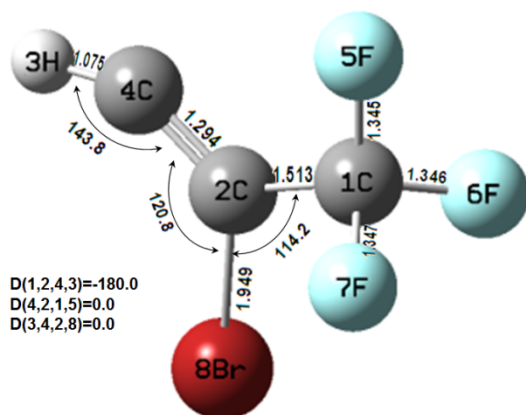
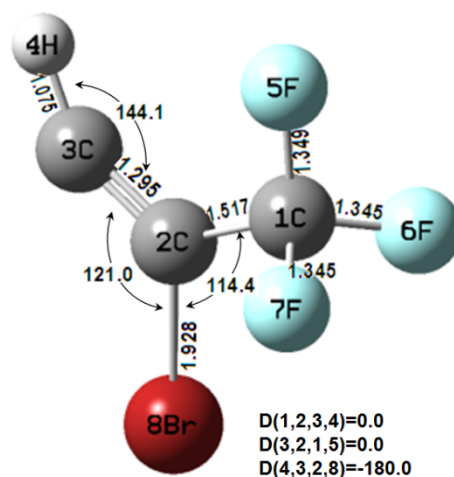




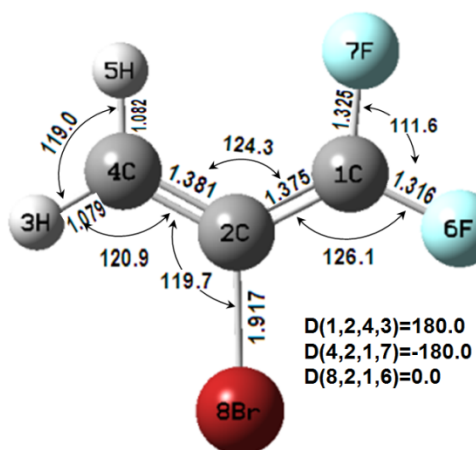
CF<sub>3</sub>CBrCH<sub>2</sub>OH (P<sub>1-3</sub>)



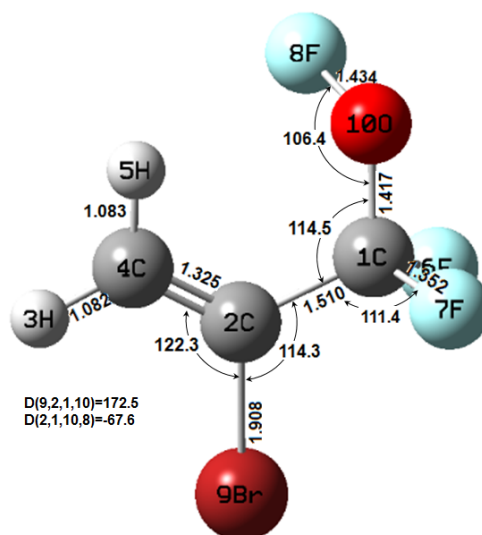
CF<sub>3</sub>C(OH)CH<sub>2</sub> (P<sub>2</sub>)



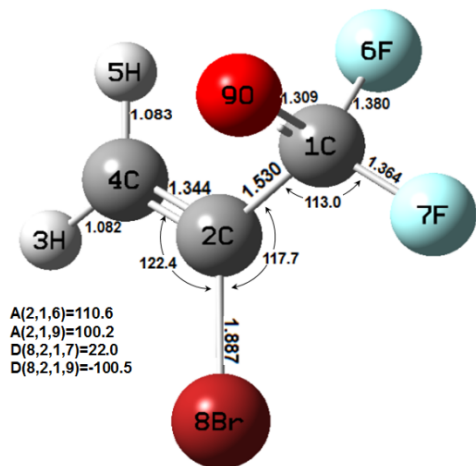
CF<sub>3</sub>CBrCH (P<sub>3-1</sub>)



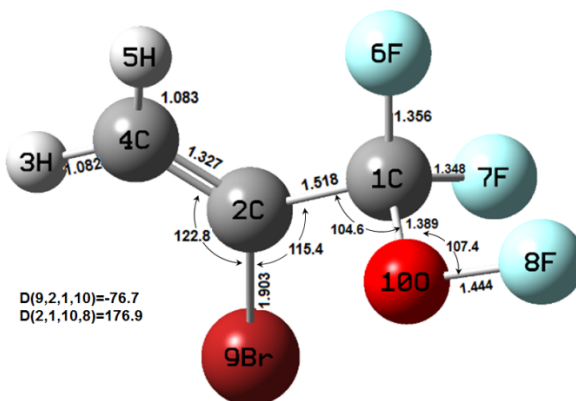
CF<sub>3</sub>CBrCH (P<sub>3-2</sub>)



CF<sub>2</sub>CBrCH<sub>2</sub> (P<sub>4</sub>)

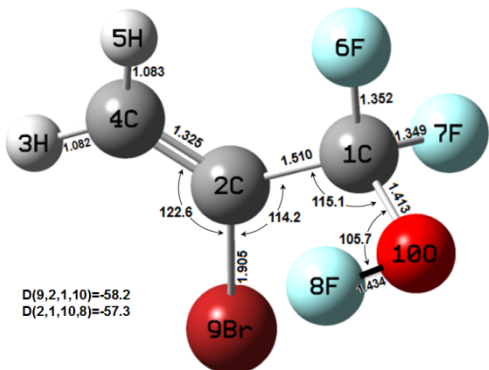


CF<sub>2</sub>(OF)CBrCH<sub>2</sub> (P<sub>5-1</sub>)

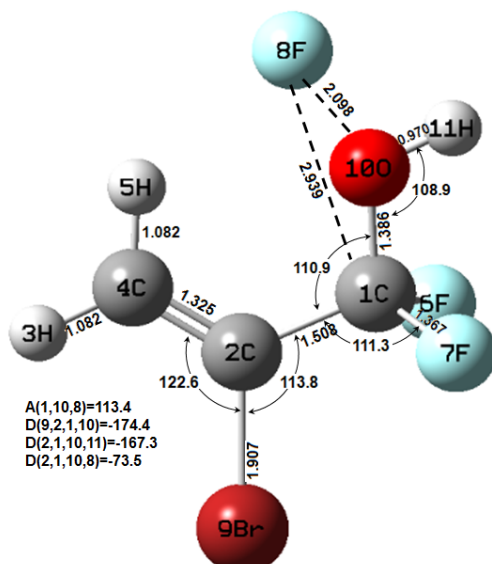


CF<sub>2</sub>(O)CBrCH<sub>2</sub> (P<sub>5-2</sub>)

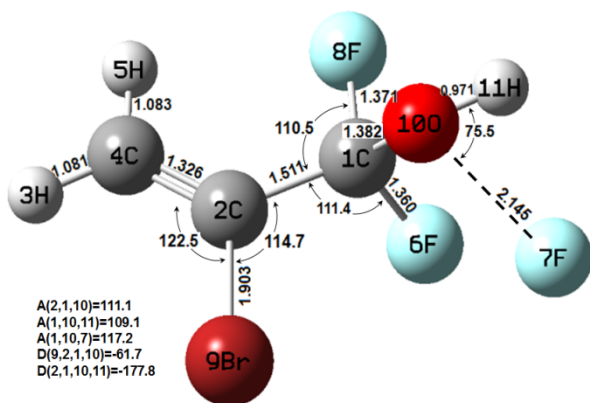
CF<sub>2</sub>(OF)CBrCH<sub>2</sub> (P<sub>5-3</sub>)



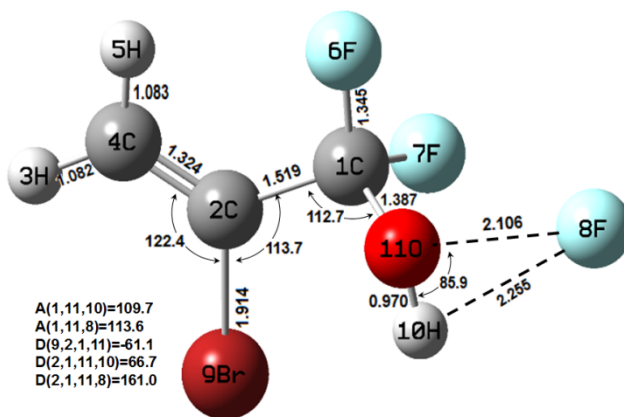
CF<sub>2</sub>(OF)CBrCH<sub>2</sub> (P<sub>5-4</sub>)



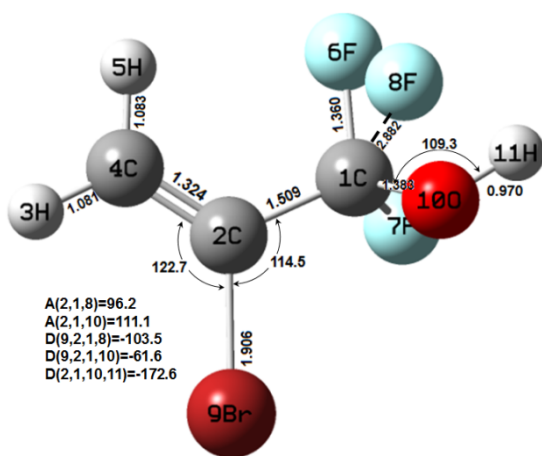
IM<sub>1</sub>



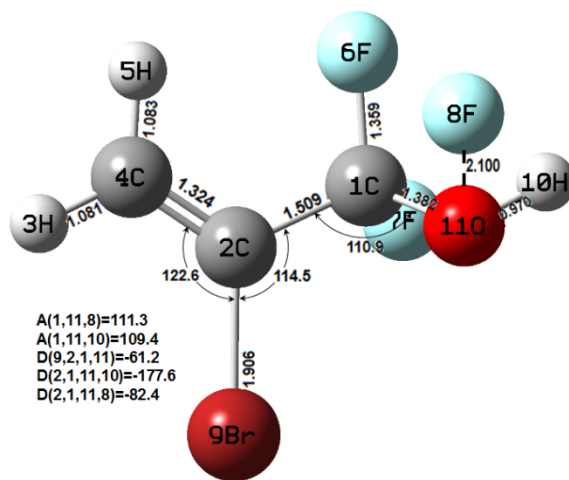
IM<sub>2</sub>



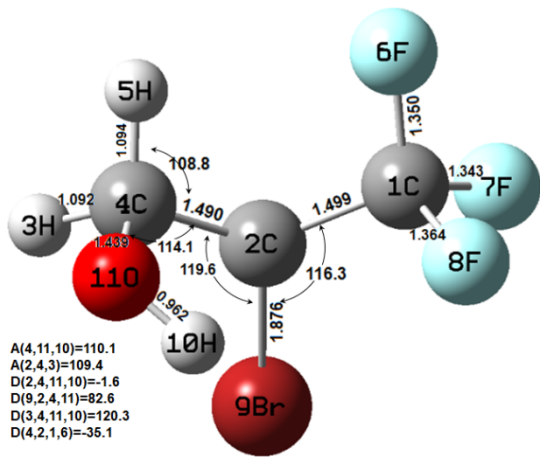
IM<sub>3</sub>



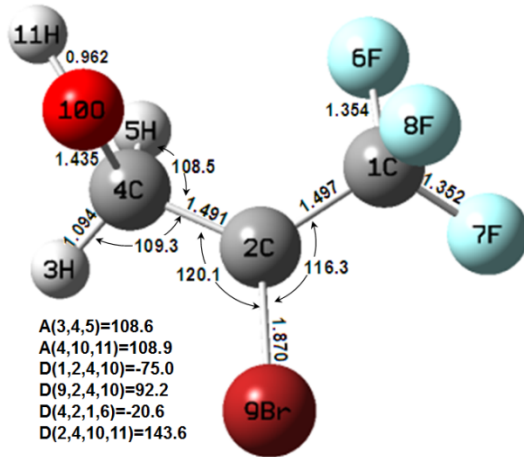
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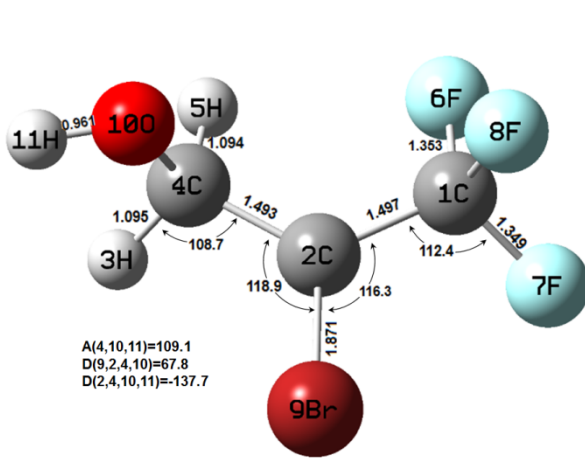
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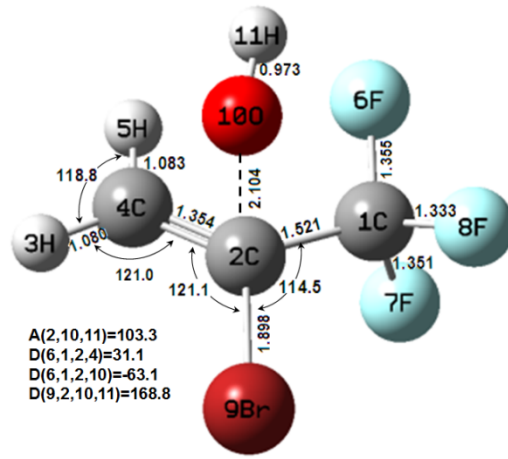
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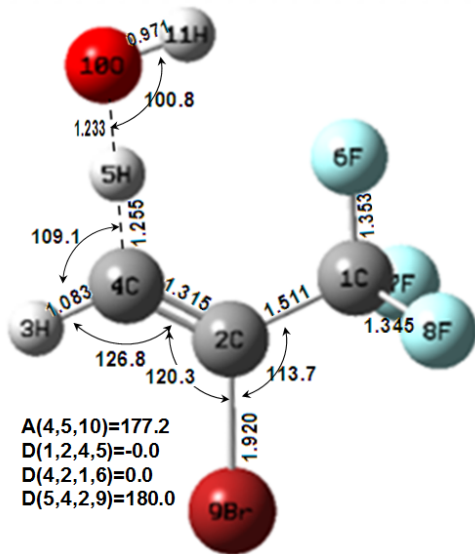
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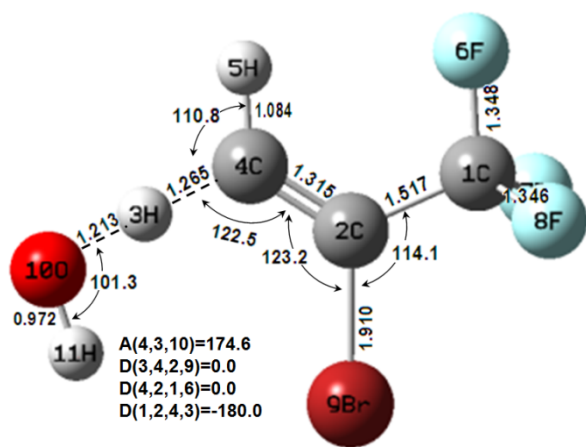
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TS<sub>4</sub>

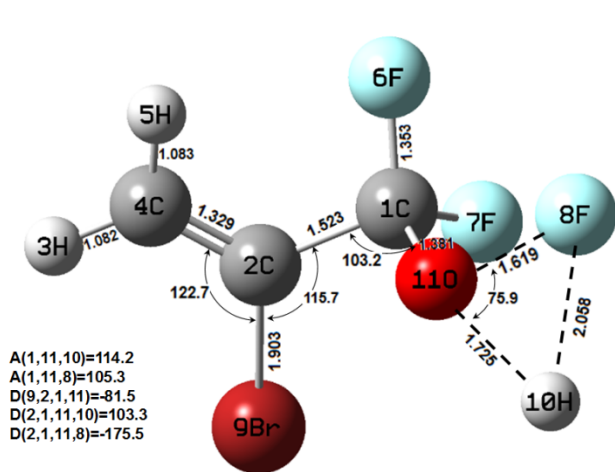


TS<sub>5</sub>

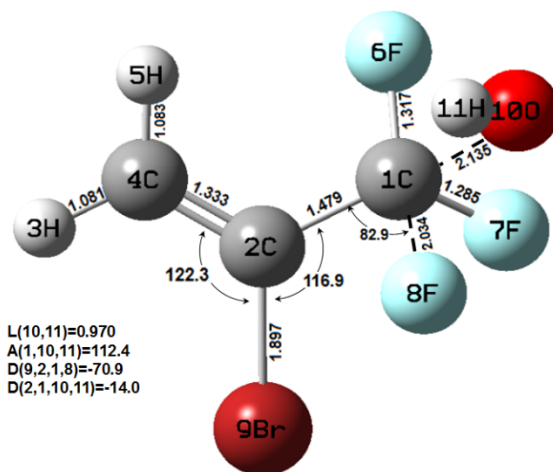


TS<sub>6</sub>

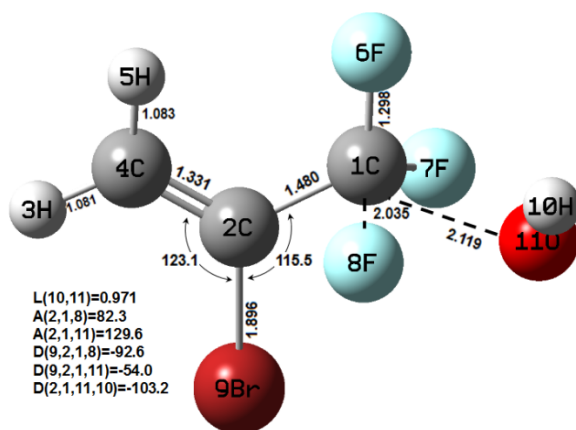




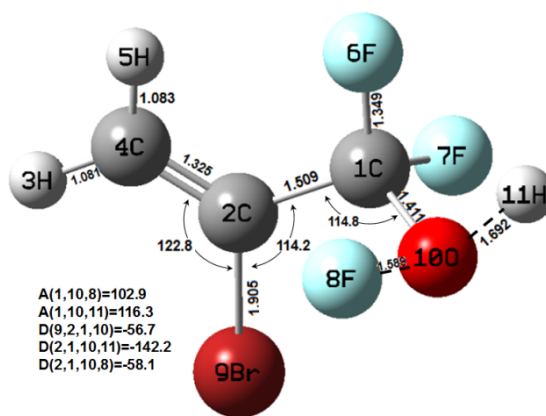
TS<sub>13</sub>



TS<sub>14</sub>



TS<sub>15</sub>

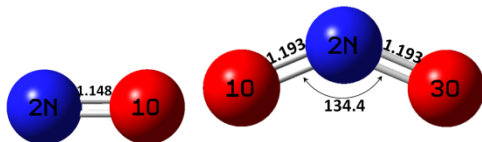


TS<sub>16</sub>

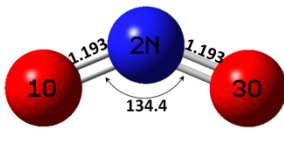
## Appendix B:

Optimized structures and geometrical parameters of various species involved in the subsequent degradation reaction of P<sub>1-1</sub> at the B3LYP/6-311++G (d, p) theory level. Bond distances and angles are in angstroms and degree, respectively.

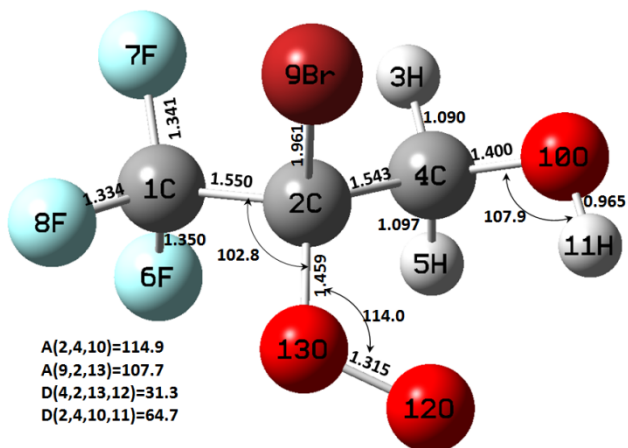




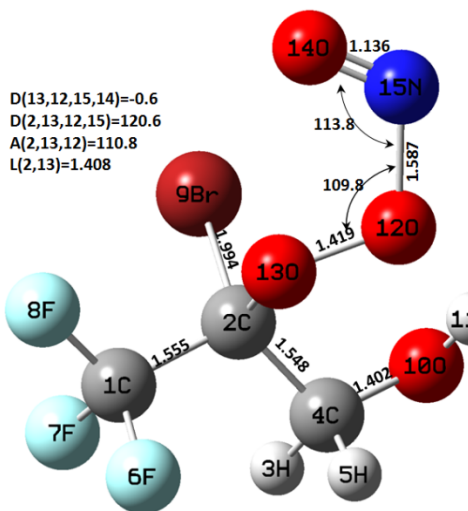
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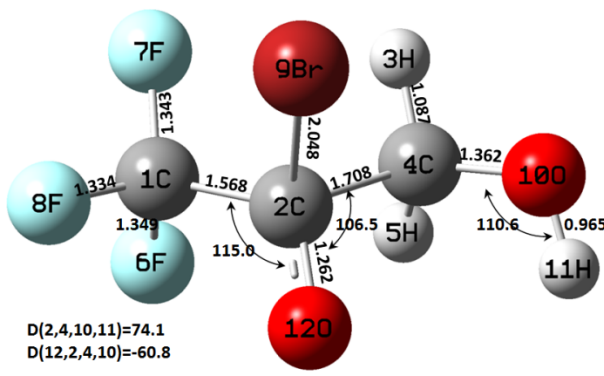
NO<sub>2</sub>



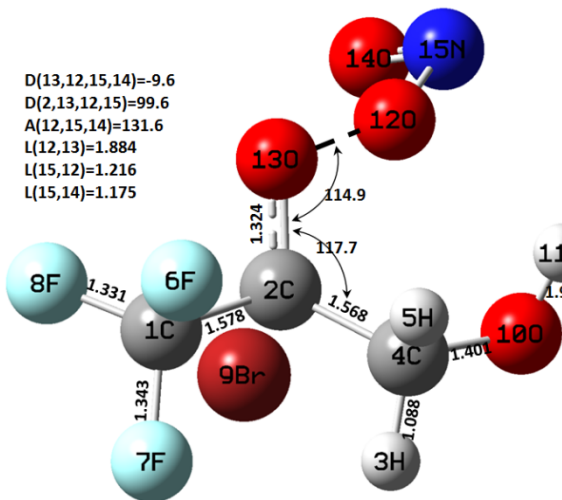
IM<sub>6</sub>



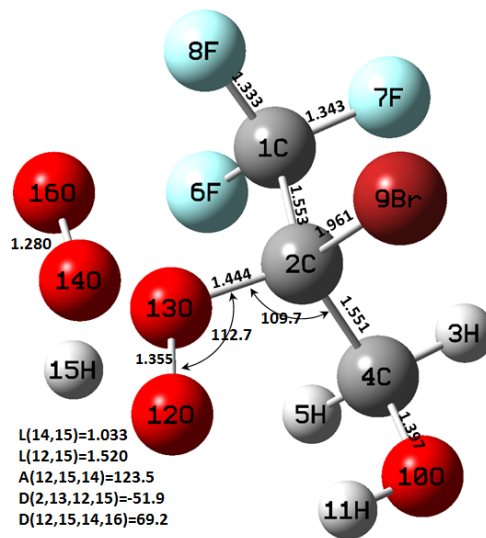
IM<sub>7</sub>



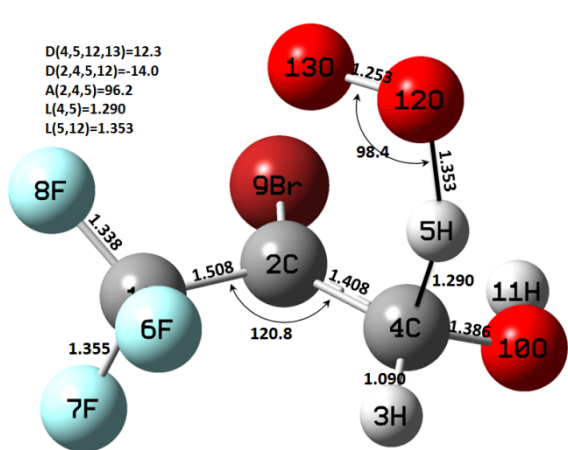
IM<sub>8</sub>



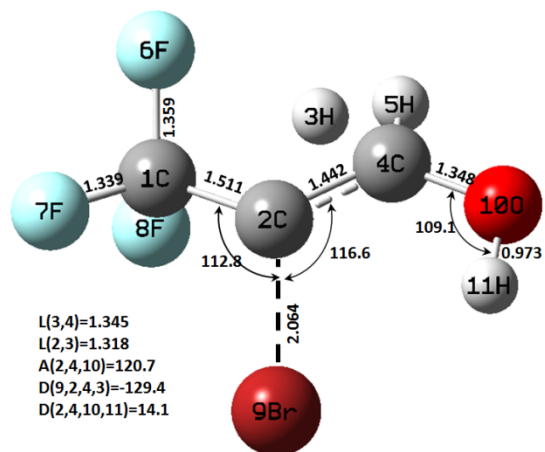
TS<sub>17</sub>



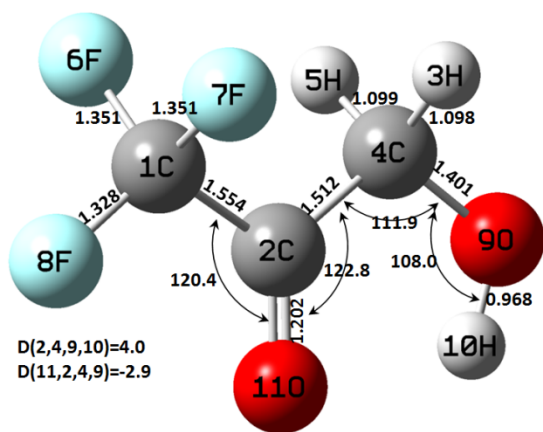
TS<sub>18</sub>



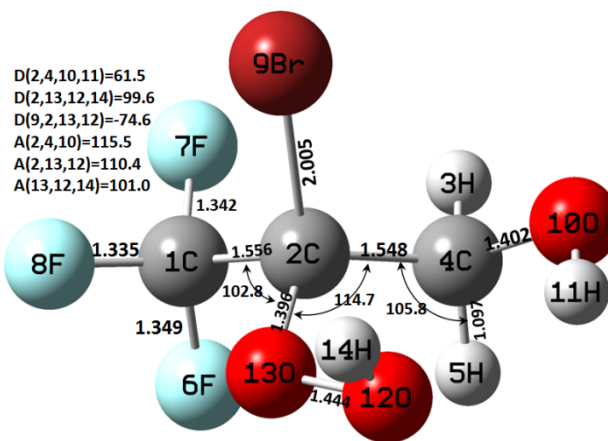
TS<sub>19</sub>



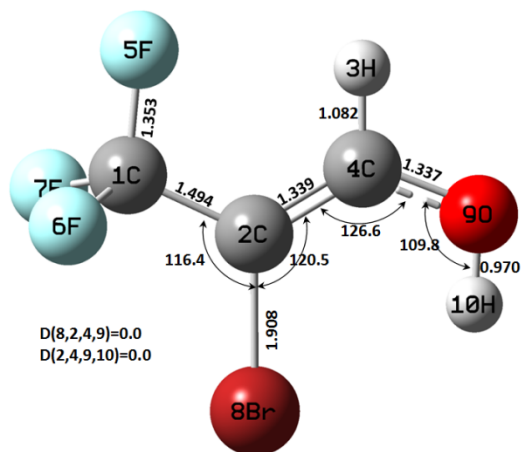
TS<sub>20</sub>



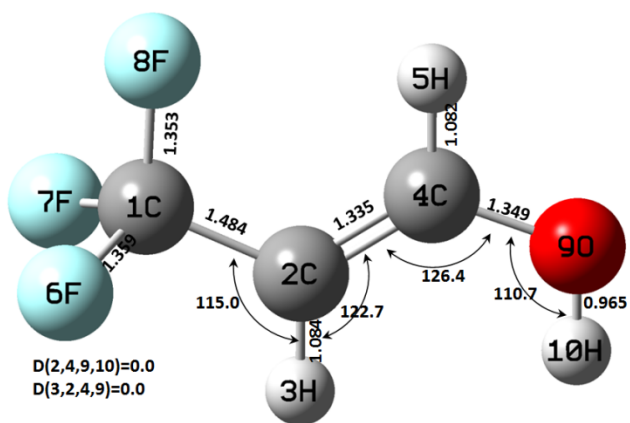
FP<sub>1</sub>



FP<sub>2</sub>



FP<sub>3</sub>



FP<sub>4</sub>