Supporting Information
for

A new intermediate in the Prins reaction

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Geometries of the precursor, intermediates and products, and other related geometries.

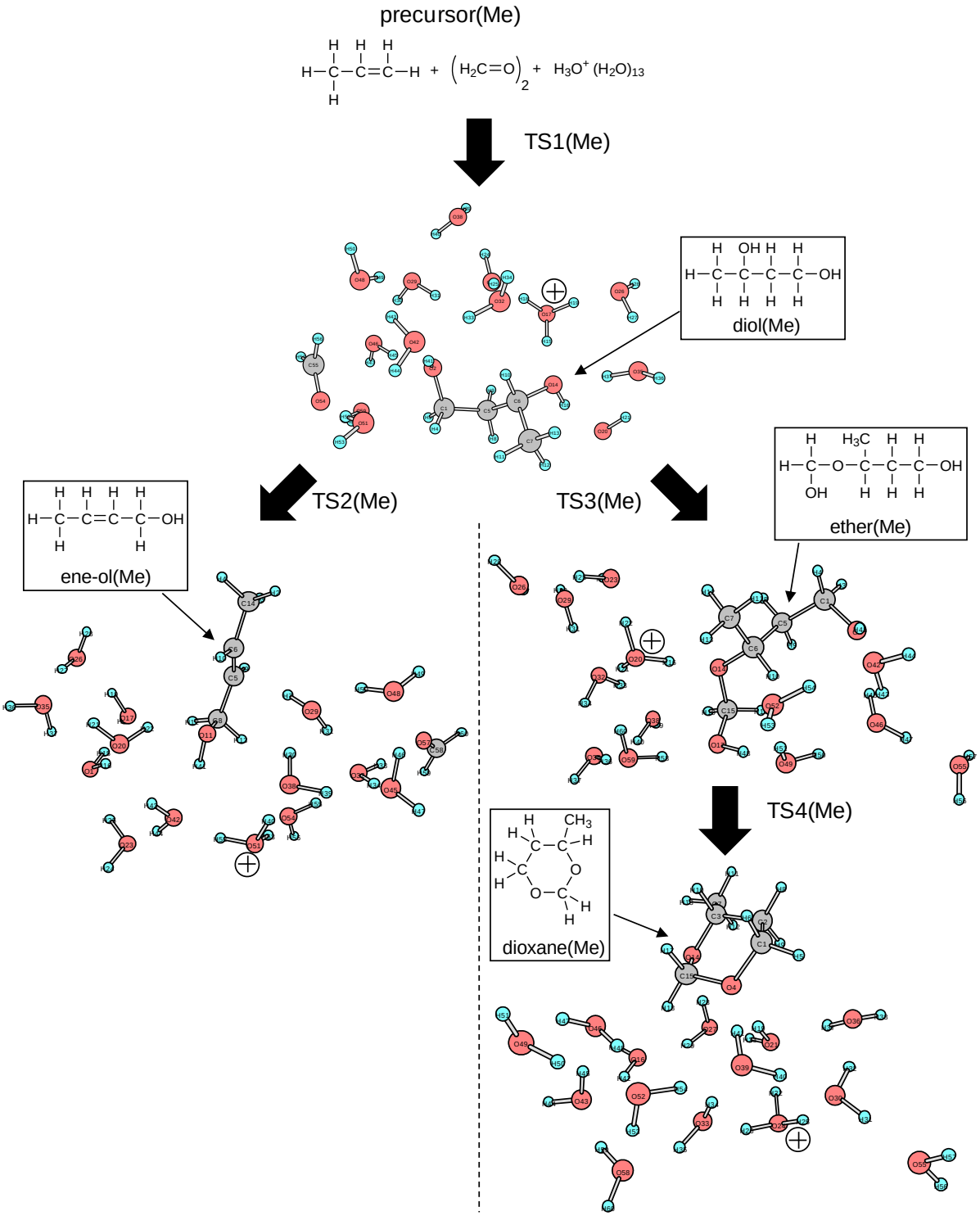
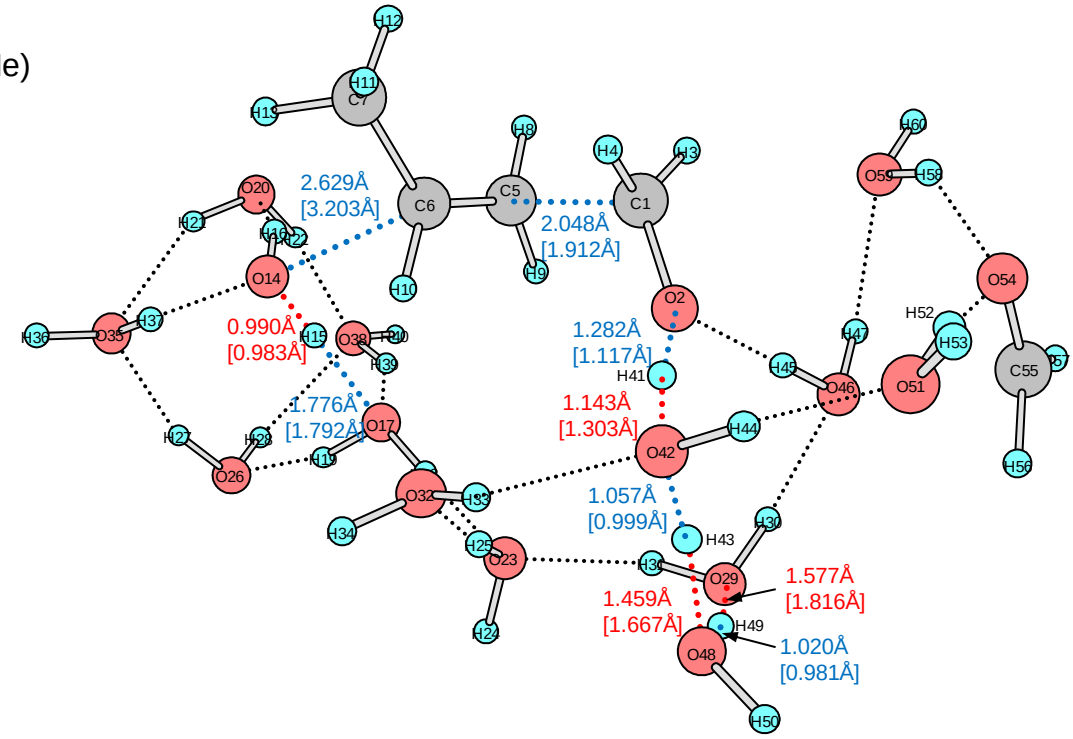


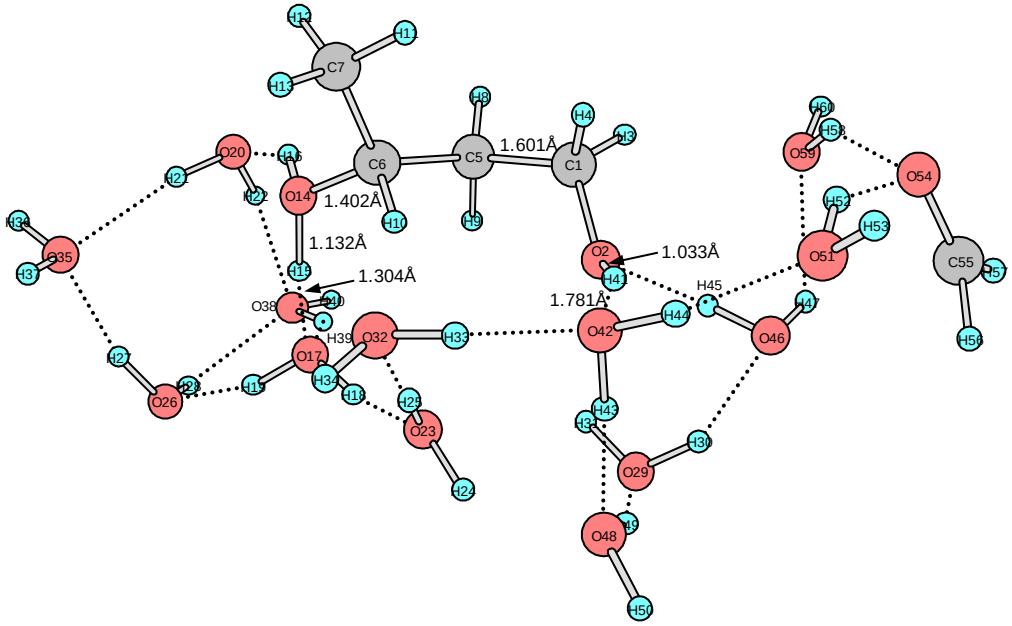
Figure S1: Geometries of intermediates and products of the propene Prins reaction. TS geometries are shown in Figure 1.

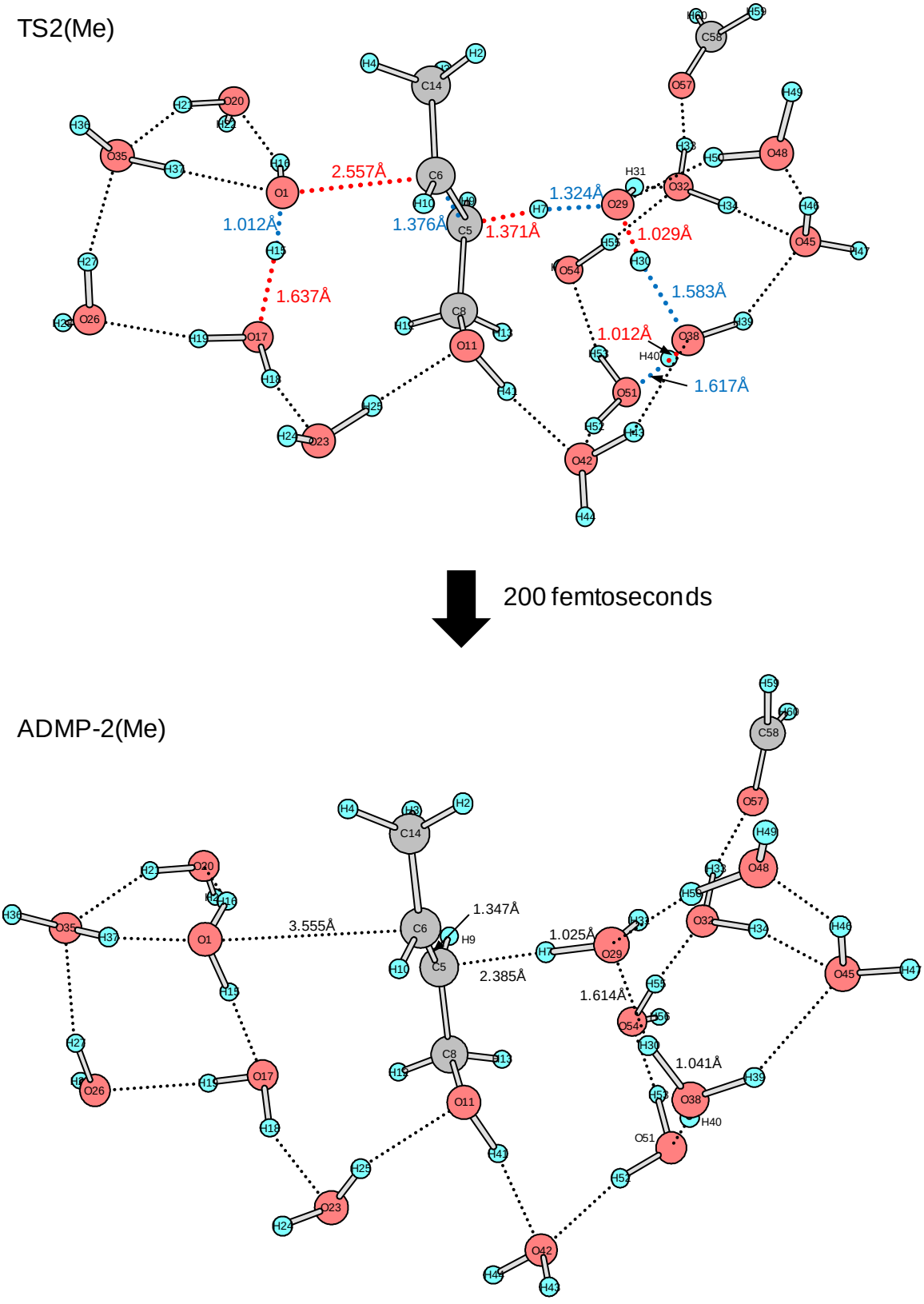
TS1(Me)



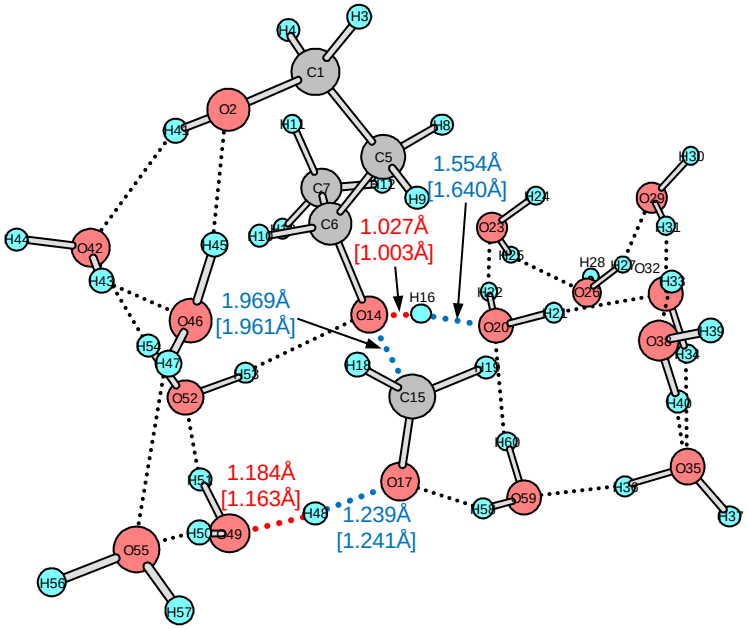
200 femtoseconds

ADMP-1(Me)



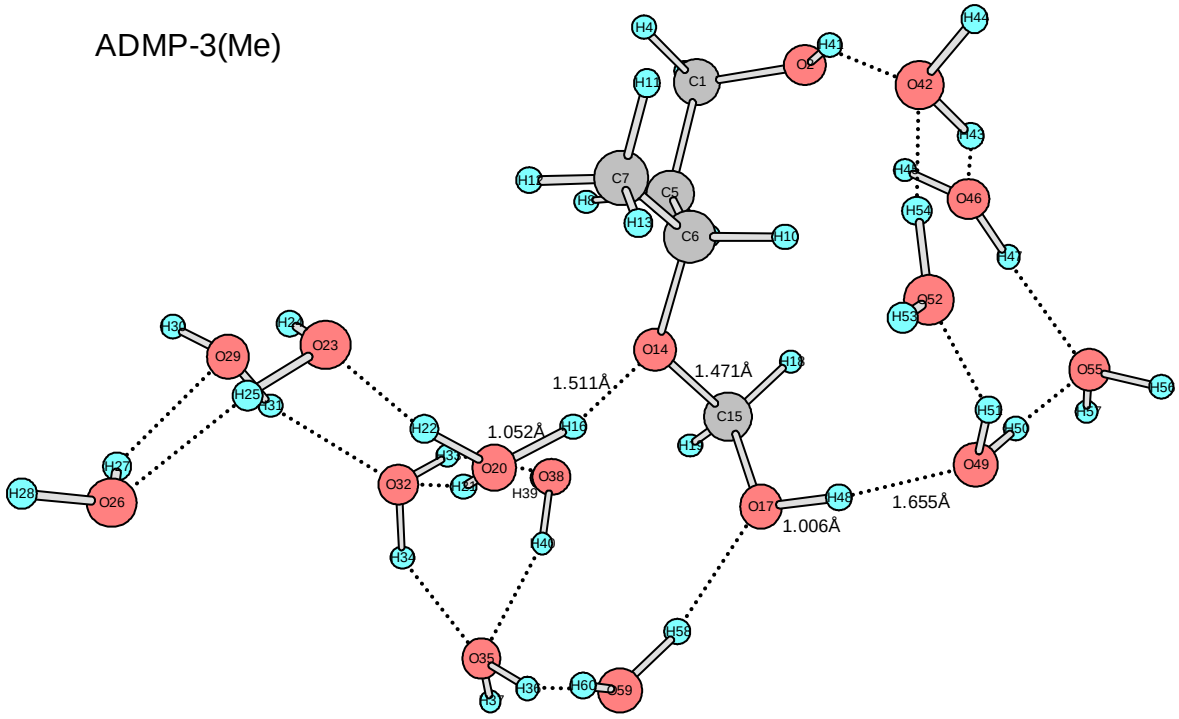

TS2(Me)
2.557Å
1.012Å
1.637Å
1.376Å
1.371Å
1.324Å
1.029Å
1.583Å
1.012Å
1.617Å
200 femtoseconds
ADMP-2(Me)
3.555Å
1.347Å
2.385Å
1.025Å
1.614Å
1.041Å

TS3(Me)

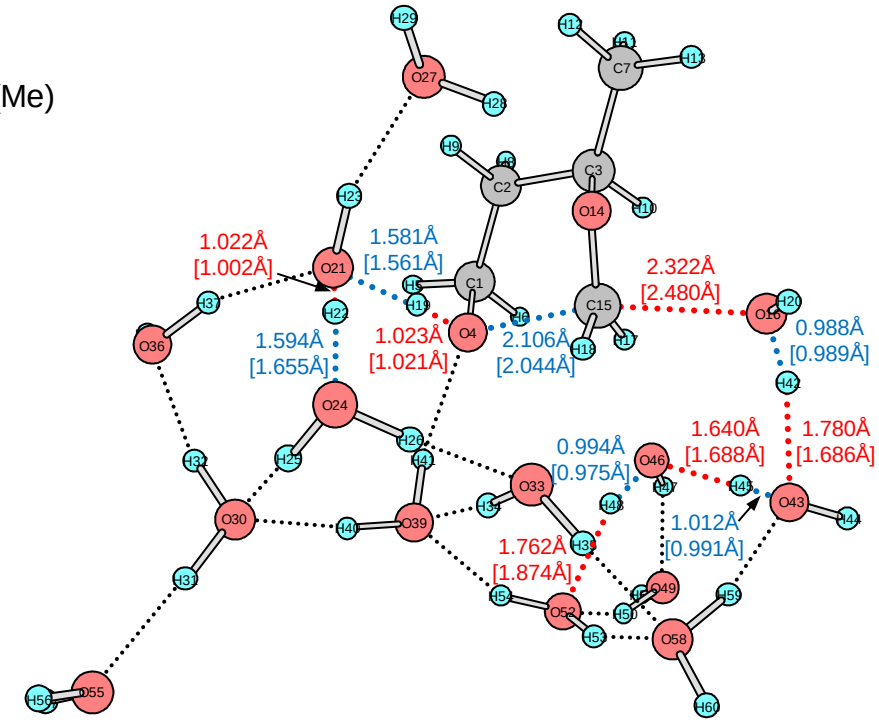


200 femtoseconds

ADMP-3(Me)

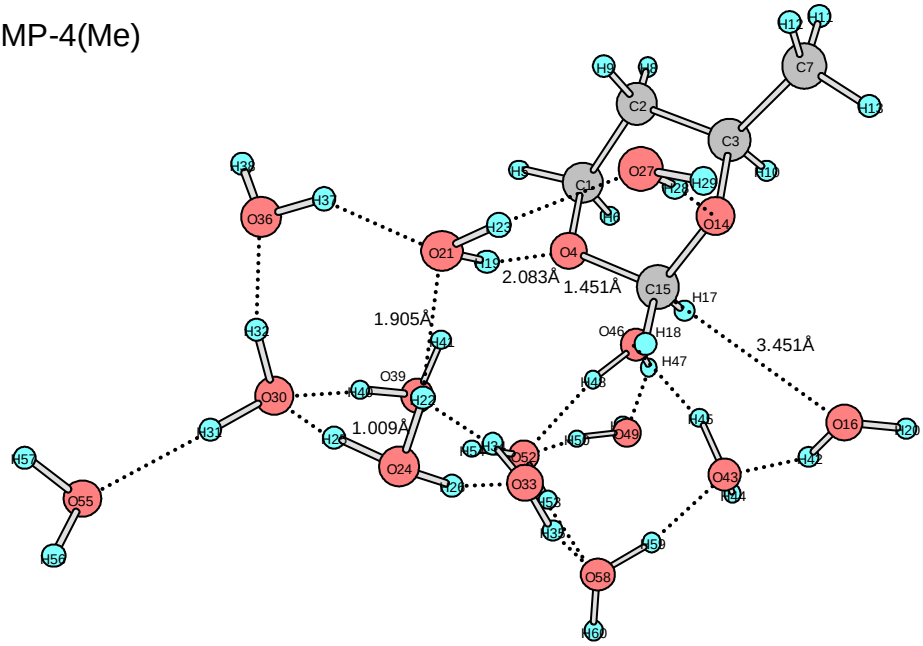


TS4(Me)



200 femtoseconds

ADMP-4(Me)



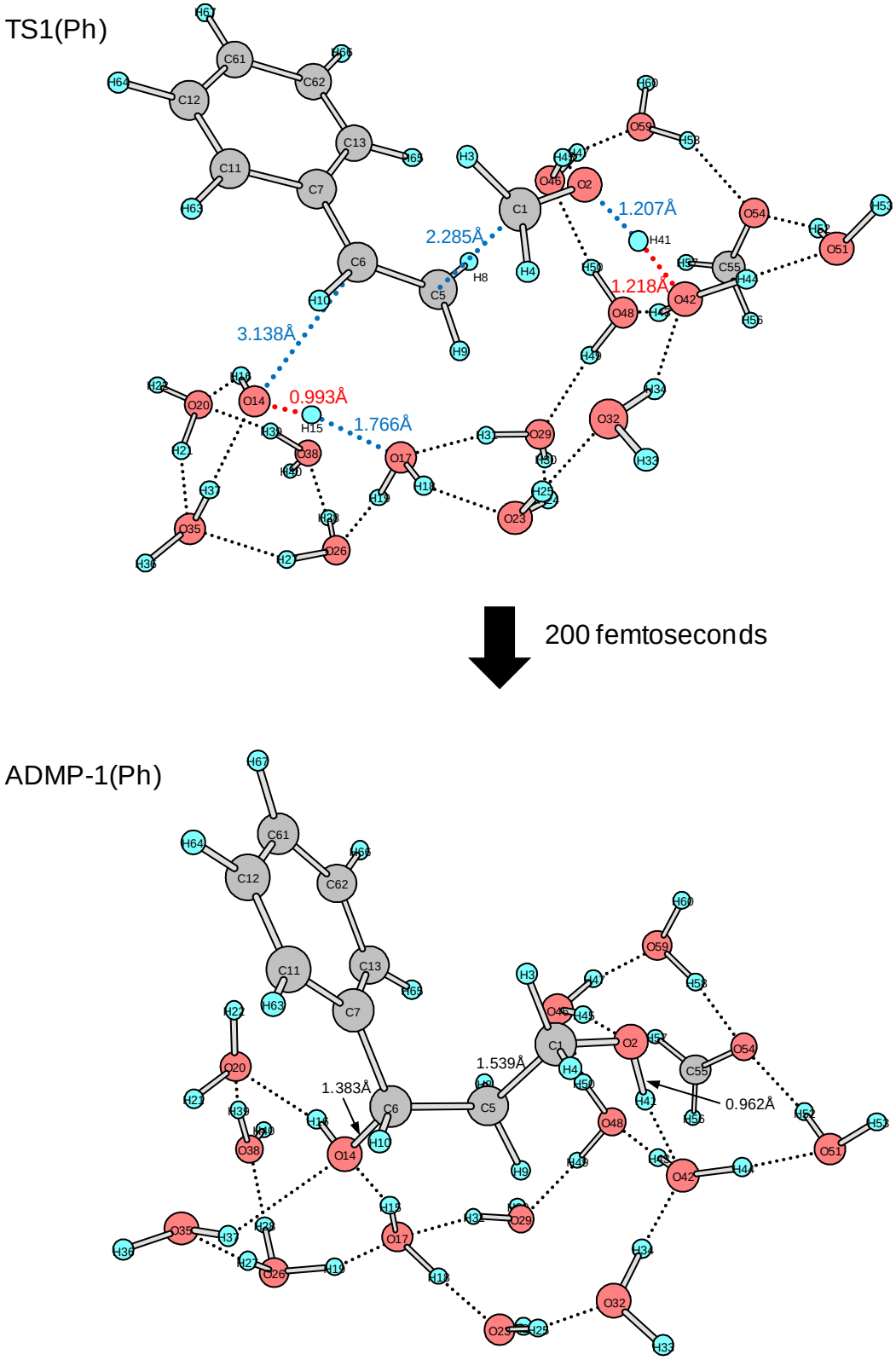
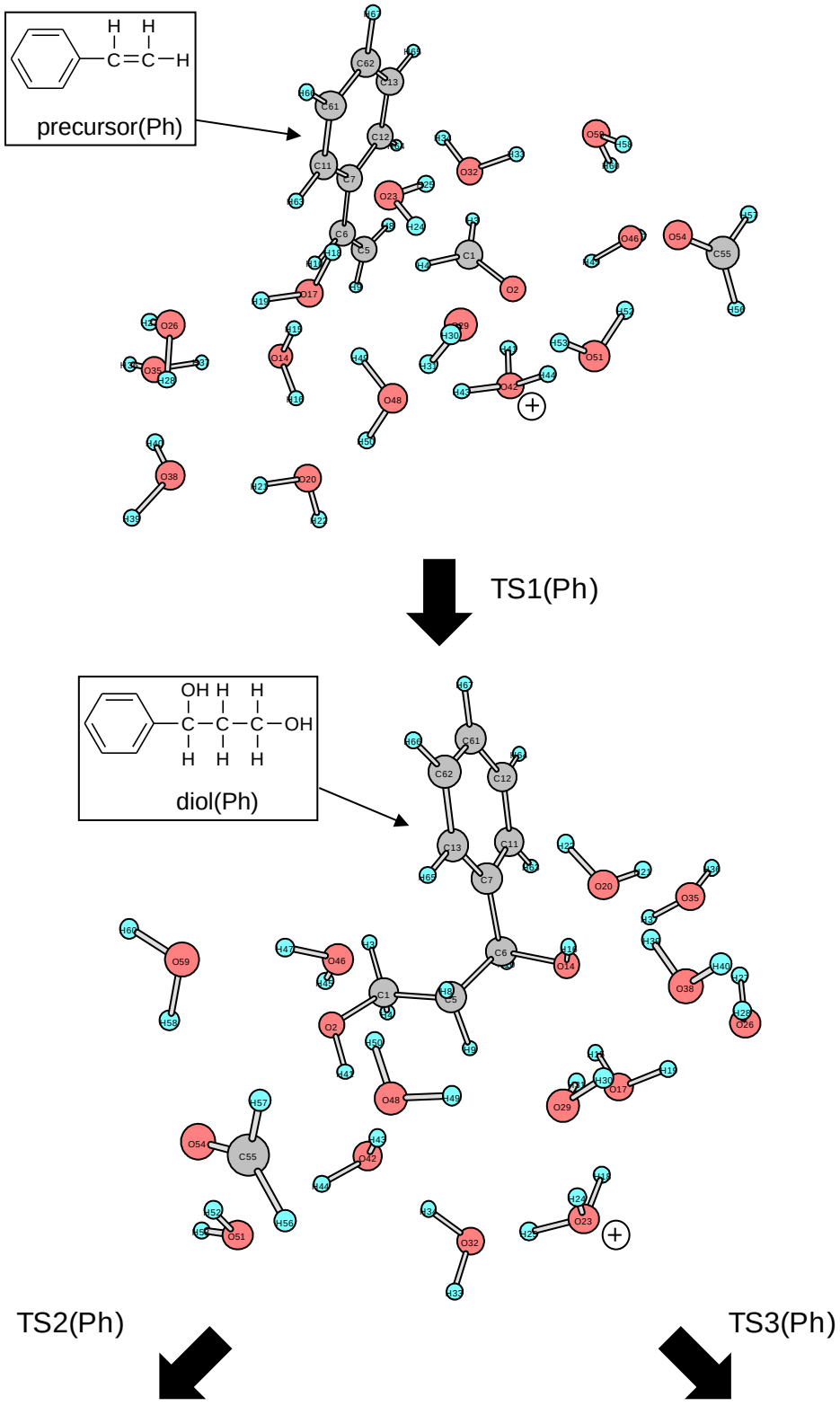


Figure S2: Geometries at the 200 femtoseconds passed from TS1(Me), TS2(Me), TS3(Me), TS4(Me) in Figure 1 and TS1(Ph) in Figure 3.


precursor(Ph)
TS1(Ph)
diol(Ph)
TS2(Ph)
TS3(Ph)

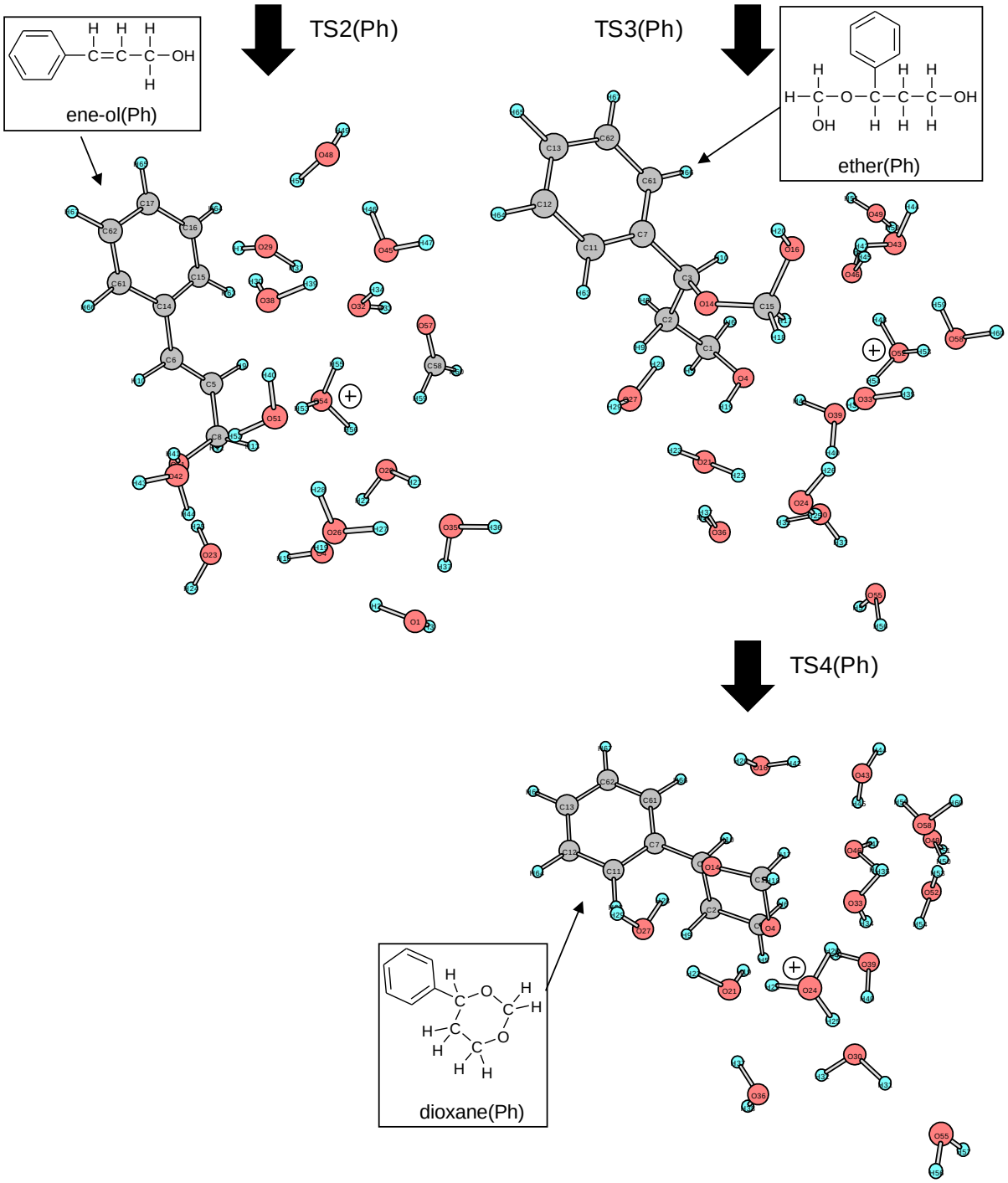


Figure S3: Geometries of the precursor, intermediates and products of the styrene Prins reaction. TS geometries are shown in Figure 3.

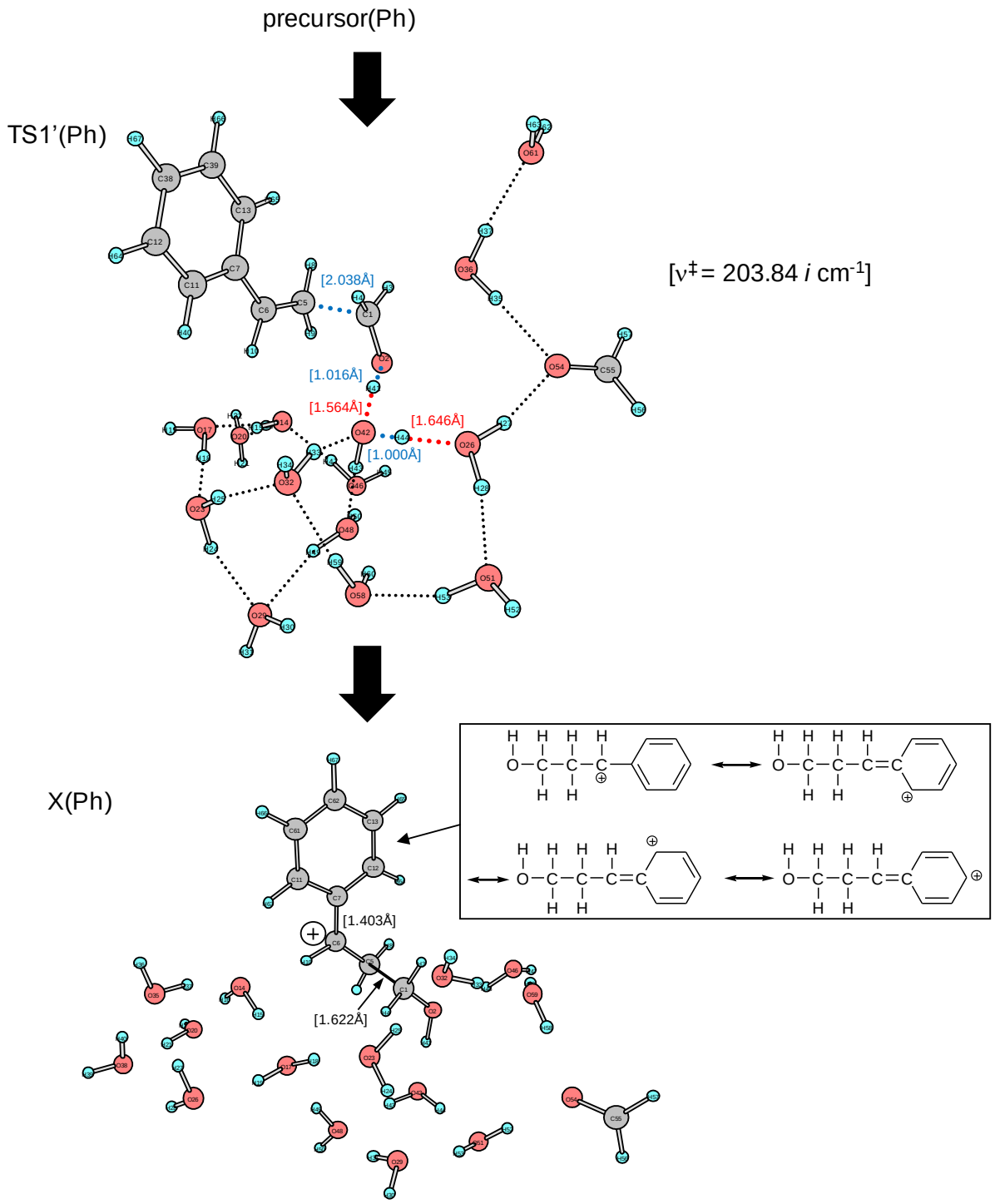
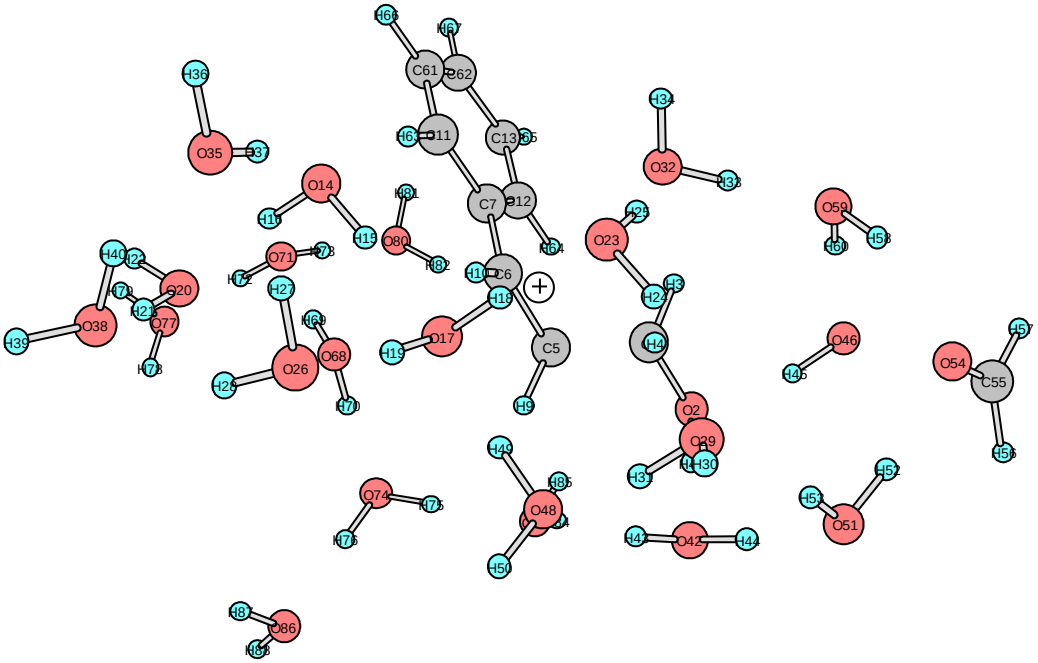


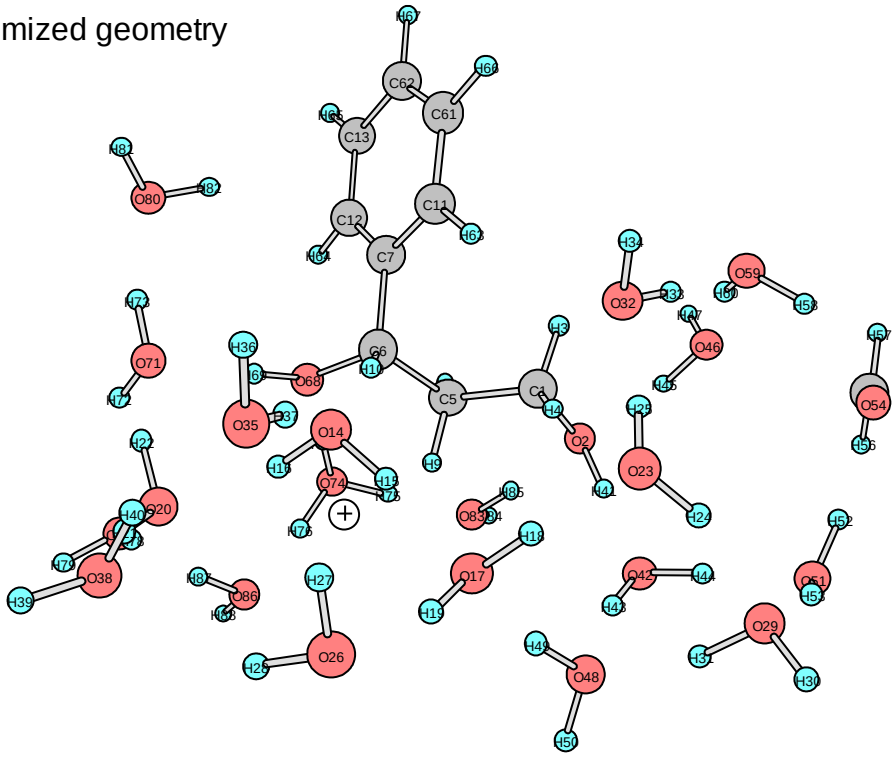
Figure S4: A carbocation [X(Ph)] formation path calculated by B3LYP/6-311+G(d,p). The geometry of precursor(Ph) is shown in Figure S3. The cation X(Ph) is stabilized by canonical resonance structures exhibited in the box.

The initial geometry



B3LYP/6-31G(d)

The optimized geometry



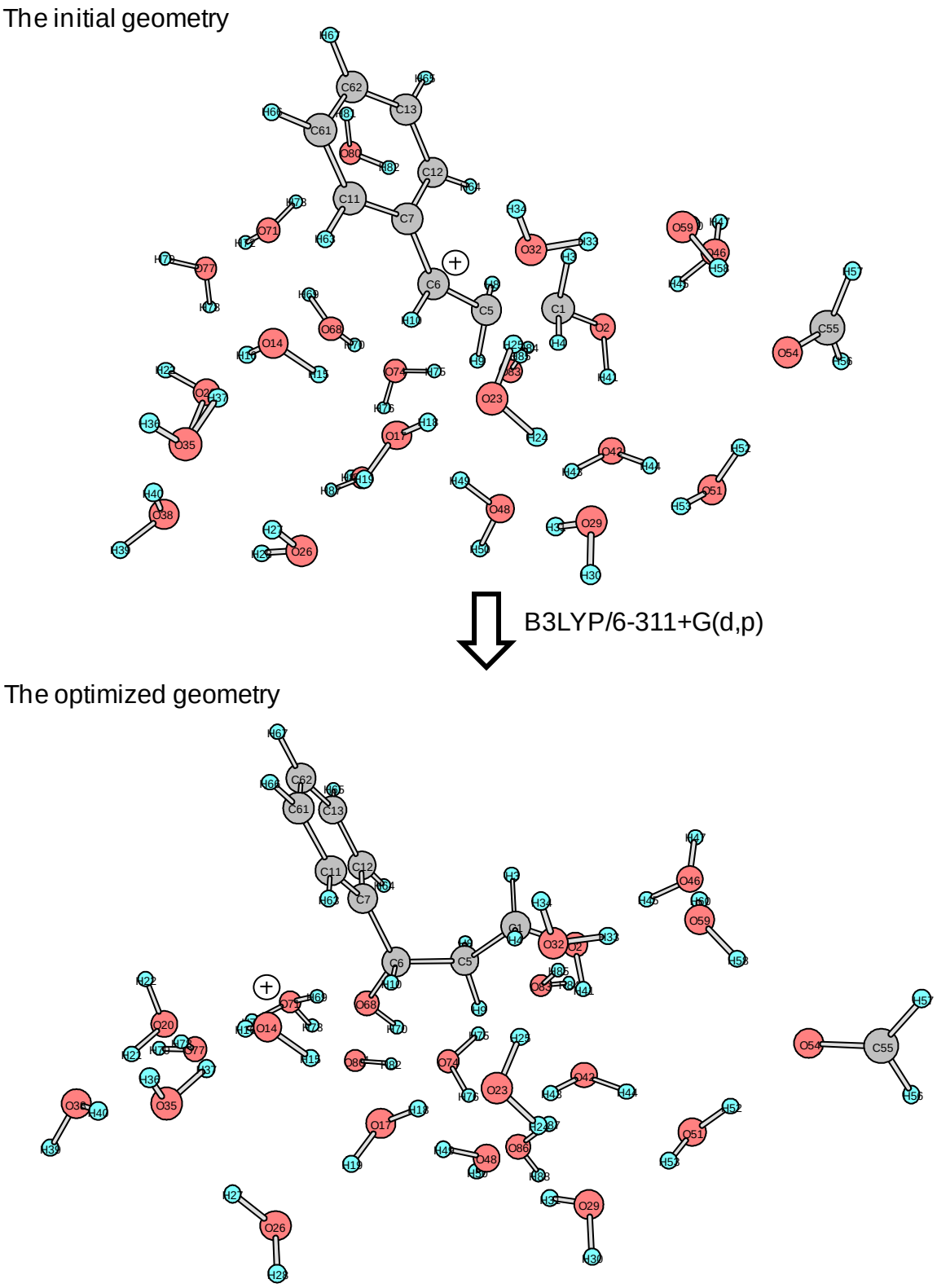


Figure S5: The initial geometry composed of that of the carbocation X(Ph) and $(H_2O)_7$ is converted into that of diol(Ph) and $(H_2O)_7$ both by B3LYP/6-31G(d) and by B3LYP/6-311+G(d,p). The molecular formula of the system is $C_{10}H_{55}O_{23}^{+}$.