

Directions of External Electric Field Control Catalyze the Hydroboration of C–O Unsaturated Compounds

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Table S1. Relative energies (kcal/mol) of reactants, transition states, and products in Markovnikov hydroboration of benzaldehyde in present of EEFs (10^{-4} au).

	-150	-100	-75	-50	-25	25	50	75	100	150
PhCHO + HBPIn	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TS2 (F_X)	–	–	88.4	89.0	89.0	88.4	87.6	86.6	85.5	79.5
P2 (F_X)	–	–	-10.7	-8.9	-7.4	-4.8	-3.7	-3.0	-9.0	-14.6
TS2 (F_Y)	–	–	87.5	87.9	88.4	89.2	89.6	90.1	–	–
P2 (F_Y)	–	–	-10.9	-9.2	-7.6	-4.9	-3.6	-2.6	–	–
TS2 (F_Z)	98.7	95.3	93.9	92.2	90.5	87.1	85.4	83.8	–	–
P2 (F_Z)	1.7	-1.2	-2.6	-3.8	-5.0	-7.2	-8.2	-9.0	–	–

Table S2. Relative energies (kcal/mol) of reactants, transition states, and products in Markovnikov hydroboration of benzophenone in present of EEFs (10^{-4} au).

	-100	-75	-50	-25	25	50	75	100
Ph ₂ CO + HBPIn	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TS2' (F_X)	–	94.0	94.4	94.4	93.1	91.9	90.1	88.1
P2' (F_X)	–	3.0	3.1	2.9	1.6	0.5	-0.9	-2.6
TS2' (F_Y)	–	93.8	93.8	93.8	94.1	94.3	94.5	–
P2' (F_Y)	–	2.9	2.8	3.0	1.6	0.9	0.1	–
TS2' (F_Z)	100.9	99.2	97.4	95.7	92.2	90.4	88.7	–
P2' (F_Z)	7.7	6.3	4.9	3.6	1.2	0.1	-0.9	–

Table S3. Relative energies (kcal/mol) of reactants, transition states, and products in anti-Markovnikov hydroboration of benzaldehyde in present of EEFs (10^{-4} au).

	-150	-100	-75	-50	-25	25	50	75	100	150
PhCHO + HBP _{in}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TS1 (F_X)	–	–	37.4	37.3	36.4	32.6	30.2	27.0	24.2	14.9
P1 (F_X)	–	–	-36.7	-34.3	-33.2	-31.5	-30.8	-30.9	-30.7	-33.8
TS1 (F_Y)	–	–	35.5	35.2	35.0	34.4	34.1	33.7	–	–
P1 (F_Y)	–	–	-33.9	-34.1	-33.2	-31.5	-30.9	-29.2	–	–
TS1 (F_Z)	22.2	26.4	29.0	31.0	33.0	36.1	37.0	37.7	–	–
P1 (F_Z)	-27.9	-29.3	-29.9	-30.8	-31.6	-33.3	-34.3	-35.1	–	–

Table S4. Relative energies (kcal/mol) of reactants, transition states, and products in anti-Markovnikov hydroboration of benzophenone in present of EEFs (10^{-4} au).

	-100	-75	-50	-25	25	50	75	100
Ph ₂ CO + HBPin	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TS1' (F_X)	–	39.9	38.6	36.9	33.2	30.5	28.1	25.1
P1' (F_X)	–	-31.7	-30.5	-29.9	-29.3	-29.3	-30.0	-30.8
TS1' (F_Y)	–	34.7	35.0	35.1	35.2	34.9	34.6	–
P1' (F_Y)	–	-29.6	-42.9	-28.5	-30.4	-31.2	-32.1	–
TS1' (F_Z)	26.6	28.7	30.7	33.1	36.8	38.2	39.2	–
P1' (F_Z)	-26.5	-27.1	-27.9	-28.6	-30.4	-31.3	-32.2	–

Table S5. Relative energies (kcal/mol) of reactants, transition states, and products in anti-Markovnikov hydroboration of benzaldehyde with and without EEFs (10^{-4} au) at the level of M06/6-311++G**//M06/6-31G*.

	-50	0	50
PhCHO + HBPin	0.0	0.0	0.0
TS1 (F_X)	31.3	28.9	24.5
P1 (F_X)	-39.6	-37.9	-36.1
TS1 (F_Y)	29.5	28.9	28.2
P1 (F_Y)	-39.2	-37.9	-37.1
TS1 (F_Z)	25.4	28.9	30.7
P1 (F_Z)	-36.7	-37.9	-39.4

Table S6. Relative energies (kcal/mol) of reactants, transition states, and products in Markovnikov hydroboration of benzaldehyde with and without EEFs (10^{-4} au) at the level of M06/6-311++G**//M06/6-31G*.

	-50	0	50
PhCHO + HBPIn	0.0	0.0	0.0
TS2 (F_X)	82.7	82.3	81.4
P2 (F_X)	-14.8	-12.4	-10.2
TS2 (F_Y)	81.5	82.3	83.2
P2 (F_Y)	-14.9	-12.4	-10.1
TS2 (F_Z)	85.6	82.3	79.1
P2 (F_Z)	-10.1	-12.4	-14.5

Table S7. Relative energies (kcal/mol) of reactants, transition states, and products in anti-Markovnikov hydroboration of benzaldehyde with and without EEFs (10^{-4} au) at the level of PBE0/6-311++G**//PBE0/6-31G*.

	-50	0	50
PhCHO + HBPIn	0.0	0.0	0.0
TS1 (F_X)	30.3	27.9	23.5
P1 (F_X)	-40.5	-38.3	-36.6
TS1 (F_Y)	28.4	27.9	27.2
P1 (F_Y)	-39.8	-38.3	-36.9
TS1 (F_Z)	24.4	27.9	29.6
P1 (F_Z)	-36.8	-38.3	-40.3

Table S8. Relative energies (kcal/mol) of reactants, transition states, and products in Markovnikov hydroboration of benzaldehyde with and without EEFs (10^{-4} au) at the level of PBE0/6-311++G**//PBE0/6-31G*.

	-50	0	50
PhCHO + HBPIn	0.0	0.0	0.0
TS2 (F_X)	79.8	79.3	78.2
P2 (F_X)	-16.5	-13.9	-11.4
TS2 (F_Y)	78.5	79.3	80.0
P2 (F_Y)	-16.7	-13.9	-11.6
TS2 (F_Z)	82.6	79.3	76.0
P2 (F_Z)	-11.7	-13.9	-15.9

Table S9. Relative energies (kcal/mol) of reactants, transition states, and products in anti-Markovnikov hydroboration of benzaldehyde with and without EEFs (10^{-4} au) at the level of BP86-D3/6-311++G**//BP86-D3/6-31+G*.

	-50	0	50
PhCHO + HBPIn	0.0	0.0	0.0
TS1 (F_X)	26.9	25.1	21.1
P1 (F_X)	-37.5	-35.5	-34.0
TS1 (F_Y)	25.7	25.1	24.4
P1 (F_Y)	-37.0	-35.5	-34.6
TS1 (F_Z)	22.1	25.1	26.5
P1 (F_Z)	-34.3	-35.5	-36.4

Table S10. Relative energies (kcal/mol) of reactants, transition states, and products in Markovnikov hydroboration of benzaldehyde with and without EEFs (10^{-4} au) at the level of BP86-D3/6-311++G**//BP86-D3/6-31+G*.

	-50	0	50
PhCHO + HBPIn	0.0	0.0	0.0
TS2 (F_X)	69.6	69.6	68.9
P2 (F_X)	-15.6	-13.1	-10.7
TS2 (F_Y)	68.8	69.6	70.5
P2 (F_Y)	-15.3	-13.1	-10.9
TS2 (F_Z)	72.8	69.6	66.4
P2 (F_Z)	-10.9	-13.1	-14.7

Table S11. Relative energies (kcal/mol) of reactants, transition states, and products in anti-Markovnikov hydroboration of benzaldehyde with and without EEFs (10^{-4} au) at the level of B3LYP/6-311++G**//B3LYP/6-311G*.

	-50	0	50
PhCHO + HBPIn	0.0	0.0	0.0
TS1 (F_X)	37.5	34.7	30.5
P1 (F_X)	-34.6	-32.2	-30.7
TS1 (F_Y)	35.2	34.7	34.2
P1 (F_Y)	-34.5	-32.2	-30.7
TS1 (F_Z)	31.1	34.7	37.0
P1 (F_Z)	-30.6	-32.2	-34.3

Table S12. Relative energies (kcal/mol) of reactants, transition states, and products in Markovnikov hydroboration of benzaldehyde with and without EEFs (10^{-4} au) at the level of B3LYP/6-311++G**//B3LYP/6-311G*.

	-50	0	50
PhCHO + HBPIn	0.0	0.0	0.0
TS2 (F_X)	89.2	88.9	87.9
P2 (F_X)	-8.7	-6.1	-3.4
TS2 (F_Y)	88.1	88.9	89.8
P2 (F_Y)	-9.1	-6.1	-3.6
TS2 (F_Z)	92.3	88.9	85.6
P2 (F_Z)	-3.5	-6.1	-8.1

Table S13. Relative energies (kcal/mol) of reactants, transition states, and products in anti-Markovnikov hydroboration of benzaldehyde with and without EEFs (10^{-4} au) at the level of M06/6-311++G**//M06/6-311G*.

	-50	0	50
PhCHO + HBPIn	0.0	0.0	0.0
TS1 (F_X)	31.9	28.6	23.7
P1 (F_X)	-38.2	-37.9	-37.4
TS1 (F_Y)	29.4	28.6	27.0
P1 (F_Y)	-39.1	-37.9	-37.4
TS1 (F_Z)	25.0	28.6	30.9
P1 (F_Z)	-33.3	-37.9	-42.3

Table S14. Relative energies (kcal/mol) of reactants, transition states, and products in Markovnikov hydroboration of benzaldehyde with and without EEFs (10^{-4} au) at the level of M06/6-311++G**//M06/6-311G*.

	-50	0	50
PhCHO + HBPIn	0.0	0.0	0.0
TS2 (F_X)	82.7	82.4	81.4
P2 (F_X)	-16.0	-12.1	-8.7
TS2 (F_Y)	81.2	82.4	83.4
P2 (F_Y)	-14.0	-12.1	-10.4
TS2 (F_Z)	85.7	82.4	78.9
P2 (F_Z)	-13.3	-12.1	-11.1

Table S15. Relative energies (kcal/mol) of reactants, transition states, and products in anti-Markovnikov hydroboration of benzaldehyde with and without EEFs (10^{-4} au) at the level of PBE0/6-311++G**//PBE0/6-311G*.

	-50	0	50
PhCHO + HBPIn	0.0	0.0	0.0
TS1 (F_X)	30.3	27.8	23.5
P1 (F_X)	-40.7	-38.2	-36.5
TS1 (F_Y)	28.4	27.8	27.2
P1 (F_Y)	-40.3	-38.2	-36.8
TS1 (F_Z)	24.5	27.8	29.5
P1 (F_Z)	-36.6	-38.2	-40.1

Table S16. Relative energies (kcal/mol) of reactants, transition states, and products in Markovnikov hydroboration of benzaldehyde with and without EEFs (10^{-4} au) at the level of PBE0/6-311++G**//PBE0/6-311G*.

	-50	0	50
PhCHO + HBPIn	0.0	0.0	0.0
TS2 (F_X)	79.9	79.4	78.3
P2 (F_X)	-16.5	-13.9	-11.2
TS2 (F_Y)	78.7	79.4	80.2
P2 (F_Y)	-16.6	-13.9	-11.4
TS2 (F_Z)	82.7	79.4	76.1
P2 (F_Z)	-11.2	-13.9	-15.8

Table S17. Relative energies (kcal/mol) of reactants, transition states, and products in anti-Markovnikov hydroboration of benzaldehyde in THF solvent with and without EEFs (10^{-4} au) at the level of B3LYP/6-311++G**//B3LYP/6-31G*.

	-50	0	50
PhCHO + HBPIn	0.0	0.0	0.0
TS1 (F_X)	38.5	34.2	29.2
P1 (F_X)	-32.5	-30.2	-28.3
TS1 (F_Y)	35.3	34.2	33.7
P1 (F_Y)	-31.0	-30.2	-28.7
TS1 (F_Z)	29.0	34.2	38.1
P1 (F_Z)	-28.3	-30.2	-32.6

Table S18. Relative energies (kcal/mol) of reactants, transition states, and products in Markovnikov hydroboration of benzaldehyde in THF solvent with and without EEFs (10^{-4} au) at the level of B3LYP/6-311++G**//B3LYP/6-31G*.

	-50	0	50
PhCHO + HBPIn	0.0	0.0	0.0
TS2 (F_X)	91.4	91.1	89.8
P2 (F_X)	-7.7	-4.5	-1.5
TS2 (F_Y)	89.9	91.1	92.2
P2 (F_Y)	-7.9	-4.5	-1.8
TS2 (F_Z)	95.4	91.1	86.5
P2 (F_Z)	-1.6	-4.5	-7.2

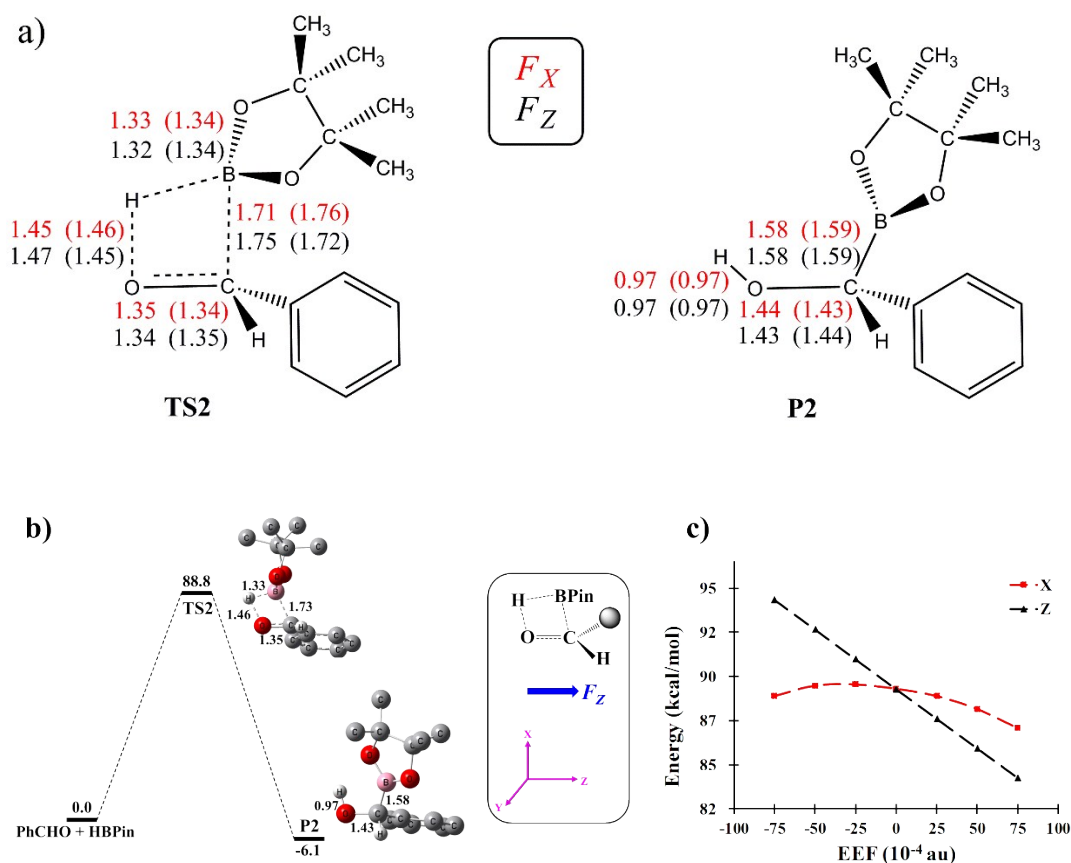


Fig. S1 a) Structures of transition states and products in Markovnikov hydroboration of benzaldehyde with HBPin in present of EEFs ($\pm 50 \times 10^{-4}$ au). Notes: The bond length are given in Å; F_X : the red, F_Z : the black; Values in brackets are those calculated when EEFs are oriented along negative directions; b) Reaction pathway of Markovnikov hydroboration of benzaldehyde with HBPin and the relative energies (kcal/mol) of stationary points at no EEf; c) The barrier variations of these hydroboration of benzaldehyde when EEFs are ± 25 , ± 50 and $\pm 75 \times 10^{-4}$ au from F_X and F_Z directions.

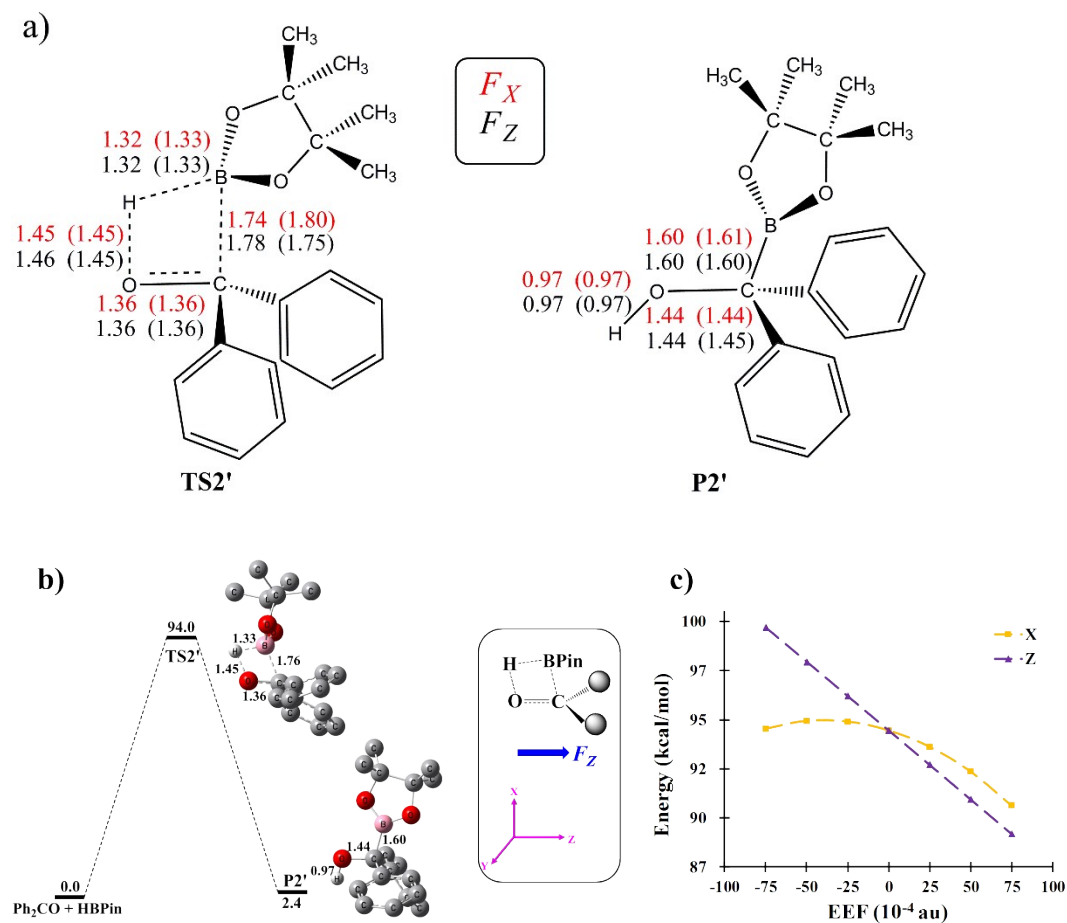


Fig. S2 a) Structures of transition states and products in Markovnikov hydroboration of benzophenone with HBPIn in present of EEFs ($\pm 50 \times 10^{-4}$ au). Notes: The bond length are given in Å; F_X : the red, F_Z : the black; Values in brackets are those calculated when EEFs are oriented along negative directions; b) Reaction pathway of Markovnikov hydroboration of benzophenone with HBPIn and the relative energies (kcal/mol) of stationary points at no EEF; c) The barrier variations of these hydroboration of benzophenone when EEFs are ± 25 , ± 50 and $\pm 75 \times 10^{-4}$ au from F_X and F_Z directions.

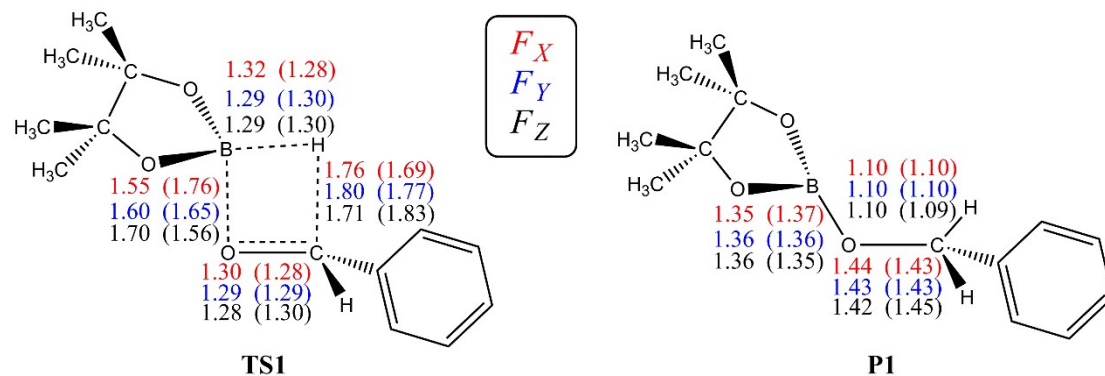


Fig. S3 Structures of transition states, and products in anti-Markovnikov hydroboration of benzaldehyde in present of EEFs ($\pm 50 \times 10^{-4}$ au). Notes: The bond length are given in Å; F_X : the red, F_Y : the blue, F_Z : the black; Values in brackets are those calculated when EEFs are oriented along negative directions.

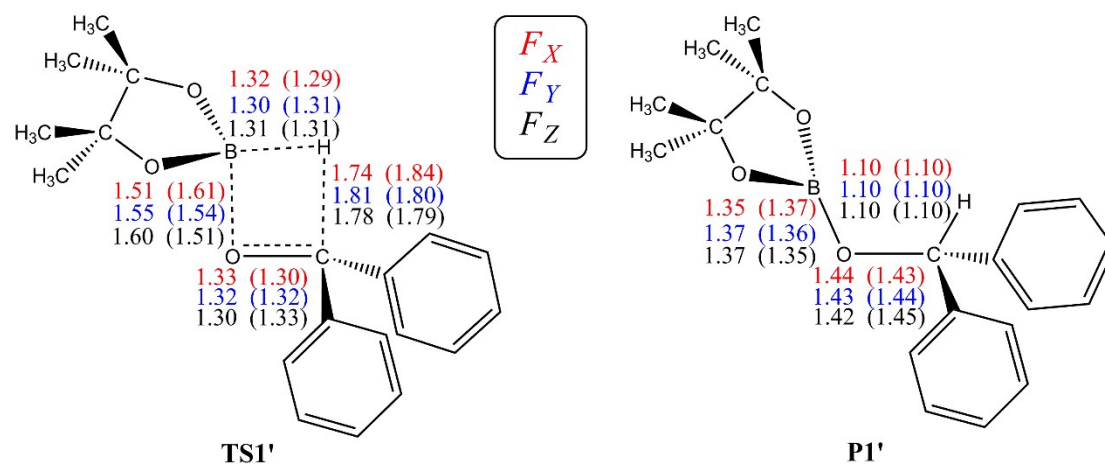


Fig. S4 Structures of transition states, and products in anti-Markovnikov hydroboration of benzophenone in present of EEFs ($\pm 50 \times 10^{-4}$ au). Notes: The bond length are given in Å; F_X : the red, F_Y : the blue, F_Z : the black; Values in brackets are those calculated when EEFs are oriented along negative directions.

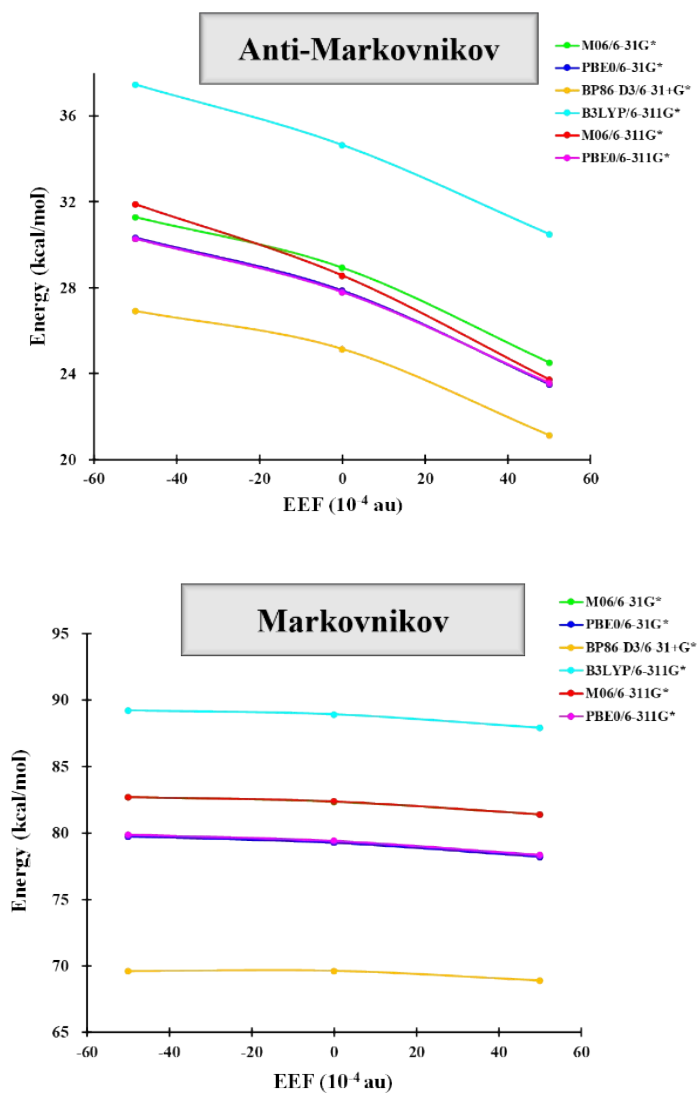


Fig. S5. The barriers of the hydroboration of benzaldehyde with HBPi according to the paths of anti-Markovnikov (the left) and Markovnikov (the right) addition when EEFs are 0 and ± 50 ($\times 10^{-4}$ au) from F_X direction on the basis of several computational methods.

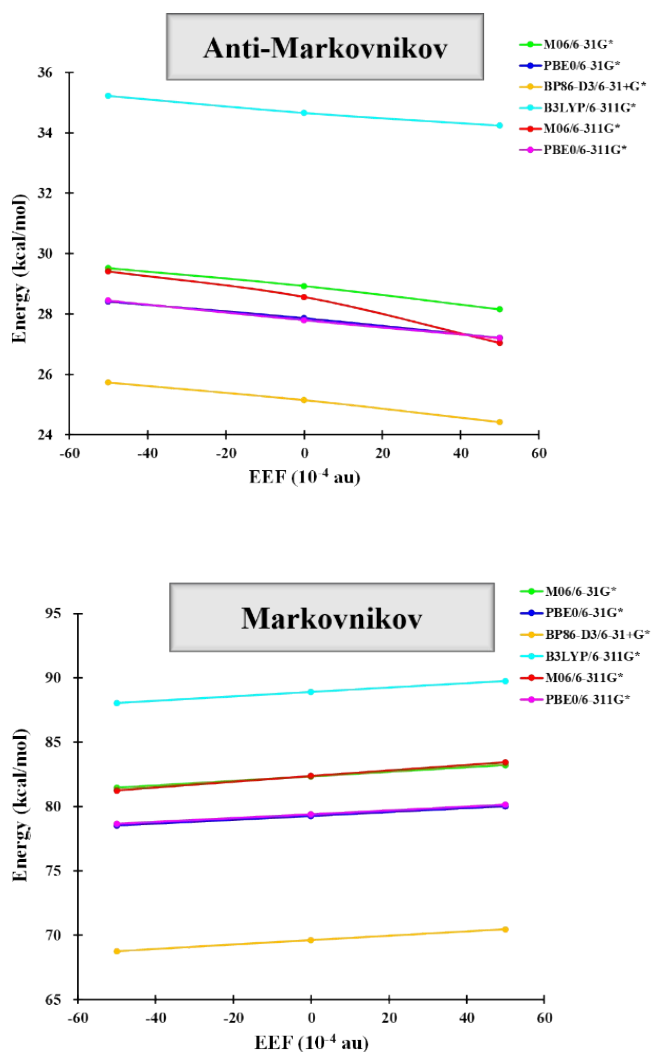


Fig. S6. The barriers of the hydroboration of benzaldehyde with HBPIn according to the paths of anti-Markovnikov (the left) and Markovnikov (the right) addition when EEFs are 0 and ± 50 ($\times 10^{-4}$ au) from F_Y direction on the basis of several computational methods.

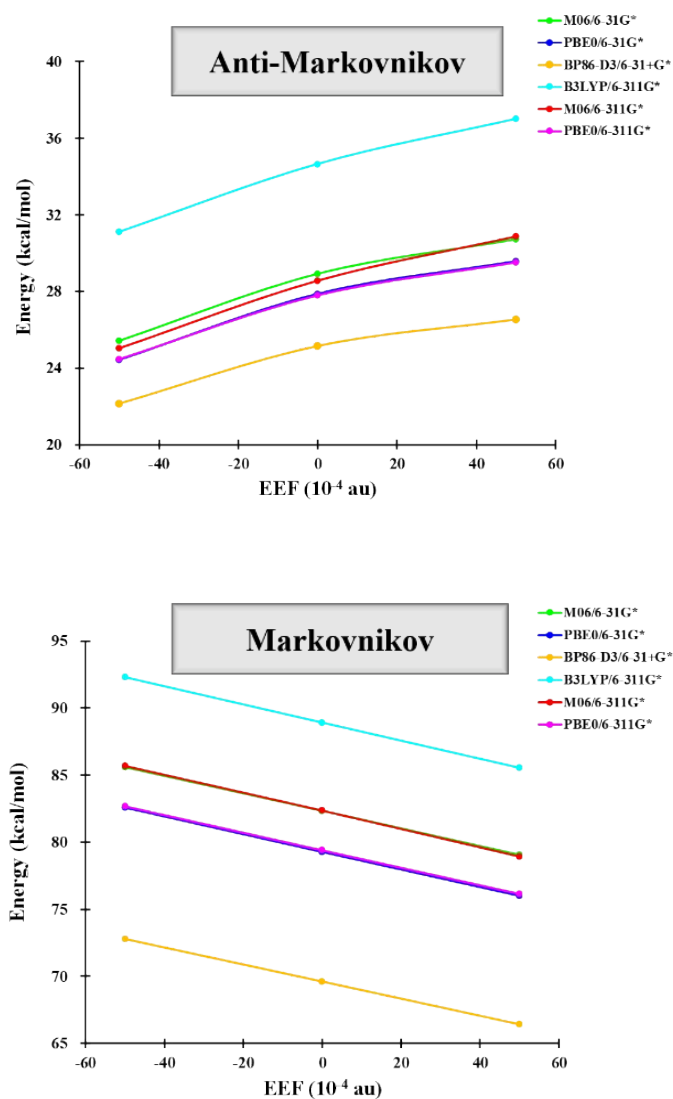


Fig. S7. The barriers of the hydroboration of benzaldehyde with HBPi according to the paths of anti-Markovnikov (the left) and Markovnikov (the right) addition when EEFs are 0 and ± 50 ($\times 10^{-4}$ au) from F_Z direction on the basis of several computational methods.

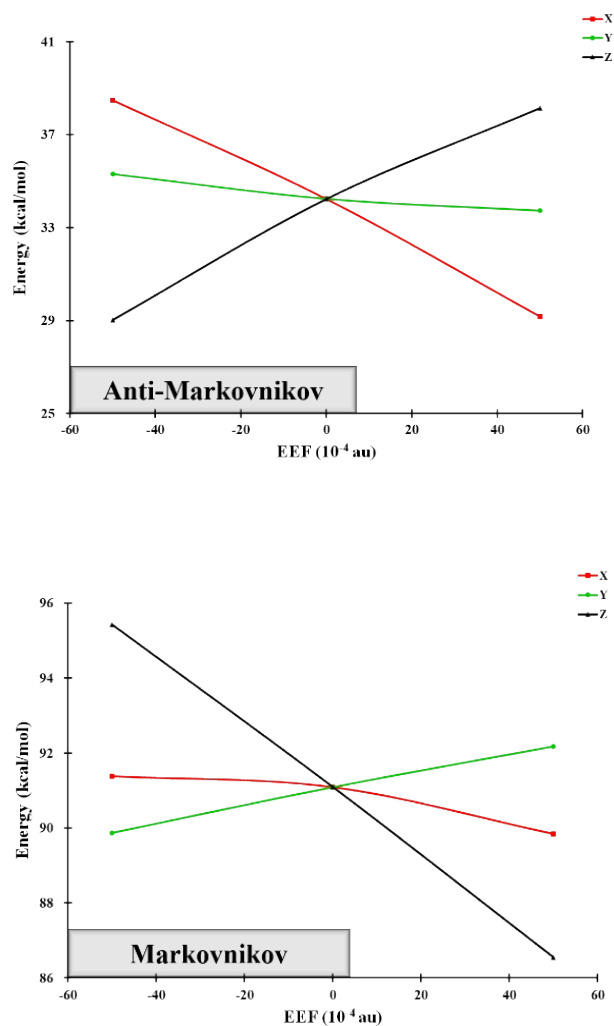


Fig. S8. The barriers of the hydroboration of benzaldehyde with HBPi according to the paths of anti-Markovnikov (the left) and Markovnikov (the right) addition when EEFs are 0 and ± 50 ($\times 10^{-4}$ au) from three directions (F_X , F_Y , and F_Z) in THF solvent.

The coordinates of TSs in hydroboration of benzaldehyde with HBPIn.

TS1

Frequency = -583.3i cm⁻¹

ZeroPoint = 0.3013689 au

E_{tot} = -757.299778 au

C,0,-0.0114084643,0.068760849,1.2600043805
B,0,1.6198415158,0.0595754014,-0.0050155445
H,0,1.7754721487,-0.0527563302,1.2697192187
O,0,-0.008657574,0.0408990143,-0.0273355206
C,0,-0.5278034861,-1.0379343196,2.061339991
C,0,-0.7470175291,-0.8610515544,3.4372009731
C,0,-0.8204440504,-2.2682897723,1.4479712882
C,0,-1.2643249658,-1.9060928215,4.1963484822
H,0,-0.5128415905,0.0941734012,3.9013169676
C,0,-1.3376607044,-3.3086475673,2.2113429986
H,0,-0.6258626089,-2.3788831769,0.3862714629
C,0,-1.5591544873,-3.1272284443,3.581662314
H,0,-1.4384862135,-1.7744955213,5.2601167583
H,0,-1.5662697325,-4.2630552353,1.7462940418
H,0,-1.9620680086,-3.9439036781,4.1747292143
O,0,2.1907385972,1.2551239067,-0.4909487494
O,0,2.063877414,-1.0701426358,-0.7377849918
C,0,3.152223931,-0.6060722087,-1.5643369155
C,0,2.804958757,0.9221765206,-1.7564336215
C,0,4.0090368262,1.8416497426,-1.9589980422
H,0,3.6680559044,2.8776954582,-2.060366304
H,0,4.6946708806,1.7969084105,-1.109378051
H,0,4.560475606,1.5770966375,-2.8693878587
C,0,4.4640527125,-0.826437776,-0.7935865787
H,0,4.4883883366,-0.2267240948,0.1216287299
H,0,4.5324957405,-1.8816726573,-0.5094970114
H,0,5.3432440755,-0.5748418459,-1.3974262408
C,0,3.1576173735,-1.4340866041,-2.850136471
H,0,2.1863489799,-1.4007382813,-3.3490055216
H,0,3.9242330019,-1.0755714866,-3.5476169033
H,0,3.3791456109,-2.4803045172,-2.6130565477
C,0,1.7694294461,1.1617554939,-2.8675001266
H,0,1.4064461176,2.1919397436,-2.79323854
H,0,2.1997182218,1.0193875874,-3.8655449124
H,0,0.9113079343,0.4922713603,-2.7580119237
H,0,0.1135114133,1.026982732,1.7855585955

TS2

Frequency = -1233.8i cm⁻¹

ZeroPoint = 0.299 au

E_{tot} = -757.2134878 au

C,0,0.0149069592,-0.0314163456,1.3550848669
B,0,1.5998788016,0.0940494901,0.6631475555
H,0,1.3218747963,-0.1411868382,-0.6173511431
O,0,0.0138244438,0.016867121,0.0097849242
C,0,-0.3461132448,-1.2608576242,2.071852775
C,0,-0.573976215,-2.4768332878,1.407257514
C,0,-0.4536160365,-1.2177400273,3.4718451335
C,0,-0.9080151402,-3.6186899457,2.1301868344
H,0,-0.4914729247,-2.5145769986,0.3257290997
C,0,-0.79245231,-2.3616960249,4.1906015213
H,0,-0.2764778433,-0.2800263338,3.9940782447
C,0,-1.0195987899,-3.5672754192,3.5227051391
H,0,-1.0853950602,-4.5537692699,1.6054072273
H,0,-0.8776790818,-2.3129153724,5.2729307619
H,0,-1.2825855553,-4.4604493577,4.0828039091
O,0,2.2389264928,1.3535634871,0.7492202385
O,0,2.4442316719,-0.9975998897,1.0151250061
C,0,3.5869831862,1.0638165122,1.2008252675
C,0,3.7760812321,-0.459270223,0.8109660044
C,0,4.5411848325,2.0320014895,0.5031348502
H,0,5.5835848722,1.8139840248,0.7635994426
H,0,4.4342317165,1.986808456,-0.5831906926
H,0,4.3209551157,3.0569218963,0.8195136741
C,0,3.6156128497,1.2895934103,2.7199921819
H,0,3.2603350104,2.3029213273,2.9324128469
H,0,2.9597143211,0.5809055618,3.2353641395
H,0,4.6266022591,1.186874637,3.1293679592
C,0,4.7243911134,-1.2442393998,1.7166081147
H,0,5.7371877146,-0.8266560823,1.6777948781
H,0,4.3805408303,-1.2398984489,2.7530221679
H,0,4.7731853504,-2.2856726576,1.3824330833
C,0,4.1719141348,-0.6566106793,-0.6596407271
H,0,5.2039460029,-0.3419335884,-0.8467977499
H,0,4.083814305,-1.7181612454,-0.9117245471
H,0,3.519880849,-0.0913256224,-1.3350695754
H,0,-0.1309816996,0.9368939087,1.8393667938

$F_X = 50 (10^{-4}) \text{ au}$

TS1

Frequency = -604.5i cm⁻¹

ZeroPoint = 0.3013537 au

E_{tot} = -757.3068589 au

C,0,0.01068462,0.04041791,1.29084367
B,0,1.56711962,0.05137491,-0.03310533
H,0,1.76745262,-0.08846209,1.25990067
O,0,0.02102762,-0.01396809,-0.01262633
C,0,-0.57353338,-1.01623309,2.09801067
C,0,-0.80328638,-0.79595909,3.46846067
C,0,-0.96185438,-2.22966309,1.49997667
C,0,-1.42214338,-1.77768909,4.23382067
H,0,-0.51003438,0.14965491,3.91842067
C,0,-1.58436638,-3.20493909,2.26976467
H,0,-0.77738638,-2.37191609,0.44041967
C,0,-1.81415838,-2.97889809,3.63240367
H,0,-1.61680938,-1.60787609,5.28835367
H,0,-1.90369038,-4.13711309,1.81386567
H,0,-2.31188938,-3.73968009,4.22727767
O,0,2.12845062,1.28064891,-0.48263633
O,0,2.08915962,-1.04030109,-0.79026333
C,0,3.13856162,-0.50951309,-1.61265133
C,0,2.72263562,1.00587591,-1.76315733
C,0,3.88107562,1.98286891,-1.97435533
H,0,3.48980162,3.00393091,-2.04039033
H,0,4.58988662,1.94865991,-1.14237833
H,0,4.41829762,1.76585191,-2.90646733
C,0,4.47246562,-0.68614909,-0.86435133
H,0,4.47784862,-0.10450309,0.06289867
H,0,4.59110562,-1.74351009,-0.60364233
H,0,5.33219662,-0.38094509,-1.47409733
C,0,3.16622362,-1.30437509,-2.92025133
H,0,2.18646162,-1.30486109,-3.40231633
H,0,3.90253062,-0.89081709,-3.62125833
H,0,3.43833562,-2.34571309,-2.71432733
C,0,1.65533662,1.22217691,-2.85007833
H,0,1.24385262,2.23069091,-2.74279533
H,0,2.06902462,1.12373891,-3.86075033
H,0,0.83098562,0.51223691,-2.74041033
H,0,0.14463762,1.01117691,1.78535267

TS2

Frequency = -1258.4i cm⁻¹

ZeroPoint = 0.2991155 au

E_{tot} = -757.2133209 au

C,0,0.0374206568,-0.0601729874,1.352570051
B,0,1.6046477489,0.0742711724,0.6774084032
H,0,1.3470240924,-0.163314434,-0.6043298017
O,0,0.0372510607,-0.0186645644,0.0037440507
C,0,-0.3342005918,-1.2882454439,2.0718239639
C,0,-0.6138864555,-2.4916580435,1.4053376659
C,0,-0.4182794431,-1.2441687126,3.4731140222
C,0,-0.9808452864,-3.6226555175,2.129623338
H,0,-0.5639182808,-2.5249583013,0.3216286166
C,0,-0.7899203005,-2.3770891451,4.1930665747
H,0,-0.2141553902,-0.311345676,3.9943696928
C,0,-1.0712906786,-3.5704104966,3.5236962473
H,0,-1.2160976582,-4.5444561361,1.6048209548
H,0,-0.8734122567,-2.3261763387,5.2751937167
H,0,-1.3756107096,-4.450394007,4.0832711368
O,0,2.2473865757,1.3438554196,0.7573591436
O,0,2.480149358,-1.0026414452,1.0348128599
C,0,3.5903629806,1.0709701102,1.2009155007
C,0,3.7940404201,-0.4518412622,0.8167173245
C,0,4.5325494713,2.0482305118,0.495360069
H,0,5.5800377892,1.8448164772,0.7521856896
H,0,4.4192284265,1.9972373475,-0.5902439656
H,0,4.2980008251,3.0714599599,0.8074695196
C,0,3.6296877252,1.3015677087,2.7207021842
H,0,3.2585162794,2.3092054103,2.9326055529
H,0,2.9858568992,0.5859114154,3.2409503441
H,0,4.6454051368,1.2144913385,3.1250706252
C,0,4.7631896467,-1.2211591173,1.7160040683
H,0,5.7716723772,-0.7915729529,1.6655112287
H,0,4.4278837586,-1.215781187,2.7552442691
H,0,4.8182601483,-2.2643347986,1.3868002475
C,0,4.1848054191,-0.6483359317,-0.6576015733
H,0,5.2132629948,-0.3234477297,-0.8532409077
H,0,4.1023694437,-1.7111812243,-0.9071022409
H,0,3.5215529055,-0.0917889981,-1.3284189233
H,0,-0.1435210885,0.9101785794,1.8219473509

$$F_X = -50 (10^{-4}) \text{ au}$$

TS1

$$\text{Frequency} = -656.1i \text{ cm}^{-1}$$

$$\text{ZeroPoint} = 0.3015401 \text{ au}$$

$$E_{\text{tot}} = -757.2994895 \text{ au}$$

C,0,0.0057779681,-0.0220852759,1.2388930409
B,0,1.7430585447,-0.0321373808,0.1714067747
H,0,1.6830567078,-0.0491218124,1.4467656014
O,0,-0.0040136022,-0.0045754302,-0.0397758198
C,0,-0.3859900291,-1.2196353439,2.0168785968
C,0,-0.6902607369,-1.1007240408,3.3789076079
C,0,-0.4533624536,-2.4689075289,1.383035211
C,0,-1.0677409122,-2.2263680872,4.1082366107
H,0,-0.6198788892,-0.1292601625,3.8636776675
C,0,-0.8257125254,-3.5916324286,2.1162594269
H,0,-0.1817893979,-2.534612331,0.3345308318
C,0,-1.1333195107,-3.4708093277,3.4758189672
H,0,-1.2942057434,-2.1386687082,5.1672370779
H,0,-0.8602146189,-4.5655624617,1.6360478312
H,0,-1.4104870236,-4.3527640501,4.047743541
O,0,2.3577409331,1.1122040296,-0.321992706
O,0,2.1829499765,-1.2176511392,-0.424669004
C,0,3.3430517891,-0.8404797896,-1.2228225788
C,0,3.0655117819,0.6855823915,-1.5231374923
C,0,4.3129577151,1.5528610464,-1.6700803493
H,0,4.0212417016,2.5920901101,-1.8544751503
H,0,4.9268592107,1.5323403783,-0.7672536763
H,0,4.925766103,1.2199076059,-2.515483108
C,0,4.5917223901,-1.0660003562,-0.3600202881
H,0,4.5897704864,-0.4184159093,0.5223034866
H,0,4.6027032413,-2.1053173905,-0.0171772638
H,0,5.5138794561,-0.8819128108,-0.9204688645
C,0,3.3856966585,-1.7440427283,-2.453662992
H,0,2.4475250333,-1.7073993901,-3.0132127237
H,0,4.2057632907,-1.4560102474,-3.1210277027
H,0,3.5563037952,-2.7799121305,-2.1426345318
C,0,2.124266582,0.9016983956,-2.7172088219
H,0,1.8097427643,1.9502834698,-2.730918781
H,0,2.621535286,0.6801181498,-3.6677962245
H,0,1.2286128577,0.2783534574,-2.6348471269
H,0,-0.02916557,0.9268809475,1.8032291024

TS2

$$\text{Frequency} = -1215.0i \text{ cm}^{-1}$$

$$\text{ZeroPoint} = 0.298664 \text{ au}$$

$$E_{\text{tot}} = -757.2193468 \text{ au}$$

C,0,-0.0009635033,-0.0166612244,1.3732383601
B,0,1.6074562758,0.1067253551,0.6606544633
H,0,1.2992487618,-0.1392896513,-0.6154673939
O,0,0.000566616,0.0436409054,0.0306141063
C,0,-0.3616801037,-1.2471017113,2.0804513201
C,0,-0.5525102489,-2.4683993788,1.4114983652
C,0,-0.4976796635,-1.212097004,3.4791112406
C,0,-0.8742581383,-3.6188212084,2.1261385215
H,0,-0.4333563422,-2.5052195651,0.3333869254
C,0,-0.8243299289,-2.3647780481,4.1893367909
H,0,-0.3359674154,-0.2753298594,4.0080489679
C,0,-1.013647413,-3.5743799266,3.5165004945
H,0,-1.0052141665,-4.559516712,1.5969873932
H,0,-0.9152091656,-2.3221910053,5.2718089117
H,0,-1.2515240905,-4.4778224091,4.071902563
O,0,2.2345989932,1.3594853633,0.74482673
O,0,2.4273264032,-0.992921532,1.0080849016
C,0,3.5936845237,1.0636831304,1.1967922714
C,0,3.7745051432,-0.4603546869,0.807194605
C,0,4.548178613,2.0255921243,0.4946346735
H,0,5.5892979429,1.8019092246,0.7518632063
H,0,4.4398509291,1.9796473712,-0.5913489697
H,0,4.3375318541,3.052115096,0.8117090065
C,0,3.6203865367,1.2931612628,2.7137213549
H,0,3.2764838125,2.3110068224,2.923575018
H,0,2.9600756641,0.5904278699,3.2324252576
H,0,4.6302407201,1.1832304644,3.1216683695
C,0,4.7118455923,-1.2511848412,1.7170265318
H,0,5.7265702525,-0.8401062254,1.6808412317
H,0,4.3665312557,-1.243935542,2.7529022608
H,0,4.7584758795,-2.2922621939,1.3828195352
C,0,4.1669604476,-0.6635908786,-0.661252059
H,0,5.1991800711,-0.3523433284,-0.8484508647
H,0,4.0796206095,-1.725756628,-0.9099749393
H,0,3.5173191274,-0.0978417711,-1.3396346528
H,0,-0.1041718451,0.9476813417,1.8747525022

$F_Y = 50 (10^{-4})$ au

TS1

Frequency = -568.2i cm⁻¹

ZeroPoint = 0.3012769 au

E_{tot} = -757.305756 au

C,0,0.0071842202,-0.0135852937,1.2505821773
B,0,1.5896453076,-0.070687773,-0.0771567659
H,0,1.8082395805,0.0293017841,1.1911732323
O,0,-0.0107586657,0.0226632293,-0.0428576696
C,0,-0.3874886958,-1.184552941,2.0126685335
C,0,-0.6301408411,-1.0641267267,3.3936996877
C,0,-0.5371810445,-2.4294172796,1.3708940766
C,0,-1.0326263386,-2.1742893503,4.1258002307
H,0,-0.5025660237,-0.0988200639,3.8793711725
C,0,-0.9358516744,-3.5365073624,2.1107436854
H,0,-0.3119944707,-2.5024669087,0.3124678689
C,0,-1.184541659,-3.4088108042,3.4826161206
H,0,-1.2245013145,-2.0894026286,5.1912425398
H,0,-1.0473558634,-4.5024213442,1.6282028271
H,0,-1.4926613319,-4.2787620022,4.0557126439
O,0,2.2199848626,0.9713827664,-0.808022855
O,0,1.9412035183,-1.3447092172,-0.5978220919
C,0,3.0448353312,-1.1313520182,-1.4969409759
C,0,2.786453695,0.3475565269,-1.9842875547
C,0,4.042238632,1.1249602136,-2.3792081871
H,0,3.7680815372,2.1427517051,-2.6815836543
H,0,4.7429474734,1.1967211093,-1.5438249175
H,0,4.5524271666,0.6463293294,-3.2237209878
C,0,4.3518408623,-1.2764236514,-0.6989682877
H,0,4.4311428105,-0.5064609346,0.0756374539
H,0,4.3551085957,-2.2537371405,-0.2068392749
H,0,5.2364505218,-1.2159874824,-1.3430967325
C,0,2.984571744,-2.1982317099,-2.5905354229
H,0,2.0091164039,-2.2142403165,-3.0822903842
H,0,3.7591148014,-2.034607859,-3.3493565871
H,0,3.1518539176,-3.1860718807,-2.149490941
C,0,1.7450190909,0.4226575685,-3.1131488388
H,0,1.4507122323,1.4687424752,-3.2545533134
H,0,2.1406267414,0.0427194767,-4.062045728
H,0,0.8494509614,-0.1501164644,-2.8566085051
H,0,0.0623597151,0.9307071387,1.8137204554

TS2

Frequency = -1242.8i cm⁻¹

ZeroPoint = 0.2989837 au

E_{tot} = -757.216969 au

C,0,0.0092342676,-0.0262885233,1.3607802691
B,0,1.5904539851,0.1066223007,0.6950634474
H,0,1.335734976,-0.1366279906,-0.5903584455
O,0,0.0182833625,0.0422832808,0.0134867425
C,0,-0.3569897718,-1.2627098603,2.0643513134
C,0,-0.5828655142,-2.4727189464,1.388276912
C,0,-0.4589954577,-1.2320020177,3.4651562808
C,0,-0.9088881639,-3.6229533171,2.101799589
H,0,-0.5012759626,-2.50352526,0.3064522702
C,0,-0.7909342825,-2.3837534738,4.1744294724
H,0,-0.2791041537,-0.2985768009,3.9955778445
C,0,-1.0147167077,-3.583982561,3.495367396
H,0,-1.0808361613,-4.5550756447,1.5714381765
H,0,-0.8698543514,-2.3489917953,5.2576794334
H,0,-1.2672673653,-4.4846227173,4.0471570542
O,0,2.2369856569,1.3719908463,0.7785195296
O,0,2.4364802322,-0.9775997124,1.0590626666
C,0,3.5902945718,1.0743604529,1.203732302
C,0,3.7676104171,-0.4563164433,0.8322949782
C,0,4.538273638,2.0265142169,0.4738600665
H,0,5.5840620954,1.8061692063,0.718613646
H,0,4.4120882886,1.9610413571,-0.6095253768
H,0,4.3282783829,3.0589747228,0.7768903022
C,0,3.6526859273,1.3212654962,2.7190089652
H,0,3.3096868004,2.3413483608,2.9248571224
H,0,2.9997156305,0.6254288998,3.2542375009
H,0,4.6698468455,1.2115407876,3.111112378
C,0,4.7192501274,-1.235677855,1.7399306637
H,0,5.735406491,-0.8272770489,1.6869536045
H,0,4.3842710561,-1.2188716372,2.7790765681
H,0,4.7576205762,-2.2809615452,1.4192086197
C,0,4.1496773192,-0.6786545832,-0.6385000424
H,0,5.1825974353,-0.3748424532,-0.839325435
H,0,4.0542581252,-1.7432680689,-0.871360336
H,0,3.4939175768,-0.1231188072,-1.3192654202
H,0,-0.1495618926,0.9372781347,1.8523469408

$F_Y = -50 (10^{-4}) \text{ au}$

TS1

Frequency = -628.5i cm⁻¹

ZeroPoint = 0.3014455 au

E_{tot} = -757.2989157 au

C,0,0.0019916425,0.0418014878,1.2465917736
B,0,1.6602636026,0.1022198019,0.063143918
H,0,1.750623062,-0.1954355349,1.3241435758
O,0,0.0217270461,-0.0462033752,-0.0363445159
C,0,-0.5994300235,-1.0028591037,2.0861693353
C,0,-0.8008027701,-0.769827856,3.4543711684
C,0,-1.0000249133,-2.2173251564,1.5079226878
C,0,-1.401846653,-1.7476573083,4.2436386396
H,0,-0.4917486894,0.1764552086,3.8913997002
C,0,-1.6036152796,-3.1889494277,2.2988161239
H,0,-0.8311134694,-2.3642031375,0.4460632199
C,0,-1.8027840487,-2.9545249922,3.6642916611
H,0,-1.5643545244,-1.5674847249,5.302148778
H,0,-1.9235047882,-4.1285974066,1.8559027746
H,0,-2.2779117508,-3.7147953151,4.2796144407
O,0,2.1289955274,1.4013860352,-0.1718103793
O,0,2.2331147718,-0.8473184538,-0.8127012725
C,0,3.283023327,-0.1386058241,-1.5196091595
C,0,2.8005089323,1.364615202,-1.4532307979
C,0,3.9178453651,2.4065735974,-1.4375968601
H,0,3.4839139376,3.4084159427,-1.362312542
H,0,4.586134774,2.2686088365,-0.5843342234
H,0,4.5098131626,2.3663006391,-2.3595535445
C,0,4.5999850183,-0.3752626356,-0.7644924143
H,0,4.555344395,0.0488499101,0.2430831154
H,0,4.7668947563,-1.4545902933,-0.6740855197
H,0,5.4566775075,0.0649134198,-1.2864529019
C,0,3.3754960435,-0.7209508565,-2.9299261162
H,0,2.4099412977,-0.6809202541,-3.4389058364
H,0,4.1114318349,-0.1752065247,-3.5320756695
H,0,3.6900812721,-1.7698975964,-2.8775669364
C,0,1.7716742039,1.7160641559,-2.5399786801
H,0,1.3238643284,2.6842445288,-2.2970490997
H,0,2.2352315674,1.794605201,-3.5297166848
H,0,0.967634965,0.9751818167,-2.5855409783
H,0,0.1554454493,1.0171964434,1.7301587904

TS2

Frequency = -1227.7i cm⁻¹

ZeroPoint = 0.2988425 au

E_{tot} = -757.2152293 au

C,0,0.018096727,-0.033148683,1.3578524719
B,0,1.6085508516,0.0867010375,0.6398016679
H,0,1.3048387004,-0.1394074634,-0.6354846359
O,0,0.0085945589,-0.0003265779,0.0143293944
C,0,-0.3382883646,-1.2580010954,2.0820308522
C,0,-0.5585511886,-2.47978898,1.4243584848
C,0,-0.4601510197,-1.2074538137,3.4810384367
C,0,-0.8992752845,-3.6170915797,2.1511415926
H,0,-0.4684069116,-2.5209556211,0.3435552016
C,0,-0.8048670758,-2.3473251184,4.2035025968
H,0,-0.2934190173,-0.2660832923,3.9989987098
C,0,-1.0251772794,-3.558006067,3.5422013058
H,0,-1.0745034599,-4.554793892,1.6280870654
H,0,-0.9036168856,-2.2879146544,5.2842626457
H,0,-1.2977678339,-4.4467733329,4.1063959912
O,0,2.2418011433,1.3395416444,0.727254213
O,0,2.4499790946,-1.0128533074,0.9791200342
C,0,3.5868986608,1.0564708215,1.1971539916
C,0,3.7831827523,-0.4616307248,0.7935338981
C,0,4.5442422611,2.0357677719,0.5214954409
H,0,5.5842329745,1.819918208,0.7930705132
H,0,4.4504780748,2.0055309259,-0.566415357
H,0,4.3169556784,3.0553991738,0.8466907459
C,0,3.5922562548,1.2673313476,2.7182355245
H,0,3.2306987594,2.2766534365,2.9350065739
H,0,2.9335913146,0.5510446264,3.2206082639
H,0,4.5989069812,1.1686524863,3.138988966
C,0,4.7276502954,-1.2519589381,1.6980890054
H,0,5.7381231272,-0.8285396817,1.6702948718
H,0,4.3767024262,-1.2558526324,2.7322074803
H,0,4.7832926199,-2.2909222898,1.3539787074
C,0,4.1892095608,-0.6406923238,-0.6764687026
H,0,5.2202681024,-0.3177836466,-0.8535222598
H,0,4.1063081509,-1.70006618,-0.9429915621
H,0,3.5401021655,-0.0677759577,-1.3474831496
H,0,-0.115512915,0.9385353738,1.8374680201

$F_z = 50 (10^{-4}) \text{ au}$

TS1

Frequency = -675.6i cm⁻¹

ZeroPoint = 0.3013763 au

E_{tot} = -757.2966758 au

C,0,0.00551056,-0.0271821,1.26107053
B,0,1.68729156,-0.0628961,0.11914053
H,0,1.70811156,-0.0748311,1.40993953
O,0,-0.00019744,0.0276009,-0.01739947
C,0,-0.42096244,-1.2375681,1.99425453
C,0,-0.72989844,-1.1585431,3.35847053
C,0,-0.54671244,-2.4546201,1.30785953
C,0,-1.17081744,-2.2919471,4.03731153
H,0,-0.63042444,-0.2071901,3.87745253
C,0,-0.98390044,-3.5857671,1.99135653
H,0,-0.28368744,-2.4885831,0.25578453
C,0,-1.29717644,-3.5040461,3.35206753
H,0,-1.41973944,-2.2329621,5.09395253
H,0,-1.08239544,-4.5308111,1.46544353
H,0,-1.64315844,-4.3896141,3.87953853
O,0,2.33121256,1.0519929,-0.41646947
O,0,2.08576956,-1.2754201,-0.46638247
C,0,3.13006956,-0.9324571,-1.42094347
C,0,2.85342756,0.5978809,-1.70215447
C,0,4.09125356,1.4303589,-2.02720747
H,0,3.80119756,2.4742129,-2.18484747
H,0,4.82223256,1.4008839,-1.21529247
H,0,4.57102356,1.0742029,-2.94564547
C,0,4.47799156,-1.1790471,-0.72750047
H,0,4.60148056,-0.5187331,0.13734053
H,0,4.50919556,-2.2154431,-0.37528747
H,0,5.32158056,-1.0228461,-1.40830647
C,0,2.98702156,-1.8475041,-2.63542947
H,0,1.98387356,-1.7922671,-3.06294047
H,0,3.71212956,-1.5849151,-3.41386847
H,0,3.17231356,-2.8858791,-2.34029547
C,0,1.77167556,0.8265019,-2.76739447
H,0,1.47869656,1.8807839,-2.75312747
H,0,2.13877456,0.5880179,-3.77099747
H,0,0.87924156,0.2256499,-2.57228747
H,0,-0.00010644,0.9053309,1.85206853

TS2

Frequency = -1191.2i cm⁻¹

ZeroPoint = 0.2988977 au

E_{tot} = -757.2141945 au

C,0,0.0151028194,-0.0349875631,1.3901613637
B,0,1.6112054537,0.1000903784,0.6922459587
H,0,1.3430853928,-0.1395381885,-0.5826154048
O,0,0.0300667787,0.0253388926,0.0499327513
C,0,-0.3569439539,-1.2698046827,2.0894688374
C,0,-0.5513377244,-2.4839337196,1.4097415705
C,0,-0.5164265885,-1.2378317811,3.4848385163
C,0,-0.9034826579,-3.6329805184,2.1122148825
H,0,-0.4309283372,-2.5147944146,0.331882375
C,0,-0.8734751643,-2.3891592655,4.1829959282
H,0,-0.3670138491,-0.3005622093,4.017332056
C,0,-1.0674490329,-3.5921800642,3.5000587902
H,0,-1.0554441424,-4.5639418979,1.5729244002
H,0,-1.0015514878,-2.347029618,5.2625596265
H,0,-1.347321406,-4.4916798914,4.0425525528
O,0,2.2422117701,1.3609047151,0.7943788463
O,0,2.4546697921,-0.9865185651,1.0619212376
C,0,3.6047355579,1.0758868787,1.1988156444
C,0,3.7845673228,-0.4527935198,0.8211688428
C,0,4.53543466,2.036204507,0.4601040001
H,0,5.5861975163,1.8235978571,0.6901881547
H,0,4.3965679041,1.9760325602,-0.6211592852
H,0,4.3218556933,3.0656272613,0.7666854164
C,0,3.6792226402,1.3210376553,2.7146938104
H,0,3.3319659194,2.3386086354,2.9220162388
H,0,3.0354870518,0.6200404995,3.256332658
H,0,4.7024321074,1.2211493832,3.0947586173
C,0,4.7483389005,-1.2291049022,1.7187006888
H,0,5.7603447163,-0.8125852664,1.6560117232
H,0,4.4224364874,-1.2142896645,2.7616824029
H,0,4.7911156041,-2.2730263388,1.3921645452
C,0,4.1538293996,-0.6686687285,-0.6524167976
H,0,5.1814626643,-0.3552567839,-0.8621617076
H,0,4.062938518,-1.7325869713,-0.8916082982
H,0,3.4925654997,-0.1134963995,-1.3268039641
H,0,-0.1210418256,0.9286327307,1.8866200216

$F_z = -50 (10^{-4}) \text{ au}$

TS1

Frequency = -499.3i cm⁻¹

ZeroPoint = 0.3015628 au

E_{tot} = -757.3101873 au

C,0,0.045300239,-0.018263824,1.2888937171
B,0,1.5691585312,0.0623927871,-0.117486367
H,0,1.8648961448,-0.1570080861,1.1259686023
O,0,0.0181151714,-0.0440133125,-0.0133500881
C,0,-0.5167758537,-1.0773449029,2.0974889142
C,0,-0.6667920658,-0.8829485579,3.4844051019
C,0,-0.9254288601,-2.2877136583,1.5031095154
C,0,-1.2280408938,-1.8845318793,4.2688214428
H,0,-0.34300339,0.0510916884,3.9366290898
C,0,-1.4876318154,-3.2819631178,2.2919152978
H,0,-0.7851638117,-2.4160055853,0.4348968288
C,0,-1.6377403844,-3.0810221237,3.671042345
H,0,-1.3463084463,-1.7405845503,5.3380084081
H,0,-1.805764421,-4.2192774762,1.8448509915
H,0,-2.0732739243,-3.8642307162,4.2851997637
O,0,2.0681636169,1.3348075686,-0.5312497742
O,0,2.0543416213,-0.95869662,-0.9926091202
C,0,3.2236403008,-0.4071190335,-1.6144321831
C,0,2.8580139824,1.1281107774,-1.7096177067
C,0,4.0532620192,2.0833351294,-1.6677361251
H,0,3.6979981064,3.119073336,-1.7075400235
H,0,4.6237570774,1.9639574627,-0.7440308973
H,0,4.7259300065,1.9207287318,-2.5197969356
C,0,4.4398386202,-0.6750527374,-0.7106459721
H,0,4.3410204129,-0.161430504,0.2499495702
H,0,4.4997534775,-1.7498399193,-0.5106231843
H,0,5.3796622106,-0.3573058146,-1.1769157511
C,0,3.4195486895,-1.1110710424,-2.9600735119
H,0,2.5167802546,-1.0533647619,-3.5739785943
H,0,4.2561175508,-0.6713151521,-3.5178921273
H,0,3.6448520044,-2.1696587062,-2.7896124123
C,0,1.973746147,1.450857176,-2.9281848967
H,0,1.5710657425,2.4622818758,-2.8088247102
H,0,2.5345663988,1.4102582009,-3.871061678
H,0,1.1304252998,0.7560890693,-2.9889573131
H,0,0.2567595204,0.9278063185,1.8008256236

TS2

Frequency = -1279.5i cm⁻¹

ZeroPoint = 0.298949 au

E_{tot} = -757.2177882 au

C,0,0.0169351831,-0.0295258482,1.3163809142
B,0,1.5899186169,0.0858417594,0.626619137
H,0,1.2959869389,-0.1444769515,-0.6606055535
O,0,-0.0038983723,0.0052030486,-0.0343868103
C,0,-0.3315665859,-1.2516461546,2.0534586429
C,0,-0.6028054701,-2.4687933481,1.4082249992
C,0,-0.3770752924,-1.1963722924,3.4568509776
C,0,-0.9186542688,-3.6009531188,2.1543961887
H,0,-0.5672187054,-2.5144498538,0.3238437371
C,0,-0.6977659041,-2.3305674097,4.1990295862
H,0,-0.1657106513,-0.2587071773,3.9657208582
C,0,-0.9679296935,-3.5377859297,3.5501942833
H,0,-1.1303973613,-4.5389914027,1.6472242603
H,0,-0.7339622358,-2.2739000176,5.2829818152
H,0,-1.2152483175,-4.4225701807,4.129642462
O,0,2.2371053642,1.3436984321,0.6953166187
O,0,2.4357360442,-1.0108809736,0.9578386904
C,0,3.5666921042,1.0497536952,1.2018810916
C,0,3.7691982708,-0.4662627946,0.7974040415
C,0,4.5461387183,2.0282539687,0.5553489434
H,0,5.5771817408,1.8057170206,0.8537730778
H,0,4.480358563,2.0003011966,-0.5357807394
H,0,4.3145245478,3.0474152831,0.8815345605
C,0,3.5388904572,1.2520435122,2.7233791119
H,0,3.1728240112,2.2600819898,2.9409130189
H,0,2.8693055838,0.533661031,3.2058839175
H,0,4.5338354638,1.1463096852,3.1684864897
C,0,4.6992907863,-1.2608130134,1.7127876243
H,0,5.7114965846,-0.840086321,1.7042707083
H,0,4.332764448,-1.2709450701,2.7407295393
H,0,4.7582973451,-2.2985099081,1.3681061647
C,0,4.1968888585,-0.6410987293,-0.6687231332
H,0,5.2331368567,-0.3240760517,-0.8296744968
H,0,4.1137508963,-1.6996651681,-0.9365436812
H,0,3.5554238604,-0.0646791559,-1.3455489034
H,0,-0.1380243858,0.9438772486,1.7874288573

The coordinates of TSs in hydroboration of benzophenone with HBPIn.

TS1'	TS2'
Frequency = -570.9i cm⁻¹	Frequency = -1246.9i cm⁻¹
ZeroPoint = 0.3826263 au	ZeroPoint = 0.379817 au
E_{tot} = -988.3299502 au	E_{tot} = -988.2361821 au
C,0,0.0800094948,-0.0452270765,1.3332305934	C,0,-0.017591777,-0.0397479059,1.3516532761
B,0,1.5164590514,-0.0978806822,-0.1793508272	B,0,1.5849792345,0.0452514223,0.6189759796
H,0,1.8664990014,-0.0966268272,1.0770416579	H,0,1.2838695413,-0.1496830536,-0.658838541
O,0,-0.0185441367,-0.0031601352,0.0209233408	O,0,-0.009816663,-0.0455003427,-0.0076831572
C,0,-0.0371647505,-1.3648392381,2.000935004	C,0,-0.3718305878,-1.3370524222,2.0063250604
C,0,0.4316335776,-1.6015998883,3.3058856074	C,0,-0.2143229124,-2.5463959546,1.3053304211
C,0,-0.6150269486,-2.4171598747,1.2726846019	C,0,-0.9074710949,-1.3885283955,3.3044422403
C,0,0.29809203,-2.8628617364,3.8772785207	C,0,-0.5693175152,-3.7600934477,1.885996027
H,0,0.9339873263,-0.8093660662,3.8518225729	H,0,0.1884263576,-2.5304517087,0.2997867238
C,0,-0.7642499942,-3.672540345,1.8574579875	C,0,-1.2619775818,-2.6074285573,3.8826896768
H,0,-0.9352964496,-2.2289303772,0.2544949388	H,0,-1.0747495858,-0.4729286786,3.8595035929
C,0,-0.3104788911,-3.8970978909,3.1584453532	C,0,-1.0925470451,-3.8001239558,3.1804864608
H,0,0.6754443986,-3.0442840832,4.8796367653	H,0,-0.4372740802,-4.6801115226,1.3224820054
H,0,-1.2230312246,-4.4791477086,1.2929011606	H,0,-1.6812378942,-2.6182608581,4.8854948353
H,0,-0.4171731033,-4.880006522,3.6094744466	H,0,-1.3698404616,-4.748678575,3.6323073204
C,0,-0.134798415,1.2249471275,2.069335463	C,0,-0.3142666389,1.285646986,1.9775670275
C,0,-0.7914907174,1.268781172,3.312691148	C,0,0.2023628055,1.6250050053,3.2385024265
C,0,0.241494941,2.4317210261,1.4456550451	C,0,-1.1022715404,2.2269074244,1.2969609188
C,0,-1.0492228781,2.4924878547,3.9281490999	C,0,-0.084203037,2.8614867102,3.8148001726
H,0,-1.1366958866,0.353695857,3.7794759251	H,0,0.8397806548,0.9204656708,3.7640148069
C,0,-0.0028143451,3.6462203164,2.0755579578	C,0,-1.3822449067,3.4651698525,1.8712245394
H,0,0.7445740026,2.394056207,0.4845144914	H,0,-1.4951624819,1.9791303212,0.315953435
C,0,-0.6479383347,3.6806342571,3.3165177117	C,0,-0.8783787685,3.7859621757,3.133678372
H,0,-1.5700798466,2.5163479592,4.8811057448	H,0,0.3232373983,3.1070182281,4.7919576034
H,0,0.3059675169,4.5713066416,1.5972489076	H,0,-2.0004692064,4.1796072381,1.3340221835
H,0,-0.8439739013,4.6335701536,3.8009301504	H,0,-1.1003137897,4.7507243859,3.5818988343
O,0,2.0831725334,1.0527338154,-0.8161062301	O,0,2.2723357711,1.2799472805,0.6603709527
O,0,1.8826747888,-1.2780773641,-0.8814225829	O,0,2.4098323917,-1.0653058071,0.9477754509
C,0,2.9677532787,-0.9157795675,-1.754075704	C,0,3.6531788586,0.9500722021,0.9608679782
C,0,2.6561072472,0.6014167371,-2.0604345116	C,0,3.7444051463,-0.5966817485,0.6254610614
C,0,3.8791300048,1.4651799223,-2.3697870159	C,0,4.5522884665,1.848123319,0.1111171947
H,0,3.5658545841,2.5003030296,-2.5453939222	H,0,5.610789136,1.6091796076,0.2681709164
H,0,4.5876537113,1.4660255579,-1.5379989741	H,0,4.3256542562,1.753343616,-0.9534295421
H,0,4.3952228277,1.1118787108,-3.2706390788	H,0,4.3960724459,2.8939205587,0.3950034265
C,0,4.2909580222,-1.1099297621,-0.9939483764	C,0,3.8745212292,1.244925362,2.4517442984
H,0,4.3547926124,-0.4364786217,-0.133564971	H,0,3.5733269973,2.2769110615,2.6547758631
H,0,4.3344745708,-2.1390162022,-0.6223186084	H,0,3.2687043474,0.5840282676,3.078597374
H,0,5.1632763837,-0.9382756299,-1.6348535949	H,0,4.9256572594,1.1270886673,2.7380109148

C,0,2.9293770101,-1.8416890737,-2.9711068271	C,0,4.7253693772,-1.388028135,1.4902890721
H,0,1.9487876934,-1.8257573156,-3.4526645201	H,0,5.7484283061,-1.0160464364,1.3622913634
H,0,3.6889544694,-1.5571844553,-3.7092014737	H,0,4.4601237553,-1.3323913387,2.5479634573
H,0,3.1329353953,-2.8709459891,-2.6561931243	H,0,4.7075986935,-2.4419088797,1.1942773072
C,0,1.5968809607,0.7772744286,-3.1613063635	C,0,4.0182631564,-0.8784756558,-0.8594974351
H,0,1.2610818481,1.8195106098,-3.1640043678	H,0,5.0433679638,-0.6153290496,-1.1403091387
H,0,1.9932499581,0.5420178107,-4.1559355154	H,0,3.8716703703,-1.9462383676,-1.0506222978
H,0,0.7270438525,0.1413688985,-2.9718522063	H,0,3.3374412979,-0.3209675359,-1.5130236089

$F_X = 50 (10^{-4})$ au

TS1'

Frequency = -631.1i cm⁻¹

ZeroPoint = 0.3823487 au

E_{tot} = -988.3367626 au

C,0,-0.0144310565,-0.0006187433,1.2842658252
 B,0,1.5005260758,-0.0873850132,-0.1057907956
 H,0,1.7244772881,-0.0470728205,1.1988822053
 O,0,-0.0065606546,-0.0017954386,-0.0465981758
 C,0,-0.2322256101,-1.2997372317,1.969260313
 C,0,0.1624945095,-1.5316254165,3.298639945
 C,0,-0.8680626888,-2.3219389388,1.2478053635
 C,0,-0.0993877966,-2.7579998124,3.9003447384
 H,0,0.6947999814,-0.7588869118,3.8453673515
 C,0,-1.1497628222,-3.5400929871,1.8638816539
 H,0,-1.1466676712,-2.1386196943,0.2165508057
 C,0,-0.76858231,-3.759530454,3.1882850881
 H,0,0.2107985958,-2.9340043709,4.9266579824
 H,0,-1.6682713494,-4.3166517294,1.3095787476
 H,0,-0.9905861575,-4.7092722361,3.6669970089
 C,0,-0.3184941377,1.2865263594,1.9535469953
 C,0,-1.0422958583,1.3497165123,3.1593642629
 C,0,0.026537136,2.4844278475,1.2949711748
 C,0,-1.3997649131,2.5831989959,3.7006492593
 H,0,-1.3712623856,0.4408058689,3.6484636026
 C,0,-0.321826394,3.709716864,1.8491621149
 H,0,0.575953479,2.4323528478,0.3611162018
 C,0,-1.0364832884,3.7633257443,3.0512224588
 H,0,-1.9815629559,2.6198522166,4.6168075723
 H,0,-0.0522267294,4.6287549801,1.3364948146
 H,0,-1.3253655817,4.7233446896,3.4703030626
 O,0,2.1516225677,1.048039355,-0.7032875001
 O,0,1.9697010221,-1.2842274168,-0.7268757299
 C,0,3.0792401537,-0.9287551266,-1.558817595

TS2'

Frequency = -1261.2i cm⁻¹

ZeroPoint = 0.3796919 au

E_{tot} = -988.2368249 au

C,0,0.0268083607,-0.0129663904,1.346849035
 B,0,1.6125528209,0.0557700469,0.6428162826
 H,0,1.3400299065,-0.1222330163,-0.6411426023
 O,0,0.0385689729,-0.014888955,-0.0151645731
 C,0,-0.3437726903,-1.3122397851,1.9953151676
 C,0,-0.2834715281,-2.5090014103,1.2599130135
 C,0,-0.8022379953,-1.3659534195,3.321861246
 C,0,-0.6691145578,-3.7168880186,1.833400463
 H,0,0.0495099109,-2.4850047784,0.228762159
 C,0,-1.1873046159,-2.5790038857,3.8925296696
 H,0,-0.8984436797,-0.4555767648,3.9017052347
 C,0,-1.1217538992,-3.7602435852,3.1541922159
 H,0,-0.6319617199,-4.6268111338,1.2402577165
 H,0,-1.5612174835,-2.5926830298,4.9126400111
 H,0,-1.4385930347,-4.7010620389,3.5954387534
 C,0,-0.3122839846,1.3085178797,1.9660060752
 C,0,0.2436229104,1.7007193803,3.1935373246
 C,0,-1.2097214275,2.1732583404,1.320952338
 C,0,-0.1103548761,2.916910529,3.7753158132
 H,0,0.9527523027,1.0472981479,3.6933719958
 C,0,-1.5592519682,3.3909797873,1.9016254402
 H,0,-1.6452786901,1.8785193026,0.3714328521
 C,0,-1.0143175839,3.7649536729,3.1319938208
 H,0,0.3180771331,3.2022806327,4.7327070567
 H,0,-2.2720297885,4.0404404114,1.4015463312
 H,0,-1.3003749484,4.7076569239,3.590105676
 O,0,2.3327609352,1.2847252008,0.6969890731
 O,0,2.4428848433,-1.0631000714,0.9715568206
 C,0,3.7013685746,0.9351486328,0.9786465366

C,0,2.7659312298,0.5765431621,-1.9137389494	C,0,3.7696737782,-0.6129444595,0.6394656132
C,0,3.9911086145,1.4464524434,-2.2028743582	C,0,4.6069436183,1.8239561479,0.122238679
H,0,3.6707708633,2.4731801965,-2.4120451692	H,0,5.6653294956,1.572145205,0.2685797972
H,0,4.6714434976,1.4745235333,-1.3473265457	H,0,4.3673348644,1.7338013764,-0.9399786762
H,0,4.5394907942,1.0786566734,-3.0794710652	H,0,4.4631777032,2.8712311342,0.4082727532
C,0,4.3726633817,-1.0877367078,-0.737749591	C,0,3.9472741538,1.2222100676,2.469048018
H,0,4.3875009748,-0.3900988672,0.1056570064	H,0,3.6559480853,2.2556908493,2.6791456583
H,0,4.4083341439,-2.1063870752,-0.3366505932	H,0,3.3397253949,0.5661735506,3.0989353717
H,0,5.271730549,-0.9227137815,-1.345047429	H,0,5.0011827079,1.0925003264,2.7449252146
C,0,3.1063629496,-1.8836010579,-2.7548509072	C,0,4.7508727116,-1.4190730515,1.4932100739
H,0,2.1476687377,-1.8907690967,-3.2779254108	H,0,5.779289278,-1.0622286399,1.3553394521
H,0,3.8939917382,-1.6068876122,-3.4674280472	H,0,4.4952248151,-1.3608463004,2.5531881927
H,0,3.303969238,-2.9039366284,-2.4075047631	H,0,4.7114950669,-2.4727495877,1.1971352248
C,0,1.7472184308,0.7136401995,-3.0587067642	C,0,4.0351213593,-0.8943618139,-0.8495266085
H,0,1.3994446725,1.7508422741,-3.0992081066	H,0,5.0637874376,-0.6467111975,-1.1358186747
H,0,2.1811955233,0.4579636451,-4.0326852019	H,0,3.8675022511,-1.958865006,-1.042480228
H,0,0.8760500529,0.0753651602,-2.8870504966	H,0,3.3590570794,-0.3258962067,-1.4974778078

$F_X = -50 (10^{-4}) \text{ au}$

TS1'

Frequency = -566.5i cm⁻¹

ZeroPoint = 0.3824617 au

E_{tot} = -988.3298258 au

C,0,0.0223169236,-0.0140718785,1.3032016318
B,0,1.5992801745,-0.0816415628,-0.0990333192
H,0,1.8531238763,-0.0811838602,1.16245322
O,0,-0.0052461923,0.02437308,0.0008874746
C,0,-0.103475146,-1.3303288,1.9805596115
C,0,0.2900633627,-1.5405159712,3.3144652584
C,0,-0.5790887051,-2.4120289155,1.2222141961
C,0,0.1838351017,-2.8062621967,3.8828211335
H,0,0.727291233,-0.727193559,3.8843401731
C,0,-0.7001228697,-3.6726096157,1.8014972932
H,0,-0.8258485765,-2.2431237839,0.1802671258
C,0,-0.3203990313,-3.8718166975,3.1305264479
H,0,0.5163802647,-2.9685825272,4.9039998998
H,0,-1.0639037338,-4.506767525,1.2077795863
H,0,-0.3908202135,-4.8614462825,3.5742877477
C,0,-0.2081198326,1.2631038881,2.030735158
C,0,-0.9520413208,1.3247362864,3.2218960994
C,0,0.263905366,2.4561182127,1.4487405416
C,0,-1.2038618468,2.5540158084,3.8294656032
H,0,-1.3544611618,0.4174083352,3.6585240147
C,0,0.0282074202,3.6755258075,2.0741806689

TS2'

Frequency = -1235.1i cm⁻¹

ZeroPoint = 0.3795164 au

E_{tot} = -988.2430786 au

C,0,-0.0539675231,-0.0575560461,1.354436919
B,0,1.5760983654,0.0412467061,0.5979252973
H,0,1.2431501913,-0.1682905068,-0.6730133136
O,0,-0.0412728899,-0.064752042,-0.0029957161
C,0,-0.3964216172,-1.3520334279,2.0119926156
C,0,-0.1725435511,-2.5684523816,1.3397756756
C,0,-0.9865331303,-1.4039514996,3.2875154096
C,0,-0.5100292651,-3.7840120143,1.9270083045
H,0,0.2851960291,-2.5569727723,0.3583918499
C,0,-1.3234075802,-2.62468199,3.8722486794
H,0,-1.1974342673,-0.4856277701,3.8233830884
C,0,-1.0848846762,-3.8227220416,3.1996268689
H,0,-0.3094774895,-4.7079248028,1.3906190547
H,0,-1.771960268,-2.6335396668,4.8630134769
H,0,-1.3339317087,-4.7743524601,3.6620644443
C,0,-0.3207191721,1.2683085184,1.9855176154
C,0,0.1686637317,1.5748292249,3.2665307084
C,0,-1.0350015714,2.2557055553,1.2877095623
C,0,-0.0727088028,2.8211037903,3.8425981358
H,0,0.7619931552,0.8411135655,3.8031440605
C,0,-1.2691070374,3.5033854204,1.8616328453

H,0,0.8419371999,2.4030218287,0.5307190405	H,0,-1.3941029472,2.0383496036,0.2865671675
C,0,-0.7049422383,3.7283011718,3.2640200639	C,0,-0.7935982486,3.7907592867,3.1431349539
H,0,-1.782500769,2.5921691318,4.7486950682	H,0,0.32551805,3.042247374,4.829209361
H,0,0.4237978126,4.5877703391,1.6370971113	H,0,-1.8189969962,4.2574352342,1.3032791066
H,0,-0.8827247137,4.6842156962,3.7500948266	H,0,-0.9678052244,4.7676840835,3.5866502375
O,0,2.1747946551,1.0698242246,-0.7034254721	O,0,2.2343873328,1.2781792335,0.6323868723
O,0,1.9695187276,-1.2592210548,-0.7859899623	O,0,2.3888071998,-1.0653046686,0.9260223317
C,0,3.1404546409,-0.9056934778,-1.5607684396	C,0,3.6283897591,0.9616087429,0.9459505864
C,0,2.8707727717,0.6149474449,-1.8905473729	C,0,3.734749548,-0.5842286146,0.6133980016
C,0,4.1235954248,1.4702270418,-2.0718203083	C,0,4.5211483202,1.8651740328,0.0987583103
H,0,3.8385517739,2.507513711,-2.2793804289	H,0,5.5797515559,1.6348566167,0.2617024716
H,0,4.7447986067,1.4679171022,-1.1735660992	H,0,4.3026743263,1.7664577868,-0.9670159079
H,0,4.7281564264,1.1136874414,-2.9137468326	H,0,4.3582182008,2.9101179606,0.3810477865
C,0,4.3854349758,-1.116109487,-0.685212823	C,0,3.8312421122,1.2633671712,2.4361399348
H,0,4.381398871,-0.4507505111,0.1837394418	H,0,3.5275438064,2.2958863209,2.6323796053
H,0,4.3896250176,-2.1481301504,-0.3202944281	H,0,3.2247547007,0.6015669529,3.0619954632
H,0,5.3122329282,-0.9476569423,-1.2432061682	H,0,4.8799173225,1.151060334,2.7298131061
C,0,3.2024793808,-1.8295845843,-2.7769514505	C,0,4.7118051314,-1.3662907276,1.488407366
H,0,2.2700443296,-1.8074246913,-3.3471526107	H,0,5.731837003,-0.9859634802,1.3676094628
H,0,4.0285174828,-1.5496160227,-3.4406009016	H,0,4.4397342084,-1.3105335823,2.5442579779
H,0,3.373184446,-2.8595980349,-2.4465896312	H,0,4.7086753627,-2.4201701453,1.1933349551
C,0,1.9241998411,0.8048833741,-3.0864725739	C,0,4.0144405087,-0.8680662228,-0.867736697
H,0,1.6042119803,1.8518777805,-3.1192628996	H,0,5.0368866055,-0.5939061006,-1.1445229735
H,0,2.4145695546,0.5672539583,-4.0371997379	H,0,3.8844657321,-1.9382413099,-1.0562384673
H,0,1.0330295011,0.1774722677,-2.9840901679	H,0,3.330247708,-0.3193142415,-1.5262935943

$F_Y = 50 (10^{-4}) \text{ au}$

TS1'

Frequency = -564.4i cm⁻¹

ZeroPoint = 0.3825564 au

E_{tot} = -988.3345125 au

C,0,0.0758119432,-0.0284674774,1.3425453416
B,0,1.4882157123,-0.0414565989,-0.1908841632
H,0,1.8606356707,-0.0117872705,1.059258953
O,0,-0.0413871632,0.0566889254,0.0325494963
C,0,-0.0322088835,-1.3488573661,1.9845230532
C,0,0.3869620175,-1.5860203601,3.3097089549
C,0,-0.5357448519,-2.4161475833,1.2176632364
C,0,0.2769986476,-2.8578147919,3.8586109038
H,0,0.8390787117,-0.7855052208,3.88685578
C,0,-0.6620606826,-3.6826664575,1.7809319412
H,0,-0.8172170264,-2.2302854541,0.1879712039
C,0,-0.2581123178,-3.9054725827,3.0993477373

TS2'

Frequency = -1252.4i cm⁻¹

ZeroPoint = 0.3797037 au

E_{tot} = -988.239422 au

C,0,-0.018170983,-0.0331817351,1.3488757271
B,0,1.5848920353,0.0561720975,0.6306381743
H,0,1.2971679176,-0.1675459848,-0.6453573365
O,0,-0.0028512818,-0.0182178254,-0.0107102925
C,0,-0.3766679833,-1.3329690628,1.9959462823
C,0,-0.2303863584,-2.5348372603,1.2795460184
C,0,-0.8940407333,-1.3954433214,3.3011852165
C,0,-0.5770702638,-3.7542302119,1.8531425841
H,0,0.157633349,-2.5119935883,0.2682473353
C,0,-1.2412412682,-2.6200448224,3.8715512494
H,0,-1.0553970852,-0.4866119025,3.8697432941
C,0,-1.0808603811,-3.8056726589,3.1549860517

H,0,0.617925079,-3.0421004288,4.8730842231	H,0,-0.45331706,-4.6692243193,1.2811280492
H,0,-1.060535127,-4.5007367965,1.1889058467	H,0,-1.6458242008,-2.6437096085,4.8798766958
H,0,-0.3441383009,-4.8979498037,3.5322303074	H,0,-1.3492656965,-4.7586979131,3.601086587
C,0,-0.1254331988,1.2415391757,2.1037444332	C,0,-0.3147340988,1.2910431995,1.9800264622
C,0,-0.8399240322,1.2809395523,3.3116547276	C,0,0.1930642093,1.6250713717,3.2457709724
C,0,0.3131900468,2.447424693,1.5242450673	C,0,-1.1005734923,2.2360083599,1.3020557542
C,0,-1.0910566977,2.5005884914,3.942384377	C,0,-0.0994836494,2.8575648888,3.8280675254
H,0,-1.2289717959,0.365665913,3.7422726618	H,0,0.8245300489,0.9162675475,3.7718369648
C,0,0.074397653,3.6565757192,2.1673761422	C,0,-1.387318406,3.470285833,1.8820800774
H,0,0.8519380405,2.4142047613,0.581884386	H,0,-1.4898280703,1.9900576438,0.3191983645
C,0,-0.6272070797,3.6876322487,3.3775333233	C,0,-0.8922825299,3.7851054292,3.149473616
H,0,-1.6545972515,2.5172901109,4.8712151062	H,0,0.2993148764,3.0937635981,4.8115072842
H,0,0.4326735375,4.5809409472,1.7208813651	H,0,-2.0095879733,4.1834669047,1.3460424982
H,0,-0.8179119673,4.6368070811,3.8735147156	H,0,-1.124023499,4.7448446633,3.6059996247
O,0,2.0474809193,1.0942192809,-0.8713987925	O,0,2.2780827068,1.2943886507,0.6609755694
O,0,1.8413947116,-1.2372830101,-0.8637067758	O,0,2.4062111208,-1.0462366469,0.9827161242
C,0,2.9381370448,-0.9133956844,-1.7350613787	C,0,3.6587008088,0.9567504597,0.9540090328
C,0,2.6310956697,0.5936707391,-2.0939304482	C,0,3.7416235061,-0.5968732294,0.6442569574
C,0,3.8602106229,1.4412496924,-2.4248229177	C,0,4.5573305078,1.834255465,0.081469964
H,0,3.5533836676,2.4718243,-2.6414473537	H,0,5.6151343902,1.5894002059,0.2339173519
H,0,4.5621145486,1.4660383689,-1.5876243441	H,0,4.3218319483,1.7190229403,-0.9792087504
H,0,4.3815445215,1.0508186582,-3.3070324343	H,0,4.4099738849,2.8871862808,0.3476129939
C,0,4.2525316042,-1.0849866127,-0.9542102038	C,0,3.8953367946,1.2756253185,2.4377692578
H,0,4.3128659367,-0.3829165795,-0.1160846114	H,0,3.6025413956,2.3137112673,2.6266941697
H,0,4.2871630923,-2.1001309787,-0.5472449407	H,0,3.2898347629,0.6288670038,3.0788648073
H,0,5.1319600991,-0.9431246296,-1.5927144209	H,0,4.9472506527,1.1518247296,2.7186989456
C,0,2.9100627515,-1.8822893923,-2.9178243619	C,0,4.7205720026,-1.3801292475,1.5188522351
H,0,1.9346202853,-1.8859881134,-3.4098926905	H,0,5.7464389191,-1.0197372743,1.3793353443
H,0,3.6784326659,-1.628185065,-3.6578707644	H,0,4.4606320345,-1.3070661556,2.5767734969
H,0,3.1083420954,-2.8987873298,-2.5635937584	H,0,4.6935884572,-2.4380793192,1.2416119672
C,0,1.5814769503,0.7317884747,-3.2090478178	C,0,4.0066094723,-0.9081300258,-0.8361262965
H,0,1.2453116889,1.7740758917,-3.2518016059	H,0,5.0333506764,-0.6617347259,-1.1266008359
H,0,1.9846346474,0.4578978226,-4.1908316988	H,0,3.8508384884,-1.977561587,-1.0053100819
H,0,0.7114807938,0.1020907397,-3.0026328018	H,0,3.3268320482,-0.3592004325,-1.4988940326

$F_Y = -50 (10^{-4}) \text{ au}$

TS1'

Frequency = -574.9i cm⁻¹

ZeroPoint = 0.3823655 au

E_{tot} = -988.3343986 au

C,0,0.0790005878,-0.0656699375,1.3284747757
 B,0,1.5175408024,-0.1556367721,-0.1844919398
 H,0,1.8602685229,-0.1876992545,1.0777261053

TS2'

Frequency = -1251.1i cm⁻¹

ZeroPoint = 0.3796682 au

E_{tot} = -988.2408982 au

C,0,-0.0252100356,-0.0531588869,1.3600003913
 B,0,1.5773264698,0.0326365224,0.6125411403
 H,0,1.2594312075,-0.143566947,-0.6660047236

O,0,-0.0115007977,-0.0684964305,0.0121992413	O,0,-0.0230661599,-0.0787039484,-0.0004943693
C,0,-0.0458285518,-1.382317165,2.0216479371	C,0,-0.3734886076,-1.3493377285,2.0182448992
C,0,0.4777542995,-1.6242055552,3.3022697193	C,0,-0.1972240556,-2.5648118026,1.3311083606
C,0,-0.6957098127,-2.4183543176,1.3357498218	C,0,-0.9319616572,-1.3962637217,3.3073872875
C,0,0.3292211307,-2.8759704969,3.8935304917	C,0,-0.5559425086,-3.7760330356,1.9149345451
H,0,1.0290098944,-0.8425874509,3.8151495311	H,0,0.2233472085,-2.551868152,0.3329325615
C,0,-0.8584224481,-3.6641933057,1.9391267249	C,0,-1.2895214343,-2.6125677782,3.8892876538
H,0,-1.0594002117,-2.2249110423,0.3329432016	H,0,-1.1122743892,-0.4759466693,3.8500618642
C,0,-0.3485533132,-3.8951497794,3.2176589056	C,0,-1.1023466353,-3.8105969259,3.2002417352
H,0,0.7471015533,-3.0576044489,4.8800720842	H,0,-0.4088887192,-4.6995278734,1.3585369926
H,0,-1.3756217246,-4.4571591757,1.404747407	H,0,-1.7271994025,-2.6149649587,4.8845594973
H,0,-0.4683567732,-4.8698604207,3.6852436958	H,0,-1.384796848,-4.757479246,3.6549916909
C,0,-0.143569526,1.2057471949,2.0361972595	C,0,-0.314983482,1.2741421243,1.9808910524
C,0,-0.7283686023,1.2641073335,3.3185994872	C,0,0.1991720541,1.6090391363,3.2450973692
C,0,0.1614170711,2.4091721073,1.3630061281	C,0,-1.0769612526,2.2283026638,1.2874121611
C,0,-0.9873198301,2.494041693,3.9153999576	C,0,-0.0645337493,2.8549957904,3.8113638176
H,0,-1.0220322524,0.3534860187,3.827785597	H,0,0.8226592866,0.8970190776,3.7783372195
C,0,-0.0842700244,3.6318014239,1.9753991779	C,0,-1.3323842193,3.476120908,1.8517886676
H,0,0.6187773657,2.3619007276,0.380484723	H,0,-1.4642860094,1.9871809066,0.3025225983
C,0,-0.6585945098,3.6782449826,3.2504385959	C,0,-0.8305857632,3.7932499591,3.1163913521
H,0,-1.4536273627,2.5317477811,4.8955053018	H,0,0.3427731503,3.1014532116,4.7879950682
H,0,0.1683790901,4.5534874406,1.4604078373	H,0,-1.9241940745,4.204305131,1.3046560152
H,0,-0.8556797823,4.6371713183,3.7212227023	H,0,-1.028649408,4.7677685576,3.5529712224
O,0,2.0895131098,1.0105924183,-0.7763801904	O,0,2.2550191574,1.2657229854,0.6551675861
O,0,1.8976320698,-1.3168952736,-0.9205957185	O,0,2.4100247344,-1.0809322203,0.9221274014
C,0,2.9844956471,-0.9162367745,-1.7755307193	C,0,3.6378102303,0.95088185,0.9628048873
C,0,2.674361716,0.6109084283,-2.0305843461	C,0,3.74200358,-0.5913505594,0.6119709763
C,0,3.8971893722,1.4895121802,-2.2950552517	C,0,4.5320094683,1.8666760152,0.1278674412
H,0,3.5812579246,2.5286504461,-2.43237827	H,0,5.5922734132,1.6383646087,0.2889421993
H,0,4.5985479371,1.4643402408,-1.4576383573	H,0,4.311982523,1.7844646085,-0.9390413373
H,0,4.4230140206,1.176293123,-3.2051829925	H,0,4.3641061926,2.9068782106,0.4223534807
C,0,4.3053418015,-1.1354763381,-1.0180989661	C,0,3.8459555363,1.2326536681,2.457858593
H,0,4.3604909391,-0.4948023956,-0.1330027377	H,0,3.534745524,2.2594645313,2.6680398137
H,0,4.3525132199,-2.1789530409,-0.6860094328	H,0,3.2420430768,0.5613423004,3.0761210525
H,0,5.1795694704,-0.9317850859,-1.6467579224	H,0,4.8969789093,1.1248784515,2.7484020698
C,0,2.9535330046,-1.7958972557,-3.0273809901	C,0,4.7280201136,-1.3818884207,1.4717560105
H,0,1.9751323087,-1.7594079417,-3.51231494	H,0,5.7470438154,-0.997061492,1.3510721034
H,0,3.7153855824,-1.4806584771,-3.7505167088	H,0,4.4588647703,-1.3362864645,2.528982575
H,0,3.1570242399,-2.8375887113,-2.751416984	H,0,4.7217480708,-2.4340339465,1.1651765418
C,0,1.6250984854,0.8270820611,-3.1340398622	C,0,4.0240204674,-0.852629935,-0.875321214
H,0,1.292570755,1.8691275604,-3.1031240926	H,0,5.0455807598,-0.5700303483,-1.1493763393
H,0,2.0308628707,0.629349782,-4.1331455971	H,0,3.8915421833,-1.9205441284,-1.0809766429
H,0,0.7504157304,0.1883685855,-2.9761053904	H,0,3.3384085082,-0.2944010295,-1.5223202689

$F_Z = 50 (10^{-4}) \text{ au}$

TS1'

Frequency = -639.6i cm⁻¹

ZeroPoint = 0.3823621 au

E_{tot} = -988.3265799 au

C,0,-0.0010826314,0.0010701716,1.2671456341
B,0,1.6078194211,-0.0953634858,-0.0511018606
H,0,1.7790799321,-0.0421008705,1.2427510703
O,0,0.0120250406,0.0066290714,-0.035939564
C,0,-0.1838640099,-1.305589357,1.96335932
C,0,0.162098252,-1.5121346716,3.309348728
C,0,-0.6938671062,-2.3727634464,1.2092287664
C,0,-0.0250510786,-2.7610583205,3.8940984512
H,0,0.6140613166,-0.7060213774,3.8792475432
C,0,-0.8956309512,-3.6171208827,1.8040647868
H,0,-0.9143863917,-2.2083316601,0.1607961318
C,0,-0.5641511778,-3.8126610874,3.1454023008
H,0,0.2616347173,-2.9205642905,4.9307529181
H,0,-1.2956321538,-4.436339909,1.2138867058
H,0,-0.708696269,-4.7879582407,3.6034329999
C,0,-0.2893310264,1.2964169231,1.94873031
C,0,-1.0534491623,1.3784231175,3.1248059238
C,0,0.1291269035,2.4809267419,1.3125108628
C,0,-1.3799211475,2.6227873391,3.6631999529
H,0,-1.4276371488,0.4757999046,3.5946370876
C,0,-0.1856303654,3.7173457154,1.8657667127
H,0,0.7134880357,2.4090204708,0.3999203679
C,0,-0.9414359923,3.7918336163,3.0400217053
H,0,-1.9904345792,2.6772690028,4.5611386803
H,0,0.1477682048,4.6258621054,1.3727129413
H,0,-1.1990820027,4.7615936833,3.4587112492
O,0,2.2172297177,1.0344406285,-0.6516425936
O,0,2.0276419742,-1.2986807566,-0.6519694906
C,0,3.0945773992,-0.9509970371,-1.5694732702
C,0,2.7738608673,0.5573443534,-1.9084184715
C,0,3.9890210747,1.4183677985,-2.2466332688
H,0,3.6696293006,2.4468654377,-2.4453339576
H,0,4.7074571923,1.4398788142,-1.423274852
H,0,4.494583132,1.0467336082,-3.1449782669
C,0,4.4294875664,-1.1254159891,-0.8282689064
H,0,4.5058595911,-0.4315706271,0.0155808024
H,0,4.4833104496,-2.1471216419,-0.4376067698
H,0,5.2881432543,-0.965423936,-1.4893464952
C,0,3.0284545753,-1.9064534093,-2.7601444836

TS2'

Frequency = -1213.6i cm⁻¹

ZeroPoint = 0.3796657 au

E_{tot} = -988.2383132 au

C,0,-0.0261579357,-0.0521726482,1.370218462
B,0,1.5871359122,0.04036842,0.6234188229
H,0,1.2854143442,-0.1577734155,-0.6481984819
O,0,-0.0073453266,-0.0603795818,0.0150186836
C,0,-0.3761794749,-1.3490929176,2.0235628914
C,0,-0.2021304615,-2.5574492196,1.3236454151
C,0,-0.9326244906,-1.4061083782,3.3130669488
C,0,-0.5613840392,-3.7738036506,1.8958134548
H,0,0.2116660095,-2.5389057725,0.3230116401
C,0,-1.2912004048,-2.6279727088,3.8828004342
H,0,-1.1178063527,-0.4905772852,3.8631377981
C,0,-1.1056853574,-3.8189586678,3.1815623849
H,0,-0.4210492076,-4.6901016132,1.3289046152
H,0,-1.7329733458,-2.6417493606,4.8770260898
H,0,-1.3918131942,-4.7702857317,3.6229420557
C,0,-0.3162444664,1.2752989435,1.9921106157
C,0,0.1719335487,1.6059432817,3.2668629576
C,0,-1.0595737425,2.2350977853,1.2866832165
C,0,-0.1018678257,2.8506959622,3.8319678447
H,0,0.7834771458,0.8894884392,3.8073718325
C,0,-1.3251516784,3.4816822189,1.8494683786
H,0,-1.4242687155,1.998190006,0.2925710967
C,0,-0.8522645772,3.7931119437,3.1261824232
H,0,0.2885512326,3.0910848752,4.818403958
H,0,-1.902967153,4.2107525271,1.2881103604
H,0,-1.0594656779,4.7672940665,3.5619167615
O,0,2.2615081845,1.2791956652,0.6765415917
O,0,2.4139096704,-1.0630268398,0.9650079515
C,0,3.6488356483,0.9581004679,0.9573429403
C,0,3.7455204618,-0.5889595126,0.6232944497
C,0,4.5332048316,1.8597724201,0.0973249419
H,0,5.5946318368,1.6261874341,0.2421725712
H,0,4.2969081662,1.7621600884,-0.9641117108
H,0,4.374191738,2.9057504074,0.3791635128
C,0,3.8804835314,1.2571915734,2.4469768583
H,0,3.5765251372,2.2890485444,2.6480187228
H,0,3.2803276087,0.5948958325,3.07889171
H,0,4.9349198265,1.1441838926,2.7245941017
C,0,4.7381175032,-1.3737112119,1.4810817618

H,0,2.0383474981,-1.9032355057,-3.2208847772	H,0,5.7576975248,-0.9969277102,1.3407880972
H,0,3.7687777521,-1.6390357339,-3.522645342	H,0,4.4823149821,-1.3174258257,2.5419127026
H,0,3.2420711625,-2.9277356088,-2.4270161501	H,0,4.7234217058,-2.4273984534,1.1848101544
C,0,1.7008953585,0.7098531646,-2.996467007	C,0,4.0057736817,-0.8727328671,-0.8622234685
H,0,1.3682324547,1.7524216577,-3.0230392013	H,0,5.0268503856,-0.6072587716,-1.1537826206
H,0,2.0879384213,0.4523929799,-3.9878393683	H,0,3.8608612062,-1.9404923038,-1.052655677
H,0,0.8301286185,0.0809925191,-2.789927296	H,0,3.3203636038,-0.3186753475,-1.5133662514

$F_z = -50 (10^{-4}) \text{ au}$

TS1'

Frequency = -548.3i cm⁻¹

ZeroPoint = 0.3824917 au

E_{tot} = -988.3421223 au

C,0,0.058770702,-0.0534705342,1.3225245216
B,0,1.3840524402,-0.0880444598,-0.2765008625
H,0,1.8099062638,-0.087100406,0.9601824817
O,0,-0.099379566,-0.0154780824,-0.0012362451
C,0,-0.0331388935,-1.3680579515,1.9929538744
C,0,0.4982531093,-1.5996554508,3.2762066818
C,0,-0.6640894716,-2.4195008346,1.3070393899
C,0,0.3708942248,-2.8508315578,3.8702511269
H,0,1.0382309525,-0.8108040956,3.7898813448
C,0,-0.8069342825,-3.663497019,1.9158407662
H,0,-1.0396044206,-2.2356872731,0.3069646266
C,0,-0.2934842428,-3.8809158513,3.1964674269
H,0,0.7893961035,-3.0255514781,4.8567395548
H,0,-1.3145646367,-4.4674377536,1.3901243971
H,0,-0.4014888039,-4.8529608972,3.6694057436
C,0,-0.1362378807,1.2109163631,2.0634664807
C,0,-0.7324371634,1.2405055814,3.3395316022
C,0,0.2002097407,2.4282865044,1.4349435177
C,0,-0.965492561,2.4555074187,3.9806791441
H,0,-1.0494134739,0.320914467,3.8163096936
C,0,-0.0198943977,3.6334878456,2.0892320274
H,0,0.659469074,2.4070972197,0.4523021674
C,0,-0.6008337159,3.651891655,3.3627755779
H,0,-1.4326628168,2.4656634251,4.9606765183
H,0,0.2641820218,4.566165064,1.6098977935
H,0,-0.7714315966,4.5971515902,3.8704621828
O,0,1.9299802512,1.068428251,-0.9480224572
O,0,1.7646237759,-1.2630860663,-1.000207067
C,0,2.9166353539,-0.9055175504,-1.7693351954
C,0,2.6283891409,0.6102344438,-2.1110709273

TS2'

Frequency = -1283.1i cm⁻¹

ZeroPoint = 0.3797539 au

E_{tot} = -988.2403623 au

C,0,-0.0097688753,-0.0236400923,1.3318793025
B,0,1.5831049963,0.0507048734,0.6105039603
H,0,1.2774202816,-0.1420294436,-0.6745900502
O,0,-0.0140177788,-0.0278665487,-0.0321481806
C,0,-0.3658037871,-1.3212325792,1.9890586333
C,0,-0.2405514141,-2.5298425307,1.2808332964
C,0,-0.8599734061,-1.3706090478,3.3035926548
C,0,-0.5858248021,-3.741749862,1.8713907748
H,0,0.1340977908,-2.5140904998,0.2638586955
C,0,-1.2039793082,-2.5875662068,3.8920970812
H,0,-0.9992820973,-0.4568621763,3.8686690748
C,0,-1.0657473613,-3.7800313344,3.1826786573
H,0,-0.4754063603,-4.6637087152,1.3055440514
H,0,-1.5846580211,-2.5976906283,4.9094220207
H,0,-1.3297333749,-4.7265505514,3.6457718108
C,0,-0.3127547519,1.3005050172,1.9599719315
C,0,0.2239185308,1.6492330808,3.2099700788
C,0,-1.140212829,2.2228756519,1.3008688441
C,0,-0.0816005759,2.8753283635,3.7985041833
H,0,0.8853912831,0.958231801,3.7229603421
C,0,-1.4393948249,3.4511262384,1.8869505297
H,0,-1.5543975043,1.9643084768,0.3308789384
C,0,-0.9156716022,3.7804272803,3.1393264058
H,0,0.3349685322,3.1249221214,4.7700700301
H,0,-2.0942282405,4.1494423635,1.3716059072
H,0,-1.1575924502,4.7334376839,3.6013006692
O,0,2.2854055115,1.2795194849,0.6380871768
O,0,2.4036655359,-1.0683674781,0.9253517965
C,0,3.6577923342,0.9390942743,0.9647665529
C,0,3.7426461201,-0.6068143623,0.6262300575

C,0,3.8733671385,1.4786927899,-2.3096051227	C,0,4.5765790258,1.8334529135,0.1310152714
H,0,3.5729901991,2.511940668,-2.5188317896	H,0,5.6307624179,1.5869796714,0.3044909794
H,0,4.4974377528,1.4901674124,-1.4131425775	H,0,4.3644757312,1.743769048,-0.9379697437
H,0,4.4788677556,1.1236614085,-3.1538395003	H,0,4.4236179232,2.8787974602,0.4181675761
C,0,4.1749106083,-1.0920994016,-0.9021228304	C,0,3.8619518291,1.2270934886,2.4585521157
H,0,4.1671304751,-0.4189225881,-0.0399844311	H,0,3.563766992,2.2592107483,2.6640171999
H,0,4.1903302941,-2.1191033103,-0.5231262732	H,0,3.2468645694,0.5671884872,3.0764969646
H,0,5.097658511,-0.9189862282,-1.4685045163	H,0,4.9081300876,1.1026762045,2.7583577593
C,0,2.9909910407,-1.8398454769,-2.9806496844	C,0,4.7088036647,-1.4070331463,1.4993022142
H,0,2.055291579,-1.8349276596,-3.5461641885	H,0,5.7358459295,-1.0408833673,1.3865548586
H,0,3.8123311848,-1.5559374288,-3.651201799	H,0,4.4318676508,-1.3530811481,2.5534227747
H,0,3.1713652846,-2.8651807107,-2.6394444024	H,0,4.6873848517,-2.4606869422,1.2021031837
C,0,1.6825013935,0.7723834504,-3.3158485263	C,0,4.0329837386,-0.8849671287,-0.8581342943
H,0,1.3426800044,1.8129650206,-3.3560329563	H,0,5.0629023512,-0.624911154,-1.1258336738
H,0,2.1737822681,0.5312039776,-4.2676184989	H,0,3.8839851132,-1.9523478947,-1.0518989774
H,0,0.8020242794,0.1329515094,-3.2011337905	H,0,3.3586585732,-0.3222068947,-1.5146864351