

**Role of Kinetics on the Site Reactivity of the Reactions between Leucine Residues
and Free Radicals in Aqueous Solution: A Theoretical Study**

Manuel E. Medina,^{a,b} Annia Galano,^b Juan Raúl Alvarez-Idaboy*^a

*^aDepartamento de Física y Química Teórica, Facultad de Química, Universidad Nacional Autónoma de México,
México D. F. 04510, México.*

*^bDepartamento de Química, División de Ciencias Básicas e Ingeniería, Universidad Autónoma Metropolitana-
Iztapalapa, Av. San Rafael Atlixco No. 186, Col. Vicentina, México D. F. 09340, México.*

Electronic Supplementary Information

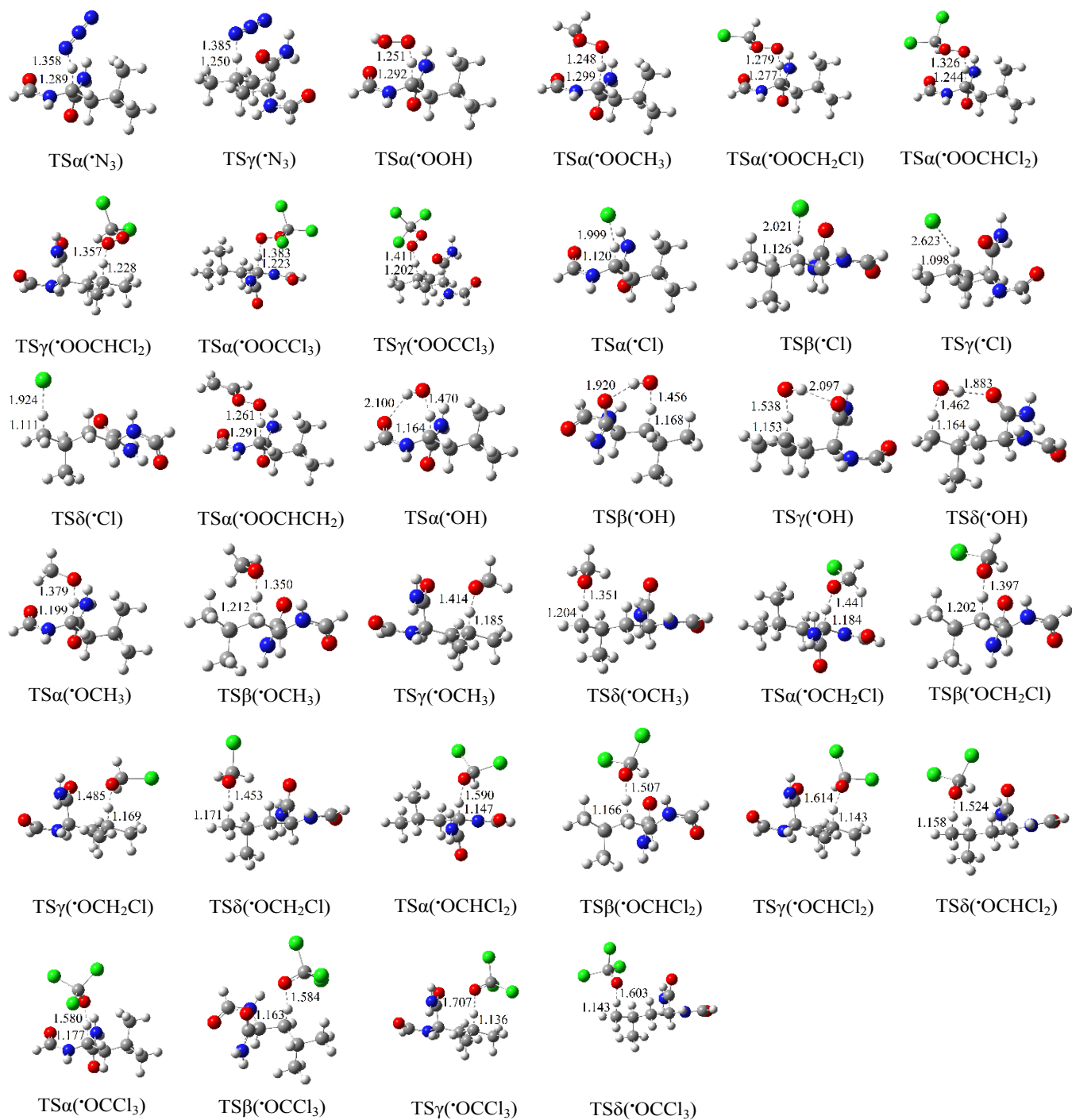


Figure S1. Optimized geometries of the transition states for the HT reactions between 1 and *N_3 , *NO_2 , *Cl , *OR and *OOR radicals.

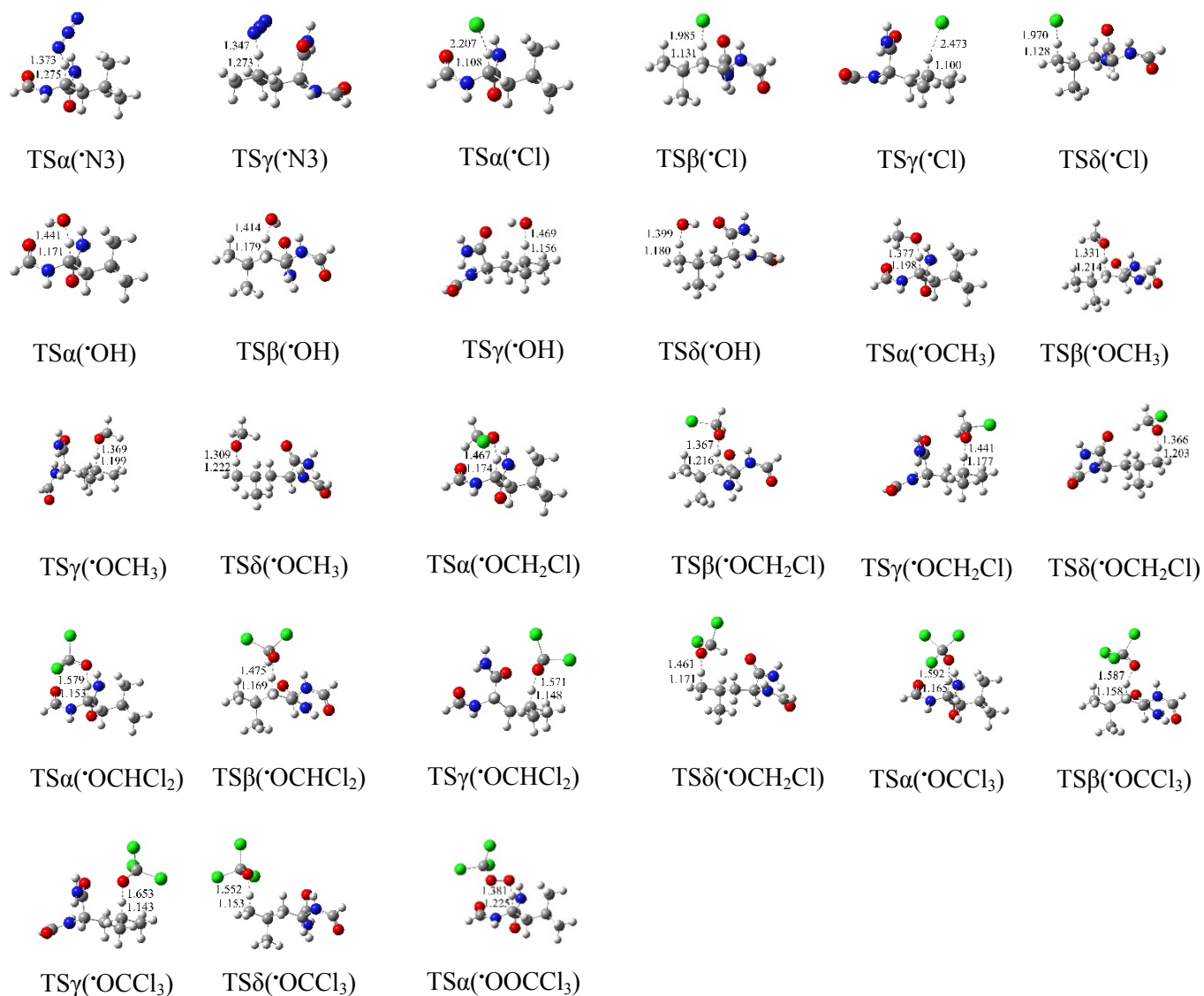


Figure S2. Optimized geometries of the transition states for the HT reactions between 1 and $\cdot N3$, $\cdot Cl$, $\cdot OR$ and $\cdot OOR$ radicals in lipid media.

Cartesian coordinates of all stationary points modelled in water solvent

•N₃

TS α

G= -699.230620

H= -699.170238

If= -1554.9029

0 2

N	0.0081257291	0.1677328703	0.1061958734
H	-0.0273566494	0.4314131074	1.0773031878
H	0.9035818991	0.1187214821	-0.3563691904
C	-1.0937767035	-0.0330460595	-0.6071236925
O	-1.0939540619	-0.2980392476	-1.8092637265
C	-2.4378851813	-0.0292408332	0.1191723629
H	-2.3230069735	0.5462399635	1.2673506561
N	-3.3954333663	0.7877236184	-0.5138951333
H	-4.3514430092	0.4609387887	-0.563972916
C	-3.1343257559	2.0562695116	-0.903401941
O	-2.0330315944	2.5764538372	-0.7931488295
H	-3.996893515	2.572104816	-1.3315684094
C	-2.9875310434	-1.4239816764	0.365916739
H	-3.3105950822	-1.8008714288	-0.6102116808
H	-3.8818831563	-1.3231837741	0.9882205351
C	-2.0330176439	-2.4346935977	1.0002243244
H	-1.1395280042	-2.5142629276	0.3744863557
C	-2.7225652253	-3.7975084191	1.0260346463
H	-3.6194449713	-3.7557340745	1.6489766256
H	-2.0570444171	-4.5554293933	1.4403407316
H	-3.0181304687	-4.1106148554	0.023763802
C	-1.6169192126	-2.0298410227	2.4118724094
H	-0.9807392555	-1.1454442187	2.4136770105
H	-2.4986849662	-1.8275042011	3.0255481286
H	-1.0523477711	-2.8348944611	2.884272932
N	-2.7008024148	1.3292962872	2.3110923819
N	-1.9643780906	1.1619613664	3.2480459228
N	-1.290396409	1.0272068302	4.1544719446

TS γ

G= -699.239996

H= -699.178523

If= -1048.1155

0 2

N	-0.1284453525	-0.0109406955	-0.5173520186
H	0.1073457566	-0.2171541377	0.4400832014
H	0.6019094367	0.0064271247	-1.2131523812
C	-1.3930016884	0.186887809	-0.8883546495
O	-1.7242692329	0.4584351294	-2.0444568338
C	-2.4470759129	0.0236963191	0.2089923723
H	-1.9568532743	0.0024270298	1.1815016942
N	-3.3713502689	1.1443954814	0.170738416
H	-4.3393280845	0.9775593536	-0.0608635542
C	-2.9579333467	2.4024141888	0.3261276262
O	-1.7849353811	2.7110982399	0.5447000758
H	-3.7536510483	3.1483963044	0.2490524972
C	-3.2642464149	-1.2488036807	-0.0239741601
H	-3.7403136524	-1.1790983972	-1.0044874225
H	-4.0648380813	-1.263047096	0.7253467848

C	-2.5382930587	-2.5738719516	0.0918500433
H	-1.7309932847	-2.612334248	-0.8611190513
C	-3.4406542408	-3.7414127521	-0.2374354644
H	-4.1983246155	-3.8382787372	0.5466877985
H	-2.873028525	-4.670570655	-0.2775573536
H	-3.9515728592	-3.5914429603	-1.1884330719
C	-1.7028368486	-2.7887242261	1.3306988927
H	-2.3584457017	-2.7381969225	2.2069437411
H	-1.2428128774	-3.7768981806	1.3130552827
H	-0.9210178723	-2.0411380055	1.4604301684
N	-0.779492599	-2.9374801081	-1.8134910597
N	0.2558192278	-3.0125050299	-1.2090869462
N	1.2473376913	-3.0834197158	-0.6519699993

Cl•

TS α

G= -995.24691

H= -995.190322

If= -200.6021

0 2

C	-3.6325985017	-0.4703812259	-0.5504326336
C	-2.2912491949	-0.1308393193	0.0969356716
C	-2.2584294314	1.3478499594	0.4789785148
C	-1.1764770016	-0.5047885721	-0.8809967469
C	0.2504882613	-0.3790163259	-0.3520751994
C	0.4375381676	-1.2088653974	0.9262626802
O	0.5221246624	-2.4330070568	0.8378319664
N	1.1755372285	-0.7878493277	-1.3658070445
C	2.5009722519	-0.7561456064	-1.1640579218
O	3.0071208904	-0.4272378226	-0.0947989289
N	0.4374302444	-0.5485651722	2.0802633821
H	-4.4565068463	-0.2346493358	0.1239743261
H	-3.6902594566	-1.5292428264	-0.8065582243
H	-3.7657193595	0.1103553286	-1.4664346403
H	-2.1852272824	-0.7359583385	1.0015793411
H	-3.1253575094	1.5942987983	1.0939924666
H	-2.294024194	1.9688630197	-0.419865479
H	-1.367928519	1.6204104712	1.0460530651
H	-1.3060004857	-1.5435628852	-1.1969675841
H	-1.2525837611	0.1235251558	-1.7730400539
H	0.8247930064	-1.0151813408	-2.2852750679
H	3.0944929112	-1.0502361264	-2.0330504753
H	0.3771522867	0.4563658823	2.1118087173
H	0.4962615683	-1.0656763659	2.9445213599
H	0.4628734814	0.6970157018	-0.0894141803
Cl	1.1103065831	2.5571997283	-0.6071543112

TS β

G= -995.248158

H= -995.190367

If= -129.218

0 2

C 3.0829556186 -0.9011070356 -0.2210040097
 C 1.6067668042 -1.2548185654 -0.0611205491
 C 1.2981081911 -2.5655669976 -0.790654594
 C 0.7558062801 -0.1184588738 -0.6152969456
 C -0.754610975 -0.2340424293 -0.4316046252
 C -1.0859357778 -0.2858185214 1.0602215983
 O -1.031706329 0.731493177 1.753504031
 N -1.3916043385 0.9137443893 -1.0478744318
 C -2.7101166757 1.1044248629 -0.9771103343
 O -3.4793437435 0.324535117 -0.4136725393
 N -1.3757261095 -1.4923020006 1.5442226974
 H 3.7111138921 -1.708100561 0.1565980962
 H 3.3342138716 0.01018381 0.3241470992
 H 3.3218572118 -0.7467311572 -1.2758119115
 H 1.3895065318 -1.3775654872 1.002045647
 H 1.970552149 -3.3485644683 -0.4381217895
 H 1.4518004136 -2.4417063141 -1.865082879
 H 0.2746748781 -2.9014035627 -0.6245459789
 H 1.0625127793 0.818475243 -0.0713128228
 H 0.9788669745 0.0436073275 -1.67165022
 H -1.1136912379 -1.1445732944 -0.9140359221
 H -0.8251165749 1.6105149754 -1.5079343767
 H -3.0576375723 2.0173326072 -1.4681934984
 H -1.4294493498 -2.2943527069 0.9373131955
 H -1.5491746134 -1.6045066714 2.5313603779
 Cl 1.7591227013 2.7156061372 -0.0474093148

TS γ

G= -995.248465

H= -995.190531

If= -524.788

O 2

H 0.0025515238 0.1290858039 -0.0619027357
 N 0.0306431075 0.1105051363 0.9445282798
 H 0.9219803471 0.1202348061 1.4164166173
 C -1.0925563344 0.0781100562 1.6620227248
 O -1.1035998577 0.0311934416 2.8944701506
 C -2.3941591559 0.1643975809 0.8667726204
 H -2.1935084002 -0.0832218072 -0.174859556
 N -3.3624706085 -0.7774671895 1.3992714972
 H -4.200639747 -0.4252203369 1.836950005
 C -3.101064415 -2.0822898328 1.4733533364
 H -3.8924982789 -2.6740390144 1.9411426255
 O -2.0630531411 -2.5932007565 1.0462874122
 C -2.9769955956 1.574648465 0.9915318601
 H -3.9287392963 1.5870271854 0.4532312662
 H -3.1902964748 1.7549047975 2.0489436817
 C -2.0936086052 2.6976091571 0.4489286421
 H -1.1223600351 2.6667150552 0.9603632888
 C -2.7500369448 4.0417429955 0.7525180166
 H -3.6992760404 4.1210355343 0.2170712549
 H -2.9495061108 4.1561139871 1.8188273665
 H -2.1105041705 4.8650795489 0.4317470612
 C -1.8432987148 2.561863886 -1.0512469019
 H -2.7976061635 2.534634289 -1.5836888899
 H -1.2743403779 3.4169511087 -1.418516839
 H -1.2883805576 1.6583199269 -1.3040457495
 Cl -0.2988260962 3.2335517592 3.3853115181

TS γ

G= -995.249896

H= -995.190061

If= -207.969

O 2

C -2.4935384382 1.1818796245 -0.3652188929
 C -0.9925731719 1.2752846338 -0.135363531
 C -0.4694605491 2.5362677895 -0.8290589538
 C -0.3226794895 0.0083878335 -0.6665010722
 C 1.1858173718 -0.0829032409 -0.4224992051
 C 1.4599602659 -0.0637680322 1.0807483029
 O 1.2155135027 -1.0481521965 1.7830438543
 N 1.6630867427 -1.3259897466 -1.0019955212
 C 2.93874636 -1.7002903877 -0.910630203
 O 3.8128030958 -1.0193141388 -0.3694926444
 N 1.9236494848 1.085584597 1.5717555997
 H -2.7338368647 1.0437663979 -1.4193135521
 H -3.0329932875 2.0439056543 0.0267460856
 H -2.8960506239 0.3005150778 0.1984212046
 H -0.8135037483 1.357157709 0.9391186732
 H -1.0039475959 3.4169783188 -0.4718533491
 H -0.6202409958 2.4587067692 -1.9081868424
 H 0.5934283846 2.6921193912 -0.6424528383
 H -0.7832030828 -0.8694173078 -0.2051553079
 H -0.4915098169 -0.0547941312 -1.7448133067
 H 1.7075858471 0.7495978395 -0.8928970584
 H 0.9974259674 -1.9686403941 -1.4049031977
 H 3.1544620594 -2.6720959661 -1.3630985744
 H 2.1242915186 1.8654970978 0.9669407506
 H 2.063784382 1.1816198061 2.5658098046
 Cl -3.7615863181 -1.539002998 0.0644747751

•OH

TS α

G= -610.847165

H= -610.791411

if= -1345.5737

O 2

N -0.0475822479 -0.0579639511 0.1497507214
 H -0.1141687413 -0.2686390417 1.1332306052
 H 0.8433828062 -0.1299742248 -0.3174671499
 C -1.1066133491 0.3761886149 -0.5275949199
 O -1.0738961597 0.7118039097 -1.7127517371
 C -2.439251617 0.3820974235 0.2228871174
 N -3.1494066224 1.6073419689 -0.0001720952
 H -4.0873863738 1.57228813 -0.373530213
 C -2.61465985 2.7969160836 0.2962380182
 H -3.2550862288 3.6507587301 0.0642427303
 O -1.4966873641 2.9236974964 0.7975661402
 H -2.1969692495 0.3131021519 1.3594587312
 C -3.3133051106 -0.8019203343 -0.178495471
 H -3.5714554514 -0.6583717039 -1.2323761685
 H -4.239651403 -0.7422260757 0.3992575145

C -2.6935728457 -2.1872752367 0.0076815001
H -1.7516354169 -2.2314436317 -0.5452762348
C -2.4268777733 -2.5018717946 1.4785158188
H -3.3506620145 -2.3998561456 2.0540200844
H -2.0713637695 -3.5275023389 1.5866932726
H -1.6792692954 -1.8425718757 1.918522832
C -3.6432337865 -3.2271882969 -0.5836377764
H -3.8339801811 -3.0344069591 -1.6403021182
H -3.2240233369 -4.229409674 -0.4869300066
H -4.5989149772 -3.2074799508 -0.0540953455
O -1.6905439149 0.6949250168 2.6852962151
H -1.3994709655 1.5851525741 2.4129552737

TS β

G= -610.848991

H= -610.792564

If= -1211.8487

0 2

N -0.4083653729 -0.4419445884 -0.3972474663
H -0.677595046 -1.1771803715 0.236643292
H 0.4036949289 -0.5652863786 -0.9830665411
C -1.1133344205 0.6807359024 -0.4807408791
O -0.8095213273 1.6161886438 -1.2309121136
C -2.377620863 0.7541367185 0.3785036552
N -2.4607784472 2.0467508443 1.0333923556
H -3.1709219335 2.6982581381 0.7327346268
C -1.4937043581 2.4854122649 1.8414530766
O -0.5110403796 1.8112771098 2.1541779182
H -1.6486059978 3.5007736289 2.2159640714
H -2.3392924867 -0.02840928 1.1384225943
C -3.6157606655 0.5687505593 -0.4906258871
H -3.6456184913 1.4671796289 -1.2368209678
H -4.511952906 0.703902299 0.1196094613
C -3.6969130287 -0.70423457 -1.3166220232
H -2.8105465814 -0.7693167051 -1.953360106
C -3.7607034776 -1.9400052835 -0.4140227995
H -4.6175857286 -1.8667568285 0.2596359236
H -3.8821891445 -2.8364089742 -1.0234428277
H -2.8619444722 -2.0636448822 0.1901036398
C -4.9332781135 -0.6460722605 -2.2112448755
H -4.9052262972 0.2238416931 -2.8683348537
H -4.9983235605 -1.5425280811 -2.8285909304
H -5.8374214745 -0.5865243137 -1.6009042717
O -3.3215859985 2.559585262 -2.1426543575
H -2.3602116819 2.4588744688 -1.9866777898

TS γ

G= -610.849807

H= -610.793009

If= -853.4205

0 2

N -0.4538404554 -0.6485376205 -0.2643844296
H -0.6191419293 -1.2412725721 0.5329555677
H 0.3412227217 -0.8271735158 -0.8593415996
C -1.2346854268 0.3985975721 -0.5092362851
O -1.0407604652 1.1792947767 -1.4497389766
C -2.4574483983 0.5620332382 0.3914028947

N -2.4981483426 1.910615325 0.934382887
H -3.2601714735 2.5188964223 0.6747214031
C -1.5257254555 2.3952314972 1.7065226831
O -0.5282199655 1.7491599203 2.03379656
H -1.6859119268 3.4264835556 2.0330538231
H -2.4027295923 -0.1504365282 1.2141880257
C -3.730781076 0.3521397906 -0.4319668148
H -3.7809219971 1.1434820881 -1.1838775894
H -4.5828359101 0.481538723 0.2423032415
C -3.8781297559 -0.9988019663 -1.1195694598
H -3.0466661648 -1.0882005816 -1.9132251789
C -3.7486750046 -2.1926688298 -0.1876981715
H -4.4988258223 -2.1098220757 0.6044686185
H -3.9320575781 -3.1191701372 -0.7320646639
H -2.7678357322 -2.2635828669 0.2798245837
C -5.1780524567 -1.0440806215 -1.9061640006
H -5.258260115 -0.1943016624 -2.5845247195
H -5.2463843707 -1.9642661318 -2.4865919304
H -6.0247319356 -1.012970759 -1.2150188837
O -2.2488948437 -0.9253784 -3.2178683699
H -1.7945169906 -0.1176965738 -2.9144574479

TS δ

G= -610.846950

H= -610.789806

If= -1192.2785

0 2

N -0.064483966 -0.1137564405 -0.0368910283
H -0.0887541436 -0.2724027485 0.9595764567
H 0.8199067118 -0.1161536392 -0.5225397726
C -1.1596581533 0.3019276989 -0.6695555226
O -1.1657202982 0.615239683 -1.8659185848
C -2.4156788351 0.3992191814 0.2040107705
N -2.3665662848 1.6612544611 0.9344396065
H -2.8404915124 2.4630633451 0.5443061682
C -1.7375500017 1.8009953775 2.1034409687
O -1.1135634917 0.8991675244 2.6680935062
H -1.8249723085 2.8021569026 2.5337257545
H -2.387865829 -0.4066271465 0.9369140048
C -3.6798873732 0.3206511032 -0.6324001693
H -3.64236847 1.1065354415 -1.3890875649
H -4.5356463685 0.5273895109 0.0135602816
C -3.8587735619 -1.0572998213 -1.2851062013
H -2.8782120079 -1.4557174951 -1.5594508836
C -4.5218233198 -2.0377198843 -0.3154921714
H -5.5354575644 -1.7058844683 -0.0813863876
H -3.9598895618 -2.103256544 0.6178089883
H -4.5792538819 -3.0364794779 -0.7491863742
C -4.6818812774 -0.9371235115 -2.5510984214
H -4.0928342647 -0.2953670965 -3.3237686503
H -4.8498913031 -1.8925133503 -3.0466285026
H -5.6232433254 -0.4079022133 -2.3971089825
O -3.048548739 0.4593560799 -4.0147664469
H -2.4430813595 0.5197581078 -3.2460088757

•OCH3

TS α

G= -650.125021

H= -650.063956

If= -1588.2943

0 2

N	0.0309871054	-0.0291989642	-0.1965113077
H	0.0527346269	0.1646303682	0.7934041625
H	0.8937637362	-0.1111318774	-0.7123732372
C	-1.1297096652	-0.0942557772	-0.8430090663
O	-1.2369680607	-0.2708581812	-2.0579084079
C	-2.3815274097	-0.0344167952	0.0277330257
N	-3.3115103933	0.9531607446	-0.4203452258
H	-4.295896926	0.7274127322	-0.378607013
C	-2.9716283163	2.1746387517	-0.8684469969
O	-1.8177916354	2.5797025067	-0.9547541293
H	-3.831381157	2.7829819522	-1.1617208327
H	-2.0258137268	0.2575199228	1.134717766
C	-3.0729937954	-1.3948480531	0.094585101
H	-3.5153438929	-1.5639662441	-0.8918015756
H	-3.8932120955	-1.3178551215	0.8141047422
C	-2.1903737199	-2.5911411779	0.4524085044
H	-1.347909545	-2.6266292816	-0.2442247669
C	-1.6519108848	-2.5161484235	1.8791905132
H	-1.1014313343	-3.4267299561	2.120591666
H	-0.9820191673	-1.6700473761	2.0255075358
H	-2.4792350805	-2.4233501259	2.587340995
C	-3.0090052312	-3.867663312	0.2689075225
H	-3.3836659064	-3.9549604276	-0.7519648077
H	-2.4030831786	-4.7472997502	0.4892765717
H	-3.8659915361	-3.868448762	0.9471633383
O	-1.6223912855	0.7303452084	2.3659891259
C	-1.6963894255	2.1347274224	2.3234295561
H	-0.9228542896	2.5695732513	1.6901136608
H	-1.537957324	2.4662422467	3.356847285
H	-2.6884335383	2.480880681	2.0217557558

TS β

G= -650.122011

H= -650.061356

If= -1598.6399

0 2

N	0.0649846112	0.0516424473	0.1374063495
H	0.0723201306	-0.2297350953	1.104392027
H	0.9390149161	0.1435334145	-0.3570190455
C	-1.0791026644	0.2930579032	-0.5036302893
O	-1.1307367932	0.661376041	-1.6768248731
C	-2.3567788782	0.0533529189	0.3066387449
N	-3.3486179723	1.0585230425	-0.0233785203
H	-4.1911952312	0.7795063447	-0.5040677361
C	-3.0956492686	2.3588829199	0.1290897092
O	-2.0492155911	2.796659157	0.6112909285
H	-3.9036527207	3.0154159249	-0.204481538
H	-2.1174061959	0.1312474975	1.3694115942
C	-2.9397143761	-1.3231802266	0.0218919562
H	-3.2129189344	-1.3508928286	-1.1583002743
H	-3.9287267112	-1.407393638	0.4791310649

C	-2.0871624753	-2.537494552	0.3353511983
H	-1.1366628103	-2.4597839706	-0.1986049425
C	-2.8085516928	-3.8057790951	-0.1200446381
H	-3.7620519036	-3.901660617	0.4045056486
H	-2.2053918363	-4.6849008778	0.1087975312
H	-3.0084509912	-3.7948620905	-1.1913410097
C	-1.8052715516	-2.6244105835	1.8413796335
H	-1.2381173411	-1.7718200894	2.2132140736
H	-1.2355791496	-3.5292884024	2.0563563945
H	-2.7469546656	-2.6751643291	2.3924616574
O	-3.5648683131	-1.4777176626	-2.455403864
C	-2.4175453655	-1.8695276777	-3.1801020862
H	-1.9659968272	-1.0261131752	-3.7014401386
H	-1.6730870825	-2.3209275371	-2.5181810225
H	-2.7233880692	-2.638373504	-3.8952674662

TS γ

G= -650.127728

H= -650.066754

If= -1232.5977

0 2

H	-0.123935588	-0.0150922248	-0.3560348891
N	-0.086293628	-0.2621686271	0.6192029143
H	0.8096904574	-0.3474088261	1.0741533388
C	-1.2007038085	-0.405271831	1.3343658368
O	-1.2036277125	-0.7121706323	2.5294039252
C	-2.5148823005	-0.143233845	0.5973077086
H	-2.3275489791	-0.0924729396	-0.4745503966
N	-3.4420528881	-1.2315174598	0.8600321934
H	-4.2663502943	-1.0520290882	1.4138927825
C	-3.1752010324	-2.4864700764	0.4995218193
H	-3.9437223076	-3.2085458543	0.7887466486
O	-2.1589218582	-2.8189880847	-0.1143258518
C	-3.1601010243	1.1479652929	1.1036114382
H	-4.1321078372	1.2438095188	0.6079475286
H	-3.3520648866	1.0353886913	2.1740188305
C	-2.3926214018	2.4385523849	0.8632145152
H	-1.3889137423	2.3788073851	1.4910705876
C	-3.1566424418	3.6182045724	1.4347255421
H	-4.0672559872	3.7778877192	0.8496656472
H	-3.4491772475	3.4408609205	2.4700075791
H	-2.5600499859	4.5297098681	1.3870310121
C	-1.9730152385	2.6823393661	-0.5754214715
H	-2.8623569449	2.6921458683	-1.2134705041
H	-1.4831765308	3.652248951	-0.664809239
H	-1.2926521254	1.9224084663	-0.9568345411
O	-0.328459531	2.4988844844	2.4187229523
C	-0.9479177472	2.6014878055	3.6779981388
H	-1.4083571309	3.5783420973	3.8343576556
H	-0.145259903	2.4723519648	4.4137599428
H	-1.6734802327	1.8006928294	3.8383890284

TS δ

G= -650.122706

H= -650.062295

If= -1442.1399

0 2

N	-0.4675277185	-0.8556174907	0.6132279758
H	-0.9261811969	-1.341696005	1.3666467698
H	0.4565675685	-1.1415905689	0.3281502503
C	-1.0454976814	0.1860262049	0.014328493
O	-0.4980455922	0.835928892	-0.8798967454
C	-2.4715796503	0.5072723907	0.4608983969
N	-2.6272973799	1.9416090634	0.62957748
H	-3.257127457	2.4430433486	0.0213317156
C	-1.8720474464	2.6348571195	1.480604273
O	-1.021162531	2.1225251555	2.211535866
H	-2.0721906763	3.7098149765	1.4842996615
H	-2.66840022	0.016864827	1.4137183325
C	-3.4665383272	0.0453630124	-0.6066440527
H	-3.2633153161	0.6119566447	-1.5188309334
H	-4.4686183308	0.3155389231	-0.2628533128
C	-3.4382032249	-1.4506838162	-0.922542028
H	-2.4354669109	-1.733514393	-1.2541320128
C	-3.8148995255	-2.3078158612	0.2921864693
H	-4.7909718663	-2.0030795536	0.6756105897
H	-3.0859856337	-2.2151807547	1.0974836146
H	-3.8692673839	-3.3603274617	0.0120986283
C	-4.4160145121	-1.7425058809	-2.040440824
H	-4.1461609749	-1.0635186564	-2.9970513911
H	-4.3689164228	-2.7656978796	-2.4090478281
H	-5.43973271	-1.4499901716	-1.8023908493
O	-3.6537676482	-0.3802526411	-4.0536791264
C	-2.2724832453	-0.6686409361	-4.0555732304
H	-1.8650685594	-0.1427405541	-4.9255090442
H	-2.081023763	-1.7361114687	-4.1804186896
H	-1.7735042777	-0.289829804	-3.1616243943

•OCH₂Cl

TS_α

G= -1109.754845

H= -1109.690438

if= -1190.0135

0 2

N	0.2392883013	-0.0181122184	-0.1944779836
H	0.4519488969	-0.0325709813	0.790114624
H	0.9887848696	-0.1046921008	-0.8638996195
C	-1.0026510697	0.1677361954	-0.6317034419
O	-1.310214396	0.2379706115	-1.8214175689
C	-2.1034004424	0.2094327942	0.4310825954
H	-1.5544777766	0.3534054143	1.4700660139
N	-2.9766513769	1.3198157512	0.2490006619
H	-3.9742231659	1.1652213661	0.3082224697
C	-2.5323397662	2.5768965333	0.0479985678
O	-1.3438692731	2.869720673	0.0065776917
H	-3.3307792444	3.3132197331	-0.0730443172
C	-2.9076308648	-1.0871914752	0.4533978641
H	-3.471028668	-1.1160138746	-0.4841366095
H	-3.6314399725	-1.0170815737	1.2699008775
C	-2.1041461066	-2.3800623884	0.594965626

H	-1.3577788203	-2.4203385341	-0.2034967042
C	-3.0561749796	-3.5614996004	0.4170457659
H	-3.8197446184	-3.5491387419	1.1987055061
H	-2.514456716	-4.5053314031	0.4867801386
H	-3.5586103541	-3.5233643665	-0.5504423916
C	-1.3975852202	-2.4796925483	1.9449230252
H	-2.1243909976	-2.3866972213	2.7559227426
H	-0.9050088947	-3.4486298189	2.0397250387
H	-0.642621886	-1.7056758165	2.0805059744
O	-0.9916312598	0.8058644009	2.7168621402
C	-1.9550443746	1.5168776018	3.3248115471
Cl	-3.2506868742	0.4538507863	4.0975473887
H	-1.5113590835	2.0811720122	4.1488382529
H	-2.4997408178	2.1909544922	2.6614111477

TS_β

G= -1109.749407

H= -1109.686096

if= -1423.2440

0 2

N	0.1325869812	0.102996712	0.3822027965
H	-0.0258439695	-0.0041461357	1.3708771882
H	1.0778004217	0.155236177	0.0344267797
C	-0.8835786311	0.155096481	-0.4781177332
O	-0.7329458228	0.3091520012	-1.6910247034
C	-2.2811737667	-0.0132128362	0.1265872195
N	-3.2085538796	0.9180755214	-0.4879184854
H	-3.880838138	0.5680658244	-1.1555348355
C	-3.0061489433	2.236311032	-0.4196641984
O	-2.0997086243	2.7522937048	0.2351005199
H	-3.7258744668	2.8304168042	-0.989240619
H	-2.2295396031	0.2011512157	1.1965580796
C	-2.8113319473	-1.4284212335	-0.0590495659
H	-3.0900930986	-1.5650287495	-1.2202942093
H	-3.80196069	-1.509811966	0.3946901026
C	-1.9196273457	-2.586066107	0.3452524563
H	-0.9333905237	-2.4593720718	-0.1071947668
C	-2.5187884898	-3.903769519	-0.1423338399
H	-3.523164798	-4.0357758391	0.2668452909
H	-1.9037616441	-4.7410096376	0.1890408575
H	-2.5823484009	-3.9312155616	-1.2296545323
C	-1.7738711043	-2.6223377495	1.8724148047
H	-1.3506845662	-1.7027199412	2.2755674308
H	-1.1246760967	-3.4509129506	2.1583350102
H	-2.7516422784	-2.7782396651	2.3331933307
O	-3.7206265476	-1.7498726556	-2.4528972512
C	-2.8680999615	-1.348981214	-3.4249004549
H	-2.3115132937	-0.4495851635	-3.1787644657
Cl	-1.5765686848	-2.6139898976	-3.8030928394
H	-3.4369780979	-1.2358536929	-4.3492134115

TS_γ

G= -1109.755577

H= -1109.692357

If= -989.4273

0 2			
H	-0.1272464312	0.0180599585	-0.3616051166
N	-0.0851441542	-0.2189088805	0.6160370944
H	0.8121239147	-0.2778964061	1.0726913987
C	-1.1967238958	-0.3745412334	1.3327019446
O	-1.1950740761	-0.6695678756	2.530646953
C	-2.5142952438	-0.1381064327	0.5933514001
H	-2.3281738637	-0.099188907	-0.4791860209
N	-3.4301756878	-1.2320184577	0.8719212784
H	-4.2571448279	-1.0527183153	1.4218160249
C	-3.1445226534	-2.490774914	0.539210887
H	-3.9039328656	-3.2171354585	0.8414061866
O	-2.1210597836	-2.8217941496	-0.0630750038
C	-3.172494248	1.1529771101	1.0827285039
H	-4.143147107	1.2367619443	0.5826465862
H	-3.3702938448	1.0513134533	2.1533978108
C	-2.4201988603	2.4507539485	0.8306201165
H	-1.4284082629	2.4068156217	1.4470943375
C	-3.2026031955	3.6236729861	1.3936941981
H	-4.1221500744	3.7511841548	0.8148824342
H	-3.4789217654	3.4536077184	2.4346737134
H	-2.6262119111	4.5460532742	1.3275735856
C	-2.0049340843	2.6865172433	-0.6109008412
H	-2.897194198	2.678463805	-1.244675967
H	-1.528505925	3.6618820438	-0.710477694
H	-1.3166530474	1.9309626021	-0.9863020443
O	-0.3080003688	2.4557660506	2.4200025686
C	-0.837016126	2.3877381817	3.6554965959
Cl	-1.1374199138	4.0533586795	4.4050733424
H	-0.1227117318	1.9065702642	4.32614411
H	-1.7989256458	1.8769106873	3.6881122899

TS δ

G= -1109.743378

H= -1109.678435

If= -1041.2059

0 2

N	-0.0537543685	-0.0165171762	-0.0145402125
H	-0.0263655853	-0.011619884	0.99216479
H	0.8109701516	-0.0253543456	-0.5335413285
C	-1.2152362605	-0.0117303994	-0.6688737364
O	-1.2972814297	0.0064834028	-1.8993539442
C	-2.4681880149	-0.0920059852	0.2026873157
N	-3.4803581832	0.8214799506	-0.2967162257
H	-4.3507466497	0.4471792746	-0.6444758503
C	-3.2443529161	2.1261731584	-0.4295006654
H	-4.0781290774	2.6926672885	-0.8530725181
O	-2.1838520987	2.6639429978	-0.1027032016
H	-2.2138397158	0.1869021162	1.2247715927
C	-3.0410250183	-1.5104474036	0.1463726601
H	-3.3321762061	-1.7090040048	-0.8887354209
H	-3.9493861831	-1.5275207402	0.7544430581
C	-2.1001190347	-2.6133540559	0.6333872705
H	-1.1624141352	-2.5686057551	0.0732233464
C	-2.7407036171	-3.962832786	0.3843948145
H	-2.9580816796	-4.0891998234	-0.7590129259
H	-3.7242377785	-4.0624467469	0.8465186581
H	-2.097506503	-4.8022556855	0.6435408495

C	-1.7823470215	-2.4833189818	2.127022841
H	-1.2467233676	-1.5587948894	2.344888496
H	-2.7069429606	-2.490270441	2.708160652
H	-1.1620948339	-3.3166719976	2.4581692038
O	-2.9972744007	-4.1430354167	-2.2106535985
C	-1.7580078706	-3.6225842451	-2.5837235034
H	-1.6339633674	-2.5791477127	-2.3088780886
H	-0.9273433943	-4.2456256729	-2.2655347299
Cl	-1.7885066275	-3.6768553326	-4.3896046272

•OCHCl₂

TS α

G=-1569.364292

H=-1569.297607

If=-788.7367

0 2

N	0.2277058094	-0.200477335	-0.5772702852
H	0.4868647557	-0.2582375794	0.3947909331
H	0.9389901951	-0.2986616574	-1.2860417765
C	-1.0233669943	0.0596109267	-0.9431051621
O	-1.3890750857	0.1892825772	-2.1097819876
C	-2.0650458698	0.1253416562	0.1809243934
H	-1.4851188329	0.2295065602	1.1653455676
N	-2.9015230182	1.273357065	0.0556438665
H	-3.9063246171	1.1542209683	0.0784123061
C	-2.3987626029	2.5237397949	-0.0497717942
O	-1.1983796417	2.756192207	-0.0558238959
H	-3.1593241733	3.3051842515	-0.1234367082
C	-2.9249971097	-1.1322327466	0.2411647679
H	-3.5347279921	-1.1469800231	-0.6666729192
H	-3.6044336521	-1.0208875811	1.0929420213
C	-2.1686045321	-2.454918862	0.365583271
H	-1.4617564402	-2.5355940275	-0.4649978873
C	-3.172678099	-3.5996869806	0.2495866574
H	-3.900570233	-3.5456320512	1.0628994175
H	-2.6653036118	-4.562850466	0.3129656662
H	-3.714621108	-3.557398814	-0.696187282
C	-1.4070745894	-2.5645634391	1.6849444955
H	-2.0927793642	-2.425083746	2.5248966703
H	-0.9570524161	-3.5542004091	1.7766150536
H	-0.6100378081	-1.8266759511	1.7744703935
O	-1.1837738985	0.6708460012	2.662536239
C	-2.3022621187	1.1868256721	3.1228120408
Cl	-2.932979663	0.2791953348	4.5607271432
Cl	-2.1042385268	2.9319197625	3.5854793797
H	-3.1072922854	1.1677168818	2.3793729226

TS β

G= -1569.361128

H= -1569.294630

If= -971.6645

0 2

N	0.1253587847	0.1104037344	0.3824905239
H	-0.0309308835	0.039348233	1.3749140555
H	1.0694896618	0.1580251607	0.0308499145
C	-0.892959168	0.1268123912	-0.4749921644
O	-0.7474012954	0.2361339773	-1.6945967382
C	-2.2878782661	-0.0316623642	0.1361938064
N	-3.218461791	0.8870136272	-0.4924442151
H	-3.8921079267	0.5245076293	-1.1524844627
C	-3.0196497565	2.2069691448	-0.4462262563
O	-2.1124823639	2.7357912543	0.1968745694
H	-3.742865422	2.7896036811	-1.0232137665
H	-2.2369539587	0.196184119	1.2029309483
C	-2.8096361884	-1.4525016958	-0.0375732241
H	-3.0430674438	-1.5981645616	-1.1703926427
H	-3.8012175528	-1.5346637212	0.4138562628
C	-1.9103446978	-2.5966470059	0.3922557897
H	-0.92388214	-2.4700762471	-0.0600626551
C	-2.4989367732	-3.9245357525	-0.0790142905
H	-3.5002420292	-4.0622335923	0.3356007494
H	-1.874535506	-4.7531501555	0.2560355988
H	-2.568044653	-3.9624117907	-1.1662124759
C	-1.7691066261	-2.6046686172	1.9195404161
H	-1.3434365482	-1.6784529505	2.3046286703
H	-1.1231102044	-3.4295701542	2.2226684123
H	-2.7482855901	-2.7483589814	2.3812623194
O	-3.6738550052	-1.8039008516	-2.5235965862
C	-2.7858307472	-1.3380527953	-3.4145817821
H	-2.2348778072	-0.4674178894	-3.0714020804
Cl	-1.5391269338	-2.5736854447	-3.870995208
Cl	-3.7285671796	-0.8821654945	-4.8801175334

TS γ

G= -1569.367044

H= -1569.299914

If= -716.7231

0 2

H	-0.0851487438	0.1560115831	-0.1784000312
N	-0.1096992942	-0.1111172489	0.7921907661
H	0.7510033712	-0.1524195564	1.3169687033
C	-1.2647254011	-0.3446716786	1.4135797629
O	-1.3374324769	-0.673536466	2.6001448072
C	-2.5317039861	-0.1256534309	0.5873491794
H	-2.2791668201	-0.0921779305	-0.4719770391
N	-3.4635857113	-1.215511515	0.8200712639
H	-4.3650081979	-1.0130881896	1.2254851274
C	-3.1318128491	-2.4882482063	0.6072155665
H	-3.9228867064	-3.2028248845	0.8502230085
O	-2.0355886613	-2.8454589458	0.1704014172
C	-3.2126241127	1.1715985917	1.0305489626
H	-4.1704820117	1.238988593	0.5044152863
H	-3.4323388165	1.0929152175	2.0986763097
C	-2.4588329708	2.4673964992	0.7647134475
H	-1.4871339296	2.4389564777	1.3651246882
C	-3.2529098539	3.645386223	1.3045020145
H	-4.1608722153	3.7723265316	0.7086062656
H	-3.5474117818	3.4808876858	2.3412271047

H	-2.6735543421	4.5667853936	1.2446564498
C	-2.050164176	2.6831952586	-0.6836354981
H	-2.944676846	2.6623296807	-1.3134399067
H	-1.5779819134	3.6590677855	-0.7987188058
H	-1.3592556342	1.9249632627	-1.0495347002
O	-0.3228799046	2.7997646066	2.4223720797
C	-0.7362496921	2.3542893994	3.6121971341
Cl	-1.4349718526	3.6677812045	4.6473326424
Cl	0.683902017	1.6426975158	4.4634060849
H	-1.4929663656	1.5760852396	3.5299985819

TS δ

G= -1569.360648

H= -1569.295194

If= -886.3476

0 2

N	-0.0656670481	-0.0105992064	-0.0029740052
H	-0.0505008877	0.0863685404	0.9995615146
H	0.8048389203	-0.0631051485	-0.5097623331
C	-1.2194894658	-0.0859246699	-0.6648686538
O	-1.2906171129	-0.1938622885	-1.8922940944
C	-2.4807221084	-0.1018482968	0.1978334029
N	-3.4785897074	0.7962243813	-0.3560971456
H	-4.34722053184	0.4121224622	-0.6977682843
C	-3.2355456014	2.0935923218	-0.5398058666
H	-4.0626893159	2.6445150267	-0.9956074104
O	-2.1761780874	2.6406675259	-0.2261038478
H	-2.2316089435	0.22173576	1.2079161453
C	-3.0660158508	-1.5155852599	0.1990389932
H	-3.387738043	-1.7371536132	-0.8224712914
H	-3.9565520304	-1.5132703752	0.8326824835
C	-2.1101564393	-2.6079819684	0.6811267903
H	-1.1700219232	-2.5472253902	0.1253251066
C	-2.7248929425	-3.9660215313	0.4225352745
H	-2.9421896708	-4.0814847274	-0.7092632942
H	-3.7069968959	-4.0880049861	0.8828289753
H	-2.0663311933	-4.7957642158	0.6742572147
C	-1.7865694459	-2.472822529	2.1732388325
H	-1.2767659052	-1.5312328177	2.3810266658
H	-2.7062979325	-2.5058098375	2.7606688426
H	-1.1389782631	-3.2868779604	2.4993221603
O	-3.0085599574	-4.0847649676	-2.2316419919
C	-1.8566639612	-3.5322487205	-2.6495392494
H	-1.5429138904	-2.6557330107	-2.090667041
Cl	-0.4717818417	-4.6951425728	-2.6191466126
Cl	-2.1565872847	-2.9971332174	-4.338526309

•OCCl₃

TS α

G= -2028.972899

H= -2028.901783

If= -540.7154

0 2

N	0.192072291	0.1225767374	-0.2054481626
H	0.2080117482	0.3516087454	0.778776402
H	1.0574404577	0.0420542341	-0.7214685052
C	-0.9461098954	0.0171826603	-0.8554340495
O	-1.1239125068	-0.1973901035	-2.0340492709
C	-2.2974691404	0.091206655	0.0252111825
H	-1.7965155674	0.355560197	1.0566635266
N	-3.1080108102	1.1545973438	-0.3241140408
H	-4.0796003086	0.9757913834	-0.562642604
C	-2.70253393	2.4766333758	-0.2729463397
O	-1.5686191198	2.7889293104	0.0057939127
H	-3.4992271028	3.1841820766	-0.508475866
C	-3.039667386	-1.2304849575	0.0062868648
H	-3.4857862852	-1.3445027127	-0.9847531017
H	-3.860455364	-1.1457972746	0.7253411016
C	-2.2010065467	-2.4642453068	0.3445239808
H	-1.3384319008	-2.5032925367	-0.3272380484
C	-3.0498421647	-3.7096421596	0.1002649925
H	-3.9282562106	-3.7009389954	0.7504087286
H	-2.476807297	-4.6115155937	0.3174504645
H	-3.3923473651	-3.7596075623	-0.9342682279
C	-1.7084918582	-2.4363533123	1.7891714108
H	-2.5585544374	-2.3628224054	2.4726796306
H	-1.1675228276	-3.3552536973	2.0199456563
H	-1.0435138036	-1.5965949613	1.9857144209
O	-1.0219155965	0.841858034	2.3446160152
C	-1.6621953103	1.1550416347	3.3691046533
Cl	-1.2559326182	0.1037482119	4.8459515566
Cl	-1.3557190053	2.903788873	3.9185191518
Cl	-3.507623662	1.0225400966	3.1734380725

TSβ

G= -2028.963671

H= -2028.893189

If= -917.2125

0 2

N	-0.0958764001	0.4322799548	1.074482064
H	-0.4265508296	0.1537336787	1.9841460889
H	0.8693046782	0.7005016148	0.9587488407
C	-0.9124575053	0.4569741618	0.0225247295
O	-0.5622580389	0.8202002714	-1.1008526389
C	-2.3387058329	-0.0409938681	0.2727992635
N	-3.3005900212	0.8432933119	-0.3571818312
H	-3.7771514101	0.5315396767	-1.1909497767
C	-3.3804687479	2.1322182519	-0.0200161496
O	-2.7197634643	2.6410633165	0.8865949819
H	-4.0951005148	2.7068186045	-0.6153603969
H	-2.5281423936	-0.059783819	1.3480470058
C	-2.5220483118	-1.4470426872	-0.2812895152
H	-2.369196411	-1.3457585311	-1.4294737225
H	-3.5666059596	-1.7475939286	-0.1765814388
C	-1.5817990538	-2.5276448684	0.2208715966
H	-0.5489709273	-2.2114681084	0.0601012429
C	-1.8282603888	-3.8283065639	-0.5384312159
H	-2.8591105274	-4.1600189837	-0.3964866713

H	-1.1639672142	-4.6098399183	-0.169147882
H	-1.6488303885	-3.7044519064	-1.6058614425
C	-1.8117396726	-2.7559416443	1.7221255598
H	-1.5511230573	-1.8844442237	2.3218519671
H	-1.1982898445	-3.5940286065	2.0551738918
H	-2.8594892364	-3.0023715078	1.9065447946
O	-2.7340800537	-0.7320787389	-2.8434072657
C	-3.1717867726	-1.6430647708	-3.6967338878
Cl	-1.8840966337	-2.7302768594	-4.316213944
Cl	-4.5013477367	-2.6443753424	-3.0376784541
Cl	-3.7944433412	-0.6506650795	-5.0661498387

TSγ

G= -2028.967169

H= -2028.898273

If= -461.3930

0 2

H	-0.128613355	0.0677896727	-0.3127638622
N	-0.1389114542	-0.2417571221	0.6451503175
H	0.7326045912	-0.339528708	1.1429556538
C	-1.2852066212	-0.4771480241	1.2811741878
O	-1.3398568499	-0.8802965346	2.4454889436
C	-2.5653796695	-0.1888975549	0.4945998153
H	-2.3226590182	-0.0527737072	-0.5585138429
N	-3.4798609853	-1.3115309256	0.6240708203
H	-4.3470573565	-1.1858097771	1.1243097162
C	-3.1534171446	-2.5345887302	0.2067788768
H	-3.9187691256	-3.2922097561	0.3950189485
O	-2.0874670591	-2.8011960958	-0.3522060491
C	-3.270760558	1.0488855207	1.0527339767
H	-4.2136997578	1.1557277156	0.5070283399
H	-3.5193992078	0.8579045494	2.0998013788
C	-2.5278790602	2.3760179363	0.9424862159
H	-1.602014995	2.2997745126	1.5964501141
C	-3.3967810732	3.4944134992	1.4989824695
H	-4.2871155792	3.59083882	0.8710255143
H	-3.7234581737	3.2844150692	2.517561574
H	-2.8678177278	4.4460996395	1.4839422325
C	-2.0400687869	2.7137202608	-0.4581806005
H	-2.8941255157	2.7182185938	-1.1420461633
H	-1.5924128482	3.7076312708	-0.4688633127
H	-1.3056981548	2.0061616422	-0.8391133997
O	-0.2206449294	2.1847657896	2.5927830077
C	-0.450276295	2.8226850725	3.7298181089
Cl	-0.6444807549	4.5886362133	3.5215619898
Cl	1.0503825258	2.4919834572	4.6661981989
Cl	-1.8663149393	2.1867863973	4.6174675028

TSδ

G= -2028.966202

H= -2028.894701

If= -729.5936

0 2

N	-0.0794743488	0.1955115583	0.1134803589
H	-0.0627717346	0.0597226046	1.1114403474
H	0.7901924457	0.2696593061	-0.3917652003

C	-1.2341778559	0.2538615571	-0.5512127462
O	-1.3031000743	0.4282787745	-1.7699138671
C	-2.493757599	0.0374023234	0.2860669128
N	-3.5376377415	0.9464403516	-0.1500916362
H	-4.366959837	0.5759288003	-0.589600579
C	-3.3714171635	2.2677899668	-0.1018990211
H	-4.217455426	2.8426042706	-0.4883768523
O	-2.3570560158	2.8090652592	0.3443545567
H	-2.2679953163	0.240074062	1.332235491
C	-2.9923651637	-1.3983491444	0.105903423
H	-3.1921332306	-1.554161324	-0.957790347
H	-3.9413023377	-1.491285202	0.640505868
C	-2.0369462318	-2.4810565844	0.609159864
H	-1.0705420896	-2.3744358324	0.1148653635
C	-2.6019891508	-3.8456441385	0.2700757825
H	-2.8324629638	-3.8902558045	-0.8487032902
H	-3.5698670229	-4.0298135219	0.7405178065
H	-1.91144022	-4.6619417242	0.4760280569
C	-1.8195563732	-2.4053868462	2.1249344386
H	-1.3192766754	-1.4790595858	2.4094298315
H	-2.7777018033	-2.4563231576	2.6460960382
H	-1.2002253798	-3.2371102261	2.4619600264
O	-3.0435918146	-3.9409575463	-2.4364700367
C	-1.8939549335	-4.3346591295	-2.9739799799
Cl	-0.5427443791	-3.2096775611	-2.6364980677
Cl	-1.4090703405	-5.9815121388	-2.4666760745
Cl	-2.2532073708	-4.3290806596	-4.733251496

•OOH

TS α

G= -686.003467

H= -685.944011

If= -1814.4249

O 2

N	0.0747856227	-0.0978511123	-0.1370250289
H	0.14180669	-0.1755955629	0.8652062798
H	0.9175235986	-0.0977308965	-0.6917920036
C	-1.0970456535	0.0900027642	-0.7369465814
O	-1.2285395689	0.2546734957	-1.9508699099
C	-2.3440374042	0.0081430039	0.1373601586
H	-1.9552186503	0.109290444	1.364936914
N	-3.211304864	1.1100847219	-0.044205608
H	-4.2083499239	0.9403726678	-0.0506441678
C	-2.7873130442	2.391095098	-0.0617960025
O	-1.6091658263	2.7129269562	0.0328235
H	-3.594363107	3.1190370957	-0.1745468957
C	-3.0898833231	-1.3074702883	-0.0167208348
H	-3.5363134146	-1.295559712	-1.0168419243
H	-3.9105585113	-1.3147784096	0.7065230933
C	-2.2612150542	-2.5825791443	0.1424599399
H	-1.4251488653	-2.548773198	-0.5616357519
C	-3.1414279475	-3.7778491693	-0.2185112874
H	-3.9912453892	-3.8397643749	0.4657718982

H	-2.5767220141	-4.7076186836	-0.1418452026
H	-3.5275435383	-3.6930202104	-1.2352058111
C	-1.715702746	-2.7499509293	1.5588822531
H	-2.5353102156	-2.7298666359	2.2813805188
H	-1.2039593743	-3.7088007711	1.6532635201
H	-1.006323707	-1.9686980141	1.8297414138
O	-1.657244281	0.3985411621	2.5454305928
O	-2.3422428534	1.5647173004	2.8190300863
H	-1.7482118644	2.2713780048	2.5246188495

•OOCH₃

TS α

G= -725.280618

H= -725.217269

If= -1908.0988

O 2

N	-0.0787089317	0.1451670532	0.016284952
H	-0.1183149621	0.2594245797	1.0169802313
H	0.8146202624	0.1701549981	-0.4517296232
C	-1.1918724945	0.1108273936	-0.7109112705
O	-1.2071720584	0.0631176918	-1.9421885701
C	-2.5105418385	0.0211287179	0.0470483293
H	-2.2935513276	0.2378018443	1.3091850524
N	-3.4386790668	1.0220875183	-0.3211940478
H	-4.4214904534	0.7840866783	-0.2945190674
C	-3.1204446585	2.3160572705	-0.5450292028
O	-1.9754038313	2.7463859885	-0.5577398443
H	-3.9916071019	2.9480580663	-0.7363254872
C	-3.1351427845	-1.363612225	-0.0393237681
H	-3.48460794	-1.4870976904	-1.0694021094
H	-4.0169476574	-1.3741694626	0.6084765425
C	-2.2238865607	-2.5375163853	0.3213349566
H	-1.3330315248	-2.4987683869	-0.312411203
C	-2.9681496905	-3.8367756278	0.018687755
H	-3.2701952744	-3.8855657824	-1.028497734
H	-3.8668820834	-3.9071030056	0.6364250766
H	-2.3386831653	-4.7004083039	0.2359091741
C	-1.795537638	-2.5151594928	1.7866242902
H	-2.67549418	-2.501205971	2.4345222847
H	-1.1778138772	-1.6508794765	2.0301431004
H	-1.2179747891	-3.4105361964	2.0215989291
O	-2.308326931	0.5426448668	2.5195585175
O	-2.6633246598	1.8705455934	2.5521256641
C	-1.4745976657	2.6669079673	2.5913416901
H	-0.8729818655	2.4684990972	1.7069575977
H	-1.8188517387	3.6983169343	2.5934062787
H	-0.9178727898	2.4466760448	3.5005507299

•OOCH₂Cl

TS α

G= -1184.896927
H= -1184.831803
If= -1754.7010

0 2

N	-0.1030482758	0.2257763326	0.1136110598
H	-0.1911525023	0.357680778	1.1087673947
H	0.8082973782	0.2748170208	-0.3160132207
C	-1.1793989474	0.0905844582	-0.6549973978
O	-1.1435187068	-0.0121577453	-1.8819322286
C	-2.5193580957	-0.0471813859	0.058060641
H	-2.3569655681	0.2438147672	1.290405461
N	-3.4945725952	0.8656160334	-0.4005971127
H	-4.4602898194	0.5643284719	-0.3976683832
C	-3.2465658218	2.1591862503	-0.7050520803
O	-2.1303359665	2.6591892755	-0.68982311
H	-4.1428436855	2.7190691639	-0.983698993
C	-3.0466313809	-1.4753356184	0.0234474314
H	-3.3457875054	-1.6708858651	-1.0113815682
H	-3.9500696141	-1.5137374439	0.6390844437
C	-2.0735024292	-2.5646646649	0.4772060061
H	-1.1594512985	-2.4899127022	-0.1188803501
C	-1.7138005012	-2.4498669859	1.9571546105
H	-1.0907613284	-3.2942296797	2.2560593571
H	-1.1627298819	-1.5374915515	2.1856795284
H	-2.6205743052	-2.4655386332	2.5667908726
C	-2.7117454599	-3.9252853083	0.2027635074
H	-2.0412573999	-4.7313118681	0.5028200559
H	-3.6395577768	-4.0260510104	0.771105897
H	-2.9445273421	-4.0475469725	-0.8558735845
O	-2.4234255895	0.6112611925	2.5133553314
O	-3.0116217289	1.8539101809	2.4788813207
C	-1.957409842	2.8114363335	2.4627545703
H	-1.3601536166	2.689655019	1.5653790826
H	-1.3795601108	2.7440022508	3.3777686172
Cl	-2.7572287678	4.3956398076	2.4078646464

•OOCHCl₂

TS α

G= -1644.510377
H= -1644.442508
If= -1590.7220

0 2

N	-0.1039893528	0.2249960577	0.1273622299
H	-0.1933803036	0.3567331485	1.1226468945
H	0.8090817528	0.2661400527	-0.2994415921
C	-1.1774302634	0.0853575471	-0.6442187648
O	-1.1399003973	-0.025450265	-1.8696143616
C	-2.5224946439	-0.0456009158	0.0663399696
H	-2.3438342306	0.2395451243	1.2639367991

N	-3.4928619819	0.8651288184	-0.4105904372
H	-4.4561072646	0.5578222722	-0.4438829944
C	-3.2318338568	2.1494671273	-0.7405364856
O	-2.1155974379	2.6475468813	-0.6889176322
H	-4.1151532271	2.7040199295	-1.066666082
C	-3.0540700866	-1.4732504312	0.0263453337
H	-3.3578681944	-1.6581922597	-1.0088547277
H	-3.9552954613	-1.5125117407	0.6448175786
C	-2.0834952608	-2.5703711321	0.4657294053
H	-1.1713907769	-2.4934087466	-0.1330362333
C	-1.7179101128	-2.4737281043	1.9453740967
H	-1.1003247717	-3.3259388266	2.2330996409
H	-1.1588781634	-1.5680829457	2.1813139641
H	-2.6225899663	-2.4886391541	2.5581415593
C	-2.7294194349	-3.9247285739	0.1778708721
H	-2.0617838478	-4.7374670596	0.4657866017
H	-3.6558175049	-4.0275739473	0.7481029229
H	-2.9663562963	-4.0332149983	-0.8813516712
O	-2.3069819619	0.6126618093	2.5361381025
O	-2.9821853888	1.8084652788	2.5784288701
C	-2.061252059	2.853290737	2.4138915096
H	-1.4347511707	2.6847893589	1.5456956093
Cl	-1.0089933285	3.0133184892	3.8458010072
Cl	-3.0366834914	4.3036463691	2.1833298212

TS γ

G= -1644.514446
H= -1644.446020
If= -1369.6981

0 2

N	-0.0331526297	0.1541107768	0.1559039323
H	-0.0424957579	-0.0539598841	1.1411608915
H	0.8399023569	0.1229432981	-0.3482925674
C	-1.1612581485	0.4110375762	-0.5035380065
O	-1.1945391192	0.6801565763	-1.7069801668
C	-2.453498714	0.3098104654	0.3073702303
H	-2.2185693856	0.3154297228	1.3712253402
N	-3.3142876253	1.440414759	0.0039118559
H	-4.2211310871	1.2710413471	-0.404570918
C	-2.9104990804	2.701207168	0.1588849253
O	-1.8023675577	3.0153377182	0.5978791385
H	-3.6531660663	3.447400337	-0.1364630495
C	-3.2158434746	-0.9608385699	-0.0746760487
H	-3.4078699288	-0.9419466913	-1.1505859052
H	-4.1889531745	-0.9162213856	0.4279789929
C	-2.5886684357	-2.2876659488	0.3082690597
H	-1.5521290281	-2.4058358016	-0.3389631822
C	-2.1691967813	-2.4328454852	1.7554131864
H	-3.0484978209	-2.2847642417	2.3913261411
H	-1.7821137867	-3.4349405447	1.937544537
H	-1.4127762385	-1.7102727102	2.0563956609
C	-3.4277280431	-3.4466449939	-0.1830493097
H	-4.3640660381	-3.4696190245	0.3839044732
H	-3.6750445039	-3.3427701421	-1.2395142643
H	-2.9147639495	-4.3953980624	-0.0269836604
O	-0.5281819367	-2.7938892186	-1.1399706105
O	-1.1395790254	-3.2921593116	-2.2670697285

C -1.3167260534 -2.2394376571 -3.1715249217
H -1.6607137423 -1.3429450533 -2.6705492697
Cl 0.2261199336 -1.8376603456 -3.9817382984
Cl -2.5174402799 -2.7881126857 -4.3400869272

•OOCCL₃

TS α

G= -2104.108147

H= -2104.037042

If= -1482.1141

0 2

N -0.0778069921 0.1401652564 -0.2833308713
H -0.0297899936 0.2112932831 0.7201348663
H 0.7756625705 0.1368059965 -0.8216357234
C -1.2445835259 0.0517631483 -0.9126295549
O -1.3650311002 -0.034436719 -2.1342759264
C -2.5004928363 -0.0475607589 -0.046159396
H -2.2330884773 0.2586488379 1.1078760666
N -3.5154076488 0.8542426317 -0.4393991633
H -4.4764849589 0.5476100774 -0.3657080477
C -3.290954661 2.1522765658 -0.7511041882
O -2.1781917516 2.6522599951 -0.8058260623
H -4.2053601648 2.7122845267 -0.9639885984
C -3.03834323 -1.4724867109 0.0172074316
H -3.4095471111 -1.7062772944 -0.9853499195
H -3.8973172731 -1.4725485039 0.6947004208
C -2.0474432393 -2.5531365528 0.4526038859
H -1.1747378197 -2.5184955491 -0.2052519071
C -1.5864896399 -2.3796036059 1.8988842802
H -0.9512552462 -3.2175077131 2.1900021155
H -1.0127451536 -1.4649052844 2.05134878
H -2.4489939719 -2.3596136229 2.5693212593
C -2.7195152243 -3.914833067 0.2837480253
H -2.0368483942 -4.7174281387 0.5647080476
H -3.6024627085 -3.9799758042 0.9244312193
H -3.0346965945 -4.075814377 -0.748014911
O -2.4509164777 0.6331265588 2.4208039084
O -3.0056945266 1.8841483387 2.310389075
C -2.1784176758 2.8564945511 2.8732392022
Cl -0.5413005503 2.8353456172 2.1970531882
Cl -2.0829680952 2.6271366101 4.6365856126
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TS γ

G= -2104.115068

H= -2104.041350

If= -1079.4415

0 2

N -0.0751975386 -0.0530816289 0.0264527898
H -0.0671081074 -0.6700253476 0.8220536731
H 0.7155140946 -0.0494506227 -0.5993513181

C -1.1697803479 0.6295722351 -0.3032944645
O -1.2314385989 1.3730935571 -1.2854629874
C -2.3891470989 0.4268882674 0.598285593
H -2.0866311492 -0.0766451905 1.516450905
N -2.9654876698 1.7185704122 0.9349530918
H -3.894941776 1.9418021828 0.6113640413
C -2.2671668502 2.6589886653 1.5709231263
O -1.1056183228 2.5051018474 1.9533168214
H -2.8155048015 3.590937114 1.7333067638
C -3.4658040903 -0.3760878766 -0.1348495861
H -3.7153102514 0.1439317655 -1.0624521487
H -4.3615391287 -0.3622989277 0.4961436484
C -3.1714618446 -1.837857207 -0.4332899855
H -2.3032264086 -1.835603976 -1.2643256373
C -2.646476713 -2.6482094055 0.7329222661
H -3.353870213 -2.5612217065 1.5647052357
H -2.5671484832 -3.7011306133 0.4667584995
H -1.6738824402 -2.3068456409 1.0852323494
C -4.3532998406 -2.481974085 -1.1293506615
H -5.2021007058 -2.5028082456 -0.4387750499
H -4.6483429408 -1.9154161628 -2.0128631272
H -4.1321540808 -3.5072997394 -1.4210658928
O -1.3523399254 -1.784842958 -2.3056956863
O -0.2618799534 -2.4673043746 -1.8388952772
C -0.1358563976 -3.7083339968 -2.4633480694
Cl -1.561317573 -4.7258703248 -2.1900123849
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•OOCHCH₂

TS α

G= -763.365093

H= -763.300032

If= -1827.5569

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H 0.7909822152 0.2419050132 -0.3299407042
C -1.1966581797 0.1127057992 -0.6921256079
O -1.1498804154 0.0367013582 -1.920868171
C -2.5474975815 -0.0015494915 0.0033453513
H -2.3798507617 0.2402759008 1.2600714166
N -3.4805985774 0.968950871 -0.422183524
H -4.4582873042 0.7087917232 -0.4335107333
C -3.1779176101 2.2596576936 -0.6887622458
O -2.0421731073 2.7123111048 -0.668506326
H -4.0521023318 2.8640392396 -0.9434063221
C -3.1304820548 -1.404491778 -0.0856129551
H -3.4368344003 -1.5514356315 -1.1263123841
H -4.0353269766 -1.4314573244 0.5288106065
C -2.1999957149 -2.5463905026 0.3255400563
H -1.2848171174 -2.4851716974 -0.270464197
C -2.8906066763 -3.8705771435 0.0040692742

H	-3.1370656102	-3.9409745904	-1.0562555019
H	-3.8165849395	-3.9596877228	0.5773622725
H	-2.2481832852	-4.7125850889	0.2641746837
C	-1.8344416162	-2.4976179727	1.8072517576
H	-2.7407422293	-2.5041818049	2.4179238965
H	-1.2525736559	-1.6134358879	2.0669625537
H	-1.2406085914	-3.372986464	2.0749856682
O	-2.3968946826	0.5699676488	2.4769721198
O	-2.778808593	1.8901263324	2.4892307563
C	-1.6743477411	2.7248130588	2.5141423424
H	-0.7330697076	2.1986490813	2.5914476436
C	-1.8392359818	4.0358618556	2.4615996713
H	-0.9691012025	4.6737009648	2.502739223
H	-2.8214900069	4.4803947085	2.3767627116