

## Long-Range Proton Relay Shows an Inverse Linear Free Energy Relationship Depending on the pKa of the Hydrogen-Bonded Wire

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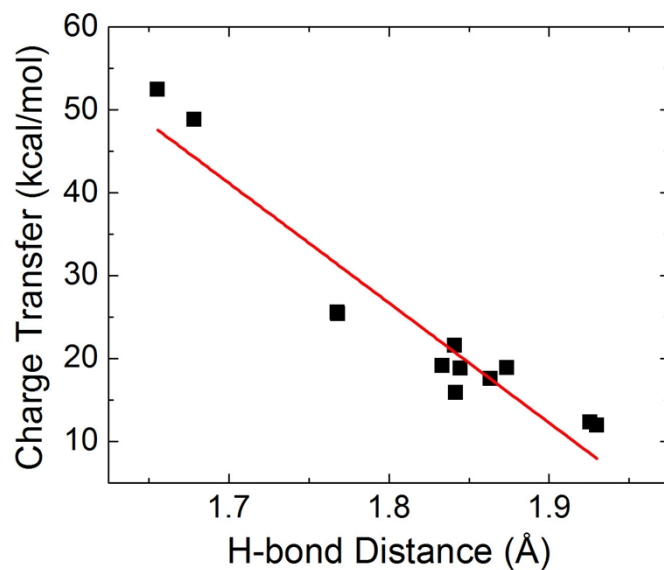
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### The relation between the H-bond strength and length in the H-bonded chain

The charge transfer interaction between the lone pair electron of oxygen (or nitrogen) and anti-bonding orbital of O–H bond is an important component of the H-bond based on the NBO analysis, which can be used to estimate the strength of H-bond; the larger the charge transfer interaction, the stronger the H-bond becomes. Table S1 listed the H-bond lengths and the charge transfer energies, which are the donor-acceptor ( $n_{O(N)} \rightarrow \sigma^*_{O-H}$ ) interaction energies obtained from the NBO analysis. A good correlation was found between the charge transfer energies of each H-bond in the H-bonded chain and its lengths as depicted in Figure S1.

**Table S1.** The H-bond lengths (Å) and charge transfer energies (kcal/mol) for H-bonded chains.

Acid-R <sub>a</sub> OH-R <sub>b</sub> OH-Base	$n_{O3} \rightarrow \sigma^*_{O1-H2}$		$n_{O5} \rightarrow \sigma^*_{O3-H4}$		$n_{N7} \rightarrow \sigma^*_{O5-H6}$	
	Distance	Energy	Distance	Energy	Distance	Energy
H <sub>2</sub> O – H <sub>2</sub> O	1.768	25.38	1.926	12.32	1.874	18.87
H <sub>2</sub> O – CF <sub>3</sub> CH <sub>2</sub> OH	1.768	25.57	1.930	11.92	1.678	48.84
CF <sub>3</sub> CH <sub>2</sub> OH – H <sub>2</sub> O	1.842	15.86	1.833	19.13	1.841	21.57
CF <sub>3</sub> CH <sub>2</sub> OH – CF <sub>3</sub> CH <sub>2</sub> OH	1.863	17.6	1.845	18.81	1.656	52.45

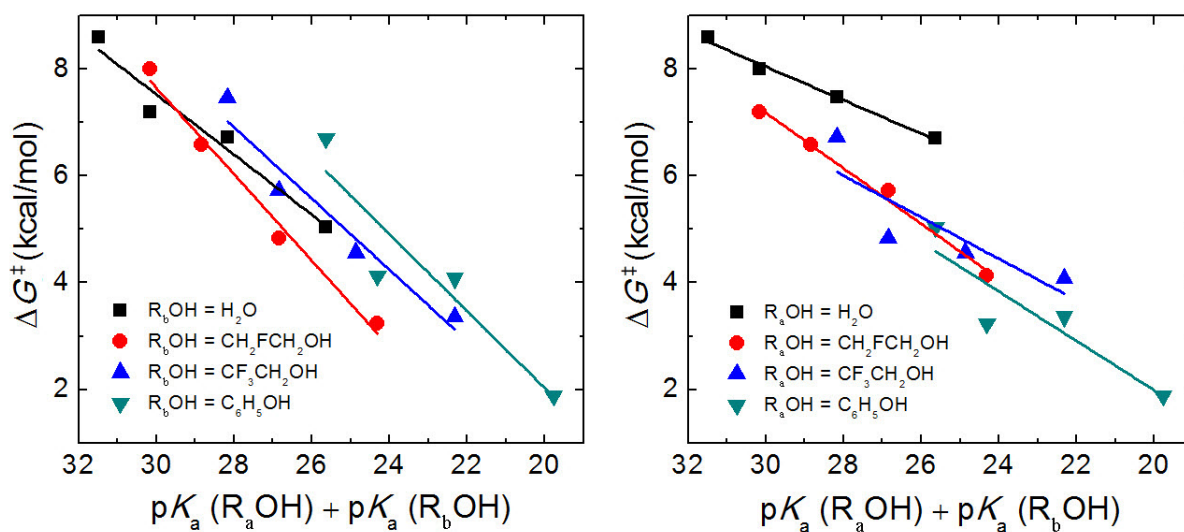


**Figure S1.** Correlation between the H-bond distance and the charge transfer energy in relay chain.

**Table S2.** Free energies of activation (kcal/mol) for the triple proton transfer in water when only one hydroxyl molecule in a wire is changed.

H-bonded chains <sup>a</sup>	Hydroxyl molecules			
	H <sub>2</sub> O	CH <sub>2</sub> FCH <sub>2</sub> OH	CF <sub>3</sub> CH <sub>2</sub> OH	C <sub>6</sub> H <sub>5</sub> OH
A-H – H <sub>2</sub> O – <b>R<sub>b</sub>OH</b> – B	7.27	6.76	5.62	5.09
A-H – <b>R<sub>a</sub>OH</b> – H <sub>2</sub> O – B	7.27	5.75	5.24	3.67
A-H – CH <sub>2</sub> FCH <sub>2</sub> OH – <b>R<sub>b</sub>OH</b> – B	5.75	4.58	3.84	3.35
A-H – <b>R<sub>a</sub>OH</b> – CH <sub>2</sub> FCH <sub>2</sub> OH – B	6.76	4.58	3.46	2.78
A-H – CF <sub>3</sub> CH <sub>2</sub> OH – <b>R<sub>b</sub>OH</b> – B	5.24	3.46	2.93	2.17
A-H – <b>R<sub>a</sub>OH</b> – CF <sub>3</sub> CH <sub>2</sub> OH – B	5.62	3.84	2.93	1.97
A-H – C <sub>6</sub> H <sub>5</sub> OH – <b>R<sub>b</sub>OH</b> – B	3.67	2.78	1.97	1.37
A-H – <b>R<sub>a</sub>OH</b> – C <sub>6</sub> H <sub>5</sub> OH – B	5.09	4.35	2.17	1.37

<sup>a</sup> A-H and B are denoted for carboxylic and imidazole groups, respectively



**Figure S2.** The correlation between the free energy of activation and the  $pK_a$  of hydroxyl molecules in a chain.

**Table S3.** Activation and reaction free energies ( $\Delta G^\ddagger$  and  $\Delta G_0$ , respectively, kcal/mol) for the triple proton relay with different pairs of chain molecules in solution with dielectric constant of 10.

Pair	Order <sup>a</sup>	$\Delta G^\ddagger$	$\Delta G_0$	Pair	Order <sup>a</sup>	$\Delta G^\ddagger$	$\Delta G_0$
H <sub>2</sub> O and CF <sub>3</sub> CH <sub>2</sub> OH	S – S	8.64	4.92	H <sub>2</sub> O and CH <sub>2</sub> FCH <sub>2</sub> OH	S – S	10.2	8.98
	S – W	9.27	4.57		S – W	10.9	8.04
	W – S	10.7	9.32		W – S	11.6	7.88
	W – W	12.0	7.39		W – W	12.0	7.39
CH <sub>2</sub> FCH <sub>2</sub> OH and CF <sub>3</sub> CH <sub>2</sub> OH	S – S	8.64	4.92	CF <sub>3</sub> CH <sub>2</sub> OH and C <sub>6</sub> H <sub>5</sub> OH	S – S	3.92	2.39
	S – W	9.23	4.15		S – W	4.93	1.36
	W – S	9.71	8.74		W – S	6.17	5.77
	W – W	10.2	8.98		W – W	8.64	4.92
H <sub>2</sub> O and C <sub>6</sub> H <sub>5</sub> OH	S – S	3.92	2.39	CH <sub>2</sub> FCH <sub>2</sub> OH and C <sub>6</sub> H <sub>5</sub> OH	S – S	3.92	2.39
	S – W	6.50	0.78		S – W	5.37	1.62
	W – S	10.1	9.34		W – S	9.45	9.03
	W – W	12.0	7.39		W – W	10.2	8.98

<sup>a</sup> S and W denote hydroxyl molecules with relatively strong and weak acidities, respectively.

## Optimized Cartesian Coordinates:

### (1) Carboxylic group – H<sub>2</sub>O – H<sub>2</sub>O – Imidazole:

#### Reactant

C	-0.66644200	-1.37564100	0.78418400
C	0.50389000	-2.29214100	1.18331500
C	1.83320600	-1.52376200	1.05196500
C	2.05573900	-1.02622800	-0.40539300
C	0.82276400	-0.24410700	-0.93288400
C	-0.52551000	-0.95750000	-0.69754000
C	-1.65054600	0.02389700	-1.09215400
C	-3.07439000	-0.48098400	-0.72246600
C	-3.16094000	-1.01226900	0.74157900
C	-2.03903800	-2.03359600	1.01409200
H	-0.61462300	-0.45963000	1.40531500
H	0.51157400	-3.18626300	0.53559300
H	0.37400700	-2.63685800	2.22056600
H	2.68555300	-2.15276800	1.35025100
H	1.81007600	-0.65229800	1.72676400
H	2.23110400	-1.90327900	-1.05045900
H	0.95872600	-0.04168300	-2.00739200
H	0.77772500	0.72887600	-0.42029700
H	-0.58412800	-1.86986400	-1.31721900
H	-1.44492000	0.97650900	-0.58088400
H	-1.61408400	0.21999200	-2.17499700
H	-3.35582600	-1.29695400	-1.40255100
H	-4.15136800	-1.46583300	0.89512600
H	-3.06245900	-0.17820700	1.45439500
H	-2.14619400	-2.90687600	0.34775000
H	-2.11537900	-2.39433900	2.05108300
C	-4.08236800	0.62671600	-0.91370300
O	-5.06971800	0.53420600	-1.62598600
O	-3.87627400	1.76741000	-0.24707000
H	-3.05639700	1.78083000	0.30933900
N	3.35323900	1.05909800	0.09698200
C	3.26108000	-0.14177000	-0.45464300
N	4.42686400	-0.47993800	-1.05287200
C	4.63488000	1.49911500	-0.16394400
C	5.31796400	0.55430800	-0.87865800
H	4.98432000	2.46358900	0.17532600
H	6.32267300	0.52083100	-1.26959700
H	4.60012000	-1.34953200	-1.54292300
O	-1.80734800	2.20971400	1.48502700
H	-1.97959800	1.71424800	2.29699700
H	-0.84579300	2.12759500	1.33607700
O	1.07732400	2.19134700	1.40956500
H	1.88782100	1.81651300	0.98555100
H	1.39275400	2.77363500	2.11263800

#### TS

C	0.68682500	1.54231800	0.63861300
C	-0.46782400	2.50665800	0.96130500
C	-1.79780000	1.73092700	0.90717000
C	-2.03432200	1.11734700	-0.50795300
C	-0.78965200	0.35393700	-1.04308400
C	0.56511000	1.05899100	-0.82283600
C	1.65917400	0.01641400	-1.15450800
C	3.09314400	0.38923500	-0.68306400
C	3.14000300	1.04244500	0.73470600
C	2.07953600	2.15211300	0.86863600
H	0.58712000	0.66222500	1.30346000
H	-0.47471700	3.34231600	0.24055900
H	-0.33477200	2.93452600	1.96677500
H	-2.65155900	2.37577600	1.16167100

H	-1.75894600	0.91883000	1.65200600
H	-2.30516400	1.92787900	-1.20103500
H	-0.93829700	0.13901800	-2.11290300
H	-0.72293800	-0.61138300	-0.52155900
H	0.65775300	1.93874400	-1.48233400
H	1.35366100	-0.92596000	-0.68090800
H	1.68285600	-0.16315500	-2.24054300
H	3.53565000	1.09785400	-1.39707200
H	4.15201400	1.44076900	0.89964800
H	2.95066800	0.28074400	1.50714200
H	2.26287600	2.95667400	0.13578000
H	2.13934400	2.59545100	1.87445500
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O	3.54280000	-1.89045100	0.02651900
H	2.60744400	-1.84210100	0.54590500
N	-3.10131300	-1.06232700	0.12028100
C	-3.16801700	0.15132500	-0.42835900
N	-4.42500600	0.34315500	-0.84328700
C	-4.34549700	-1.65308300	0.05140900
C	-5.18525000	-0.77175500	-0.55585800
H	-4.52646600	-2.64506100	0.43435200
H	-6.23115300	-0.83266000	-0.80920100
H	-4.75335100	1.18651400	-1.30305800
O	1.44545500	-1.99419500	1.33243300
H	1.67394300	-2.48176300	2.13469500
H	0.27728200	-2.06283200	1.20130900
O	-0.96332400	-2.15210800	1.11078900
H	-2.19170600	-1.51442800	0.55078100
H	-1.23361400	-2.86858400	1.70002400

#### Product

C	-0.68041900	-1.36472300	0.81588100
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C	2.02688400	-1.06582000	-0.39722800
C	0.80320700	-0.25688200	-0.91225400
C	-0.54472200	-0.96677700	-0.67224400
C	-1.67191500	0.00731600	-1.07944800
C	-3.09474200	-0.48486300	-0.71101200
C	-3.16894000	-0.97450400	0.76426800
C	-2.05918100	-2.00191100	1.06621500
H	-0.61291100	-0.43990400	1.42292400
H	0.47501400	-3.19297700	0.58361300
H	0.35858800	-2.61853300	2.26234200
H	2.66809300	-2.18504400	1.36193600
H	1.81933600	-0.66884500	1.74120200
H	2.18381500	-1.94599200	-1.03994500
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H	-0.59846400	-1.88744700	-1.28010500
H	-1.48203600	0.96504100	-0.57296100
H	-1.62454500	0.19577700	-2.16423300
H	-3.36931600	-1.32555600	-1.36615100
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H	-2.17567300	-2.89127600	0.42255600
H	-2.13255900	-2.33688100	2.11246200
C	-4.10801600	0.64280500	-0.90827700
O	-5.13045200	0.41983500	-1.61223900
O	-3.87384700	1.74746800	-0.32412300
H	-2.50164800	2.07974600	0.79241500
N	3.36867100	1.01130300	0.04633700

C	3.24432800	-0.21330100	-0.47223900	<b>TS</b>			
N	4.41574500	-0.51824600	-1.03229100	C	-1.78158000	-1.67484300	0.97668200
C	4.64117800	1.49202500	-0.18706100	C	-1.04750500	-2.89366100	1.56175000
C	5.30622800	0.52478100	-0.87034000	C	0.45897900	-2.76276100	1.26744300
H	4.95450900	2.46766500	0.14733600	C	0.72729100	-2.71042000	-0.26884200
H	6.31313400	0.48279900	-1.25204400	C	-0.18431600	-1.68090900	-0.99720100
H	4.60311500	-1.39643300	-1.50674300	C	-1.66554400	-1.68679400	-0.56269600
O	-1.80389800	2.35298500	1.43324000	C	-2.30295600	-0.41583200	-1.17052700
H	-1.98078900	1.83647800	2.23058000	C	-3.70478900	-0.04467800	-0.60535100
H	0.10557500	2.26156500	1.26881100	C	-3.84074300	-0.24187300	0.93687200
O	1.07929600	2.30135200	1.34625100	C	-3.26408500	-1.60129300	1.37939600
H	2.60984200	1.50530400	0.53490500	H	-1.27715800	-0.76336200	1.35275800
H	1.25372300	2.91213300	2.07397800	H	-1.45139300	-3.82304100	1.12440800
				H	-1.20370400	-2.94235000	2.65003500
				H	1.02805800	-3.59869700	1.69931000
				H	0.82686800	-1.83170100	1.73098100
				H	0.57407100	-3.71549000	-0.68966800
				H	-0.10539500	-1.84232800	-2.08350100
				H	0.19555200	-0.67026100	-0.78820100
				H	-2.17577200	-2.59138200	-0.93541800
				H	-1.60677900	0.41306200	-0.98279600
				H	-2.38549700	-0.52720900	-2.26333100
				H	-4.46601200	-0.66921700	-1.09326900
				H	-4.90485200	-0.15933500	1.20344300
				H	-3.30513600	0.55585000	1.47331300
				H	-3.81899100	-2.43089400	0.90804600
				H	-3.36660100	-1.70683800	2.47051600
				C	-4.00959100	1.40064800	-0.94723900
				O	-5.01843600	1.72196300	-1.57851700
				O	-3.16399000	2.32069900	-0.53989400
				H	-2.27065300	2.04277000	0.03162600
				N	2.62343500	-1.07524900	-0.30356400
				C	2.14447200	-2.30672500	-0.49501300
				N	3.16660400	-3.07323700	-0.88192800
				C	3.97651700	-1.06010800	-0.57032000
				C	4.32392500	-2.32241400	-0.93632800
				H	4.56878500	-0.16327000	-0.48320400
				H	5.26909700	-2.74740300	-1.23258000
				H	3.08436700	-4.06073800	-1.10323000
				O	-1.14165900	1.94570000	0.78148300
				H	-1.39560300	1.72177600	1.68670800
				H	-0.07193800	1.44862500	0.59026100
				O	1.06582400	1.02097800	0.49306200
				H	2.02770800	-0.25673900	-0.00369000
				C	1.90314600	1.87384600	1.20934300
				H	1.37791500	2.40422300	2.01626500
				H	2.75640000	1.33922900	1.65048400
				C	2.48307200	2.93113700	0.29632200
				F	3.29600500	3.77950600	0.95927000
				F	1.52890800	3.68231200	-0.29041200
				F	3.21227700	2.39590100	-0.70504200
				<b>Product</b>			
				C	-1.15723700	-1.06267700	1.45759200
				C	-0.12090700	-1.70926400	2.39408200
				C	1.26813400	-1.68956100	1.72871500
				C	1.24404500	-2.45533100	0.37129300
				C	0.08781200	-1.97252200	-0.55143200
				C	-1.27956400	-1.89100100	0.15776500
				C	-2.27811200	-1.22916600	-0.81727800
				C	-3.65142300	-0.89416000	-0.18100700
				C	-3.48380000	-0.14229800	1.17010900
				C	-2.53926800	-0.90988200	2.11757700
				H	-0.79294300	-0.05130500	1.18439300
				H	-0.42184100	-2.74609400	2.62353100
				H	-0.07709200	-1.15778700	3.34577100
				H	2.02918700	-2.14104900	2.38143400

**(2) Carboxylic group – H<sub>2</sub>O – CF<sub>3</sub>CH<sub>2</sub>OH – Imidazole**

**Reactant**

C	-1.58566900	-1.04506600	1.37631100
C	-0.68686100	-1.96186000	2.22436400
C	0.72808500	-1.99934000	1.61660500
C	0.70588900	-2.52869300	0.15208500
C	-0.35701500	-1.79691500	-0.71512000
C	-1.73797200	-1.63315200	-0.04429700
C	-2.57573700	-0.68922500	-0.93505300
C	-3.92444900	-0.25741900	-0.29129700
C	-3.75968400	0.21590200	1.18550000
C	-2.97286700	-0.82511400	2.00568600
H	-1.08518700	-0.05903400	1.28746400
H	-1.11875200	-2.97719100	2.25932100
H	-0.63594100	-1.58745400	3.25837500
H	1.39884400	-2.63299100	2.21615800
H	1.14162200	-0.97725300	1.62358000
H	0.47711800	-3.60652200	0.17493100
H	-0.46480700	-2.33174400	-1.67221100
H	0.01564500	-0.78800600	-0.94576700
H	-2.23898400	-2.61312900	0.04434500
H	-1.95827400	0.19822400	-1.14037300
H	-2.78196300	-1.17309900	-1.90252900
H	-4.61936800	-1.10833700	-0.30715600
H	-4.75721800	0.38338500	1.61775500
H	-3.21569100	1.17313200	1.22049900
H	-3.52192100	-1.78171400	2.03905600
H	-2.86437300	-0.46751000	3.04088000
C	-4.55340500	0.84798100	-1.10585200
O	-5.66747900	0.77896700	-1.60079000
O	-3.84282800	1.96795600	-1.27620500
H	-2.94362000	1.95805600	-0.85911800
N	2.58811900	-1.14874700	-0.74741000
C	2.05416300	-2.32837500	-0.46503600
N	2.91305400	-3.31911100	-0.79046700
C	3.83763600	-1.40243100	-1.27323300
C	4.05613500	-2.75169000	-1.30795800
H	4.49338100	-0.60558200	-1.59328100
H	4.89236400	-3.34483600	-1.64297500
H	2.73253900	-4.30928400	-0.67292000
O	-1.33674100	2.40066400	-0.26955800
H	-1.39457600	2.57729800	0.67940400
H	-0.55122000	1.82993600	-0.37379000
O	1.23921300	1.12236100	-0.23862300
H	1.75479900	0.27950200	-0.45995000
C	1.85366300	1.75302300	0.85201400
H	1.11583400	2.33332300	1.41535000
H	2.34374500	1.04267900	1.52811400
C	2.91225400	2.71303600	0.35819100
F	3.53643700	3.33068400	1.37883500
F	2.40035900	3.67575200	-0.43253000
F	3.86047800	2.08685300	-0.36698000

H	1.55948300	-0.64084700	1.55120000	O	-3.69953200	-3.37866900	-1.73771500
H	1.12907300	-3.53120700	0.57302700	O	-3.29010800	-1.22179100	-1.58260900
H	0.02562200	-2.64121800	-1.42405900	H	-2.67740600	-0.56233700	-1.18438400
H	0.32341200	-0.96244700	-0.92252500	N	3.49128300	1.22181800	-0.71973100
H	-1.62656800	-2.90363800	0.42834700	C	3.87457400	0.03927600	-0.26208400
H	-1.81857600	-0.29878800	-1.18269000	N	5.21017200	-0.11631800	-0.41327400
H	-2.43404200	-1.88381700	-1.69033400	C	4.63482800	1.84147800	-1.17992300
H	-4.20160400	-1.82838600	0.00835100	C	5.71535700	1.02362300	-0.99603600
H	-4.47404400	-0.00379700	1.63106700	H	4.60903900	2.83168300	-1.61146300
H	-3.06014500	0.85826000	0.98132000	H	6.76381900	1.13903600	-1.22174200
H	-2.95275100	-1.90872800	2.34213000	H	5.73737300	-0.93712900	-0.13993100
H	-2.44198100	-0.36831300	3.07115500	O	-1.82707500	0.98488300	-0.66010600
C	-4.46838700	-0.02633400	-1.13267600	H	-0.86551300	1.18277900	-0.68046200
O	-5.62670200	-0.40329600	-1.46181400	O	0.77364900	1.97973800	-0.48275200
O	-3.93350600	1.05308400	-1.54474300	H	1.73362100	1.75117100	-0.57804900
H	-2.34277300	1.67576100	-1.08716400	H	0.72095400	2.94408400	-0.50134100
N	2.95641500	-1.08535800	-0.84698000	C	-2.38202200	1.51626800	0.51852700
C	2.53909000	-2.24528900	-0.33183600	H	-3.33451700	1.01826500	0.71817900
N	3.50524100	-3.13672000	-0.55503600	H	-1.71962900	1.40068200	1.38343500
C	4.20721300	-1.24197600	-1.40830000	C	-2.67358400	2.99051400	0.34607800
C	4.55669300	-2.54148500	-1.22408300	F	-1.55618200	3.70976300	0.12134300
H	4.72663500	-0.42683300	-1.88544100	F	-3.25803900	3.49981100	1.44552000
H	5.44052400	-3.09035900	-1.50546000	F	-3.49701000	3.23087600	-0.69012000
H	3.45534700	-4.11079600	-0.27150100	<b>TS</b>			
O	-1.47434900	2.11602300	-0.92041200	C	0.42318100	-1.82104100	1.24094100
H	-1.59370000	2.62782000	-0.10929400	C	1.69693400	-1.91757700	2.09763300
H	0.21972600	1.40974000	-0.80855600	C	2.68890800	-0.82701500	1.64924100
O	1.16697800	1.28624100	-0.57937100	C	3.07293100	-0.99586900	0.14619600
H	2.40383700	-0.21994200	-0.82287500	C	1.82956600	-1.18865900	-0.76744100
C	1.42808800	1.97270100	0.61952300	C	0.76319400	-2.16422100	-0.22652500
H	0.58533700	1.93010700	1.31869900	C	-0.47374900	-2.01815300	-1.14510700
H	2.31536600	1.54411000	1.09345600	C	-1.79499600	-2.61719700	-0.58112800
C	1.72590400	3.42971300	0.34057800	C	-1.99762500	-2.37661300	0.94753400
F	2.01117600	4.09082900	1.47782600	C	-0.71971300	-2.72257500	1.73534000
F	0.68590600	4.06214700	-0.23683100	H	0.06540800	-0.77318400	1.27755800
F	2.77668000	3.58690000	-0.48525800	H	2.14579100	-2.92041600	1.99083100
				H	1.45192300	-1.77331000	3.16082800
				H	3.60659400	-0.84524500	2.25529600
				H	2.21437600	0.15817300	1.79271200
				H	3.74531100	-1.86225800	0.05162100
				H	2.16816800	-1.50886500	-1.76528600
				H	1.32999400	-0.21644800	-0.88849700
				H	1.13797000	-3.20162700	-0.25281600
				H	-0.60855900	-0.94478000	-1.33285400
				H	-0.26754300	-2.48929000	-2.11872900
				H	-1.80632300	-3.70130300	-0.75696200
				H	-2.85157600	-2.98257000	1.28389700
				H	-2.24333800	-1.31993400	1.13619700
				H	-0.45236500	-3.78403100	1.59649300
				H	-0.89496100	-2.55852400	2.80957500
				C	-2.97884900	-2.02834900	-1.31787700
				O	-3.83007300	-2.71358500	-1.87183700
				O	-3.10301900	-0.70547800	-1.33235300
				H	-2.36746400	-0.16175700	-0.87303900
				C	3.23208700	1.41235300	-0.53359400
				N	3.79830800	0.22814800	-0.30242000
				N	5.11704200	0.35440900	-0.49708900
				C	4.21791500	2.31218400	-0.88026100
				C	5.40834500	1.65288300	-0.85956800
				H	3.99302600	3.34070700	-1.11564600
				H	6.41437900	1.97741700	-1.07048300
				H	5.78615300	-0.40087100	-0.39049400
				O	-1.45380000	0.89766000	-0.20521200
				H	-0.40271800	1.34937800	-0.30961500
				O	0.73548700	1.91523700	-0.35373800
				H	2.12636600	1.63536400	-0.44840700
<b>(3) Carboxylic group – CF<sub>3</sub>CH<sub>2</sub>OH – H<sub>2</sub>O – Imidazole</b>							
<b>Reactant</b>							
C	0.21177300	-1.46764900	1.40608500				
C	1.42049100	-1.38501500	2.35642100				
C	2.49341300	-0.45699600	1.75378300				
C	2.97341000	-0.97552700	0.36722600				
C	1.77529400	-1.25391700	-0.57993300				
C	0.64591600	-2.08851400	0.05902300				
C	-0.53532500	-2.11543300	-0.93688500				
C	-1.83377700	-2.73519400	-0.34658500				
C	-2.17880900	-2.17333900	1.06739600				
C	-0.95731300	-2.27125300	2.00130500				
H	-0.14437600	-0.43600600	1.21007300				
H	1.83456900	-2.39632600	2.51457400				
H	1.10131600	-0.99962400	3.33694500				
H	3.36137600	-0.36953400	2.42463000				
H	2.06414700	0.55091700	1.63035500				
H	3.53790600	-1.90997100	0.52128500				
H	2.14455700	-1.75349500	-1.48991300				
H	1.33943100	-0.29137800	-0.88922200				
H	0.99645900	-3.11722100	0.25476500				
H	-0.72080100	-1.07632100	-1.24858400				
H	-0.25187400	-2.68035700	-1.83863800				
H	-1.70867500	-3.82420200	-0.26325200				
H	-3.03371200	-2.73406100	1.47248300				
H	-2.47812400	-1.11546700	0.99613700				
H	-0.65639200	-3.32468700	2.13242600				
H	-1.22134900	-1.87437400	2.99354500				
C	-3.00035600	-2.49365000	-1.27374000				

H	0.59102600	2.86998500	-0.31847900	C	2.54249100	-2.27182000	0.26881000
C	-2.07643500	1.46523300	0.90713200	C	1.36061300	-1.98280800	-0.69948500
H	-2.79573500	0.77441500	1.36361300	C	0.06803800	-2.75863400	-0.36876300
H	-1.35382600	1.77661300	1.67331300	C	-1.04316400	-2.23668400	-1.30787300
C	-2.85147700	2.69775800	0.49792600	C	-2.47217500	-2.72672500	-0.93031500
F	-2.06058000	3.63717500	-0.05962800	C	-2.76924700	-2.60735000	0.59581200
F	-3.46565900	3.27443000	1.55011900	C	-1.64310600	-3.25940800	1.42035600
F	-3.80746800	2.41847500	-0.41053900	H	-0.44706000	-1.46852100	1.29135900
<b>Product</b>				H	1.05171500	-4.10539600	1.80091300
C	0.58155300	-1.69261900	1.27734800	H	0.55043600	-2.96814700	3.07261600
C	1.86984100	-1.73259500	2.11979100	H	2.93017100	-2.49590000	2.40113200
C	2.84057700	-0.63261100	1.64856300	H	1.86092500	-1.13417700	1.99821100
C	3.19803500	-0.81558400	0.14164500	H	2.92844400	-3.28644400	0.07742100
C	1.92415600	-0.95685900	-0.73753900	H	1.68061600	-2.20102600	-1.73116000
C	0.91818400	-1.99565200	-0.20122500	H	1.12191100	-0.90772100	-0.65217000
C	-0.34564300	-1.92372600	-1.08722200	H	0.22132000	-3.83956200	-0.53426500
C	-1.56326100	-2.71666300	-0.53940500	H	-1.00544100	-1.13842900	-1.28080900
C	-1.79126900	-2.47550300	0.98061300	H	-0.82774100	-2.54194800	-2.34362600
C	-0.48984900	-2.67430600	1.78315200	H	-2.58194600	-3.78050000	-1.22180300
H	0.16112700	-0.66837400	1.33300100	H	-3.73914700	-3.08228800	0.80389300
H	2.34144200	-2.72620900	2.02499200	H	-2.84681200	-1.54798000	0.88686600
H	1.63235800	-1.57686800	3.18307700	H	-1.56156200	-4.33297200	1.17801300
H	3.76693200	-0.63997300	2.24125800	H	-1.87762600	-3.17695000	2.49264900
H	2.36078800	0.35022700	1.78934500	C	-3.50832600	-1.94219200	-1.69920700
H	3.82535000	-1.71368300	0.03191600	O	-4.33496800	-2.44360100	-2.44251400
H	2.22303500	-1.21093200	-1.76659500	O	-3.52257800	-0.61198000	-1.53029900
H	1.40284100	0.01385700	-0.77513500	H	-2.80933500	-0.27998800	-0.94007200
H	1.35780700	-3.00760900	-0.25070200	N	3.48551400	0.03599200	0.08868900
H	-0.61797600	-0.86448100	-1.18752500	C	3.63031500	-1.27887100	0.00910400
H	-0.10598000	-2.29303400	-2.09742400	N	4.89729900	-1.58675900	-0.34543000
H	-1.38982200	-3.79219900	-0.69364900	C	4.70961900	0.58450700	-0.23110600
H	-2.57620200	-3.16004000	1.33649600	C	5.60198800	-0.41472100	-0.50328800
H	-2.15063900	-1.44655000	1.14108600	H	4.87179200	1.65258100	-0.24281900
H	-0.12352800	-3.70980900	1.67440300	H	6.64254000	-0.40357900	-0.78691900
H	-0.68251000	-2.50040600	2.85318000	H	5.25893500	-2.52530400	-0.46725200
C	-2.82507200	-2.31341000	-1.30108000	O	-1.57588000	0.66830000	0.08535900
O	-3.50152400	-3.19990200	-1.87891600	H	-0.59941900	0.74751600	0.04902300
O	-3.14203500	-1.07547300	-1.29920500	O	1.11923000	1.18403600	0.55745100
H	-2.29365400	0.06354500	-0.62548500	H	2.01092200	0.73168700	0.37632900
N	3.50160900	1.60001100	-0.47094400	C	-2.02502400	1.19540100	1.30970300
C	3.98151600	0.36278900	-0.31909800	H	-2.72696400	0.50592700	1.78951000
N	5.28003100	0.41040800	-0.62031600	H	-1.19805100	1.40860000	1.99394300
C	4.51309800	2.44892900	-0.87053100	C	1.33177800	2.56749800	0.65020700
C	5.64065400	1.69759500	-0.96728200	H	0.52522400	3.03068400	1.22581800
H	4.34058500	3.49722000	-1.05348300	H	2.29417700	2.80978600	1.11606000
H	6.64939600	1.95407800	-1.24694700	C	-2.76503100	2.48553800	1.04539600
H	5.89705500	-0.39555300	-0.59113100	C	1.32304900	3.18822300	-0.72901200
O	-1.81486800	0.84060500	-0.18546400	F	-1.98026500	3.42606900	0.48918600
H	-0.08396100	1.62785100	-0.07974100	F	-3.26538400	3.00425200	2.18182800
O	0.70352800	2.16913200	0.12232600	F	-3.80024600	2.30219100	0.20241200
H	2.51787300	1.85786800	-0.30314100	F	1.46832900	4.52542900	-0.66794400
H	0.40317800	3.08585100	0.06397600	F	0.17829500	2.94225200	-1.39250100
C	-2.61720500	1.34810900	0.84488400	F	2.32121300	2.71631800	-1.50299100
H	-3.35772300	0.62044500	1.19598300	<b>TS</b>			
H	-1.99812700	1.66656800	1.69028800	C	0.07320000	-2.71771000	0.97855300
C	-3.36984800	2.56120000	0.34927100	C	1.27438700	-3.15081400	1.83682200
F	-2.53946100	3.53972500	-0.06393600	C	2.42121200	-2.13822200	1.65662600
F	-4.15132500	3.08867500	1.31047000	C	2.86860500	-2.05323700	0.16406000
F	-4.16751700	2.27002400	-0.69658400	C	1.66545800	-1.87088400	-0.80432000
				C	0.45360100	-2.78028100	-0.51703700
				C	-0.70400300	-2.26370200	-1.40294900
				C	-2.10297600	-2.84463000	-1.05030000
				C	-2.37603300	-2.92906400	0.48332400
				C	-1.18583700	-3.56508900	1.22630000
				H	-0.16813000	-1.66497000	1.22950600
				H	1.59984100	-4.16293200	1.54102100
<b>(4) Carboxylic group – CF<sub>3</sub>CH<sub>2</sub>OH – CF<sub>3</sub>CH<sub>2</sub>OH – Imidazole</b>							
<b>Reactant</b>							
C	-0.31024700	-2.55464000	1.11586700				
C	0.84132100	-3.04262100	2.01351300				
C	2.09517200	-2.18423000	1.75602000				

H	0.98627200	-3.18986400	2.89866500	H	-1.56026900	-4.13779800	-1.23507100
H	3.29160600	-2.40451500	2.27392700	H	-2.75069600	-3.85032800	0.88320000
H	2.06863400	-1.14650900	1.98580000	H	-2.23262400	-2.15577700	1.01899500
H	3.42483900	-2.96700000	-0.09273000	H	-0.33851500	-4.58928500	1.09713400
H	2.01576800	-2.01729000	-1.83788800	H	-0.82793900	-3.59677900	2.48969200
H	1.30340400	-0.83487200	-0.72613600	C	-2.94150100	-2.52388600	-1.54485000
H	0.68940300	-3.82968400	-0.76491000	O	-3.64920400	-3.26067000	-2.27497800
H	-0.72325200	-1.17036000	-1.29663300	O	-3.21143500	-1.29754900	-1.31080500
H	-0.48940100	-2.48279600	-2.46057000	H	-2.35356800	-0.33374800	-0.41456800
H	-2.19209000	-3.85648200	-1.46938500	N	3.58885300	0.81095500	-0.00341700
H	-3.29800700	-3.50701000	0.64239500	C	4.00467900	-0.45457700	-0.10443400
H	-2.54093400	-1.92139900	0.89449800	N	5.29840700	-0.41084600	-0.42397700
H	-1.01749300	-4.59824400	0.87700000	C	4.63299100	1.67397500	-0.26665000
H	-1.40713100	-3.60825500	2.30370200	C	5.71764100	0.90060800	-0.53171000
C	-3.18169300	-1.99731900	-1.68950000	H	4.51446700	2.74511400	-0.23936600
O	-4.03259100	-2.45788000	-2.44149600	H	6.73308600	1.15742400	-0.78571500
O	-3.21010100	-0.70246500	-1.39618800	H	5.87374000	-1.23463400	-0.57335100
H	-2.47331800	-0.33894600	-0.78614100	O	-1.89034700	0.35654600	0.16633200
N	3.36779300	0.39342300	0.00502200	O	-0.10619800	0.78005400	0.46853400
C	3.77179100	-0.87854800	0.00112700	H	0.69367200	1.25993000	0.77238300
N	5.10029400	-0.87340500	-0.13293100	H	2.62472700	1.06811200	0.23203800
C	4.46133000	1.22367700	-0.12723100	C	-2.74413100	0.71766600	1.21723300
C	5.55895600	0.42642900	-0.21635200	H	-3.36344700	-0.11917000	1.56124200
H	4.36722800	2.29759200	-0.15172100	H	-2.15795300	1.09906000	2.05940800
H	6.60510700	0.65761700	-0.33377000	C	0.38563600	2.63083500	0.85595400
H	5.67167000	-1.71188500	-0.17059100	H	-0.62993100	2.81324400	1.21944100
O	-1.52225300	0.48759100	0.13367300	H	1.10233600	3.11679100	1.52237800
H	-0.39662300	0.79837300	0.15222700	C	-3.67732500	1.82301500	0.77360000
O	0.78763500	1.17429600	0.25091700	C	0.52032900	3.27414300	-0.50640400
H	2.35317900	0.68926600	0.09215200	F	-3.01427600	2.91855100	0.35439200
C	-2.11401500	0.80847700	1.35585100	F	-4.49015200	2.21282700	1.77415900
H	-2.72222100	-0.01477000	1.75344500	F	-4.46532500	1.44068000	-0.25042400
H	-1.37024100	1.08630800	2.11488000	F	0.27123400	4.59411000	-0.45228900
C	0.85298000	2.53241300	0.55718600	F	-0.32243000	2.74365900	-1.41138800
H	0.02697600	2.87391400	1.19547000	F	1.76371000	3.12365300	-1.00901000
H	1.79666400	2.79122200	1.05938700				
C	-3.04864400	1.98616300	1.18547500				
C	0.79754500	3.36600300	-0.70333300				
F	-3.64575000	2.32195100	2.34665100				
F	-4.03258300	1.72371100	0.30092600				
F	-2.41957800	3.08838100	0.73352400				
F	0.86000600	4.68669000	-0.43382600				
F	-0.33419600	3.16189100	-1.40620900				
F	1.81931600	3.09060300	-1.54209900				
<b>Product</b>				<b>(5) Carboxylic group – H<sub>2</sub>O – CH<sub>2</sub>FCH<sub>2</sub>OH – Imidazole</b>			
C	0.48757100	-2.57890300	1.08727900	<b>Reactant</b>			
C	1.76658700	-2.85814600	1.89717300	C	-1.12791900	-0.91647300	1.40975300
C	2.79878600	-1.74325600	1.64279000	C	-0.08083900	-1.64986400	2.26688200
C	3.15793800	-1.65683600	0.12818400	C	1.30896900	-1.48207600	1.62506500
C	1.88765800	-1.55830100	-0.76352100	C	1.34415500	-2.06194900	0.17963900
C	0.80726000	-2.60600800	-0.42510800	C	0.15675800	-1.55236900	-0.68441200
C	-0.45207100	-2.26602900	-1.25177400	C	-1.21733800	-1.58492500	0.01919500
C	-1.69990500	-3.10735600	-0.87480700	C	-2.22019100	-0.83376300	-0.88455500
C	-1.92792000	-3.15325400	0.66355000	C	-3.60328600	-0.60266600	-0.21455300
C	-0.64306700	-3.57390500	1.40474100	C	-3.47530700	-0.01767100	1.22464000
H	0.13227800	-1.55967600	1.34097500	C	-2.51732600	-0.87932800	2.07036500
H	2.18067000	-3.83927000	1.60686800	H	-0.78322000	0.12842200	1.26753600
H	1.53201400	-2.89967000	2.97172000	H	-0.34623800	-2.71898300	2.34007300
H	3.71946800	-1.91344700	2.21951000	H	-0.07154400	-1.23907900	3.28807900
H	2.36978900	-0.78149400	1.97081500	H	2.08878000	-1.97548500	2.22452700
H	3.73863600	-2.54909600	-0.15123500	H	1.55017100	-0.40685200	1.58588700
H	2.18528400	-1.64520000	-1.82009800	H	1.30104300	-3.16148900	0.24608700
H	1.43141300	-0.56339500	-0.63140300	H	0.11759400	-2.13933200	-1.61598400
H	1.16888300	-3.61738700	-0.68134100	H	0.35498700	-0.50772700	-0.96553900
H	-0.67115700	-1.20009100	-1.09354300	H	-1.54987900	-2.62792400	0.16355400
H	-0.23856700	-2.40041200	-2.32439600	H	-1.76344300	0.13292200	-1.14494200
				H	-2.36659200	-1.38927700	-1.82398600
				H	-4.13833600	-1.56082900	-0.15088300
				H	-4.47503800	0.02387100	1.68133800
				H	-3.08453500	1.01130800	1.18364300
				H	-2.91128500	-1.90577600	2.16561400
				H	-2.43982200	-0.45729100	3.08396800
				C	-4.44816800	0.31857600	-1.06119700



O	-5.55868300	0.02652600	-1.47714100	H	2.10432900	0.40142300	-0.05209500
O	-3.94960700	1.52366200	-1.35299200	C	1.85649100	2.49023100	0.99386900
H	-3.04809800	1.70596800	-0.98174500	H	1.27842800	2.96220900	1.80189800
N	2.93893500	-0.42984100	-0.85103500	H	2.76802300	2.06833000	1.44424400
C	2.62953900	-1.66175300	-0.47364000	C	2.24928400	3.54195000	-0.02517200
N	3.66071600	-2.50136900	-0.71880800	F	3.02565800	4.53147100	0.60572700
C	4.22106200	-0.49220200	-1.35573800	H	2.85763900	3.10889600	-0.82494300
C	4.68700400	-1.77556800	-1.28029700	H	1.36999000	4.03625000	-0.44790900
H	4.72356500	0.38283700	-1.74240200	<b>Product</b>			
H	5.62112000	-2.22989800	-1.57110600	C	-0.84222900	-0.72734100	1.48302700
H	3.66656900	-3.49325000	-0.51172400	C	0.29956100	-1.06536900	2.45849700
O	-1.55051100	2.47231300	-0.47713700	C	1.65948700	-0.87505200	1.76143000
H	-1.64104200	2.73168800	0.44995200	C	1.76899300	-1.77960200	0.49590900
H	-0.67402600	2.04401300	-0.53695700	C	0.54101600	-1.61250900	-0.44553800
O	1.19128600	1.67493600	-0.45452500	C	-0.81593000	-1.70024800	0.28312900
H	1.82039200	0.91997300	-0.63440700	C	-1.91965900	-1.33474100	-0.73428300
C	1.72042600	2.44641700	0.60974300	C	-3.33005300	-1.16800600	-0.11170400
H	0.91393200	3.06851900	1.01192000	C	-3.29825000	-0.27477200	1.16170600
H	2.09502500	1.80346800	1.41644000	C	-2.22553600	-0.76029800	2.15743400
C	2.84381300	3.32139100	0.08787700	H	-0.67420000	0.29668500	1.09230100
F	3.36805100	4.06649300	1.15633200	H	0.19113200	-2.10593300	2.80979900
H	3.65816900	2.71665700	-0.32272500	H	0.24865700	-0.41028400	3.34189600
H	2.48374200	4.02943000	-0.66253800	H	2.49187200	-1.10936500	2.44064700
<b>TS</b>				H	1.75970500	0.18171800	1.46315100
C	-1.34637600	-1.65913000	0.96486600	H	1.84785800	-2.82997000	0.81538900
C	-0.44075700	-2.77289000	1.51758900	H	0.59612200	-2.37065500	-1.24230800
C	1.02662400	-2.41240000	1.21868800	H	0.59126900	-0.62189800	-0.92585200
C	1.27586200	-2.27673200	-0.31735200	H	-0.97306300	-2.72327400	0.66764700
C	0.20051200	-1.40272600	-1.02658000	H	-1.62807600	-0.38743100	-1.21138100
C	-1.25750500	-1.63922700	-0.57572800	H	-1.96344000	-2.10017900	-1.52625600
C	-2.09008400	-0.47539600	-1.16448500	H	-3.72097800	-2.15751800	0.17000000
C	-3.51431700	-0.30614300	-0.56218700	H	-4.29556900	-0.27939000	1.62752200
C	-3.57104100	-0.50787800	0.98331900	H	-3.07009400	0.76507300	0.87494100
C	-2.81544200	-1.78415300	1.40224000	H	-2.44903300	-1.78912000	2.48986900
H	-0.96253000	-0.69171300	1.34498900	H	-2.22350200	-0.11613400	3.05051400
H	-0.70753700	-3.73930200	1.05654900	C	-4.27496300	-0.53533300	-1.13427200
H	-0.57867200	-2.87088400	2.60524300	O	-5.35717800	-1.12235100	-1.40683300
H	1.71875500	-3.16407700	1.62507800	O	-3.91827000	0.57324300	-1.64491600
H	1.25268600	-1.45047700	1.70832000	H	-2.44673600	1.49454100	-1.22699000
H	1.29639200	-3.28351600	-0.76062000	N	3.21302500	-0.26273600	-0.88500400
H	0.29085600	-1.54448300	-2.11491600	C	3.00404400	-1.42109200	-0.25333200
H	0.41703200	-0.34533700	-0.81694000	N	4.10570200	-2.15499900	-0.41422400
H	-1.62894000	-2.60776100	-0.95151700	C	4.46771600	-0.26159100	-1.45951000
H	-1.51613700	0.44517100	-0.99378500	C	5.03547600	-1.45915900	-1.16162000
H	-2.18317000	-0.60074800	-2.25485600	H	4.83830400	0.58046300	-2.02154500
H	-4.19325600	-1.03743900	-1.02287200	H	5.99787700	-1.87575500	-1.41049000
H	-4.62643300	-0.55285300	1.29023100	H	4.22352500	-3.08931700	-0.03450200
H	-3.11361500	0.35272900	1.49509400	O	-1.66752100	2.08321500	-1.08282500
H	-3.27272600	-2.67531500	0.93914600	H	-1.80426600	2.48144300	-0.21215000
H	-2.87622700	-1.90624600	2.49457400	H	0.18774700	1.67882300	-1.06837700
C	-4.03881000	1.07746600	-0.89581300	O	1.13451300	1.78340600	-0.84268100
O	-5.11556900	1.24526600	-1.47049200	H	2.51778600	0.49679600	-0.92510200
O	-3.31416900	2.11581100	-0.53786700	C	1.21601300	2.58715400	0.32597600
H	-2.37859600	1.97637600	-0.00186900	H	0.50502500	2.24396200	1.08829800
N	2.85571300	-0.33299200	-0.33220500	H	2.22985500	2.48660300	0.72446800
C	2.60509300	-1.62953500	-0.52033900	C	0.93923000	4.03691000	-0.02360400
N	3.75660700	-2.21866500	-0.85830800	F	1.03377500	4.79477000	1.15457500
C	4.19595200	-0.09405200	-0.55197300	H	1.67611200	4.42812900	-0.72897400
C	4.76975800	-1.28121300	-0.88705800	H	-0.07080000	4.16939900	-0.42052000
H	4.62507900	0.89118800	-0.45825200				
H	5.78465000	-1.54067900	-1.14093700				
H	3.85157400	-3.20802700	-1.06477700				
O	-1.20626700	2.06611200	0.71571300	<b>(6) Carboxylic group – CH<sub>2</sub>FCH<sub>2</sub>OH – H<sub>2</sub>O –</b>			
H	-1.39484800	1.84018000	1.63619600	<b>Imidazole</b>			
H	-0.08665500	1.73392700	0.50194700	<b>Reactant</b>			
O	1.10541500	1.48175000	0.35783600	C	-0.24656200	-1.06803900	1.42778200
				C	0.94685000	-1.18539200	2.39227300

C	2.18218200	-0.50263000	1.77623600	H	1.06028800	-0.26712400	-0.92162000
C	2.56207700	-1.14469700	0.41008400	H	0.23136200	-3.06750100	-0.01702100
C	1.33754200	-1.22448700	-0.54227600	H	-0.97988300	-0.60601100	-1.35639200
C	0.06963300	-1.81426700	0.11232000	H	-0.96057800	-2.25566700	-1.99134700
C	-1.09159200	-1.67193600	-0.89653600	H	-2.74328400	-2.98207000	-0.57694100
C	-2.48652400	-2.00902600	-0.29411000	H	-3.64771400	-1.85800100	1.34709200
C	-2.72650200	-1.31843000	1.08249700	H	-2.69409700	-0.38679100	1.06913500
C	-1.55325600	-1.60191600	2.03952900	H	-1.48426000	-3.12087900	1.81459000
H	-0.39263300	0.00445800	1.18793500	H	-1.67335800	-1.72057200	2.89657800
H	1.15576100	-2.25047200	2.59388900	C	-3.52224100	-1.16409800	-1.34374600
H	0.70063700	-0.70824500	3.35337000	O	-4.47894800	-1.72157800	-1.87572000
H	3.04673000	-0.56384000	2.45441700	O	-3.36765000	0.14175500	-1.48099900
H	1.95866200	0.56545200	1.61917700	H	-2.53348300	0.60216400	-1.03091700
H	2.94067800	-2.16318600	0.59716100	N	3.22361400	0.99070700	-0.60164800
H	1.61301900	-1.81197600	-1.43313900	C	3.54038300	-0.26081800	-0.26886200
H	1.09107500	-0.20733700	-0.88460900	N	4.85553000	-0.41555200	-0.46000700
H	0.22870000	-2.88010100	0.35283500	C	4.36556000	1.64590600	-1.01154400
H	-1.08289000	-0.63449600	-1.26149900	C	5.39834600	0.76444100	-0.92551400
H	-0.91337300	-2.32559500	-1.76463300	H	4.34857000	2.67539200	-1.33266600
H	-2.56595100	-3.09639400	-0.15415200	H	6.44784400	0.86327500	-1.15061200
H	-3.67596600	-1.68322400	1.50140300	H	5.36070900	-1.27850200	-0.28675200
H	-2.81717600	-0.22831600	0.95032700	O	-1.53536200	1.48094800	-0.46469800
H	-1.46267600	-2.68624900	2.22398500	H	-0.38582300	1.67159900	-0.51565900
H	-1.74232500	-1.11421500	3.00822000	O	0.83290100	1.96974900	-0.50996900
C	-3.58018300	-1.60263200	-1.25260900	H	2.20083900	1.41620700	-0.55488800
O	-4.43531000	-2.36446200	-1.67444000	H	0.88417100	2.93466200	-0.49074600
O	-3.61437300	-0.32126900	-1.63811800	C	-2.05885200	2.17961100	0.64328800
H	-2.87950400	0.23237300	-1.27500000	H	-3.07693300	1.82740700	0.85412700
N	3.49652600	0.88771100	-0.71802300	H	-1.44725800	2.00797600	1.54181100
C	3.64183400	-0.33782000	-0.23707300	C	-2.10255600	3.66454700	0.33605600
N	4.92099500	-0.75523400	-0.38197100	F	-2.64550900	4.33925800	1.44369000
C	4.73926700	1.26262500	-1.18651000	H	-1.10132000	4.07046300	0.16521800
C	5.63828500	0.25194600	-0.98577800	H	-2.74534600	3.87311400	-0.52314900
H	4.90751500	2.22977100	-1.63812900	<b>Product</b>			
H	6.68882800	0.15523400	-1.21060400	C	-0.22747500	-1.09258400	1.42383100
H	5.27901100	-1.65748500	-0.09142300	C	0.96561000	-1.19605700	2.39045000
O	-1.81108500	1.57960900	-0.81956200	C	2.19551700	-0.49484700	1.78467800
H	-0.83204700	1.60490200	-0.82282800	C	2.58015500	-1.14032000	0.41842800
O	0.93917800	2.15017000	-0.57633200	C	1.36193700	-1.21119000	-0.54538400
H	1.84185100	1.74968700	-0.63260100	C	0.10054900	-1.82064400	0.10073300
H	1.06986400	3.10728700	-0.58591500	C	-1.06382900	-1.67295000	-0.90372600
C	-2.27551700	2.29711700	0.31554000	C	-2.45655100	-2.04232800	-0.32346800
H	-3.33890800	2.06916700	0.43281500	C	-2.69972800	-1.38841600	1.06515400
H	-1.74582200	1.98155800	1.22283700	C	-1.52562200	-1.65762400	2.02652300
C	-2.08964300	3.78524600	0.09066100	H	-0.39499000	-0.02097300	1.19180200
F	-2.59447600	4.46225900	1.21127400	H	1.18940700	-2.25818300	2.59055400
H	-1.03281200	4.04901700	-0.00576200	H	0.71329400	-0.72310700	3.35174600
H	-2.64724100	4.12819200	-0.78414900	H	3.05881800	-0.54944200	2.46373800
<b>TS</b>				H	1.95921700	0.57059800	1.62737700
C	-0.20176400	-1.43142500	1.31878400	H	2.96681000	-2.15487400	0.60079700
C	1.00653300	-1.71091300	2.22851500	H	1.64568900	-1.78353100	-1.44260300
C	2.20994800	-0.89048500	1.72690800	H	1.10356400	-0.19085800	-0.87168200
C	2.58047800	-1.27246700	0.25962000	H	0.27307100	-2.88720100	0.32862200
C	1.34301900	-1.30292200	-0.68353100	H	-1.08103900	-0.62442800	-1.23554800
C	0.08419400	-1.97681300	-0.09812800	H	-0.86813100	-2.29463900	-1.79251800
C	-1.07806400	-1.66206800	-1.07147900	H	-2.52010600	-3.13536100	-0.21012800
C	-2.50704600	-1.91145700	-0.50379700	H	-3.64397100	-1.77172000	1.48183200
C	-2.67825200	-1.48435900	0.98580300	H	-2.81120400	-0.29952700	0.94076200
C	-1.51936000	-2.01849000	1.84807100	H	-1.41131700	-2.74162800	2.20108300
H	-0.32582800	-0.33229100	1.24917200	H	-1.72315800	-1.18379000	3.00087900
H	1.23958700	-2.78977400	2.22230600	C	-3.54660300	-1.58382900	-1.29127900
H	0.77416100	-1.42625600	3.26618700	O	-4.34863900	-2.43592300	-1.75577800
H	3.09283900	-1.03851900	2.36576100	O	-3.59181600	-0.34195600	-1.57138800
H	1.94290400	0.17879000	1.76625500	H	-2.47220900	0.84105200	-1.08560000
H	3.07165700	-2.25745100	0.26637100	N	3.50839200	0.88484000	-0.73759500
H	1.63032200	-1.78917200	-1.62909200	C	3.65861500	-0.33574800	-0.21655700

N	4.94623200	-0.65806100	-0.34805800	H	-1.50584800	1.91297200	1.74590800
C	4.72163400	1.34788600	-1.20453600	C	1.31065600	2.85468000	0.45330300
C	5.63368200	0.37198000	-0.95849300	H	0.59153000	3.31645300	1.13811900
H	4.82640000	2.31689000	-1.66516800	H	2.32080900	3.03640500	0.84016000
H	6.69027500	0.31408600	-1.16271900	C	-2.41509000	3.46383200	0.54463100
H	5.34666100	-1.53737200	-0.03423300	C	1.16804700	3.45573600	-0.93146000
O	-1.89966400	1.61943900	-0.85560300	F	-2.97859000	4.11046800	1.65550000
H	0.00306400	1.82814300	-0.72789200	F	1.38190300	4.84044300	-0.84373100
O	0.89780200	2.18403600	-0.56054700	H	1.91142900	3.04977600	-1.62331800
H	2.61020800	1.38918300	-0.75968300	H	0.16099300	3.30089700	-1.32978900
H	0.83377400	3.12622900	-0.76553700	H	-1.47619700	3.97180200	0.30802400
C	-2.42084000	2.24897100	0.30391200	H	-3.11672200	3.56418500	-0.28748400
H	-3.47529600	1.98646900	0.44763000	<b>TS</b>			
H	-1.86006400	1.94302500	1.19824500	C	-0.48921700	-2.14764500	1.11674500
C	-2.28609200	3.74459700	0.10974000	C	0.66245400	-2.70719000	1.96929400
F	-2.70965600	4.38377800	1.28510200	C	1.95491200	-1.94164700	1.62887500
H	-1.24475000	4.03095500	-0.06394800	C	2.32489300	-2.10024900	0.12095300
H	-2.91670300	4.10241100	-0.70767500	C	1.11658400	-1.82678100	-0.82116100

**(7) Carboxylic group – CH<sub>2</sub>FCH<sub>2</sub>OH – CH<sub>2</sub>FCH<sub>2</sub>OH – Imidazole**

**Reactant**

C	-0.46827900	-1.96885200	1.23709800	C	-1.86908900	-2.69502400	1.51514300
C	0.69312900	-2.46225500	2.11849900	H	-0.50751000	-1.04770600	1.25013100
C	1.99559600	-1.75279900	1.70090000	H	0.78553900	-3.78666400	1.77527500
C	2.33620200	-2.01518700	0.20450800	H	0.43678000	-2.58385200	3.03942500
C	1.11932200	-1.74039900	-0.72209800	H	2.80143400	-2.28685300	2.24002900
C	-0.20477600	-2.36439600	-0.23442100	H	1.79496700	-0.87354700	1.85114000
C	-1.33039000	-1.85060900	-1.16034600	H	2.70855300	-3.11828000	-0.04262800
C	-2.76295700	-2.18113800	-0.65197100	H	1.37437100	-2.16496800	-1.83681700
C	-2.95065900	-1.85242000	0.86039000	H	0.95190800	-0.74057600	-0.87139700
C	-1.83353300	-2.50863900	1.69379400	H	-0.20601500	-3.54333000	-0.50336500
H	-0.49975400	-0.86200500	1.29508100	H	-1.10651900	-0.73940000	-1.31713100
H	0.79711800	-3.55651800	2.01377700	H	-1.22720600	-2.20724000	-2.29605300
H	0.47884300	-2.24975300	3.17739500	H	-3.11153100	-3.04038700	-1.08234100
H	2.84282600	-2.08018600	2.32225700	H	-3.96214200	-2.26372200	1.02537500
H	1.87106500	-0.66845300	1.85504900	H	-2.88964300	-0.84946100	1.06015200
H	2.64335500	-3.06792500	0.09540800	H	-1.93008700	-3.77100900	1.27737000
H	1.35553200	-2.09839500	-1.73705900	H	-2.02266700	-2.58386300	2.59970200
H	0.96560700	-0.65162900	-0.78862200	C	-3.69329300	-1.03486100	-1.45870000
H	-0.14993500	-3.46608600	-0.28698800	O	-4.68730000	-1.37189900	-2.09750100
H	-1.20716800	-0.76129300	-1.25029000	O	-3.40690500	0.24833000	-1.32569600
H	-1.20448300	-2.27596000	-2.16830300	H	-2.54422700	0.52646200	-0.78415400
H	-2.96140200	-3.25179300	-0.79965800	N	3.20080000	0.19778000	-0.31600000
H	-3.94150800	-2.20493100	1.18157600	C	3.39626800	-1.11679400	-0.21066100
H	-2.91568200	-0.76220400	1.01950900	N	4.69711800	-1.35123700	-0.41016000
H	-1.86048200	-3.60537800	1.57435200	C	4.40442900	0.81367200	-0.58654000
H	-1.99020600	-2.28603800	2.76021300	C	5.35355700	-0.15966700	-0.64563900
C	-3.79188500	-1.42309900	-1.45677600	H	4.48525600	1.88130700	-0.71845500
O	-4.71130300	-1.95492900	-2.05818800	H	6.41296200	-0.11841000	-0.83956300
O	-3.69072100	-0.08880600	-1.48573200	H	5.12038400	-2.27374700	-0.39095100
H	-2.91337800	0.27206400	-0.99148800	O	-1.49125900	1.17245700	-0.04334900
N	3.40427200	0.19327400	-0.27616300	H	-0.32005400	1.22727400	-0.01838500
C	3.46772400	-1.12830100	-0.20889800	O	0.91054900	1.36338300	0.08685300
N	4.70294500	-1.55811500	-0.55097100	O	2.22779600	0.67372800	-0.17550900
C	4.65387600	0.61892200	-0.67554600	C	-2.03229600	1.82209700	1.08704200
C	5.47571700	-0.45974200	-0.85310900	H	-2.92556300	1.28863400	1.43986900
H	4.87984500	1.66646700	-0.81463600	H	-1.30301200	1.83677700	1.90935000
H	6.50615400	-0.54725100	-1.15960400	C	1.23017400	2.70675900	0.36856300
H	4.99845600	-2.52706500	-0.57616200	H	0.55018700	3.13512900	1.11951800
O	-1.70120600	1.31624500	-0.23557300	H	2.24995000	2.77555400	0.77697600
H	-0.72804600	1.23410500	-0.15737200	C	-2.42228500	3.23907100	0.71028900
O	1.03739100	1.46386500	0.39105100	C	1.14980500	3.52431300	-0.90629600
H	1.87612100	0.99601200	0.11801300	F	-2.98574700	3.87219600	1.83201500
C	-2.20023000	2.00645000	0.90324200	F	1.44186300	4.86882100	-0.61147800
H	-3.15729900	1.55571500	1.18704600	H	-1.55535500	3.83031500	0.40092600

H	-3.17773800	3.23881700	-0.08088800	C	1.00320800	-2.50749100	1.73344600
H	1.88345800	3.18218300	-1.64246400	C	1.27660000	-2.86578700	0.24221900
H	0.14411300	3.49390400	-1.33664700	C	0.24322600	-2.19969500	-0.70840300
<b>Product</b>				C	-1.22629300	-2.34962100	-0.26048800
C	-0.36538400	-1.54005600	1.44734100	C	-2.08873100	-1.47132800	-1.19450300
C	0.83454900	-1.76454800	2.38491400	C	-3.56556700	-1.32847500	-0.73091300
C	2.11510100	-1.21098300	1.73276800	C	-3.68637500	-0.98694700	0.78577700
C	2.39102500	-1.90558900	0.36377400	C	-2.86229500	-1.97759700	1.62985200
C	1.14159900	-1.89891600	-0.56230600	H	-1.05654200	-0.84769300	1.28541900
C	-0.16094800	-2.33707300	0.13816300	H	-0.72257800	-3.82409800	1.98576100
C	-1.32806200	-2.08108000	-0.83937800	H	-0.63204400	-2.49804400	3.16701200
C	-2.72876600	-2.30328100	-0.21516200	H	1.67882100	-3.09634900	2.37188800
C	-2.87100400	-1.57667600	1.15331000	H	1.23477800	-1.44167500	1.89417100
C	-1.70447400	-1.93247100	2.09754800	H	1.22066700	-3.96111600	0.13050100
H	-0.40655000	-0.46153600	1.18909200	H	0.37317700	-2.61059500	-1.72241100
H	0.94436500	-2.84281400	2.59346200	H	0.45810800	-1.12156200	-0.76311400
H	0.66476800	-1.25599100	3.34616900	H	-1.54378100	-3.40466600	-0.33461900
H	2.98847600	-1.35249500	2.38604500	H	-1.61169400	-0.48129800	-1.23784200
H	1.98917100	-0.12731700	1.57234300	H	-2.07535700	-1.88393300	-2.21528900
H	2.70764900	-2.94308400	0.55124400	H	-4.09482200	-2.27394700	-0.91450900
H	1.34063900	-2.54535000	-1.43130200	H	-4.74836100	-1.01062700	1.07176400
H	0.97998100	-0.87714200	-0.93902100	H	-3.31181200	0.03205000	0.97542400
H	-0.11207400	-3.40986600	0.39594900	H	-3.23946700	-3.00531900	1.49181600
H	-1.24680700	-1.04020600	-1.18569900	H	-2.96490600	-1.72640200	2.69658400
H	-1.22040100	-2.73014100	-1.72380600	C	-4.27319400	-0.26293300	-1.53399400
H	-2.88458500	-3.38046100	-0.05103400	O	-5.30682100	-0.45560400	-2.15366400
H	-3.83625100	-1.85025300	1.60601200	O	-3.74250900	0.96630800	-1.54070600
H	-2.87739700	-0.48674800	0.99146100	H	-2.90219000	1.05697400	-1.02975100
H	-1.70459700	-3.01531100	2.31201100	N	3.01948400	-1.14021600	-0.25067600
H	-1.82491100	-1.40486000	3.05633300	C	2.64987600	-2.40724000	-0.13340700
C	-3.81461000	-1.79371600	-1.16057900	N	3.69980900	-3.22342200	-0.37152000
O	-4.76359500	-2.56118500	-1.46803800	C	4.35962800	-1.15361600	-0.57645400
O	-3.71334200	-0.59424600	-1.57887700	C	4.79989700	-2.44539600	-0.65619700
H	-2.53559800	0.49612900	-1.13878500	H	4.91766600	-0.24182700	-0.73305200
N	3.42563100	0.03717000	-0.84105700	H	5.76341500	-2.87343200	-0.88392400
C	3.50453300	-1.18954600	-0.31760100	H	3.66819800	-4.23569300	-0.34452500
N	4.75966400	-1.60478700	-0.49354000	O	-1.40730000	1.66326900	-0.24318800
C	4.65011900	0.40810700	-1.35822000	H	-0.50870200	1.28197700	-0.27865300
C	5.49671300	-0.63113600	-1.13872100	O	1.28762700	0.84812800	0.24910700
H	4.80541700	1.36486200	-1.83033600	H	1.93369100	0.09744800	0.03435400
H	6.53831200	-0.76786000	-1.37935200	H	-1.57878200	2.29869900	1.01823200
H	5.10574400	-2.51024700	-0.18978300	C	-2.61264100	2.14519600	1.34313700
O	-1.95054400	1.25747300	-0.87023800	H	-0.90711600	1.85989900	1.76504200
H	-0.07978600	1.30156700	-0.76687800	C	2.02591400	1.94594200	0.71322300
O	0.86805900	1.47444200	-0.59473200	H	1.40565700	2.56918100	1.36424800
H	2.56309200	0.59702800	-0.84572100	H	2.92542600	1.64162400	1.26142300
C	-2.64793700	2.02615400	0.09735500	C	-1.30317500	3.78236400	0.86777400
H	-3.69953900	1.72041900	0.14504900	C	2.47222100	2.79976000	-0.45282500
H	-2.20353200	1.89058100	1.09252300	F	-1.46696200	4.39008600	2.12252900
C	0.98624900	2.43987100	0.44254900	F	3.11167800	3.90914100	-0.03686900
H	0.02725500	2.58917500	0.95015700	F	1.43884100	3.20081400	-1.21796600
H	1.71363400	2.08261300	1.17999300	F	3.31668800	2.13852300	-1.26977200
C	-2.55497500	3.48124300	-0.31030100	H	-0.27803400	3.97260500	0.53910500
C	1.47325000	3.73997100	-0.16583900	H	-2.01108600	4.24934700	0.17841000
F	-3.14964600	4.26392600	0.69175300	<b>TS</b>			
F	1.63259000	4.68152500	0.86254600	C	-0.66402800	-2.54486700	0.91088200
H	2.44659200	3.60759000	-0.64667100	C	0.43980000	-3.29865500	1.67292400
H	0.75325300	4.14675300	-0.88075500	C	1.76931900	-2.53514400	1.52213700
H	-1.51389000	3.80348100	-0.40535200	C	2.18038100	-2.41864200	0.02117300
H	-3.09247300	3.67221800	-1.24247300	C	1.01760800	-1.90332600	-0.87355100
				C	-0.35325800	-2.55682200	-0.60176600
				C	-1.39846900	-1.73511100	-1.39315000
				C	-2.88104300	-2.00013500	-1.00064900
				C	-3.11134700	-2.16193100	0.53448800
				C	-2.07111700	-3.11440000	1.15466000
				H	-0.65873200	-1.49168900	1.25520200
<b>(8) Carboxylic group – CH<sub>2</sub>FCH<sub>2</sub>OH – CF<sub>3</sub>CH<sub>2</sub>OH – Imidazole</b>							
<b>Reactant</b>							
C	-1.38378100	-1.90504300	1.21109100				
C	-0.46966200	-2.75666700	2.10945300				

H	0.53479900	-4.32561000	1.28057000	H	-1.05857600	-1.89816700	-2.35129100
H	0.17987700	-3.37169900	2.74015400	H	-2.74088000	-3.35093600	-1.35677600
H	2.58201000	-3.02773800	2.07535800	H	-3.79699400	-2.98074900	0.81255300
H	1.64220700	-1.52378900	1.94309300	H	-2.90525600	-1.46457400	1.06687300
H	2.51750600	-3.40499600	-0.33067200	H	-1.61014000	-4.26042500	0.89078500
H	1.29861300	-2.03165800	-1.93063300	H	-1.84747700	-3.30661300	2.37340500
H	0.88906800	-0.82466100	-0.69774400	C	-3.70940600	-1.43667400	-1.48994300
H	-0.35397000	-3.60689900	-0.94116900	O	-4.58414000	-1.92954200	-2.24835400
H	-1.15998100	-0.67455000	-1.23385600	O	-3.67562100	-0.20765700	-1.15322100
H	-1.28349800	-1.92963000	-2.47086400	H	-2.52172700	0.44780200	-0.15062800
H	-3.22585300	-2.91943500	-1.49399500	N	3.42565800	0.18511800	0.10442300
H	-4.13327200	-2.53588800	0.69363900	C	3.54111200	-1.12656100	-0.11596700
H	-3.03125500	-1.18410300	1.03577900	N	4.80273000	-1.34633700	-0.48722500
H	-2.15138200	-4.12105600	0.70897800	C	4.63120400	0.81228700	-0.13244300
H	-2.25914400	-3.21102200	2.23477400	C	5.50596400	-0.15757200	-0.50673300
C	-3.74784100	-0.86253900	-1.49993000	H	4.75974200	1.87603600	-0.01232100
O	-4.71705900	-1.04300400	-2.23405600	H	6.54643300	-0.11315300	-0.78416500
O	-3.44534600	0.35961100	-1.10195300	H	5.17337200	-2.26242800	-0.72178600
H	-2.59776500	0.49968800	-0.47739200	O	-1.90975100	0.92922600	0.47445100
N	3.20203900	-0.13273300	0.05156000	H	-0.09370700	0.99471400	0.74758800
C	3.31192100	-1.45547200	-0.09036000	O	0.79102200	1.34065100	0.99562200
N	4.60209700	-1.72680600	-0.30088200	H	2.55167500	0.63327400	0.40308200
C	4.44724100	0.44803400	-0.07229300	C	-2.70094700	1.66642000	1.38964200
C	5.33534700	-0.55699400	-0.29633900	H	-3.53665800	1.05968800	1.76119500
H	4.59363200	1.51372200	0.00306100	H	-2.06926200	1.94284600	2.24013900
H	6.40137600	-0.54856100	-0.45519400	C	0.75216400	2.74368200	0.88407700
H	4.97144400	-2.66185600	-0.44315300	H	-0.21161800	3.16133600	1.19326900
O	-1.55755500	0.93475300	0.39676600	H	1.54839800	3.17621700	1.49461100
H	-0.38527500	0.99837600	0.40484500	C	-3.22756100	2.91251200	0.70404100
O	0.83879300	1.13917300	0.51631700	C	1.00252700	3.15317000	-0.55053500
H	2.28372800	0.36533400	0.22524600	F	-3.96842300	3.66016100	1.63317300
C	-2.08449500	1.59565600	1.52724500	F	0.96649000	4.48907700	-0.69462400
H	-2.85721400	0.98148300	2.00981000	F	0.09345700	2.63361300	-1.39643400
H	-1.29298600	1.77527100	2.26738400	F	2.21062100	2.73871500	-0.98660000
C	1.12990400	2.48372300	0.73855500	H	-2.40883100	3.54420900	0.34682000
H	0.35824600	3.00174500	1.32620100	H	-3.89592700	2.65944300	-0.12390300
H	2.09279800	2.61441100	1.25201700				
C	-2.68885000	2.91740100	1.09112400				
C	1.23736200	3.22511300	-0.57537600				
F	-3.18765500	3.58808100	2.22128300				
F	1.52171000	4.53109400	-0.39554300				
F	0.09556100	3.16708200	-1.29126700				
F	2.20623200	2.71967900	-1.36816100				
H	-1.94048900	3.56580200	0.62585400				
H	-3.52735200	2.76276100	0.40589900				
<b>Product</b>				<b>(9) Carboxylic group – CF<sub>3</sub>CH<sub>2</sub>OH – CH<sub>2</sub>FCH<sub>2</sub>OH –</b>			
C	-0.35251200	-2.49267700	1.01850100	<b>Imidazole</b>			
C	0.84057400	-3.11624200	1.76575100	<b>Reactant</b>			
C	2.09575000	-2.24469200	1.56637200	C	0.39740300	-2.33430800	1.15883700
C	2.44422500	-2.11750100	0.05258500	C	1.68188800	-2.55931500	1.97720300
C	1.21677100	-1.65166700	-0.78127200	C	2.71711700	-1.47230000	1.62391900
C	-0.06349000	-2.46346400	-0.49952500	C	3.06270500	-1.48401800	0.10534600
C	-1.22415900	-1.79245000	-1.26682500	C	1.78063800	-1.47286900	-0.77167900
C	-2.62858300	-2.34979100	-0.91300300	C	0.71109400	-2.50006600	-0.34552900
C	-2.83942500	-2.47186800	0.62392800	C	-0.54229700	-2.25175000	-1.21333400
C	-1.67457100	-3.23282000	1.28859600	C	-1.80856800	-3.01278200	-0.72880900
H	-0.46596700	-1.44610800	1.36494800	C	-2.03091300	-2.88372600	0.80963800
H	1.01968500	-4.13828800	1.38948700	C	-0.74815900	-3.27498400	1.56972200
H	0.61569100	-3.19165100	2.84036400	H	0.06058100	-1.29120700	1.32651200
H	2.96137300	-2.66407500	2.09947700	H	2.08611300	-3.56355500	1.76064700
H	1.90124400	-1.24013300	1.97897700	H	1.45501300	-2.51892900	3.05363600
H	2.79535200	-3.09271400	-0.31741600	H	3.64352900	-1.60147400	2.20322400
H	1.47124300	-1.69831500	-1.85178700	H	2.29536300	-0.48744000	1.88517900
H	0.99690000	-0.59752300	-0.54098800	H	3.64664400	-2.39183100	-0.11701800
H	0.06648100	-3.50419000	-0.84505900	H	2.06431200	-1.63433500	-1.82413200
H	-1.19249300	-0.71706200	-1.03894000	H	1.31876500	-0.47437900	-0.70590800
				H	1.08272500	-3.52741000	-0.50473800
				H	-0.73196300	-1.16900300	-1.20393700
				H	-0.33357800	-2.53533200	-2.25662200
				H	-1.70989800	-4.07952300	-0.97370000
				H	-2.87537100	-3.52500300	1.10093200
				H	-2.29298200	-1.84495100	1.07194900
				H	-0.47460900	-4.32028400	1.34382400
				H	-0.92534400	-3.20341200	2.65364400

C	-3.03219500	-2.50275900	-1.45209900	H	4.14695000	2.82046700	-0.68792800
O	-3.79737400	-3.21081400	-2.08518600	H	6.51046700	1.36004300	-0.78020400
O	-3.29397800	-1.19132200	-1.36574400	H	5.78983400	-1.04243400	-0.31159000
H	-2.61778400	-0.68566100	-0.86039600	O	-1.46081000	0.58777700	-0.06914700
N	3.43364600	0.96775300	-0.20233100	O	-0.36036700	0.96516300	-0.07960200
C	3.88368700	-0.27780700	-0.22593700	O	0.79951500	1.43860000	-0.00984600
N	5.19075400	-0.29684000	-0.57063300	H	2.24466800	1.09591700	-0.16977400
C	4.49867100	1.77233900	-0.54780600	C	-2.06918200	0.98781200	1.12127200
C	5.60294500	0.99986200	-0.78087400	H	-2.66159500	0.18220100	1.57478000
H	4.40470600	2.84733000	-0.60639100	H	-1.33883000	1.33699800	1.86354600
H	6.61375300	1.24231000	-1.06900400	C	0.75069200	2.82879800	0.21776900
H	5.75751600	-1.13138000	-0.66573100	H	0.01808400	3.08534700	0.99584600
O	-1.62906700	0.58324200	0.02447400	H	1.73109600	3.18959200	0.56378300
H	-0.67393800	0.81357100	0.08951100	C	-3.03063800	2.12740900	0.86233700
O	0.88083600	1.55441600	0.58990000	C	0.38040900	3.54369500	-1.06768400
H	1.80038600	1.30152800	0.28139100	F	-3.64288600	2.52671600	1.99523200
C	-2.30612500	1.11996000	1.13465400	F	-4.00226000	1.78270500	-0.00730000
H	-2.96967300	0.36887700	1.57535600	F	-2.42574600	3.21334300	0.34023100
H	-1.61529400	1.49081300	1.89819200	F	0.25816700	4.92113500	-0.80774200
C	0.76078200	2.96440900	0.47553000	H	1.15494600	3.42250900	-1.83047300
H	-0.08240800	3.28450900	1.09522000	H	-0.58235400	3.19499500	-1.45145500
H	1.66881900	3.46224900	0.83729700	<b>Product</b>			
C	-3.16937300	2.27307500	0.67672000	C	0.73157000	-2.30517300	1.10067700
C	0.50501200	3.33198900	-0.97374100	C	2.05081000	-2.47605300	1.87566100
F	-2.44937400	3.28080000	0.14863600	C	2.98745500	-1.28814900	1.58057300
F	-3.88082600	2.78530100	1.69690800	C	3.29237600	-1.18622500	0.05527800
F	-4.04803700	1.89357400	-0.27108200	C	1.99001800	-1.20366000	-0.79840800
F	0.26392100	4.71278300	-1.04923400	C	1.01133600	-2.33283700	-0.41853300
H	1.37281700	3.11331700	-1.60294200	C	-0.29000200	-2.11473900	-1.22171700
H	-0.37936300	2.81822000	-1.36041000	C	-1.46864000	-3.02615000	-0.78728200
<b>TS</b>				C	-1.64602900	-3.05758400	0.75821300
C	0.32703100	-2.38282000	1.11140500	C	-0.31254600	-3.37592100	1.46376600
C	1.57161300	-2.60260200	1.98787000	H	0.30823300	-1.31136700	1.35080400
C	2.61009200	-1.51046300	1.66821600	H	2.53001800	-3.42670200	1.58433800
C	3.03981300	-1.57007500	0.17023800	H	1.85062700	-2.52128200	2.95677600
C	1.81967900	-1.62195000	-0.79359400	H	3.93529600	-1.38001100	2.13022200
C	0.69282800	-2.58953300	-0.37471700	H	2.49320500	-0.36141100	1.91619300
C	-0.51471200	-2.28203000	-1.29079600	H	3.93714600	-2.02808000	-0.23902400
C	-1.86140500	-2.91408400	-0.83627100	H	2.26276000	-1.27562600	-1.86298000
C	-2.10137500	-2.84341900	0.70432500	H	1.45876300	-0.24701500	-0.65915800
C	-0.85220200	-3.29603800	1.48386800	H	1.45077800	-3.31494900	-0.66721800
H	-0.00030600	-1.33213700	1.24484900	H	-0.58103600	-1.06191900	-1.09713800
H	1.99247100	-3.60568200	1.80036400	H	-0.09191500	-2.27225400	-2.29408600
H	1.29848300	-2.55037300	3.05289900	H	-1.27559400	-4.05294300	-1.13339300
H	3.50523000	-1.60657800	2.29981700	H	-2.41256800	-3.80530800	1.01338500
H	2.15732400	-0.52607300	1.87476900	H	-2.00787900	-2.07681900	1.10827100
H	3.67497900	-2.45606000	0.01910300	H	0.05611600	-4.36966300	1.15556800
H	2.17726800	-1.86937200	-1.80542200	H	-0.46177100	-3.39944000	2.55421500
H	1.36911800	-0.61958200	-0.84356700	C	-2.76581200	-2.53239700	-1.42373000
H	1.01549700	-3.63683000	-0.50245700	O	-3.44789100	-3.32199800	-2.12399500
H	-0.61497600	-1.18866400	-1.32623300	O	-3.10504000	-1.32394100	-1.19211300
H	-0.29840700	-2.61968400	-2.31615300	H	-2.25193100	-0.28868200	-0.33827200
H	-1.88648100	-3.97080200	-1.13699600	N	3.50069300	1.30575200	-0.04088100
H	-2.97140200	-3.46893800	0.95185100	C	4.01445400	0.08618100	-0.21992200
H	-2.34108200	-1.81065400	1.00129100	N	5.25350200	0.25202600	-0.68395500
H	-0.60570500	-4.34548900	1.24666000	C	4.42557100	2.26351200	-0.40003400
H	-1.05281500	-3.23680800	2.56448100	C	5.53804900	1.59819000	-0.80734200
C	-3.01265200	-2.21824600	-1.52907800	H	4.21207200	3.31851200	-0.33644000
O	-3.86723700	-2.81507900	-2.17211700	H	6.48953000	1.95193100	-1.16904200
O	-3.10608500	-0.89829700	-1.40032600	H	5.87838400	-0.51464900	-0.91451300
H	-2.37668200	-0.42767100	-0.86639300	O	-1.80378800	0.43902000	0.20171500
N	3.31584400	0.87640400	-0.27013300	O	0.03458300	0.93859600	0.65305900
C	3.83039900	-0.34787800	-0.15260200	H	0.74053300	1.56225800	0.91354400
N	5.15042800	-0.25502100	-0.34420500	H	2.54081600	1.46840400	0.29689900
C	4.33222900	1.76762800	-0.54371100	C	-2.69614800	0.88716100	1.18416200
C	5.49273900	1.05910000	-0.59180200	H	-3.31504900	0.07816100	1.59040700

H	-2.14108300	1.35984700	2.00036400	C	-2.55737400	-2.26765400	-1.62166000
C	0.29882000	2.87568300	0.59100600	C	-3.37198200	-1.02538500	0.29369600
H	-0.67203000	3.08714400	1.05252000	C	-3.47950300	-3.27695500	-1.35468900
H	1.03680900	3.57326800	0.99634800	H	-1.86862100	-2.34162000	-2.45827100
C	-3.63038300	1.92892100	0.60729700	C	-4.29701600	-2.03878900	0.54543900
C	0.20844600	3.02769000	-0.91538100	H	-3.31517400	-0.15098400	0.93658400
F	-2.96809900	2.97731300	0.08048100	C	-4.35491400	-3.16857000	-0.27222000
F	-4.46024600	2.41854200	1.54824800	H	-3.51394000	-4.15233100	-1.99658900
F	-4.40077200	1.43235200	-0.38077200	H	-4.97154200	-1.94438100	1.39147100
F	-0.25252600	4.32102600	-1.20122900	H	-5.07360800	-3.95560600	-0.06771300
H	1.18853100	2.91265600	-1.38730200	<b>TS</b>			
H	-0.50396200	2.31863700	-1.34641400	C	-1.26093700	-2.37063900	1.06849200

**(10) Carboxylic group – CF<sub>3</sub>CH<sub>2</sub>OH – C<sub>6</sub>H<sub>5</sub>OH – Imidazole**  
**Reactant**

C	1.93248700	1.69198900	1.20677500	C	-1.04412100	-2.77774300	-0.40683200
C	1.24705600	2.69878500	2.14728400	C	-1.89739500	-1.89909600	-1.35644400
C	-0.23043300	2.85997800	1.73861000	C	-3.37520400	-1.68200900	-0.91097900
C	-0.35727300	3.36627700	0.27051000	C	-3.55172300	-1.47162300	0.62467000
C	0.48504900	2.49988300	-0.70106200	C	-2.74830400	-2.50567600	1.43329900
C	1.93415600	2.24229000	-0.23585100	H	-0.97921600	-1.30474700	1.17566600
C	2.55895200	1.22650600	-1.22041200	H	-0.51260800	-4.27079700	1.82551800
C	3.91392800	0.62332800	-0.74610500	H	-0.54561600	-2.96686200	3.03654400
C	3.90405300	0.20184100	0.75536800	H	1.82745800	-3.37796400	2.31943100
C	3.36371800	1.33927300	1.64244200	H	1.27666100	-1.75439900	1.84064300
H	1.33185900	0.76248400	1.21273700	H	1.52206300	-4.25167400	0.05547800
H	1.76847300	3.67037000	2.09461000	H	0.62191800	-2.94727100	-1.81837000
H	1.30766500	2.34398200	3.18756700	H	0.57776800	-1.46654300	-0.84268200
H	-0.75316500	3.55880600	2.40843200	H	-1.32197300	-3.84080300	-0.51042300
H	-0.73237500	1.87991100	1.82133400	H	-1.39455400	-0.92492400	-1.42139900
H	-0.00674100	4.41060100	0.23107500	H	-1.89651700	-2.32966600	-2.37013400
H	0.48290200	2.96770900	-1.69850500	H	-3.97763500	-2.55318600	-1.20430200
H	0.00262800	1.51548300	-0.80013500	H	-4.62491800	-1.52591800	0.86069100
H	2.51416800	3.18140700	-0.24402700	H	-3.20413900	-0.46648300	0.90486800
H	1.82474700	0.42091900	-1.36526400	H	-3.09849900	-3.52994000	1.21740400
H	2.71063600	1.70402900	-2.20080000	H	-2.89387000	-2.32337600	2.50951800
H	4.71072900	1.36536700	-0.89200400	C	-3.94990400	-0.46682600	-1.61001800
H	4.92643800	-0.07749100	1.04889400	O	-4.97057800	-0.49882900	-2.28951400
H	3.26622900	-0.68568600	0.89686500	O	-3.31060600	0.67990100	-1.43091900
H	4.01046700	2.23006400	1.56445000	H	-2.41292900	0.65579400	-0.90576100
H	3.36898000	1.01551900	2.69486800	N	3.08731000	-1.29343300	-0.36326000
C	4.25997000	-0.58002200	-1.59066900	C	2.82090800	-2.58278300	-0.12392300
O	5.27736100	-0.68296800	-2.25416200	N	3.98781700	-3.23222200	-0.13708700
O	3.39300900	-1.60435000	-1.58208000	C	4.44671500	-1.12511200	-0.52583900
H	2.58163200	-1.43695500	-1.05279200	C	5.01973800	-2.34913200	-0.38485100
N	-2.45151100	2.23110800	-0.51552600	H	4.88247200	-0.16032200	-0.73395000
C	-1.79526400	3.31943200	-0.13871700	H	6.04727400	-2.66987200	-0.44040800
N	-2.63691100	4.37615800	-0.10121600	H	4.08143800	-4.23168500	0.01665400
C	-3.76083100	2.61295900	-0.72258000	O	-1.15693800	0.99108000	-0.12859000
C	-3.89283000	3.94911600	-0.46912500	H	-0.07893100	0.82443100	-0.46949800
H	-4.51342800	1.90812400	-1.04619700	O	1.13235900	0.66009300	-0.75288000
H	-4.73610200	4.61958200	-0.52035000	H	2.36935500	-0.55298400	-0.43183500
H	-2.37638600	5.32163900	0.15475900	C	-1.14575300	1.44847700	1.19247500
O	0.83145800	-1.46296500	-0.31827100	H	-1.85740600	0.90364300	1.82457900
H	0.08820500	-0.95376900	-0.70218900	H	-0.14492800	1.36160600	1.63969500
O	-1.55579400	-0.19151200	-1.05972600	C	-1.53856200	2.90897800	1.25250300
H	-1.87875300	0.73906100	-0.77208500	F	-0.65283700	3.71296700	0.63343400
C	0.53097800	-1.75089700	1.02703800	F	-1.63116000	3.33938300	2.52785200
H	1.36712800	-1.47546600	1.67736500	F	-2.73541000	3.13513000	0.67221200
H	-0.37586900	-1.23778700	1.36538500	C	1.77473300	1.84393400	-0.65269100
C	0.31681800	-3.23855200	1.18360900	C	1.44688000	2.90966700	-1.50902100
F	-0.76146600	-3.68411600	0.51623400	C	2.77489200	2.03603300	0.31537300
F	0.14708400	-3.56971500	2.47783800	C	2.09508200	4.13749600	-1.38810600
F	1.37136300	-3.94269400	0.72840700	H	0.67055800	2.75897300	-2.25565500
C	-2.50130200	-1.14329000	-0.79446200	C	3.42547300	3.26610000	0.42435600

H	3.02216800	1.21834400	0.99092800
C	3.08930300	4.32499400	-0.42294100
H	1.82363800	4.95335200	-2.05341500
H	4.19470300	3.39937700	1.18103700
H	3.59372600	5.28243400	-0.33224300
<b>Product</b>			
C	0.40448800	-2.32117400	1.36935500
C	1.68487800	-2.40957500	2.21965100
C	2.76815700	-1.48220200	1.63613000
C	3.10067400	-1.88591400	0.16708200
C	1.81877200	-1.96422900	-0.70859200
C	0.69199300	-2.80261300	-0.07203100
C	-0.56810400	-2.64801200	-0.95075000
C	-1.83431700	-3.30786200	-0.34625300
C	-2.03825900	-2.89621500	1.13877600
C	-0.75963500	-3.13095800	1.96793800
H	0.09355100	-1.25761400	1.31893800
H	2.04553500	-3.45257400	2.23861000
H	1.46859200	-2.11456900	3.25789200
H	3.68833900	-1.51835600	2.23715900
H	2.39655800	-0.44384600	1.65277500
H	3.60606900	-2.86411600	0.17360700
H	2.08236500	-2.37071800	-1.69740600
H	1.42460000	-0.94674100	-0.86203200
H	0.99302000	-3.86442700	-0.02579000
H	-0.75020700	-1.57073000	-1.08286300
H	-0.37996300	-3.07537700	-1.94928400
H	-1.72881100	-4.40248200	-0.39359700
H	-2.88451600	-3.46075400	1.55884500
H	-2.29678300	-1.82607700	1.18286300
H	-0.49887700	-4.20381900	1.97270100
H	-0.93109000	-2.82659800	3.01218700
C	-3.06764400	-2.90203900	-1.14966200
O	-3.80178900	-3.79752200	-1.63888700
O	-3.30426100	-1.65414400	-1.27174600
H	-2.41553700	-0.42235600	-0.76874300
N	3.72520500	0.37935800	-0.71669900
C	4.03391000	-0.88529700	-0.41707400
N	5.32425500	-1.04533000	-0.71261200
C	4.83646100	1.03641500	-1.20485400
C	5.85047300	0.13275400	-1.20451000
H	4.80380200	2.07037800	-1.50810300
H	6.88115700	0.21620700	-1.50823500
H	5.82900900	-1.91817300	-0.58919200
O	-1.94118000	0.42949600	-0.50777200
H	-0.08768000	0.84477500	-0.41063200
O	0.76451600	1.18699900	-0.06483200
H	2.79250000	0.77639000	-0.58518100
C	-2.57006200	0.99411800	0.61192900
H	-2.92280000	0.23975400	1.32441300
H	-1.87633800	1.67000000	1.12299700
C	-3.77346100	1.81013000	0.19269800
F	-3.45573200	2.80563300	-0.65670500
F	-4.37164200	2.37646400	1.25850300
F	-4.70229300	1.06044200	-0.43167000
C	0.73386600	2.55179200	0.03970100
C	-0.22526000	3.32217800	-0.62041900
C	1.71547400	3.16162900	0.82349400
C	-0.20656600	4.70915400	-0.47851900
H	-0.97567300	2.83174900	-1.23388200
C	1.72931700	4.54950000	0.94818400
H	2.45029000	2.54243000	1.33069600
C	0.76846800	5.33050700	0.30292800
H	-0.95926500	5.30388200	-0.98789100
H	2.49300900	5.02120300	1.55938100
H	0.77989500	6.41036700	0.40847400

**(11) Carboxylic group – C<sub>6</sub>H<sub>5</sub>OH – CF<sub>3</sub>CH<sub>2</sub>OH – Imidazole**

<b>Reactant</b>			
C	-0.87682200	-2.03934400	1.03126200
C	0.03820200	-2.53711400	2.16271600
C	1.46828700	-2.00789200	1.94410800
C	2.04249200	-2.48650900	0.57860800
C	1.06718600	-2.17205300	-0.58920600
C	-0.39523600	-2.59388800	-0.32652000
C	-1.25617900	-2.02637900	-1.47753100
C	-2.78789500	-2.17153600	-1.24268700
C	-3.22629500	-1.72765800	0.18669700
C	-2.35335000	-2.40452400	1.26019300
H	-0.80131000	-0.93563700	0.98921900
H	0.03472700	-3.64070200	2.18446700
H	-0.34340200	-2.18541000	3.13438600
H	2.14070300	-2.33541100	2.75101800
H	1.44608100	-0.90492200	1.95611700
H	2.20804800	-3.57498300	0.63049200
H	1.43997200	-2.65094600	-1.50866400
H	1.06726500	-1.08481300	-0.76320200
H	-0.47641800	-3.69460900	-0.30024900
H	-0.99037700	-0.96348600	-1.58664400
H	-0.99370600	-2.52522700	-2.42311300
H	-3.07515700	-3.22304200	-1.38213900
H	-4.28807300	-1.97726100	0.32551100
H	-3.12843100	-0.63467800	0.29728300
H	-2.47647600	-3.50058800	1.22358900
H	-2.67533000	-2.06610800	2.25743200
C	-3.54785600	-1.36343100	-2.26696500
O	-4.38575400	-1.82453500	-3.02230500
O	-3.28648300	-0.04822200	-2.32638900
H	-2.59108700	0.24096100	-1.69802200
N	3.49776100	-0.51105800	0.08583900
C	3.34966000	-1.80711200	0.32056000
N	4.55257300	-2.42171900	0.31333300
C	4.85029600	-0.29595000	-0.07634900
C	5.52315600	-1.47763300	0.06352200
H	5.25103100	0.68656200	-0.28036100
H	6.57055100	-1.72927700	0.00955100
H	4.70299600	-3.41148500	0.47051000
O	-1.34613400	1.25859200	-0.58672300
H	-0.41549400	1.00459000	-0.39971700
O	1.37513700	1.10541800	0.00773200
H	2.19596400	0.50548200	0.02116200
C	1.75165000	2.42762700	0.27749200
H	0.91676300	2.97098000	0.73289200
H	2.62223300	2.48648600	0.94070900
C	2.10555000	3.13367200	-1.01150100
F	2.43344100	4.42177700	-0.79780000
F	1.08603900	3.12540800	-1.89157000
F	3.15300500	2.55661200	-1.63423300
C	-1.96734600	1.69431000	0.55381800
C	-3.24597900	2.23998400	0.41889200
C	-1.37353200	1.58251200	1.81363200
C	-3.93183600	2.67198400	1.55170200
H	-3.68702000	2.31668300	-0.57087700
C	-2.06993800	2.02635800	2.93810600
H	-0.37626000	1.16040200	1.90727700
C	-3.35029800	2.56711600	2.81704400
H	-4.92647000	3.09365900	1.44223700
H	-1.60555200	1.93904800	3.91589200
H	-3.88810600	2.90371500	3.69738500
<b>TS</b>			
C	-1.00477500	-2.22224700	0.75568700



C	-0.14780000	-2.93340600	1.81629700	C	0.53030600	-1.90975700	1.50991500
C	1.29173900	-2.38827600	1.75399300	C	1.97089300	-2.47906300	1.40167000
C	1.92298700	-2.63852400	0.35012500	C	2.52667400	-2.43332400	-0.05214000
C	0.99622600	-2.16085100	-0.80390600	C	1.51635500	-3.01118600	-1.06433200
C	-0.48676800	-2.56300200	-0.65833900	H	0.40252700	-1.16136700	-1.11485900
C	-1.26793300	-1.76780500	-1.73070700	H	-1.08781100	-3.72732700	-1.92360700
C	-2.81527900	-1.80061900	-1.56320800	H	-0.35307100	-2.57208900	-3.06035100
C	-3.29130000	-1.63268200	-0.08660600	H	-2.79210800	-2.04659000	-2.78232500
C	-2.50120400	-2.55791900	0.85846500	H	-1.77291000	-0.72873200	-2.15941800
H	-0.89136900	-1.13127900	0.90550800	H	-3.18967100	-2.91799500	-0.51328500
H	-0.15743300	-4.02289800	1.64142700	H	-2.25103200	-1.90966000	1.51201300
H	-0.56465900	-2.75417800	2.81977700	H	-1.51339000	-0.58301300	0.59371900
H	1.93048200	-2.85151100	2.51992800	H	-0.61751500	-3.51365000	0.56867200
H	1.26464200	-1.30306400	1.95165500	H	0.56278400	-0.81294600	1.42241800
H	2.13322600	-3.71362200	0.24409800	H	0.12885600	-2.14430600	2.50924300
H	1.39854500	-2.53038400	-1.76026000	H	1.96284900	-3.52912600	1.73167800
H	1.02043900	-1.06165700	-0.84170400	H	3.47271500	-2.99434900	-0.08744500
H	-0.61099600	-3.64780600	-0.81881400	H	2.75163100	-1.39303500	-0.33430700
H	-0.91258800	-0.72805400	-1.67995200	H	1.33406500	-4.08032200	-0.85893300
H	-1.01719200	-2.14572700	-2.73388300	H	1.92879400	-2.93466200	-2.08259400
H	-3.19971000	-2.75875500	-1.93967900	C	2.89931000	-1.69074300	2.32322900
H	-4.36898800	-1.84659500	-0.04165000	O	3.56126600	-2.30131500	3.19791200
H	-3.14837000	-0.59306800	0.24860100	O	2.96531100	-0.42598700	2.14876000
H	-2.66910600	-3.61719300	0.59883100	H	2.23668000	0.35413700	1.02812400
H	-2.85243100	-2.40812400	1.89136800	N	-3.69861400	0.40931300	-0.46807800
C	-3.43811500	-0.70651300	-2.39978500	C	-3.86497000	-0.91528800	-0.50514500
O	-4.29628600	-0.90302000	-3.24672000	N	-5.17711500	-1.14118500	-0.43248700
O	-3.03314700	0.54651200	-2.17482000	C	-4.92214700	1.03711800	-0.36382200
H	-2.32979000	0.65023600	-1.47767700	C	-5.86142900	0.05555400	-0.34369200
N	3.30409400	-0.56031800	0.14372300	H	-5.01565100	2.11019100	-0.31716200
C	3.20692300	-1.88586700	0.25999500	H	-6.93595100	0.09672700	-0.27247100
N	4.44921500	-2.37382200	0.32152000	H	-5.59405300	-2.06754500	-0.43488100
C	4.63454100	-0.19818000	0.13178500	O	1.78399700	0.88545500	0.28084300
C	5.36231500	-1.34144600	0.24517000	O	-0.09239400	0.94631000	-0.25879700
H	4.94892300	0.82967000	0.04349100	O	-0.88329300	1.44615100	-0.54310200
H	6.42562800	-1.51537800	0.27095700	H	-2.77842300	0.86254600	-0.49707800
H	4.67170300	-3.36068700	0.40690000	C	-0.72034200	2.77786400	-0.11712700
O	-1.16778800	1.22445400	-0.29993400	H	0.32395700	3.10383300	-0.16711300
H	-0.01297900	1.08799500	-0.19902200	H	-1.33969900	3.43041000	-0.73648700
O	1.22668700	1.07297900	-0.07268200	C	-1.19314800	2.91104700	1.31318800
H	2.46061500	0.09571700	0.06183900	F	-1.08129800	4.17633200	1.75383700
C	1.64716000	2.35717900	0.26349400	F	-0.49304400	2.12945500	2.15661500
H	0.85488600	2.95210800	0.74241800	F	-2.48667700	2.55370200	1.44829100
H	2.51825800	2.34602500	0.93413200	C	2.68018400	1.23864700	-0.67904600
C	2.06541100	3.11071700	-0.97908000	C	2.20385700	1.56762700	-1.95299300
F	2.47961400	4.36244800	-0.69461400	C	4.05515000	1.28525100	-0.41744900
F	1.05983600	3.22367200	-1.87055400	C	3.09839700	1.94694900	-2.95221200
C	3.08048500	2.50128100	-1.62722400	H	1.13644100	1.51973600	-2.15007400
C	-1.75666200	1.53028200	0.87491200	C	4.93989500	1.65474400	-1.42949000
C	-1.13113300	1.26737500	2.10626900	H	4.41943000	1.03254700	0.57385600
C	-3.03592400	2.10954400	0.87472200	C	4.47057400	1.99119600	-2.70010600
C	-1.77302400	1.59029300	3.30132100	H	2.71728200	2.20325600	-3.93652600
H	-0.14011300	0.82109800	2.11667100	H	6.00477600	1.68349800	-1.21754000
C	-3.67126300	2.41616600	2.07578900	H	5.16352600	2.28239100	-3.48282500
H	-3.51883100	2.31127600	-0.07783500				
C	-3.04674600	2.16067500	3.29881100				
H	-1.27169400	1.38614100	4.24347100				
H	-4.66226700	2.86104000	2.05382100				
H	-3.54339900	2.40427800	4.23242700				
<b>Product</b>				<b>(12) Carboxylic group – C<sub>6</sub>H<sub>5</sub>OH – C<sub>6</sub>H<sub>5</sub>OH – Imidazole</b>			
C	0.18618600	-2.24025700	-0.97755300	<i>Reactant</i>			
C	-0.81500900	-2.66740700	-2.06563200	C	-1.07801300	-1.60731100	1.38129200
C	-2.07090400	-1.77852100	-1.99665400	C	-0.02697000	-1.90162300	2.46370500
C	-2.76066900	-1.90877000	-0.60603100	C	1.38588500	-1.76040400	1.86687500
C	-1.76015200	-1.65673300	0.55937000	C	1.59056000	-2.74607400	0.67973900
C	-0.43428200	-2.43421600	0.42410400	C	0.46501800	-2.58439300	-0.37582200
				C	-0.96098400	-2.61439600	0.21649300
				C	-1.94508000	-2.24095600	-0.91594900
				C	-3.40130500	-1.98325700	-0.43080100

C	-3.47585300	-1.08568100	0.84405300	C	-2.15476800	-2.20716500	1.81533600
C	-2.51409400	-1.59949100	1.93159000	H	-0.61774400	-0.91178100	1.04371600
H	-0.86884300	-0.60153500	0.97170100	H	0.33001800	-3.36369200	2.63807100
H	-0.17377400	-2.91971700	2.86435700	H	0.10874900	-1.73654800	3.32212600
H	-0.14910700	-1.19591000	3.30048900	H	2.50879400	-2.04604300	2.63753300
H	2.15937400	-1.94055100	2.62840200	H	1.71363900	-0.77803000	1.67667900
H	1.51861000	-0.72792000	1.49509100	H	2.30064800	-3.68258500	0.82750200
H	1.58137100	-3.77592900	1.07264000	H	1.19775900	-3.23880500	-1.31281800
H	0.57298500	-3.36599800	-1.14467800	H	0.94645600	-1.52890400	-0.90530400
H	0.59371500	-1.61062900	-0.87596900	H	-0.55484400	-3.89120300	0.33069500
H	-1.19086800	-3.62272800	0.60331900	H	-1.14020700	-1.47113600	-1.44587000
H	-1.54712700	-1.33828800	-1.40381200	H	-1.35680700	-3.17094300	-1.89408400
H	-1.96335600	-3.03774200	-1.67567600	H	-3.31993800	-3.42856200	-0.51945700
H	-3.88139400	-2.94525000	-0.20341800	H	-4.18516300	-1.84183100	1.07916700
H	-4.51393200	-1.07503100	1.20647900	H	-2.99644200	-0.59695500	0.64875800
H	-3.20181200	-0.04524300	0.59980000	H	-2.32120300	-3.28188800	2.00279700
H	-2.79941400	-2.61619300	2.25167300	H	-2.31847800	-1.67437900	2.76497000
H	-2.57576600	-0.94206800	2.81323200	C	-3.76404600	-1.70482200	-1.66207300
C	-4.20675700	-1.33459600	-1.53132600	O	-4.75155700	-2.20100600	-2.18434800
O	-5.25566300	-1.77805500	-1.96614800	O	-3.40055200	-0.47079300	-2.01404100
O	-3.73981500	-0.18334800	-2.03926500	H	-2.58641200	-0.11121400	-1.55456000
H	-2.88761400	0.10385400	-1.64641200	N	3.38826600	-0.83510800	-0.59424600
N	3.20720000	-1.40895100	-0.68188500	C	3.33120900	-2.02920600	-0.00080900
C	2.91667000	-2.47757500	0.04514400	N	4.57133000	-2.52076900	0.00824200
N	4.01187300	-3.25672400	0.18383200	C	4.68820800	-0.55589100	-0.96015400
C	4.54205300	-1.51111600	-1.01355300	C	5.43937200	-1.62393900	-0.58355800
C	5.05845200	-2.65974400	-0.48308700	H	4.95914600	0.36206200	-1.45713200
H	5.03900900	-0.75871000	-1.60908300	H	6.49274500	-1.82845400	-0.68455100
H	6.04273800	-3.09905600	-0.52110600	H	4.82043700	-3.42442200	0.39906400
H	4.04548500	-4.13135000	0.69485700	O	-1.33272400	0.82380100	-0.90001800
O	-1.28271700	1.04873900	-1.12850900	H	-0.13226600	0.76417900	-0.84503700
H	-0.38336100	0.66113500	-1.08919400	O	1.07296600	0.80990900	-0.74516300
O	1.53877100	0.56937300	-1.26028700	H	2.56101700	-0.21722400	-0.70707000
H	2.17486600	-0.18622400	-0.99238700	C	-1.83366500	1.63238900	0.05638800
C	2.06046400	1.78762300	-0.93750800	C	-1.17422900	1.82451900	1.28419600
C	3.07363200	1.92398500	0.01800800	C	-3.05367100	2.29241000	-0.16509100
C	1.52756900	2.92012900	-1.56088700	C	-1.72551400	2.66194400	2.25298400
C	3.54449000	3.19621800	0.34338400	H	-0.22812800	1.32158500	1.46793700
H	3.47954700	1.04004200	0.50225200	C	-3.60020300	3.11786700	0.81559200
C	2.00006300	4.18509000	-1.21931000	H	-3.56059600	2.14885200	-1.11557200
H	0.74111600	2.79452300	-2.29971600	C	-2.94140000	3.31159800	2.03133900
C	3.01064200	4.33212100	-0.26633600	H	-1.19961000	2.80177000	3.19344800
H	4.33056800	3.29738200	1.08603400	H	-4.54596000	3.61729100	0.62434300
H	1.57660600	5.06034500	-1.70333000	H	-3.36626500	3.95925500	2.79145900
H	3.37730200	5.31902800	-0.00333300	C	1.48828700	2.08962600	-0.65752900
C	-1.49627000	1.90655000	-0.08093100	C	2.55221300	2.42478500	0.19694400
C	-0.61820500	1.99025600	1.00267200	C	0.87704200	3.11127300	-1.40607600
C	-2.64881300	2.69224400	-0.12116900	C	2.99589700	3.74295200	0.29158800
C	-0.89816500	2.87573400	2.04278300	H	3.01707900	1.64199100	0.79208300
H	0.27679400	1.37362400	1.02328800	C	1.32113500	4.42747800	-1.29552100
C	-2.92051100	3.56671000	0.92955400	H	0.05323300	2.85934500	-2.06859300
H	-3.31899300	2.60826100	-0.97196000	C	2.38395100	4.75486500	-0.45049000
C	-2.04794100	3.66604000	2.01479700	H	3.82175700	3.98026700	0.95655300
H	-0.21091300	2.94156500	2.88114900	H	0.83330800	5.20378300	-1.87866700
H	-3.81923200	4.17512800	0.89599400	H	2.72895400	5.78074600	-0.37134300
H	-2.26193800	4.35074200	2.82891500	<b>Product</b>			
<b>TS</b>				C	-0.62953600	-2.21599300	1.16098600
C	-0.71588800	-1.97850500	1.32328700	C	0.39616300	-2.59937100	2.24353000
C	0.34076800	-2.28658100	2.39703600	C	1.78242000	-2.02845400	1.88358600
C	1.72919800	-1.86235400	1.88408800	C	2.25928500	-2.59017100	0.51059700
C	2.09656000	-2.63060700	0.57642800	C	1.20017000	-2.33343100	-0.59463300
C	0.96504500	-2.54762700	-0.48796200	C	-0.21321500	-2.81004000	-0.20386500
C	-0.45083000	-2.82628500	0.06076000	C	-1.18695200	-2.35835400	-1.31472300
C	-1.44649800	-2.45502600	-1.06244000	C	-2.68942800	-2.55216200	-0.97603200
C	-2.93383400	-2.40383200	-0.61012700	C	-3.04946600	-2.10924100	0.47410300
C	-3.14532700	-1.68331200	0.75815800	C	-2.05644800	-2.67755300	1.50774000

H	-0.63655500	-1.11125000	1.06851500	C	-2.55097100	-0.05298900	2.26266100
H	0.44945700	-3.69856300	2.33143200	H	-0.87045400	0.40076500	0.98685000
H	0.07679400	-2.20337100	3.21962100	H	-0.51129400	-1.90002400	2.99504600
H	2.52581500	-2.27339400	2.65605800	H	0.01183000	-0.22312900	3.27464500
H	1.71207200	-0.92846700	1.81895100	H	1.93341300	-1.57735600	2.37087300
H	2.43918500	-3.67200300	0.61129400	H	1.45435600	-0.29330100	1.23977000
H	1.52100800	-2.82374500	-1.52702400	H	0.74609000	-3.28170000	1.06621600
H	1.14137000	-1.25054300	-0.79112400	H	-0.52749400	-2.80165200	-0.97142400
H	-0.22296600	-3.91051000	-0.11314300	H	-0.06223700	-1.08968100	-0.93146100
H	-0.99207800	-1.29528900	-1.50960300	H	-1.96365000	-2.46482000	1.04506600
H	-0.96160000	-2.90382800	-2.24538800	H	-2.16223300	-0.36112800	-1.16960500
H	-2.94404900	-3.61785500	-1.07881100	H	-2.96520400	-1.93980200	-1.15362100
H	-4.07595400	-2.43710700	0.69776700	H	-4.51211800	-1.26764700	0.60484300
H	-3.03545400	-1.01031400	0.54403500	H	-4.46510500	0.88440500	1.76109600
H	-2.09474700	-3.78053600	1.51449000	H	-3.07978800	1.45629900	0.80592600
H	-2.33231500	-2.32951500	2.51537300	H	-3.00614600	-0.92752100	2.75854300
C	-3.55160500	-1.75378000	-1.95229200	H	-2.31309100	0.68604100	3.04300200
O	-4.48056400	-2.33297700	-2.56508800	C	-4.76694800	0.19511900	-0.89927000
O	-3.29738800	-0.50632400	-2.08212300	O	-5.94381300	-0.07164100	-1.08486500
H	-2.27489300	0.27425800	-1.25018200	O	-4.19867200	1.14404400	-1.65138400
N	3.68478400	-0.67766200	-0.28164700	H	-3.24294000	1.31244400	-1.45535100
C	3.54319800	-1.93958500	0.13236800	N	2.49487700	-1.44766500	-1.14658200
N	4.76729200	-2.46678800	0.18272600	C	2.13190000	-2.37030400	-0.26746800
C	5.01861000	-0.39569300	-0.49427600	N	3.06133000	-3.34978900	-0.20813500
C	5.70596500	-1.52998700	-0.20234700	C	3.70963900	-1.85414100	-1.65774100
H	5.35400900	0.56974300	-0.83718700	C	4.07575600	-3.04059800	-1.08611600
H	6.75939900	-1.75510700	-0.23420700	H	4.23584900	-1.27546400	-2.40324600
H	4.95819200	-3.42529800	0.46034000	H	4.93322700	-3.68057400	-1.22222600
O	-1.59047100	0.79741500	-0.69269200	H	3.00673900	-4.17141600	0.38242800
H	0.30815900	0.92622400	-0.75498800	O	-1.59914100	1.97267800	-1.39146000
O	1.25333000	1.14174800	-0.60711300	H	-0.77286800	1.45866600	-1.36929300
H	2.90439900	-0.02526500	-0.40669300	O	1.28257800	0.95989200	-1.22909500
C	1.45299400	2.49486100	-0.67753800	H	1.74525400	0.05818600	-1.20680800
C	2.70486400	2.98819000	-0.30578800	C	1.99361300	1.89214800	-0.53613700
C	0.44978300	3.36547700	-1.10952400	C	1.50699300	3.20360300	-0.50218700
C	2.95011000	4.35842800	-0.36785800	C	3.18485200	1.57527400	0.12990600
H	3.47329500	2.29933800	0.03354900	C	2.20268300	4.18527700	0.20006800
C	0.70830400	4.73451300	-1.16417100	H	0.59204400	3.44282200	-1.03559400
H	-0.51846300	2.96735800	-1.39916300	C	3.87196100	2.56895300	0.82673400
C	1.95548700	5.23959800	-0.79531100	H	3.56769500	0.55949900	0.09655900
H	3.92481900	4.73704500	-0.07489100	C	3.38759100	3.87655200	0.87090800
H	-0.07444700	5.40799400	-1.50022700	H	1.81580100	5.19996600	0.21862700
H	2.15031900	6.30613700	-0.83970500	H	4.79394400	2.31248000	1.34052000
C	-2.18558300	1.47161000	0.32761700	H	3.92643500	4.64505700	1.41546200
C	-1.40533300	1.84651700	1.42775800	H	-1.54553800	2.55764000	-0.62274500
C	-3.54593000	1.79988400	0.29313800	<b>TS</b>			
C	-1.98370000	2.55605400	2.47858400	C	-2.03682800	-1.50568800	0.99318500
H	-0.35174800	1.57999100	1.44688500	C	-1.46888400	-2.82620300	1.54088600
C	-4.11468700	2.49899100	1.35713700	C	0.03699200	-2.90371900	1.22438100
H	-4.14422600	1.50671400	-0.56478500	C	0.28668300	-2.84841400	-0.31553600
C	-3.34068700	2.88404900	2.45294600	C	-0.46855300	-1.67158100	-0.99533200
H	-1.36988400	2.84549600	3.32651700	C	-1.93336900	-1.49016900	-0.54821400
H	-5.17169700	2.74693400	1.32464200	C	-2.40141700	-0.12803900	-1.10904600
H	-3.78968900	3.43083000	3.27583600	C	-3.75773600	0.37473600	-0.54415200
				C	-3.90427400	0.17608200	0.99581600
				C	-3.49416600	-1.24855500	1.41646200
				H	-1.41401700	-0.67711300	1.38547700
				H	-2.00294300	-3.68024700	1.08959800
				H	-1.61530500	-2.87830400	2.63029200
				H	0.48245500	-3.82621000	1.62403900
				H	0.54402800	-2.05113000	1.70651200
				H	-0.02808600	-3.80504700	-0.75933200
				H	-0.41844500	-1.80082400	-2.08772000
				H	0.04911900	-0.73140500	-0.75292900
				H	-2.56263700	-2.30681100	-0.94155700
				H	-1.61570300	0.60314200	-0.87399600
<b>(13) Carboxylic group – H<sub>2</sub>O – C<sub>6</sub>H<sub>5</sub>OH – Imidazole</b>							
<b>Reactant</b>							
C	-1.26655200	-0.48055200	1.53196800				
C	-0.17205700	-0.97694300	2.49338900				
C	1.12574700	-1.23838300	1.70483500				
C	0.90693800	-2.30152500	0.58789200				
C	-0.31857000	-1.95425700	-0.29893500				
C	-1.58768300	-1.58291000	0.49660000				
C	-2.64935100	-1.09925600	-0.51597500				
C	-3.90739300	-0.47156200	0.14788200				
C	-3.54207700	0.56371500	1.25654300				

H	-2.47600500	-0.18296400	-2.20686000
H	-4.57623800	-0.17039400	-1.03567600
H	-4.94823100	0.38210000	1.27578600
H	-3.27118800	0.89693400	1.53480700
H	-4.15620100	-1.99640800	0.94697100
H	-3.59447900	-1.35280400	2.50800000
C	-3.92488000	1.84744300	-0.87073100
O	-4.92131600	2.26358400	-1.47246700
O	-2.98651200	2.67276100	-0.48446900
H	-2.08124300	2.32307200	0.11145600
N	2.41194100	-1.52080300	-0.37519400
C	1.74547200	-2.66461800	-0.55666300
N	2.63940900	-3.75899900	-0.93511400
C	3.75297700	-1.71221800	-0.63865700
C	3.89891000	-3.01491400	-0.99500500
H	4.47398800	-0.91437100	-0.55692500
H	4.76773400	-3.58243000	-1.28598400
H	2.40941500	-4.54533200	-1.14794700
O	-1.01947500	2.14802600	0.81914500
H	-0.00673900	1.55159400	0.55869200
O	1.05819400	0.99597300	0.40778100
H	1.96519400	-0.64184800	-0.06846600
C	2.06885700	1.88398100	0.35602000
C	1.91472200	3.14117500	-0.25709500
C	3.31986100	1.55652000	0.90881500
C	2.98067300	4.03734000	-0.30774100
H	0.95438800	3.40069100	-0.69431700
C	4.38266000	2.45551700	0.84239600
H	3.44215100	0.59378000	1.40022100
C	4.22284100	3.70345600	0.23655100
H	2.83898700	5.00420000	-0.78301300
H	5.34074300	2.18004000	1.27488600
H	5.05086600	4.40342900	0.18988200
H	-1.28141200	1.88773200	1.71231400
<b>Product</b>			
C	-1.44156000	-0.79752300	1.50204600
C	-0.51046600	-1.61216200	2.41884700
C	0.83553700	-1.86493600	1.71168700
C	0.61972000	-2.63595200	0.37363400
C	-0.44939300	-1.94878500	-0.52384600
C	-1.75427700	-1.60746300	0.22304500
C	-2.64855400	-0.78951700	-0.73423000
C	-3.92201000	-0.21728700	-0.06170600
C	-3.57937800	0.51741600	1.26579500
C	-2.74918800	-0.38427000	2.20177200
H	-0.90715300	0.12473300	1.19930700
H	-0.99225100	-2.57106300	2.67691500
H	-0.33167800	-1.06713600	3.35810400
H	1.51520400	-2.44579200	2.35210700
H	1.31741500	-0.89475700	1.50397600
H	0.30186600	-3.66423700	0.60499600
H	-0.66340700	-2.59841800	-1.38698500
H	-0.03792800	-1.00350500	-0.91443900
H	-2.27349900	-2.53542600	0.52180200
H	-2.04301900	0.04151600	-1.12514300
H	-2.94014400	-1.41465300	-1.59394100
H	-4.61352300	-1.04311300	0.16567700
H	-4.51238500	0.83424100	1.75641900
H	-2.99643100	1.42449800	1.03624900
H	-3.32499600	-1.28595500	2.47398500
H	-2.51889900	0.15579800	3.13305000
C	-4.62164100	0.76246600	-1.00319900
O	-5.84727400	0.59588900	-1.24787200
O	-3.92602100	1.71666300	-1.47553400
H	-2.23394300	2.06325700	-1.12068400
N	2.52049500	-1.65445400	-0.93452200

C	1.90314700	-2.70001600	-0.37755500
N	2.66027200	-3.76939500	-0.62523700
C	3.69140300	-2.06271100	-1.53913300
C	3.77993800	-3.40420400	-1.34680600
H	4.34503900	-1.37136500	-2.04622400
H	4.52242800	-4.12217700	-1.65445100
H	2.42668100	-4.71139800	-0.32509500
O	-1.28894700	2.33549500	-1.02196800
H	0.31526500	1.44979800	-0.78122400
O	1.18569300	1.07852600	-0.51451000
H	2.16216900	-0.69582300	-0.88932100
C	2.03981200	2.07427100	-0.12712900
C	1.79310900	3.41800600	-0.41945000
C	3.19685400	1.70583900	0.56424100
C	2.70653100	4.38909100	-0.01040000
H	0.89999000	3.69615500	-0.97043400
C	4.10625100	2.68512400	0.95742900
H	3.37350100	0.65736800	0.78679100
C	3.86674000	4.03170000	0.67685400
H	2.50746200	5.43202000	-0.23840000
H	5.00380200	2.39171500	1.49372200
H	4.57492600	4.79152300	0.99092200
H	-1.30492000	3.16203200	-0.52167700

**(14) Carboxylic group – C<sub>6</sub>H<sub>5</sub>OH – H<sub>2</sub>O – Imidazole  
Reactant**

C	0.00021700	-0.63334900	1.50549400
C	1.06357300	-0.13577000	2.49979900
C	2.27889600	0.41499100	1.72843000
C	2.90823700	-0.67876700	0.81888900
C	1.83870800	-1.33072900	-0.09775800
C	0.56455500	-1.78570900	0.64586000
C	-0.47051400	-2.21135100	-0.41818200
C	-1.88045000	-2.50861100	0.16746100
C	-2.37390000	-1.40169700	1.15074400
C	-1.29536300	-1.08203300	2.20364700
H	-0.24738400	0.20188600	0.82334600
H	1.37060000	-0.96581300	3.15974500
H	0.63700400	0.65414800	3.13762100
H	3.04574000	0.79729700	2.41881100
H	1.94783900	1.25865600	1.09820600
H	3.35549900	-1.45342000	1.46370900
H	2.29062000	-2.18374500	-0.62894900
H	1.53413700	-0.59411500	-0.85816900
H	0.79594200	-2.63564100	1.31165500
H	-0.53153900	-1.39258100	-1.15204400
H	-0.11423600	-3.10427700	-0.95531600
H	-1.85249600	-3.46388500	0.70983500
H	-3.30272000	-1.74465700	1.62948700
H	-2.61006500	-0.47682600	0.59945300
H	-1.09070100	-1.96940100	2.82731600
H	-1.66067300	-0.28453500	2.86947300
C	-2.89085700	-2.65576500	-0.94476500
O	-3.62350400	-3.61977500	-1.08373400
O	-2.99798400	-1.63992800	-1.81494600
H	-2.37520400	-0.90369600	-1.63585900
N	3.78893000	0.82216500	-0.98368900
C	3.98296600	-0.07235900	-0.02604400
N	5.30108500	-0.34851700	0.10356500
C	5.03972600	1.12616600	-1.48049300
C	5.99345700	0.40636900	-0.81567000
H	5.17542200	1.83869500	-2.28124600
H	7.06711100	0.35933800	-0.90814600
H	5.69864700	-1.00208200	0.76770300
O	-1.45307600	0.81939900	-1.55260000
H	-0.48193900	0.97280300	-1.49602200

O	1.19332600	1.66709000	-1.71735700	H	-4.86066900	3.08007500	-0.10272400
H	2.10383500	1.39602300	-1.43205900	H	-3.60291500	4.37353700	1.61594200
C	-2.13030000	1.69906000	-0.75049500	H	1.20881800	2.29524000	-2.02119800
C	-3.52033200	1.74700100	-0.87747300	<b>Product</b>			
C	-1.47728600	2.50292000	0.18689100	C	0.09632100	-0.76184800	1.52632400
C	-4.25640600	2.60292400	-0.06136000	C	1.16458700	-0.30318000	2.53485000
H	-4.00615400	1.10968600	-1.61095400	C	2.34279100	0.35068200	1.78837600
C	-2.22668900	3.36291100	0.99021600	C	2.99098000	-0.66578600	0.80106700
H	-0.39597700	2.45834000	0.28115500	C	1.93137800	-1.27955600	-0.15612200
C	-3.61591000	3.41482700	0.87690800	C	0.68303200	-1.82334600	0.56996700
H	-5.33709100	2.63486600	-0.16251400	C	-0.35525400	-2.20542200	-0.50873400
H	-1.71548100	3.98927000	1.71526200	C	-1.75677000	-2.57886400	0.05067700
H	-4.19390400	4.08088300	1.50915200	C	-2.24927400	-1.60186700	1.15888500
H	1.11899000	2.60677100	-1.50329700	C	-1.15865400	-1.32850400	2.21341400
<b>TS</b>				H	-0.20682000	0.11583500	0.92148900
C	-0.09793800	-0.85592800	1.56897800	H	1.51758800	-1.16903500	3.12163300
C	0.99128500	-0.48456800	2.58912600	H	0.72952800	0.42074100	3.24103400
C	2.19975300	0.11558000	1.84447900	H	3.10776200	0.71241600	2.49053800
C	2.78798700	-0.90124400	0.82057400	H	1.96870600	1.22017200	1.22009300
C	1.69146200	-1.50300000	-0.10081800	H	3.47413500	-1.46641300	1.38185200
C	0.41299300	-1.96729100	0.62963600	H	2.40242100	-2.07838100	-0.74997900
C	-0.62994900	-2.28308200	-0.46919000	H	1.59224400	-0.50104100	-0.85791900
C	-2.09337300	-2.43706200	0.03622500	H	0.95595700	-2.70946100	1.16981900
C	-2.50141100	-1.38919800	1.12085900	H	-0.45425900	-1.34629300	-1.18749200
C	-1.42420800	-1.28520900	2.21722200	H	0.02297600	-3.05033500	-1.10669600
H	-0.30121600	0.04026900	0.95370400	H	-1.70802100	-3.59034500	0.48122800
H	1.29314000	-1.37795200	3.16295500	H	-3.14812300	-2.02762700	1.63019200
H	0.59851600	0.25313900	3.30634600	H	-2.54338900	-0.64260800	0.70645600
H	2.99234700	0.41635800	2.54496400	H	-0.89651700	-2.25611700	2.75064200
H	1.86831800	1.02016800	1.30575400	H	-1.53835300	-0.61012700	2.95723100
H	3.29372100	-1.70710900	1.37451700	C	-2.76731000	-2.58501200	-1.09577400
H	2.12540600	-2.33502400	-0.67749500	O	-3.41251100	-3.63343000	-1.34331100
H	1.37931500	-0.73115000	-0.82011500	O	-2.91381500	-1.49865900	-1.75355300
H	0.61978200	-2.86580500	1.23610800	H	-2.13816600	-0.17116900	-1.49463300
H	-0.57627400	-1.46197900	-1.19790200	N	3.81112700	0.94344700	-0.94507500
H	-0.34545700	-3.20321600	-1.00221300	C	4.03699400	0.02223700	-0.00443100
H	-2.22696700	-3.43926600	0.46607200	N	5.35970700	-0.12886800	0.08045400
H	-3.47254400	-1.68727000	1.54216900	C	5.00982900	1.38629900	-1.46532400
H	-2.63012300	-0.39278900	0.66567400	C	5.99202500	0.70804200	-0.81769200
H	-1.29848600	-2.25219500	2.73369400	H	5.05576300	2.13181000	-2.24288800
H	-1.73803800	-0.54243800	2.96721200	H	7.06487300	0.73988400	-0.91412200
C	-3.04984500	-2.31564700	-1.12736400	H	5.81565200	-0.77386700	0.71895200
O	-3.90389000	-3.14557600	-1.39599300	O	-1.63726600	0.70355800	-1.33745000
O	-2.96500200	-1.21400700	-1.88176800	H	0.25885600	1.22787900	-1.58438700
H	-2.25094600	-0.57913300	-1.61774600	O	1.10289200	1.68844500	-1.74652800
N	3.50382700	0.66744600	-1.00120400	H	2.87085600	1.25714800	-1.22589200
C	3.79206100	-0.20408400	-0.03578800	C	-2.39442000	1.58026800	-0.62226900
N	5.12513800	-0.30777100	0.04844900	C	-1.74810600	2.58472400	0.10656400
C	4.68578600	1.12810600	-1.54220100	C	-3.79177500	1.49523200	-0.60339700
C	5.71130900	0.51950100	-0.88642700	C	-2.49913600	3.50645800	0.83383500
H	4.70129600	1.84519700	-2.34825200	H	-0.66266800	2.63516900	0.09539800
H	6.78090300	0.59048500	-1.00011900	C	-4.53016100	2.41423300	0.14065300
H	5.61140800	-0.91244600	0.70235300	H	-4.28667400	0.71071700	-1.16865600
O	-1.15174100	0.84788900	-1.40862700	C	-3.89252400	3.42598000	0.86062400
H	-0.02179000	1.06821400	-1.53455300	H	-1.98829300	4.28688100	1.39027400
O	1.18675000	1.36546900	-1.75690100	H	-5.61355600	2.33816900	0.15238300
H	2.44822200	0.98594800	-1.32104500	H	-4.47297800	4.14131600	1.43418000
C	-1.75989900	1.77048200	-0.63367300	H	0.88295300	2.62870300	-1.70059900
C	-1.05564400	2.49688600	0.34249300				
C	-3.13842500	1.99559500	-0.78112000	<b>(15) Carboxylic group – CH<sub>2</sub>FCH<sub>2</sub>OH – C<sub>6</sub>H<sub>5</sub>OH –</b>			
C	-1.71987500	3.43260900	1.13451100	<b>Imidazole</b>			
H	0.00966800	2.32581100	0.46963500	<b>Reactant</b>			
C	-3.79353500	2.92202600	0.02661800	C	-1.21119300	-1.57228700	1.40485400
H	-3.68238000	1.43593700	-1.53731000	C	-0.17100400	-2.21707500	2.33794700
C	-3.09125400	3.64898700	0.99066800	C	1.22740200	-2.12152600	1.69930800
H	-1.15842100	3.98871700	1.88032400	C	1.26647100	-2.84350700	0.31950100

C	0.11348100	-2.36396200	-0.60404300	C	-3.20149700	-1.75916900	1.40906900
C	-1.27506900	-2.34575500	0.06942200	H	-1.22676900	-0.91189100	1.22636100
C	-2.25648200	-1.66192200	-0.90754500	H	-1.37338200	-3.95265500	1.66740800
C	-3.65366600	-1.36969000	-0.28797800	H	-1.14766400	-2.75775100	2.96653500
C	-3.56654600	-0.71413000	1.12372400	H	1.09320900	-3.60225000	2.20540500
C	-2.61068600	-1.50102800	2.04056200	H	0.89356700	-1.87041800	1.85335100
H	-0.87630000	-0.53988600	1.18170300	H	0.64713900	-4.22806900	-0.11393900
H	-0.43890500	-3.27230200	2.52067800	H	0.02411800	-2.66700000	-1.88000100
H	-0.17044900	-1.70120300	3.31052600	H	0.29333700	-1.25837000	-0.83481800
H	1.99461000	-2.55692500	2.35659400	H	-2.05394100	-3.20806400	-0.62750600
H	1.47910500	-1.05684000	1.55149900	H	-1.55318800	-0.26431900	-1.29540800
H	1.17344700	-3.92863000	0.48807100	H	-2.25916100	-1.47797000	-2.37310400
H	0.08879100	-2.99566900	-1.50649800	H	-4.36497500	-1.48438800	-1.21606000
H	0.33270300	-1.33520900	-0.93135500	H	-4.86751300	-0.43334200	0.89369100
H	-1.60935200	-3.37601000	0.28384900	H	-3.28242100	0.35782600	0.99476600
H	-1.78706100	-0.72179800	-1.23515500	H	-3.73613800	-2.68641100	1.14103600
H	-2.39235000	-2.28719500	-1.80374100	H	-3.31625400	-1.60980000	2.49392100
H	-4.21356400	-2.31115800	-0.20127000	C	-4.03220900	0.58479900	-1.55600500
H	-4.57754000	-0.67012400	1.55443200	O	-5.06409000	0.69762100	-2.21949800
H	-3.20172400	0.32046400	1.03738300	O	-3.23444400	1.61832200	-1.39630200
H	-2.99432900	-2.52255800	2.20580100	H	-2.33722200	1.52602300	-0.78691600
H	-2.55321000	-1.00455700	3.02177700	N	2.74554400	-1.60055100	-0.23464000
C	-4.43781600	-0.46353600	-1.20630200	C	2.24069200	-2.83630300	-0.19357200
O	-5.51815200	-0.75090400	-1.69440200	N	3.25526400	-3.67746900	-0.39709500
O	-3.90603500	0.73437200	-1.48389000	C	4.10500300	-1.65522300	-0.46414100
H	-3.02871800	0.89459500	-1.06224700	C	4.42976700	-2.97048800	-0.56905900
N	2.93405200	-1.37568700	-0.81959500	H	4.71143100	-0.76618100	-0.53446900
C	2.57362700	-2.55982800	-0.34785400	H	5.37219500	-3.46081400	-0.75082300
N	3.57179100	-3.45328200	-0.52105100	H	3.15687900	-4.68795900	-0.42178000
C	4.21518100	-1.52133300	-1.30766800	O	-1.21480400	1.66365400	-0.02662600
C	4.62698700	-2.81318200	-1.13287000	H	-0.09267100	1.18361100	-0.03403500
H	4.75068900	-0.69754900	-1.75758400	O	1.02547200	0.78389700	0.06275200
H	5.54273600	-3.32542000	-1.38255100	H	2.17351800	-0.75285800	-0.09794000
H	3.53787300	-4.42897800	-0.24938300	C	-1.50760900	2.23583600	1.22878600
O	-1.40239600	1.56497500	-0.49403900	H	-2.56196400	2.54194600	1.25640000
H	-0.53838900	1.13478900	-0.63642400	H	-1.34514700	1.51250200	2.04234700
O	1.40948500	0.80978300	-0.70106700	C	-0.63985500	3.45949000	1.46040400
H	1.98517800	-0.03325000	-0.70356500	F	-1.02361000	4.05131600	2.67722000
C	-1.37258700	2.24599100	0.75674100	C	1.92625600	1.75129000	-0.20183800
H	-1.52542300	1.54672800	1.58983400	C	1.66304800	2.77453600	-1.13075200
H	-0.40569400	2.74209800	0.89616200	C	3.16909000	1.74224200	0.45466900
C	-2.48107000	3.25882700	0.77719100	C	2.61627200	3.75996200	-1.38132000
F	-2.20163600	4.27690000	-0.15211400	H	0.70763600	2.78747800	-1.64786100
C	2.15034000	1.88439700	-0.30645400	C	4.11995800	2.72531200	0.18699000
C	1.71873400	3.16258700	-0.67594900	H	3.37205900	0.96153500	1.18455100
C	3.30929500	1.73283300	0.46358400	C	3.85104200	3.74435300	-0.72874700
C	2.43942900	4.28282200	-0.26781900	H	2.39217700	4.54478200	-2.09866100
H	0.81714200	3.26020000	-1.27545600	H	5.07398700	2.69828200	0.70632700
C	4.02893000	2.86214800	0.85426800	H	4.59019200	4.51301500	-0.93016200
H	3.63660700	0.73815300	0.75271600	H	-0.78358200	4.20382800	0.67242300
C	3.59981900	4.14067700	0.49604700	H	0.42006100	3.20305100	1.54696300
H	2.09419200	5.27155200	-0.55567300	<b>Product</b>			
H	4.92932300	2.73823400	1.44908800	C	-0.84977200	-1.92984400	1.39400600
H	4.16208100	5.01538300	0.80656900	C	0.27437200	-2.45690800	2.30466300
H	-3.43576100	2.81282200	0.48228400	C	1.65099600	-2.09527500	1.71209600
H	-2.56656000	3.72600900	1.76066200	C	1.80976000	-2.71216300	0.29055800
<b>TS</b>				C	0.62324900	-2.32140800	-0.63481200
C	-1.71227600	-1.89292400	1.04917200	C	-0.75665300	-2.58857200	-0.00180100
C	-0.97884900	-2.94753700	1.89583400	C	-1.83188400	-2.00551700	-0.94465900
C	0.53051800	-2.87986700	1.59688400	C	-3.26820900	-2.03841800	-0.35947400
C	0.81373800	-3.15938000	0.08752200	C	-3.31249000	-1.49472900	1.09677500
C	-0.07808600	-2.29468500	-0.84894900	C	-2.24990300	-2.17027900	1.98660500
C	-1.56696000	-2.23369000	-0.45013000	H	-0.71062600	-0.83667300	1.26573700
C	-2.21805000	-1.13841500	-1.32617400	H	0.18191000	-3.55222600	2.40935200
C	-3.64846400	-0.71955300	-0.88456500	H	0.18003800	-2.01889700	3.31007500
C	-3.79982300	-0.55342800	0.65867900	H	2.46557500	-2.45729400	2.35573200

H	1.73663900	-0.99728700	1.64645000	H	1.53835900	-2.77614200	-1.13187300
H	1.85983300	-3.80816400	0.38294300	H	1.14715100	-1.07176300	-0.83160800
H	0.71463600	-2.86454600	-1.58829800	H	-0.23976600	-3.48585300	0.45570100
H	0.68092700	-1.24416000	-0.85871000	H	-0.97212800	-1.21213100	-1.46035400
H	-0.90954900	-3.67555900	0.12122800	H	-0.95228000	-2.93786100	-1.86458300
H	-1.55441700	-0.96272900	-1.15878500	H	-2.91751200	-3.40919800	-0.52412900
H	-1.82064000	-2.55225800	-1.90133600	H	-4.07801600	-1.82649400	0.90406500
H	-3.63078900	-3.07745500	-0.35413600	H	-3.02442100	-0.48040000	0.43162700
H	-4.32176400	-1.64829700	1.50842400	H	-2.11541300	-2.95277700	2.03028900
H	-3.12120800	-0.41046200	1.08442200	H	-2.33223900	-1.29763600	2.64781400
H	-2.43891600	-3.25552600	2.05469400	C	-3.54911600	-1.85671200	-1.81115800
H	-2.30279500	-1.76008100	3.00707400	O	-4.42489600	-2.51928800	-2.33983300
C	-4.20229100	-1.19926800	-1.23074900	O	-3.35352700	-0.59940600	-2.23935800
O	-5.23043300	-1.73838300	-1.71714300	H	-2.62543500	-0.13254900	-1.77703800
O	-3.89594100	0.02507000	-1.40852300	N	3.61096300	-0.24058800	-0.38685400
H	-2.49528200	0.81002500	-0.89907400	C	3.53088400	-1.40775700	0.23431000
N	3.33136000	-0.98122900	-0.70010900	N	4.75804800	-1.96233300	0.35252400
C	3.08052900	-2.23732600	-0.32149700	C	4.94646900	-0.04745500	-0.67467800
N	4.17967600	-2.94476400	-0.58532900	C	5.67566000	-1.11121100	-0.22027700
C	4.61001500	-0.88664100	-1.21046400	H	5.29653700	0.83583500	-1.18958000
C	5.14895800	-2.13098000	-1.13810900	H	6.72960200	-1.33835600	-0.25210800
H	5.01299500	0.04416200	-1.57555900	H	4.95397300	-2.85547300	0.78872400
H	6.11549800	-2.50832100	-1.42949700	O	-1.36030800	1.18948400	-1.07712200
H	4.27234900	-3.93849600	-0.39617800	H	-0.39705800	1.04820700	-0.92756900
O	-1.71632200	1.36373200	-0.61917100	O	1.39042400	1.29944500	-0.87225800
H	0.10664300	1.03297700	-0.50077400	H	2.19133100	0.72503700	-0.69010900
O	1.03571000	1.01887500	-0.18095800	C	1.71082200	2.63739500	-0.52911800
H	2.65530900	-0.21849600	-0.60754700	H	0.78550700	3.22241100	-0.55134900
C	-2.10748700	2.19898500	0.45770100	H	2.13427900	2.69436000	0.48250700
H	-2.78654000	1.67349800	1.13960300	C	2.69996200	3.19610900	-1.53441900
H	-1.20832400	2.47822100	1.01800100	F	3.01011100	4.51538600	-1.16857800
C	-2.78976700	3.44082600	-0.08171300	C	-1.92985800	1.85843700	-0.02650500
F	-3.16150800	4.24942800	1.00515300	C	-3.24221400	2.30742700	-0.18840100
C	1.53282300	2.28916000	-0.07098100	C	-1.25268300	2.07162900	1.17711900
C	0.92785700	3.37813400	-0.70307400	C	-3.87755300	2.96950800	0.85967500
C	2.69165000	2.46536000	0.68765900	H	-3.74884600	2.13024800	-1.13279900
C	1.48306700	4.64925600	-0.55885600	C	-1.89875800	2.74345200	2.21510100
H	0.03306400	3.22224400	-1.29949800	H	-0.23011500	1.72209900	1.29420200
C	3.24115900	3.73958900	0.81590700	C	-3.21169600	3.19077800	2.06693200
H	3.14459100	1.60488400	1.17244900	H	-4.89831000	3.31610400	0.72906600
C	2.63975700	4.83810900	0.19863500	H	-1.36824800	2.91169500	3.14759100
H	1.00654000	5.49393600	-1.04758200	H	-3.70952800	3.70816500	2.88043200
H	4.14219900	3.87329900	1.40725600	H	2.27524600	3.22293300	-2.54093100
H	3.06854700	5.82902900	0.30660500	H	3.63383800	2.62604100	-1.53433700
H	-2.11819600	4.02787300	-0.71411600	<b>TS</b>			
H	-3.70045600	3.18699000	-0.63138300	C	-0.76600400	-1.87981100	1.09003900

**(16) Carboxylic group – C<sub>6</sub>H<sub>5</sub>OH – CH<sub>2</sub>FCH<sub>2</sub>OH – Imidazole**

**Reactant**

C	-0.62797300	-1.53792600	1.31344700	C	-0.32129300	-2.48936600	-0.25548300
C	0.39110500	-1.65121000	2.45984800	C	-1.21201700	-1.97401700	-1.41050000
C	1.77144000	-1.16660600	1.97888900	C	-2.74115900	-2.02496700	-1.12733300
C	2.27195500	-2.00966700	0.76986700	C	-3.12432600	-1.55467400	0.31056200
C	1.20759200	-2.06454200	-0.35854100	C	-2.23524700	-2.23638700	1.36812600
C	-0.21116300	-2.43248800	0.12571000	H	-0.70001900	-0.77823100	1.00331500
C	-1.17610000	-2.21847100	-1.06167600	H	0.23487800	-3.42185000	2.25749100
C	-2.67808300	-2.34815900	-0.67967600	H	-0.17391700	-1.95738000	3.18206400
C	-3.04821600	-1.56621400	0.61838100	H	2.30021000	-1.99823800	2.73039800
C	-2.05979200	-1.88511900	1.75658200	H	1.50945300	-0.63299600	1.90891600
H	-0.62505800	-0.49068400	0.95736000	H	2.42484700	-3.29681300	0.66686600
H	0.45018300	-2.69880600	2.80357500	H	1.48838100	-2.60357400	-1.47485500
H	0.06047200	-1.04064800	3.31513900	H	1.07920500	-0.99333500	-0.85507800
H	2.51520600	-1.22128200	2.78804000	H	-0.39068200	-3.58809200	-0.17748100
H	1.69422100	-0.10943400	1.66839900	H	-0.90778700	-0.93514000	-1.60511700
H	2.48473500	-3.03273800	1.12146100	H	-1.00476700	-2.54805700	-2.32688400

H	-3.10196400	-3.05428100	-1.25813600	H	-1.66419800	-3.05596500	-2.36991400
H	-4.18750300	-1.77709200	0.48097200	H	-0.85817500	-1.82893900	-3.37311200
H	-2.99632800	-0.46335400	0.40369600	H	-3.21018300	-1.10379200	-2.87338600
H	-2.37003600	-3.33126100	1.34454800	H	-2.02690700	-0.00075700	-2.13234100
H	-2.52686600	-1.88512600	2.37012200	H	-3.60090200	-2.25014600	-0.73220700
C	-3.47347500	-1.16291900	-2.13037400	H	-2.45562100	-1.64705600	1.35807600
O	-4.38151300	-1.56733600	-2.83929200	H	-1.60850300	-0.29720700	0.57472700
O	-3.11514000	0.12292800	-2.22152800	H	-1.06860300	-3.27142200	0.08710000
H	-2.36527400	0.39856000	-1.63323700	H	0.45527300	-0.87149600	1.24071600
N	3.36970600	-0.17852100	-0.17278400	H	-0.08876100	-2.28611800	2.16265000
C	3.37106700	-1.44774000	0.23447000	H	1.53352100	-3.74241600	1.05759200
N	4.64508900	-1.84384800	0.33561100	H	3.04056700	-3.03915000	-0.72670900
C	4.67333100	0.24082800	-0.33366100	H	2.44984900	-1.36590200	-0.66913100
C	5.48330400	-0.80497000	-0.01437700	H	0.76314800	-3.80514900	-1.51736900
H	4.91715500	1.23959200	-0.66106300	H	1.42023800	-2.55081200	-2.59316600
H	6.55615000	-0.90764200	-0.00741100	C	2.71036800	-2.14993300	1.88579200
H	4.93252900	-2.77313800	0.62582300	O	3.38807400	-2.98076000	2.54093600
O	-1.10385700	1.28145400	-0.70285200	O	2.86983500	-0.88583500	1.97484500
H	0.05187900	1.21372800	-0.67939800	H	2.21109700	0.17780300	1.02351900
O	1.30772400	1.26521200	-0.67589600	N	-3.74045300	1.05563500	-0.11500800
H	2.45601800	0.42252600	-0.37379200	C	-4.04670200	-0.21165400	-0.40742500
C	1.71709500	2.60752300	-0.55157600	N	-5.37793100	-0.29593700	-0.41604600
H	0.86881800	3.25320600	-0.27898700	C	-4.89525100	1.78821800	0.06559700
H	2.47921900	2.71307900	0.23652000	C	-5.93404500	0.93417600	-0.12503700
C	2.29803300	3.07013200	-1.87385700	H	-4.87494500	2.83750800	0.31212400
F	2.75304200	4.39514200	-1.74515200	H	-7.00012400	1.08463000	-0.07738100
C	-1.61162100	1.79361500	0.43782300	H	-5.89097700	-1.15134300	-0.60745300
C	-0.87247400	1.81396700	1.63382700	O	1.80423400	0.92263900	0.46427800
C	-2.91940700	2.30498900	0.44095300	H	-0.17703800	1.29854000	-0.08738400
C	-1.43466100	2.34221100	2.79527800	O	-0.93255300	1.90773900	-0.00230400
H	0.14141900	1.42293000	1.64235900	H	-2.77493400	1.40860100	-0.05374000
C	-3.47409500	2.81794400	1.61133000	C	-0.68760600	2.73225900	1.13047000
H	-3.48971000	2.29024800	-0.48408000	H	0.29132900	3.22004900	1.05036400
C	-2.73785600	2.84224800	2.79811500	H	-1.46544300	3.50061500	1.14281800
H	-0.84644500	2.35471300	3.70871600	C	-0.75437400	1.90289000	2.39940700
H	-4.48913100	3.20485000	1.59285200	F	-0.51010000	2.75359700	3.48801500
H	-3.17088400	3.24580400	3.70764100	C	2.69918900	1.42756700	-0.42341200
H	3.15677000	2.45757100	-2.16455300	C	2.27465200	2.44790900	-1.28248700
H	1.54310500	3.05775000	-2.66493200	C	4.01790100	0.96119800	-0.49550300
<b>Product</b>				C	3.16475100	2.99624900	-2.20326700
C	-0.19208000	-1.86568000	-1.30019300	H	1.25028300	2.80389900	-1.21509400
C	-1.28222100	-2.02049900	-2.37555200	C	4.89765500	1.51893800	-1.42260200
C	-2.42836200	-1.02770300	-2.10365900	H	4.34469000	0.17211100	0.17544600
C	-3.06367600	-1.28971700	-0.70408600	C	4.48080200	2.53595500	-2.28217500
C	-1.98694500	-1.31915700	0.41681700	H	2.82448000	3.78883600	-2.86340800
C	-0.76977200	-2.20804800	0.09294000	H	5.91851700	1.15106400	-1.47051900
C	0.29551900	-1.95843600	1.18270800	H	5.17127500	2.96465200	-3.00119200
C	1.65153700	-2.65795500	0.90988100	H	-1.74486000	1.46151900	2.53948300
C	2.14920300	-2.41908100	-0.54648300	H	0.01316900	1.12309500	2.41025700
C	1.04511500	-2.73940600	-1.57521400				
H	0.13165800	-0.80430100	-1.28725400				