

*Supporting Information*

**Effects of Electrostatic Drag on the Velocity of Hydrogen Migration – Pre- and Post-Transition State Enthalpy/Entropy Compensation**

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## 1. Molecular dynamics simulations

### Molecular Dynamics Trajectory Configuration File (used for all TSSs).

```
method b3lyp/6-31+g(d,p)
method2 restricted
charge 1
multiplicity1
processors 16
memory 50GB
killcheck 1
diagnostics 0
title hydrogen migration dynamics
initialdis 2
timestep 1E-15
scaling 1.0
temperature 298.15
method 3 empiricaldispersion=gd3bj*
numimag 1
searchdir positive
classical 0
keepevery 1
highlevel 999
boxon 0
boxsize 7.5
etolerance 1.0
damping 1
reversetrajectory true
```

\*used for B3LYP-D3(BJ) only. For M06-2X, this line is not present.

## 2. Energies, Enthalpies, and Free Energies of the Calculated Structures

**Zero-point correction (ZPE), thermal correction to enthalpy ( $\Delta H$ ), thermal correction to Gibbs free energy ( $G$ ), energies ( $E$ ), enthalpies ( $H$ ), Gibbs free energies ( $G$ ) (in Hartree) and imaginary frequencies of the transition states calculated at the B3LYP/6-31+G(d,p)**

Structures	ZPE	TCH	TCG	E	H	G	Imaginary Frequency
<b>Reactant</b>	0.520867	0.546241	0.466743	-950.908919	-950.907975	-950.987473	
<b>TS-N(CH<sub>3</sub>)<sub>2</sub></b>	0.518006	0.543364	0.464832	-950.867736	-950.866792	-950.945324	-497.87i
<b>Reactant</b>	0.480698	0.503986	0.429509	-931.500819	-931.499875	-931.574352	
<b>TS-OCH<sub>3</sub></b>	0.477426	0.500950	0.426587	-931.458299	-931.457354	-931.531718	-463.96i
<b>Reactant</b>	0.448087	0.469012	0.399742	-817.005499	-817.004555	-817.073825	
<b>TS-H</b>	0.444953	0.465878	0.397357	-816.962262	-816.961317	-817.029838	-460.85i

<b>Reactant</b>	0.452731	0.477434	0.397527	-1154.058851	-1154.057907	-1154.137814	
<b>TS-CF<sub>3</sub></b>	0.449503	0.474083	0.395693	-1154.007050	-1154.006106	-1154.084495	-450.86i
<b>Reactant</b>	0.447083	0.469882	0.396230	-909.250435	-909.249491	-909.323143	
<b>TS-CN</b>	0.443296	0.466162	0.392439	-909.197963	-909.197019	-909.270742	-450.00i
<b>Reactant</b>	0.450080	0.473732	0.396389	-1021.504128	-1021.503184	-1021.580527	
<b>TS-NO<sub>2</sub></b>	0.447522	0.470952	0.396079	-1021.457307	-1021.456363	-1021.531236	-431.16i
<b>TS<sub>CHO</sub></b>	0.372903	0.391194	0.329238	-699.297586	-699.296642	-699.358598	-340.63i
<b>TS<sub>NO2</sub></b>	0.367268	0.386030	0.322638	-790.481289	-790.480344	-790.543736	-345.43i
<b>TS<sub>CN</sub></b>	0.362732	0.380803	0.319439	-678.220960	-678.220016	-678.281380	-347.27i
<b>TS<sub>OCH3</sub></b>	0.396527	0.415622	0.351973	-700.498568	-700.497624	-700.561273	-371.32i
<b>TS<sub>F</sub></b>	0.356531	0.373849	0.313976	-685.227600	-685.226656	-685.286528	-391.91i
<b>TS<sub>SCH3</sub></b>	0.392377	0.412190	0.346176	-1023.456973	-1023.456029	-1023.522043	-393.15i
<b>TS<sub>CH=CH2</sub></b>	0.396852	0.415592	0.352523	-663.345003	-663.344059	-663.407128	-427.26i
<b>TS<sub>NO</sub></b>	0.360459	0.378792	0.316443	-715.264195	-715.263251	-715.325600	-428.57i
<b>TS<sub>H</sub></b>	0.363293	0.379866	0.322053	-585.980904	-585.979960	-586.037773	-465.44i
<b>TS<sub>NMe2</sub></b>	0.437308	0.457600	0.391900	-719.881684	-719.880740	-719.946440	-348.46i
<b>TS<sub>Furan</sub></b>	0.414336	0.434560	0.367515	-814.789644	-814.788700	-814.855745	-446.96i

### 3. Velocity of hydrogen migration

The velocity effects were measured in two ways: (1) distances between starting and ending positions of the migrating hydrogen divided by total trajectory time, (2) total distance traversed by the migrating hydrogen during a trajectory divided by total trajectory time (since the migrating hydrogen does not necessarily take a direct path and can move back and forth). We refer to the former as “velocity<sub>endpoints</sub>” and the latter as “velocity<sub>allpoints</sub>.”

Table S1. Results of the average velocity<sub>endpoints</sub> and average velocity<sub>allpoints</sub> for hydrogen migration in Figure 1.

X	TSS	Average velocity <sub>endpoints</sub> (Å/ps)	Average velocity <sub>allpoints</sub> (Å/ps)	Total trajectories
N(CH <sub>3</sub> ) <sub>2</sub>	<b>TS-N(CH<sub>3</sub>)<sub>2</sub></b>	22.5	48.5	104
OCH <sub>3</sub>	<b>TS-OCH<sub>3</sub></b>	20.6	48.9	122
H	<b>TS-H</b>	20.2	47.4	117
CF <sub>3</sub>	<b>TS-CF<sub>3</sub></b>	20.7	48.8	143
CN	<b>TS-CN</b>	19.9	49.0	131
NO <sub>2</sub>	<b>TS-NO<sub>2</sub></b>	20.9	49.4	109

Table S2. Results of the average velocity<sub>endpoints</sub> and average velocity<sub>allpoints</sub> for hydrogen migration in Figure 4.

X	TSS	Average velocity <sub>endpoints</sub> (Å/ps)	Average velocity <sub>allpoints</sub> (Å/ps)	Total trajectories
CHO	TS <sub>CHO</sub>	17.3	47.4	86
NO <sub>2</sub>	TS <sub>NO2</sub>	17.0	48.0	85
CN	TS <sub>CN</sub>	14.4	46.6	74
OCH <sub>3</sub>	TS <sub>OCH3</sub>	16.5	46.8	92
F	TS <sub>F</sub>	18.5	48.9	89
SCH <sub>3</sub>	TS <sub>SCH3</sub>	16.2	45.3	82
CH=CH <sub>2</sub>	TS <sub>CH=CH2</sub>	20.4	48.5	119
NO	TS <sub>NO</sub>	21.0	48.4	111
H	TS <sub>H</sub>	21.4	48.6	105
NMe <sub>2</sub>	TS <sub>NMe2</sub>	24.3	56.3	93
Furan	TS <sub>Furan</sub>	20.6	48.4	90

#### 4. Cartesian Coordinates of Optimized Structures

##### Reactant

C	-1.10223400	0.19560800	0.93352300
H	-0.02492700	0.02713300	0.88070000
C	-1.65728500	-0.86631500	1.99653400
H	-2.66247800	-0.53033000	2.27283300
H	-1.01328000	-0.89345500	2.87709800
C	-1.72618900	-2.12759300	1.26829000
C	-0.71918600	-3.18459000	1.46148500
H	-0.50235400	-3.34002600	2.52381800
H	-0.97641000	-4.12287200	0.96717800
H	0.22761900	-2.81960700	1.02031900
C	-2.73441200	-2.18287600	0.21357000
H	-3.66660900	-2.52828000	0.69486300
C	-2.50694600	-2.90303400	-1.14539000
H	-3.01980900	-3.85654500	-1.28299200
H	-1.44860400	-3.03742600	-1.38389300
C	-3.13717300	-1.66342800	-1.84300500
H	-4.18092600	-1.83733800	-2.11852700
H	-2.60155900	-1.27901500	-2.71492400
C	-3.01770700	-0.80860700	-0.53907100
C	-1.70040300	0.02561100	-0.49391500
H	-0.97059000	-0.54539700	-1.08202000
C	-4.29337700	-0.06766400	-0.13559700

H	-4.19452500	0.47363900	0.81074000
H	-4.57759200	0.66064600	-0.90040400
H	-5.13036500	-0.76660000	-0.03751700
C	-1.78248900	1.47217300	-1.06027600
H	-1.21620500	1.56145100	-1.99118600
H	-2.81413400	1.73388600	-1.30793200
C	-1.24415200	2.46439300	0.02434200
C	0.22503100	2.91994400	-0.26201200
H	0.21810200	3.41647900	-1.24076200
H	0.46968300	3.69796600	0.47118300
C	-1.35852500	1.65264400	1.34609200
H	-0.66075800	1.99713400	2.11587300
C	-2.11450400	3.73299300	0.08712300
H	-2.05979100	4.29245200	-0.85322800
H	-3.16620800	3.48476300	0.26723400
H	-1.78469300	4.40185000	0.88949600
H	-2.37160900	1.76163000	1.75277300
C	1.32916600	1.88386200	-0.24181300
C	1.65738600	1.11245000	-1.36937900
C	2.12018700	1.68474400	0.90261000
C	2.68289700	0.17033800	-1.35411200
H	1.12032300	1.26878900	-2.30189600
C	3.15132100	0.75033800	0.94440000
H	1.94376800	2.29492200	1.78570000
C	3.46157900	-0.04616700	-0.18777200
H	2.90272600	-0.36890700	-2.26718000
H	3.73816700	0.66851600	1.85071700
N	4.48395200	-0.97653500	-0.16076300
C	4.91490700	-1.61126100	-1.40085400
C	5.39081300	-1.01698200	0.98052800
H	5.70956700	-2.32348600	-1.17839400
H	4.09314200	-2.16757600	-1.86549200
H	5.29736300	-0.88510000	-2.13311200
H	4.84505400	-1.21318600	1.90996500
H	6.10368200	-1.82958800	0.84006200
H	5.95434100	-0.08027000	1.10244400

**TS-N(CH<sub>3</sub>)<sub>2</sub>**

C	-1.83541700	0.30479700	-0.83534200
H	-0.84617600	0.42186900	-1.28495700
C	-2.68967600	1.53150900	-1.29928100
H	-3.61003500	1.60507200	-0.70949200
H	-2.97316100	1.34934000	-2.34211300
C	-1.78261300	2.71313600	-1.10998000

C	-0.79347100	3.00738600	-2.20672200
H	-1.33375600	3.40748800	-3.07399000
H	-0.05331600	3.75546900	-1.91581300
H	-0.26367500	2.11239200	-2.55865700
C	-1.70857500	3.17749200	0.14574900
H	-2.55057900	2.96093800	0.80706400
C	-0.41866800	3.41997100	0.85649400
H	-0.36092300	4.34916800	1.43625100
H	0.42672200	3.41417000	0.16480100
C	-0.31196700	2.25381300	1.87494300
H	-0.80465300	2.59984200	2.79333600
H	0.72994300	2.08187000	2.17689100
C	-0.95490800	0.85176300	1.73824500
C	-1.58829000	0.09918300	0.70099800
H	-0.30902000	-0.02880300	0.89645400
C	-0.91988200	0.19565500	3.12080600
H	-1.93280500	0.18022200	3.53903800
H	-0.55421900	-0.83093600	3.09609100
H	-0.28045200	0.75915500	3.79994500
C	-2.25240300	-1.23568100	1.04547600
H	-1.84697900	-1.74750500	1.91628000
H	-3.29481100	-0.97570500	1.28981800
C	-2.22812200	-2.10239700	-0.22957300
C	-0.87524900	-2.87027900	-0.38279300
H	-0.92357100	-3.41336200	-1.33433500
H	-0.84691700	-3.63669700	0.40173700
C	-2.45390800	-1.03256100	-1.31818200
H	-2.04825400	-1.32444000	-2.29146000
C	-3.36114800	-3.14201500	-0.21512700
H	-3.24072000	-3.85559300	0.60734500
H	-4.34009000	-2.66263100	-0.10642500
H	-3.37332500	-3.71501700	-1.14813200
H	-3.53243200	-0.89129000	-1.45693000
C	0.41679300	-2.07907700	-0.32895100
C	1.14870800	-1.94200800	0.86399100
C	0.99064200	-1.50569700	-1.47808100
C	2.34979000	-1.23396800	0.93077000
H	0.79888300	-2.44458700	1.76412700
C	2.18831500	-0.79988400	-1.44072300
H	0.50085900	-1.63558600	-2.44052700
C	2.90578200	-0.62838200	-0.22610900
H	2.87805900	-1.20031500	1.87547900
H	2.58594400	-0.40978200	-2.36906100
N	4.09022900	0.07433300	-0.17937100

C	4.90409600	0.03922900	1.03108900
C	4.72112500	0.51226200	-1.42069100
H	5.78081700	0.67064700	0.88844300
H	4.35082900	0.43385100	1.89065600
H	5.24690200	-0.97646100	1.27622400
H	4.05433800	1.16913300	-1.98955700
H	5.61794500	1.08326300	-1.18105000
H	5.01129100	-0.33099200	-2.06392900

**Reactant**

C	-1.44602100	-0.50546400	-1.04318600
H	-1.20098400	0.22357800	-1.82207500
C	-3.05564400	-0.72591700	-1.03972100
H	-3.27666700	-1.34639700	-0.16841000
H	-3.36328700	-1.21705800	-1.96281800
C	-3.51188000	0.64324400	-0.91962800
C	-3.94304900	1.39335500	-2.12085800
H	-4.85392800	1.96226200	-1.88998900
H	-3.19322500	2.15638600	-2.37579500
H	-4.11052700	0.75206200	-2.98628600
C	-3.33778900	1.29324700	0.37214800
H	-4.09129200	0.86539500	1.05267100
C	-3.09075700	2.81804300	0.42605600
H	-3.49772100	3.25745500	1.33804800
H	-3.43114400	3.41933400	-0.41869600
C	-1.56800700	2.53224800	0.52618300
H	-0.98842500	3.14981400	1.21709200
H	-1.08794000	2.56023800	-0.45838200
C	-1.83672300	1.06795100	0.99498800
C	-1.00645500	-0.06513800	0.36451400
H	0.01598700	0.32617800	0.26348500
C	-1.89168600	0.99813100	2.52399200
H	-2.34770000	0.07228800	2.88395600
H	-0.87359200	1.05135200	2.92444200
H	-2.45175100	1.83763700	2.94578700
C	-0.91014100	-1.40544000	1.12647900
H	-0.27987300	-1.32735000	2.01507300
H	-1.90059200	-1.71914000	1.48184500
C	-0.36633600	-2.45131400	0.10919200
C	1.17858600	-2.67117100	0.24773300
H	1.47390700	-3.38690600	-0.52936600
H	1.34530200	-3.17824300	1.20607400
C	-0.73383700	-1.85478100	-1.29407100
H	0.16331600	-1.65259600	-1.88524300

C	-1.04632500	-3.81742700	0.32272900
H	-0.85576500	-4.19745700	1.33224600
H	-2.13295400	-3.75049900	0.19229200
H	-0.67176600	-4.56192000	-0.38801800
H	-1.34732700	-2.54394400	-1.88246600
C	2.08320800	-1.45734200	0.17248400
C	2.42413600	-0.72765300	1.32858400
C	2.64972100	-1.03459300	-1.03682600
C	3.25024500	0.38891400	1.27273500
H	2.05881100	-1.05655200	2.29847400
C	3.48599600	0.08585800	-1.11730600
H	2.46853000	-1.60538300	-1.94464000
C	3.78383300	0.81155200	0.04341000
H	3.52131100	0.93380700	2.17138200
H	3.91208300	0.36176700	-2.07455100
O	4.58267300	1.91202300	0.08967300
C	5.23770900	2.33830200	-1.10380800
H	4.51280400	2.63645200	-1.87122100
H	5.83870100	3.20152400	-0.81839400
H	5.89162200	1.55211200	-1.49884600
<b>TS-OCH<sub>3</sub></b>			
C	1.42530000	-0.22293200	-0.99673900
H	0.36488500	-0.29030900	-1.25405200
C	2.13856400	-1.41434100	-1.71319400
H	3.16516600	-1.52293200	-1.34669200
H	2.18735500	-1.16162200	-2.77867900
C	1.28713600	-2.61101900	-1.40581100
C	0.06413900	-2.83219800	-2.25658200
H	0.38067400	-3.16928500	-3.25174700
H	-0.59602900	-3.60205200	-1.85177400
H	-0.52327400	-1.91775600	-2.41232800
C	1.51109900	-3.17361200	-0.20962400
H	2.48819900	-3.00106900	0.24742500
C	0.42776800	-3.48840800	0.76649000
H	0.50728900	-4.45777700	1.27313800
H	-0.55971400	-3.44280600	0.30149400
C	0.57530500	-2.40252500	1.86248100
H	1.31106500	-2.78449400	2.58431100
H	-0.34755600	-2.30160300	2.45012800
C	1.11639600	-0.96701100	1.67273500
C	1.47080200	-0.12087500	0.57341100
H	0.26114200	-0.08600500	1.01079600
C	1.34112500	-0.37556900	3.06677200
H	2.41410300	-0.23177700	3.23459000



H	0.85449700	0.59226800	3.19894600
H	0.96035700	-1.04383500	3.83821900
C	2.11806500	1.23542600	0.87825100
H	1.80638700	1.69339900	1.81556700
H	3.19408200	1.02186200	0.97804800
C	1.89138500	2.15443000	-0.34024200
C	0.52370700	2.90989100	-0.26529100
H	0.44375400	3.51358300	-1.17660500
H	0.59195100	3.62262200	0.56609300
C	1.96851600	1.13876700	-1.49646600
H	1.43019700	1.46919200	-2.38989200
C	3.00184300	3.21412000	-0.44181400
H	2.98818400	3.89283000	0.41789900
H	3.99216200	2.74861600	-0.48956700
H	2.87609200	3.82211400	-1.34356100
H	3.01794400	1.01303000	-1.78949700
C	-0.74436300	2.09532600	-0.10199700
C	-1.23681000	1.75772400	1.17592800
C	-1.50192200	1.67913700	-1.20527400
C	-2.39449300	1.00018800	1.34171500
H	-0.73481000	2.14390800	2.06100900
C	-2.67215100	0.92564700	-1.06355100
H	-1.18632800	1.96087400	-2.20692400
C	-3.12088600	0.56904900	0.21758800
H	-2.78176100	0.77065800	2.32944300
H	-3.23084700	0.64293900	-1.94787300
O	-4.23585900	-0.15745100	0.47668200
C	-5.09319700	-0.52803500	-0.60661500
H	-4.57874300	-1.19357200	-1.30965400
H	-5.92876500	-1.05773400	-0.15037500
H	-5.46474900	0.35726800	-1.13436400
<b>Reactant</b>			
C	0.27661500	0.17929700	-0.96883700
H	-0.52226200	-0.56218700	-0.90866300
C	1.35252000	-0.42198900	-1.99314500
H	2.04518000	0.38984700	-2.23631300
H	0.85406600	-0.78577000	-2.89281300
C	2.01651500	-1.45697000	-1.21362800
C	1.69057200	-2.88266000	-1.37947300
H	1.56043600	-3.15009700	-2.43253500
H	2.39898500	-3.54515700	-0.87851300
H	0.70315200	-3.04099600	-0.90659800
C	2.87018000	-0.97061100	-0.13889100
H	3.85885100	-0.79766800	-0.60075000

C	3.00337200	-1.67303500	1.24028900
H	3.92746200	-2.22563900	1.41781400
H	2.15556900	-2.32368200	1.47061700
C	2.89194400	-0.26809000	1.89993400
H	3.86936200	0.12243000	2.19559200
H	2.20886100	-0.19110400	2.74971600
C	2.39173700	0.37782800	0.56635300
C	0.83454600	0.42541600	0.46767600
H	0.47311700	-0.39951600	1.09350400
C	3.12543100	1.65522300	0.15473400
H	2.77230900	2.06779100	-0.79604900
H	3.00098300	2.43299800	0.91360900
H	4.20087100	1.47172900	0.06408000
C	0.15242600	1.74303500	0.93381000
H	-0.32269900	1.62097900	1.91109200
H	0.89275500	2.53810600	1.05205600
C	-0.87896000	2.17694200	-0.15614800
C	-2.34212400	1.72965500	0.17636900
H	-2.61570100	2.22395900	1.11648600
H	-2.99247500	2.15894400	-0.59468500
C	-0.32021500	1.51252100	-1.44663100
H	-1.08125400	1.37736900	-2.22175300
C	-0.90472900	3.70961700	-0.30773400
H	-1.24975000	4.18805400	0.61535800
H	0.09192500	4.10273300	-0.53562300
H	-1.58034200	4.01864200	-1.11248300
H	0.46593700	2.15178900	-1.86736200
C	-2.65449100	0.25043800	0.29247600
C	-2.46451500	-0.44688000	1.49752900
C	-3.17837500	-0.45877600	-0.80200200
C	-2.75117700	-1.81153900	1.59606200
H	-2.11653200	0.08752700	2.37798300
C	-3.46832000	-1.82305900	-0.70982300
H	-3.38281300	0.06791500	-1.73118700
C	-3.24691200	-2.50758800	0.48913700
H	-2.61315400	-2.32451000	2.54371600
H	-3.88895600	-2.34434600	-1.56500400
H	-3.49011800	-3.56279600	0.57035400

**TS-H**

C	-0.44175200	-0.99546600	-0.88541400
H	-0.31532600	0.01445100	-1.28532600
C	-1.74579700	-1.57156700	-1.52614500
H	-2.03691300	-2.50372600	-1.02981900

H	-1.50944100	-1.80652800	-2.57033200
C	-2.76763900	-0.48528700	-1.35833100
C	-2.77023000	0.63064300	-2.36949900
H	-3.17826600	0.25148300	-3.31497500
H	-3.39443300	1.47358200	-2.06591200
H	-1.76460300	1.00784200	-2.59685900
C	-3.35302900	-0.44266600	-0.15314900
H	-3.35435000	-1.36466600	0.43263500
C	-3.46660300	0.80024700	0.66333300
H	-4.43348600	0.96408300	1.15419900
H	-3.24445200	1.69177400	0.07243800
C	-2.42304600	0.60888000	1.79239400
H	-2.92756300	0.05248200	2.59517300
H	-2.15860400	1.56782300	2.25888400
C	-1.10738600	-0.19777400	1.70459100
C	-0.34454400	-0.84384700	0.67882400
H	-0.09284100	0.38828600	0.95224800
C	-0.55893800	-0.33316600	3.12754800
H	-0.60854600	-1.38171000	3.44084900
H	0.48083700	-0.01247900	3.21245500
H	-1.14548600	0.26075800	3.82746000
C	0.87457800	-1.67447200	1.09740400
H	1.38606800	-1.32248500	1.99177500
H	0.47025300	-2.66965600	1.34157300
C	1.81380800	-1.79201400	-0.12139500
C	2.81424100	-0.59327100	-0.21823700
H	3.41496200	-0.75232600	-1.12085300
H	3.50615100	-0.67834500	0.62862700
C	0.79626100	-1.83965200	-1.27798200
H	1.21583600	-1.49685100	-2.22853800
C	2.64799100	-3.08262400	-0.04699600
H	3.31934400	-3.07671800	0.81846700
H	2.00520500	-3.96610500	0.02941400
H	3.26636700	-3.19758400	-0.94308000
H	0.48010000	-2.87877700	-1.43005100
C	2.25537100	0.81637700	-0.24411800
C	2.04941300	1.53438700	0.94939600
C	1.96239900	1.46304000	-1.45660400
C	1.53225700	2.83579200	0.93453100
H	2.35439700	1.09375600	1.89652200
C	1.44903200	2.76254400	-1.47747300
H	2.15885300	0.95188900	-2.39574100
C	1.22003500	3.44998200	-0.28127500
H	1.40688600	3.37846200	1.86725000

H	1.24491300	3.24577600	-2.42835900
H	0.83559800	4.46499600	-0.29853900
<b>Reactant</b>			
C	1.99929200	0.36485400	-1.12201500
H	1.71605900	-0.25145900	-1.98339900
C	3.54073400	0.37751000	-1.04082300
H	3.88193600	1.25070500	-0.45199200
H	4.00169900	0.53325600	-2.02414400
C	4.19905300	-0.74013400	-0.32291800
C	5.67075400	-0.91394300	-0.44674800
H	6.02332900	-1.86025500	-0.03222700
H	6.01475600	-0.79392300	-1.47849500
H	6.14169500	-0.10321700	0.13108400
C	3.44212000	-1.63522600	0.47837900
H	4.00529900	-2.15580300	1.25459700
C	3.10348100	-2.73421500	-0.74548000
H	3.67888900	-3.64329700	-0.57120600
H	3.28508200	-2.38296800	-1.76306900
C	1.63643800	-2.66877000	-0.28160600
H	1.33323300	-3.58434200	0.23195600
H	0.92223800	-2.45860200	-1.08109200
C	1.90884100	-1.48422600	0.70643000
C	1.34874700	-0.14863300	0.18507300
H	0.28619500	-0.32006700	-0.02631800
C	1.49452300	-1.78669400	2.14729100
H	1.87032900	-1.03231400	2.84497300
H	0.40254800	-1.80971000	2.22571500
H	1.87037600	-2.76313100	2.47145800
C	1.44530000	1.08069000	1.11241300
H	0.75337900	1.01721200	1.95494300
H	2.45127800	1.15981400	1.54854800
C	1.16401800	2.32000000	0.20224400
C	-0.29601300	2.86683300	0.36578200
H	-0.42200700	3.67791600	-0.36135800
H	-0.36207600	3.32991900	1.35728600
C	1.42652200	1.79346600	-1.25457100
H	0.49406600	1.74217900	-1.82061000
C	2.11281700	3.48212500	0.55742800
H	1.99092700	3.78548400	1.60305300
H	3.16505700	3.20634900	0.41691600
H	1.91857700	4.35926700	-0.06908200
H	2.09414000	2.45862000	-1.81391300
C	-1.44092000	1.88610800	0.21376100
C	-1.94972200	1.19531000	1.32606200

C	-2.05055700	1.66028000	-1.03173700
C	-2.98925700	0.27416700	1.19642300
H	-1.54705700	1.39657500	2.31509200
C	-3.09068200	0.74148200	-1.17505700
H	-1.72994100	2.22876600	-1.90040900
C	-3.55268200	0.03528400	-0.06051400
H	-3.37384600	-0.24032400	2.07061700
H	-3.55221500	0.58873500	-2.14499300
C	-4.62580000	-1.01015900	-0.22360300
F	-5.49933800	-0.70052000	-1.20810000
F	-4.08505500	-2.22085700	-0.54942600
F	-5.33738400	-1.19773900	0.91072400

**TS-CF<sub>3</sub>**

C	-1.88751600	0.19334700	-0.95028100
H	-0.83856500	0.22193400	-1.25887500
C	-2.60179300	1.37100800	-1.68616900
H	-3.61566200	1.50691200	-1.29450000
H	-2.68503500	1.08077000	-2.73991300
C	-1.72708400	2.56608800	-1.44650000
C	-0.52484800	2.74082500	-2.33621400
H	-0.86394100	3.04561700	-3.33435300
H	0.15611400	3.51554800	-1.97843300
H	0.04779600	1.81439200	-2.47532400
C	-1.91838200	3.17859900	-0.26943300
H	-2.88577800	3.03390200	0.21719400
C	-0.81126700	3.52885900	0.66644300
H	-0.87937300	4.51610600	1.13880400
H	0.16555300	3.46598700	0.18133300
C	-0.93362600	2.48549700	1.80429400
H	-1.66884300	2.88275000	2.51947500
H	-0.00383000	2.42216900	2.38598700
C	-1.45624400	1.03633400	1.68039500
C	-1.85335900	0.14997900	0.62418300
H	-0.62436600	0.16211300	1.00048800
C	-1.60491500	0.48190900	3.10058900
H	-2.66378300	0.30494900	3.31746300
H	-1.07752100	-0.46341700	3.24227600
H	-1.21814700	1.18770000	3.83440300
C	-2.46283600	-1.20338400	1.01287100
H	-2.07286600	-1.63564700	1.93330100
H	-3.52760800	-0.99119500	1.19816500
C	-2.33893800	-2.15698500	-0.19382200
C	-0.98680500	-2.94590400	-0.19796200

H	-0.99067700	-3.57907300	-1.09204200
H	-1.00545800	-3.62760200	0.66090400
C	-2.48385700	-1.17241000	-1.36983400
H	-2.01728200	-1.53463300	-2.29080500
C	-3.47238500	-3.19836200	-0.18414000
H	-3.41137900	-3.85056300	0.69381800
H	-4.45440200	-2.71372600	-0.17741700
H	-3.42261700	-3.83616300	-1.07248000
H	-3.54961800	-1.03753600	-1.59071700
C	0.31024900	-2.16298000	-0.16183300
C	0.90741100	-1.80954900	1.06364500
C	0.97554700	-1.79869200	-1.34257800
C	2.09836800	-1.08231000	1.10816100
H	0.46400800	-2.15375900	1.99522200
C	2.16820700	-1.07245500	-1.31046700
H	0.56737100	-2.09943600	-2.30358100
C	2.72233400	-0.69736000	-0.08382400
H	2.55182100	-0.83451900	2.06297000
H	2.66756000	-0.80486900	-2.23529600
C	4.01901400	0.07332800	-0.01836000
F	4.34998600	0.61876500	-1.20855400
F	3.93738000	1.08932300	0.88290300
F	5.04962100	-0.71153300	0.37086700

**Reactant**

C	-1.39318400	-0.43302100	-1.10679800
H	-1.20558100	0.19926500	-1.98259800
C	-2.91682000	-0.66002700	-1.01031100
H	-3.12746400	-1.55345400	-0.39158800
H	-3.35570300	-0.90837300	-1.98437400
C	-3.71934900	0.37741500	-0.31897700
C	-5.20016600	0.35764500	-0.45551100
H	-5.67952100	1.24108400	-0.03006400
H	-5.51346500	0.21484400	-1.49454700
H	-5.56647900	-0.52140200	0.09710700
C	-3.08967800	1.37897200	0.46492700
H	-3.71931000	1.83988400	1.22753200
C	-2.90226300	2.48234000	-0.78873100
H	-3.60958100	3.30010800	-0.65271400
H	-3.00831600	2.07517000	-1.79610200
C	-1.44922900	2.64668700	-0.30412700
H	-1.30170100	3.60179900	0.20554900
H	-0.69862900	2.54599600	-1.09160100
C	-1.55072200	1.44435000	0.69440500
C	-0.80995900	0.19369100	0.18273600

H	0.21405100	0.51246300	-0.04805300
C	-1.18193300	1.81312300	2.13220800
H	-1.44833900	1.01942800	2.83642100
H	-0.10405200	1.98958600	2.20961000
H	-1.69080500	2.72982600	2.44883900
C	-0.71530100	-1.01816000	1.13313300
H	-0.02891600	-0.83948600	1.96345500
H	-1.69334200	-1.23188500	1.58706500
C	-0.27159300	-2.22247600	0.24185100
C	1.25417300	-2.55291500	0.39413800
H	1.48070200	-3.36506200	-0.30687100
H	1.39977400	-2.96432100	1.39986400
C	-0.62629700	-1.76976600	-1.21937800
H	0.28052200	-1.60030300	-1.80373800
C	-1.03855100	-3.50119200	0.63424700
H	-0.85729800	-3.76458400	1.68207900
H	-2.12151300	-3.38064100	0.50970300
H	-0.73132300	-4.35321900	0.01851700
H	-1.20153200	-2.53415800	-1.75386500
C	2.24864500	-1.43003200	0.18267200
C	2.67033300	-0.62848700	1.25810800
C	2.80197300	-1.17299800	-1.08365900
C	3.56557900	0.42262700	1.07417900
H	2.31118700	-0.84164700	2.26119900
C	3.69824000	-0.12538100	-1.28680900
H	2.54920000	-1.81516500	-1.92278300
C	4.07462200	0.69179500	-0.20788000
H	3.88504400	1.02739500	1.91656600
H	4.11738500	0.05655500	-2.27086600
C	4.97809500	1.78819700	-0.41041200
N	5.69504300	2.68942600	-0.57625900

**TS-CN**

C	-1.46571600	0.08396700	-0.88943800
H	-0.46510900	0.27296100	-1.28893700
C	-2.40304400	1.17014500	-1.51066500
H	-3.37918800	1.16301900	-1.01362900
H	-2.55822400	0.89118100	-2.55921300
C	-1.66792000	2.46446000	-1.32323300
C	-0.60657700	2.81535500	-2.33203600
H	-1.09384800	3.11314800	-3.26909900
H	0.01783200	3.65317900	-2.01547300
H	0.04857900	1.97025000	-2.58182100
C	-1.80005500	3.01820300	-0.10938800

H	-2.68178800	2.74030000	0.47280300
C	-0.64614200	3.48233900	0.71386700
H	-0.77601800	4.44598300	1.22066800
H	0.27145900	3.54440800	0.12447300
C	-0.51984000	2.41124700	1.82595400
H	-1.20601200	2.71059200	2.63125700
H	0.47202300	2.44097400	2.29727700
C	-0.89320500	0.91456400	1.71379400
C	-1.28842100	0.00898000	0.67270600
H	-0.03843300	0.15015900	0.95009800
C	-0.85761400	0.32745600	3.12788300
H	-1.87612100	0.07357500	3.44182400
H	-0.25567200	-0.57995800	3.19778900
H	-0.45186400	1.04838400	3.83653300
C	-1.71452500	-1.40960700	1.06948700
H	-1.21482500	-1.81001900	1.95009400
H	-2.78064100	-1.32086100	1.33198000
C	-1.57058600	-2.32204400	-0.16694000
C	-0.14214200	-2.95297800	-0.28204000
H	-0.12470100	-3.53476100	-1.21041900
H	-0.04012700	-3.67650300	0.53546000
C	-1.90866200	-1.34078300	-1.30660400
H	-1.45920000	-1.62577700	-2.26258200
C	-2.57556800	-3.48642000	-0.10674600
H	-2.38336900	-4.13750000	0.75271600
H	-3.60354700	-3.11733500	-0.02837300
H	-2.51154500	-4.10304700	-1.00898500
H	-2.99428400	-1.33805700	-1.46055500
C	1.06080400	-2.03241300	-0.25683000
C	1.70774100	-1.72747400	0.95584300
C	1.59169900	-1.48673100	-1.43874600
C	2.80935800	-0.87214400	0.99980000
H	1.37446900	-2.20366500	1.87497200
C	2.69144900	-0.63143000	-1.41378200
H	1.14924800	-1.74776000	-2.39614100
C	3.29822700	-0.30284500	-0.18852600
H	3.30700800	-0.66150800	1.94098000
H	3.09197400	-0.22430000	-2.33637300
C	4.41237400	0.60060700	-0.14899600
N	5.29887300	1.35260200	-0.10850200
<b>Reactant</b>			
C	-1.06355800	0.22658300	0.99131000
H	0.01500700	0.05781300	1.02617300
C	-1.69710200	-0.82724800	2.00399400



H	-2.74744500	-0.54214800	2.13685100
H	-1.17724300	-0.80332600	2.96336600
C	-1.61929500	-2.11481000	1.31902500
C	-0.67232500	-3.16105200	1.73202000
H	-0.67719300	-3.29120500	2.82039700
H	-0.81645800	-4.10955100	1.21285500
H	0.34291000	-2.79343100	1.49411000
C	-2.43960800	-2.23273100	0.12288200
H	-3.38306100	-2.69171300	0.47574100
C	-1.95798400	-2.93276700	-1.18566100
H	-2.33807200	-3.93858800	-1.36996600
H	-0.86918700	-2.94336900	-1.28177200
C	-2.63258900	-1.77019600	-1.96890800
H	-3.61265600	-2.05889600	-2.35807000
H	-2.04365100	-1.33473200	-2.78006500
C	-2.75847600	-0.90278600	-0.67208100
C	-1.54143100	0.06035100	-0.48636200
H	-0.71353900	-0.40782400	-1.03205500
C	-4.14025700	-0.28830700	-0.43803000
H	-4.20639000	0.28133200	0.49517000
H	-4.40871400	0.38896100	-1.25363700
H	-4.90886500	-1.06743700	-0.40999900
C	-1.72524900	1.51299700	-1.01019800
H	-1.22763300	1.65976500	-1.97307800
H	-2.78283600	1.72694400	-1.18055000
C	-1.19397700	2.50167300	0.07498000
C	0.27750500	2.97378800	-0.18890100
H	0.27180400	3.50434400	-1.14837200
H	0.51877800	3.72165500	0.57490000
C	-1.34924500	1.68490500	1.38899600
H	-0.69393800	2.03717400	2.19211900
C	-2.05928000	3.77571100	0.12632900
H	-1.99373900	4.33252900	-0.81462200
H	-3.11278300	3.53019600	0.29684400
H	-1.73566700	4.44482400	0.93063900
H	-2.38161600	1.78212200	1.74727700
C	1.38396200	1.94126200	-0.21169400
C	1.69211400	1.22672000	-1.38332800
C	2.15011400	1.68684400	0.94040400
C	2.68516100	0.24871900	-1.39684400
H	1.16123700	1.44862800	-2.30444800
C	3.14878900	0.71431500	0.94942600
H	1.97130700	2.26623500	1.84198900
C	3.38616400	-0.00861300	-0.21914600

H	2.92870200	-0.30261300	-2.29724900
H	3.74290300	0.51671000	1.83371400
N	4.41037000	-1.07108200	-0.21138600
O	5.00181000	-1.28357300	0.84705800
O	4.59379600	-1.69254900	-1.25803800

**TS-NO<sub>2</sub>**

C	-1.59422800	0.15507500	-0.97846400
H	-0.53433600	0.20194600	-1.24635800
C	-2.30359200	1.30041800	-1.76841200
H	-3.33739800	1.41628600	-1.42541000
H	-2.33127900	0.98838200	-2.81884500
C	-1.47301100	2.52347700	-1.51335300
C	-0.23742900	2.71719700	-2.35183800
H	-0.53950400	2.99864300	-3.36853800
H	0.40699600	3.51473800	-1.97697500
H	0.36476000	1.80446600	-2.45233100
C	-1.73561000	3.15073200	-0.35799400
H	-2.71984300	2.98546100	0.08640200
C	-0.68464000	3.55270300	0.62044800
H	-0.80341500	4.54652800	1.06822000
H	0.31529000	3.50981900	0.18254100
C	-0.83014800	2.52853500	1.77238000
H	-1.61189100	2.91457400	2.44317500
H	0.07112900	2.50672700	2.40020500
C	-1.29914300	1.06100000	1.65289200
C	-1.62146400	0.14273100	0.59704300
H	-0.41067200	0.20982800	1.02263300
C	-1.48969300	0.52634400	3.07592200
H	-2.55032700	0.31679500	3.25133700
H	-0.93765400	-0.39749500	3.25934700
H	-1.15889800	1.25804600	3.81167600
C	-2.19917600	-1.22371900	0.98914000
H	-1.82335100	-1.62882600	1.92773400
H	-3.27466800	-1.04191700	1.14180000
C	-2.01443800	-2.19355900	-0.19707600
C	-0.64691000	-2.95534000	-0.14449900
H	-0.61636400	-3.61424700	-1.01902200
H	-0.67351800	-3.61096500	0.73413900
C	-2.14177400	-1.23221800	-1.39399800
H	-1.63460900	-1.59736000	-2.29203400
C	-3.12465700	-3.25989800	-0.20559300
H	-3.07532900	-3.89875100	0.68280800
H	-4.11636700	-2.79640300	-0.23365200

H	-3.03573100	-3.90794600	-1.08331100
H	-3.20202100	-1.12790700	-1.65401200
C	0.63224400	-2.14552300	-0.10184700
C	1.17873400	-1.72371300	1.12641900
C	1.32852500	-1.82347200	-1.27966000
C	2.34891200	-0.96434500	1.18124400
H	0.71313100	-2.03946300	2.05696100
C	2.50268000	-1.07109000	-1.24699100
H	0.95868400	-2.17986800	-2.23680600
C	2.98354500	-0.63281000	-0.01438600
H	2.78280800	-0.64962900	2.12319000
H	3.04656400	-0.82722200	-2.15206500
N	4.21017200	0.19125200	0.03088800
O	4.78010700	0.41692600	-1.03378300
O	4.56792400	0.60955500	1.13162400

**TS<sub>CHO</sub>**

C	-3.57121700	-0.78175900	-1.34899400
H	-4.23530200	0.08263000	-1.45800200
H	-3.22068000	-1.06515600	-2.34636800
H	-4.16815600	-1.61241800	-0.95851600
C	-2.38349300	-0.46890100	-0.41773700
C	-1.38237100	-1.64258400	-0.36716000
C	0.03611400	-1.06772200	-0.13228000
C	1.13559700	-1.95256200	-0.80447800
H	0.87950800	-2.99859400	-0.60005900
C	2.41957700	-1.50059100	-0.16822800
C	2.93297100	-0.37153500	-0.67671200
C	3.36682100	0.78693100	0.15581500
H	3.45051800	0.51514100	1.21052600
H	4.31416900	1.25439400	-0.13807200
C	2.26100100	1.85477300	-0.05442300
C	0.76419700	1.58847800	-0.37297100
C	-1.50131400	0.65133500	-1.00939200
H	-1.43749000	0.51035700	-2.10027800
H	-1.90781700	1.64902000	-0.85524000
C	2.78496900	-2.10826700	1.16048000
H	3.60956800	-1.58682200	1.65041100
H	1.94054000	-2.15454100	1.86152000
H	3.10794300	-3.14476500	1.00070000
H	-1.63511800	-2.39182300	0.38935000
C	-2.99017700	-0.11641400	0.96987400
H	-3.80853100	0.61340700	0.83753800

H	-3.50193400	-1.00122000	1.37467000
H	2.64091800	-0.10610100	-1.69512300
H	1.12867900	-1.81141500	-1.89074300
C	-0.07285500	0.44948900	-0.50780400
H	0.02933200	1.13576300	0.64834900
C	0.13718700	2.94124500	-0.75238800
H	-0.76354200	3.16450600	-0.17614900
H	0.84266300	3.75123800	-0.57108800
H	-0.12716400	2.95470900	-1.81449800
H	2.54691700	2.43238400	-0.94391300
H	2.26997500	2.58737200	0.76285700
H	-1.39907400	-2.15730600	-1.33487600
H	0.24498200	-1.07999400	0.94292400
C	-2.19099300	0.46490500	2.10444800
O	-1.06896900	0.95304800	2.05781800
H	-2.72522100	0.47392700	3.07323800

**TS<sub>NO2</sub>**

C	-3.36597100	0.03770800	-1.87616000
H	-3.98708100	0.92651200	-1.72241000
H	-2.94099500	0.09409300	-2.88289300
H	-4.01810400	-0.84028300	-1.83907600
C	-2.24040800	-0.05902900	-0.82783100
C	-1.31008700	-1.26239800	-1.07276100
C	0.09907900	-0.90657500	-0.53347500
C	1.21181600	-1.66278700	-1.32637100
H	0.88132500	-2.70319100	-1.42545200
C	2.45444200	-1.49020900	-0.50144700
C	3.09012100	-0.32368100	-0.68073000
C	3.52862200	0.55809300	0.43896000
H	3.50145000	0.03709300	1.39871900
H	4.52632200	1.00063500	0.33419500
C	2.51893700	1.73300900	0.41945100
C	1.04289800	1.67678500	-0.03328400
C	-1.25795100	1.12509300	-0.95356900
H	-1.11488700	1.34645500	-2.02209600
H	-1.63257600	2.03632900	-0.49213400
C	2.65560600	-2.42872600	0.65901800
H	3.47450200	-2.12139600	1.31221500
H	1.75482900	-2.55871600	1.27346700
H	2.90855300	-3.42350100	0.27109200
H	-1.67709000	-2.19108500	-0.62570300
C	-2.96509600	-0.11276900	0.54541700
H	-3.49469400	0.82223200	0.74152900

H	-3.65463400	-0.95543600	0.58184200
H	2.91213200	0.20282200	-1.62124700
H	1.31277100	-1.24380300	-2.33347200
C	0.11707900	0.66804000	-0.44533700
H	0.18822900	0.98376000	0.79821700
C	0.51365200	3.11563600	-0.06137100
H	-0.37706200	3.24081900	0.55911600
H	1.26783800	3.80970600	0.30670500
H	0.25498800	3.40274600	-1.08566800
H	2.90246600	2.47091300	-0.30037600
H	2.51897200	2.26918200	1.37790300
H	-1.24358700	-1.43494100	-2.15322800
H	0.17652900	-1.25660400	0.50159100
O	-1.31414400	0.65935700	2.03032900
N	-2.03977800	-0.30324700	1.71972500
O	-2.02563000	-1.38445200	2.28292300

**TS<sub>CN</sub>**

C	-3.67890800	-0.60212200	-1.27448800
H	-4.32080700	0.28524800	-1.28322900
H	-3.37338600	-0.80815200	-2.30493100
H	-4.28370400	-1.44814600	-0.93206500
C	-2.45076600	-0.40307300	-0.37202800
C	-1.46648400	-1.58417100	-0.45675400
C	-0.04241900	-1.06234100	-0.14353600
C	1.04298700	-1.92959600	-0.85400400
H	0.77572200	-2.97852100	-0.68025100
C	2.34199400	-1.51587700	-0.22545600
C	2.88129900	-0.39952900	-0.73466600
C	3.36864700	0.73628100	0.09861600
H	3.47221600	0.45384300	1.14872000
H	4.31867600	1.18429200	-0.21589900
C	2.28498000	1.82936000	-0.07313000
C	0.77945500	1.60694200	-0.33547600
C	-1.56439200	0.76530100	-0.85631600
H	-1.52928200	0.75470400	-1.95599100
H	-1.95836300	1.73974200	-0.56966700
C	2.71267700	-2.14806300	1.08995300
H	3.56449300	-1.66012500	1.56745100
H	1.88230900	-2.17199300	1.80801900
H	2.99688500	-3.19316300	0.91355100
H	-1.73343200	-2.41504700	0.20328000
C	-2.98371000	-0.15732700	1.08193800
H	-3.80705300	0.56632400	1.05450200

H	-3.39069300	-1.08683400	1.49448000
H	2.58154600	-0.11627400	-1.74621600
H	1.02412500	-1.75241500	-1.93483900
C	-0.11779300	0.49289100	-0.40058100
H	0.07256500	1.06926300	0.72889900
C	0.15628400	2.97705800	-0.62329000
H	-0.67681100	3.20515300	0.04570300
H	0.89451300	3.76861800	-0.50392400
H	-0.21886200	3.00978800	-1.65136300
H	2.54426800	2.39779700	-0.97868300
H	2.34164500	2.57173500	0.73431700
H	-1.48275200	-1.97658100	-1.48059200
H	0.13400400	-1.16475100	0.93221500
C	-1.96661700	0.37407200	1.99035300
N	-1.08731800	0.84095200	2.59138700

**TS<sub>oCH<sub>3</sub></sub>**

C	-3.24471400	-1.67493300	-1.23065700
H	-3.88100700	-1.03346300	-1.84971200
H	-2.76377200	-2.40666500	-1.88702200
H	-3.89457700	-2.22444700	-0.54157000
C	-2.19333100	-0.86070300	-0.46178400
C	-1.23367400	-1.75998400	0.36361700
C	0.15811400	-1.06704100	0.40014800
C	1.32640400	-2.02567900	-0.03725200
H	1.23890900	-2.94232900	0.55661600
C	2.60301300	-1.26122500	0.21109800
C	2.93054900	-0.33473200	-0.70743200
C	3.29898700	1.07809500	-0.33661600
H	4.09010200	1.16384300	0.41255400
H	3.60553400	1.67235800	-1.20217500
C	1.97480000	1.64632900	0.29651300
C	0.76505200	1.34042600	-0.58935900
C	-1.21310600	-0.12156700	-1.40742000
H	-0.88489100	-0.80149000	-2.20600100
H	-1.65478400	0.75446300	-1.88373500
C	3.17642200	-1.33198000	1.60285300
H	4.00259200	-0.63450400	1.75625300
H	2.42547900	-1.15616300	2.38492900
H	3.56692700	-2.34225900	1.77857000
H	-1.61438500	-1.95045800	1.37103200
C	-2.93851900	0.15480500	0.42476000
H	-3.61759600	0.76496600	-0.18939600
H	-3.54212100	-0.37911900	1.17215100

H	2.49415600	-0.44185200	-1.70161800
H	1.20629700	-2.29985500	-1.09200600
C	-0.00367800	0.16197000	-0.52993000
H	-0.38328000	1.16481700	0.19814800
C	0.50042100	2.40637900	-1.62617500
H	-0.33327100	2.20136400	-2.29342700
H	0.35797600	3.38153800	-1.15033000
H	1.40824800	2.48930900	-2.23610700
H	2.03852300	2.73002700	0.44347600
H	1.85056900	1.17850200	1.27650100
H	-1.14282800	-2.73316400	-0.13089800
H	0.37947500	-0.71757400	1.41282100
C	-2.64821400	1.95224300	1.98621900
H	-3.19766800	1.41816900	2.77018800
H	-1.85961800	2.55208800	2.44305800
H	-3.33695200	2.60545700	1.43649100
O	-2.01364900	1.02150300	1.09996500

**TS<sub>F</sub>**

C	-3.76544500	-0.54980400	-1.00704500
H	-4.40384300	0.33967900	-0.98064200
H	-3.53894300	-0.77122500	-2.05432500
H	-4.34523800	-1.38925600	-0.60964600
C	-2.46891400	-0.34571000	-0.20560100
C	-1.50499200	-1.54244600	-0.31776500
C	-0.06258200	-1.02360400	-0.08544000
C	0.98162100	-1.82540000	-0.92634700
H	0.72222100	-2.88635000	-0.83492600
C	2.30716700	-1.46533900	-0.31785500
C	2.81379400	-0.29086300	-0.72000900
C	3.30750800	0.75812900	0.21956100
H	3.42676800	0.36575400	1.23189500
H	4.25149400	1.24252000	-0.05735500
C	2.21639000	1.85836800	0.17818800
C	0.72062400	1.65717000	-0.13779800
C	-1.59898100	0.79413200	-0.77058700
H	-1.55111400	0.70501400	-1.86631600
H	-2.00097100	1.78206700	-0.55219900
C	2.73877900	-2.22838200	0.90646600
H	3.60318600	-1.78022200	1.40043800
H	1.93720600	-2.34518800	1.64769400
H	3.02954500	-3.24314800	0.60677000
H	-1.74727700	-2.35224400	0.37707900
C	-2.86955900	-0.04311800	1.24205600

H	-3.55015100	0.81101400	1.30394400
H	-3.32028300	-0.91196700	1.72871500
H	2.47441500	0.09482600	-1.68425200
H	0.91377600	-1.55304300	-1.98545300
C	-0.16772100	0.54045900	-0.27512900
H	-0.05813800	1.04094800	0.86986900
C	0.10338200	3.03854000	-0.36460500
H	-0.81134500	3.19610300	0.20904200
H	0.80505600	3.82624200	-0.09242900
H	-0.14527900	3.15358200	-1.42573400
H	2.48273900	2.53566700	-0.64655800
H	2.25852700	2.50160200	1.06816900
H	-1.57775000	-1.95794800	-1.32984800
H	0.19374400	-1.17839900	0.96673400
F	-1.72830800	0.30902100	2.02231000
<b>TS<sub>SCH3</sub></b>			
C	-2.90570100	-2.06761700	-1.40638300
H	-3.63386800	-1.47584100	-1.97121800
H	-2.36247300	-2.70066900	-2.11549100
H	-3.46212200	-2.72548400	-0.73149100
C	-1.93352000	-1.17060500	-0.61819800
C	-0.85346900	-1.99538900	0.11517500
C	0.44021300	-1.13954600	0.19062800
C	1.73360600	-2.00398100	0.00031600
H	1.59024500	-2.93259800	0.56375300
C	2.83474200	-1.12814900	0.53040900
C	3.24685000	-0.16592400	-0.30801700
C	3.36925900	1.26899100	0.08318500
H	3.33114400	1.38968000	1.16795900
H	4.27199300	1.78067200	-0.27097400
C	2.16135600	1.97626700	-0.59581600
C	0.82318000	1.30719400	-1.01763300
C	-1.06439800	-0.31445600	-1.56282300
H	-0.71247800	-0.94367400	-2.39673800
H	-1.59900000	0.52109500	-2.00954800
C	3.07956900	-1.15709500	2.01622700
H	3.74536900	-0.35860800	2.34944700
H	2.15495800	-1.10696300	2.60695800
H	3.55978700	-2.10827900	2.27831800
H	-1.16974600	-2.32071700	1.11066400
C	-2.79336800	-0.28914300	0.32110100
H	-3.45973100	0.33359000	-0.28492200
H	-3.41427600	-0.93295100	0.95111300
H	3.07859000	-0.32838100	-1.37496400



H	1.86819700	-2.26754900	-1.05456300
C	0.20403700	0.04430700	-0.80158200
H	-0.07257600	1.15687700	-0.04279200
C	0.13675100	2.24969900	-2.01788500
H	-0.93212100	2.36692600	-1.83261600
H	0.58668400	3.24161500	-1.97253500
H	0.26515800	1.86858000	-3.03680400
H	2.51827500	2.33124300	-1.57068200
H	1.89027400	2.89329400	-0.05577400
H	-0.64740900	-2.90162800	-0.46560200
H	0.51527800	-0.69187600	1.18688000
C	-3.14566600	2.10854900	1.78584400
H	-3.99130300	1.64359300	2.29681500
H	-2.69450300	2.84845100	2.44970700
H	-3.47935800	2.59723700	0.86797600
S	-1.85910200	0.85523400	1.44186500

**TS<sub>CH=CH2</sub>**

C	0.10270200	-1.11328700	0.00741200
H	0.32267100	-1.01311800	1.07482400
C	1.24313200	-2.00286800	-0.59037100
H	1.22757500	-1.96166600	-1.68492500
H	1.03543500	-3.03602800	-0.29014800
C	2.50443300	-1.43569700	-0.00401200
C	2.89875900	-1.90317000	1.37221500
H	3.27588500	-2.93125800	1.30220900
H	3.69475900	-1.29909700	1.81211400
H	2.05653100	-1.93401000	2.07659100
C	2.96768100	-0.33515800	-0.61415000
H	2.67022700	-0.17893500	-1.65357300
C	3.33997600	0.91475000	0.11094500
H	4.26704200	1.39847700	-0.21889600
H	3.42714400	0.74358800	1.18620700
C	2.18637800	1.90507700	-0.20228200
H	2.47178600	2.43713400	-1.12002900
H	2.12374100	2.69879200	0.55490100
C	0.72692700	1.53353100	-0.56047400
C	-0.07436300	0.34930200	-0.53698500
H	-0.07252700	1.15121600	0.48740700
C	0.05919300	2.78865600	-1.13239100
H	-0.09373700	2.66342300	-2.20997200
H	-0.91225900	2.99653300	-0.68046400
H	0.68942800	3.66410300	-0.97843100

C	-1.46904300	0.38447100	-1.16096300
H	-1.93702200	1.36635700	-1.20384200
H	-1.31583400	0.06367400	-2.20394900
C	-2.32903800	-0.66230700	-0.42381700
C	-2.94197500	-0.06751600	0.88184000
H	-3.55724400	-0.85480800	1.33699100
H	-3.62941400	0.73815300	0.59598800
C	-1.29099400	-1.77339000	-0.16462200
H	-1.54134500	-2.39740600	0.69915000
C	-3.48568700	-1.15363100	-1.30903000
H	-4.18741400	-0.34424300	-1.53732800
H	-3.11456500	-1.55675600	-2.25728100
H	-4.04857100	-1.94702100	-0.80701000
H	-1.26006300	-2.43958600	-1.03466100
C	-1.99290100	0.45036900	1.93292700
C	-1.86374600	1.73804500	2.28658500
H	-1.41489100	-0.29427200	2.48183700
H	-1.20456100	2.04414100	3.09417200
H	-2.46136900	2.51954300	1.82114500

**TS<sub>NO</sub>**

C	-3.49843200	-0.56746500	-1.50873400
H	-4.15450600	0.30768200	-1.56722600
H	-3.07678200	-0.73994300	-2.50400100
H	-4.11895300	-1.43347700	-1.25711600
C	-2.37223900	-0.36711400	-0.47035300
C	-1.38481500	-1.55431300	-0.48576200
C	0.03828900	-1.03350800	-0.16691500
C	1.12683100	-1.88101000	-0.89882900
H	0.85219800	-2.93446500	-0.77047100
C	2.41811800	-1.49996500	-0.23348400
C	2.96456800	-0.35933300	-0.67748600
C	3.42851700	0.73747600	0.21975000
H	3.49958600	0.40636900	1.25834700
H	4.38860300	1.19660200	-0.04439400
C	2.35207600	1.84073400	0.06383700
C	0.85503500	1.63261400	-0.25911300
C	-1.46235600	0.80929700	-0.88541800
H	-1.39129300	0.82831200	-1.98397900
H	-1.86096300	1.77836500	-0.58921200
C	2.76761000	-2.19400800	1.05641200
H	3.60811300	-1.72638900	1.57292900
H	1.92364100	-2.25797000	1.75610200

H	3.06068500	-3.22792500	0.83452000
H	-1.67020400	-2.35843000	0.19922200
C	-3.10501600	-0.17476000	0.88287100
H	-3.87548700	0.61143600	0.80724400
H	-3.67633300	-1.07751300	1.13835200
H	2.68204000	-0.02817500	-1.67931100
H	1.12488000	-1.66200300	-1.97217000
C	-0.03732700	0.52351900	-0.39544500
H	0.08857500	1.06194000	0.75011500
C	0.24793600	3.01468300	-0.52928700
H	-0.61700400	3.22536300	0.10402400
H	0.98117200	3.79935000	-0.34825400
H	-0.07725100	3.08392000	-1.57239500
H	2.64293600	2.44628600	-0.80707200
H	2.38634800	2.54768900	0.90373700
H	-1.38151000	-1.98844300	-1.49227600
H	0.21916400	-1.15601900	0.90560400
O	-1.30003900	0.55726100	2.11810300
N	-2.45573000	0.18260900	2.16294100

**TS<sub>H</sub>**

C	-3.96057300	-0.22140200	-0.66826600
H	-4.55983300	0.64378400	-0.36444100
H	-3.82427300	-0.17549200	-1.75440600
H	-4.54327300	-1.12017900	-0.44270700
C	-2.61322200	-0.25272700	0.06692600
C	-1.70589200	-1.39756700	-0.41011800
C	-0.25392500	-1.00546000	-0.05651100
C	0.77930600	-1.80308100	-0.90521500
H	0.48938700	-2.85824400	-0.84079600
C	2.11896900	-1.49503500	-0.30409900
C	2.67999900	-0.35788700	-0.73816800
C	3.25995800	0.67668100	0.16375500
H	3.41313000	0.29582800	1.17649900
H	4.20657600	1.12140200	-0.16564600
C	2.21113600	1.81324500	0.15467600
C	0.68093100	1.66090400	0.03756600
C	-1.74321300	0.96711400	-0.29505000
H	-1.81911900	1.16978400	-1.37505500
H	-2.06383100	1.87374100	0.21764600
C	2.53311700	-2.26422200	0.92244200
H	3.42491600	-1.85215500	1.39881500
H	1.73862400	-2.33605400	1.67682500

H	2.77125700	-3.29494200	0.63104700
H	-1.96463000	-2.36269000	0.03553100
C	-2.85216200	-0.31342400	1.58924500
H	-3.44537100	0.54337500	1.92614400
H	-1.92034200	-0.31929700	2.16860900
H	-3.40196400	-1.22140600	1.85534600
H	2.33926800	0.03081700	-1.70047500
H	0.71739900	-1.50246600	-1.95646000
C	-0.27283800	0.58184600	-0.05469000
H	0.07719500	0.98457300	1.09532100
C	0.08334100	3.06941200	-0.02737000
H	-0.64936100	3.25453200	0.76131800
H	0.86199200	3.82514700	0.06415400
H	-0.42569100	3.20979800	-0.98632300
H	2.39893200	2.41849000	-0.74609500
H	2.38039100	2.51346900	0.98361100
H	-1.79313900	-1.50900300	-1.49865200
H	-0.07782600	-1.28320500	0.98946000

**TS<sub>NMe2</sub>**

C	-3.09230700	-1.81803500	-1.40423000
H	-3.81371800	-1.14665100	-1.88216400
H	-2.64681400	-2.44399000	-2.18400400
H	-3.64942800	-2.47504000	-0.72817400
C	-2.01260600	-1.03913400	-0.63728000
C	-0.92421900	-1.97323100	-0.06239500
C	0.39654400	-1.16205900	0.00153200
C	1.66075600	-2.00414500	-0.39756400
H	1.54053600	-3.00269200	0.03647000
C	2.80504800	-1.21491100	0.18224300
C	3.14318100	-0.11554300	-0.50745200
C	3.29583700	1.23340000	0.11273500
H	3.34199100	1.16367600	1.20182400
H	4.17262400	1.80447800	-0.21472300
C	2.04344500	2.04249500	-0.34106700
C	0.65845000	1.43975200	-0.76918000
C	-1.15220300	-0.16342100	-1.57862700
H	-0.82458800	-0.78053600	-2.43459200
H	-1.66433700	0.69988500	-1.99609000
C	3.16793200	-1.49415700	1.61717800
H	3.85816300	-0.75495800	2.02819800
H	2.29320400	-1.55812700	2.27906700
H	3.66690200	-2.46974100	1.67504000

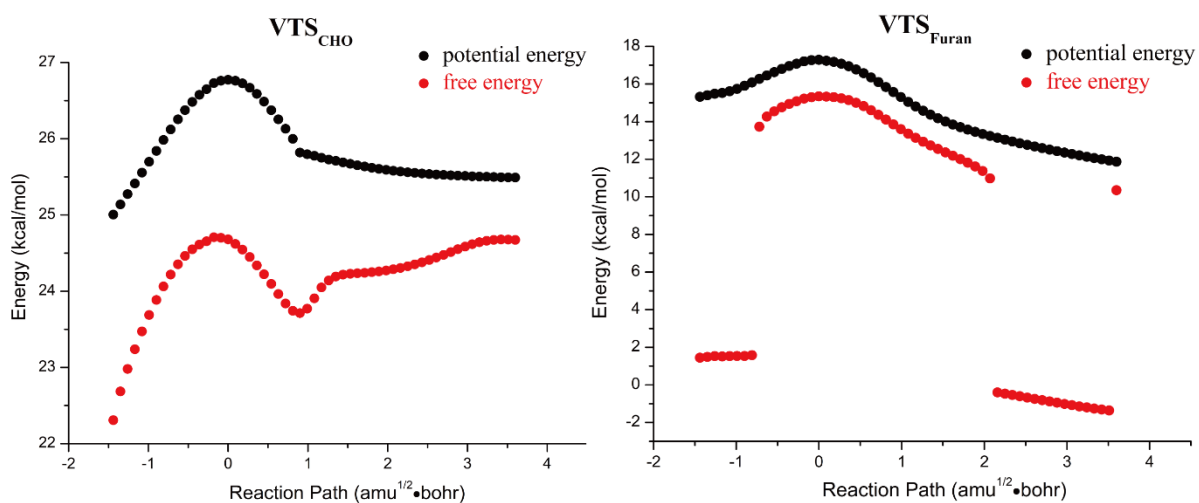
H	-1.18597100	-2.39673200	0.91160500
C	-2.73238300	-0.14918000	0.41353000
H	-3.46628000	0.45240000	-0.13358500
H	-3.31025800	-0.79863500	1.08854900
H	2.88767500	-0.09599600	-1.56956900
H	1.72477700	-2.11730400	-1.48554400
C	0.12234100	0.11318900	-0.82912700
H	-0.13677300	1.24696600	0.16009200
C	-0.02271300	2.50764000	-1.64980800
H	-1.10967100	2.51193200	-1.57644400
H	0.32368400	3.49963600	-1.35556400
H	0.25090900	2.35988000	-2.69991100
H	2.33596800	2.56551500	-1.25851800
H	1.82579700	2.84050200	0.37868400
H	-0.79165800	-2.82008300	-0.74532200
H	0.57372000	-0.81940300	1.02558100
N	-1.87987200	0.78415700	1.20021500
C	-2.52886600	2.10220900	1.34632000
H	-3.48624300	2.03809900	1.88698000
H	-1.87015700	2.77527800	1.90283200
H	-2.71898900	2.54215900	0.36389800
C	-1.57549800	0.25233900	2.54207500
H	-0.87971000	0.92157600	3.05633500
H	-2.48331700	0.16062200	3.15955100
H	-1.11537600	-0.73505800	2.47469500

**TS<sub>Furan</sub>**

C	-0.43093500	-0.98724700	-0.73481100
H	-0.46297400	-0.19076500	-1.48334600
C	-1.75902200	-1.82693300	-0.87823100
H	-1.80681000	-2.57741400	-0.08059400
H	-1.69454300	-2.36079100	-1.83284100
C	-2.90176100	-0.84894500	-0.80562300
C	-3.28932900	-0.15956800	-2.08861400
H	-3.76179500	-0.88875500	-2.75873100
H	-4.00525400	0.65053800	-1.93494400
H	-2.42571900	0.24126200	-2.63617300
C	-3.25624100	-0.43637800	0.42456900
H	-2.96953600	-1.06879600	1.26632900
C	-3.43435300	1.01975300	0.76770800
H	-3.78463700	1.16947300	1.79290900
H	-4.11447400	1.56675700	0.10980800
C	-1.99136900	1.60709700	0.56824700
H	-1.91282200	2.62427300	0.96758100

H	-1.79576300	1.65070000	-0.50538200
C	-0.93915800	0.73275500	1.25948200
C	-0.25993800	-0.36369300	0.67222400
H	0.24640100	0.84747000	0.60435400
C	-0.73000100	1.09421500	2.71140000
H	-1.70636500	1.00938100	3.20337100
H	-0.02895900	0.45835500	3.24664600
H	-0.42471600	2.14071500	2.80760800
C	0.77693700	-1.20530200	1.39607200
H	1.27372600	-0.70348900	2.22775000
H	0.23913500	-2.06960400	1.81284500
C	1.76162300	-1.68586900	0.29928700
C	2.87784000	-0.62279800	0.04344500
H	3.52504500	-1.00226700	-0.75640600
H	3.50079700	-0.55684200	0.94243000
C	0.83019500	-1.87634900	-0.93016000
H	1.33931100	-1.64356700	-1.86855400
C	2.45125900	-2.99782400	0.70420900
H	3.06566200	-2.86789700	1.60177000
H	1.71630300	-3.78325200	0.90876100
H	3.10644900	-3.35565100	-0.09658700
H	0.52140100	-2.92530100	-0.98724500
C	2.45828800	0.76941400	-0.30330600
C	2.45795500	1.95423800	0.38872500
O	2.01675400	1.00096000	-1.58408000
C	1.99031300	2.96917700	-0.51508100
H	2.79999000	2.09504200	1.40528300
C	1.74254100	2.33681500	-1.69594100
H	1.88672200	4.02677900	-0.31872500
H	1.41032700	2.67061400	-2.66687900

## 5. Free energy profiles calculated using the RODS algorithm.



## 6. Tunneling results.

Table. Results of the Wigner tunneling correction (transmission coefficient) to the rate constant  $k$  for hydrogen migration in Figure 1.

X	TSS	TSS barrier(kcal/ mol)	$k$ ( $s^{-1}$ )	Wigner correction
$N(CH_3)_2$	<b>TS-<math>N(CH_3)_2</math></b>	26.4	$2.34 \times 10^{-7}$	1.23
$OCH_3$	<b>TS-<math>OCH_3</math></b>	26.8	$1.40 \times 10^{-7}$	1.20
H	<b>TS-H</b>	27.6	$3.32 \times 10^{-8}$	1.20
$CF_3$	<b>TS-<math>CF_3</math></b>	33.5	$1.68 \times 10^{-12}$	1.19
CN	<b>TS-CN</b>	32.9	$4.40 \times 10^{-12}$	1.19
$NO_2$	<b>TS-<math>NO_2</math></b>	30.9	$1.21 \times 10^{-10}$	1.17

Tunneling calculations were performed with the KiSTheIP program<sup>1</sup> and Wigner method<sup>2</sup> is used to estimate the tunneling correction to the rate constant  $k$ . Reaction path degeneracy<sup>3</sup> is set to 1. We also considered the frequency scale factor<sup>4</sup> and estimate it to 0.98.

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