Electronic Supplementary Material (ESI) for RSC Advances.


# Supporting information

# Additive Effect of Fluoroethylene and Difluoroethylene Carbonates for the Solid Electrolyte Interphase Film Formation in Sodium-Ion Batteries: A Quantum Chemical Study

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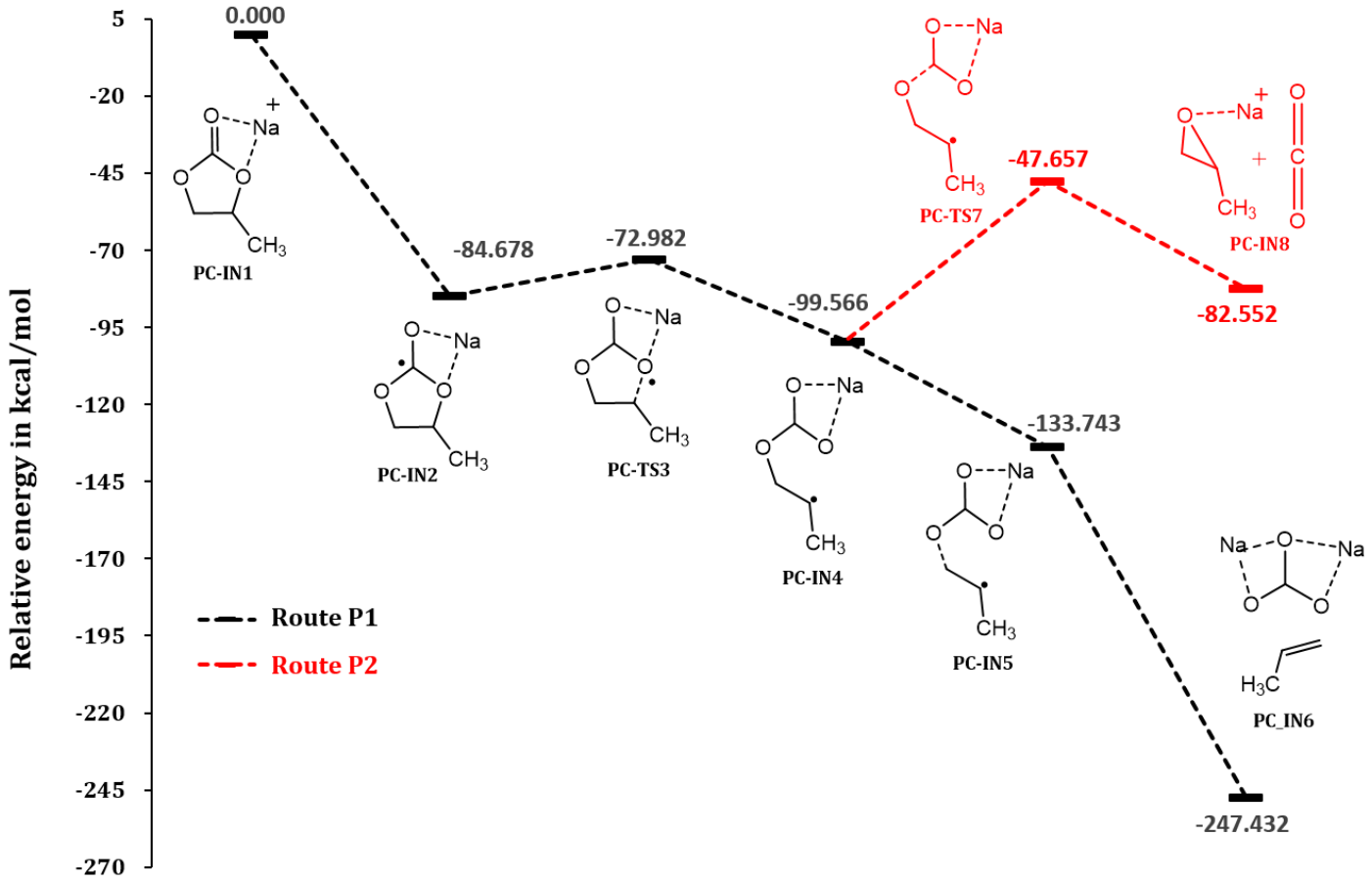



**Figure S1**: Potential energy profiles (ΔE in kcal/mol) for the possible reductive decomposition of $Na^+$- propylene carbonate ($Na^+$-PC) in gas phase.

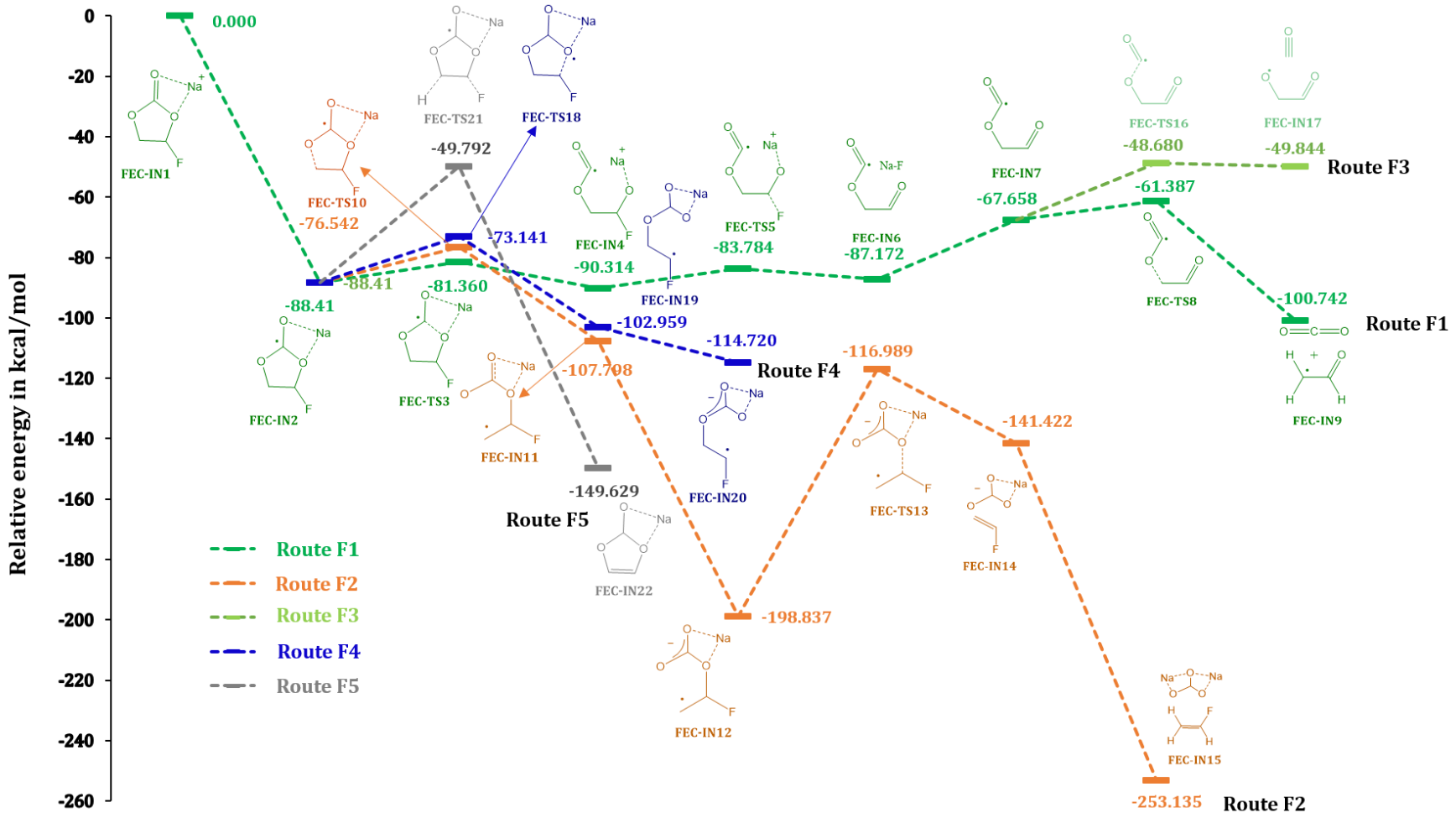



**Figure S2**: Potential energy profiles (ΔE in kcal/mol) for the possible reductive decomposition of $Na^+$- FEC in gas phase.

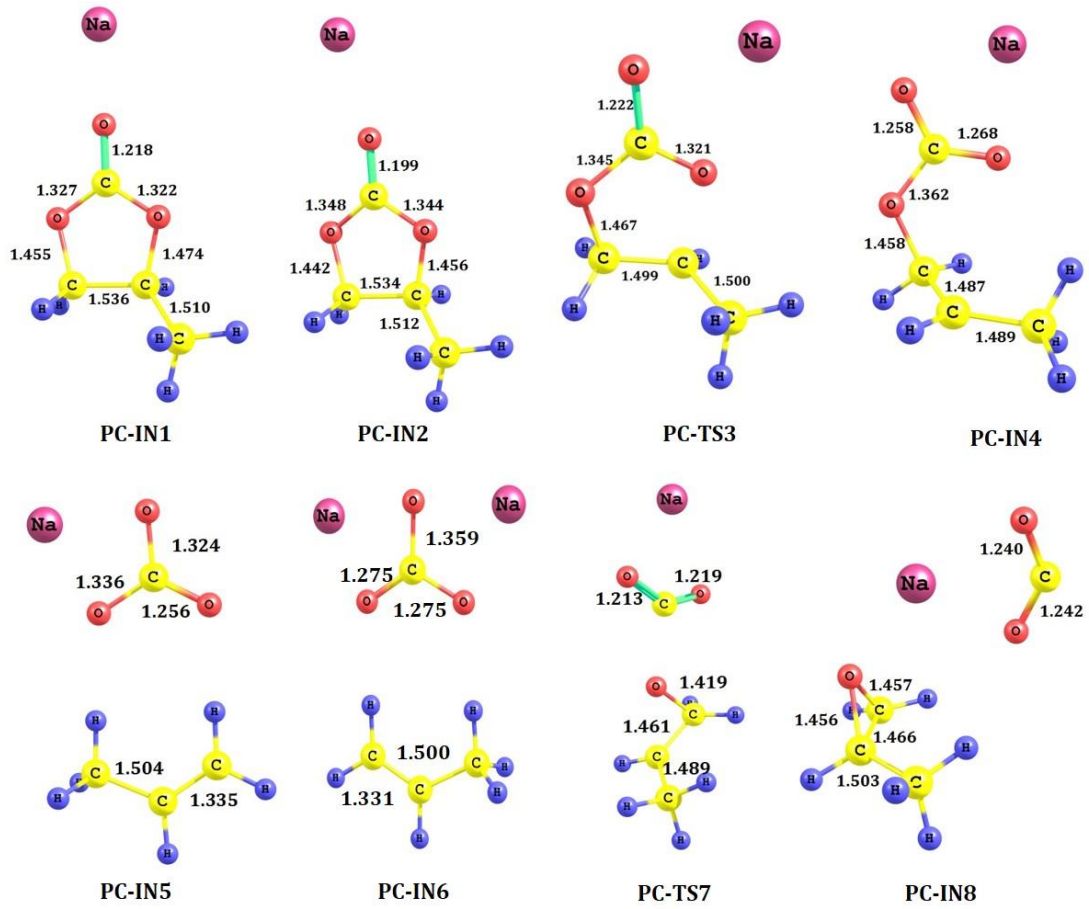
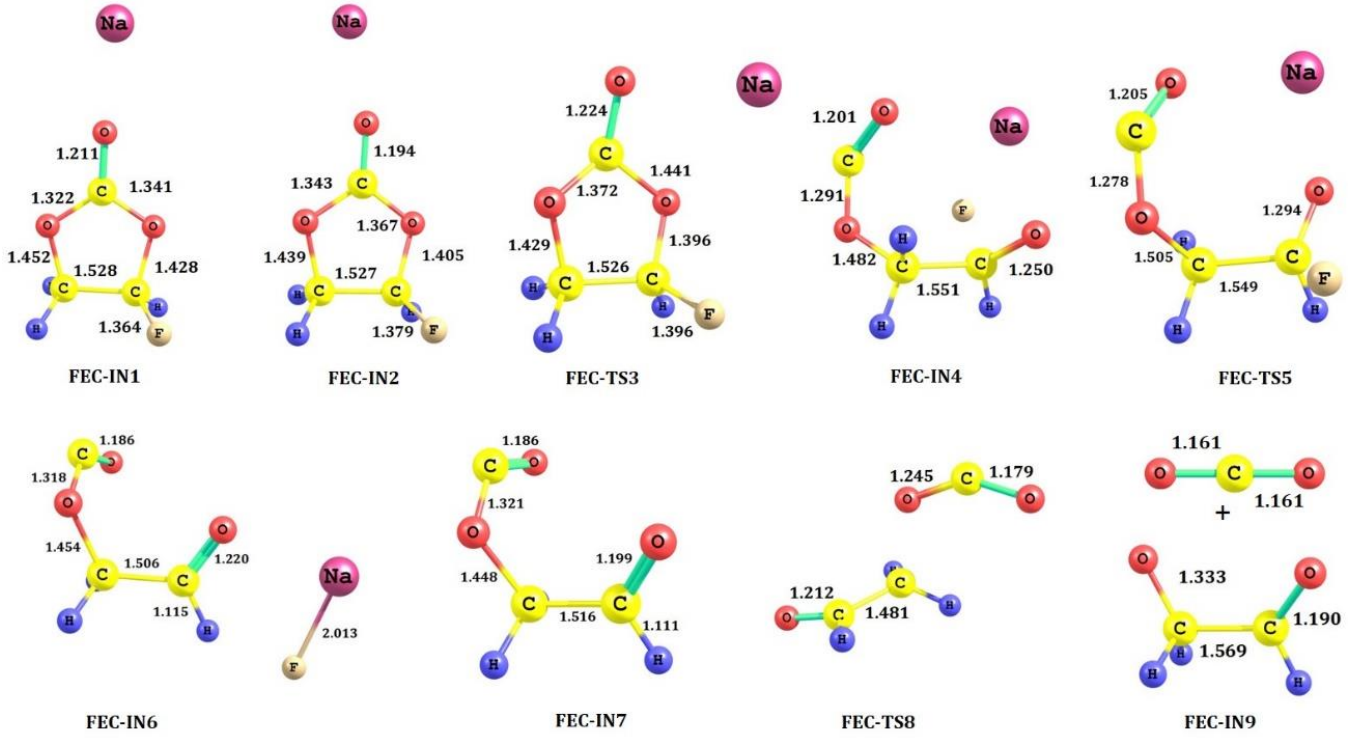



**Figure S3**: Optimized geometries with respective bond lengths of intermediates, products and transition states in the $Na^+$- propylene carbonate ($Na^+$- PC) reductive decomposition mechanism calculated at B3LYP/6-311++G(d,p) level of theory.


FEC-IN1
FEC-IN2
FEC-TS3
FEC-IN4
FEC-TS5
FEC-IN6
FEC-IN7
FEC-TS8
FEC-IN9

**Route 1**

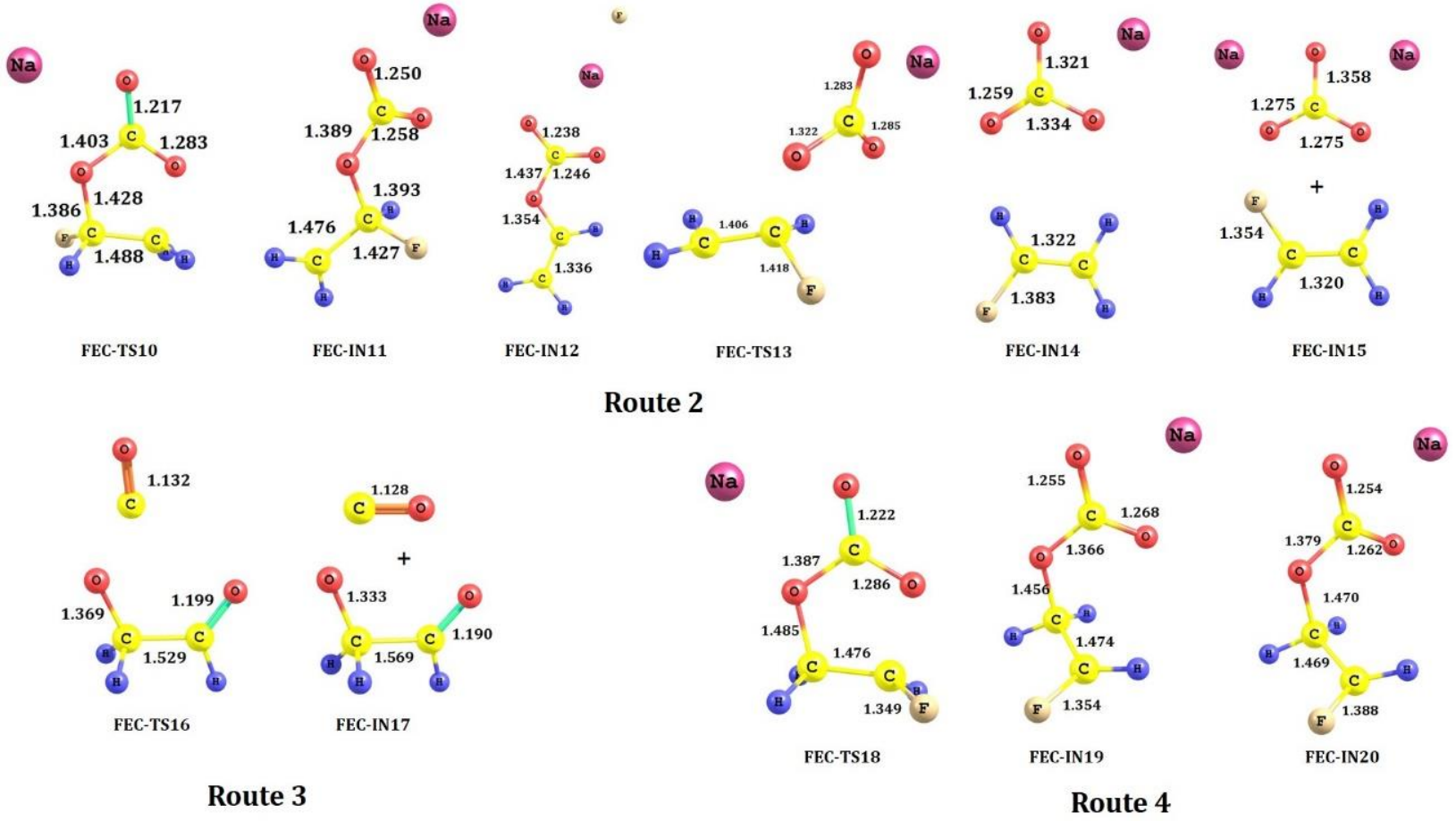
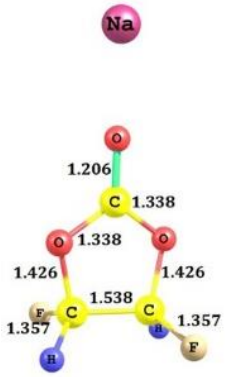
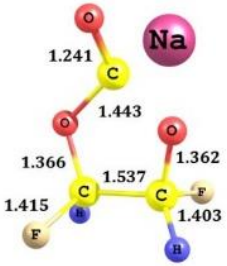


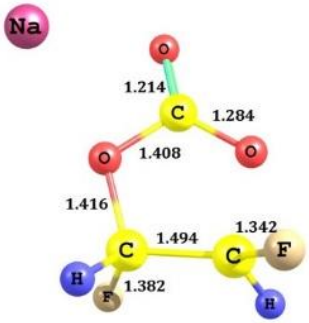

**Figure S4**: Optimized geometries with respective bond lengths of intermediates, products and transition states formed in the $Na^+$-fluoroethylene carbonate ($Na^+$-FEC) reductive decomposition mechanism calculated at B3LYP/6-311++G(d,p) level of theory.



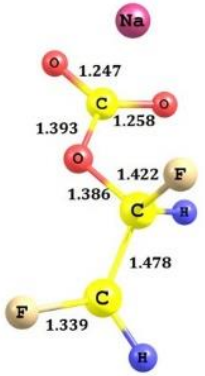

DFEC-IN1




DFEC-IN2




DFEC-TS3

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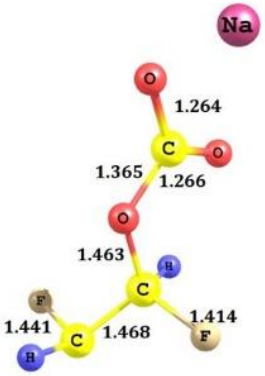


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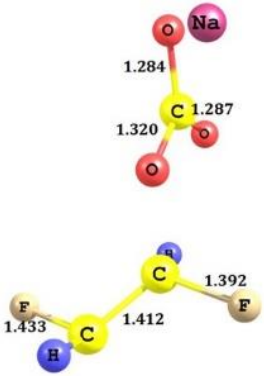


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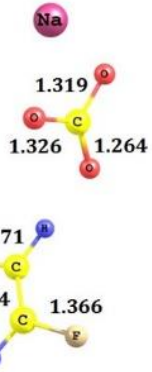


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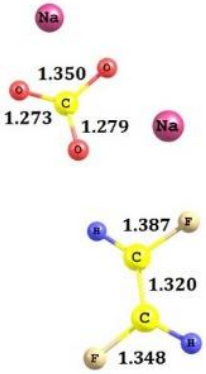


DFEC-IN8

**Route 1**

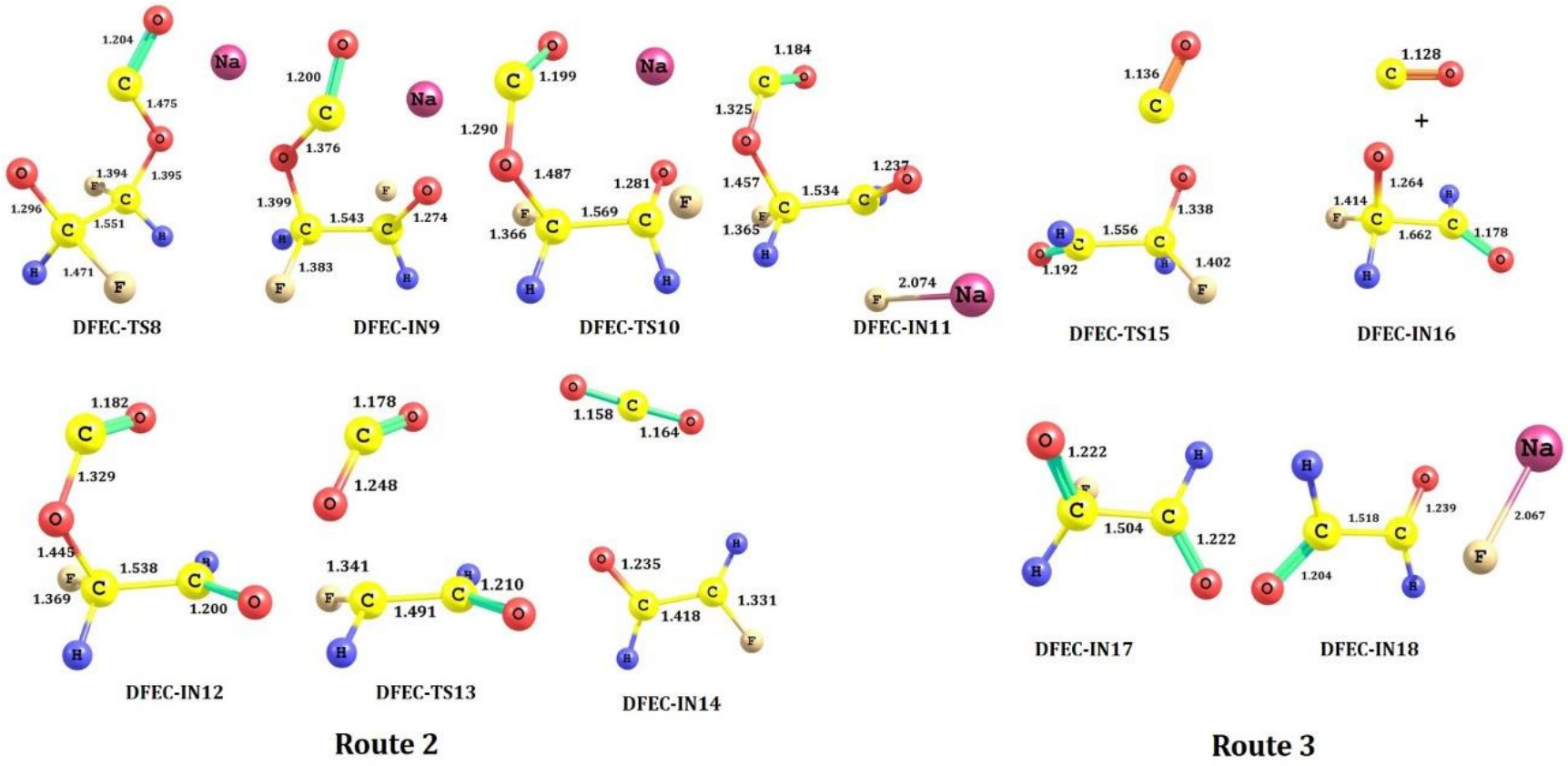


**Figure S5**: Optimized geometries with respective bond lengths of intermediates, products and transition states formed in the $Na^+$-difluoroethylene carbonate ($Na^+$-DFEC) reductive decomposition mechanism calculated at B3LYP/6-311++G(d,p) level of theory.