

## SUPPORTING INFORMATION

### **Acid-catalysed esterification of betaines : theoretical exploration of the impact of the carbon chain-length on the reaction mechanism**

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**Table S1.** Total electronic energies (Ee), zero-point corrected electronic energies (EZPE), enthalpies (H298) and Gibbs free energies (G298) for gas phase structures involved in the reaction profiles.

a): Reaction profile for **GB2** + HCl + primary hydroxyl glycerol

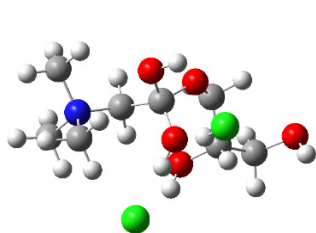
Structures	Ee <sup>a</sup>	EZPE	H <sub>298</sub>	G <sub>298</sub>	ΔG <sup>b</sup>
<b>R</b>	-1707.784197	-1707.808108	-1707.783253	-1707.864355	0.0
<b>TS1</b>	-1707.754699	-1707.775822	-1707.753755	-1707.826890	23.5
<b>IR1</b>	-1707.767086	-1707.789126	-1707.766142	-1707.842322	13.8
<b>IR2</b>	-1707.769797	-1707.792242	-1707.768853	-1707.845971	11.5
<b>TS2</b>	-1707.756182	-1707.777324	-1707.755237	-1707.82729	23.1
<b>P</b>	-1707.786830	-1707.810958	-1707.785886	-1707.866875	-1.6

b): Reaction profile for **GB3** + HCl + primary hydroxyl glycerol

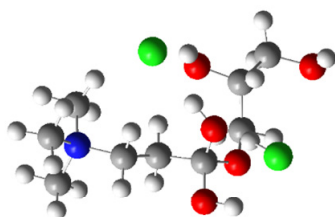
Structures	Ee <sup>a</sup>	EZPE	H <sub>298</sub>	G <sub>298</sub>	ΔG <sup>b</sup>
<b>R</b>	-1747.067537	-1747.092906	-1747.066593	-1747.152808	0.0
<b>TS1</b>	-1747.052364	-1747.074680	-1747.051420	-1747.127698	20.6
<b>IR1</b>	-1747.053115	-1747.076673	-1747.052171	-1747.132037	13.0
<b>IR2</b>	-1747.053763	-1747.077454	-1747.052819	-1747.132580	12.7
<b>TS2</b>	-1747.041059	-1747.063490	-1747.040114	-1747.115085	23.7
<b>P</b>	-1747.071143	-1747.096295	-1747.070199	-1747.154539	-1.1

<sup>a</sup> Electronic structure calculations at the B3LYP/6-31+G(d,p) level. All values are in atomic units (1a.u. = 627.51kcal/mol).

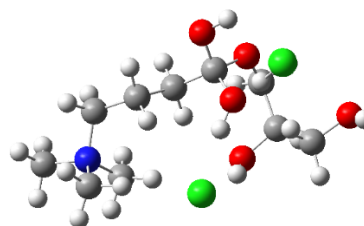
<sup>b</sup> Relative energies in kcal/mol.



**IR1-1**



**IR1-2**



**IR1-3**

**Figure S1:** Structure of the IR1 intermediate species for betaines 1, 2 and 3, showing the molecular backbone folding in IR1-3

## Optimized structures

Betaine (zwitterion) GB2 et GB3

Gas phase HCl

Betaine hydrochloride GB2 (two structures, GB2-1 to GB2-2)

Equilibrium structures (R, IR1, IR2, P) and transition structures (TS1, TS2) for HCl-catalyzed esterification reaction profiles:

GB2 + HCl + prim-glycerol

**R1** : Betaine hydrochloride GB2-3 + HCl

**R2** : Glycerol

**R**: Pre-reactant structure, i.e., (GB2 ou GB3 + HCl + glycerol) van der Waals complexe

**TS2**: HCl-catalyzed nucleophilic addition transition structure

**IR1**: tetrahedral intermediate resulting from nucleophilic addition

**IR2**: rearranged tetrahedral intermediate

**TS2**: HCl-catalyzed H<sub>2</sub>O elimination transition structure

**P**: Product structure, i.e., (ester + HCl + H<sub>2</sub>O) Van der Waals complexe

## Cartesian Coordinates in Å

### HCl

H	-0.0933901188	0.	0.
Cl	1.1933901188	0.	0.

### H<sub>2</sub>O

O	-2.8690237817	-0.4159257006	0.0039920116
H	-1.9044683755	-0.4459520434	-0.0062353048
H	-3.1606378428	-1.286722256	-0.2927367067

### Glycerol

O	-0.54915800	1.61917400	0.03209600
C	0.01272500	0.34713000	-0.27521500
C	1.44738300	0.36037200	0.25730300
O	2.17262200	-0.81555500	-0.10109600
C	-0.82425900	-0.77188900	0.33025800
O	-2.14262000	-0.63178500	-0.21965700
H	-2.74678200	-1.23680500	0.22701800
H	-0.84774300	-0.65670600	1.42329900
H	-0.38869600	-1.74602800	0.07799300
H	0.03594900	0.20335600	-1.36959100
H	-1.50099500	1.55689800	-0.13728500
H	1.94590200	1.27062500	-0.09903200
H	1.43832200	0.39192800	1.35098700

H	2.40219100	-0.77161300	-1.03819900
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• 2CH<sub>2</sub>

Glycine Betaine (zwitterion) **GB(CH<sub>2</sub>)**

N	1.20652300	-0.02715900	0.06698100
C	0.34026400	1.22208300	-0.24918100
H	0.19874200	1.72045200	0.71298100
C	-1.00704700	0.94857200	-0.90442900
C	-1.85927000	-0.03555900	-0.03412500
O	-2.35054700	0.46125000	1.00121300
O	-1.83457400	-1.23974400	-0.42121700
H	0.97654300	1.84411600	-0.88638800
H	-1.50981100	1.92046300	-0.95201200
H	-0.88100100	0.57636800	-1.92558200
C	2.61175500	0.44397500	0.29302800
C	0.73459600	-0.73137300	1.32368000
C	1.17808200	-1.00586800	-1.08187200
H	1.45233600	-1.52297900	1.54716800
H	0.70249600	-0.00517900	2.13573100
H	-0.25491000	-1.15215600	1.14698900
H	1.87382800	-1.81571200	-0.85379400
H	0.15182600	-1.38108000	-1.17281000
H	1.49483700	-0.48660700	-1.98808100
H	3.23394700	-0.40758000	0.57232100
H	2.99210300	0.89479800	-0.62462300
H	2.61407900	1.18218400	1.09666000

**GB2-1**

N	0.62086800	0.29761000	0.00094200
C	-0.85182300	0.64098500	0.00150700
H	-1.03238800	1.26031200	0.88217100
C	-1.80751600	-0.55233500	0.00043500
C	-3.25254300	-0.05348100	-0.00070300
O	-3.56052600	1.11232800	-0.00213000
O	-4.20711200	-1.01496700	-0.00017900
H	-1.03270200	1.26212700	-0.87779100
Cl	4.13965800	-0.39605100	-0.00133500
H	-1.66134600	-1.18620800	-0.88173700
H	-1.66264900	-1.18670100	0.88245900
C	1.40567400	1.59571100	0.00263300
C	1.01905900	-0.48723200	1.23144800
H	-3.82779800	-1.90643400	0.00122400
C	1.01894800	-0.48390400	-1.23174400
H	2.11109400	-0.61463800	1.18581800
H	0.71526100	0.07944100	2.11369600
H	0.52510500	-1.45864200	1.21096900
H	2.11103300	-0.61136200	-1.18636100
H	0.52501900	-1.45537700	-1.21389600

H	0.71512000	0.08517900	-2.11242300
H	2.47092900	1.32708600	0.00225100
H	1.13667700	2.15989900	-0.89181400
H	1.13668700	2.15756800	0.89855400

# **GB2-2**

N	-1.12230300	-0.06323400	0.13207300
C	0.37872000	-0.17126000	0.27188600
H	0.80821800	0.64553500	-0.31077300
C	0.98157400	-1.50761500	-0.16496500
C	2.49614400	-1.49937000	0.01910800
O	3.13819600	-0.53068100	0.35948100
O	3.12899900	-2.66374100	-0.22606200
H	0.61072000	0.01649300	1.32252900
Cl	-4.67714000	0.28087500	-0.15544300
Cl	3.01436200	2.66542000	-0.14251800
H	0.56934500	-2.34284900	0.41245200
H	0.77727800	-1.71480600	-1.22214000
H	3.25854000	1.42311700	0.14517200
C	-1.53865600	1.31538500	0.61269400
C	-1.56669700	-0.20548500	-1.30758900
H	2.51590500	-3.36990900	-0.48039600
C	-1.84639600	-1.08851200	0.97646900
H	-2.65339200	-0.03142500	-1.32049700
H	-1.03141000	0.53323000	-1.90698900
H	-1.34444400	-1.21538800	-1.65274500
H	-2.92222500	-0.87613600	0.87727900
H	-1.62498200	-2.08622700	0.59708700
H	-1.50741300	-0.98497500	2.00910400
H	-2.62929300	1.37685700	0.49973300
H	-1.24073000	1.41807500	1.65733600
H	-1.02846900	2.06054800	0.00071300

# **Betaine 2CH<sub>2</sub> protonated**

C	-2.5569680683	-0.7738854115	1.5049543813
N	-2.491260696	-0.4930608191	0.0235356447
C	-3.4650312089	0.6058161443	-0.3257882919
C	-2.8868151512	-1.7463040179	-0.7246973266
C	-1.0695872569	-0.1300045751	-0.407964116
C	-0.4802192059	1.120531901	0.2403467673
C	0.9305256499	1.3287510241	-0.3004878305
O	1.4941221455	2.4183847686	0.2392134797
O	1.4610839459	0.6006936369	-1.109480469
H	-3.561575858	-1.1201700558	1.7498374693
H	-1.8274972399	-1.5465291935	1.7506082138
H	-2.3409272908	0.1379886049	2.059299116
H	-3.8992022436	-2.0264490455	-0.4328292169
H	-2.8483135534	-1.5456383178	-1.7955836184
H	-2.1896775302	-2.544871354	-0.4700709876
H	-0.4506819892	-1.0010234668	-0.1852129259
H	-1.0989074388	-0.0173232471	-1.4932227666

H	-1.0536158746	2.0266855294	0.0204055902
H	-0.4065100648	1.0430877867	1.3297666657
H	-4.4738858547	0.2653095303	-0.090456196
H	-3.2357187919	1.4959140835	0.2578535423
H	-3.385306806	0.8226699446	-1.3916589178
H	2.3914930118	2.5230873797	-0.1257115171

**GB (2CH2):** Active specie in Watson

C	1.8190518416	-1.3729963466	1.0068654609
N	1.6655701906	-0.0345649732	0.3116017081
C	2.1153428401	-0.1541640065	-1.1311855163
C	2.5642679548	0.9775096078	1.0130804465
C	0.2421651328	0.4945899233	0.4160242776
C	-0.839632364	-0.3913340114	-0.2386046911
C	-2.2215112296	0.1838371165	-0.1023180342
O	-2.3629962036	1.2963213875	0.5123801455
O	-3.2816217606	-0.3709422909	-0.5655378879
H	2.8753370606	-1.6431377715	1.0006278562
H	1.4702114658	-1.2839692191	2.0367355331
H	1.2571172659	-2.1371995107	0.4698756241
H	3.5925679251	0.6215200489	0.9524606827
H	2.4744288875	1.9412450719	0.5108086245
H	2.2603524093	1.0595649275	2.0571300577
H	0.0350270069	0.6157251883	1.4813391158
H	0.2462515522	1.4849350499	-0.0440658138
H	-0.6706265649	-0.5296318745	-1.3155742595
H	-0.8813682912	-1.3959002505	0.204820828
H	3.1718148106	-0.4235348349	-1.139492937
H	1.5483314742	-0.9380031214	-1.6334139196
H	1.9787061742	0.8064348236	-1.6300082365
H	-3.2908980999	1.6222653131	0.5697035418
H	-3.179395878	-1.2224559568	-1.0369111265

**GB (2CH2):** Active specie in Ingold

C	2.13196800	1.28690600	-0.00069900
H	1.93025400	1.87154800	-0.89911100
H	1.93038100	1.87250700	0.89711700
H	3.16921500	0.95178600	-0.00058800
C	1.54732700	-0.77179500	-1.24284300
H	2.61396100	-0.99834900	-1.24162000
H	0.99243300	-1.71059600	-1.22092900
H	1.29915100	-0.18683300	-2.12990500
C	1.54761400	-0.77056200	1.24361400
H	1.29965600	-0.18471500	2.13015100
H	0.99271500	-1.70938200	1.22278600
H	2.61424100	-0.99714000	1.24235000
C	-0.19179600	0.55456900	-0.00009900
H	-0.31217900	1.17659200	-0.88966100
H	-0.31224000	1.17686300	0.88926500
C	-1.26985400	-0.58347700	-0.00004200

H	-1.22651100	-1.22920200	0.89231400
H	-1.22660200	-1.22912800	-0.89246400
N	1.23723800	0.04478100	0.00001400
C	-2.61660900	-0.04455600	0.00011900
O	-3.66462900	0.35700900	-0.00001200

**R (Esterification of GB2 + HCl + primary glycerol)**

C	4.06550000	0.93403700	1.57559000
N	3.48436100	0.22982300	0.38514800
C	2.91752100	-1.10911100	0.81100700
C	4.56560600	-0.02282500	-0.63387700
C	2.42372700	1.10312200	-0.30109500
C	1.15344800	1.32194100	0.51509200
C	0.00322000	1.89940900	-0.31488400
O	-0.33290200	1.30867600	-1.44388200
O	-0.62065300	2.86796600	0.10443300
O	-0.27932400	-1.28353700	2.06218100
C	-0.76621100	-2.29239100	1.15027600
C	-1.84582400	-1.78040600	0.17734600
C	-3.22172200	-1.71345500	0.84274300
O	-4.20788600	-1.02300900	0.10152800
O	-1.91986300	-2.65452600	-0.93546600
Cl	-3.68993900	2.58322600	0.01377400
Cl	0.97117700	-1.30689300	-2.08936000
H	4.83563300	0.30101000	2.01893600
H	4.50061600	1.88151900	1.25359800
H	3.27615500	1.11435400	2.30433600
H	5.36220800	-0.60381400	-0.16709600
H	4.12679800	-0.57715600	-1.46478400
H	4.95574100	0.93461300	-0.98215800
H	2.92444800	2.04949600	-0.52440800
H	2.19383000	0.57535400	-1.22869100
H	0.76872100	0.37885900	0.92269100
H	1.30436700	2.01464600	1.34533900
H	-2.39448300	2.80496900	-0.09404400
H	3.75135000	-1.73062300	1.14154800
H	2.20975600	-0.96769800	1.62685400
H	2.40861100	-1.54688800	-0.05277900
H	-0.98673100	-1.04657400	2.67602300
H	0.10065400	-2.59924000	0.56292600
H	-1.12916600	-3.16664700	1.70797600
H	-1.55972700	-0.76810300	-0.14416100
H	-1.17149100	-2.44932400	-1.52431500
H	0.12722600	0.42763700	-1.65373700
H	-3.59519300	-2.73551300	0.96783600
H	-3.11234100	-1.27147700	1.85080400
H	-3.95512800	-0.09230500	0.00270000

**TS1-2 (Esterification of GB2 + HCl + primary glycerol)**

C	-4.41822700	-1.36501200	1.01009300
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N	-3.84735600	-0.25364200	0.17635700
C	-3.71733800	1.00243200	1.01176500
C	-4.77796100	0.03787700	-0.97318400
C	-2.50222700	-0.66624200	-0.43112200
C	-1.33950800	-0.72501200	0.55893500
C	-0.05785300	-1.00345600	-0.23000800
O	0.21265700	-0.20985900	-1.25710900
O	0.10494900	-2.30726300	-0.45723700
O	1.14413800	-0.69419900	0.97416400
C	1.51988700	0.70126200	1.22947600
C	2.57423100	1.27138200	0.26221800
C	4.02020300	0.87065400	0.62913000
O	4.79668800	0.48145300	-0.48844300
O	2.47449900	2.69514900	0.32152700
Cl	3.07226000	-2.38759800	-0.30605900
Cl	-1.05953600	2.42119700	-0.82185300
H	-5.36911400	-1.03681800	1.43246100
H	-4.57105500	-2.24154300	0.37894000
H	-3.72216000	-1.60412900	1.81317000
H	-5.77135700	0.25450200	-0.57803400
H	-4.39138600	0.89950300	-1.51844300
H	-4.81631300	-0.83414700	-1.62729400
H	-2.66932700	-1.63311000	-0.91195600
H	-2.28740800	0.09124500	-1.18544100
H	-1.22897500	0.23820900	1.05593000
H	-1.44154500	-1.51859700	1.30154200
H	1.04385800	-2.49487300	-0.75744100
H	-4.72178100	1.37649200	1.21488700
H	-3.22356000	0.75398200	1.95015200
H	-3.11742800	1.73132000	0.45567100
H	1.95713300	-1.27208800	0.63971600
H	0.60246700	1.28672800	1.14881800
H	1.86577300	0.73190200	2.26737200
H	2.36920200	0.91080400	-0.75108700
H	1.65308000	2.96835200	-0.11954800
H	-0.15803100	0.73337700	-1.14227200
H	4.50359800	1.74897400	1.06766600
H	4.01276300	0.07121900	1.38425700
H	4.52605900	-0.42254700	-0.72608500

**IR1-2 (Esterification of GB2 + HCl + primary glycerol)**

C	-4.23988000	-1.10338400	0.29221600
N	-3.55304200	0.22125700	0.12717300
C	-3.19844800	0.78986400	1.48460500
C	-4.48279300	1.18611600	-0.55921100
C	-2.30982200	0.08234500	-0.76428500
C	-1.13864100	-0.64264900	-0.11547400
C	0.10503600	-0.56437100	-1.03193600
O	0.31566400	0.67647600	-1.59126100
O	-0.08055300	-1.49333800	-2.04967000



O	1.26943900	-1.01971300	-0.29904400
C	1.79886400	-0.13699600	0.72247900
C	2.85367900	0.86510700	0.20717400
C	4.22059000	0.20317800	0.07187300
O	5.20249200	1.01050000	-0.56935400
O	2.94812000	1.93973500	1.13138000
Cl	0.83199100	-3.79260500	0.90840800
Cl	-0.46249100	2.76649200	0.44520300
H	-5.11238200	-0.97207100	0.93425800
H	-4.54752300	-1.46911000	-0.68850600
H	-3.54852200	-1.81019500	0.74936200
H	-5.41306700	1.24781700	0.00748600
H	-3.99787400	2.16212200	-0.59724700
H	-4.68236000	0.82699800	-1.56969900
H	-2.64317800	-0.42412900	-1.67305000
H	-2.01531100	1.10502600	-0.99829300
H	-0.88362500	-0.16103400	0.82798500
H	-1.33723900	-1.70252900	0.06309900
H	0.61314700	-1.33893500	-2.70925900
H	-4.12518800	1.09043700	1.97594000
H	-2.70597200	0.01795400	2.07394100
H	-2.52033000	1.63914500	1.34182900
H	1.06623100	-2.63950100	0.29500200
H	0.99212200	0.43409400	1.18849000
H	2.23269700	-0.79531200	1.48206600
H	2.53382300	1.22765700	-0.77947300
H	2.12650500	2.45918800	1.07583500
H	0.13526100	1.42125800	-0.94291800
H	4.61580400	-0.01115500	1.07019900
H	4.09207000	-0.75173800	-0.46132600
H	4.82191500	1.35459600	-1.38836900

**IR2-2 (Esterification of GB1 + HCl + primary glycerol)**

C	-4.27443000	0.32056400	0.67179500
N	-3.34396300	-0.37780900	-0.28523100
C	-2.99935500	-1.73056600	0.29718900
C	-2.10145900	0.51757100	-0.43372900
C	-0.89995400	-0.15661500	-1.08425300
C	0.33058400	0.76883800	-1.00448500
O	0.00201700	1.92414800	-1.72204200
C	-4.02339200	-0.55542100	-1.61026700
O	1.46303700	0.23516000	-1.64143300
C	1.94659500	-1.09605500	-1.37404700
C	2.13920300	-1.52402400	0.08626800
O	0.93929500	-2.12151000	0.58583400
O	0.66477000	1.13077400	0.31852300
C	3.24824100	-2.58596800	0.18497700
O	4.52299400	-2.11428200	-0.24926600
Cl	-0.74074100	-0.34513300	2.57782000
Cl	2.05997200	3.84324300	0.64460800
H	-2.42740000	1.39242300	-0.99973900

H	-1.85079700	0.81077200	0.58553000
H	-0.63816800	-1.08305500	-0.57110400
H	-1.06316200	-0.36040400	-2.14700300
H	0.78471200	2.49720700	-1.74529600
H	1.45992000	2.66696000	0.63728100
H	1.29058100	-1.83375100	-1.85838000
H	2.91428600	-1.11063500	-1.87943100
H	0.19383200	0.63692900	1.04911500
H	2.41990700	-0.65113700	0.68778900
H	0.61082800	-1.66016400	1.38660600
H	3.28197200	-2.95439100	1.21809200
H	3.00524100	-3.43564700	-0.46175600
H	4.84949500	-1.45986600	0.38238000
H	-3.93478200	-2.23687700	0.54155700
H	-2.44842200	-2.30879700	-0.44255300
H	-2.38490700	-1.57206300	1.18956600
H	-5.20474900	-0.24571800	0.73945200
H	-3.78451700	0.36922200	1.64549000
H	-4.47307600	1.32642200	0.29911300
H	-4.89530700	-1.19845400	-1.47941500
H	-4.33130800	0.42107100	-1.98679900
H	-3.32645600	-1.01749300	-2.30877800

**TS2-2 (Esterification of GB2 + HCl + primary glycerol)**

C	-4.19328700	-0.12945400	0.54472500
N	-3.19129400	-0.58353400	-0.48872100
C	-2.76600500	-1.99315400	-0.14196700
C	-2.02040500	0.40762600	-0.43317800
C	-0.73576200	-0.08395300	-1.09086000
C	0.36325500	0.96140200	-0.93371300
O	-0.03592200	2.17815400	-1.21036100
C	-3.82730400	-0.56754100	-1.84759200
O	1.59086100	0.66783200	-1.37396900
C	2.16134500	-0.67125400	-1.33600400
C	2.34243800	-1.31692300	0.04166700
O	1.16556600	-2.03761400	0.41563800
O	0.67970100	0.98697300	0.84376200
C	3.49755800	-2.33401900	-0.01334700
O	4.74377200	-1.74834000	-0.37970100
Cl	-0.93559000	-0.79914300	2.57238700
Cl	1.25827800	3.85617500	0.66861300
H	-2.37809200	1.33095000	-0.89094600
H	-1.84275800	0.56948500	0.62899600
H	-0.38782900	-1.01920500	-0.65176600
H	-0.85252400	-0.21706600	-2.17427900
H	0.53457600	2.91555000	-0.72070300
H	0.86976100	1.95923100	1.06840300
H	1.56671200	-1.33591300	-1.97403600
H	3.13912500	-0.52075400	-1.79401500
H	0.07123200	0.53167500	1.50959700
H	2.57400100	-0.53690000	0.77417400

H	0.78724500	-1.71770000	1.25936400
H	3.55241100	-2.84116800	0.95781300
H	3.28519900	-3.09517100	-0.77146400
H	5.07179700	-1.20854400	0.35171900
H	-3.66856700	-2.59841900	-0.04295800
H	-2.14427700	-2.38720200	-0.94444200
H	-2.20780500	-1.95838400	0.79891500
H	-5.08081500	-0.76023500	0.47537000
H	-3.72831900	-0.22347600	1.52785100
H	-4.45437900	0.91104500	0.34663400
H	-4.65074800	-1.28319600	-1.86205400
H	-4.20054100	0.43618100	-2.05498800
H	-3.08484500	-0.84801000	-2.59447000

**P (Esterification of GB2 + HCl + primary glycerol)**

C	-3.71362800	0.47480100	0.88277700
N	-3.04453900	0.17644300	-0.44049100
C	-3.05320600	-1.32118600	-0.64026000
C	-1.61691600	0.72078900	-0.34492400
C	-0.72784800	0.45351300	-1.56269700
C	0.59453300	1.18028300	-1.31020300
O	0.58270700	2.38476800	-1.09406500
C	-3.80467600	0.84524300	-1.54530800
O	1.75879100	0.54398100	-1.36197600
C	1.95216200	-0.88901800	-1.54211400
C	1.66912700	-1.71599800	-0.29009500
O	0.29271400	-2.08118800	-0.27101500
O	0.82498300	0.62290700	1.81824800
C	2.52447100	-2.99583700	-0.29327500
O	3.92616700	-2.72849500	-0.28378000
Cl	-1.26132700	-1.64078200	2.39182800
Cl	2.35309900	3.80336100	1.04395100
H	-1.71286900	1.79494900	-0.17716700
H	-1.18659200	0.25962100	0.54461600
H	-0.57946300	-0.61530900	-1.69684200
H	-1.13837200	0.90140200	-2.47489000
H	1.71909600	3.18266200	0.07420900
H	1.15623300	1.30867500	2.41137600
H	1.35459800	-1.24754900	-2.38691500
H	3.00977900	-0.95694600	-1.79767300
H	0.26515200	0.01062400	2.34034900
H	1.91564500	-1.10245400	0.58633200
H	-0.06413200	-2.06295500	0.65014000
H	2.22226600	-3.61402800	0.56134800
H	2.33147600	-3.57302400	-1.20379800
H	4.17523200	-2.38130500	0.58305000
H	-4.09311900	-1.65239200	-0.64944000
H	-2.57722500	-1.55993900	-1.58978900
H	-2.51034300	-1.77445500	0.19331900
H	-4.74253000	0.11409000	0.83790800
H	-3.15405800	-0.04661100	1.66560000

H	-3.69899900	1.55369200	1.04378100
H	-4.83955500	0.50101800	-1.51849000
H	-3.76753200	1.92591600	-1.39956200
H	-3.36004600	0.58404700	-2.50497000

• 3CH<sub>2</sub>

**Betaine 3CH<sub>2</sub> protonated**

C	-0.4148643654	-1.1851689344	0.252868444
C	-1.8666857962	-1.219484012	-0.2506948373
C	-2.5810475405	0.1058390222	-0.0543801844
O	-3.8728398304	0.0296082485	-0.4007710873
O	-2.0523941348	1.1203940342	0.3632619771
H	-0.0274132502	-2.2079196132	0.2745467113
H	-0.426563429	-0.8118179115	1.2802983281
H	-1.9309580737	-1.4939052737	-1.3112665099
H	-2.4308204837	-1.9904905148	0.2843668829
C	0.4570992011	-0.2991433691	-0.6427654131
H	-0.0706272075	0.6207733409	-0.8960379331
H	0.7230746949	-0.823304213	-1.564939822
N	1.783728198	0.1615647759	-0.0286415787
C	2.615205289	-1.0147115642	0.4128333018
H	2.0959841382	-1.546022502	1.208918713
H	2.7731494404	-1.6766572891	-0.4397015578
H	3.574060647	-0.647854385	0.7807754244
C	1.5396937359	1.082975882	1.1448411443
H	0.8806945247	1.8909046926	0.8275244549
H	1.0716794669	0.5271713413	1.9544691635
H	2.500078841	1.4780739998	1.4772865103
C	2.5405814701	0.9273443661	-1.0871007623
H	2.7334312587	0.2679006318	-1.9337638615
H	1.937636087	1.7781508107	-1.4055861005
H	3.4834998013	1.2765311947	-0.6652481716
H	-4.2898694329	0.8977768513	-0.2558646861

**Active specie in Watson**

C	-0.0458564067	-0.7074658614	-0.0011808044
H	0.1475667999	-1.3217725532	-0.8845700385
H	0.1511177851	-1.3218612718	0.8813610954
C	0.9285336348	0.4924836987	-0.0030786471
H	0.7765391894	1.138553956	0.8750439901
H	0.7731759171	1.1385166313	-0.8806356189
C	2.3794990803	0.1223473038	-0.0058301481
O	3.3423705799	0.9752398438	-0.0077777227
H	3.0932375149	1.920898398	-0.0073951663
O	2.7041983405	-1.1157204357	-0.0063388256
H	3.6741627921	-1.2800640388	-0.0081843308
N	-2.5859899066	-1.2574466627	0.0034414776
C	-2.5083689519	-2.1285588656	1.2389009406
H	-3.3675829334	-2.7996509216	1.241021152
H	-1.5933394761	-2.7188918734	1.216718633

H	-2.5364893166	-1.4936539364	2.1254375339
C	-2.5134302877	-2.1271689099	-1.2332979726
H	-1.5983526882	-2.7175762614	-1.2155118824
H	-3.3726763585	-2.7982240029	-1.2326814619
H	-2.5451263207	-1.4912700453	-2.1190004914
C	-3.9239647786	-0.5371751989	0.006570033
H	-4.718974396	-1.2828577986	0.0078277234
H	-3.993996971	0.0805158173	0.9024778426
H	-3.9976889625	0.0814306865	-0.8884106494
C	-1.4940500849	-0.1894861585	0.001812738
H	-1.6807289739	0.4250410816	0.887046127
H	-1.6841640309	0.425853798	-0.8821254365

#### Active specie in Ingold

C	-0.3718835412	0.6513065808	0.0005448375
H	-0.6052829948	1.2434777838	-0.8876365996
H	-0.6035917213	1.2455123363	0.8878097293
C	-1.2794201628	-0.6293952466	0.002902819
H	-1.1256617669	-1.2620795578	0.8931220308
H	-1.1269901804	-1.2644142659	-0.8858846446
C	-2.6912113761	-0.3123697116	0.003524923
O	-3.7865931127	-0.062925219	0.0040188933
C	1.1011317685	0.192986132	-0.0004336453
H	1.3110662084	-0.4131529822	-0.8861278084
H	1.3125795178	-0.4124579635	0.8853759374
N	2.1368756416	1.3117285741	-0.0017474724
C	2.0219844855	2.1783236241	-1.2400212204
H	2.078768971	1.5452669326	-2.1266492681
H	1.084508605	2.7331490904	-1.2181328848
H	2.8524726961	2.884668234	-1.2412695618
C	2.025073671	2.1783561053	1.2368002976
H	1.0871467672	2.732516816	1.2177016555
H	2.0849662239	1.5454049005	2.1232934104
H	2.8550494549	2.8853034103	1.2354793746
C	3.5085109689	0.6497918556	-0.0034187748
H	4.2668164631	1.432772672	-0.0040449654
H	3.6078124152	0.0370236311	-0.9000348918
H	3.6097779183	0.0365615478	0.892661008

#### R (Esterification of GB3 + HCl + primary glycerol)

C	2.50434000	0.99263100	1.52336700
C	0.97470900	0.84662800	1.76407400
C	0.13592300	1.36478600	0.60580100
O	-0.06039500	0.59685200	-0.45246800
O	-0.30469100	2.51222100	0.61641800
O	-2.07344700	-0.36602200	2.21079000
C	-2.37908000	-1.60391600	1.54697500
C	-2.79202700	-1.41574700	0.07542700
C	-4.24202900	-0.94860700	-0.05963400
O	-4.55112000	-0.35533400	-1.31114100

O	-2.64681400	-2.64633500	-0.62515000
Cl	-2.85665000	2.97843600	-1.01656400
Cl	0.83232600	-2.22792300	-0.58836800
H	2.97906300	1.16096200	2.49452500
H	2.69454400	1.90782200	0.95158100
H	0.71297600	-0.19236700	1.98189400
H	0.69241800	1.44856400	2.62877400
H	-1.70327800	2.78736700	-0.38879300
H	-2.87643300	0.16715300	2.27436400
H	-1.45614400	-2.18734200	1.57720400
H	-3.15061700	-2.16211100	2.09748000
H	-2.14241000	-0.64567000	-0.35936200
H	-1.69957000	-2.78207800	-0.79617900
H	0.22748300	-0.37086600	-0.36970600
H	-4.90045400	-1.81755700	0.04060800
H	-4.48059900	-0.25041900	0.76199000
H	-4.05121000	0.47045100	-1.39474600
C	5.08393600	0.86831400	-0.25284500
H	5.62000300	0.95511600	-1.19913000
H	4.73596100	1.85177600	0.06179200
H	5.74078100	0.44562500	0.50891200
C	4.38634300	-1.40254000	-0.89242700
H	4.92290800	-1.28745300	-1.83540800
H	5.05195700	-1.80987300	-0.13015500
H	3.50967900	-2.04287000	-1.01897800
C	3.00148200	0.50838100	-1.51781300
H	2.62088900	1.48160300	-1.21335900
H	3.58884600	0.61057100	-2.43165100
H	2.18038500	-0.19448600	-1.66318900
C	3.16073300	-0.25001700	0.88564000
H	2.41854300	-1.02319600	0.66171400
H	3.91340200	-0.67707500	1.55323200
N	3.90716400	-0.04184400	-0.44122000

**TS1-3 (Esterification of GB3 + HCl + primary glycerol)**

C	-2.28067400	-1.34118800	1.14721000
C	-0.81657400	-1.08458400	1.59742000
C	0.14551600	-1.18177800	0.42121900
O	0.00853900	-0.34168000	-0.60154200
O	0.34769900	-2.44618400	0.06038700
O	1.67141700	-0.77495200	1.18249000
C	1.99547500	0.64201600	1.37972700
C	2.67620000	1.30861500	0.16943800
C	4.18339700	0.99023200	0.07847200
O	4.62962900	0.75879800	-1.24510400
O	2.51944700	2.71870300	0.30930500
Cl	3.14832500	-2.22831100	-0.84870900
Cl	-0.91723800	2.42855500	-0.13512500
H	-2.79803800	-1.89309900	1.93724300
H	-2.26290700	-2.01030000	0.28185900
H	-0.72852800	-0.10620600	2.07678700

H	-0.50511300	-1.84151700	2.31831700
H	1.14973900	-2.51334700	-0.54561900
H	2.35508600	-1.24673500	0.55808500
H	1.05317800	1.14821500	1.59603300
H	2.62618600	0.68703600	2.27314500
H	2.19875900	0.95508300	-0.75113800
H	1.59700900	2.94678200	0.09960700
H	-0.24807800	0.60941900	-0.35770300
H	4.72790400	1.86136000	0.45586100
H	4.42873700	0.12977100	0.71785900
H	4.34303800	-0.13853400	-1.48903000
C	-4.94676000	-1.04751700	-0.39299200
H	-5.56496400	-0.95061300	-1.28675300
H	-4.47611800	-2.03015200	-0.37768900
H	-5.56021500	-0.91498300	0.49961400
C	-4.52898500	1.37723700	-0.47058100
H	-5.12161100	1.44826800	-1.38377700
H	-5.17130100	1.49859200	0.40269600
H	-3.73338600	2.12579000	-0.46756600
C	-3.02980300	-0.14186300	-1.65402500
H	-2.51680800	-1.10093300	-1.63035900
H	-3.68610900	-0.08811600	-2.52398200
H	-2.30130100	0.66979800	-1.66485700
C	-3.03958900	-0.03111900	0.86238900
H	-2.35552200	0.81712900	0.75858200
H	-3.74219900	0.19375700	1.66938400
N	-3.88557000	0.01165500	-0.41648200

**IR1-3 (Esterification of GB3 + HCl + primary glycerol)**

C	-2.22053600	-1.49382100	0.98401600
C	-0.77275400	-1.32110400	1.49721600
C	0.25725600	-1.26712000	0.34862400
O	-0.12491200	-0.50267500	-0.74958600
O	0.39817100	-2.57467600	-0.10232500
O	1.54786500	-0.86979100	0.85784300
C	1.70365500	0.51280100	1.27302900
C	2.50730500	1.35786800	0.26175000
C	4.01678400	1.18544700	0.46143000
O	4.79571000	1.54056500	-0.67407100
O	2.19995600	2.73086200	0.44720500
Cl	3.73306200	-2.23873500	-0.89473600
Cl	-1.00586100	2.41441500	-0.43875900
H	-2.78409300	-2.13080400	1.67367000
H	-2.17312300	-2.02661700	0.03061000
H	-0.69108300	-0.42387800	2.11757700
H	-0.48461400	-2.16942300	2.12254100
H	0.85220700	-2.54529200	-0.95937300
H	2.86378200	-1.67819800	-0.07196500
H	0.72568400	0.98050900	1.40514000
H	2.20228900	0.48933100	2.24838100
H	2.23573200	1.02794500	-0.75183500

H	1.29220600	2.89061700	0.12697300
H	-0.27256500	0.46326600	-0.56172900
H	4.32546000	1.85755000	1.26861100
H	4.23853700	0.15526100	0.77152500
H	4.71347100	0.83539500	-1.33011700
C	-5.02355600	-1.01182800	-0.14002500
H	-5.77106000	-0.84345500	-0.91697700
H	-4.59346100	-2.00671200	-0.25179500
H	-5.48338900	-0.91464700	0.84491900
C	-4.52826600	1.39977900	-0.16708900
H	-5.24312600	1.53979000	-0.97954900
H	-5.03280500	1.49292000	0.79571300
H	-3.70857600	2.11905900	-0.24410100
C	-3.28142100	-0.10237500	-1.63164500
H	-2.81007500	-1.07814200	-1.72513700
H	-4.05563300	0.02046000	-2.39096400
H	-2.52729300	0.68352800	-1.70693100
C	-2.90771300	-0.12780000	0.85086300
H	-2.19034700	0.67295000	0.64946300
H	-3.44965300	0.12346500	1.76764700
N	-3.93996100	0.01331400	-0.27491900

**IR2-3 (Esterification of GB3 + HCl + primary glycerol)**

C	-1.68293900	1.14486200	-0.87874100
C	-0.54207000	0.20426900	-1.29678000
C	0.84286300	0.83416400	-1.08877700
O	0.86585600	2.02453100	-1.82159200
O	1.89734700	0.05723200	-1.61219700
C	2.03044200	-1.34714500	-1.33554400
C	2.05133500	-1.79586300	0.13182000
O	0.73166500	-2.13144100	0.57165300
O	1.12051700	1.12505500	0.26767000
C	2.90975200	-3.06217800	0.29213700
O	4.27547400	-2.87244800	-0.07609100
Cl	-0.72020700	-0.03917200	2.41074100
Cl	3.01614500	3.44536200	0.85488900
H	-1.58064700	2.07548500	-1.44654200
H	-1.58588200	1.42012800	0.17466000
H	-0.56082800	-0.73728600	-0.74787700
H	-0.61931600	-0.01981100	-2.36734500
H	1.76839600	2.37776400	-1.78820300
H	2.16873000	2.43990600	0.70013800
H	1.24055000	-1.91184600	-1.85158900
H	2.98892300	-1.59670000	-1.79581900
H	0.46707300	0.77420700	0.93103000
H	2.47248100	-0.99206000	0.74804200
H	0.45417200	-1.57180000	1.32685100
H	2.81477300	-3.41529300	1.32696500
H	2.52946100	-3.85234000	-0.36400600
H	4.68924600	-2.26590700	0.55233900
C	-3.09339500	0.63073700	-1.17559800



C	-3.95641200	0.49531600	1.17740300
H	-4.45571100	1.44131200	0.96196100
H	-4.57561000	-0.11445900	1.83703300
H	-2.97960700	0.64614900	1.64525800
C	-2.98696500	-1.52026900	0.15511200
H	-3.60575700	-2.17378500	0.77216200
H	-2.75812900	-2.00578700	-0.79400500
H	-2.08125300	-1.25948200	0.70671200
C	-5.12363800	-0.63591600	-0.66089400
H	-5.69880200	0.27037900	-0.85604500
H	-4.99350700	-1.20062300	-1.58520300
H	-5.64100500	-1.24995700	0.07687200
N	-3.77356700	-0.25894700	-0.12012500
H	-3.78227100	1.47151500	-1.29369900
H	-3.11219500	0.04638200	-2.10090400

**TS2-3 (Esterification of GB3 + HCl + primary glycerol)**

C	1.60140300	-1.16643000	-0.72272800
C	0.41739900	-0.31191100	-1.19782600
C	-0.92267400	-1.00016300	-0.98266400
O	-0.91525200	-2.27815300	-1.27208500
O	-2.04156000	-0.36591600	-1.35768500
C	-2.20048100	1.07761200	-1.31454500
C	-2.17173400	1.73707000	0.06839500
O	-0.84061300	2.12325100	0.41812100
O	-1.14930000	-0.95649200	0.81262000
C	-3.02130900	3.02095400	0.05182400
O	-4.38660700	2.78932500	-0.28484900
Cl	0.90845800	0.39212000	2.48674800
Cl	-2.57469900	-3.51544800	0.68691700
H	1.48095800	-2.17188000	-1.13738000
H	1.57224300	-1.27956700	0.36393100
H	0.38421000	0.66882600	-0.72506000
H	0.48295100	-0.16128100	-2.28545900
H	-1.65653400	-2.81104700	-0.76505700
H	-1.60085500	-1.83507400	1.04927100
H	-1.44899600	1.54961500	-1.95840100
H	-3.18669600	1.21676300	-1.75852900
H	-0.40074600	-0.71103100	1.43424400
H	-2.58027700	1.03572300	0.80371000
H	-0.53360400	1.67734100	1.23361200
H	-2.91827000	3.51125200	1.02790700
H	-2.63606600	3.71065800	-0.70665400
H	-4.81802900	2.31516000	0.43849000
C	2.97914800	-0.68578100	-1.18438900
C	4.02870700	-0.23686800	1.04956300
H	4.54597400	-1.18746700	0.91101100
H	4.67337800	0.46844700	1.57593500
H	3.09866300	-0.35536700	1.61204200
C	2.91345300	1.61163200	-0.13197800
H	3.55626000	2.35144500	0.34757900

H	2.59795000	1.96938000	-1.11270000
H	2.06228500	1.40266500	0.52009100
C	5.00548900	0.67570800	-1.00823600
H	5.58727500	-0.23748800	-1.14166900
H	4.78382300	1.12154100	-1.97893600
H	5.56484800	1.38364200	-0.39604800
N	3.71567400	0.34357800	-0.31176100
H	3.66922700	-1.53187400	-1.23460200
H	2.92663600	-0.23589300	-2.18076500

**P (Esterification of GB3 + HCl + primary glycerol)**

C	-1.63334400	0.50526900	-1.49953400
C	-0.21984500	-0.04495400	-1.74995800
C	0.81388600	1.05088500	-1.54083500
O	0.49784500	2.23275500	-1.54870000
O	2.09924700	0.73755600	-1.35595400
C	2.63289400	-0.61611600	-1.33928400
C	2.59541800	-1.25463900	0.04762300
O	1.32715100	-1.84466900	0.28451800
O	-1.46172500	1.66600300	1.62659600
C	3.67580200	-2.34491800	0.16497800
O	5.00117200	-1.84388800	-0.01213700
Cl	0.14240400	-0.72753300	2.81397500
Cl	0.65409500	4.41403000	0.62417200
H	-1.84711600	1.28537100	-2.23578400
H	-1.65173900	1.00904600	-0.52760400
H	0.02537500	-0.87979000	-1.08882400
H	-0.12135200	-0.40916000	-2.78349300
H	0.76003100	3.54435900	-0.35421700
H	-0.97929900	2.50524500	1.62319100
H	2.10823200	-1.24508000	-2.06528300
H	3.66754500	-0.48537300	-1.65910600
H	-0.89530500	1.02556200	2.12266600
H	2.79368500	-0.46967500	0.79236700
H	0.99355600	-1.55489100	1.17937600
H	3.55397100	-2.84235600	1.13465900
H	3.52913900	-3.09900700	-0.61582300
H	5.25543700	-1.34291800	0.77400500
C	-2.75166700	-0.53828800	-1.60553600
C	-3.85940600	-0.13206200	0.60646200
H	-4.68071100	0.34012800	0.06411900
H	-4.23988200	-0.64172000	1.49272700
H	-3.11124800	0.60484800	0.90825900
C	-2.09840300	-1.84415000	0.45184000
H	-2.52268800	-2.39037400	1.29474700
H	-1.58646800	-2.53020700	-0.22353300
H	-1.40560700	-1.10349300	0.85208200
C	-4.26374900	-2.20493300	-0.63802100
H	-5.07747800	-1.73012400	-1.18853000
H	-3.80261100	-2.98178300	-1.24939600
H	-4.64677700	-2.64214300	0.28446200

N	-3.22917000	-1.17223300	-0.29216700
H	-3.65327800	-0.09102800	-2.03212800
H	-2.46074600	-1.37887800	-2.24324000