

Supporting Information for: Why HS- and CN- can be detected by  
different chemosensors with similar structures:  
a quantum mechanics and molecular dynamics study

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Table S1. The calculated main excitations of COUMC compared to other functionals and the experimental result.

<b>Methods</b>	<b>Excitation (nm)</b>
Wb97xd	493
PBE	522
M062X	498
LC-BLYP	452
B3LYP	533
BLYP	586
Exp. <sup>1</sup>	588

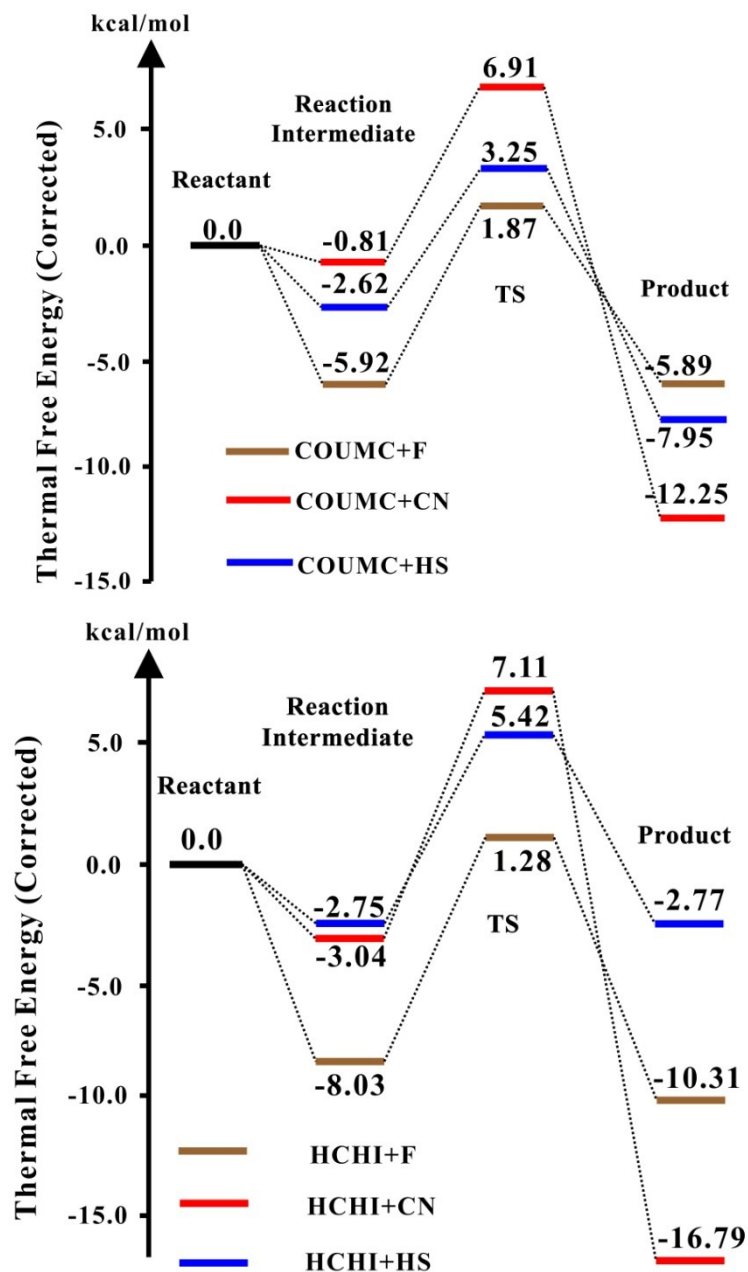


Figure S1 DFT-calculated free energy diagrams for COUMC (upper)/ HCHI (bottom) reacting with anions at 298.15K. Values of imaginary frequency are -113.9 (COUMC+F), -245.8 (COUMC+CN), -171.9 (COUMC+HS), -122.6 (HCHI+F), -276.6 (HCHI+CN), and -189.0 (HCHI+HS).

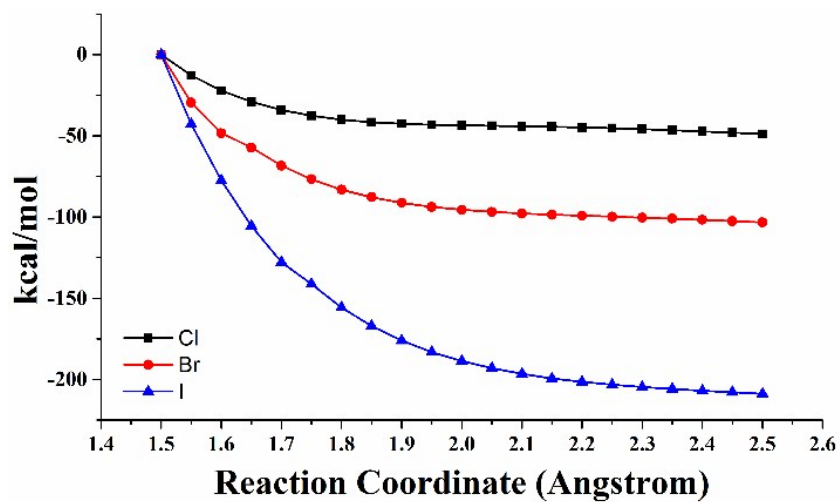


Figure S2 Flexible scanning the potential energy changes along reaction distances (X-C18) in COUMC system. Where X represents halogen anions (Cl<sup>-</sup>, Br<sup>-</sup>, and I<sup>-</sup>). This result indicates that COUMC is not intend to bind other halogen anions.

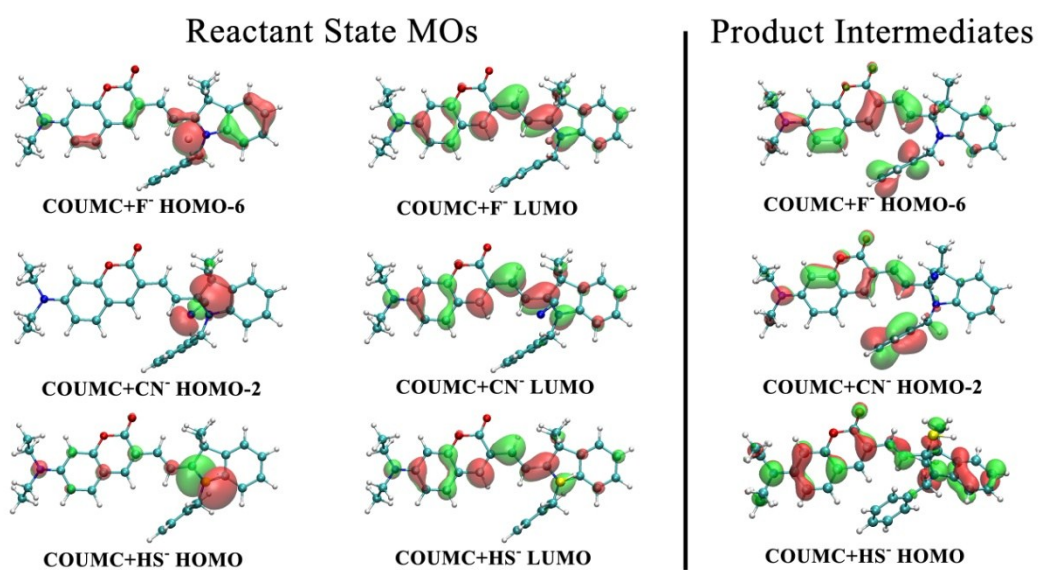


Figure S3 Geometries and Involved MOs for COUMC reacting with anions F<sup>-</sup>, CN<sup>-</sup>, and HS<sup>-</sup>.

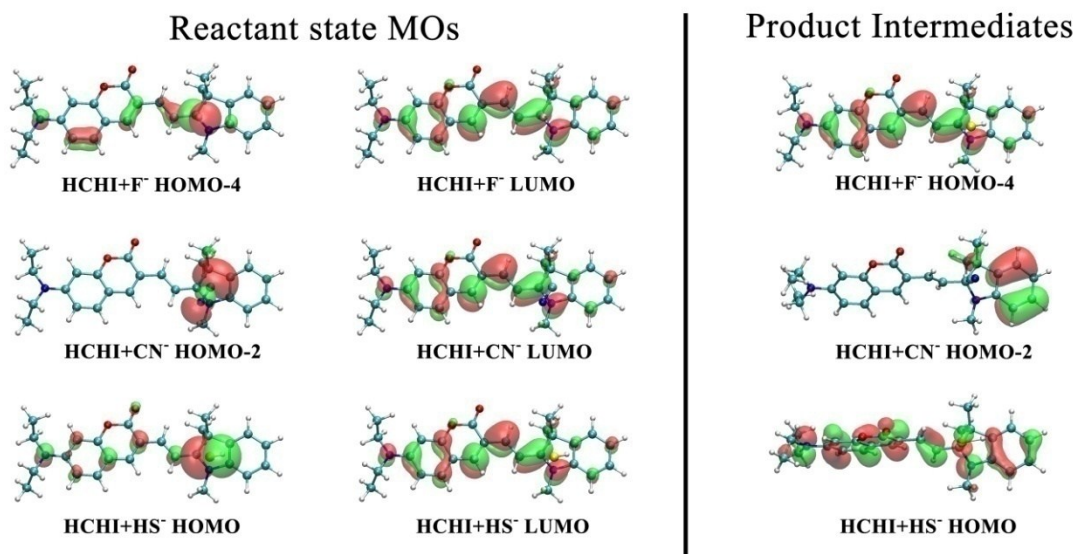


Figure S4 Geometries and involved MOs for HCHI reacting with anions F<sup>-</sup>, CN<sup>-</sup>, and HS<sup>-</sup>.

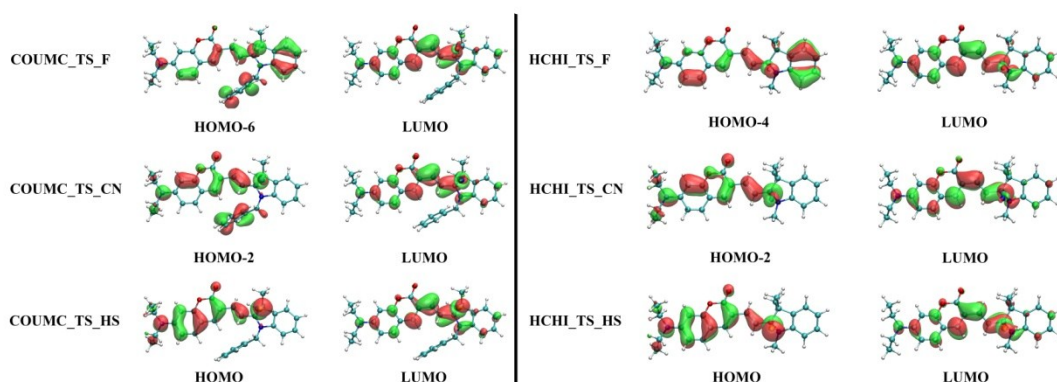


Figure S5 Geometries and involved MOs of TS states for COUMC/HCHI reacting with anions F<sup>-</sup>, CN<sup>-</sup>, and HS<sup>-</sup>.

Table S2 Reaction involved MOs in terms of a percentage contribution from each part for a single COUMC/HCHI and the corresponding reaction intermediates and product intermediates.

System	MO		Anion	BP	SP	SB
<b>COUMC</b>	HOMO		/	87.4	12.0	0.6
	LUMO		/	66.3	32.7	1.0
<b>COUMC+HS<sup>-</sup></b>	HOMO	REA	81.8	20.8	-2.6	0.0
		PRO	0.9	91.4	7.3	0.4
<b>COUMC+CN<sup>-</sup></b>	HOMO-2	REA	95.0	0.5	3.9	0.6
		PRO	0.0	45.4	3.4	51.2
<b>COUMC+F<sup>-</sup></b>	HOMO-6	REA	60.1	16.1	19.4	4.4
		PRO	0.6	62.3	6.9	30.2
<b>HCHI</b>	HOMO		/	87.8	12.2	0.0
	LUMO		/	66.8	33.2	0.0
<b>HCHI+HS<sup>-</sup></b>	HOMO	REA	88.6	10.1	10.3	0.0
		PRO	4.4	71.6	22.7	1.3
<b>HCHI+CN<sup>-</sup></b>	HOMO-2	REA	94.4	1.6	3.6	0.4
		PRO	1.0	92.7	6.1	0.3
<b>HCHI+F<sup>-</sup></b>	HOMO-4	REA	69.4	22.4	8.2	0.0
		PRO	0.1	96.1	3.3	0.5

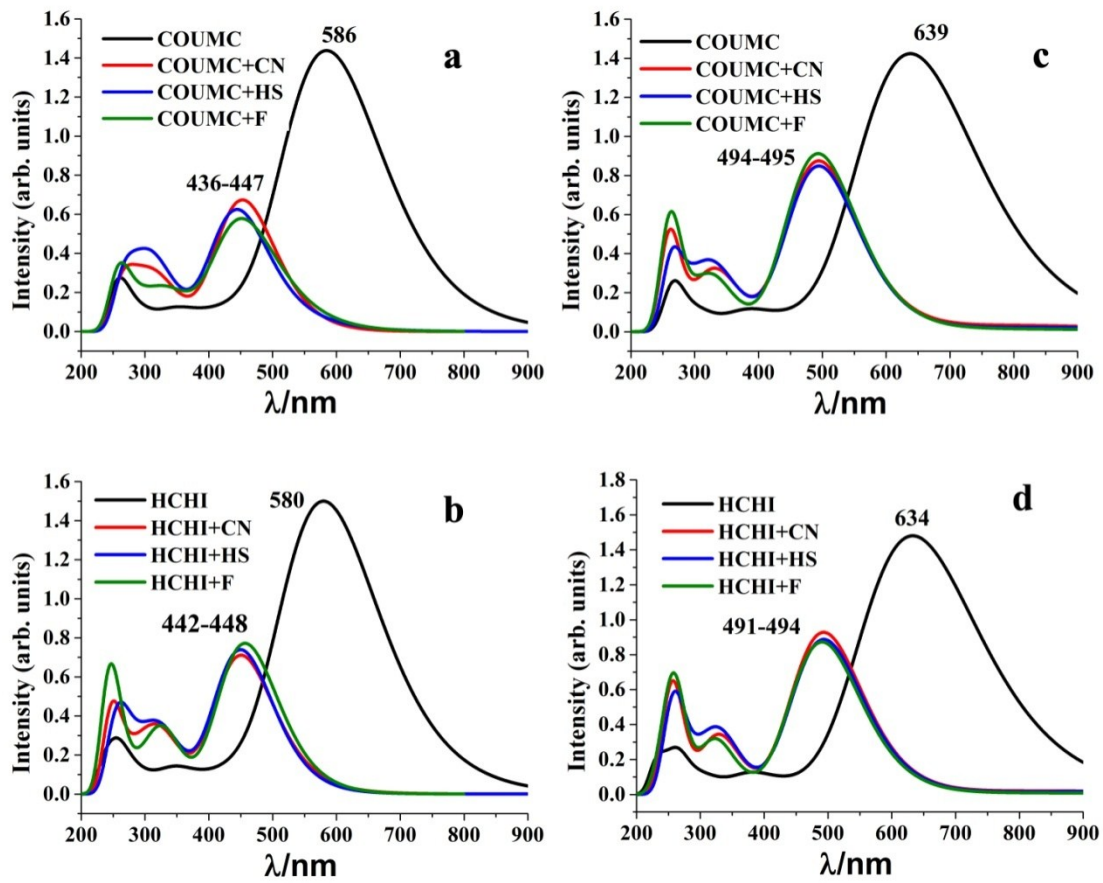
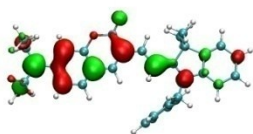


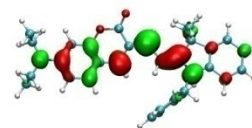
Figure S6 The computed absorption spectra for COUMC (a) and HCHI (b). The computed emission spectra for COUMC (c) and HCHI (d).

## Excitation

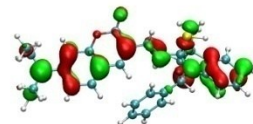
COUMC



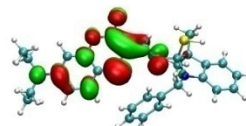
586 nm  
HOMO to LUMO



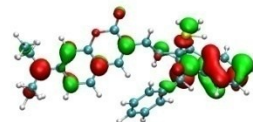
COUMC\_HS



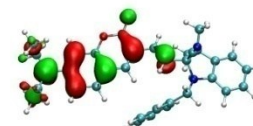
436 nm



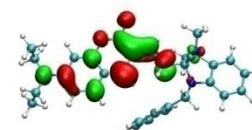
HOMO\_1 & HOMO to LUMO



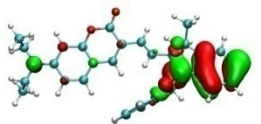
COUMC\_CN



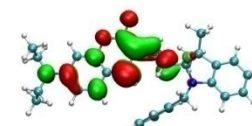
447 nm  
HOMO to LUMO



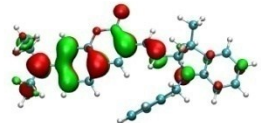
COUMC\_F



439 nm



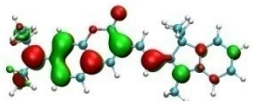
HOMO\_1 & HOMO to LUMO



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## Excitation

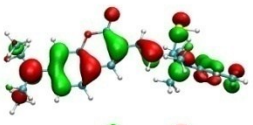
HCHI



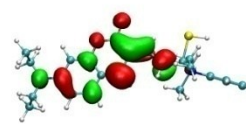
580 nm  
HOMO to LUMO



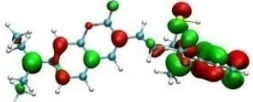
HCHI\_HS



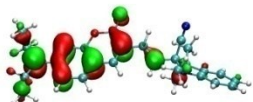
443 nm



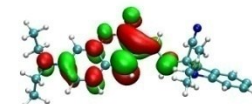
HOMO\_1 & HOMO to LUMO



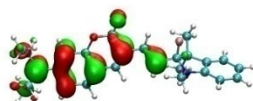
HCHI\_CN



442 nm  
HOMO to LUMO



HCHI\_F



448 nm  
HOMO to LUMO

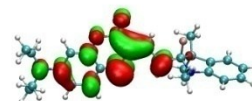
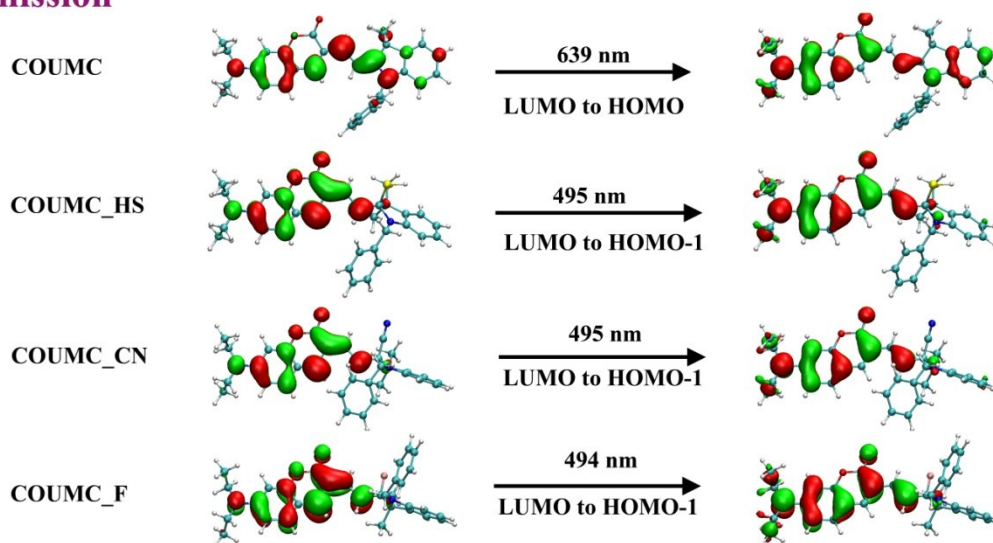


Figure S7 List of excitations.

## Emission



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## Emission

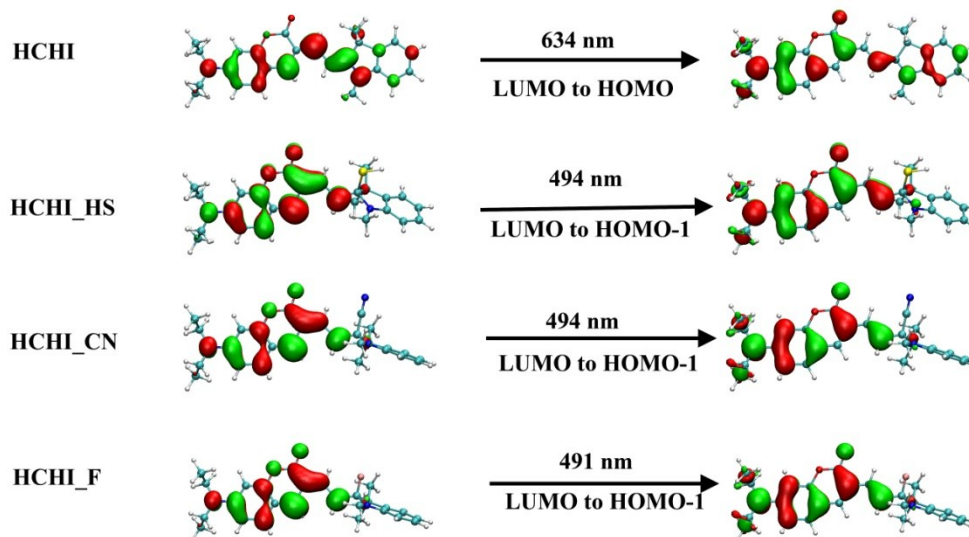


Figure S8 List of emissions



Table S3 MO contributions from each group

<b>Excitation</b>				
<b>Systems</b>	<b>MOs</b>	<b>BP</b>	<b>SP</b>	<b>Anion</b>
COUMC	LUMO	64.6%	34.4%	-
	HOMO	84.5%	14.8%	-
COUMC_HS <sup>-</sup>	LUMO	97.9%	1.3%	0.1%
	HOMO	59.5%	34.1%	4.7%
	HOMO-1	39.5%	52.0%	5.6%
COUMC_CN <sup>-</sup>	LUMO	99.0%	-0.6%	0.9%
	HOMO	98.4%	0.7%	0.6%
COUMC_F <sup>-</sup>	LUMO	95.1%	4.2%	0.0%
	HOMO	88.9%	10.2%	0.3%
	HOMO-1	11.4%	81.9%	2.3%
HCHI	LUMO	64.7%	33.8%	-
	HOMO	85.0%	14.3%	-
HCHI_HS <sup>-</sup>	LUMO	96.7%	2.1%	1.0%
	HOMO	70.7%	23.3%	4.7%
	HOMO-1	28.9%	61.6%	5.8%
HCHI_CN <sup>-</sup>	LUMO	97.5%	2.0%	0.1%
	HOMO	93.2%	6.1%	0.3%
HCHI_F <sup>-</sup>	LUMO	97.9%	1.7%	0.0%
	HOMO	96.4%	3.1%	0.2%
<b>Emission</b>				
<b>System</b>	<b>MOs</b>	<b>BP</b>	<b>SP</b>	<b>Anion</b>
COUMC	LUMO	63.1%	35.4%	-
	HOMO	80.3%	18.7%	-
COUMC_HS <sup>-</sup>	LUMO	97.1%	1.6%	0.7%
	HOMO-1	94.5%	4.7%	0.3%
COUMC_CN <sup>-</sup>	LUMO	96.8%	2.7%	0.1%
	HOMO-1	93.9%	5.2%	0.0%
COUMC_F <sup>-</sup>	LUMO	89.0%	1.7%	0.1%
	HOMO-1	90.1%	3.4%	0.0%
HCHI	LUMO	63.4%	35.0%	-
	HOMO-1	80.2%	18.9%	-
HCHI_HS <sup>-</sup>	LUMO	97.1%	1.6%	0.2%
	HOMO-1	95.4%	3.5%	0.1%
HCHI_CN <sup>-</sup>	LUMO	96.7%	1.9%	0.3%
	HOMO-1	96.6%	2.7%	0.2%
HCHI_F <sup>-</sup>	LUMO	97.9%	0.6%	0.1%
	HOMO-1	96.9%	1.2%	0.2%

**Appendix: List of coordinates**

**Coordinates for COUMC**

**Coordinates for COUMC\_HS<sup>-</sup> TS**

**Coordinates for COUMC\_CN<sup>-</sup> TS**

**Coordinates for COUMC\_F<sup>-</sup> TS**

**Coordinates for HCHI**

**Coordinates for HCHI\_HS<sup>-</sup> TS**

**Coordinates for HCHI\_CN<sup>-</sup> TS**

**Coordinates for HCHI\_F<sup>-</sup> TS**

**Coordinates for COUMC\_HS<sup>-</sup> Reactant Complex**

**Coordinates for COUMC\_CN<sup>-</sup> Reactant Complex**

**Coordinates for COUMC\_F<sup>-</sup> Reactant Complex**

**Coordinates for HCHI\_HS<sup>-</sup> Reactant Complex**

**Coordinates for HCHI\_CN<sup>-</sup> Reactant Complex**

**Coordinates for HCHI\_F<sup>-</sup> Reactant Complex**

**Coordinates for COUMC**

C	0.70858500	-1.37055800	0.03235100
C	-0.71095700	-1.20329900	0.03499800
C	-1.49853300	-2.35401800	0.46911500
C	-1.36324600	-0.03946900	-0.32272700
C	-3.49968800	-1.06172700	0.13236000
C	-2.75543300	0.06169700	-0.28365700
C	-3.48563600	1.22356000	-0.63212200
H	-2.94041900	2.10717000	-0.94495700
C	-5.59377900	0.10235000	-0.15580200
C	-4.87024500	-1.06256600	0.19975400
H	-0.79617600	0.83166800	-0.63489800
H	1.04051000	-2.32500400	0.42091000
H	-5.36288600	-1.97195000	0.50950500
O	-2.86233900	-2.21037400	0.48484600
O	-1.06036600	-3.42517300	0.81470600
C	1.62377400	-0.46151300	-0.40374100
H	1.27942400	0.48031800	-0.80992000
C	3.02438500	-0.65350900	-0.34564000
C	3.80892500	-1.82618800	0.23292600
C	3.54269800	-3.13291300	-0.53908900
H	3.69737300	-2.99020400	-1.61029100
H	4.24132300	-3.89527900	-0.18915200
H	2.53068900	-3.50469500	-0.37863600

C	3.54187500	-1.97988400	1.74356900
H	2.52165400	-2.30799400	1.94340200
H	4.22590300	-2.72802700	2.14851000
H	3.71309400	-1.03623400	2.26575000
C	5.22852700	-1.36220800	0.00552900
C	5.21567700	-0.11736600	-0.60249100
C	6.43308800	-1.96759500	0.31236800
C	6.37032400	0.57869500	-0.91584400
C	7.61302600	-1.29352100	0.00090300
H	6.46492400	-2.94179300	0.78699200
C	7.57902000	-0.03784700	-0.60181700
H	6.35644600	1.55714200	-1.37834600
H	8.56794100	-1.75013800	0.23192000
H	8.50671200	0.47261600	-0.83076500
N	3.86480600	0.26452300	-0.80508900
C	3.47039800	1.53909800	-1.40589200
H	2.73854200	1.33937700	-2.18961500
H	4.35007900	1.94656100	-1.90209400
C	2.92441700	2.51988900	-0.38976500
C	1.85756900	3.34388500	-0.73908100
C	3.48238000	2.62345500	0.88313900
C	1.35560500	4.26690100	0.17221900
H	1.41033700	3.26019900	-1.72448300
C	2.97882000	3.54367400	1.79454800
H	4.30917000	1.98275000	1.17296900
C	1.91544200	4.36847700	1.44060400
H	0.52298400	4.90163500	-0.10874100
H	3.41928600	3.61710800	2.78224400
H	1.52318500	5.08476100	2.15341700
C	-4.84636600	1.25312500	-0.57366100
H	-5.35738300	2.16892400	-0.83103000
N	-6.94021800	0.13264200	-0.09989400
C	-7.71961300	-0.99459600	0.41073900
H	-7.19966300	-1.44317400	1.25905500
H	-8.64797500	-0.58327000	0.81168400
C	-8.02698800	-2.03509700	-0.66130000
H	-8.58506700	-1.58469500	-1.48582100
H	-7.11078800	-2.46977900	-1.06741600
H	-8.63136100	-2.84044900	-0.23808500
C	-7.71730100	1.28632000	-0.55417200
H	-7.24260000	1.72467900	-1.43297900
H	-8.68158200	0.90373300	-0.89457400
C	-7.92295800	2.32923100	0.53889500
H	-6.96918500	2.74056200	0.87761300

H	-8.53768600	3.14965100	0.16196000
H	-8.43005300	1.88915400	1.40104600

**Coordinates for COUMC\_HS- TS**

C	-0.80421900	-1.47294100	-0.22941700
C	0.64563800	-1.32893200	-0.16645400
C	1.45005700	-2.52802300	-0.35519200
C	1.26774300	-0.12480300	-0.00962000
C	3.43595000	-1.18444500	-0.14957700
C	2.67933500	-0.01748200	0.01392700
C	3.38841800	1.18814600	0.16996700
H	2.83048100	2.11115800	0.28589000
C	5.52120400	0.02209300	0.01019200
C	4.81512300	-1.18949800	-0.15023100
H	0.68037500	0.78595200	0.07304200
H	-1.17093200	-2.30118200	-0.82317500
H	5.31846600	-2.13866300	-0.26188300
O	2.81209400	-2.38546900	-0.32240900
O	1.02004600	-3.64537700	-0.53535900
C	-1.63584600	-0.61531900	0.37806100
H	-1.20781600	0.13251200	1.03228300
C	-3.07270200	-0.53465100	0.20946200
C	-3.94274200	-1.38703100	-0.72038400
C	-4.00747800	-2.88741100	-0.44826500
H	-4.43446600	-3.08404600	0.53269400
H	-4.62581200	-3.35932200	-1.21613400
H	-3.01895300	-3.34738700	-0.48979700
C	-3.45501400	-1.13560600	-2.17703700
H	-2.49702300	-1.61968000	-2.36631700
H	-4.19388200	-1.55079800	-2.86486700
H	-3.35306400	-0.06875900	-2.38598500
C	-5.26656400	-0.67579600	-0.57387200
C	-5.05001500	0.55678300	0.03205100
C	-6.53214800	-1.02598700	-1.00398300
C	-6.06778700	1.47699700	0.21959100
C	-7.57663700	-0.12082600	-0.81229600
H	-6.71191300	-1.98330700	-1.48043400
C	-7.34233000	1.11408400	-0.21368600
H	-5.90447800	2.44026200	0.68530900
H	-8.57883200	-0.37923400	-1.13357700
H	-8.16235800	1.80905500	-0.07572700
N	-3.68738900	0.65121400	0.38461100
C	-3.12495000	1.75879300	1.14416000

H	-2.84965500	1.37396900	2.13154300
H	-3.91878300	2.48852600	1.29894200
C	-1.94151400	2.43020900	0.47819400
C	-0.92563100	2.95737400	1.27331400
C	-1.84112300	2.53030200	-0.90735100
C	0.17673600	3.57493100	0.69216100
H	-0.98841300	2.87062300	2.35335100
C	-0.73388000	3.13681400	-1.49016100
H	-2.62384100	2.12145100	-1.53713000
C	0.27850900	3.66097900	-0.69234500
H	0.96186600	3.97599200	1.32332400
H	-0.66136800	3.19948900	-2.56995000
H	1.14396100	4.12879100	-1.14763100
C	4.75753000	1.21799800	0.17060800
H	5.25314000	2.17217900	0.27551800
N	6.87988500	0.05251300	0.00555500
C	7.67561200	-1.13518300	-0.28425000
H	7.17348600	-1.73325300	-1.04747500
H	8.60907100	-0.79437000	-0.73809000
C	7.97748600	-1.97222000	0.95558600
H	8.52320200	-1.38015600	1.69470500
H	7.05834500	-2.33580500	1.42102600
H	8.59178000	-2.83520400	0.68751100
C	7.63214400	1.27094400	0.28769300
H	7.11458600	1.85298100	1.05220800
H	8.57954900	0.96547300	0.73793900
C	7.89691900	2.11372000	-0.95643200
H	6.96193800	2.44104000	-1.41743600
H	8.48049400	2.99988300	-0.69526800
H	8.45943800	1.53971900	-1.69722500
S	-3.54037900	-1.49613200	2.61497200
H	-4.86404300	-1.28316400	2.48777400

**Coordinates for COUMC\_CN TS**

C	-0.86453300	-1.45312200	-0.14904600
C	0.58524000	-1.31824700	-0.08954700
C	1.37920800	-2.51149500	-0.34718900
C	1.21704600	-0.12568200	0.11483800
C	3.37542900	-1.18707300	-0.12058800
C	2.62811000	-0.02644400	0.11833500
C	3.34644700	1.16671700	0.32431600
H	2.79560400	2.08451400	0.50012200
C	5.46891900	0.00188500	0.05625500

C	4.75373700	-1.19719300	-0.15285300
H	0.63798000	0.78354300	0.25099400
H	-1.23181600	-2.28131800	-0.74197600
H	5.25019500	-2.14111100	-0.32371100
O	2.74227400	-2.37569400	-0.33740000
O	0.94022900	-3.61791600	-0.56757700
C	-1.69849700	-0.59203000	0.44737100
H	-1.28289100	0.16542200	1.09910300
C	-3.13714100	-0.52058900	0.26068400
C	-4.01235100	-1.46369100	-0.56683200
C	-4.03327200	-2.92894800	-0.14156700
H	-4.44754000	-3.03530900	0.85949500
H	-4.64857900	-3.49687800	-0.84348700
H	-3.03255100	-3.36419700	-0.15164000
C	-3.57405000	-1.34728300	-2.05483800
H	-2.61586700	-1.83409500	-2.23388900
H	-4.32782500	-1.83814000	-2.67289500
H	-3.49993600	-0.30447200	-2.36950100
C	-5.34071500	-0.75567800	-0.44668500
C	-5.12033400	0.53352800	0.02557600
C	-6.61405600	-1.15782400	-0.80295900
C	-6.14396000	1.45606800	0.15969600
C	-7.66331300	-0.24898800	-0.66450700
H	-6.79602400	-2.15780800	-1.18066300
C	-7.42685700	1.03941400	-0.19294400
H	-5.97959600	2.46085100	0.52686600
H	-8.67196800	-0.54738700	-0.92512100
H	-8.25166400	1.73513400	-0.09265500
N	-3.74502400	0.67848500	0.31622900
C	-3.19179900	1.84633700	0.98775300
H	-2.97538600	1.57257100	2.02719700
H	-3.97430600	2.60332000	1.01947300
C	-1.96286800	2.43053700	0.32144200
C	-1.00027800	3.05900300	1.10898900
C	-1.77340900	2.36058600	-1.05665100
C	0.13715800	3.60983800	0.52779700
H	-1.13318100	3.10910300	2.18495800
C	-0.63032600	2.89883000	-1.63719400
H	-2.51270000	1.86991400	-1.67998800
C	0.32819200	3.52560100	-0.84722700
H	0.87931100	4.09308300	1.15331300
H	-0.48767400	2.82470000	-2.70917600
H	1.22108700	3.94104500	-1.30022800
C	4.71499000	1.19044700	0.29903500

H	5.21809400	2.13507600	0.44542500
N	6.82645900	0.02849300	0.02170800
C	7.61102900	-1.14545300	-0.34569500
H	7.09336000	-1.69804500	-1.13256000
H	8.53852800	-0.78365300	-0.79533300
C	7.92867300	-2.05062000	0.84123400
H	8.48552900	-1.50151300	1.60484600
H	7.01594300	-2.43936300	1.29883000
H	8.53797700	-2.89748200	0.51658900
C	7.58990800	1.22529300	0.36246000
H	7.09482800	1.75575300	1.17809600
H	8.54803300	0.88886800	0.76530400
C	7.82409700	2.14914500	-0.82892500
H	6.87951800	2.51642100	-1.23725600
H	8.42528600	3.00974000	-0.52573800
H	8.35693900	1.62322800	-1.62537100
C	-3.66683000	-1.20559400	2.37264800
N	-3.76290600	-1.34216200	3.52653500

#### Coordinates for COUMC\_F-TS

C	-0.80885200	-1.42259300	-0.17933300
C	0.63721900	-1.27031100	-0.14794400
C	1.43393000	-2.45898100	-0.42318100
C	1.26859200	-0.07881400	0.07285600
C	3.42774200	-1.13968800	-0.15335500
C	2.67826800	0.02102500	0.08340800
C	3.39708900	1.21097300	0.31102100
H	2.84750600	2.13004000	0.48387700
C	5.52078600	0.03959400	0.08205700
C	4.80569500	-1.15454900	-0.15556500
H	0.68783400	0.82728700	0.22391800
H	-1.17273800	-2.27641400	-0.73682800
H	5.30186900	-2.09895100	-0.32391600
O	2.79664000	-2.32374300	-0.39605400
O	0.99808700	-3.56108500	-0.66832400
C	-1.65372100	-0.57489000	0.42870200
H	-1.24282300	0.21547100	1.04174700
C	-3.08818800	-0.59208200	0.31641300
C	-3.95927900	-1.57136800	-0.46108100
C	-3.86961400	-3.02838400	-0.00630500
H	-4.06465800	-3.09012600	1.06225900
H	-4.60119600	-3.61985700	-0.56220300
H	-2.88278900	-3.44971800	-0.20497600

C	-3.62718300	-1.43691300	-1.97090500
H	-2.64482200	-1.84798800	-2.20299400
H	-4.37489500	-1.99253500	-2.54009100
H	-3.65500900	-0.39371000	-2.29399900
C	-5.32277000	-0.96104800	-0.24028100
C	-5.17220500	0.28177200	0.35861300
C	-6.58091800	-1.41194600	-0.59137600
C	-6.24305200	1.11796200	0.62099900
C	-7.68013900	-0.59511100	-0.32402600
H	-6.71475700	-2.37866900	-1.06402400
C	-7.50963000	0.65274900	0.26967300
H	-6.12511300	2.08987700	1.08252000
H	-8.67663200	-0.93367200	-0.58236300
H	-8.37377100	1.27596400	0.46737300
N	-3.79597300	0.48876900	0.61472500
C	-3.26005900	1.66717100	1.29020700
H	-2.77410200	1.33396100	2.20906700
H	-4.10552500	2.28655500	1.58673500
C	-2.30920500	2.46484000	0.42306600
C	-1.17248300	3.03600400	0.99086500
C	-2.55136900	2.63726100	-0.93795300
C	-0.28597300	3.76787700	0.20760400
H	-0.97070800	2.89668400	2.04829400
C	-1.66349400	3.36363500	-1.72257600
H	-3.43208900	2.19546200	-1.39258800
C	-0.52744600	3.92977900	-1.15210200
H	0.59818300	4.20284500	0.65971600
H	-1.85853900	3.48733100	-2.78175700
H	0.16611700	4.49323200	-1.76571000
C	4.76545100	1.23025600	0.31329400
H	5.26847000	2.17234700	0.47544000
N	6.87789100	0.05881300	0.08576200
C	7.66568300	-1.12042700	-0.25850400
H	7.17054500	-1.66723700	-1.06365500
H	8.61019900	-0.76452400	-0.67611100
C	7.93598700	-2.03014400	0.93651400
H	8.47147600	-1.48720600	1.71959700
H	7.00526300	-2.41186000	1.36283400
H	8.54851100	-2.88161300	0.63063700
C	7.63949200	1.25214400	0.44345800
H	7.12570700	1.78982000	1.24239900
H	8.58342800	0.91078500	0.87439000
C	7.91286900	2.16751000	-0.74603300
H	6.98216100	2.53903600	-1.18146800



H	8.51191100	3.02542400	-0.43140700
H	8.46325300	1.63296100	-1.52456300
F	-3.26920600	-1.43614100	2.41112100

### Coordinates for HCHI

C	1.20073100	-0.59168000	0.05545600
C	-0.22901800	-0.53584800	0.03888800
C	-0.92277500	-1.81759100	0.13591200
C	-0.97142400	0.62427200	-0.05110000
C	-3.02059000	-0.64508100	0.03874300
C	-2.36926100	0.60176900	-0.05301000
C	-3.19130900	1.75129900	-0.13622100
H	-2.71979300	2.72548600	-0.20141600
C	-5.20251500	0.38276600	-0.03569300
C	-4.38715000	-0.77275800	0.04406700
H	-0.47474000	1.58689800	-0.11791200
H	1.59569900	-1.59162800	0.18204400
H	-4.80502100	-1.76703000	0.09531600
O	-2.29317400	-1.79121200	0.12218300
O	-0.40053300	-2.90323100	0.22479500
C	2.05822800	0.45706400	-0.07162500
H	1.66415400	1.45494300	-0.21496200
C	3.46953900	0.32850300	-0.03786200
C	4.31237100	-0.93158400	0.13058200
C	4.09184900	-1.92970400	-1.02273800
H	4.21980600	-1.44193200	-1.99101800
H	4.83061800	-2.72917400	-0.94030200
H	3.10053000	-2.38164300	-0.98792700
C	4.07962400	-1.58327500	1.50831000
H	3.08360700	-2.01922500	1.58914400
H	4.81112700	-2.38144200	1.64787000
H	4.20788100	-0.85414200	2.31079900
C	5.70592800	-0.35388900	0.05883500
C	5.62865400	1.01847600	-0.11612300
C	6.93998100	-0.97185900	0.14204800
C	6.74856200	1.82535000	-0.22184200
C	8.08525700	-0.18316800	0.04349000
H	7.02054300	-2.04400700	0.28145900
C	7.98752500	1.19489500	-0.13750000
H	6.68678500	2.89579200	-0.36707100
H	9.06231700	-0.64681000	0.10764800
H	8.88900300	1.79074000	-0.21494700
N	4.25841500	1.38485300	-0.15966600

C	3.79659500	2.75867900	-0.32439900
H	3.30458000	2.87358800	-1.29056500
H	4.64846700	3.42950000	-0.27816800
C	-4.55074500	1.65641400	-0.12849800
H	-5.13445000	2.56381500	-0.17451700
N	-6.54777900	0.29091000	-0.02145500
C	-7.23327800	-0.98671700	0.16594200
H	-6.67393100	-1.59807600	0.87564600
H	-8.19013500	-0.76918000	0.64458600
C	-7.45993500	-1.73147700	-1.14572900
H	-8.06704500	-1.13173700	-1.82825600
H	-6.51222100	-1.95766800	-1.63987300
H	-7.98315300	-2.67159400	-0.95765400
C	-7.41501000	1.45558400	-0.19965700
H	-6.97232000	2.13450500	-0.92992300
H	-8.34112700	1.09372100	-0.65047100
C	-7.71702900	2.17507900	1.11036700
H	-6.80486600	2.56730000	1.56595800
H	-8.39862900	3.00938000	0.93000300
H	-8.18979700	1.49476000	1.82301100
H	3.10849400	3.01694500	0.47966100

#### Coordinates for HCHI\_HS

C	-0.94552500	-0.73091800	-0.01830900
C	0.50822500	-0.63831800	-0.04560000
C	1.22785300	-1.88786600	-0.27243900
C	1.22002100	0.51057500	0.14310800
C	3.30433900	-0.68224700	-0.13614500
C	2.63539200	0.52538200	0.09971300
C	3.43410600	1.67110300	0.28176200
H	2.94937400	2.62526500	0.45792900
C	5.47296000	0.36991500	-0.00955900
C	4.67833400	-0.78218900	-0.19154600
H	0.70554800	1.44487100	0.34586600
H	-1.32677400	-1.73740100	0.09246700
H	5.11024300	-1.75920500	-0.35164700
O	2.59503900	-1.83367500	-0.30758300
O	0.72181100	-2.97545600	-0.43626300
C	-1.78793300	0.30685800	-0.12596800
H	-1.38779000	1.30494800	-0.25863100
C	-3.23728700	0.22252700	-0.05528000
C	-4.08226000	-1.06373900	-0.04957200
C	-3.93186100	-2.02565900	1.12641400

H	-4.19203200	-1.53697300	2.06286200
H	-4.59440100	-2.88023700	0.96648000
H	-2.91515500	-2.41106800	1.21238000
C	-3.79515500	-1.81201200	-1.38267600
H	-2.80447400	-2.26765000	-1.38060100
H	-4.53730100	-2.60377700	-1.50158500
H	-3.86753300	-1.13847800	-2.23945800
C	-5.46659200	-0.46903200	-0.16309400
C	-5.35201600	0.86283100	-0.54567000
C	-6.71321100	-1.04530800	-0.01538000
C	-6.45944600	1.66029600	-0.78360200
C	-7.84442200	-0.26056600	-0.24703400
H	-6.81572800	-2.08465500	0.27667700
C	-7.71441100	1.07235200	-0.62678000
H	-6.37309800	2.70102200	-1.06867700
H	-8.83130000	-0.69176200	-0.12674300
H	-8.60211800	1.66985100	-0.79905600
N	-3.98660600	1.19659700	-0.61431400
C	-3.51737900	2.54001900	-0.88952500
H	-3.28581400	3.04797300	0.05159300
H	-4.29295700	3.08687700	-1.41957200
C	4.80083300	1.60713600	0.22712100
H	5.36562400	2.51991800	0.34967400
N	6.82905100	0.30655300	-0.05955200
C	7.52915200	-0.92277400	-0.41440600
H	6.96947600	-1.44958300	-1.19012500
H	8.47624700	-0.63253500	-0.87500300
C	7.79179300	-1.83164200	0.78327900
H	8.39839200	-1.31549700	1.53181000
H	6.85743900	-2.14156500	1.25711700
H	8.33001600	-2.72783300	0.46564900
C	7.67400300	1.45325800	0.25978000
H	7.21513300	2.03397800	1.06197900
H	8.60554600	1.05912100	0.67274300
C	7.97408200	2.33269700	-0.95026600
H	7.05762700	2.75702500	-1.36737100
H	8.63534700	3.15424800	-0.66440000
H	8.46840000	1.75313500	-1.73420200
S	-3.30552600	1.03990900	2.37400400
H	-4.64954200	1.12455700	2.39074500
H	-2.63345900	2.51181500	-1.52507600

**Coordinates for HCHI\_CN<sup>-</sup>**

C	1.00328900	0.68029000	-0.07774400
C	-0.44981300	0.59752300	-0.08838500
C	-1.16141300	1.86232100	-0.24623700
C	-1.17061900	-0.55497700	0.04869800
C	-3.24654100	0.66934100	-0.12505400
C	-2.58401800	-0.55547300	0.03368600
C	-3.38940100	-1.70406400	0.16961600
H	-2.90929500	-2.66945100	0.28728700
C	-5.42084300	-0.37231300	-0.01259500
C	-4.61963500	0.78251900	-0.14752000
H	-0.66419900	-1.50606500	0.18028200
H	1.38479000	1.69250500	-0.08486900
H	-5.04634800	1.76950200	-0.24938500
O	-2.53000900	1.82090000	-0.25464100
O	-0.65031500	2.95227300	-0.37221700
C	1.85023900	-0.35865700	-0.06446100
H	1.46274200	-1.36978800	-0.05292800
C	3.30136500	-0.24797900	-0.02430400
C	4.12772300	1.04437300	-0.11515900
C	3.94125900	2.08035900	0.99057500
H	4.18465800	1.65602700	1.96318700
H	4.60562000	2.92602100	0.79659600
H	2.92239700	2.46752100	1.02449800
C	3.85502500	1.68783200	-1.50284900
H	2.86130900	2.13384500	-1.55307700
H	4.59203400	2.47563000	-1.66910400
H	3.94843800	0.95307700	-2.30537100
C	5.51873600	0.45538800	-0.15943600
C	5.42076600	-0.90394200	-0.43271800
C	6.75951100	1.05293300	-0.04619100
C	6.53626200	-1.71064200	-0.58560300
C	7.89860700	0.25998800	-0.19376300
H	6.85144200	2.11389300	0.15826800
C	7.78440300	-1.10187400	-0.45972000
H	6.45969200	-2.77196300	-0.78456200
H	8.88056300	0.70756700	-0.09512400
H	8.67899600	-1.70437100	-0.56577100
N	4.05802800	-1.25687400	-0.50043100
C	3.62553600	-2.63761200	-0.58428000
H	3.52551700	-3.05673300	0.42342700
H	4.36217500	-3.20813800	-1.14471100
C	-4.75535100	-1.62641300	0.14620200
H	-5.32630200	-2.53941700	0.23235100
N	-6.77565300	-0.29664400	-0.03511100

C	-7.47183300	0.95702500	-0.30404900
H	-6.91772400	1.52723500	-1.05215500
H	-8.42665500	0.70205500	-0.76947300
C	-7.71073200	1.78938000	0.95260200
H	-8.31387400	1.23186400	1.67366200
H	-6.76705300	2.05788700	1.43322700
H	-8.24279400	2.70970700	0.70052200
C	-7.62510100	-1.45290500	0.23616000
H	-7.16119400	-2.07740100	1.00172700
H	-8.54841000	-1.07375700	0.67998400
C	-7.94655200	-2.26694100	-1.01340600
H	-7.03873100	-2.67611600	-1.46309100
H	-8.61038500	-3.09727400	-0.76091200
H	-8.44636900	-1.64431200	-1.75982000
C	3.51053500	-0.72112600	2.14788100
N	3.42852000	-1.22227600	3.19699200
H	2.67687000	-2.71049200	-1.11161400

#### Coordinates for HCHI\_F-

C	-1.07151800	-0.64658800	-0.14271200
C	0.38029100	-0.56869900	-0.14775100
C	1.08990900	-1.82639200	-0.36233300
C	1.10400600	0.57487300	0.04550000
C	3.17756800	-0.64747400	-0.16333300
C	2.51657400	0.57142700	0.04321100
C	3.32342000	1.70979800	0.24370900
H	2.84443200	2.67063500	0.39744500
C	5.35291200	0.37903700	0.03561700
C	4.55030600	-0.76466300	-0.17008900
H	0.59929300	1.52101600	0.21371000
H	-1.45748000	-1.65324600	-0.23212500
H	4.97559700	-1.74720500	-0.31239500
O	2.45910300	-1.78854300	-0.35766100
O	0.57756100	-2.90736400	-0.54578400
C	-1.91507300	0.39303500	-0.03787200
H	-1.52363700	1.39747500	0.05684800
C	-3.35317600	0.28213800	0.00072100
C	-4.19536200	-0.99404000	-0.04599400
C	-3.94904300	-1.99744100	1.08057600
H	-4.03609900	-1.49501400	2.04162600
H	-4.68499000	-2.80186800	1.00528100
H	-2.95824100	-2.44862900	1.00847000
C	-4.00561800	-1.65933800	-1.43520500

H	-3.01323000	-2.09796500	-1.54280100
H	-4.74414000	-2.45660900	-1.54040600
H	-4.15869800	-0.94000300	-2.24302800
C	-5.58491900	-0.40210200	-0.01299900
C	-5.49292700	0.97027600	-0.19400100
C	-6.82372700	-1.00182200	0.10461400
C	-6.60472600	1.79148800	-0.25567800
C	-7.96314400	-0.19636800	0.05099700
H	-6.91495800	-2.07358800	0.24221600
C	-7.85171500	1.17961400	-0.12754200
H	-6.52654800	2.86349700	-0.38455100
H	-8.94350100	-0.64671500	0.15313500
H	-8.74618200	1.79053700	-0.16288300
N	-4.12738700	1.32273200	-0.28406300
C	-3.69244500	2.70237000	-0.41306300
H	-3.58257600	3.15311800	0.57494200
H	-4.43412600	3.25259700	-0.98815300
C	4.68901600	1.62784800	0.23915200
H	5.26155200	2.53354500	0.37675900
N	6.70723500	0.29790700	0.03848800
C	7.40455800	-0.94544600	-0.27287000
H	6.87238600	-1.47237500	-1.06750400
H	8.37483700	-0.67307800	-0.69409500
C	7.59974500	-1.84351700	0.94537200
H	8.17955700	-1.32703000	1.71459900
H	6.64085900	-2.13437200	1.38062900
H	8.13834500	-2.75096400	0.66241200
C	7.55540100	1.43893000	0.37225400
H	7.07969600	2.03327200	1.15428200
H	8.46910200	1.03808600	0.81681400
C	7.90172500	2.30068100	-0.83808700
H	7.00331200	2.73063900	-1.28727000
H	8.56371800	3.11777000	-0.54154100
H	8.41261600	1.70601500	-1.59968700
F	-3.34953700	0.64623200	2.16032400
H	-2.74951000	2.75141300	-0.95223400

**Coordinates for COUMC\_HS<sup>-</sup> Reactant Complex**

C	-0.59352200	-1.28671200	-0.42889400
C	0.83234300	-1.16110600	-0.34400600
C	1.61629500	-2.31263800	-0.77962200
C	1.48721500	-0.02557500	0.08265600
C	3.62397400	-1.08244100	-0.28609700

C	2.88428000	0.04426700	0.12320400
C	3.61929700	1.17742600	0.54318300
H	3.07781200	2.06418200	0.85394800
C	5.72565600	0.02256800	0.14431700
C	4.99691900	-1.11438400	-0.28056700
H	0.92252800	0.85283100	0.38056500
H	-0.93444600	-2.17849200	-0.93947200
H	5.48493500	-2.02590500	-0.59165600
O	2.98135600	-2.20390300	-0.71115500
O	1.17306100	-3.35821100	-1.19206200
C	-1.48980900	-0.39524000	0.06758400
H	-1.12475800	0.46447400	0.61116500
C	-2.89434800	-0.48485700	-0.09868100
C	-3.70603800	-1.57020900	-0.79316800
C	-3.52512200	-2.94419700	-0.12270200
H	-3.70535700	-2.87542600	0.95199600
H	-4.24206400	-3.64472000	-0.55541600
H	-2.52414100	-3.34565600	-0.28258000
C	-3.38552300	-1.61645700	-2.30189000
H	-2.37284300	-1.97435700	-2.48854500
H	-4.08368900	-2.30020100	-2.78855200
H	-3.49645100	-0.62946600	-2.75604800
C	-5.10938600	-1.05245200	-0.58626800
C	-5.05931400	0.16053100	0.08275800
C	-6.32908600	-1.58506000	-0.96078100
C	-6.19218200	0.89008800	0.39989900
C	-7.48716800	-0.87430800	-0.64942800
H	-6.38867900	-2.53363400	-1.48239000
C	-7.41636000	0.34595000	0.01928000
H	-6.15142400	1.83950000	0.91753400
H	-8.45366700	-1.27541700	-0.93026200
H	-8.32765700	0.88407600	0.25094500
N	-3.70048400	0.46481000	0.35036900
C	-3.26662000	1.65877400	1.07906800
H	-2.73636700	1.32292500	1.97339900
H	-4.16454100	2.16800300	1.42442800
C	-2.41906100	2.58822000	0.23814300
C	-1.31655400	3.21504700	0.81423300
C	-2.72020300	2.82696300	-1.10095100
C	-0.52103900	4.07083400	0.06000800
H	-1.07138800	3.02425100	1.85429200
C	-1.92307000	3.67895500	-1.85605200
H	-3.57275600	2.33945800	-1.56322300
C	-0.82130600	4.30223200	-1.27760400

H	0.33881400	4.54764900	0.51657400
H	-2.16073600	3.85439600	-2.89901700
H	-0.19728600	4.96156900	-1.86990800
C	4.98267700	1.17649700	0.55750000
H	5.49892000	2.07186800	0.87043100
N	7.07530200	0.02422700	0.15563600
C	7.85388100	-1.10411900	-0.35196800
H	7.36086200	-1.52060700	-1.23218500
H	8.80617200	-0.70202100	-0.70344500
C	8.09563100	-2.17853300	0.70333300
H	8.62590600	-1.76066100	1.56256400
H	7.15431700	-2.60466000	1.05795900
H	8.70227400	-2.98481900	0.28499700
C	7.85204300	1.14940100	0.67546400
H	7.34942200	1.57117000	1.54711500
H	8.79489300	0.74008000	1.04375200
C	8.12062800	2.21943600	-0.37737700
H	7.18886400	2.65580800	-0.74473300
H	8.73121700	3.01915600	0.04788900
H	8.65706700	1.79475600	-1.22947400
S	-3.53130900	-1.13101300	3.62474300
H	-4.43463200	-1.08365800	2.62771800

**Coordinates for COUMC\_CN<sup>-</sup> Reactant Complex**

C	-0.68422200	-1.33230600	-0.31934900
C	0.74486800	-1.19713300	-0.25601200
C	1.53024300	-2.35773000	-0.66297600
C	1.39690800	-0.04541400	0.12333800
C	3.53660700	-1.10020200	-0.23689200
C	2.79572800	0.03402900	0.14510900
C	3.52843700	1.18364900	0.51907900
H	2.98558500	2.07707600	0.80772700
C	5.63722600	0.02910300	0.13170200
C	4.91036200	-1.12413600	-0.24820500
H	0.83035900	0.83990500	0.39681300
H	-1.02896300	-2.23495700	-0.80787900
H	5.39986300	-2.04249800	-0.53597800
O	2.89524600	-2.23874200	-0.61727400
O	1.08775600	-3.41937800	-1.03394200
C	-1.57215400	-0.43309100	0.17197500
H	-1.20004000	0.43370500	0.69848500
C	-2.98148100	-0.52385100	0.03250200
C	-3.80723600	-1.63576300	-0.59812600



C	-3.60747800	-2.97984000	0.12447400
H	-3.76246600	-2.85973700	1.19839700
H	-4.33232600	-3.69944200	-0.26161300
H	-2.60888600	-3.38461100	-0.04366100
C	-3.52212200	-1.74140600	-2.11123100
H	-2.51475700	-2.10867000	-2.30769800
H	-4.23269800	-2.44207100	-2.55397400
H	-3.64215700	-0.77218700	-2.60011200
C	-5.20528800	-1.10867000	-0.38151200
C	-5.13908800	0.13295300	0.23126300
C	-6.43323100	-1.65571600	-0.70439100
C	-6.26437900	0.87725300	0.54086000
C	-7.58400400	-0.93070900	-0.39820000
H	-6.50475900	-2.62594900	-1.18294900
C	-7.49732800	0.31795200	0.21383700
H	-6.21183300	1.84759400	1.01694500
H	-8.55690700	-1.34315200	-0.63747000
H	-8.40295900	0.86660700	0.44322900
N	-3.77454500	0.44768800	0.45206200
C	-3.32241700	1.67960800	1.10367000
H	-2.79247100	1.38748700	2.01352300
H	-4.21318700	2.22133900	1.41661900
C	-2.46800000	2.54610500	0.20468500
C	-1.34274100	3.17384300	0.73428500
C	-2.78200900	2.72645300	-1.14074900
C	-0.53711800	3.97156600	-0.07105000
H	-1.08779100	3.02793400	1.77931700
C	-1.97494800	3.52039100	-1.94707200
H	-3.65315600	2.23885600	-1.56721800
C	-0.85030300	4.14374700	-1.41461000
H	0.33996800	4.44913400	0.35066100
H	-2.22323500	3.65148600	-2.99414200
H	-0.21964600	4.75882200	-2.04625100
C	4.89257400	1.19083300	0.51678300
H	5.40705600	2.09891700	0.79417500
N	6.98796800	0.03851000	0.12692300
C	7.76643300	-1.10003700	-0.35650600
H	7.26710200	-1.54220500	-1.22074700
H	8.71380200	-0.70408800	-0.72792100
C	8.02330000	-2.14546200	0.72422500
H	8.56077300	-1.70328500	1.56674100
H	7.08767900	-2.56592100	1.10011700
H	8.62893000	-2.96019600	0.32099600
C	7.76339100	1.18210100	0.60589700

H	7.26692900	1.62586300	1.47029100
H	8.71231400	0.78885200	0.97636200
C	8.01595300	2.22422000	-0.47855000
H	7.07840100	2.64563200	-0.84876500
H	8.62629500	3.03846900	-0.08136400
H	8.54654900	1.77926400	-1.32400200
C	-3.55386400	-1.21089800	3.42541800
N	-2.72815200	-0.39929300	3.60087700

**Coordinates for COUMC\_F<sup>-</sup> Reactant Complex**

C	-0.62859300	-1.39771900	-0.19981800
C	0.79682600	-1.21943800	-0.18795000
C	1.58266900	-2.18038900	-0.95268800
C	1.43491000	-0.20342200	0.49406900
C	3.57543300	-0.99197000	-0.31860800
C	2.83218300	-0.07299000	0.44356500
C	3.55770800	0.94084500	1.10886800
H	3.00935500	1.66818300	1.69724900
C	5.66307200	0.08497000	0.23616100
C	4.94497900	-0.93404500	-0.43234600
H	0.85689500	0.50974400	1.09853800
H	-0.96658400	-2.28041000	-0.72914100
H	5.43914700	-1.69392500	-1.01969100
O	2.94319700	-2.00297400	-0.97550300
O	1.15014200	-3.12317800	-1.57586800
C	-1.51863400	-0.53938100	0.36557800
H	-1.14239200	0.34107100	0.88572300
C	-2.92299100	-0.72513600	0.35301700
C	-3.73497600	-1.92361500	-0.12488400
C	-3.36587400	-3.20962300	0.63318600
H	-3.46220800	-3.06651200	1.71127600
H	-4.04456500	-4.00906700	0.32899900
H	-2.34577700	-3.52637600	0.41373100
C	-3.60649500	-2.09684400	-1.65364400
H	-2.60941000	-2.42815800	-1.94314200
H	-4.32434000	-2.85052000	-1.98314700
H	-3.82718500	-1.16061600	-2.17085900
C	-5.13736800	-1.47624000	0.21326700
C	-5.09272200	-0.19894000	0.74970500
C	-6.35307400	-2.11404300	0.04867700
C	-6.22827100	0.49203900	1.13673500
C	-7.51303300	-1.44333600	0.43476300
H	-6.40865200	-3.11157700	-0.37255300

C	-7.44843900	-0.15835200	0.96969200
H	-6.18915400	1.49161300	1.55029900
H	-8.47602500	-1.92533100	0.31558000
H	-8.36070700	0.34808700	1.26139300
N	-3.73852200	0.21434600	0.81175800
C	-3.32754700	1.56952800	1.20848900
H	-2.42417300	1.50701800	1.82140300
H	-4.12640100	1.97743900	1.82641300
C	-3.06687400	2.43492300	-0.00710200
C	-1.80143200	2.98811400	-0.19220600
C	-4.06823500	2.67313400	-0.94995700
C	-1.54324800	3.77839700	-1.30921000
H	-1.02927900	2.77268100	0.54398700
C	-3.80538200	3.45565300	-2.06744900
H	-5.05693800	2.24519400	-0.81766700
C	-2.54142800	4.01172700	-2.24822900
H	-0.55693700	4.20743000	-1.44876800
H	-4.58753700	3.63437200	-2.79679500
H	-2.33735000	4.62280500	-3.12051300
C	4.91709700	1.02673000	1.01461500
H	5.42284700	1.83403600	1.52367700
N	7.00996000	0.17031800	0.14208000
C	7.78141300	-0.71528500	-0.72616500
H	7.22793600	-0.89255700	-1.65023400
H	8.68348800	-0.17253500	-1.01637000
C	8.15882800	-2.02993000	-0.05000300
H	8.74535600	-1.84266500	0.85296100
H	7.27029800	-2.59888800	0.23330800
H	8.75878600	-2.64266000	-0.72670700
C	7.78865200	1.13087300	0.92120100
H	7.33757400	1.25388600	1.90699100
H	8.76795900	0.67952800	1.09456200
C	7.95155800	2.47595600	0.22083700
H	6.98398400	2.95636500	0.05766700
H	8.56917200	3.14185800	0.82798300
H	8.43743500	2.34837300	-0.74978200
F	-0.28507300	1.59839300	2.17052700

**Coordinates for HCHI<sub>2</sub>HS<sup>-</sup> Reactant Complex**

C	1.17316500	-0.91127700	-0.00225800
C	-0.25960700	-0.85172300	-0.00766000
C	-0.96298500	-2.13032600	-0.00456800
C	-0.98858200	0.31825300	-0.00468200
C	-3.05143600	-0.93541100	0.00968900

C	-2.38907100	0.30624700	0.00225600
C	-3.19631300	1.46742400	0.00763700
H	-2.70818500	2.43663500	0.00773100
C	-5.22268100	0.11730100	0.03203800
C	-4.42057100	-1.04914400	0.02094700
H	-0.48268700	1.28206000	-0.00290500
H	1.56770400	-1.91831600	0.03747900
H	-4.84949400	-2.03990300	0.00418400
O	-2.33398400	-2.09191000	0.00040900
O	-0.45093000	-3.22562500	-0.00723900
C	2.02055300	0.15157700	-0.04171200
H	1.60949100	1.15425800	-0.09822400
C	3.43450400	0.02685100	-0.01170600
C	4.26736100	-1.25253900	0.09533800
C	4.07231100	-2.16747600	-1.12958900
H	4.23372900	-1.61624700	-2.05817600
H	4.80188200	-2.97819500	-1.08070200
H	3.07724600	-2.61124300	-1.15738500
C	3.99789200	-1.99255900	1.42030800
H	2.99810900	-2.42530200	1.45201300
H	4.72152800	-2.80357800	1.52307600
H	4.11318500	-1.31893300	2.27188700
C	5.66786400	-0.68833300	0.09916700
C	5.60173300	0.69039100	0.00491700
C	6.89837300	-1.31375600	0.18185100
C	6.72151100	1.50350100	-0.01156400
C	8.04621400	-0.52167800	0.16773600
H	6.97599200	-2.39238400	0.25891600
C	7.95702400	0.86601400	0.07230700
H	6.65275400	2.58135400	-0.08410600
H	9.02051200	-0.99103300	0.23382900
H	8.86190000	1.46183800	0.06381800
N	4.24034900	1.07629500	-0.06292500
C	3.88258700	2.48595600	-0.15724000
H	2.81089200	2.61924300	-0.28367000
H	4.39627300	2.91770900	-1.01675900
C	-4.55816100	1.38647500	0.02164700
H	-5.13134900	2.30156700	0.04487200
N	-6.57117300	0.03734000	0.05617500
C	-7.26521100	-1.24341200	0.17135700
H	-6.70634300	-1.89972300	0.84081100
H	-8.21811200	-1.04833500	0.66727600
C	-7.50603800	-1.91054100	-1.17928400
H	-8.11413300	-1.26915700	-1.82205700

H	-6.56372700	-2.11423200	-1.69314600
H	-8.03383000	-2.85690700	-1.04120800
C	-7.42661500	1.22077300	-0.01969400
H	-6.99159000	1.94453900	-0.71075600
H	-8.36746800	0.90304100	-0.47349600
C	-7.69026700	1.85074800	1.34402700
H	-6.76314100	2.19928100	1.80489900
H	-8.36455000	2.70380700	1.23915300
H	-8.15572200	1.12772600	2.01858500
H	4.20596300	2.99276300	0.75319800
S	0.24946600	3.70303200	-0.49479000
H	1.18547600	4.61396700	-0.16820400

**Coordinates for HCHI\_CN<sup>-</sup> Reactant Complex**

C	1.17379400	-0.79848300	0.01975300
C	-0.26253600	-0.72399300	0.00622300
C	-0.97835800	-1.99125200	0.09666300
C	-0.97086100	0.45631500	-0.07735200
C	-3.05239200	-0.77669400	0.02748400
C	-2.37671600	0.45239400	-0.06764100
C	-3.17543600	1.61578100	-0.13829300
H	-2.68301500	2.57956500	-0.20585600
C	-5.21580100	0.29273500	-0.01636600
C	-4.42420300	-0.87724200	0.04878300
H	-0.44222200	1.41644100	-0.15321100
H	1.56482500	-1.80433700	0.10884900
H	-4.86077700	-1.86358300	0.10134500
O	-2.34886400	-1.94000000	0.09703000
O	-0.47875100	-3.09108900	0.17096700
C	2.00925100	0.26973800	-0.06434700
H	1.57921400	1.26823200	-0.15803800
C	3.42408100	0.16743700	-0.03443600
C	4.28763400	-1.08669800	0.10281800
C	4.09636700	-2.04502500	-1.08836400
H	4.23731200	-1.52212900	-2.03655400
H	4.84002000	-2.84174700	-1.02186700
H	3.10747200	-2.50347200	-1.08800600
C	4.04650200	-1.79041600	1.45264700
H	3.05487200	-2.23984800	1.50606800
H	4.78630600	-2.58426800	1.57392800
H	4.15582200	-1.08830400	2.28173900
C	5.67425400	-0.49008600	0.07265300
C	5.57298900	0.88411200	-0.06062800

C	6.92006000	-1.08353200	0.15948000
C	6.67354700	1.72172500	-0.11512400
C	8.04881900	-0.26548600	0.10881900
H	7.02343200	-2.15740100	0.26736300
C	7.92516500	1.11605900	-0.02711500
H	6.57753000	2.79483600	-0.22054700
H	9.03462800	-0.70991600	0.17733600
H	8.81537500	1.73263700	-0.06429500
N	4.20276200	1.23566200	-0.12136800
C	3.80116400	2.63267600	-0.25380200
H	2.71423700	2.73993700	-0.29091500
H	4.24068200	3.03170400	-1.16953300
C	-4.53958300	1.55010200	-0.11312400
H	-5.10349400	2.47067400	-0.14812200
N	-6.56741500	0.22750000	0.01523900
C	-7.27335400	-1.03510100	0.21557800
H	-6.71613400	-1.65514300	0.92004200
H	-8.22028000	-0.79994200	0.70624900
C	-7.53245000	-1.78310400	-1.08868800
H	-8.13854900	-1.17579400	-1.76557900
H	-6.59606600	-2.02803900	-1.59541500
H	-8.06929300	-2.71337500	-0.88917700
C	-7.41093900	1.40940800	-0.14923200
H	-6.96266400	2.08166200	-0.88265300
H	-8.35064700	1.07044500	-0.59049500
C	-7.68301800	2.13376900	1.16518200
H	-6.75672900	2.50132700	1.61294400
H	-8.34482000	2.98606400	0.99434800
H	-8.16586700	1.46363500	1.88089900
H	4.19463300	3.18477000	0.60154500
C	0.67886700	2.96012400	-0.32698700
N	1.82546700	2.96012400	-0.32698700

**Coordinates for HCHI\_F- Reactant Complex**

C	-0.62859300	-1.39771900	-0.19981800
C	0.79682600	-1.21943800	-0.18795000
C	1.58266900	-2.18038900	-0.95268800
C	1.43491000	-0.20342200	0.49406900
C	3.57543300	-0.99197000	-0.31860800
C	2.83218300	-0.07299000	0.44356500
C	3.55770800	0.94084500	1.10886800
H	3.00935500	1.66818300	1.69724900
C	5.66307200	0.08497000	0.23616100

C	4.94497900	-0.93404500	-0.43234600
H	0.85689500	0.50974400	1.09853800
H	-0.96658400	-2.28041000	-0.72914100
H	5.43914700	-1.69392500	-1.01969100
O	2.94319700	-2.00297400	-0.97550300
O	1.15014200	-3.12317800	-1.57586800
C	-1.51863400	-0.53938100	0.36557800
H	-1.14239200	0.34107100	0.88572300
C	-2.92299100	-0.72513600	0.35301700
C	-3.73497600	-1.92361500	-0.12488400
C	-3.36587400	-3.20962300	0.63318600
H	-3.46220800	-3.06651200	1.71127600
H	-4.04456500	-4.00906700	0.32899900
H	-2.34577700	-3.52637600	0.41373100
C	-3.60649500	-2.09684400	-1.65364400
H	-2.60941000	-2.42815800	-1.94314200
H	-4.32434000	-2.85052000	-1.98314700
H	-3.82718500	-1.16061600	-2.17085900
C	-5.13736800	-1.47624000	0.21326700
C	-5.09272200	-0.19894000	0.74970500
C	-6.35307400	-2.11404300	0.04867700
C	-6.22827100	0.49203900	1.13673500
C	-7.51303300	-1.44333600	0.43476300
H	-6.40865200	-3.11157700	-0.37255300
C	-7.44843900	-0.15835200	0.96969200
H	-6.18915400	1.49161300	1.55029900
H	-8.47602500	-1.92533100	0.31558000
H	-8.36070700	0.34808700	1.26139300
N	-3.73852200	0.21434600	0.81175800
C	-3.32754700	1.56952800	1.20848900
H	-2.42417300	1.50701800	1.82140300
H	-4.12640100	1.97743900	1.82641300
C	4.91709700	1.02673000	1.01461500
H	5.42284700	1.83403600	1.52367700
N	7.00996000	0.17031800	0.14208000
C	7.78141300	-0.71528500	-0.72616500
H	7.22793600	-0.89255700	-1.65023400
H	8.68348800	-0.17253500	-1.01637000
C	8.15882800	-2.02993000	-0.05000300
H	8.74535600	-1.84266500	0.85296100
H	7.27029800	-2.59888800	0.23330800
H	8.75878600	-2.64266000	-0.72670700
C	7.78865200	1.13087300	0.92120100
H	7.33757400	1.25388600	1.90699100

H	8.76795900	0.67952800	1.09456200
C	7.95155800	2.47595600	0.22083700
H	6.98398400	2.95636500	0.05766700
H	8.56917200	3.14185800	0.82798300
H	8.43743500	2.34837300	-0.74978200
F	-0.28507300	1.59839300	2.17052700
H	-3.06687400	2.43492300	-0.00710200