602	-382.62966	-382.63147	-382.62674	-382.62784
TS-AA'	-382.59097	-382.59086	-382.59121	-382.58930	-382.59167	-382.59089	-382.59082	-382.59178	-382.59215	-382.59298	-382.58806
A'	-382.62801	-382.62820	-382.63009	-382.62526	-382.62626	-382.62922	-382.62764	-382.62730	-382.62999	-382.62714	-382.62903
F	-382.57709	-382.57457	-382.57910	-382.57436	-382.57397	-382.58024	-382.57953	-382.57161	-382.57763	-382.58231	-382.57755
TS-FG	-382.57624	-382.57532	-382.57314	-382.57575	-382.57600	-382.57314	-382.57648	-382.57794	-382.57881	-382.57728	-382.57850
G	-382.63174	-382.63460	-382.63315	-382.62828	-382.63307	-382.62995	-382.63406	-382.62968	-382.63107	-382.63377	-382.62979
TS-GG'	-382.61752	-382.62090	-382.61871	-382.61870	-382.61851	-382.61384	-382.61461	-382.61761	-382.61811	-382.61831	-382.61595
G'	-382.63094	-382.63217	-382.62328	-382.62902	-382.63293	-382.63203	-382.63293	-382.63341	-382.63063	-382.63095	-382.63200
J	-382.63233	-382.63200	-382.63441	-382.62753	-382.62970	-382.63452	-382.63283	-382.63282	-382.63256	-382.63435	-382.63259
TS-JK	-382.57162	-382.57391	-382.56928	-382.57155	-382.57108	-382.57517	-382.57539	-382.56977	-382.57178	-382.56973	-382.56853
K	-382.60561	-382.60514	-382.60636	-382.60616	-382.60404	-382.60686	-382.60443	-382.60527	-382.60829	-382.60671	-382.60286
TS-KL	-382.60589	-382.60492	-382.60611	-382.60462	-382.60586	-382.60494	-382.60672	-382.60683	-382.60832	-382.60491	-382.60567
L	-382.61317	-382.61468	-382.61418	-382.61116	-382.60852	-382.61427	-382.61200	-382.61292	-382.61499	-382.61708	-382.61189
TS-LM	-382.51546	-382.51514	-382.51508	-382.51739	-382.51631	-382.51599	-382.51429	-382.51335	-382.51529	-382.51699	-382.51476
TS-LN	-382.57880	-382.58337	-382.58236	-382.57608	-382.57503	-382.57250	-382.57890	-382.57801	-382.57439	-382.58310	-382.58423
TS-MN	-382.55281	-382.55517	-382.55245	-382.55564	-382.54908	-382.55250	-382.55310	-382.54915	-382.55445	-382.55424	-382.55233
M	-382.63737	-382.63660	-382.63576	-382.63597	-382.63749	-382.63875	-382.63515	-382.64063	-382.63873	-382.63735	-382.63723
N	-382.61599	-382.61599	-382.61583	-382.61486	-382.61494	-382.61630	-382.61506	-382.61777	-382.61726	-382.61598	-382.61589

Table S41: Total energies (in Hartee) of various molecules in the reaction set for ESU2-RYRZ(2,2)/STO-3G calculations on noisy *FakeQuito* backend without any error mitigation

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
A	-382.62834	-382.62418	-382.62958	-382.62983	-382.62873	-382.62952	-382.62947	-382.62831	-382.62929	-382.62606	-382.62841
TS-AA'	-382.58987	-382.58848	-382.58787	-382.59040	-382.59360	-382.58828	-382.58879	-382.58944	-382.58905	-382.59082	-382.59195
A'	-382.62794	-382.62875	-382.62996	-382.62768	-382.62618	-382.62910	-382.62840	-382.62831	-382.62633	-382.62749	-382.62717
F	-382.57626	-382.57477	-382.57457	-382.57876	-382.57413	-382.57644	-382.57631	-382.57705	-382.57904	-382.57615	-382.57541
TS-FG	-382.57583	-382.57948	-382.57020	-382.57457	-382.57552	-382.57445	-382.57441	-382.57787	-382.57516	-382.57849	-382.57817
G	-382.63169	-382.62672	-382.63606	-382.63209	-382.63167	-382.63143	-382.63362	-382.62976	-382.63280	-382.63221	-382.63057
TS-GG'	-382.61619	-382.62059	-382.61432	-382.61935	-382.61997	-382.61536	-382.61320	-382.61454	-382.61795	-382.61414	-382.61248
G'	-382.63044	-382.63181	-382.62733	-382.62795	-382.63428	-382.63157	-382.62659	-382.63253	-382.62995	-382.63149	-382.63087
J	-382.63049	-382.63063	-382.63147	-382.63198	-382.63104	-382.62865	-382.62240	-382.63178	-382.63122	-382.63360	-382.63211
TS-JK	-382.57108	-382.56803	-382.57177	-382.57174	-382.57421	-382.56863	-382.57385	-382.56742	-382.56986	-382.57395	-382.57133
K	-382.60542	-382.60309	-382.60811	-382.60198	-382.60463	-382.60582	-382.60633	-382.60450	-382.60563	-382.60574	-382.60838
TS-KL	-382.60531	-382.60559	-382.60603	-382.60648	-382.60658	-382.59792	-382.60392	-382.60551	-382.60840	-382.60636	-382.60635
L	-382.61400	-382.61343	-382.61297	-382.61166	-382.61339	-382.61350	-382.61287	-382.61549	-382.61564	-382.61465	-382.61642
TS-LM	-382.51569	-382.51373	-382.51264	-382.51666	-382.51784	-382.51458	-382.51810	-382.51909	-382.51643	-382.51545	-382.51234
TS-LN	-382.57885	-382.57756	-382.58167	-382.57675	-382.57949	-382.58140	-382.57880	-382.57792	-382.57806	-382.57892	-382.57798
TS-MN	-382.55313	-382.55084	-382.55258	-382.55316	-382.55240	-382.55416	-382.55342	-382.55400	-382.55382	-382.55304	-382.55385
M	-382.63670	-382.63714	-382.63862	-382.63935	-382.63821	-382.63563	-382.63688	-382.63456	-382.63391	-382.63340	-382.63926
N	-382.61548	-382.61585	-382.61513	-382.61346	-382.61322	-382.61663	-382.61615	-382.61748	-382.61615	-382.61361	-382.61708

Table S42: Total energies (in Hartee) of various molecules in the reaction set for EXCT. PRESERV.(2,2)/STO-3G calculations on noisy *FakeQuito* backend without any error mitigation

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
A	-382.61140	-382.60922	-382.60963	-382.61226	-382.61148	-382.60912	-382.61275	-382.61236	-382.61325	-382.61246	-382.61143
TS-AA'	-382.57504	-382.57329	-382.57637	-382.57423	-382.57635	-382.57600	-382.57633	-382.57141	-382.57534	-382.57527	-382.57581
A'	-382.61139	-382.61354	-382.60835	-382.60983	-382.61064	-382.61204	-382.61205	-382.61257	-382.61383	-382.61062	-382.61038
F	-382.55390	-382.55530	-382.55526	-382.55090	-382.55444	-382.54887	-382.55809	-382.55534	-382.55390	-382.55180	-382.55506
TS-FG	-382.55821	-382.55879	-382.55657	-382.55780	-382.55886	-382.55980	-382.55804	-382.55911	-382.55845	-382.55632	-382.55836
G	-382.61716	-382.61779	-382.61744	-382.61612	-382.61756	-382.61886	-382.61605	-382.61648	-382.61693	-382.61823	-382.61616
TS-GG'	-382.59926	-382.60031	-382.59944	-382.60222	-382.59999	-382.60039	-382.60220	-382.59914	-382.59904	-382.59240	-382.59748
G'	-382.61647	-382.61618	-382.61691	-382.61614	-382.61719	-382.61585	-382.61626	-382.61751	-382.61360	-382.61807	-382.61703
J	-382.61796	-382.61702	-382.61960	-382.61687	-382.61991	-382.61648	-382.61805	-382.61855	-382.61690	-382.61598	-382.62020
TS-JK	-382.55434	-382.55371	-382.55594	-382.55434	-382.55410	-382.55538	-382.55342	-382.55438	-382.55295	-382.55351	-382.55571
K	-382.58730	-382.58689	-382.58738	-382.58555	-382.58624	-382.58783	-382.58856	-382.58759	-382.58776	-382.58685	-382.58835
TS-KL	-382.58963	-382.58998	-382.58905	-382.59122	-382.58772	-382.59071	-382.59129	-382.58896	-382.58739	-382.58980	-382.59022
L	-382.59503	-382.59490	-382.59589	-382.59558	-382.59296	-382.59389	-382.59445	-382.59504	-382.59479	-382.59536	-382.59745
TS-LM	-382.50363	-382.50351	-382.50262	-382.50344	-382.50334	-382.50185	-382.50439	-382.50359	-382.50395	-382.50465	-382.50491
TS-LN	-382.55695	-382.55319	-382.55688	-382.55891	-382.55949	-382.55769	-382.55465	-382.55839	-382.55475	-382.55836	-382.55718
TS-MN	-382.53666	-382.53619	-382.53728	-382.53623	-382.53649	-382.53934	-382.53697	-382.53685	-382.53396	-382.53710	-382.53618
M	-382.62293	-382.62507	-382.62350	-382.62447	-382.62329	-382.62190	-382.62217	-382.62141	-382.62029	-382.62326	-382.62393
N	-382.60016	-382.60038	-382.59973	-382.60101	-382.60159	-382.60014	-382.59890	-382.60021	-382.60071	-382.59872	-382.60024

Table S43: Total energies (in Hartee) of various molecules in the isomer set for HWE-1(2,2)/STO-3G calculations on noisy *FakeQuito* backend with state tomography correction applied

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
1	-383.51203	-383.51222	-383.51288	-383.51278	-383.51092	-383.51177	-383.51260	-383.51107	-383.51269	-383.51253	-383.51082
exo-2	-383.48188	-383.48166	-383.48220	-383.48252	-383.48209	-383.48175	-383.48142	-383.48193	-383.48099	-383.48176	-383.48249
endo-2	-383.47490	-383.47455	-383.47528	-383.47500	-383.47520	-383.47554	-383.47447	-383.47445	-383.47432	-383.47563	-383.47458
3	-383.49133	-383.49253	-383.49123	-383.49166	-383.49079	-383.49255	-383.48790	-383.49212	-383.49208	-383.49168	-383.49078
4	-383.48305	-383.48388	-383.48372	-383.48350	-383.48288	-383.48377	-383.48268	-383.48252	-383.48171	-383.48348	-383.48235
syn-5	-383.49216	-383.48854	-383.49262	-383.49316	-383.49238	-383.49258	-383.49251	-383.49105	-383.49349	-383.49242	-383.49282
anti-5	-383.39295	-383.39299	-383.39373	-383.39232	-383.39340	-383.39254	-383.39341	-383.39316	-383.39229	-383.39271	-383.39296
syn-6	-383.48697	-383.48706	-383.48733	-383.48557	-383.48731	-383.48672	-383.48689	-383.48758	-383.48767	-383.48711	-383.48648
anti-6	-383.40061	-383.40127	-383.39742	-383.40095	-383.40177	-383.40139	-383.40165	-383.40133	-383.40082	-383.40038	-383.39913
7	-383.46731	-383.46728	-383.46824	-383.46777	-383.46816	-383.46601	-383.46790	-383.46822	-383.46795	-383.46590	-383.46569
exo-8	-383.47922	-383.47849	-383.47963	-383.47855	-383.47946	-383.47936	-383.47866	-383.47936	-383.47945	-383.47962	-383.47960
endo-8	-383.46332	-383.46367	-383.46376	-383.46120	-383.46366	-383.46372	-383.46306	-383.46327	-383.46311	-383.46412	-383.46365
9	-383.46021	-383.46020	-383.46006	-383.46015	-383.46074	-383.45890	-383.46070	-383.46054	-383.46059	-383.45973	-383.46053
10	-383.46985	-383.46878	-383.46939	-383.47067	-383.46986	-383.46827	-383.47029	-383.47059	-383.47001	-383.47039	-383.47022
syn-11	-383.45363	-383.45376	-383.45368	-383.45299	-383.45392	-383.45368	-383.45298	-383.45425	-383.45378	-383.45364	-383.45362
anti-11	-383.47005	-383.47073	-383.47051	-383.46963	-383.46937	-383.46978	-383.46904	-383.47009	-383.47060	-383.47056	-383.47018
12	-383.48905	-383.48214	-383.48974	-383.49051	-383.48876	-383.49014	-383.49022	-383.49038	-383.49023	-383.48907	-383.48931
13	-383.47817	-383.47905	-383.47716	-383.47852	-383.47864	-383.47595	-383.47880	-383.47807	-383.47745	-383.47891	-383.47915
14	-383.47733	-383.47770	-383.47786	-383.47821	-383.47784	-383.47227	-383.47802	-383.47803	-383.47820	-383.47737	-383.47777
18	-383.48723	-383.48708	-383.48755	-383.48760	-383.48762	-383.48681	-383.48699	-383.48747	-383.48743	-383.48660	-383.48711
19	-383.49053	-383.49109	-383.49075	-383.49057	-383.49049	-383.49132	-383.49070	-383.49109	-383.49071	-383.48863	-383.48992

Table S44: Total energies (in Hartee) of various molecules in the isomer set for HWE-2(2,2)/STO-3G calculations on noisy *FakeQuito* backend with state tomography correction applied

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
1	-383.51174	-383.51182	-383.51055	-383.51275	-383.51302	-383.51253	-383.51110	-383.51274	-383.51014	-383.51035	-383.51239
exo-2	-383.48134	-383.48164	-383.48024	-383.48241	-383.48016	-383.48187	-383.48222	-383.48264	-383.48051	-383.48096	-383.48071
endo-2	-383.47465	-383.47522	-383.47551	-383.47571	-383.47483	-383.47564	-383.47134	-383.47483	-383.47264	-383.47510	-383.47570
3	-383.49182	-383.49058	-383.49223	-383.49252	-383.49243	-383.49198	-383.49030	-383.49172	-383.49231	-383.49204	-383.49207
4	-383.48332	-383.48257	-383.48307	-383.48367	-383.48352	-383.48318	-383.48354	-383.48316	-383.48388	-383.48299	-383.48367
syn-5	-383.49237	-383.49335	-383.49305	-383.49315	-383.49238	-383.49200	-383.49255	-383.49192	-383.49326	-383.49222	-383.48985
anti-5	-383.39262	-383.39340	-383.38746	-383.39359	-383.39096	-383.39268	-383.39352	-383.39369	-383.39358	-383.39368	-383.39362
syn-6	-383.48680	-383.48706	-383.48705	-383.48742	-383.48732	-383.48767	-383.48627	-383.48667	-383.48684	-383.48519	-383.48653
anti-6	-383.40074	-383.40168	-383.39544	-383.40049	-383.40158	-383.40111	-383.40142	-383.40161	-383.40168	-383.40136	-383.40102
7	-383.46758	-383.46728	-383.46770	-383.46828	-383.46817	-383.46825	-383.46752	-383.46842	-383.46711	-383.46549	-383.46763
exo-8	-383.47876	-383.47715	-383.47944	-383.47946	-383.47812	-383.47959	-383.47954	-383.47931	-383.47756	-383.47786	-383.47953
endo-8	-383.46393	-383.46416	-383.46413	-383.46393	-383.46396	-383.46390	-383.46424	-383.46406	-383.46403	-383.46356	-383.46332
9	-383.46011	-383.46058	-383.45868	-383.46027	-383.46077	-383.45909	-383.46052	-383.46019	-383.45975	-383.46078	-383.46044
10	-383.46938	-383.47045	-383.46993	-383.46767	-383.47020	-383.47031	-383.47008	-383.46823	-383.46962	-383.46989	-383.46744
syn-11	-383.45266	-383.45359	-383.45347	-383.45235	-383.45397	-383.45391	-383.45429	-383.44480	-383.45386	-383.45206	-383.45434
anti-11	-383.47035	-383.47077	-383.46927	-383.47037	-383.46982	-383.47093	-383.47091	-383.47004	-383.47064	-383.47015	-383.47062
12	-383.48971	-383.49038	-383.49014	-383.48856	-383.48820	-383.48998	-383.49007	-383.48911	-383.49061	-383.48952	-383.49051
13	-383.47809	-383.47802	-383.47617	-383.47813	-383.47891	-383.47816	-383.47901	-383.47838	-383.47853	-383.47715	-383.47847
14	-383.47712	-383.47748	-383.47789	-383.47453	-383.47787	-383.47824	-383.47778	-383.47620	-383.47753	-383.47605	-383.47765
18	-383.48697	-383.48721	-383.48687	-383.48719	-383.48640	-383.48621	-383.48712	-383.48706	-383.48688	-383.48731	-383.48744
19	-383.49014	-383.48906	-383.49090	-383.48769	-383.49084	-383.49051	-383.48983	-383.49040	-383.49041	-383.49067	-383.49110

Table S45: Total energies (in Hartee) of various molecules in the isomer set for ESU2-RY(2,2)/STO-3G calculations on noisy *FakeQuito* backend with state tomography correction applied

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
1	-383.51191	-383.51141	-383.51149	-383.51189	-383.51205	-383.51215	-383.51211	-383.51199	-383.51245	-383.51185	-383.51168
exo-2	-383.48164	-383.48203	-383.48191	-383.48186	-383.48180	-383.48211	-383.48183	-383.48025	-383.48199	-383.48063	-383.48199
endo-2	-383.47337	-383.47355	-383.46884	-383.47293	-383.46839	-383.47514	-383.47510	-383.47498	-383.47465	-383.47502	-383.47506
3	-383.49161	-383.49170	-383.49194	-383.49167	-383.49199	-383.49162	-383.49049	-383.49148	-383.49126	-383.49208	-383.49187
4	-383.48292	-383.48293	-383.48114	-383.48341	-383.48327	-383.48334	-383.48203	-383.48308	-383.48325	-383.48353	-383.48318
syn-5	-383.49209	-383.49277	-383.49252	-383.48942	-383.49273	-383.49220	-383.49287	-383.49176	-383.49251	-383.49156	-383.49260
anti-5	-383.39301	-383.39303	-383.39293	-383.39317	-383.39314	-383.39284	-383.39316	-383.39269	-383.39295	-383.39316	-383.39297
syn-6	-383.48686	-383.48698	-383.48716	-383.48676	-383.48668	-383.48697	-383.48675	-383.48700	-383.48679	-383.48674	-383.48678
anti-6	-383.40095	-383.40097	-383.40092	-383.40128	-383.40113	-383.40091	-383.40123	-383.40093	-383.39964	-383.40113	-383.40138
7	-383.46715	-383.46745	-383.46735	-383.46812	-383.46680	-383.46317	-383.46729	-383.46768	-383.46782	-383.46797	-383.46784
exo-8	-383.47797	-383.47883	-383.47916	-383.47897	-383.47912	-383.47833	-383.47928	-383.46922	-383.47880	-383.47905	-383.47897
endo-8	-383.46327	-383.46378	-383.46300	-383.46358	-383.46365	-383.46358	-383.46377	-383.46371	-383.46338	-383.46070	-383.46359
9	-383.46007	-383.45984	-383.46047	-383.46000	-383.45999	-383.45984	-383.45999	-383.46013	-383.46002	-383.46017	-383.46029
10	-383.46974	-383.46989	-383.46941	-383.46998	-383.46992	-383.46991	-383.46953	-383.46962	-383.46986	-383.47002	-383.46926
syn-11	-383.45339	-383.45184	-383.45349	-383.45359	-383.45348	-383.45381	-383.45350	-383.45292	-383.45384	-383.45347	-383.45395
anti-11	-383.46991	-383.46987	-383.47050	-383.46999	-383.46986	-383.47028	-383.47019	-383.46891	-383.46939	-383.47020	-383.46986
12	-383.48969	-383.48873	-383.48951	-383.48931	-383.48971	-383.49021	-383.48991	-383.49004	-383.48988	-383.48981	-383.48978
13	-383.47806	-383.47792	-383.47770	-383.47876	-383.47834	-383.47863	-383.47887	-383.47522	-383.47835	-383.47842	-383.47844
14	-383.47707	-383.47771	-383.47750	-383.47774	-383.47627	-383.47728	-383.47463	-383.47792	-383.47694	-383.47708	-383.47764
18	-383.48643	-383.48649	-383.48676	-383.48643	-383.48675	-383.48681	-383.48358	-383.48703	-383.48677	-383.48690	-383.48676
19	-383.49022	-383.49083	-383.49056	-383.49047	-383.49068	-383.49047	-383.49024	-383.48812	-383.49052	-383.48994	-383.49036

Table S46: Total energies (in Hartee) of various molecules in the isomer set for ESU2-RYRZ(2,2)/STO-3G calculations on noisy *FakeQuito* backend with state tomography correction applied

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
1	-383.51164	-383.51243	-383.51267	-383.51147	-383.50596	-383.51251	-383.51173	-383.51208	-383.51223	-383.51282	-383.51253
exo-2	-383.48183	-383.48162	-383.48224	-383.48259	-383.48234	-383.48160	-383.48105	-383.48218	-383.48256	-383.48251	-383.47959
endo-2	-383.47477	-383.47484	-383.47522	-383.47433	-383.47563	-383.47510	-383.47569	-383.47435	-383.47426	-383.47469	-383.47360
3	-383.49155	-383.49009	-383.49243	-383.49218	-383.49204	-383.49113	-383.49106	-383.49085	-383.49149	-383.49189	-383.49231
4	-383.48305	-383.48326	-383.48291	-383.48320	-383.48385	-383.48289	-383.48342	-383.48188	-383.48314	-383.48258	-383.48341
syn-5	-383.49269	-383.49282	-383.49294	-383.49264	-383.49229	-383.49344	-383.49018	-383.49332	-383.49308	-383.49274	-383.49341
anti-5	-383.39248	-383.39185	-383.39363	-383.39238	-383.39184	-383.39365	-383.39343	-383.39350	-383.39376	-383.38751	-383.39326
syn-6	-383.48672	-383.48738	-383.48738	-383.48719	-383.48607	-383.48733	-383.48752	-383.48658	-383.48766	-383.48675	-383.48339
anti-6	-383.40101	-383.40096	-383.40148	-383.40031	-383.40093	-383.40102	-383.40127	-383.40106	-383.40073	-383.40141	-383.40097
7	-383.46773	-383.46852	-383.46693	-383.46813	-383.46710	-383.46746	-383.46819	-383.46782	-383.46767	-383.46836	-383.46707
exo-8	-383.47815	-383.47903	-383.47852	-383.47020	-383.47850	-383.47961	-383.47945	-383.47884	-383.47886	-383.47889	-383.47961
endo-8	-383.46272	-383.46366	-383.46373	-383.46321	-383.46401	-383.46237	-383.45748	-383.46383	-383.46310	-383.46319	-383.46261
9	-383.46017	-383.46054	-383.46023	-383.46028	-383.46043	-383.45979	-383.46041	-383.45968	-383.45920	-383.46066	-383.46053
10	-383.46989	-383.46984	-383.46984	-383.46962	-383.47006	-383.47053	-383.47019	-383.46979	-383.46900	-383.47059	-383.46946
syn-11	-383.45378	-383.45407	-383.45305	-383.45418	-383.45418	-383.45372	-383.45427	-383.45329	-383.45428	-383.45323	-383.45350
anti-11	-383.47001	-383.47065	-383.47077	-383.46883	-383.47082	-383.47021	-383.47018	-383.46998	-383.47083	-383.46708	-383.47078
12	-383.48952	-383.48967	-383.48924	-383.48998	-383.48935	-383.48829	-383.48951	-383.48993	-383.48976	-383.48947	-383.49004
13	-383.47850	-383.47864	-383.47885	-383.47820	-383.47834	-383.47699	-383.47868	-383.47900	-383.47873	-383.47873	-383.47881
14	-383.47699	-383.47791	-383.47807	-383.47788	-383.47782	-383.46880	-383.47815	-383.47780	-383.47826	-383.47804	-383.47718
18	-383.48710	-383.48648	-383.48753	-383.48679	-383.48752	-383.48758	-383.48731	-383.48668	-383.48728	-383.48735	-383.48644
19	-383.49011	-383.48931	-383.49052	-383.48920	-383.49112	-383.49085	-383.49120	-383.49133	-383.48815	-383.48967	-383.48976

Table S47: Total energies (in Hartee) of various molecules in the isomer set for EXCT. PRESERV.(2,2)/STO-3G calculations on noisy *FakeQuito* backend with state tomography correction applied

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
1	-383.51112	-383.51186	-383.51083	-383.51134	-383.51052	-383.51060	-383.51100	-383.51110	-383.51168	-383.51120	-383.51107
exo-2	-383.48087	-383.48085	-383.48170	-383.48138	-383.48015	-383.48108	-383.48064	-383.48050	-383.48078	-383.48119	-383.48049
endo-2	-383.47387	-383.47381	-383.47466	-383.47341	-383.47429	-383.47443	-383.47365	-383.47368	-383.47370	-383.47384	-383.47318
3	-383.49078	-383.49040	-383.49100	-383.49118	-383.49054	-383.49066	-383.49081	-383.49097	-383.49103	-383.49015	-383.49106
4	-383.48187	-383.48190	-383.48211	-383.48051	-383.48198	-383.48149	-383.48176	-383.48267	-383.48182	-383.48232	-383.48213
syn-5	-383.49195	-383.49166	-383.49222	-383.49191	-383.49239	-383.49242	-383.49226	-383.49205	-383.49203	-383.49096	-383.49157
anti-5	-383.39217	-383.39151	-383.39249	-383.39230	-383.39244	-383.39209	-383.39177	-383.39190	-383.39260	-383.39231	-383.39226
syn-6	-383.48619	-383.48561	-383.48667	-383.48676	-383.48648	-383.48613	-383.48609	-383.48625	-383.48600	-383.48610	-383.48578
anti-6	-383.39996	-383.39971	-383.39993	-383.40058	-383.39961	-383.39866	-383.40008	-383.40040	-383.40022	-383.40034	-383.40008
7	-383.46671	-383.46639	-383.46637	-383.46726	-383.46680	-383.46649	-383.46674	-383.46715	-383.46618	-383.46698	-383.46671
exo-8	-383.47789	-383.47767	-383.47794	-383.47751	-383.47824	-383.47800	-383.47735	-383.47781	-383.47849	-383.47755	-383.47832
endo-8	-383.46256	-383.46201	-383.46225	-383.46322	-383.46218	-383.46295	-383.46243	-383.46278	-383.46314	-383.46236	-383.46231
9	-383.45928	-383.45890	-383.45909	-383.45983	-383.45920	-383.45907	-383.45923	-383.45913	-383.45932	-383.45971	-383.45933
10	-383.46877	-383.46902	-383.46914	-383.46846	-383.46853	-383.46918	-383.46864	-383.46903	-383.46888	-383.46850	-383.46832
syn-11	-383.45282	-383.45238	-383.45216	-383.45285	-383.45245	-383.45298	-383.45253	-383.45361	-383.45304	-383.45349	-383.45269
anti-11	-383.46915	-383.46914	-383.46923	-383.46914	-383.46973	-383.46894	-383.46836	-383.46970	-383.46952	-383.46906	-383.46872
12	-383.48863	-383.48894	-383.48844	-383.48816	-383.48904	-383.48820	-383.48890	-383.48820	-383.48829	-383.48848	-383.48968
13	-383.47741	-383.47709	-383.47728	-383.47715	-383.47713	-383.47780	-383.47773	-383.47715	-383.47740	-383.47766	-383.47769
14	-383.47640	-383.47605	-383.47603	-383.47593	-383.47634	-383.47635	-383.47633	-383.47715	-383.47655	-383.47639	-383.47686
18	-383.48587	-383.48647	-383.48580	-383.48547	-383.48575	-383.48607	-383.48546	-383.48568	-383.48636	-383.48606	-383.48562
19	-383.48967	-383.48957	-383.49004	-383.48999	-383.48996	-383.48912	-383.48911	-383.48950	-383.48966	-383.49003	-383.48970

Table S48: Total energies (in Hartee) of various molecules in the reaction set for HWE-1(2,2)/STO-3G calculations on noisy *FakeQuito* backend with state tomography correction applied

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
A	-382.65886	-382.65868	-382.65862	-382.65901	-382.65909	-382.65907	-382.65889	-382.65875	-382.65903	-382.65890	-382.65854
TS-AA'	-382.62589	-382.62527	-382.62610	-382.62604	-382.62598	-382.62634	-382.62597	-382.62552	-382.62531	-382.62658	-382.62573
A'	-382.65861	-382.65794	-382.65893	-382.65917	-382.65912	-382.65867	-382.65895	-382.65730	-382.65880	-382.65851	-382.65871
F	-382.61940	-382.61988	-382.61949	-382.61879	-382.61925	-382.61965	-382.61992	-382.61977	-382.61933	-382.61907	-382.61880
TS-FG	-382.61167	-382.61265	-382.60962	-382.61239	-382.61235	-382.61019	-382.60997	-382.61210	-382.61281	-382.61213	-382.61252
G	-382.66068	-382.66151	-382.66169	-382.66037	-382.65947	-382.66179	-382.65889	-382.66040	-382.66166	-382.66074	-382.66032
TS-GG'	-382.65069	-382.64872	-382.65230	-382.65104	-382.65059	-382.64988	-382.65021	-382.65143	-382.65226	-382.64827	-382.65220
G'	-382.66068	-382.66162	-382.66054	-382.66162	-382.66103	-382.66128	-382.66158	-382.65568	-382.66118	-382.66074	-382.66151
J	-382.66095	-382.65934	-382.66113	-382.66179	-382.66210	-382.66264	-382.66268	-382.66051	-382.66229	-382.65747	-382.65958
TS-JK	-382.60632	-382.60651	-382.60688	-382.60707	-382.60678	-382.60656	-382.60419	-382.60663	-382.60681	-382.60486	-382.60696
K	-382.64020	-382.64002	-382.64034	-382.64011	-382.64036	-382.64037	-382.63990	-382.64064	-382.64053	-382.63925	-382.64050
TS-KL	-382.63656	-382.63471	-382.63562	-382.63679	-382.63819	-382.63815	-382.63077	-382.63781	-382.63741	-382.63811	-382.63805
L	-382.64887	-382.64981	-382.64994	-382.64975	-382.64146	-382.64966	-382.64944	-382.64957	-382.64949	-382.64990	-382.64966
TS-LM	-382.54187	-382.54162	-382.54210	-382.54200	-382.54137	-382.54185	-382.54201	-382.54194	-382.54191	-382.54223	-382.54171
TS-LN	-382.62193	-382.62325	-382.62283	-382.62271	-382.62209	-382.62285	-382.61388	-382.62314	-382.62324	-382.62268	-382.62262
TS-MN	-382.58419	-382.58621	-382.57797	-382.58450	-382.58274	-382.58610	-382.58611	-382.58076	-382.58536	-382.58605	-382.58611
M	-382.66705	-382.66719	-382.66641	-382.66701	-382.66684	-382.66726	-382.66706	-382.66726	-382.66729	-382.66691	-382.66721
N	-382.64441	-382.64479	-382.64459	-382.64425	-382.64373	-382.64489	-382.64452	-382.64449	-382.64423	-382.64359	-382.64497

Table S49: Total energies (in Hartee) of various molecules in the reaction set for HWE-2(2,2)/STO-3G calculations on noisy *FakeQuito* backend with state tomography correction applied

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
A	-382.65833	-382.65837	-382.65891	-382.65897	-382.65903	-382.65807	-382.65733	-382.65891	-382.65891	-382.65582	-382.65900
TS-AA'	-382.62543	-382.62451	-382.62591	-382.62417	-382.62660	-382.62533	-382.62631	-382.62406	-382.62508	-382.62638	-382.62592
A'	-382.65810	-382.65892	-382.65891	-382.65865	-382.65444	-382.65852	-382.65841	-382.65847	-382.65882	-382.65843	-382.65742
F	-382.61912	-382.61876	-382.61751	-382.61734	-382.61970	-382.61989	-382.61986	-382.61944	-382.61958	-382.61939	-382.61977
TS-FG	-382.61136	-382.61230	-382.61216	-382.61229	-382.60892	-382.61231	-382.61262	-382.61272	-382.60529	-382.61230	-382.61271
G	-382.66176	-382.66192	-382.66092	-382.66182	-382.66196	-382.66172	-382.66197	-382.66208	-382.66176	-382.66186	-382.66162
TS-GG'	-382.65106	-382.64626	-382.65250	-382.65116	-382.65241	-382.64675	-382.65221	-382.65225	-382.65248	-382.65226	-382.65232
G'	-382.66133	-382.66213	-382.66146	-382.66143	-382.66199	-382.66070	-382.66162	-382.66155	-382.66054	-382.66169	-382.66020
J	-382.66123	-382.65583	-382.66258	-382.66110	-382.66260	-382.66216	-382.66031	-382.66160	-382.66228	-382.66127	-382.66253
TS-JK	-382.60634	-382.60527	-382.60690	-382.60710	-382.60690	-382.60708	-382.60586	-382.60509	-382.60587	-382.60641	-382.60695
K	-382.64000	-382.64046	-382.63996	-382.63940	-382.64048	-382.64025	-382.64043	-382.64001	-382.64023	-382.63854	-382.64028
TS-KL	-382.63751	-382.63808	-382.63790	-382.63716	-382.63797	-382.63786	-382.63788	-382.63696	-382.63711	-382.63602	-382.63813
L	-382.64927	-382.64980	-382.64819	-382.64894	-382.64973	-382.64981	-382.64916	-382.64855	-382.64991	-382.64936	-382.64926
TS-LM	-382.54144	-382.54202	-382.54181	-382.53844	-382.54230	-382.54223	-382.54030	-382.54181	-382.54236	-382.54084	-382.54226
TS-LN	-382.62198	-382.62255	-382.62310	-382.62306	-382.62035	-382.62158	-382.62199	-382.61954	-382.62216	-382.62307	-382.62242
TS-MN	-382.58529	-382.58427	-382.58606	-382.58408	-382.58588	-382.58512	-382.58559	-382.58363	-382.58632	-382.58585	-382.58608
M	-382.66552	-382.66657	-382.66732	-382.66715	-382.66664	-382.66720	-382.66491	-382.66704	-382.66503	-382.65831	-382.66499
N	-382.64338	-382.63906	-382.64497	-382.64310	-382.64470	-382.64418	-382.64510	-382.64337	-382.64516	-382.63962	-382.64459

Table S50: Total energies (in Hartee) of various molecules in the reaction set for ESU2-RY(2,2)/STO-3G calculations on noisy *FakeQuito* backend with state tomography correction applied

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
A	-382.65854	-382.65886	-382.65824	-382.65872	-382.65832	-382.65870	-382.65897	-382.65892	-382.65885	-382.65697	-382.65890
TS-AA'	-382.62505	-382.62607	-382.62597	-382.62613	-382.62617	-382.62398	-382.62614	-382.62607	-382.61799	-382.62605	-382.62596
A'	-382.65843	-382.65865	-382.65846	-382.65875	-382.65833	-382.65604	-382.65864	-382.65868	-382.65885	-382.65900	-382.65891
F	-382.61886	-382.61896	-382.61530	-382.61946	-382.61926	-382.61966	-382.61940	-382.61894	-382.61911	-382.61963	-382.61892
TS-FG	-382.61134	-382.61195	-382.61172	-382.61254	-382.61251	-382.61180	-382.61233	-382.61210	-382.60535	-382.61199	-382.61110
G	-382.66149	-382.66173	-382.66180	-382.66162	-382.66189	-382.66133	-382.66128	-382.66167	-382.66058	-382.66179	-382.66126
TS-GG'	-382.65155	-382.65221	-382.65204	-382.65198	-382.64679	-382.65220	-382.65207	-382.65231	-382.65181	-382.65201	-382.65206
G'	-382.66062	-382.66188	-382.66168	-382.65620	-382.66182	-382.66191	-382.66196	-382.65941	-382.66147	-382.65987	-382.66001
J	-382.66203	-382.66217	-382.66236	-382.66227	-382.66237	-382.66248	-382.66248	-382.66161	-382.65977	-382.66240	-382.66240
TS-JK	-382.60647	-382.60671	-382.60671	-382.60523	-382.60646	-382.60669	-382.60678	-382.60657	-382.60659	-382.60673	-382.60624
K	-382.63990	-382.64012	-382.64038	-382.64035	-382.63999	-382.64019	-382.64005	-382.63976	-382.63751	-382.64022	-382.64040
TS-KL	-382.63764	-382.63768	-382.63751	-382.63793	-382.63790	-382.63770	-382.63785	-382.63786	-382.63737	-382.63712	-382.63744
L	-382.64944	-382.64936	-382.64956	-382.64936	-382.64935	-382.64950	-382.64948	-382.64904	-382.64964	-382.64953	-382.64956
TS-LM	-382.54201	-382.54157	-382.54203	-382.54195	-382.54210	-382.54167	-382.54213	-382.54219	-382.54219	-382.54221	-382.54205
TS-LN	-382.62261	-382.62288	-382.62277	-382.62229	-382.62276	-382.62282	-382.62276	-382.62187	-382.62277	-382.62241	-382.62276
TS-MN	-382.58580	-382.58613	-382.58585	-382.58601	-382.58613	-382.58593	-382.58592	-382.58506	-382.58474	-382.58611	-382.58610
M	-382.66605	-382.65830	-382.66693	-382.66656	-382.66708	-382.66710	-382.66695	-382.66683	-382.66683	-382.66703	-382.66693
N	-382.64476	-382.64475	-382.64484	-382.64462	-382.64489	-382.64474	-382.64487	-382.64447	-382.64480	-382.64480	-382.64480

Table S51: Total energies (in Hartee) of various molecules in the reaction set for ESU2-RYRZ(2,2)/STO-3G calculations on noisy *FakeQuito* backend with state tomography correction applied

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
A	-382.65841	-382.65919	-382.65900	-382.65795	-382.65869	-382.65727	-382.65911	-382.65649	-382.65902	-382.65818	-382.65915
TS-AA'	-382.62552	-382.62410	-382.62613	-382.62646	-382.62614	-382.62626	-382.62590	-382.62561	-382.62565	-382.62607	-382.62289
A'	-382.65791	-382.65766	-382.65672	-382.65911	-382.65864	-382.65580	-382.65635	-382.65855	-382.65871	-382.65852	-382.65899
F	-382.61940	-382.61740	-382.61991	-382.61963	-382.61990	-382.61976	-382.61979	-382.61965	-382.61976	-382.61959	-382.61858
TS-FG	-382.61103	-382.61270	-382.61254	-382.61119	-382.61230	-382.61243	-382.61008	-382.60403	-382.60991	-382.61268	-382.61248
G	-382.66010	-382.65387	-382.66044	-382.66188	-382.65921	-382.66090	-382.66072	-382.66099	-382.66134	-382.66133	-382.66028
TS-GG'	-382.65022	-382.64955	-382.64798	-382.65152	-382.65107	-382.64786	-382.65240	-382.65169	-382.65069	-382.65152	-382.64791
G'	-382.66101	-382.66083	-382.66024	-382.66119	-382.66135	-382.66086	-382.66152	-382.66134	-382.66057	-382.66106	-382.66113
J	-382.66099	-382.66110	-382.65968	-382.66239	-382.66250	-382.66139	-382.66070	-382.66194	-382.65925	-382.66147	-382.65951
TS-JK	-382.60622	-382.60686	-382.60661	-382.60490	-382.60689	-382.60623	-382.60704	-382.60665	-382.60689	-382.60378	-382.60633
K	-382.63938	-382.63784	-382.64052	-382.63926	-382.63881	-382.63972	-382.64060	-382.64037	-382.64027	-382.63695	-382.63949
TS-KL	-382.63710	-382.63711	-382.63813	-382.63796	-382.63741	-382.63473	-382.63788	-382.63809	-382.63619	-382.63699	-382.63656
L	-382.64906	-382.64894	-382.64838	-382.64972	-382.64865	-382.64791	-382.64949	-382.64881	-382.64931	-382.64990	-382.64954
TS-LM	-382.54168	-382.54210	-382.54153	-382.54197	-382.54189	-382.54164	-382.54193	-382.54168	-382.54150	-382.54127	-382.54131
TS-LN	-382.62266	-382.62320	-382.62022	-382.62275	-382.62309	-382.62314	-382.62262	-382.62316	-382.62323	-382.62243	-382.62277
TS-MN	-382.58581	-382.58553	-382.58640	-382.58632	-382.58523	-382.58609	-382.58637	-382.58620	-382.58567	-382.58427	-382.58601
M	-382.66690	-382.66553	-382.66725	-382.66717	-382.66723	-382.66665	-382.66674	-382.66705	-382.66695	-382.66730	-382.66716
N	-382.64392	-382.64437	-382.63971	-382.64478	-382.64480	-382.64515	-382.64469	-382.64267	-382.64428	-382.64429	-382.64448

Table S52: Total energies (in Hartee) of various molecules in the reaction set for EXCT. PRESERV.(2,2)/STO-3G calculations on noisy *FakeQuito* backend with state tomography correction applied

Molecule	**Average**	**Run1**	**Run2**	**Run3**	**Run4**	**Run5**	**Run6**	**Run7**	**Run8**	**Run9**	**Run10**
A	-382.65827	-382.65803	-382.65768	-382.65816	-382.65830	-382.65821	-382.65860	-382.65817	-382.65846	-382.65869	-382.65841
TS-AA'	-382.62525	-382.62534	-382.62529	-382.62466	-382.62533	-382.62507	-382.62561	-382.62483	-382.62536	-382.62567	-382.62532
A'	-382.65832	-382.65820	-382.65869	-382.65808	-382.65837	-382.65858	-382.65807	-382.65858	-382.65763	-382.65865	-382.65834
F	-382.61880	-382.61855	-382.61907	-382.61905	-382.61867	-382.61899	-382.61862	-382.61878	-382.61857	-382.61856	-382.61910
TS-FG	-382.61193	-382.61183	-382.61154	-382.61194	-382.61207	-382.61191	-382.61188	-382.61186	-382.61215	-382.61209	-382.61207
G	-382.66142	-382.66178	-382.66156	-382.66107	-382.66145	-382.66135	-382.66171	-382.66072	-382.66128	-382.66172	-382.66155
TS-GG'	-382.65095	-382.65161	-382.65045	-382.65119	-382.65081	-382.65088	-382.65086	-382.65058	-382.65116	-382.65136	-382.65063
G'	-382.66117	-382.66075	-382.66144	-382.66155	-382.66155	-382.66104	-382.66154	-382.66057	-382.66163	-382.66078	-382.66085
J	-382.66122	-382.66168	-382.65810	-382.66079	-382.66232	-382.66227	-382.66150	-382.66066	-382.66024	-382.66231	-382.66237
TS-JK	-382.60609	-382.60632	-382.60618	-382.60607	-382.60631	-382.60521	-382.60623	-382.60598	-382.60659	-382.60623	-382.60576
K	-382.63977	-382.63966	-382.64010	-382.63963	-382.63997	-382.63986	-382.63940	-382.64007	-382.64002	-382.63969	-382.63928
TS-KL	-382.63727	-382.63724	-382.63709	-382.63763	-382.63744	-382.63717	-382.63725	-382.63753	-382.63696	-382.63718	-382.63716
L	-382.64900	-382.64904	-382.64925	-382.64883	-382.64845	-382.64912	-382.64882	-382.64896	-382.64929	-382.64916	-382.64907
TS-LM	-382.54127	-382.54151	-382.54149	-382.54162	-382.54095	-382.54116	-382.54078	-382.54083	-382.54191	-382.54060	-382.54181
TS-LN	-382.62199	-382.62244	-382.62154	-382.62223	-382.62166	-382.62143	-382.62175	-382.62186	-382.62235	-382.62219	-382.62242
TS-MN	-382.58546	-382.58491	-382.58602	-382.58526	-382.58558	-382.58524	-382.58565	-382.58584	-382.58548	-382.58523	-382.58544
M	-382.66647	-382.66638	-382.66638	-382.66633	-382.66671	-382.66640	-382.66616	-382.66623	-382.66655	-382.66692	-382.66663
N	-382.64438	-382.64443	-382.64397	-382.64478	-382.64434	-382.64376	-382.64432	-382.64465	-382.64459	-382.64448	-382.64453

Table S53: Total energies (in Hartee) of various molecules in the isomer set for EXCT. PRESERV.(2,2)/STO-3G calculations on noisy *ibmq_quito* device

Molecule	**None**	**STC**	**Statevector**
1	-383.42524	-383.51013	-383.51279
exo-2	-383.41282	-383.47895	-383.48273
endo-2	-383.39876	-383.47209	-383.47575
3	-383.41010	-383.49152	-383.49253
4	-383.43132	-383.48088	-383.48392
syn-5	-383.42507	-383.48572	-383.49351
anti-5	-383.32827	-383.39145	-383.39376
syn-6	-383.40219	-383.48697	-383.48779
anti-6	-383.34609	-383.39930	-383.40164
7	-383.41133	-383.46299	-383.46813
exo-8	-383.42402	-383.47477	-383.47964
endo-8	-383.40416	-383.45788	-383.46422
9	-383.38677	-383.45618	-383.46075
10	-383.41130	-383.46589	-383.47071
syn-11	-383.37798	-383.45167	-383.45443
anti-11	-383.39940	-383.46288	-383.47093
12	-383.42184	-383.48988	-383.49041
13	-383.41147	-383.47509	-383.47913
14	-383.40750	-383.47764	-383.47845
18	-383.39546	-383.48609	-383.48745
19	-383.42818	-383.49040	-383.49132

Table S54: Total energies (in Hartee) of various molecules in the reaction set for EXCT. PRESERV.(2,2)/STO-3G calculations on noisy *ibmq_quito* device

Molecule	**None**	**STC**	**Statevector**
A	-382.60557	-382.65688	-382.65921
TS-AA'	-382.55739	-382.62574	-382.62629
A'	-382.60342	-382.65485	-382.65915
F	-382.54360	-382.61811	-382.61999
TS-FG	-382.53630	-382.61255	-382.61290
G	-382.61620	-382.65854	-382.66174
TS-GG'	-382.59765	-382.64752	-382.65037
G'	-382.61122	-382.66030	-382.66121
J	-382.61043	-382.65805	-382.66163
TS-JK	-382.55401	-382.60634	-382.60710
K	-382.58724	-382.63934	-382.64066
TS-KL	-382.58363	-382.63595	-382.63820
L	-382.58723	-382.64911	-382.65000
TS-LM	-382.49882	-382.54111	-382.54203
TS-LN	-382.53977	-382.62226	-382.62330
TS-MN	-382.53296	-382.58413	-382.58636
M	-382.61950	-382.66527	-382.66722
N	-382.59739	-382.64413	-382.64514

Table S55: Comparison of literature molecular mechanics (MM) data of various molecules in the isomer set with reference (Ref) data computed using composite methods

MM order	ΔH_f^{iso}	**Ref order**	ΔE_{ref}^{iso}
1	0.0	1	0.0
syn-5	8.9	3	10.6
3	11.5	12	12.0
14	12.4	19	13.2
18	13.2	syn-5	13.4
19	13.9	18	14.1
12	13.9	syn-6	14.2
syn-6	14.7	4	14.7
exo-2	15.8	exo-2	15.1
exo-8	15.9	exo-8	17.3
13	16.8	13	17.6
4	19.3	14	19.1
endo-2	20.3	endo-2	19.2
7	21.7	anti-11	19.2
endo-8	22.2	10	20.9
anti-11	23.9	7	22.3
10	24.1	endo-8	23.9
9	26.0	9	25.5
syn-11	33.6	syn-11	28.6
–	–	anti-6	51.4
–	–	anti-5	58.8