BBr_3-assisted cleavage of most ethers does not follow the commonly assumed mechanism

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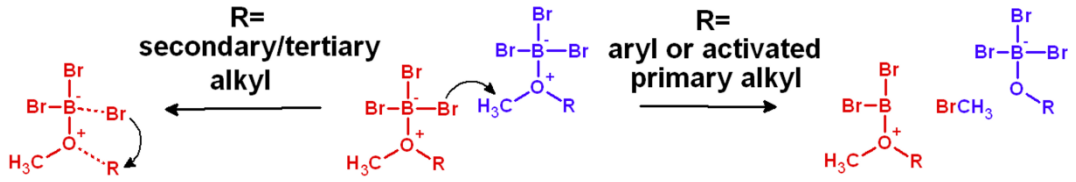
Abstract: Density-functional computations were used to probe the reaction mechanism of BBr_3-assisted ether cleavage. After the initial formation of an ether-BBr_3 adduct, secondary and tertiary alkyl ethers are cleaved through Br^- transfer from the activated BBr_3 to the alkyl moiety, as postulated in the literature. In contrast, all other ethers studied react through a novel pathway involving two ether-BBr_3 adducts, one of which acts as Br^- donor, and the other as the reaction substrate. The identification of the novel bimolecular mechanism for this classical reaction has further applications, as it implies that BBr_3-assisted ether cleavage may become impossible if the ether is surrounded by bulky portions of the molecule which prevent the approach of the attacking BBr_3-adduct. Our data also allow the construction of an order of reactivity of alkyl ether deprotection: tertiary alkyls, allyl, benzyl, isopropyl, isobutyl and ethyl can be removed sequentially as their bromo derivatives; phenyl, cyanomethyl and cloromethyl groups can be sequentially removed as their corresponding alcohols.

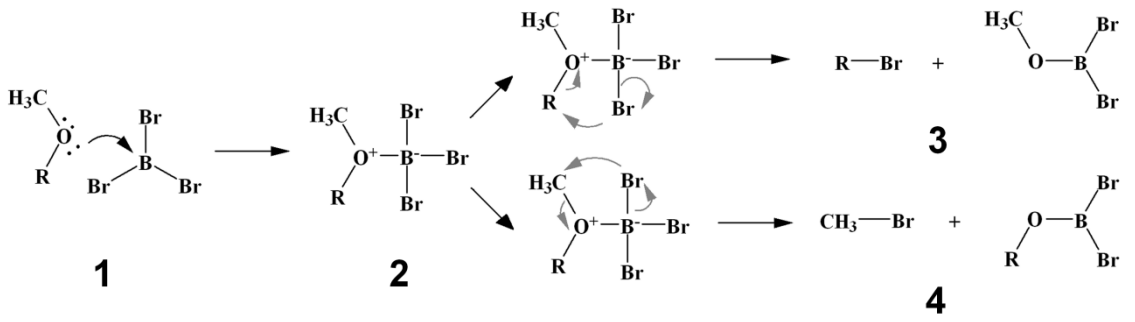
TOC graphic abstract:



Introduction

BBr_3 has long been used widely as an ether-cleaving reagent[1] due to its tolerance of several other functional groups in the target molecule. The reaction is usually performed at low temperatures (-78 ºC to 0ºC) in dichloromethane, and yields an alcohol and a brominated compound. Aryl ethers are cleaved into aromatic alcohols and bromoalkenes, whereas mixed alkyl ethers become brominated in the most substituted carbon of the ether bond and release the alcohol from the least substituted C-O bond. In analogy to the behavior of BCl3 with alcohols[2], the reaction is supposed to proceed through initial nucleophilic attack on boron by the ether oxygen atom (Scheme1). Bromine attack on one of the ether carbons is then supposed to occur, yielding a bromide and an alkoxydibromoborane which is converted to hydroxyl during reaction workup.

In spite of the synthetic importance of this reaction, the proposed mechanism has not yet been studied thoroughly either experimentally or computationally. Here we report density functional computations on the BBr_3-assisted cleavage of aromatic and mixed alkyl ethers, aiming at a solid understanding of the factors governing the bromine transfer and the severing of the C-O bond.



Scheme 1: Proposed reaction mechanism of BBr3-catalyzed ether cleavage. a) R= CH_3; b) R= CH_2Ph; c) R= CH_2-CH=CH_2; d) R= CH_2Cl; e) R= $CH_2CH(CH_3)_2$; f) R= CH_2-CN ; g) R= CH_2CH_3 ; h) R= $C(CH_3)_3$; i) R= Ph ; j) R= $CH(CH_3)_2$

Computational methods

Geometry optimizations were performed with the Firefly[3] quantum chemistry package, which is partially based on the GAMESS (US)[4] source code, at the B3LYP[5] level with the SBKJ pseudo-potential (and associated basis set[6]) for Br and a medium-sized basis set, 6-31G(d), for all other elements, using autogenerated delocalized coordinates[7]. Zero-point and thermal effects on the enthalpies at 210-298 K were computed at the optimized geometries using a scaling factor of 0.9857. Single-point energies were computed using the triple-zeta 6-311G(d,p) basis set for Cl and Br, and the 6-311+G(2d,p) basis set for all other elements. The core-electrons of Br were again treated with the SBKJ pseudo-potential. All energy values described in the text include solvation effects in dichloromethane computed using the Polarizable Continuum Model[8] implemented in Firefly.

Results

Table 1: Computed activation enthalpies (in kcal•mol^{-1}) at 250 K in the two pathways of BBr_3-assisted cleavage of methyl ethers. Values at other temperatures in the 210 K-298 K range differ from these in less than 0.8 kcal•mol^{-1}.

	R=	**2 → 3**	**2 → 4**
1a	-CH_3	39.8	39.8
1b	-CH_2-Ph	15.7	42.1

1c	$-CH_2-CH=CH_2$	18.7	41.1
1d	$-CH_2-Cl$	35.4	37.8
1e	$-CH_2-CH(CH_3)_2$	25.2	40.1
1f	$-CH_2-CN$	36.3	34.4
1g	$-CH_2-CH_3$	30.0	42.4
1h	$-C(CH_3)_3$	6.4	37.3
1i	-Ph	36.0	36.2
1j	$-CH(CH_3)_2$	16.6	43.9

Our computations show that the initial formation of the BBr_3-ether adduct **2** from the pre-reactional complex occurs very readily for all ethers studied as the activation enthalpies of this reaction step always remais very low (< 8 kcal•mol^{-1}). This step is moderately exothermic (by 6-9 kcal•mol^{-1}) for almost all ethers. The few exceptions (for ethers **1d**, **1f**, **1h** and **1i**) are endothermic by less than 3 kcal•mol^{-1}. The transition states observed in the **2→4** transformation (elimination of bromomethane) are very similar for all ethers, with methyl-O bonds between 2.15 and 2.25 Å and very high activation enthalpies (Table 1). The alternative internal bromine transfer from the boron atom to the ether alkyl or aryl group (the pathway depicted as **2→3** in scheme 1) is highly sensitive to the identity of the ether substituent, as the respective activation enthalpies range from <1 kcal•mol^{-1} (**2h**) to ≈40 kcal•mol^{-1}. Further analysis of the transition states for this reaction steps reveals that such large differences are due to markedly different reaction modes (Figure 1).

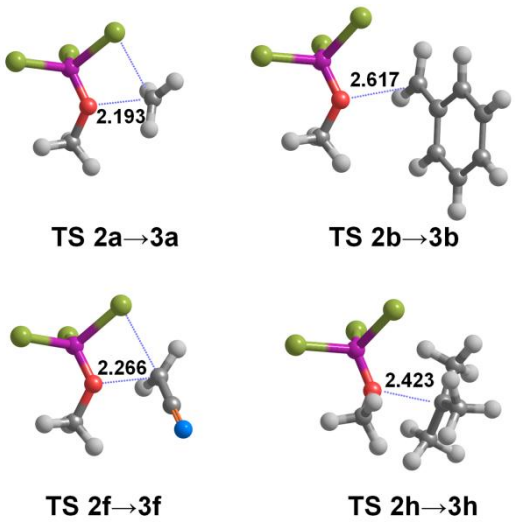


Figure 1: Transition states for the conversion of some of the ethers studied in this work. All distances in Å.

For most ether substitutents, the transition state contains a moderately elongated (2.0-2.35 Å) C-O bond and corresponds to concerted C-O bond breaking/C-Br bond formation. Such transition states all lie >30 kcal•mol^{-1} and are effectively inaccessible at the very low temperatures commonly used for this reaction. A very different behavior is observed in those ethers where the substituents are able to yield a strongly stabilized carbocation (**1b, 1c, 1e, 1h, 1j**): upon formation of the BBr_3 adduct, these ethers break through the formation of low-lying transition states with very elongated C-O bonds (Figure 1), substantial carbocationic character in the leaving group and activation enthalpies well under 25 kcal.mol^{-1}. The **2h** adduct yields such a strongly stabilized tertiary carbocation *en route* to **3h** that this step proceeds with hardly any barrier and the initial formation of the adduct becomes the rate-determining step. In all these instances, a bromide ion is then transferred from the alkoxyboron intermediate to the nascent carbocation without any further energetic barriers. Interestingly, Br^- does not add to the carbocation produced from **2j** , but rather removes a H^+, yielding HBr and H_2C=CH-CH_3 (Figure 2). The alkene may react with HBr, yielding the expected **3h** product, though only if at

least one additional HBr molecule is present to stabilize the nascent Br^- (Figure 2), in agreement with the experimental observation of kinetics of second-order in HBr when halohydrogenation of alkenes is performed in aprotic solvents[9]. We expect therefore that the alkene may be isolated in the intermediate steps of the reaction, i.e., before enough HBr has accumulated to enable the catalysis of the bromohydrogenation step. The full pathway, including the bromohydrogenation step, has an enthalpic activation barrier of 18.2 kcal•mol^{-1} (Table 2).

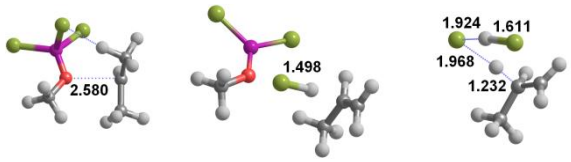
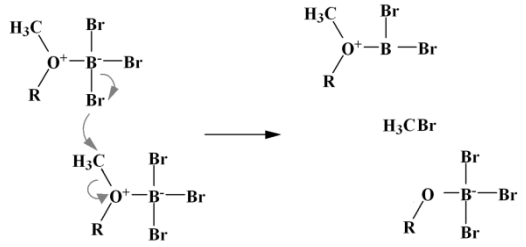


Figure 2: Transition states for the conversion of some of the ethers studied in this work. All distances in Å.

Table 2: Computed enthalpies (in kcal·mol^{-1}) at 250 K of the intermediates of BBr_3-assisted cleavage of ether **1j**. Values at other temperatures in the 210 K-298 K range differ from these in less than 0.8 kcal·mol^{-1}.

Separated reactants	0
Pre-reactional complex (**1j** + BBr3)	2.8
TS Pre-reactional complex →**2j**	2.3
2j	-8.3
TS **2j**→alkene	8.4
Alkene + HBr + methoxyborane	-8.2
TS HBr-assisted bromohydrogenation	9.9
3j	-39.4

The computations described above clearly explain why methyl ethers containing a secondary/ tertiary alkyl group yield methanol and a secondary/tertiary bromoalkane upon treatment with BBr_3, but erroneously predict that other ethers should not be substrates for this reaction. A different reaction mechanism must therefore be operative in the experimentally observed cleavage of aryl or methyl ethers. We therefore computed the feasibility of a bimolecular reaction between two ether-BBr_3 adducts. This reaction would formally be a nucleophilic substitution on the methyl (or alkyl) moiety of the ether, with a bromine from one BBr_3-ether molecule acting as attacking species and the BBr_3-O-alkyl (or methyl) moiety of the attacked ether as the leaving group (Scheme 2).



Scheme 2: Proposed SN_2 mechanism for BBr_3 ether cleavage

Investigation of the mechanism for this attack reveals very striking geometric similarities in their transition states, irrespective of the identity of the ether: the leaving group, attacked carbon and attacking Br^- are always almost perfectly collinear, and the total distance between the attacking Br^- and the leaving O remains in the 4.56-4.60 Å range (Figure 3), which entails that C-O bond distance and C-Br distances in the C atom undergoing substitution are very elegantly anti-correlated. The shortest C-O bonds are observed in those ethers bearing electron-withdrawing alkyl moieties, whereas ethers with secondary or tertiary alkyl groups have more elongated C-O bonds in the transition state.

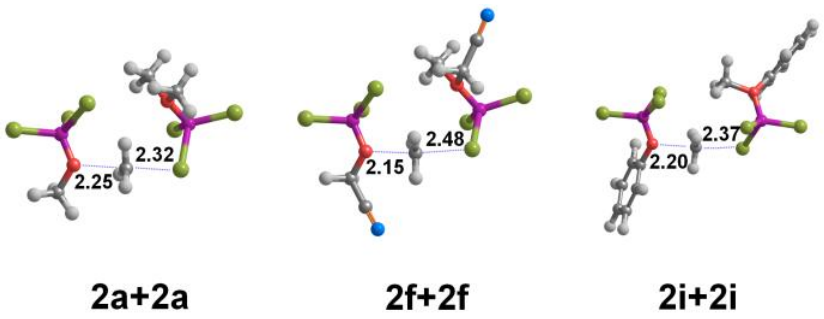


Figure 3: Transition states of the SN_2 transfer of Br^- from the adduct to the methyl group in some representative ethers. All distances in Å.

Table 3: Computed activation enthalpies (in kcal•mol^{-1}) at 250 K in the two pathways of $BBr3^-$ assisted cleavage of methyl ethers. Values at other temperatures in the 210 K-298 K range differ from these in less than 0.8 kcal•mol^{-1}. nd: not computed, as secondary/tertiary carbons or unactivated phenyl rings are usually much less prone than methyl groups to SN_2/SN_{Ar} reactivity.

	R=	Attack on CH_3	Attack on R
1a	$-CH_3$	20.9	20.9
1b	$-CH_2$-Ph	21.6	12.3
1c	$-CH_2-CH=CH_2$	22.5	10.9
1d	$-CH_2$-Cl	19.2	23.8
1e	$-CH_2-CH(CH_3)_2$	21.8	18.5
1f	$-CH_2$-CN	16.2	21.0
1g	$-CH_2-CH_3$	22.0	19.9
1h	$-C(CH_3)_3$	19.6	nd
1i	-Ph	12.5	nd
1j	$-CH(CH_3)_2$	27.5	nd

Analysis of the relative energies of the transition states shows that this mechanism affords a low-energy pathway for the methanol-yielding cleavage of all ethers (Table 3). Surprisingly, the alternative attack on the more hindered alkyl substituent was found to be more favorable than the attack on the unhindered methyl group in the adducts of allyl methyl ether (**2c**), benzyl methyl ether (**2b**) and activated primary alkyl ethers (**2e** and **2g**). In the benzyl methyl ether adduct (**2b**), Br^- attack to the benzyl moiety occurs only after the benzyl has completely detached itself from the adduct. The smaller number of resonatable double bonds in the allyl methyl ether (**2c**) provide smaller stabilization of a detached allyl moiety, and as a result Br^- attack to the allyl occurs before it has detached (Figure 4). In **2e** and **2g**, the bulky group attached to the methylene contribute to a significant lengthening of the transition state C-Br distance (2.63 Å in **2e**; 2.51 Å in **2g**) vs. the observed distances in the instances of Br^- attack to the methyl group (2.36-2.38 Å). Overall, the positive effect of charge delocalization in these four systems clearly offsets the negative steric influence that might have been expected from the replacement of a methyl H by a bulkier group.

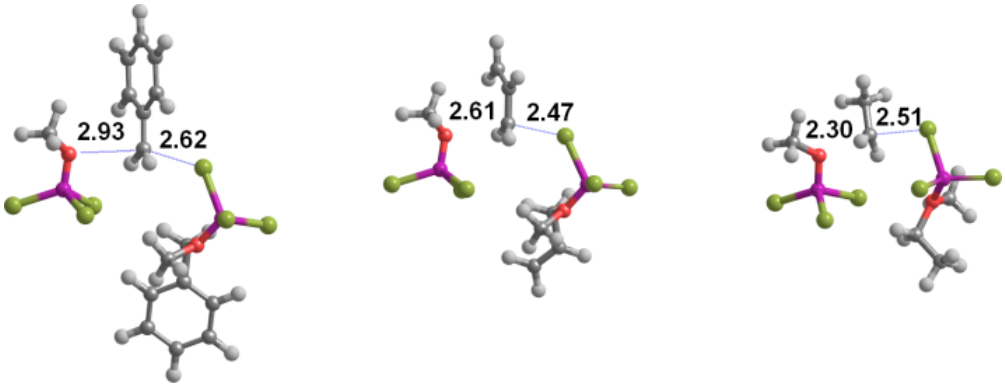


Figure 4: Transition states of the SN_2 (or SN_2-like) transfer of Br^- from the adduct to the alkyl group in **2b** (left), **2c** (center) and **2g** (right). All distances in Å.

Conclusions

Combining the results of all mechanisms, we can conclude that the originally postulated reaction sequence is the most favored mechanism only for ethers of secondary (**1j**) or tertiary (**1h**) alkyl groups. A bimolecular reaction involving two ether-BBr_3 adducts with formation of methanol and haloalkanes is the most favorable pathway for mixed ethers of methyl and activated primary alkyl groups (**1b, 1c, 1e, 1g**). Competition between monomolecular and bimolecular mechanisms may be detectable in the reaction of **1b**, as the relevant barriers are quite close. Mixed ethers of methyl and deactivated primary alkyl or aryl groups (**1a, 1d, 1f, 1i**) also follow a bimolecular mechanism involving two ether-BBr_3 adducts, though yielding bromomethane and alkyl (or aryl) alcohol.

Our data also allow the construction of an order of reactivity of alkyl ether deprotection to complement the hierarchy of reactivity for aryl ethers obtained by Punna et al.[10]: tertiary alkyls, allyl, benzyl, isopropyl, isobutyl and ethyl can be removed sequentially as their bromo derivatives; phenyl, cyanomethyl and cloromethyl groups can be sequentially removed as their corresponding alcohols. The identification of the novel bimolecular mechanism for this classical reaction has further applications, as it implies that BBr_3-assisted ether cleavage may become impossible if the ether is surrounded by bulky portions of the molecule which prevent the approach of the attacking BBr_3-adduct. In this regard, previous reports of the inability of BBr_3 to cleave ethers in thiocrown ethers derived from 1,1'-binaphthalene-2,2'-diol[11] and attributed at the time to probable preferential addition of BBr_3 to the sulfur atoms present in the molecule may simply be one example of steric crowding preventing the Br^--donating molecule of BBr_3-ether adduct from approaching the site of nucleophilic substitution in the other BBr_3-activated ether molecule.

Acknowledgments Research at REQUIMTE is supported by Fundação para a Ciência e a Tecnologia through grant no. PEst-C/EQB/LA0006/2011. This work has been financed by FEDER through Programa Operacional Factores de Competitividade – COMPETE and by Portuguese Funds through FCT – Fundação para a Ciência e a Tecnologia under project PTDC/QUI-QUI/111288/2009

Supporting Information Available Geometries, solution energies, zero-point and vibrational contributions to enthalpy for all species.

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Supplementary Material

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Gas-phase geometries, zero-point and vibrational contributions to enthalpy, and solution energies for the reactants, transition states and products of all the reactions considered in this work.

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Contents

Geometries

BBr3

B	-0.287526989	-1.361805807	-4.216111385
Br	-1.975590612	-2.294810881	-4.191731943
Br	1.336046244	-2.293388825	-3.750735817
Br	-0.223233855	0.502715665	-4.705924886

a

1a

O	-0.476047551	-0.454380832	-1.530359975
C	-0.777308389	-1.379597612	-0.510078441
H	-1.808307217	-1.258536630	-0.137630519
H	-0.669978099	-2.380025090	-0.937811943
H	-0.090069242	-1.282169522	0.347055789
C	-0.600449565	0.881046279	-1.095762318
H	-1.629291600	1.112876845	-0.773076169
H	0.079241168	1.103670078	-0.256166977
H	-0.339427363	1.523062382	-1.941304927

Pre-reaction complex (1a+BBr_3)

O	-0.475685876	-0.454212586	-1.530595496
C	-0.778152696	-1.384885214	-0.507936051
H	-1.808461864	-1.259432312	-0.141092746
H	-0.671155652	-2.384507571	-0.935211148
H	-0.086445533	-1.280748170	0.341998162
C	-0.600512130	0.886671861	-1.096524811
H	-1.629796138	1.111753760	-0.776461749
H	0.081787971	1.098881082	-0.258926866
H	-0.338703206	1.526236818	-1.941932710
B	-0.254885003	-1.324026682	-4.171094306
Br	-2.013182983	-2.134050273	-4.167212155
Br	1.298404446	-2.393012946	-3.741183414
Br	-0.027012077	0.466781386	-4.870830860

TS Pre-reactional complex→ 2a

O	-0.409062397	-0.486031816	-1.638489915
C	-0.727591054	-1.451605673	-0.650303241
H	-1.802502893	-1.445848194	-0.416229946
H	-0.451049724	-2.429606408	-1.049359107
H	-0.161138984	-1.268420992	0.274727528
C	-0.740414748	0.831226002	-1.233345356
H	-1.815404184	0.926509125	-1.018084088
H	-0.171958080	1.119053071	-0.336567143
H	-0.476800934	1.499920975	-2.054732433
B	-0.256281063	-1.298350827	-4.104245828
Br	-2.020380451	-2.110813492	-4.122605662
Br	1.298285304	-2.395504663	-3.731045174
Br	-0.013977664	0.472722867	-4.859233183

2a

O	-0.353669152	-0.600717067	-2.107133000
C	-0.437387421	-1.601015725	-1.032732391
H	-1.471148814	-1.938677726	-0.940545396
H	0.220440150	-2.419332088	-1.307016342
H	-0.088828209	-1.109554654	-0.123980823
C	-1.222758656	0.544084908	-1.802429933
H	-2.265082262	0.228379731	-1.883027807
H	-0.976998077	0.859763921	-0.788498760
H	-0.990625112	1.322198989	-2.522039829
B	-0.272415557	-1.126991781	-3.625896394
Br	-2.061618963	-2.037912343	-3.992813776
Br	1.303747030	-2.400824752	-3.706320905
Br	0.050893973	0.489490988	-4.802951142

TS 2a→3a

O	-0.245908233	-0.669843770	-2.192256812
C	-0.510807360	-1.462095877	-1.030254824
H	-1.472137525	-1.978025244	-1.113766776
H	0.294918701	-2.192415523	-0.907926371
H	-0.513171491	-0.785907201	-0.169938384
C	-1.370090653	1.206371764	-2.356066330
H	-2.252291068	0.646878293	-2.642405989
H	-1.039475184	1.165665540	-1.328491644
H	-1.168869593	2.129909563	-2.878428638
B	-0.235453459	-1.262596720	-3.495554032
Br	-2.040649002	-2.101312006	-4.013989401
Br	1.324489846	-2.520073357	-3.786200432
Br	0.023142251	0.557144323	-4.600172163

3a (=4a)

O	0.349232453	-2.979007750	-1.270202054
C	0.850040229	-3.813017888	-0.218790875
H	0.072174586	-3.883940401	0.544717541
H	1.111734865	-4.808048859	-0.584193498
H	1.730742040	-3.322926802	0.202883050
C	-0.807048106	2.624488834	-3.947709487
H	-0.863077837	1.578515316	-4.240837941
H	0.216284506	2.929313704	-3.740942929
H	-1.468923433	2.844270019	-3.113071843
B	0.213669881	-3.258830950	-2.556572109
Br	-0.504697724	-1.853935811	-3.711260681
Br	0.688843395	-4.989020360	-3.356198777
Br	-1.441731070	3.713646145	-5.507998738

2a+2a

O	-1.169891703	-0.776760662	-1.914899885
C	-1.678061787	-1.955734103	-1.188417640
H	-2.575689970	-2.319256737	-1.690992349
H	-0.892495294	-2.702744040	-1.195762110
H	-1.884676813	-1.626944318	-0.170330436
C	-2.183409284	0.288294008	-1.923118649
H	-3.016003466	-0.019928283	-2.559273065
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B	-0.292452095	-1.025678889	-3.222215907
Br	-1.499986802	-1.973865772	-4.559278450
Br	1.292463486	-2.173436814	-2.630838636
Br	0.364233880	0.770306216	-3.885396486
O	1.849990925	-6.031804186	0.897378558
C	3.037460554	-6.799577149	1.299700752
H	3.656074058	-6.176930770	1.949573075
H	2.686777971	-7.684702109	1.819467376
H	3.560211163	-7.063265903	0.380657449
C	2.222874102	-4.994037082	-0.082248180
H	3.015001273	-4.376355156	0.342976946
H	2.550531999	-5.519089267	-0.979413048
H	1.335772648	-4.404518880	-0.283665896
B	0.747682131	-5.667812883	1.989027058
Br	1.509597892	-4.128053283	3.087566422
Br	0.392159700	-7.324564061	3.093038584
Br	-0.926429324	-5.143997679	0.943004243

Bimolecular TS

O	-0.791268545	-0.890624045	-1.821658556
C	-0.593097318	-1.954422135	0.151538157
H	-1.484423480	-2.503379763	-0.117063935
H	0.347112844	-2.233973754	-0.295663661
H	-0.684543534	-0.957854763	0.559907460
C	-2.142880545	-0.450706736	-2.009257419
H	-2.786194320	-1.281965201	-2.318809631
H	-2.488490222	-0.048924927	-1.052774745
H	-2.174492491	0.335488994	-2.766782077
B	-0.094095108	-1.517966759	-2.884288881
Br	-0.799124796	-3.512892002	-3.123247365
Br	1.948867383	-1.617463237	-2.274444047
Br	-0.200124192	-0.527199095	-4.664537982
O	1.572208248	-4.531870972	0.396501076
C	1.726666659	-5.286548747	-0.882312029
H	2.308538775	-6.184561899	-0.668301456
H	0.730224826	-5.507727700	-1.246986257
H	2.229078446	-4.602351410	-1.563281213
C	2.822131418	-3.816823121	0.754784560
H	3.607636963	-4.558548143	0.900846250
H	3.023889718	-3.142107143	-0.075990661
H	2.627229160	-3.265649818	1.669804885
B	0.615492640	-4.961337622	1.503089261
Br	1.593941735	-5.745186295	3.060730296
Br	-0.901693856	-6.042262315	0.830423007
Br	-0.194471245	-2.998849443	2.184021835

Bimolecular product

O	-0.789373210	-0.145674200	-2.393761714
C	-1.073432793	-1.151866676	0.948399696
H	-1.701089502	-1.717593926	0.265513404
H	-0.215334421	-0.724600681	0.436811334
H	-1.625480173	-0.422330148	1.535325345
C	-2.018713250	0.313856156	-2.941798386
H	-2.796323492	-0.453827409	-2.847982759
H	-2.313143270	1.202459217	-2.376832388

H	-1.900390317	0.575779544	-3.998579426
B	-0.130218228	-1.225249326	-2.893826529
Br	-1.255246664	-3.086876516	-2.372752576
Br	1.747537298	-1.329111332	-1.875094203
Br	0.202089793	-1.302000248	-4.921132733
O	1.756202718	-4.934450370	0.153202721
C	1.585708499	-5.048276034	-1.360412349
H	1.549007213	-6.112145868	-1.577262951
H	0.672178716	-4.506687038	-1.619461286
H	2.470430758	-4.573245614	-1.774224258
C	2.749309197	-3.877416582	0.573348018
H	3.733626396	-4.338351319	0.502741293
H	2.595574716	-3.056715781	-0.128013100
H	2.488655410	-3.582262625	1.583690802
B	1.004607748	-5.724677500	1.065177431
Br	1.661739467	-5.929368322	2.854210629
Br	-0.525537217	-6.655774760	0.422777816
Br	-0.354037948	-2.489386342	2.291992225

b

1b

O	-0.613182316	-0.662555880	-1.401364849
C	-0.833023006	-1.703193102	-0.466529516
H	-1.779833110	-1.578731943	0.077624284
H	-0.867821156	-2.636482706	-1.034535997
H	-0.013496734	-1.761787768	0.267924444
C	-0.515893287	0.620010876	-0.803095255
H	0.237999398	0.616100798	0.002171728
H	-0.138957763	1.272987537	-1.599702996
C	-1.833466330	1.156296677	-0.270632722
C	-3.006415381	1.012622120	-1.023748249
C	-1.895932919	1.826403916	0.955261167
C	-4.213839275	1.533695022	-0.560910081
C	-3.102245518	2.357459777	1.417745496
C	-4.264727998	2.211418087	0.660384083
H	-2.963752961	0.478979871	-1.969374841
H	-0.993520669	1.934629518	1.553921042
H	-5.117086829	1.412880340	-1.153599556
H	-3.134114331	2.876554084	2.372227560
H	-5.205841482	2.619167009	1.019842582

Pre-reaction complex (1b+BBr_3)

O	-0.609568031	-0.664120734	-1.399536380
C	-0.831770298	-1.706954002	-0.461507932
H	-1.781121541	-1.575470059	0.073653859
H	-0.863171024	-2.640931082	-1.027263410
H	-0.012739812	-1.758292609	0.271722021
C	-0.516388037	0.625802381	-0.804629201
H	0.234472096	0.616749281	0.001440002
H	-0.135945612	1.274654047	-1.601775766
B	-0.265118305	-1.316295160	-4.178490049
Br	-1.990257259	-2.189157787	-4.253568117
Br	1.323388497	-2.355614135	-3.817049284
Br	-0.107340080	0.541341461	-4.692886058
C	-1.836054845	1.155998228	-0.274752219
C	-3.009815728	1.015842504	-1.027300376
C	-1.895899511	1.822115717	0.953708793

C	-4.215817060	1.536917305	-0.560493060
C	-3.100498252	2.354426679	1.418609007
C	-4.264053310	2.211767950	0.662307088
H	-2.972350457	0.488184627	-1.976291334
H	-0.992772536	1.927843181	1.551615813
H	-5.119664473	1.418932927	-1.152607346
H	-3.130049498	2.872085536	2.373853289
H	-5.203847040	2.621047705	1.023289904

TS Pre-reactional complex → 2b

O	-1.136413345	-0.649997538	-1.770363397
C	-1.259982781	-1.726685317	-0.846676380
H	-2.054716952	-1.530244981	-0.117216952
H	-1.516645366	-2.615570353	-1.425510859
H	-0.313769029	-1.899102730	-0.314345836
C	-0.773857632	0.583516096	-1.145845281
H	0.128886499	0.443127371	-0.532024331
H	-0.514268308	1.250844781	-1.973425920
B	-0.270686181	-1.321913480	-4.131214463
Br	-1.856926561	-2.371432386	-4.512043185
Br	1.331808064	-2.208398336	-3.482208567
Br	-0.149792173	0.493783113	-4.806965307
C	-1.889088044	1.184964355	-0.313374690
C	-3.192208482	1.253925261	-0.824787626
C	-1.630930165	1.708242818	0.957531493
C	-4.213788517	1.839916035	-0.079159618
C	-2.651022230	2.304536196	1.702597574
C	-3.945012616	2.370615092	1.185728286
H	-3.399959522	0.836474819	-1.806455992
H	-0.624730174	1.651244925	1.367955778
H	-5.220786416	1.885835160	-0.485461104
H	-2.435277256	2.708432801	2.688193054
H	-4.741503906	2.829882267	1.765137225

2b

O	-1.219010742	-0.854769124	-2.186300255
C	-1.726415988	-1.954681261	-1.353142227
H	-2.178183681	-1.493554817	-0.476643798
H	-2.469612401	-2.484726294	-1.939632077
H	-0.891289540	-2.606069420	-1.086377710
C	-0.548288011	0.200984302	-1.343059769
H	0.156388056	-0.325811765	-0.696227539
H	-0.001463997	0.802164853	-2.064711976
B	-0.568255921	-1.197449224	-3.590216628
Br	-1.757104912	-2.551429402	-4.521517642
Br	1.298827122	-1.935444485	-3.198085508
Br	-0.520019590	0.550263754	-4.638662651
C	-1.570340949	0.991277566	-0.584137855
C	-2.513335486	1.773124546	-1.269162395
C	-1.566355286	0.987288506	0.816323630
C	-3.438404596	2.533458146	-0.557887803
C	-2.487958668	1.758196392	1.527450461
C	-3.425124325	2.529826262	0.840449709
H	-2.517761741	1.778947694	-2.355736015
H	-0.831719356	0.390533758	1.352467837
H	-4.166573729	3.135428942	-1.093754913
H	-2.473093636	1.753251992	2.613557992

H	-4.144719935	3.128715048	1.391525389

TS 2b→3b

O	-1.288708720	-1.247618865	-2.155151263
C	-1.390345151	-2.337957362	-1.247347708
H	-1.828846249	-1.953040644	-0.320270379
H	-2.049854419	-3.111057946	-1.655909592
H	-0.407750915	-2.779871166	-1.042393053
C	-0.137027684	0.983785605	-1.416528269
H	0.378903956	0.112421764	-1.033859107
H	0.306073615	1.466774023	-2.277565002
B	-0.727099821	-1.441480619	-3.428196882
Br	-1.653106017	-2.901135156	-4.544701022
Br	1.342747181	-1.814724562	-3.299315409
Br	-1.001007556	0.433486947	-4.399332851
C	-1.213888186	1.561060566	-0.736132734
C	-1.843822982	2.732126489	-1.247642025
C	-1.661794897	1.014336381	0.500754195
C	-2.865839459	3.336607995	-0.538857519
C	-2.682146953	1.629969160	1.204062158
C	-3.282919242	2.786170525	0.683291497
H	-1.524397196	3.121615593	-2.209306060
H	-1.182177011	0.119934563	0.886060218
H	-3.351859173	4.225360750	-0.927720829
H	-3.021667848	1.220815252	2.150146570
H	-4.090392822	3.261081701	1.233712267

3b

O	-0.891025888	-1.316776345	-4.026590310
C	-1.560904397	-0.890763546	-5.230079788
H	-2.362808359	-0.223467965	-4.915422292
H	-0.853067400	-0.358455409	-5.870499886
H	-1.967635130	-1.751539216	-5.765204996
C	-2.511520181	0.604621034	-1.305674151
H	-3.102306767	0.331380652	-0.434059389
H	-2.075990427	-0.272034054	-1.779469979
B	-0.009762965	-2.303979443	-3.922358782
Br	0.567635791	-3.386181346	-5.451760340
Br	0.731952256	-2.667299641	-2.153221677
Br	-3.986066619	1.161670184	-2.666656089
C	-1.536356568	1.694977026	-1.056434845
C	-1.783227393	2.668365942	-0.076569380
C	-0.338634596	1.750118425	-1.784514405
C	-0.852078855	3.674443236	0.170874511
C	0.594005513	2.755498866	-1.535739642
C	0.338491157	3.720405970	-0.559046051
H	-2.710752139	2.634546242	0.489797206
H	-0.141526695	0.995120477	-2.540859532
H	-1.052783889	4.421503777	0.933812802
H	1.521353601	2.784358900	-2.101189257
H	1.066218738	4.503551640	-0.364619287

TS 2b→4b

O	-1.325727576	-0.424175485	-2.545208230

C	-1.198352167	-2.180697275	-1.135751955
H	-1.835241189	-1.442777308	-0.671375087
H	-1.630097730	-2.839895126	-1.878995849
H	-0.336177764	-2.518835352	-0.579301142
C	-0.905905927	0.795346179	-1.887495860
H	0.141866321	0.701496964	-1.580324118
H	-0.967495123	1.594235415	-2.632904434
B	-0.697599325	-0.896717944	-3.731866200
Br	-1.891821461	-2.266617275	-4.638152532
Br	1.029123189	-1.997169619	-2.814645559
Br	0.021177166	0.496512505	-5.002897822
C	-1.804667447	1.081986868	-0.710223314
C	-3.200087966	1.069518501	-0.857163751
C	-1.253870039	1.402521595	0.536056555
C	-4.024659988	1.369435880	0.226139544
C	-2.080081256	1.714349857	1.618256789
C	-3.466516214	1.695703788	1.465655088
H	-3.633451168	0.818481818	-1.821435691
H	-0.173248369	1.413876001	0.659474331
H	-5.103976758	1.355337404	0.101959126
H	-1.639274465	1.965467263	2.579026550
H	-4.110964056	1.933950549	2.307290164

4b

O	-1.618126626	0.749419187	-3.490289097
C	1.284769572	-0.661724194	-0.992458403
H	0.459725155	-0.361057553	-0.351178274
H	2.219424954	-0.186559378	-0.703554854
H	1.057889949	-0.501148298	-2.043821332
C	-2.830390525	0.980243071	-2.720552595
H	-3.065665024	2.040241697	-2.848062690
H	-3.641920341	0.382338829	-3.141488770
B	-1.476877467	0.092178990	-4.630879622
Br	-2.958202054	-0.781337133	-5.584267389
Br	1.532632789	-2.638226985	-0.733617472
Br	0.320283652	-0.002267353	-5.395948330
C	-2.583802097	0.644903653	-1.274405830
C	-2.752211579	-0.668135475	-0.816313464
C	-2.160962395	1.632455455	-0.376771495
C	-2.497680058	-0.990389917	0.516626598
C	-1.908458585	1.313784362	0.958264217
C	-2.075014407	0.001136448	1.405869947
H	-3.082195706	-1.441166786	-1.506390264
H	-2.030564071	2.654507675	-0.724632093
H	-2.629651525	-2.011830843	0.861067709
H	-1.586476788	2.088830719	1.648267156
H	-1.881225830	-0.248073458	2.445515899

2b+2b

O	-0.646140899	-0.864875326	-2.803940786
C	-0.831391499	-1.050691813	-1.350972532
H	-1.149770835	-2.077282611	-1.164813539
H	0.119448557	-0.839539505	-0.874547198
H	-1.586078958	-0.329756667	-1.044001987
C	-1.978958825	-0.664527489	-3.497333187
H	-1.746942025	-0.797613471	-4.550418375
H	-2.620403265	-1.478669923	-3.155378775
B	0.439825778	-1.714889836	-3.541919135

Br	-0.306698517	-3.621078837	-3.712880975
Br	2.152006892	-1.668518198	-2.428730808
Br	0.764437026	-0.845724171	-5.349686630
O	1.389590647	-5.208707113	1.028548252
C	0.923532870	-5.541463367	-0.329850999
H	0.234374928	-6.373844714	-0.237056110
H	0.440411144	-4.665361268	-0.764547506
H	1.808723079	-5.826501966	-0.894269092
C	2.660058003	-4.380250728	0.978749951
H	2.455470182	-3.562105438	0.286260016
H	2.756788381	-3.997148796	1.991018320
B	0.350648046	-4.893275168	2.152873626
Br	1.320005124	-5.110793718	3.931547846
Br	-1.191570316	-6.203525901	2.016506052
Br	-0.280085007	-2.947787005	1.862377527
C	-2.526556952	0.694279456	-3.189499079
C	-1.867392090	1.844428263	-3.650591920
C	-3.721252490	0.826595773	-2.470128803
C	-2.397229504	3.105211111	-3.387720604
C	-4.256069535	2.090908553	-2.216763326
C	-3.592491158	3.229983872	-2.672856531
H	-0.940849929	1.744909141	-4.209261857
H	-4.239695713	-0.061541112	-2.115954163
H	-1.881739575	3.991971853	-3.744915360
H	-5.185131805	2.183509148	-1.661949977
H	-4.004855953	4.214988617	-2.472998877
C	3.820785052	-5.228805397	0.561633918
C	4.287269513	-6.256223478	1.396290109
C	4.471554872	-4.977258182	-0.653635585
C	5.386166504	-7.021376154	1.013401470
C	5.579085524	-5.739507455	-1.029890566
C	6.034569413	-6.762581770	-0.198228847
H	3.785498712	-6.451682546	2.339935565
H	4.114172963	-4.181398151	-1.303058237
H	5.741577855	-7.816793363	1.662201855
H	6.080585256	-5.534035843	-1.971176417
H	6.894368106	-7.358774514	-0.491406838

Bimolecular attack on methyl (TS)

O	-0.443916331	-1.157123085	-2.726617636
C	-0.515905222	-1.810269549	-0.641910410
H	-0.984945561	-2.712649725	-1.008343118
H	0.551252648	-1.689993701	-0.726052333
H	-1.131711001	-0.948304718	-0.425535065
C	-1.772768945	-0.772307919	-3.151837489
H	-1.718598617	-0.519801646	-4.215093835
H	-2.446478077	-1.630343093	-3.044699153
B	0.378763095	-1.957628070	-3.571659661
Br	-0.398215405	-3.926599690	-3.678593031
Br	2.293404781	-2.038096814	-2.650283318
Br	0.608649491	-1.198365614	-5.458143246
O	1.408010611	-4.702742513	0.716144922
C	1.291993438	-5.339649680	-0.626014461
H	1.563160455	-6.387779710	-0.514684302
H	0.272417490	-5.217609571	-0.972498216
H	1.973478397	-4.806284591	-1.282867614
C	2.727175779	-3.929580389	0.916497093
H	2.671145674	-3.129471037	0.178255055
H	2.628902000	-3.537360835	1.924689014

B	0.287909703	-4.622875602	1.707182087
Br	0.939131786	-4.878194642	3.592979310
Br	-1.244323329	-5.803820843	1.230996571
Br	-0.401244487	-2.497952994	1.640853078
C	-2.251904435	0.408880752	-2.344757860
C	-1.432418415	1.534889928	-2.175747811
C	-3.537025610	0.413203011	-1.789599530
C	-1.893849337	2.641152755	-1.464352361
C	-4.003002439	1.525707731	-1.084937756
C	-3.181355031	2.640762584	-0.919686590
H	-0.432765542	1.533366702	-2.600888178
H	-4.179091810	-0.456180497	-1.913726211
H	-1.250420147	3.507776854	-1.338866762
H	-5.003572910	1.516317168	-0.661516988
H	-3.540108313	3.505598780	-0.368285475
C	3.912847480	-4.815513931	0.727838703
C	4.279676737	-5.748372964	1.711309800
C	4.692113909	-4.690443397	-0.432020070
C	5.405389781	-6.547480319	1.529295221
C	5.823464153	-5.487433918	-0.606940617
C	6.178059202	-6.417388515	0.371196761
H	3.682758632	-5.845010362	2.613361785
H	4.416829518	-3.965235063	-1.194070351
H	5.684636444	-7.267814403	2.292668236
H	6.423571623	-5.381202115	-1.505592728
H	7.058122407	-7.039654365	0.234561399

Bimolecular attack on methyl (product)

O	0.386900383	-0.130849860	-3.257428345
C	-1.361149850	-0.949662731	-0.137361952
H	-1.781953408	-1.745958398	-0.745473419
H	-0.410904730	-0.605165875	-0.537025873
H	-2.062654418	-0.130590408	0.000260117
C	-0.647588844	-0.287515882	-4.267167219
H	-0.389194716	0.342325584	-5.123612160
H	-0.636082827	-1.333052946	-4.585317562
B	1.689716654	-0.017216582	-3.467631678
Br	-0.020331242	-4.132993770	-2.594648651
Br	2.848313296	0.089764068	-1.892488344
Br	2.501871898	0.053492572	-5.252299273
O	-0.482140781	-6.047495670	1.252545880
C	-1.813292964	-5.814363910	0.750681294
H	-2.435079381	-6.698133626	0.912560184
H	-2.250834382	-4.950145246	1.255307262
H	-1.709726204	-5.612315196	-0.315382308
C	1.534229632	-4.202953870	-1.183679771
H	1.812617746	-3.154118342	-1.111960842
H	1.009471209	-4.540108531	-0.293147944
B	-0.171061020	-6.390287802	2.497215083
Br	1.717234929	-6.633160995	2.926305364
Br	-1.519987944	-6.675336312	3.892146930
Br	-1.002303214	-1.727895997	1.682461121
C	-1.982877143	0.088377267	-3.681483621
C	-2.208710201	1.384680038	-3.198096773
C	-3.023618751	-0.845200812	-3.640611875
C	-3.452429481	1.736499184	-2.676822137
C	-4.274391801	-0.490772628	-3.129427352
C	-4.489661499	0.799387823	-2.644924126
H	-1.404824708	2.116167918	-3.223645020
H	-2.855062949	-1.853706618	-4.010447237

H	-3.616152444	2.743253419	-2.302424479
H	-5.075901154	-1.223870041	-3.106246168
H	-5.460861291	1.076398050	-2.244188679
C	2.629470958	-5.098519498	-1.619096146
C	2.621276159	-6.453856098	-1.254707933
C	3.701450951	-4.600824817	-2.375601501
C	3.664318039	-7.293416374	-1.639262163
C	4.743915855	-5.440836350	-2.760363663
C	4.725977880	-6.789130348	-2.394417942
H	1.797372710	-6.840325928	-0.660807232
H	3.714575833	-3.551266903	-2.659195383
H	3.652481540	-8.339314293	-1.345589244
H	5.571333836	-5.044694458	-3.342391170
H	5.539728189	-7.444180900	-2.693626721

Bimolecular attack on alkyl (TS)

O	-0.793842509	-0.862314688	-2.271872310
C	-0.971109803	-1.715533397	0.333173301
H	-1.742513798	-2.463830264	0.185202423
H	-0.029703549	-1.864795348	-0.177976020
C	-2.065798219	-0.524678701	-2.819560073
H	-2.570730512	-1.413173659	-3.216162675
H	-2.663711228	-0.093417526	-2.010885714
H	-1.955060057	0.212547084	-3.621056087
B	0.165086316	-1.490703926	-3.057458803
Br	-0.383260899	-3.508027230	-3.470465509
Br	1.954961013	-1.547841508	-1.836809151
Br	0.629298022	-0.535728335	-4.816885437
O	1.447444273	-4.987134904	0.784135821
C	1.092289387	-5.275110083	-0.634139201
H	1.483809534	-6.263349401	-0.867667636
H	0.013627164	-5.237859159	-0.723769647
H	1.545019660	-4.497040644	-1.243083548
C	2.794335223	-4.252241185	0.920021900
H	2.628470924	-3.310969021	0.396190126
H	2.878805292	-4.091554456	1.990767360
B	0.491312420	-5.061137010	1.939070631
Br	1.420073345	-5.742976783	3.598455714
Br	-1.164326143	-6.103613687	1.503470861
Br	-0.061896173	-2.988845078	2.380645333
C	-1.309124422	-0.428708655	0.827777964
C	-2.594406703	-0.169951374	1.365294250
C	-0.362325373	0.622760232	0.738111903
C	-2.923859547	1.105911084	1.795068858
C	-0.701834488	1.896209358	1.169781050
C	-1.976925471	2.135642870	1.698209314
H	-3.313662947	-0.981097794	1.438920863
H	0.610866950	0.418790823	0.302393082
H	-3.908471895	1.308289766	2.204508724
H	0.016331529	2.706200500	1.091945672
H	-2.238409542	3.135207620	2.034576384
C	3.911023722	-5.059159317	0.346803916
C	4.451171496	-6.140253671	1.061401972
C	4.451550853	-4.714267399	-0.900877953
C	5.509505450	-6.871161173	0.527973079
C	5.515428289	-5.445784290	-1.429276942
C	6.041454557	-6.525152665	-0.717975059
H	4.041801181	-6.400280574	2.033293578
H	4.045361998	-3.869956521	-1.452533811
H	5.924644382	-7.705553003	1.085585727

H	5.930649160	-5.170813914	-2.394305098
H	6.869453368	-7.095042445	-1.130498298

c

1c

O	-0.759633602	-0.610325915	-1.529235987
C	-0.776717301	-1.675661483	-0.595227746
H	-1.445726661	-1.474235519	0.252509660
H	-1.134030605	-2.560208846	-1.128983665
H	0.233325862	-1.880432131	-0.205487993
C	-0.347531213	0.620610643	-0.966728191
H	0.515845389	0.469727712	-0.294747137
H	0.016122477	1.231014008	-1.805256624
C	-1.435052748	1.374227670	-0.237588004
H	-1.089952221	2.226815318	0.349276315
C	-2.733756976	1.083630952	-0.294847848
H	-3.095361863	0.246080282	-0.884629991
H	-3.473677740	1.673537628	0.238400530

Pre-reaction complex (1c+BBr_3)

O	-0.762067183	-0.609613602	-1.531352454
C	-0.777509989	-1.678157080	-0.591885681
H	-1.448557945	-1.461954144	0.247959614
H	-1.137464823	-2.563161736	-1.120502274
H	0.233054731	-1.874805728	-0.205351038
C	-0.343633974	0.626539880	-0.966742206
H	0.516330064	0.463408664	-0.296042521
H	0.019647271	1.234543037	-1.804736470
B	-0.292278451	-1.327394946	-4.130451323
Br	-1.983003577	-2.263330346	-4.233010099
Br	1.326084183	-2.311616792	-3.714313285
Br	-0.169709596	0.500736915	-4.756352949
C	-1.434843588	1.371561392	-0.237809918
H	-1.089097624	2.219647493	0.354598894
C	-2.733538450	1.081513795	-0.295763003
H	-3.100221551	0.249585818	-0.890256008
H	-3.470580544	1.669801915	0.242913123

TS pre-reactional complex →2c

O	-0.555491386	-0.691335677	-1.618109204
C	-0.668645059	-1.739956434	-0.659236350
H	-1.488494713	-1.544225262	0.041311848
H	-0.876700302	-2.658266968	-1.210889669
H	0.269928183	-1.857583246	-0.100473468
C	-0.312522154	0.587225324	-1.037598288
H	0.408270537	0.485828852	-0.210957325
H	0.178294200	1.185971334	-1.814228812
B	-0.300658911	-1.287080425	-4.002161114
Br	-2.014539092	-2.203008046	-4.105552528
Br	1.321568417	-2.335472063	-3.761344258
Br	-0.164741760	0.535756754	-4.662986579
C	-1.558257683	1.289675179	-0.559583508
H	-1.372004634	2.179475469	0.043096922

C	-2.806695967	0.918367452	-0.837995470
H	-3.015745653	0.043059313	-1.446616979
H	-3.659526488	1.483092684	-0.472966473

2c

O	-0.811019228	-0.810784529	-2.056682792
C	-1.248498588	-1.870204765	-1.131705027
H	-1.528833803	-1.369269681	-0.206797005
H	-2.103245781	-2.358691096	-1.587973990
H	-0.422440270	-2.569506150	-0.988630478
C	0.065100895	0.166376321	-1.362808961
H	0.724885062	-0.411259769	-0.708467040
H	0.673673254	0.623146884	-2.143064904
B	-0.462901200	-1.192761576	-3.568575086
Br	-1.957571865	-2.376173140	-4.257150499
Br	1.339448461	-2.152080167	-3.503283169
Br	-0.396357401	0.560728232	-4.587927339
C	-0.743233533	1.182951983	-0.616449753
H	-0.166959087	1.734194207	0.125972579
C	-2.031498457	1.459318029	-0.811863753
H	-2.627515956	0.936232529	-1.553571304
H	-2.528562310	2.233251245	-0.235560306

TS 2c→3c

O	-1.076981343	-1.164042431	-2.121414816
C	-1.260231710	-2.249254722	-1.214063400
H	-1.605433072	-1.827782726	-0.264343116
H	-2.023417734	-2.933325287	-1.599686708
H	-0.325724684	-2.801592388	-1.062343233
C	0.318611432	0.828730952	-1.448669049
H	0.208383025	0.069570429	-0.686938875
H	1.142793058	0.707132613	-2.140871175
B	-0.625726878	-1.412995171	-3.431438916
Br	-1.871813634	-2.609725194	-4.533275165
Br	1.336889178	-2.122960068	-3.471115324
Br	-0.631018803	0.554459830	-4.286035083
C	-0.395864422	2.038027347	-1.336813362
H	-0.218433826	2.820374411	-2.068520974
C	-1.276873587	2.226807074	-0.317404656
H	-1.503955355	1.430582508	0.386530926
H	-1.793223619	3.171542772	-0.176539428

3c

O	-1.682914777	-4.071671272	-2.300879078
C	-1.632078708	-3.265373548	-1.116593508
H	-1.922995969	-2.235885980	-1.340516701
H	-2.334609483	-3.705817761	-0.408139319
H	-0.622758595	-3.277696373	-0.696735667
C	0.504527033	2.578682486	-2.276028417
H	0.068696369	1.628487837	-2.581040891
H	1.592567887	2.534190347	-2.308452007
B	-1.057601875	-3.827546710	-3.444307667
Br	-1.290964818	-5.097902455	-4.902628503
Br	0.082481958	-2.247921719	-3.712692560

Br	0.066335201	3.861904855	-3.823800439
C	-0.033200290	3.092632312	-0.994959629
H	0.423776303	4.001397413	-0.607866663
C	-1.013568291	2.491403749	-0.316274458
H	-1.496433724	1.590149818	-0.687608176
H	-1.367661254	2.878304692	0.634765726

TS 2c→4c

O	-0.871429602	-0.566961804	-2.257086528
C	-0.455320534	-2.416956066	-1.061920381
H	-0.859233381	-1.691460101	-0.369807861
H	-1.143505319	-2.982276704	-1.678521455
H	0.505458788	-2.851593518	-0.829323979
C	-0.236187678	0.547782725	-1.608353090
H	0.801615622	0.279444162	-1.365420932
H	-0.189953377	1.380587002	-2.319247784
B	-0.597336719	-0.950482874	-3.603317699
Br	-2.056967871	-2.204370776	-4.253579283
Br	1.247603334	-2.160520222	-3.278525498
Br	-0.191817466	0.536457168	-4.906547671
C	-0.999527785	0.952384486	-0.379703694
H	-0.457188756	1.636706067	0.272406397
C	-2.242198937	0.577176406	-0.073551693
H	-2.814617577	-0.081060180	-0.720940972
H	-2.732055548	0.937450234	0.826048304

4c

O	-0.371716082	-0.021944019	-3.228982731
C	1.810342403	-3.082625797	-3.011698619
H	1.511750156	-3.791778185	-3.780293588
H	1.120875275	-2.243795928	-2.950880494
H	2.838575901	-2.754241997	-3.147293963
C	-0.193807148	0.874054481	-2.117639158
H	0.884737388	1.060902661	-2.052341265
H	-0.686100610	1.829832846	-2.328970926
B	-1.146396175	0.129872356	-4.296030306
Br	-1.160651596	-1.321590479	-5.603963406
Br	1.732287164	-4.049387773	-1.254196084
Br	-2.250078357	1.717457729	-4.627371618
C	-0.705283257	0.278184405	-0.838964887
H	-0.544839032	0.914980501	0.030641039
C	-1.301217026	-0.904724745	-0.708304294
H	-1.466393927	-1.564677328	-1.554114259
H	-1.636890793	-1.258070969	0.261408714

2c+2c

O	-0.974279734	-0.538347552	-2.394688144
C	-1.024950223	-0.771837185	-0.940483352
H	-1.304402997	-1.810052513	-0.753706558
H	-0.039175182	-0.551565575	-0.544869187
H	-1.760769162	-0.078594780	-0.538095404
C	-2.366960833	-0.342024492	-2.965625505
H	-2.271792854	-0.570431787	-4.022620076
H	-2.982050737	-1.101363682	-2.477557462
B	0.057460453	-1.339837229	-3.261220515

Br	-0.685854203	-3.249044359	-3.440856693
Br	1.856179205	-1.313434433	-2.298099436
Br	0.203313539	-0.395872321	-5.050157526
O	1.520361423	-5.347448158	0.688763319
C	0.972811528	-5.707659195	-0.636266886
H	0.447132660	-6.649116591	-0.517562578
H	0.306755214	-4.910521350	-0.968540616
H	1.831726548	-5.815978839	-1.295257885
C	2.590025569	-4.319500801	0.550616915
H	2.243558692	-3.607864852	-0.203862020
H	2.635340317	-3.811688667	1.514005161
B	0.569992976	-5.282677507	1.941122223
Br	1.766296049	-5.281266855	3.580191107
Br	-0.630549833	-6.913824409	1.915554828
Br	-0.508343747	-3.532493105	1.767528708
C	-2.830542101	1.056131277	-2.732303171
H	-3.122753167	1.332840916	-1.721094671
C	-2.940849281	1.942194868	-3.723784263
H	-2.662259864	1.695222799	-4.745046302
H	-3.315206227	2.946329227	-3.547068798
C	3.898751150	-4.951561246	0.187934860
H	4.614104658	-4.248696086	-0.237362840
C	4.229758850	-6.229698897	0.364466895
H	3.539782917	-6.950475147	0.793179568
H	5.213446500	-6.593561630	0.084959431

Bimolecular attack on the methyl substituent (TS)

O	-0.765477207	-0.964810884	-2.205905195
C	-0.601048340	-1.882986428	-0.226138938
H	-1.011634617	-2.774023629	-0.679552514
H	0.434555163	-1.631586642	-0.383813968
H	-1.277724800	-1.136653339	0.165474558
C	-2.046029538	-0.394783787	-2.604507243
H	-1.862035520	0.639770331	-2.908133026
H	-2.420710635	-0.950114269	-3.470235881
B	0.058972485	-1.572203060	-3.194312906
Br	-0.639226364	-3.559411120	-3.539440483
Br	2.030619863	-1.694259369	-2.413259292
Br	0.135133803	-0.553500959	-4.963610027
O	1.635778287	-4.880491588	0.563033078
C	1.431388459	-5.343320554	-0.845113689
H	1.139901011	-6.387876412	-0.795202143
H	0.669811202	-4.726152107	-1.317504137
H	2.394761249	-5.224867706	-1.332396496
C	2.835094044	-3.995455637	0.730272875
H	2.744607296	-3.240821313	-0.056704454
H	2.701769528	-3.518212280	1.701597229
B	0.566869531	-4.950639308	1.630179132
Br	1.383540386	-5.435100474	3.390639681
Br	-0.968818262	-6.082866522	1.069466047
Br	-0.177529156	-2.865509645	1.907015874
C	-3.047500154	-0.459351821	-1.490696733
H	-3.418372972	-1.451066604	-1.231400512
C	-3.534111646	0.616709738	-0.869153797
H	-3.195280730	1.619809916	-1.118552585
H	-4.299104900	0.538050106	-0.101353302
C	4.116141341	-4.763801852	0.645540003
H	4.975298558	-4.125539434	0.442572759
C	4.273705616	-6.076863345	0.801453795
H	3.441682581	-6.743965865	1.006368047
H	5.256985421	-6.530125412	0.728470459

Bimolecular attack on the methyl substituent (product)

O	-0.683402918	-0.300251082	-2.639537060
C	-1.215728459	-1.201206828	0.652060080
H	-1.759691163	-1.856801215	-0.021694363
H	-0.369820406	-0.733847324	0.156359298
H	-1.854598167	-0.489810950	1.168679406
C	-1.846664126	0.211502857	-3.307535687
H	-1.571464179	1.152958309	-3.796748254
H	-2.171981311	-0.491242895	-4.083456640
B	0.015165470	-1.377793700	-3.092308021
Br	-1.126697135	-3.245230625	-2.640359782
Br	1.822747491	-1.471648965	-1.955347514
Br	0.479947788	-1.453207646	-5.093234569
O	1.750389576	-5.022769800	0.281567929
C	1.566405417	-5.203120103	-1.222950779
H	1.474092829	-6.272546620	-1.388058665
H	0.679127104	-4.636443816	-1.514168304
H	2.475403386	-4.799660528	-1.658690023
C	2.725438226	-3.894631589	0.629132172
H	2.476540732	-3.121860625	-0.106466485
H	2.413848311	-3.551955760	1.614806270
B	0.954311222	-5.703994724	1.238887251
Br	1.526897313	-5.728250181	3.067905178
Br	-0.564634417	-6.687149206	0.637640166
Br	-0.457740096	-2.397304476	2.105169441
C	-2.949446889	0.432203917	-2.313462562
H	-3.288847314	-0.458117378	-1.785053387
C	-3.526410400	1.612011616	-2.086283475
H	-3.202675672	2.513275227	-2.603282099
H	-4.348198437	1.724834055	-1.383907339
C	4.138114109	-4.360783430	0.558315321
H	4.840792964	-3.529417567	0.610893310
C	4.582373259	-5.609369721	0.430969176
H	3.919532852	-6.467756131	0.365498225
H	5.645868444	-5.817292850	0.382532255

Bimolecular attack on the bulkier substituent (TS)

O	-0.749576216	-0.526890686	-2.106917567
C	-0.760382091	-1.619206195	0.268092314
H	-1.136132726	-2.450348105	-0.318064804
H	0.232775680	-1.270726834	0.015548084
C	-2.014111990	0.014011542	-2.485105578
H	-2.706492150	-0.779245932	-2.790249490
H	-2.416410901	0.537015147	-1.612880862
H	-1.893213179	0.722731778	-3.309594037
B	-0.033662051	-1.333027288	-2.988724128
Br	-0.973501887	-3.277808148	-3.107768368
Br	1.898703133	-1.605146359	-2.119727884
Br	0.192185498	-0.597865154	-4.887043609
O	1.631117294	-5.090242557	0.450269911
C	1.252848159	-5.424106558	-0.952929507
H	0.871274718	-6.440377785	-0.942938264
H	0.514053940	-4.705807642	-1.305467929
H	2.174062912	-5.356678109	-1.525169724
C	2.897234907	-4.235198388	0.551701102

H	2.716753881	-3.395305911	-0.120974422
H	2.900531109	-3.906366021	1.588325099
B	0.682738152	-5.183331853	1.601519326
Br	1.655764392	-5.790689667	3.251127129
Br	-0.959727214	-6.215828849	1.174822002
Br	0.077573118	-3.071818008	2.077026556
C	-1.670229980	-0.754672030	0.968165066
C	-1.301846831	0.490309385	1.332719597
H	-0.299432905	0.862437057	1.137436913
C	4.089381312	-5.047899857	0.195507851
C	4.870192925	-4.739769772	-0.843723031
H	4.643412517	-3.904843803	-1.503327569
H	-1.997495996	1.173779474	1.810118666
H	-2.677100768	-1.115737218	1.160757705
H	4.327433359	-5.879740444	0.855001960
H	5.773524991	-5.302984024	-1.059259158

d

1d

O	-0.491509917	-0.513380431	-1.243072868
C	-0.725259243	-1.485576847	-0.226701336
H	-1.731625598	-1.376696556	0.192747871
H	-0.629470473	-2.461526693	-0.704970781
H	0.016510244	-1.396544435	0.579796178
C	-0.439722057	0.777983541	-0.800865659
H	0.184684997	0.909198343	0.089875791
H	-0.109330931	1.408998072	-1.623826588
Cl	-2.097394403	1.458187806	-0.298502486

Pre-reaction complex (1d+BBr_3)

O	-0.492732875	-0.512343927	-1.243201175
C	-0.727070738	-1.486712666	-0.225265926
H	-1.733414049	-1.375709995	0.191823836
H	-0.629881169	-2.462542867	-0.702330124
H	0.016104814	-1.394883819	0.578609800
C	-0.441881747	0.783888360	-0.800264459
H	0.186135439	0.906263035	0.088447578
H	-0.109618577	1.412003341	-1.623918923
B	-0.260219333	-1.357018851	-4.254665255
Br	-2.002697824	-2.180782033	-4.237176220
Br	1.307027413	-2.400938883	-3.820445978
Br	-0.065370010	0.483973246	-4.806249444
Cl	-2.095430701	1.456028139	-0.299114145

TS pre-reactional complex→2d

O	-0.260172409	-0.682783108	-1.771712732
C	-0.565538032	-1.732232922	-0.823705627
H	-1.634379982	-1.736743747	-0.602168600
H	-0.265064039	-2.668464705	-1.288910132
H	0.018112997	-1.562583954	0.086387935
C	-0.415689569	0.615229504	-1.272056211
H	0.108139445	0.712460477	-0.319100701
H	-0.032509713	1.303896199	-2.018786933

B	-0.284117650	-1.189029496	-3.786181493
Br	-2.059878652	-2.023476499	-3.926514520
Br	1.285939621	-2.385708008	-3.766686802
Br	-0.042129941	0.569443340	-4.639180889
Cl	-2.147912532	1.070831136	-0.959974000

2d

O	-0.473464781	-0.778345324	-1.964161275
C	-0.816316062	-1.842012339	-1.009868309
H	-1.829542856	-1.664429235	-0.651184841
H	-0.745443824	-2.781885824	-1.547576928
H	-0.085726121	-1.804391902	-0.200255625
C	-0.287051041	0.510752833	-1.371456953
H	0.330809858	0.387746201	-0.482982787
H	0.180069823	1.141776488	-2.118787413
B	-0.342698764	-1.150529530	-3.584309638
Br	-2.047852474	-2.126205394	-4.043406073
Br	1.314963820	-2.312615300	-3.657705691
Br	-0.144716760	0.575416230	-4.602477586
Cl	-1.841200129	1.251533763	-0.877754269

TS 2d→3d

O	-1.090406737	-0.924276756	-2.183918258
C	-1.334681044	-1.906160470	-1.173757106
H	-2.128786240	-2.580243166	-1.510512430
H	-0.431906015	-2.489689344	-0.961826259
H	-1.669227833	-1.373255729	-0.279374675
C	0.302860067	0.889291284	-1.614720359
H	0.758309127	-0.017519777	-1.244910983
H	0.817004471	1.494155206	-2.345686082
B	-0.628530239	-1.312553937	-3.471499336
Br	-1.927263239	-2.510852309	-4.476230050
Br	1.283325776	-2.123758375	-3.390032346
Br	-0.516178850	0.597299673	-4.417866570
Cl	-0.841447836	1.660953883	-0.678288290

3d

O	-0.435519878	-1.534542945	-2.719939672
C	-0.549005905	-1.534431996	-1.283547412
H	-1.538888005	-1.885498350	-0.983603859
H	0.219680472	-2.179676766	-0.851452111
H	-0.399422672	-0.504078592	-0.961128729
C	-0.318029916	1.735083401	-3.720193936
H	0.151804311	2.161776334	-4.601163018
H	-0.215884092	0.655737735	-3.662557025
B	-0.626085300	-2.579635347	-3.518971050
Br	-1.122103744	-4.352048381	-2.852006765
Br	-0.389903950	-2.297439816	-5.435549860
Br	0.712221455	2.461441162	-2.147152332
Cl	-2.036641595	2.168733217	-3.695807079

TS 2d→4d

O	-0.171445816	-0.339902156	-2.225300206
C	0.446343882	-1.939769704	-0.818832147
H	-0.443237926	-1.509719581	-0.381321899
H	0.427577052	-3.001055227	-1.020693313

H	1.403400004	-1.467590265	-0.641578327
C	-0.863258498	0.779784207	-1.754428941
H	-0.187205746	1.382672971	-1.149717848
H	-1.279501454	1.354024797	-2.582029702
B	-0.358790314	-0.880511091	-3.566542291
Br	-2.148217187	-1.785425453	-3.852899790
Br	1.191763577	-2.348276426	-3.466776688
Br	0.072139180	0.501641216	-4.993862975
Cl	-2.254386282	0.342461329	-0.653257981

4d

O	-1.744644333	1.304561333	-3.583496146
C	4.941880774	-5.998606751	-0.014630463
H	5.731651987	-5.365193761	-0.412494834
H	3.960535222	-5.682113989	-0.360909520
H	4.985153976	-6.058636684	1.070623577
C	-1.312669209	2.288445188	-2.674867152
H	-0.353779715	1.961509447	-2.278421267
H	-1.248451096	3.270710572	-3.142629240
B	-2.541991315	1.481142741	-4.647305045
Br	-2.994260741	-0.101872971	-5.675972662
Br	5.250517222	-7.848341866	-0.722476704
Br	-3.214551147	3.230588023	-5.200756629
Cl	-2.448085059	2.425096673	-1.282763316

2d+2d

O	-1.173614783	-1.174890642	-2.217087284
C	-1.228504726	-1.557621653	-0.783048217
H	-1.387679000	-2.634772389	-0.716238084
H	-0.282586895	-1.264387941	-0.342897961
H	-2.049256678	-0.990378518	-0.348551664
C	-2.502157010	-1.097145684	-2.810076233
H	-2.376664172	-1.135888348	-3.886050682
H	-3.100466522	-1.923983583	-2.431316872
B	0.021851783	-1.707353006	-3.157188575
Br	-0.452240509	-3.650236527	-3.588236875
Br	1.747353141	-1.541012427	-2.101236359
Br	0.046677928	-0.516233693	-4.783008657
O	1.742641659	-4.642539253	0.548725951
C	1.695768112	-5.522267506	-0.642735794
H	1.738480804	-6.556456979	-0.303818865
H	0.773246426	-5.297859313	-1.167248580
H	2.559816479	-5.268541261	-1.252587732
C	3.044089462	-4.058085939	0.814112513
H	3.274292855	-3.411235264	-0.030313579
H	2.952857485	-3.505776018	1.742498325
B	0.636371650	-4.737054854	1.729824026
Br	1.325028841	-6.033349188	3.103274848
Br	-1.099608926	-5.342466379	0.873358393
Br	0.459780310	-2.826441424	2.445472651
Cl	-3.277975506	0.441404008	-2.370742184
Cl	4.344196419	-5.270536829	0.977790319

Bimolecular attack on the alkyl (TS)

O	-0.828070209	-0.632796685	-2.012389009

C	-0.733631130	-1.493116574	0.231294143
H	-1.368630650	-2.250175803	-0.211117393
H	0.295683183	-1.367101001	-0.076798314
Cl	-1.474203899	-0.203694918	1.035605352
C	-2.129172072	-0.165044116	-2.386690161
H	-2.791756726	-1.003078586	-2.629538056
H	-2.529777057	0.393929658	-1.537271937
H	-2.048343352	0.499102753	-3.250620414
B	-0.101044301	-1.466120596	-2.883123794
Br	-0.924748572	-3.446092426	-2.803548582
Br	1.880858720	-1.556749878	-2.085749819
Br	-0.006111294	-0.844980589	-4.817345314
O	1.669423410	-4.631198915	0.305011696
C	1.695313976	-5.252412077	-1.028189614
Cl	2.626327990	-6.765025420	-1.016357774
H	0.666753494	-5.440682649	-1.309175891
H	2.163862593	-4.522014908	-1.683071617
C	2.958305671	-3.977375275	0.660561709
H	3.717587220	-4.754461666	0.730261350
H	3.152822150	-3.257930083	-0.132960788
H	2.806567169	-3.480608237	1.612968122
B	0.660812796	-4.990924536	1.425091086
Br	1.597460955	-5.806662846	2.989553030
Br	-0.893371815	-6.012384672	0.747786934
Br	-0.017389546	-3.004301605	2.096077498

Bimolecular attack on methyl (TS)

O	-0.791914748	-1.007276488	-2.114918423
C	-0.614539857	-1.863684895	-0.148151766
H	-0.965462814	-2.788527936	-0.585474938
H	0.415805124	-1.570068492	-0.261624425
H	-1.329748223	-1.146960973	0.232637514
C	-2.135014684	-0.693247932	-2.410268961
H	-2.221504730	-0.314575276	-3.427028349
H	-2.785923861	-1.554643725	-2.249345706
B	0.032037878	-1.637905988	-3.128020772
Br	-0.648755445	-3.619818125	-3.408407891
Br	1.993283965	-1.687927263	-2.367434052
Br	0.032265705	-0.634712230	-4.898514825
O	1.641708899	-4.592580804	0.478802347
C	1.686393147	-5.290820748	-0.848280324
H	1.858351569	-6.347527370	-0.656643579
H	0.742239805	-5.095808439	-1.346849275
H	2.505897746	-4.833836352	-1.396383243
C	2.856893092	-3.845687767	0.812681659
H	2.999544635	-3.126120810	0.008012438
H	2.675275447	-3.372671762	1.772126182
B	0.551728601	-4.856443331	1.553556229
Br	1.360424800	-5.562480316	3.232780064
Br	-0.930563127	-5.938817868	0.798487632
Br	-0.194711958	-2.849266990	2.017188659
Cl	-2.700135545	0.615319896	-1.299979833
Cl	4.277170350	-4.901940053	0.929396058

Bimolecular attack on methyl (product)

O	-0.537771289	-0.350846318	-2.465791803
C	-1.399402623	-1.307269320	0.672701096

H	-1.858892237	-1.961146499	-0.062986500
H	-0.569178392	-0.747596033	0.252864586
H	-2.113783378	-0.676996966	1.193888823
C	-1.769304956	0.119184260	-2.909762247
H	-1.667990406	0.730635593	-3.807972704
H	-2.487172875	-0.689587204	-3.065369938
B	0.084481916	-1.417851255	-3.088309324
Br	-1.037169217	-3.266154755	-2.658494435
Br	1.995242296	-1.607369073	-2.201487225
Br	0.274844670	-1.288074227	-5.123619575
O	1.705221220	-4.943279602	0.287101111
C	1.661279346	-5.230429145	-1.215796425
H	1.610569547	-6.310854752	-1.309062254
H	0.787745334	-4.706357792	-1.608680587
H	2.595910150	-4.830416328	-1.598954179
C	2.587663356	-3.774066741	0.656283543
H	2.444460359	-3.059268081	-0.157545695
H	2.218836159	-3.412569932	1.609672820
B	0.918513082	-5.670474420	1.241417210
Br	1.486194658	-5.692044732	3.065997329
Br	-0.550851114	-6.694046858	0.601205729
Br	-0.621770091	-2.531968702	2.097782690
Cl	-2.482949614	1.196317540	-1.630430209
Cl	4.259814116	-4.304650394	0.762483028

e

1e

O	-1.076520934	-0.844823964	-0.932822395
C	-0.126684281	-1.858684288	-1.169188278
H	0.484141451	-2.064400637	-0.274552581
H	-0.677319960	-2.764412416	-1.437692357
H	0.553482541	-1.596147584	-1.996328851
C	-0.485024114	0.395794331	-0.588038909
H	0.131720172	0.280175792	0.321316845
H	0.188408507	0.729517944	-1.397928022
C	-1.581498026	1.437915808	-0.351733229
H	-1.057183088	2.368023442	-0.084360198
C	-2.486679676	1.041730627	0.824045891
C	-2.394632558	1.694767254	-1.629300184
H	-1.751602855	2.043709669	-2.446631842
H	-2.891761381	0.777668670	-1.961351336
H	-3.162813398	2.457694601	-1.457777495
H	-3.004933735	0.100868894	0.612825415
H	-3.241455725	1.813541686	1.014114584
H	-1.905957474	0.905714103	1.744694149

Pre-reaction complex (1e+BBr_3)

O	-0.771935721	-0.706475283	-1.417517040
C	-0.518477497	-1.828445500	-0.584418933
H	-1.092170180	-1.779508408	0.349481934
H	-0.830194002	-2.715210650	-1.141791408
H	0.550613731	-1.916862489	-0.342490608
C	-0.385852695	0.553772868	-0.854259226
H	0.335215998	0.389951444	-0.040279550
H	0.131724599	1.103058486	-1.650310341
B	-0.303586934	-1.337098714	-4.121770546
Br	-1.980243171	-2.297795521	-4.196343187

Br	1.341254538	-2.294916260	-3.754430340
Br	-0.221549186	0.503781036	-4.710779913
C	-1.577076891	1.385960558	-0.352604104
H	-1.132385962	2.320185459	0.025577847
C	-2.326041352	0.716083936	0.808614742
C	-2.536467675	1.742582479	-1.496770944
H	-2.024992741	2.301089967	-2.288991343
H	-2.958851048	0.836454180	-1.944065767
H	-3.365708657	2.359635731	-1.131870042
H	-2.825484560	-0.200779685	0.475929074
H	-3.098296069	1.384496340	1.206350497
H	-1.651063728	0.459392919	1.634435382

TS pre-reactional complex → 2e

O	-0.639203400	-0.712604106	-1.621546150
C	-0.630355699	-1.811236046	-0.714299898
H	-1.585727169	-1.908562534	-0.187828084
H	-0.454507046	-2.716206121	-1.299228360
H	0.177853100	-1.703688722	0.021361624
C	-0.391400118	0.576990444	-1.044967412
H	0.381894217	0.478487826	-0.268203635
H	0.027463939	1.173624050	-1.860519686
B	-0.306242389	-1.292493133	-3.996828483
Br	-2.002124394	-2.237216395	-4.125421814
Br	1.333328175	-2.314169825	-3.738603510
Br	-0.177847377	0.520049161	-4.691472440
C	-1.625786895	1.305439960	-0.482867084
H	-1.251808632	2.316882008	-0.256525366
C	-2.163990411	0.719044694	0.832102896
C	-2.736078359	1.433954621	-1.534546132
H	-2.376866301	1.938922278	-2.438210418
H	-3.106902765	0.446923516	-1.831324449
H	-3.581184280	2.009024520	-1.139279273
H	-2.681716753	-0.232693474	0.670378383
H	-2.887756484	1.405454561	1.286379016
H	-1.362513398	0.550747707	1.561802719

2e

O	-0.926795699	-0.846477317	-2.061207452
C	-1.303815849	-2.001146653	-1.221945544
H	-2.297474845	-2.312455563	-1.530604405
H	-0.572926257	-2.795906780	-1.375640030
H	-1.302934668	-1.663142535	-0.190950554
C	-0.115451614	0.177206326	-1.318213784
H	0.550345269	-0.386352199	-0.660158712
H	0.477159025	0.661856641	-2.089437983
B	-0.505525685	-1.195090266	-3.559088840
Br	-1.929213838	-2.437183496	-4.299663415
Br	1.335485192	-2.088518132	-3.436917152
Br	-0.443293315	0.536919019	-4.612759618
C	-0.964093693	1.204629826	-0.566634648
H	-0.192829901	1.905599804	-0.207587648
C	-1.697409659	0.676896109	0.678342593
C	-1.916795996	1.985838161	-1.483053800
H	-1.384595281	2.463313922	-2.309969002
H	-2.679271350	1.328345250	-1.914105028
H	-2.429403068	2.765568539	-0.909554328
H	-2.565947952	0.063172036	0.413892307

H	-2.072524365	1.519824840	1.268159767
H	-1.038566497	0.089889951	1.330462960

TS 2e → 3e

O	-1.036198771	-1.258660761	-2.061999430
C	-1.091160775	-2.382609440	-1.179281964
H	-1.429315051	-2.018728682	-0.205282904
H	-1.811428337	-3.113528741	-1.560372199
H	-0.109348098	-2.860287954	-1.086384764
C	0.216780170	0.708371426	-1.364511227
H	0.461031091	-0.191732639	-0.818267338
H	0.944834428	1.022325522	-2.104038131
B	-0.626835867	-1.448253849	-3.407207761
Br	-1.858863432	-2.683011498	-4.472062092
Br	1.363116235	-2.057432891	-3.536521335
Br	-0.765806733	0.534178886	-4.163558275
C	-0.709813227	1.669918761	-0.773731626
H	0.007659880	1.997484476	0.031024480
C	-1.924043568	1.054442437	-0.061734485
C	-1.046987216	2.906472318	-1.609615721
H	-0.162413654	3.312441463	-2.109721370
H	-1.783634335	2.648422817	-2.375428268
H	-1.469591104	3.686310694	-0.968525386
H	-2.597332165	0.622623849	-0.806998445
H	-2.459930182	1.826509705	0.497235884
H	-1.629645316	0.265349094	0.637144062

3e

O	-0.489564053	-3.999832536	-2.772586166
C	0.144126811	-3.520484248	-1.582387305
H	-0.373477449	-3.968464878	-0.731166954
H	1.204643090	-3.779312778	-1.557915089
H	0.023124244	-2.434864723	-1.551195350
C	-0.797856896	4.522127931	-1.383839520
H	-0.522598305	3.473618524	-1.269084959
H	0.073096404	5.109111728	-1.675598418
B	0.056942769	-4.591759765	-3.823167352
Br	-1.129499158	-5.109945385	-5.284016057
Br	1.981748167	-4.971492287	-3.978487827
Br	-1.958656008	4.528871927	-3.061253204
C	-1.489702448	5.081623925	-0.146643946
H	-0.713018875	4.984613065	0.632266278
C	-2.696936547	4.245804908	0.297389963
C	-1.834107231	6.571263740	-0.272039111
H	-0.956148927	7.162638675	-0.557350291
H	-2.609610827	6.733540213	-1.027802322
H	-2.206038930	6.959365730	0.682560487
H	-3.506484781	4.303113776	-0.437596237
H	-3.083519328	4.611289293	1.255105999
H	-2.429348331	3.189927017	0.422776435

TS 2e → 4e

O	-0.805231481	-0.696726492	-2.135889193
C	-0.285975486	-2.627744875	-1.117370173
H	-0.816231960	-2.007687911	-0.411832732

H	-0.871089028	-3.257272687	-1.776128472
H	0.716919587	-2.935041786	-0.859054857
C	-0.214953254	0.437121757	-1.443780788
H	0.581550929	0.049585490	-0.797480198
H	0.242629213	1.095038287	-2.184642100
B	-0.605501034	-0.992602410	-3.509786468
Br	-2.048762154	-2.270144791	-4.158124200
Br	1.309358846	-2.162864298	-3.351207967
Br	-0.313301267	0.556765014	-4.770400756
C	-1.270675750	1.186690559	-0.626824518
H	-0.710444955	1.998024814	-0.136788720
C	-1.893114804	0.314237876	0.472827824
C	-2.349354537	1.816241851	-1.519547566
H	-1.909693411	2.481407144	-2.270046208
H	-2.918319379	1.044700758	-2.049240777
H	-3.053018709	2.401073418	-0.916908197
H	-2.482796353	-0.502489894	0.038169580
H	-2.571919158	0.903888674	1.098256329
H	-1.129172499	-0.115408949	1.134418976

4e

O	-1.084997491	-0.299458307	-2.644219592
C	0.500254867	-3.715365089	-1.876125201
H	0.148220890	-3.372023588	-0.906183662
H	-0.218599768	-3.499488245	-2.662998039
H	0.780995039	-4.765832743	-1.855968067
C	-0.271595637	0.715104881	-2.003524457
H	0.743743402	0.309532529	-1.962975946
H	-0.272258161	1.617712746	-2.621032220
B	-1.445145162	-0.392634197	-3.911797166
Br	-2.526525445	-1.946639880	-4.425974410
Br	2.167797166	-2.677218164	-2.295316447
Br	-0.971218572	0.921678848	-5.290774842
C	-0.809857484	1.000173697	-0.601461106
H	-0.122744679	1.755369206	-0.190594735
C	-0.751605739	-0.242395534	0.298591570
C	-2.219870414	1.606527156	-0.645282683
H	-2.245983894	2.518575128	-1.253559743
H	-2.939847641	0.897049835	-1.068131626
H	-2.560619421	1.866357994	0.362747665
H	-1.409340675	-1.030224620	-0.084918674
H	-1.076930416	0.001368269	1.315843589
H	0.266147878	-0.645900307	0.357749180

2e+2e

O	-1.017068161	-0.580074854	-2.215320639
C	-1.130398753	-1.060708754	-0.823369234
H	-1.502963098	-2.085310326	-0.834935119
H	-0.142352070	-1.006053558	-0.379813113
H	-1.820423953	-0.392588908	-0.314221341
C	-2.359863876	-0.178180851	-2.758861734
H	-2.250316499	-0.217986368	-3.839769963
H	-3.055008727	-0.956876357	-2.435528720
B	-0.010920546	-1.329133521	-3.166874284
Br	-0.809883808	-3.185576911	-3.526750154
Br	1.785703150	-1.441060775	-2.192714313
Br	0.195960045	-0.240732079	-4.861358739
O	1.592381608	-5.246404254	0.724397126

C	0.945850714	-5.333868098	-0.605940647
H	0.810769050	-6.388473245	-0.831954943
H	-0.007580234	-4.812253037	-0.563488166
H	1.605626784	-4.852362892	-1.319886091
C	2.824188804	-4.379926563	0.742318645
H	2.578149309	-3.507141041	0.134002327
H	2.922022282	-4.080878432	1.782488739
B	0.636122814	-5.247267444	1.967933340
Br	1.724937161	-5.599001025	3.640966087
Br	-0.737762902	-6.711256790	1.675794748
Br	-0.236601617	-3.369527348	2.029985994
C	4.083645374	-5.106098336	0.268127243
H	4.861515873	-4.352602593	0.474335730
C	-2.763896314	1.215677247	-2.287738104
H	-2.834989777	1.217296935	-1.191094167
C	4.408445470	-6.354117947	1.101192655
H	3.641032041	-7.125538321	0.975865935
H	5.365427779	-6.777664030	0.778437939
H	4.476350593	-6.126071468	2.168419647
C	4.145774419	-5.404609164	-1.239157081
H	5.160169658	-5.715705087	-1.510119932
H	3.476124613	-6.223812884	-1.523878901
H	3.896906248	-4.525716409	-1.845542574
C	-1.765126207	2.299378473	-2.712961877
H	-0.759349696	2.099089875	-2.331873194
H	-1.699409109	2.367311694	-3.804351493
H	-2.084004905	3.274938947	-2.330741795
C	-4.174521395	1.494729979	-2.840165040
H	-4.173984129	1.508871290	-3.936624621
H	-4.901586698	0.744101901	-2.509358516
H	-4.523489716	2.473217838	-2.495815702

Bimolecular attack on alkyl (TS)

O	-1.076368873	-1.239913465	-1.954873107
C	-0.714551575	-1.669054113	0.245342952
H	-1.352178819	-2.529385270	0.079745183
H	0.292597133	-1.706358240	-0.142851044
C	-2.474974145	-1.301707781	-2.272280373
H	-2.798165727	-2.340421424	-2.391690663
H	-3.021996230	-0.830613677	-1.450509289
H	-2.671340690	-0.749116999	-3.194065118
B	-0.132863635	-1.618232177	-2.957229638
Br	-0.402992498	-3.637344554	-3.510216531
Br	1.804861129	-1.418950510	-2.119788007
Br	-0.244798155	-0.420587060	-4.623757614
O	1.776710458	-4.761830807	0.544655807
C	1.695851542	-5.314108332	-0.872988120
H	0.689953558	-5.080968284	-1.210582123
H	2.397959059	-4.687011714	-1.423886850
C	3.013397713	-4.002382378	0.813207057
H	3.849387900	-4.627476907	0.507007418
H	2.959986936	-3.080495504	0.233394939
H	3.054500998	-3.806871912	1.880376408
B	0.728463137	-4.923350065	1.627303633
Br	1.523325533	-5.927317053	3.187406091
Br	-0.965052256	-5.726869769	0.913733522
Br	0.285141061	-2.924045366	2.323861461
C	-1.250091934	-0.417473124	0.841532825
H	-1.620087926	0.094734424	-0.064336363
C	2.023853601	-6.797692889	-0.948597656

H	1.283282862	-7.337899492	-0.347358518
C	-2.450987909	-0.629568834	1.777875277
H	-3.215619154	-1.265252440	1.318016826
H	-2.139271645	-1.099213831	2.715978222
H	-2.910732773	0.333942726	2.018288840
C	-0.162992020	0.495736949	1.433838952
H	0.246105547	0.075992747	2.358654939
H	0.657870717	0.643877443	0.725145666
H	-0.590789218	1.474927370	1.669950517
C	1.838756973	-7.215162764	-2.421262979
H	2.555473389	-6.703447842	-3.074494573
H	2.002922766	-8.292764206	-2.522261976
H	0.831387037	-6.988863969	-2.785285031
C	3.425638561	-7.156669204	-0.437020239
H	3.542230438	-6.938374194	0.629739116
H	3.605488213	-8.228880552	-0.567847958
H	4.205966948	-6.623831812	-0.996193207

Bimolecular attack on methyl (TS)

O	-0.786380102	-0.827027126	-2.057475602
C	-0.668042447	-1.911764608	-0.149064352
H	-1.012538258	-2.755441293	-0.728531544
H	0.364094866	-1.608025369	-0.202781538
H	-1.397441618	-1.230530231	0.265124911
C	-2.155132528	-0.425891492	-2.314219981
H	-2.256888679	-0.205253676	-3.380175049
H	-2.809604337	-1.275480312	-2.082152404
B	-0.007131115	-1.436531678	-3.077851994
Br	-0.746283327	-3.400160495	-3.474925620
Br	1.970341240	-1.616398307	-2.319211132
Br	0.071871532	-0.378945386	-4.825518121
O	1.569455848	-4.981204058	0.567939034
C	1.100182659	-5.201897682	-0.835178078
H	1.249410477	-6.254885603	-1.062139618
H	0.051578714	-4.931611191	-0.894381311
H	1.690858288	-4.549838558	-1.470655358
C	2.845767139	-4.151503733	0.676919276
H	2.676255797	-3.305460087	0.008075170
H	2.845964754	-3.821412741	1.712195669
B	0.606419664	-5.123863253	1.709030589
Br	1.499162185	-5.367790348	3.476149772
Br	-0.802171047	-6.476088876	1.327102998
Br	-0.392319365	-3.084355981	1.901001831
C	4.116973799	-4.923456591	0.332309229
H	4.885607571	-4.178540088	0.598204831
C	-2.524143765	0.806428430	-1.485952889
H	-2.406362120	0.557314973	-0.419232602
C	4.344570757	-6.163598142	1.208669772
H	3.573924534	-6.922754790	1.033107590
H	5.312864718	-6.613901618	0.967457764
H	4.339336468	-5.920319694	2.274748813
C	4.308325247	-5.241052207	-1.160816593
H	5.344312732	-5.548827542	-1.335433962
H	3.671106754	-6.068863843	-1.489909300
H	4.107351098	-4.373597059	-1.799166620
C	-1.613542501	2.000094652	-1.800662310
H	-0.561325128	1.750281680	-1.637025234
H	-1.722490861	2.307664013	-2.847481966
H	-1.868235583	2.857844343	-1.167711371

C	-4.004875461	1.142065410	-1.723439797
H	-4.184434476	1.401198846	-2.774148478
H	-4.660367929	0.300659106	-1.468221758
H	-4.307973269	2.000361026	-1.114258704

Bimolecular attack on methyl (product)

O	-0.849674155	-0.211715429	-2.546381523
C	-1.487984826	-1.245480602	0.723976842
H	-1.937599991	-1.853295381	-0.056863330
H	-0.602323299	-0.729392503	0.364625805
H	-2.201689340	-0.582647297	1.206500289
C	-2.027841702	0.228548973	-3.228012263
H	-1.784237814	0.438777756	-4.277467412
H	-2.771272699	-0.579124160	-3.207211367
B	-0.048734386	-1.207942941	-3.006998498
Br	-1.120159334	-3.172968323	-2.820170920
Br	1.643319787	-1.290757338	-1.691224519
Br	0.617531726	-1.104064244	-4.943185262
O	1.528238619	-5.037149413	0.540050231
C	0.563280143	-4.664740969	-0.649159487
H	0.535844740	-5.536667452	-1.293171243
H	-0.379815484	-4.425731965	-0.173530765
H	1.031219854	-3.797511058	-1.098135180
C	2.832963018	-4.193094271	0.572866818
H	2.504503679	-3.231811148	0.179106216
H	3.060756561	-4.112762769	1.632289594
B	1.111817081	-5.919503065	1.548568560
Br	1.970958537	-5.930614112	3.267877959
Br	-0.325167815	-7.131825300	1.171408498
Br	-0.873379936	-2.521652196	2.176262827
C	3.946251773	-4.835184242	-0.237686312
H	4.755462576	-4.098870887	-0.095643499
C	-2.570112238	1.483549653	-2.543324802
H	-2.750316376	1.226420871	-1.488696959
C	4.426914453	-6.175776461	0.336660124
H	3.661119477	-6.954894375	0.233249074
H	5.308032765	-6.520926702	-0.212672770
H	4.698769628	-6.100086880	1.394669550
C	3.663484415	-4.922186656	-1.745735646
H	4.579945457	-5.202577064	-2.274082635
H	2.916460755	-5.691582617	-1.972807409
H	3.316560589	-3.969350939	-2.157317885
C	-1.555939190	2.633696867	-2.590255237
H	-0.603104566	2.332417785	-2.145548945
H	-1.363507617	2.939838160	-3.626679828
H	-1.930276631	3.508982484	-2.045977932
C	-3.909088666	1.882001006	-3.180352158
H	-3.781539654	2.128395068	-4.242261249
H	-4.647235084	1.073696106	-3.111390567
H	-4.330846649	2.763771768	-2.684800684

f

1f

O	-0.487772834	-0.475448352	-1.292533167
C	-0.755480318	-1.417829376	-0.261150422
H	-1.771448779	-1.301483093	0.139735686

H	-0.656548346	-2.405912963	-0.714516569
H	-0.032687023	-1.322396736	0.563295419
C	-0.507839655	0.859712795	-0.855167137
H	0.185498913	1.026576070	-0.014429124
H	-0.173021814	1.474053473	-1.696739339
C	-1.854899020	1.316470772	-0.438362479
N	-2.915771235	1.647588791	-0.104230266

Pre-reaction complex (1f+BBr_3)

O	-0.486751125	-0.475527843	-1.292203895
C	-0.755852793	-1.421328588	-0.260265927
H	-1.772568570	-1.303224624	0.135921542
H	-0.654480388	-2.408499383	-0.714080272
H	-0.032575150	-1.321341223	0.561937397
C	-0.508583052	0.863168118	-0.855868724
H	0.185237284	1.024130298	-0.015505460
H	-0.173080149	1.475185805	-1.698287539
B	-0.257551066	-1.352433627	-4.234691491
Br	-2.006898063	-2.161991698	-4.196324349
Br	1.307416656	-2.407869184	-3.826923329
Br	-0.057399215	0.485885165	-4.800704513
C	-1.855753586	1.315484024	-0.439182057
N	-2.915302963	1.648892852	-0.103531036

TS pre-reactional complex→2f

O	-0.204810253	-0.608161991	-1.776702645
C	-0.483175389	-1.627196694	-0.793899937
H	-1.554966896	-1.673482476	-0.579882197
H	-0.140522437	-2.569349752	-1.217922576
H	0.080181697	-1.405101778	0.118709953
C	-0.516642037	0.709161445	-1.327293663
H	0.048997694	0.919993118	-0.410672492
H	-0.184360950	1.395356435	-2.107987334
B	-0.276655063	-1.196448251	-3.828961230
Br	-2.071390687	-1.984976673	-3.890370442
Br	1.268363295	-2.411057113	-3.780647906
Br	-0.013597031	0.546944968	-4.702634211
C	-1.953252742	0.910470661	-1.064206133
N	-3.078988333	1.066952534	-0.832380570

2f

O	-0.457907122	-0.705647820	-2.014160338
C	-0.711302703	-1.739443342	-1.002141102
H	-1.702071118	-1.569108310	-0.579485960
H	-0.662641555	-2.697781527	-1.508960043
H	0.073776647	-1.661157277	-0.247904668
C	-0.386728573	0.637566449	-1.468652437
H	0.378246069	0.639816399	-0.686165360
H	-0.078661790	1.289950527	-2.285135330
B	-0.332056312	-1.140407650	-3.611773083
Br	-2.058808512	-2.093734741	-4.028240699
Br	1.301052838	-2.334831870	-3.654686297
Br	-0.092068336	0.547067645	-4.691936825
C	-1.680481545	1.059218565	-0.924085039
N	-2.691493146	1.394887212	-0.465679458

TS 2f→3f

O	-0.989138345	-0.829408305	-2.196894037
C	-1.141617959	-1.731587846	-1.094621759
H	-1.485967029	-1.140529777	-0.242627802
H	-1.905880427	-2.471834667	-1.352510403
H	-0.199760258	-2.242064277	-0.869555093
C	0.309116631	0.985474256	-1.800174449
H	0.917770900	0.174335637	-1.421100253
H	0.777794544	1.649873275	-2.512492984
B	-0.560540186	-1.298864080	-3.480658685
Br	-1.919284595	-2.535892340	-4.341551275
Br	1.334914382	-2.096646741	-3.443401715
Br	-0.520816165	0.568820853	-4.509712688
C	-0.713787059	1.522189801	-0.999043219
N	-1.528715208	1.988460137	-0.305933882

3f

O	-0.189921115	-1.731794365	-2.241072253
C	-0.334939897	-2.033195984	-0.837368090
H	-1.182323916	-2.706476422	-0.687884242
H	0.578553407	-2.502081610	-0.463722507
H	-0.507953901	-1.081503719	-0.336739120
C	-0.379348487	1.784669095	-3.267331739
H	-0.337529792	0.826729691	-3.786433023
H	0.474961189	2.406107928	-3.534830403
B	0.033947113	-2.608910419	-3.208060411
Br	0.199352777	-1.908000932	-5.030849684
Br	0.210779967	-4.533624434	-2.903080812
Br	-2.005966926	2.743549282	-3.980804313
C	-0.467229933	1.595177142	-1.833411091
N	-0.522751148	1.429506693	-0.685603579

TS 2f→4f

O	-0.803756120	-0.631602964	-2.249797918
C	-3.023732016	-0.432835802	-2.410193150
H	-3.732680555	-1.241902701	-2.505084006
H	-2.794031216	-0.105102625	-1.406493849
H	-2.926886985	0.267205353	-3.231719435
C	-0.059953531	0.373471613	-1.552166388
H	0.950727368	-0.004797306	-1.358182307
H	0.019481268	1.289312345	-2.150718569
B	-0.333779236	-1.068020350	-3.548194709
Br	-1.885096878	-2.438780503	-3.972132766
Br	1.464936282	-1.993274685	-3.448318984
Br	-0.364236559	0.460591810	-4.925169863
C	-0.737007344	0.663819875	-0.282269929
N	-1.303482152	0.903374383	0.701541810

4f

O	-0.363124848	-0.877449306	-2.922638957
C	-3.781198157	-1.020508646	-3.826885355
H	-3.099183598	-0.920169462	-4.667553658
H	-4.818419521	-0.880209783	-4.121580441
H	-3.500666148	-0.367794584	-3.003867602
C	-0.248114523	-1.589950700	-1.685031211

H	-1.012441805	-2.371679207	-1.704405660
H	0.740699934	-2.045974172	-1.580211352
B	0.634798828	-0.452747067	-3.704355018
Br	-3.622230988	-2.911955368	-3.163208783
Br	2.523235356	-0.732570275	-3.286368352
Br	0.130695153	0.472308509	-5.339608970
C	-0.497269098	-0.683665700	-0.556867154
N	-0.696152228	0.025713133	0.338636057

2f+2f

O	-1.205045566	-1.223784900	-2.255598645
C	-1.284600215	-1.392687729	-0.781416723
H	-1.342868598	-2.458184254	-0.552310303
H	-0.390860948	-0.939352089	-0.367967811
H	-2.176129238	-0.855028801	-0.461397484
C	-2.484555869	-1.564844711	-2.897589549
H	-2.293303385	-1.615448369	-3.968914518
H	-2.807073695	-2.543169054	-2.530760707
B	0.136664822	-1.609275497	-3.059533340
Br	0.113695905	-3.662018813	-3.196990886
Br	1.712085639	-0.921948768	-2.001304052
Br	-0.005385650	-0.707831067	-4.856965205
O	1.342942073	-5.040754208	0.270769144
C	1.239782302	-6.365293605	-0.374639873
H	2.051908241	-6.995278078	-0.011685470
H	0.270414262	-6.768963674	-0.100246131
H	1.298212288	-6.189071407	-1.448712962
C	2.577423230	-4.343213363	-0.098337205
H	2.564187886	-4.256829449	-1.187547516
H	2.515415808	-3.349461743	0.340826073
B	0.543764290	-4.803651772	1.667633948
Br	1.183575273	-6.202255678	2.961678530
Br	-1.421838183	-5.017603004	1.150481046
Br	0.919718251	-2.909817049	2.287435443
C	3.774443871	-5.052183650	0.358598031
N	4.741932818	-5.607193902	0.676303101
C	-3.471399559	-0.528821524	-2.599526062
N	-4.273050962	0.273858276	-2.359203369

Bimolecular attack on alkyl (TS)

O	-0.789396464	-0.736722194	-1.905855757
C	-0.607572761	-1.662198793	0.183023542
H	-1.198569304	-2.462227332	-0.248383460
H	0.427828823	-1.554303057	-0.116359119
C	-2.111093745	-0.256135989	-2.215380530
H	-2.778863328	-1.089994233	-2.455104440
H	-2.472861924	0.282343977	-1.338135169
H	-2.054913841	0.427854725	-3.064201548
B	-0.080772586	-1.513916626	-2.859028327
Br	-0.887613015	-3.489800157	-2.898369959
Br	1.931228405	-1.644620879	-2.142757673
Br	-0.051261813	-0.740994629	-4.733675306
O	1.675611002	-4.570518556	0.365407240
C	1.726178273	-5.226336481	-0.969630253
H	0.696271479	-5.380903652	-1.285155552
H	2.185795664	-4.490367838	-1.633160367

C	2.985207704	-3.968775500	0.740216291
H	3.710548750	-4.775610355	0.841273372
H	3.228896042	-3.272388055	-0.060377554
H	2.835090675	-3.448662343	1.680930589
B	0.658963539	-4.942258212	1.473991463
Br	1.562339932	-5.793384604	3.029316656
Br	-0.908414801	-5.911055607	0.756224320
Br	0.005128670	-2.944926303	2.172164647
C	-1.259113021	-0.570802363	0.819829201
N	-1.794272166	0.322502448	1.339043763
C	2.488650959	-6.468790027	-0.896205780
N	3.113368346	-7.444927497	-0.849370456

Bimolecular attack on methyl (TS)

O	-0.758524456	-0.976112486	-2.112181443
C	-0.588930924	-1.816451078	-0.143608737
H	-0.834638549	-2.770519250	-0.588856419
H	0.414061052	-1.430071766	-0.211601889
H	-1.380814373	-1.182290655	0.232312463
C	-2.108353377	-0.639648047	-2.463075577
H	-2.106356190	-0.054935440	-3.388066940
H	-2.702040420	-1.547296475	-2.629687952
B	0.059008747	-1.647262462	-3.105722953
Br	-0.627682697	-3.630470065	-3.323620648
Br	2.020274060	-1.674564710	-2.349227277
Br	0.054749913	-0.696137516	-4.904998726
O	1.572774626	-4.542714348	0.404334464
C	1.696829271	-5.389229817	-0.824256043
H	2.108619669	-6.353081392	-0.527396492
H	0.704540491	-5.465237686	-1.253192968
H	2.354052672	-4.838781229	-1.494349136
C	2.822803923	-3.822341817	0.730886703
H	2.977449103	-3.121807006	-0.094901235
H	2.636223066	-3.275030265	1.653672643
B	0.522159734	-4.806967461	1.529126409
Br	1.402760384	-5.580925385	3.141724300
Br	-1.022479821	-5.832626355	0.821559849
Br	-0.136410532	-2.797363372	2.041632768
C	3.951956087	-4.738500013	0.873815556
N	4.871389404	-5.440806823	0.952411703
C	-2.704905636	0.152063169	-1.381554628
N	-3.180427562	0.752689488	-0.510000428

Bimolecular attack on methyl (product)

O	-0.451474052	-0.929056320	-2.666694158
C	-0.621457284	0.257323764	2.166178930
H	-1.285033425	-0.560976742	1.900121844
H	-0.310632484	0.824681867	1.293389138
H	-1.047139977	0.895650951	2.936413334
C	-1.880887798	-0.944530696	-2.725532770
H	-2.246013692	-0.349069650	-3.568478076
H	-2.236638465	-1.973277260	-2.844143869
B	0.374428238	-1.113747008	-3.701035139
Br	-0.663291499	-4.216610185	-0.914689166
Br	2.280606671	-1.094820887	-3.321107609
Br	-0.263599440	-1.375299112	-5.528013900
O	1.596899520	-5.130877464	0.696084963

C	2.705345721	-5.166351452	-0.279214697
H	2.713286053	-6.162182877	-0.706826224
H	2.536125026	-4.411198346	-1.047055535
H	3.618125216	-4.979028677	0.284429505
C	1.641293341	-3.898539634	1.504053124
H	1.693612104	-3.036005379	0.835038453
H	0.714860711	-3.860466413	2.074298492
B	0.129577611	-5.685173946	0.274328803
Br	-0.890844032	-5.930249610	2.001272287
Br	0.392198301	-7.426926284	-0.698875675
Br	1.043835068	-0.555447325	2.960106129
C	2.792736174	-3.955145435	2.403546021
N	3.713641489	-3.992457932	3.107567773
C	-2.393754571	-0.385243642	-1.468788523
N	-2.801391848	0.061510898	-0.479914875

g

1g

O	-0.531016428	-0.515567818	-1.494535853
C	-0.719751599	-1.505731818	-0.506367611
H	-1.715124949	-1.458389344	-0.039152556
H	-0.616683659	-2.473575058	-1.005271171
H	0.040248116	-1.434705196	0.289492096
C	-0.496899518	0.812161206	-0.993459761
H	0.201512119	0.876793331	-0.141243867
H	-0.079154034	1.414857655	-1.807510164
C	-1.868283003	1.357321269	-0.594529610
H	-2.567194829	1.279919688	-1.434217826
H	-2.294366037	0.815733937	0.256961759
H	-1.786939934	2.412807041	-0.309009105

Pre-reaction complex (1g+BBr_3)

O	-0.517586059	-0.516934914	-1.497235163
C	-0.735268075	-1.502910432	-0.502864883
H	-1.751765897	-1.458251462	-0.088594922
H	-0.595271310	-2.474721394	-0.982119003
H	-0.011076857	-1.402789945	0.320027156
C	-0.495816350	0.820736442	-1.004225257
H	0.219493617	0.889294393	-0.168611024
H	-0.102360254	1.422290323	-1.828914888
B	-0.263529458	-1.320484643	-4.154379375
Br	-2.013691149	-2.146841786	-4.167689325
Br	1.301261661	-2.387991684	-3.758383553
Br	-0.051415554	0.486966995	-4.814874346
C	-1.866462779	1.346741621	-0.584083521
H	-2.578744576	1.264216646	-1.411647935
H	-2.272370490	0.802634067	0.275278853
H	-1.788575250	2.402738661	-0.300432340

TS pre-reactional complex→2g

O	-0.492155978	-0.586067744	-1.645358540
C	-0.771172326	-1.579333465	-0.669275961
H	-1.798995326	-1.507308099	-0.290571806

H	-0.639806032	-2.549956291	-1.151801800
H	-0.070362053	-1.502158080	0.174365288
C	-0.435217386	0.747670829	-1.133901626
H	0.227167846	0.763860622	-0.254655805
H	0.042769122	1.336263097	-1.921471639
B	-0.275962097	-1.285627025	-4.046864213
Br	-2.019693768	-2.142973025	-4.127916436
Br	1.304523400	-2.372572271	-3.734298075
Br	-0.067782322	0.507430618	-4.768574425
C	-1.804232236	1.331468927	-0.796507432
H	-2.458606739	1.307392833	-1.673806677
H	-2.296470317	0.788030608	0.016889071
H	-1.692918317	2.374694154	-0.478861698

2g

O	-0.569090248	-0.741829058	-2.062481958
C	-0.964508493	-1.770134548	-1.097443121
H	-1.998889977	-1.591816842	-0.803834071
H	-0.861673247	-2.735491053	-1.583744384
H	-0.287959121	-1.703476294	-0.244477434
C	-0.133728142	0.537930243	-1.449140946
H	0.471963685	0.257460711	-0.584411331
H	0.501042115	1.012250575	-2.192230689
B	-0.357042066	-1.149372519	-3.582140682
Br	-2.031880423	-2.175251867	-4.123605977
Br	1.327257242	-2.298838213	-3.609051799
Br	-0.161050513	0.541698734	-4.685731881
C	-1.329973903	1.392366589	-1.085204988
H	-1.917722890	1.631991832	-1.975137755
H	-1.976789080	0.908000626	-0.347048064
H	-0.967645769	2.330047826	-0.648501079

TS 2g→3g

O	-0.889781685	-0.829322696	-2.176285518
C	-1.099365946	-1.762541470	-1.115209018
H	-1.369400294	-1.188218528	-0.223330117
H	-1.927164954	-2.430073600	-1.374800357
H	-0.199187020	-2.357767529	-0.927020135
C	0.528261645	0.991924581	-1.759906203
H	0.895692421	0.129835819	-1.220147230
H	1.210221382	1.395154120	-2.496775448
B	-0.537513466	-1.289932604	-3.474353626
Br	-1.992498443	-2.402322272	-4.363765340
Br	1.299496308	-2.247506461	-3.499071917
Br	-0.332766066	0.591908846	-4.473487474
C	-0.502165241	1.855560395	-1.174043660
H	-0.931652796	2.552480310	-1.894906436
H	-1.286599657	1.297029529	-0.661361733
H	0.034699285	2.452939751	-0.408934457

3g

O	-0.208881007	-1.442275976	-2.551472437
C	1.018173738	-0.843952173	-2.097803456
H	1.589204691	-1.557507521	-1.498955308
H	1.610551774	-0.518862322	-2.955810230
H	0.738924409	0.020681946	-1.496339506
C	-1.900270274	2.629255571	-3.530605611
H	-2.024384436	2.758007015	-2.455930139
H	-2.273729942	3.505544647	-4.058777262
B	-0.324337632	-2.582204595	-3.218602399
Br	-2.120389232	-3.157388264	-3.726976411
Br	1.216834808	-3.695438382	-3.704623355
Br	0.116057729	2.722895761	-3.807453906
C	-2.468582373	1.325957530	-4.046428214
H	-2.298187829	1.210757532	-5.120528685
H	-2.039185027	0.464228484	-3.528619657
H	-3.552926552	1.324947955	-3.870044366

TS 2g→4g

O	-0.839451576	-0.510456166	-2.281075054
C	-0.522952244	-2.441534971	-1.155289108
H	-1.528954630	-2.091661522	-0.987431889
H	-0.407101562	-3.408310354	-1.622620508
H	0.270004342	-2.086775418	-0.510192917
C	-0.132831434	0.577588140	-1.642948469
H	0.913280034	0.281597539	-1.496269329
H	-0.146601456	1.426291112	-2.331519464
B	-0.592595158	-0.914513949	-3.618546751
Br	-2.058631680	-2.173890525	-4.229564756
Br	1.260434457	-2.169169734	-3.282212876
Br	-0.164449839	0.534123128	-4.950978518
C	-0.823220586	0.931037703	-0.336495558
H	-1.870494319	1.194444066	-0.513133946
H	-0.789706188	0.110156635	0.388046947
H	-0.322612126	1.793478415	0.116443353

4g

O	-0.210043107	-0.596359735	-3.488421986
C	0.639074598	-3.942685490	-2.506680023
H	0.132341564	-3.047410000	-2.858767110
H	0.938980941	-4.591439844	-3.326397317
H	0.054721319	-4.477854633	-1.761757863
C	0.860481803	0.259306257	-3.008781159
H	1.744499753	-0.381008340	-2.987018649
H	1.019191767	1.068856940	-3.725828112
B	-1.216379724	-0.276224241	-4.287227230
Br	-2.502066543	-1.684946058	-4.727208271
Br	2.327375728	-3.338315109	-1.595956278
Br	-1.478245823	1.516532644	-5.045394352
C	0.527491082	0.786008682	-1.624269522
H	-0.356214266	1.431652336	-1.649205618
H	0.344995758	-0.039860559	-0.930213981
H	1.371800253	1.372959637	-1.246375290

2g+2g

O	-1.049746189	-0.577749797	-2.314900351
C	-1.147154061	-0.937980576	-0.888709001

H	-1.503620111	-1.965700913	-0.808299035
H	-0.157441852	-0.829823395	-0.458164624
H	-1.843322817	-0.234011021	-0.436336846
C	-2.394109202	-0.232912897	-2.887800855
H	-2.351093016	-0.525909980	-3.933028370
H	-3.111170599	-0.870452059	-2.366998847
B	-0.020259222	-1.325910908	-3.232572802
Br	-0.787874175	-3.202776721	-3.560346964
Br	1.768258381	-1.391101197	-2.250800327
Br	0.152031207	-0.244720842	-4.938383199
O	1.521605433	-5.288248078	0.636017032
C	0.898444832	-5.479188242	-0.686605047
H	0.476144797	-6.479150526	-0.702595516
H	0.132936176	-4.716491439	-0.828787471
H	1.690119111	-5.378974404	-1.425784456
C	2.712749474	-4.375194944	0.577770672
H	2.466159668	-3.608118543	-0.158424080
H	2.775031309	-3.923339928	1.563672706
B	0.613708811	-5.247903242	1.910113660
Br	1.825676664	-5.588725554	3.504260906
Br	-0.799106292	-6.687881661	1.737970254
Br	-0.225608802	-3.358853845	1.969598237
C	3.948022122	-5.179216580	0.238856610
H	4.135685518	-5.937738878	1.003063679
H	3.874410954	-5.666488601	-0.738480494
H	4.805023875	-4.496931598	0.206688142
C	-2.651394051	1.247408780	-2.715925754
H	-2.654052611	1.551455190	-1.664466858
H	-1.901515741	1.832134200	-3.254423858
H	-3.637917373	1.477827447	-3.133892674

Bimolecular attack on alkyl (TS)

O	-0.9356388855	-0.9307111993	-1.9340833422
C	-0.6353681872	-1.6478263649	0.2312229055
H	-1.4383464883	-2.3276959413	-0.0206565854
H	0.3385873346	-1.8546647683	-0.1878834719
C	-2.3281907307	-0.7184948139	-2.2081785161
H	-2.8313746736	-1.6673898221	-2.4210967154
H	-2.7689478052	-0.2521007831	-1.3225355423
H	-2.4394294733	-0.0471758152	-3.0627876869
B	-0.1219489463	-1.5317067021	-2.9329384240
Br	-0.6910134519	-3.5543378373	-3.2078330515
Br	1.8729959488	-1.4982480519	-2.1958189084
Br	-0.1700666402	-0.5456686681	-4.7270496275
O	1.5945921265	-4.6086635234	0.4198357041
C	1.6434854859	-5.3225305391	-0.9231432164
H	0.6049494662	-5.3878615742	-1.2300120126
H	2.1482499959	-4.6007892513	-1.5644508488
C	2.8606517227	-3.9198861755	0.7420333240
H	3.6400071124	-4.6680161125	0.8803984141
H	3.0621650358	-3.2520131681	-0.0944536327
H	2.6996010459	-3.3571733414	1.6568662149
B	0.6304798840	-4.9582030037	1.5412904047
Br	1.5985233477	-5.8337895739	3.0733061821
Br	-0.9581885216	-5.9714480556	0.8874365596
Br	-0.0543564471	-3.0082119422	2.2570004104
C	-0.8940776656	-0.3380899611	0.8847135880
H	-1.8130668417	-0.3329052906	1.4742752019
H	-0.0478209895	-0.0244878525	1.5014525543
H	-0.9826844513	0.4001376385	0.0771911036

C	2.3384287951	-6.6596656211	-0.8263341534
H	1.8083658849	-7.3462788355	-0.1618016723
H	2.3409354809	-7.0954059009	-1.8323208669
H	3.3795454134	-6.5741421026	-0.5013097670

Bimolecular attack on methyl (TS)

O	-0.819364849	-0.911725952	-1.961929709
C	-0.602885162	-1.910083441	-0.011222826
H	-0.948334173	-2.788540808	-0.538374631
H	0.415857894	-1.580059964	-0.129432349
H	-1.334722623	-1.223573855	0.390121696
C	-2.201904986	-0.530730059	-2.170540988
H	-2.398692932	-0.489718267	-3.243343750
H	-2.838952650	-1.314165848	-1.742808671
B	-0.072702983	-1.525429473	-3.000085259
Br	-0.797483570	-3.506356058	-3.329397087
Br	1.937679325	-1.657369278	-2.323582969
Br	-0.092623568	-0.491101950	-4.765141554
O	1.652886041	-4.729051462	0.494404788
C	1.542769728	-5.237200371	-0.903795959
H	1.704923643	-6.312979910	-0.878548098
H	0.560735534	-4.975778691	-1.287015783
H	2.306225947	-4.714519426	-1.473520050
C	2.901714149	-3.925197515	0.773176080
H	2.886039900	-3.144207004	0.011035976
H	2.728898708	-3.489912704	1.754383098
B	0.637469270	-5.004086900	1.566370724
Br	1.501998513	-5.610718075	3.270050678
Br	-0.844051741	-6.160646412	0.929171863
Br	-0.210966476	-2.982045101	2.054779943
C	4.137179524	-4.795022783	0.732120071
H	4.098186096	-5.581464234	1.489231116
H	4.298834108	-5.243422935	-0.252140317
H	4.999154652	-4.152600891	0.946037062
C	-2.453050262	0.822149835	-1.526630346
H	-2.248855753	0.807995413	-0.449484423
H	-1.817150239	1.585473447	-1.984334250
H	-3.500968874	1.110327086	-1.667037362

Bimolecular attack on methyl (product)

O	-1.171066159	-1.758843655	-3.555958146
C	0.517113611	-0.105242140	1.513014648
H	-0.052057159	-0.980894191	1.208731324
H	0.741379799	0.544867118	0.671054574
H	0.038620141	0.430928350	2.329047935
C	-1.279462532	-3.129193271	-4.028328176
H	-0.703760607	-3.215102510	-4.954884341
H	-0.836178529	-3.784699534	-3.274829198
B	-0.066924235	-1.102134072	-3.263561501
Br	-1.085915534	-3.777120925	0.022960461
Br	-0.234857335	0.742801299	-2.620503327
Br	1.736154932	-1.872970973	-3.452697026
O	1.299026605	-5.251586053	0.844449715
C	2.339932689	-4.583630876	0.045034834
H	2.490331207	-5.180437024	-0.848910841
H	2.005943246	-3.573781176	-0.198376673

H	3.239481483	-4.567886890	0.657668480
C	1.331315151	-4.796381737	2.278692890
H	1.647201510	-3.752011264	2.252834672
H	0.302888582	-4.853919880	2.623993219
B	-0.087819642	-5.571896462	0.190581550
Br	-1.044865254	-6.870091558	1.423739752
Br	0.247808031	-6.425156159	-1.624515062
Br	2.282854567	-0.767620273	2.219774947
C	2.253148554	-5.696605331	3.070151452
H	1.893025988	-6.728265319	3.055100791
H	3.282217168	-5.670964871	2.697813769
H	2.266294282	-5.346974812	4.108754532
C	-2.747198121	-3.439387605	-4.243769525
H	-3.304038113	-3.339325027	-3.307498184
H	-3.185764233	-2.767136423	-4.987917838
H	-2.852697041	-4.469916825	-4.599159670

h

1h

O	-0.416540023	-0.438475729	-1.025265642
C	-0.924342175	-1.589829230	-0.383733480
H	-2.004138358	-1.526444191	-0.184193362
H	-0.753790394	-2.420681230	-1.074622115
H	-0.409059628	-1.817047468	0.561111841
C	-0.490237337	0.816904242	-0.319876836
C	-1.946914970	1.187655303	0.004687282
H	-2.558411123	1.157394699	-0.903731107
H	-2.389964700	0.509245939	0.741808663
H	-1.998502243	2.200175129	0.420192142
C	0.098172757	1.817407430	-1.320906910
H	1.125273661	1.536952122	-1.576180830
H	-0.492787423	1.821497592	-2.242558670
H	0.105260846	2.830679831	-0.904925186
C	0.365006775	0.779881670	0.957831676
H	-0.046567465	0.096891742	1.708902094
H	1.385104360	0.458452588	0.721391370
H	0.414535810	1.775071582	1.413563079

Pre-reaction complex (1h+BBr_3)

O	-0.419833404	-0.440917707	-1.031088376
C	-0.926279574	-1.589068045	-0.375987944
H	-2.016581797	-1.552351904	-0.240733096
H	-0.687741005	-2.438967083	-1.020919617
H	-0.458204097	-1.761209870	0.602855448
C	-0.490435470	0.817902426	-0.323178529
B	-0.237223439	-1.346495136	-4.374225557
Br	-2.010929448	-2.086489996	-4.188166173
Br	1.299060523	-2.356318151	-3.796060426
Br	0.000099549	0.370898215	-5.223238852
C	-1.946758676	1.184675420	0.004531732
H	-2.559825081	1.161814183	-0.902949520
H	-2.387784221	0.499476098	0.736468616
H	-1.998150851	2.193531097	0.428820128
C	0.099106776	1.824854635	-1.315910866
H	1.128706089	1.551177752	-1.568490659
H	-0.487090537	1.839000809	-2.239913655

H	0.101309615	2.833769365	-0.889701983
C	0.368305220	0.775056124	0.952157569
H	-0.050572599	0.108746843	1.713605433
H	1.382003994	0.435075062	0.714589793
H	0.436323382	1.774198748	1.396551630

TS pre-reactional complex →2h

O	-0.170656765	-0.665501991	-1.702010465
C	-0.588464486	-1.811542114	-0.940425525
H	-1.663553023	-1.792262953	-0.733621629
H	-0.355029228	-2.691732506	-1.535491999
H	-0.026592248	-1.868070951	-0.006463573
C	-0.430685001	0.661730006	-1.065467449
B	-0.268777017	-1.178020673	-3.808217024
Br	-2.043024721	-2.048391431	-3.877573088
Br	1.327864814	-2.332507729	-3.786658646
Br	-0.116704072	0.489254097	-4.847854400
C	-1.811306444	1.156631462	-1.506687067
H	-1.862326163	1.290492261	-2.589063029
H	-2.594891838	0.451788165	-1.208518717
H	-2.029578113	2.120253195	-1.032951130
C	0.707132163	1.576532044	-1.526705934
H	1.672089925	1.163043523	-1.216447486
H	0.719793528	1.707526568	-2.607410684
H	0.590318805	2.563422954	-1.065817462
C	-0.369408574	0.558607446	0.467414877
H	-1.181087491	-0.039279794	0.890951998
H	0.589015031	0.153506508	0.807507382
H	-0.463992321	1.570106529	0.874920973

2h

O	-0.223181939	-0.727521485	-1.938349513
C	-0.430987571	-1.904729888	-1.081092836
H	-1.467980677	-1.936150878	-0.749286271
H	-0.203247644	-2.779667743	-1.679071555
H	0.264895457	-1.843768620	-0.248482590
C	-0.456943897	0.674131537	-1.245959904
B	-0.270116496	-1.088582850	-3.493988920
Br	-2.063165601	-2.039672476	-3.814815132
Br	1.343596606	-2.322347957	-3.791000143
Br	-0.117610410	0.500180120	-4.754889374
C	-1.793448917	1.213573124	-1.742381033
H	-1.796418831	1.395838802	-2.815804644
H	-2.607511021	0.524651224	-1.498281684
H	-1.989144261	2.163801318	-1.232705565
C	0.761821078	1.523367972	-1.593154852
H	1.679344984	1.027139863	-1.262766270
H	0.840310456	1.735626744	-2.656444810
H	0.676489352	2.475401965	-1.057319988
C	-0.504281121	0.477761094	0.272359682
H	-1.343678075	-0.135937147	0.605649736
H	0.429248215	0.080015156	0.678682208
H	-0.643953220	1.474808333	0.701757734

TS 2h→3h

O	0.288175765	-0.623963785	-2.147749202
C	0.724866652	-1.538196475	-1.135758216
H	-0.035193147	-2.301364590	-0.934276810
H	1.648616691	-2.025789456	-1.450983262
H	0.924379360	-0.963261563	-0.227543420
C	-1.115248866	1.060816023	-1.117517689
B	-0.038567345	-1.142961170	-3.443004235
Br	-2.027690109	-1.878545036	-3.411478165
Br	1.214793310	-2.631809113	-4.104403183
Br	0.095991331	0.464185534	-4.793694537
C	-1.923480113	1.563112545	-2.229374081
H	-1.412972873	1.295450124	-3.180398088
H	-2.936625655	1.162361869	-2.255669006
H	-1.918526840	2.661441118	-2.229816724
C	0.123860426	1.796564469	-0.768485071
H	0.811827088	1.209428328	-0.159398625
H	0.628448350	2.176228306	-1.660297232
H	-0.193108102	2.665630088	-0.166488968
C	-1.738157144	0.110262924	-0.170902342
H	-2.206879968	-0.713406822	-0.724019946
H	-1.062320493	-0.265265381	0.596810424
H	-2.560762551	0.657212920	0.319455352

3h

O	0.319356043	-4.381319591	-1.650556889
C	0.426725568	-5.470291292	-0.722853927
H	0.827803410	-5.053391808	0.201818737
H	-0.558100405	-5.907695265	-0.538980021
H	1.101300983	-6.238231125	-1.109870025
C	-0.555658972	3.909509512	-2.369956322
B	-0.070733963	-4.464859456	-2.915071476
Br	-0.132268153	-2.816328414	-3.957104976
Br	-0.583493829	-6.161719460	-3.759008585
Br	-0.363894730	5.045774146	-4.117712378
C	-1.900305576	3.201627170	-2.470357540
H	-2.726893429	3.914520418	-2.532229221
H	-1.941616784	2.540626650	-3.340208759
H	-2.042436558	2.588965198	-1.568769857
C	-0.499090935	4.900619852	-1.214803048
H	0.452719446	5.438342290	-1.193546192
H	-1.311491062	5.630342018	-1.270213291
H	-0.599948118	4.345701389	-0.271248954
C	0.617607691	2.938361183	-2.365703543
H	0.558845047	2.319548097	-1.459048057
H	0.592080210	2.272533362	-3.232398605
H	1.575311994	3.465826014	-2.356751025

TS 2h→4h

O	-0.103725436	-0.567782641	-2.088955910
C	0.212015882	-2.565059949	-1.144313578
H	-0.664278890	-2.166425830	-0.664660828
H	0.092970762	-3.505444701	-1.661537251
H	1.185775870	-2.313364035	-0.748040861
C	-0.543976174	0.641496760	-1.337550788
B	-0.329776843	-0.914990097	-3.450430719
Br	-2.096207274	-1.952124154	-3.739596382

Br	1.301151931	-2.339405569	-3.677440852
Br	-0.081310696	0.526754646	-4.867991504
C	-1.917368777	1.132199315	-1.802906705
H	-1.906126905	1.447065050	-2.847541124
H	-2.677984055	0.356298970	-1.682285766
H	-2.204558861	1.995306338	-1.191533058
C	0.550528469	1.698874840	-1.523460996
H	1.520275735	1.306029805	-1.201557223
H	0.630760200	2.008655206	-2.566055284
H	0.313866694	2.579395790	-0.915273336
C	-0.616569711	0.234889261	0.139990087
H	-1.425499507	-0.478608757	0.332019613
H	0.331677029	-0.183867072	0.492413441
H	-0.825668589	1.126523013	0.738797097

4h

O	-0.634828762	-0.041517243	-2.669434845
C	2.724620420	-1.685509034	-3.998316124
H	3.655626166	-1.125072722	-4.042932558
H	2.541074033	-2.238768755	-4.916289087
H	1.880739249	-1.052153312	-3.735588313
C	-0.814714209	-0.237452429	-1.212116465
B	-1.408281113	-0.094388691	-3.733504050
Br	-3.318561220	-0.576076356	-3.776272896
Br	2.928145365	-3.041096841	-2.528384972
Br	-0.569595161	0.346877692	-5.461832789
C	-1.858927396	0.756825815	-0.701307226
H	-1.570798566	1.782487904	-0.954026876
H	-2.849992684	0.557118912	-1.114661808
H	-1.924245471	0.680926728	0.389318591
C	0.565293498	0.075180975	-0.630733631
H	1.316065367	-0.623207365	-1.012341858
H	0.868949426	1.094926634	-0.887388210
H	0.537052330	-0.013815252	0.460105646
C	-1.204398442	-1.693390619	-0.954205929
H	-2.185517046	-1.930195074	-1.372970288
H	-0.459956599	-2.371571602	-1.383016664
H	-1.243529789	-1.870846581	0.125878698

2h+2h

O	-0.127231512	-1.319698605	-2.469422448
C	0.990759580	-1.907817533	-1.708269739
H	0.880806118	-2.990507031	-1.680911928
H	1.905061100	-1.633110935	-2.221531583
H	0.985595205	-1.472898579	-0.713154565
C	-1.571474751	-1.568620582	-1.856668351
B	0.269965997	-0.966256677	-3.956416894
Br	1.048129611	-2.678317184	-4.796477050
Br	1.674077645	0.529944976	-3.789712306
Br	-1.252474820	-0.294932334	-5.134893194
O	1.126188750	-6.452245051	3.379816000
C	1.850865553	-7.500910296	2.641943109
H	1.146943063	-8.053151559	2.020934642
H	2.610508003	-7.016650468	2.035581161
H	2.318544235	-8.157890943	3.365582773
C	0.955729371	-6.789490848	4.936910298
B	0.277889867	-5.443926237	2.523113692

Br	0.888833232	-5.510828732	0.551221601
Br	-1.695610421	-6.003922648	2.601982734
Br	0.616996422	-3.548799288	3.201184359
C	0.248999825	-8.140096722	5.019743773
H	-0.742384317	-8.088655274	4.564268981
H	0.811450394	-8.956340776	4.561063539
H	0.127925734	-8.388373162	6.079435704
C	-2.276695169	-0.216206310	-1.877228160
H	-1.682307829	0.531825164	-1.344260616
H	-2.479524527	0.143964352	-2.882424120
H	-3.232294181	-0.328662699	-1.352845080
C	2.378203103	-6.782815024	5.493836402
H	2.311172619	-6.869347936	6.583469656
H	2.998344004	-7.611956859	5.144721268
H	2.876217517	-5.838008697	5.260078936
C	0.132559919	-5.713120086	5.635344105
H	0.657704529	-4.761638661	5.696773691
H	-0.844290837	-5.562291814	5.178335998
H	-0.030370642	-6.079222931	6.655449843
C	-2.229705394	-2.662759452	-2.687750067
H	-2.371757408	-2.366398364	-3.726245760
H	-1.640800824	-3.584125620	-2.658585366
H	-3.212843475	-2.876123674	-2.253149496
C	-1.416727133	-2.022696971	-0.404042269
H	-2.432804427	-2.168180324	-0.023303867
H	-0.895809912	-2.974578929	-0.290695206
H	-0.943414972	-1.266111602	0.227246529

Bimolecular attack on methyl (TS)

O	-0.967854528	-0.945044347	-1.874647648
C	-0.468313563	-2.036296935	0.029051407
H	-1.145356099	-2.810973138	-0.301787030
H	0.515941538	-1.981535890	-0.407270546
H	-0.865187789	-1.147741944	0.499407977
C	-2.282289299	-0.276928561	-2.002994505
B	-0.131770546	-1.460958322	-2.910441414
Br	-0.483725764	-3.540834363	-3.129166429
Br	1.885937151	-1.186300772	-2.272856229
Br	-0.227017741	-0.613987816	-4.803997759
O	1.426953857	-5.627607851	2.824022432
C	2.771154783	-6.210350961	2.610890764
H	2.696184422	-7.004773637	1.872368451
H	3.431396485	-5.417463433	2.268531535
H	3.112735253	-6.606835291	3.558669611
C	0.847397240	-5.882010429	4.319484760
B	0.676626538	-5.172698571	1.560260603
Br	1.820627232	-5.145645782	-0.069343068
Br	-1.028068964	-6.204160860	1.259396583
Br	0.215513755	-3.052050874	1.999164394
C	0.638488775	-7.386152446	4.421645299
H	-0.128795906	-7.725786176	3.722892107
H	1.555905604	-7.955187496	4.250875892
H	0.301634807	-7.610971875	5.439701010
C	-2.056513936	1.174565068	-2.451983018
H	-1.332164733	1.662140675	-1.791150822
H	-1.683693939	1.231540480	-3.473803258
H	-3.002963451	1.725391794	-2.395953877
C	1.908539748	-5.322554532	5.266680488
H	1.454477990	-5.255791759	6.260738277
H	2.797999520	-5.947896647	5.367241239

H	2.205096206	-4.312548716	4.970100086
C	-0.450839793	-5.111329084	4.512951313
H	-0.291290865	-4.033441801	4.548003193
H	-1.208775622	-5.348508535	3.769591376
H	-0.837357838	-5.423471489	5.489712060
C	-3.215442196	-1.048673890	-2.944224980
H	-2.832264397	-1.076497281	-3.964515914
H	-3.350218221	-2.078339686	-2.599880313
H	-4.195043138	-0.556343590	-2.959119047
C	-2.913223047	-0.248749258	-0.602925828
H	-3.881173903	0.258799284	-0.662287749
H	-3.094993467	-1.255620640	-0.213334353
H	-2.296293605	0.313940350	0.107543551

Bimolecular attack on methyl (product)

O	-0.159608229	0.731477905	-3.366567346
C	-1.096381080	-0.215965576	0.668006124
H	-1.132757224	-1.193391777	0.192023197
H	-0.338044054	0.424355232	0.223293406
H	-2.071199083	0.265503005	0.693531892
C	-1.121980779	0.177678534	-4.342013274
B	1.045049654	1.255332278	-3.412838939
Br	-0.717125015	-3.867706806	-1.485680913
Br	1.823354261	1.846395527	-1.699905380
Br	2.154402166	1.515667616	-5.021933713
O	-0.840338167	-7.863828489	0.953486973
C	-1.989526395	-7.533843369	0.148035728
H	-2.077493956	-8.235471912	-0.684772091
H	-2.894845813	-7.572019846	0.758609266
H	-1.829651796	-6.523179184	-0.227124911
C	1.854627029	-4.456712916	1.175315978
B	-0.627376960	-9.022281963	1.566885480
Br	-1.883631378	-10.524312258	1.471145619
Br	1.015536564	-9.210628216	2.603532303
Br	-0.557328852	-0.522781992	2.582796906
C	1.846097769	-5.281311832	0.102136530
H	1.308866632	-6.226611269	0.128054622
H	0.480810786	-4.406446592	-0.635472193
H	2.513978012	-5.115875538	-0.740503719
C	-1.515018431	1.281260868	-5.325875987
H	-1.897590364	2.155415985	-4.788743498
H	-0.671170947	1.591390435	-5.946726069
H	-2.307774777	0.913920327	-5.986300330
C	2.677851638	-3.199306552	1.207039046
H	3.385580817	-3.234250788	2.046134551
H	3.245512285	-3.051783787	0.284096084
H	2.041706823	-2.321011975	1.376828354
C	1.002607334	-4.729122417	2.384005094
H	0.324178967	-3.887128696	2.575174294
H	0.416003788	-5.644596312	2.273967374
H	1.634572209	-4.827489692	3.276717570
C	-0.495269845	-1.035840765	-5.030043068
H	0.363660257	-0.754537170	-5.643791083
H	-0.178324169	-1.776285545	-4.288803124
H	-1.240046030	-1.504945799	-5.681919700
C	-2.313279897	-0.237716722	-3.476525753
H	-3.100069095	-0.667872894	-4.104660931
H	-2.008714465	-0.987189374	-2.739761728
H	-2.725694635	0.627790637	-2.948205803

i

1i

O	-8.104347311	1.041720931	-11.100420850
C	-7.946710057	-0.334436599	-11.402076235
H	-8.499624738	-0.970335728	-10.697632925
H	-8.272713846	-0.564875712	-12.425301618
H	-6.878559499	-0.540640681	-11.310660197
C	-9.363657223	1.572013515	-11.142345978
C	-9.455332277	2.938675161	-10.838398501
C	-10.519894154	0.850566004	-11.461555004
C	-10.692218384	3.572861153	-10.852697853
C	-11.756894424	1.503875227	-11.472560084
C	-11.853829288	2.859869567	-11.170471977
H	-8.544261492	3.476370635	-10.594513454
H	-10.470887093	-0.205812194	-11.700243023
H	-10.750486987	4.631736729	-10.614327958
H	-12.649911798	0.936470209	-11.722078939
H	-12.818787112	3.358152588	-11.182635795

Pre-reactional complex (1i + BBr_3)

B	-6.350810041	1.201267032	-14.208512049
O	-10.022863865	1.250980875	-10.313799366
C	-8.953589481	0.746321264	-9.529420423
H	-9.003586277	1.114554527	-8.496055759
H	-8.941965270	-0.351609381	-9.519895500
H	-8.040191419	1.111366806	-10.001358374
C	-11.301984181	0.943980268	-9.938545860
C	-12.316521296	1.498350403	-10.732740952
C	-11.635959498	0.137672192	-8.844267618
C	-13.650300375	1.243576130	-10.434987774
C	-12.982819278	-0.109487492	-8.558333771
C	-13.994257253	0.436913177	-9.344425662
H	-12.032215997	2.123676384	-11.573409416
H	-10.867178368	-0.298471151	-8.216744789
H	-14.427538154	1.678305634	-11.058076325
H	-13.233945539	-0.737105890	-7.707048263
H	-15.037049041	0.238885532	-9.114434154
Br	-4.812697002	0.798304930	-13.109371350
Br	-8.089377094	1.380364589	-13.401770526
Br	-6.132373961	1.420614697	-16.113441999

TS pre-reactional complex →2i

B	-7.2161394387	0.8112823329	-13.4407249401
O	-8.2777465888	0.9389408275	-11.3673087367
C	-8.0654212048	-0.1726476495	-10.4799636994
H	-8.1780831548	0.1612348501	-9.4434100512
H	-8.7671289459	-0.9870507964	-10.6861243129
H	-7.0441245073	-0.5145379855	-10.6499753129
C	-9.5164274731	1.5663268848	-11.2198244198
C	-9.5295050795	2.8781286904	-10.7485635935
C	-10.6999229085	0.9106429821	-11.5621707924
C	-10.7493729944	3.5427056511	-10.6141774099

C	-11.9140507404	1.5834744178	-11.4192241956
C	-11.9422654812	2.8969129024	-10.9450899882
H	-8.5893813841	3.3602974381	-10.5004493012
H	-10.6681933026	-0.1037212779	-11.9471432346
H	-10.7652531384	4.5660842662	-10.2499425433
H	-12.8390570827	1.0805930068	-11.6872031647
H	-12.8903450627	3.4161685170	-10.8384899812
Br	-5.4034843910	0.9326426464	-12.7182467101
Br	-7.8920776366	-0.9511152964	-13.9677435754
Br	-8.0113965599	2.3941966238	-14.2397490694

2i

B	-7.4239752606	0.8436117357	-13.0977566068
O	-8.1499956598	0.9319805982	-11.6577342220
C	-7.8857541429	-0.1196935537	-10.6584928793
H	-8.0229356646	0.3421730784	-9.6816449439
H	-8.5817370972	-0.9426582178	-10.8190665020
H	-6.8558958435	-0.4340214554	-10.8045560710
C	-9.4205689558	1.5786533981	-11.4529018780
C	-9.4071797268	2.7956204355	-10.7868904224
C	-10.5846023900	0.9519808098	-11.8753437478
C	-10.6312760154	3.4173025663	-10.5348790644
C	-11.7986884804	1.5920134246	-11.6185495113
C	-11.8224888507	2.8174438557	-10.9493420250
H	-8.4653930607	3.2472303609	-10.4933599017
H	-10.5410215237	0.0082960621	-12.4076639453
H	-10.6501110206	4.3714679800	-10.0174892114
H	-12.7246994270	1.1297632523	-11.9465617865
H	-12.7711552459	3.3082225048	-10.7533554943
Br	-5.4347613555	0.9573215650	-12.6834642826
Br	-7.9540332363	-0.9620911931	-13.8916729007
Br	-8.0612179210	2.4029252989	-14.1928912676

TS 2i→3i

B	-7.287300633	0.691595683	-12.934125851
O	-7.948453362	0.952689821	-11.692823335
C	-7.951087180	0.010139159	-10.612603490
H	-8.469128708	0.490016190	-9.779682963
H	-8.462243330	-0.911528591	-10.903823142
H	-6.916316311	-0.205422894	-10.331694588
C	-9.631027297	2.050443037	-11.979313762
C	-9.582242606	3.096178739	-11.090518879
C	-10.701620622	1.246738690	-12.285083554
C	-10.800988452	3.396315308	-10.462472626
C	-11.896976702	1.583317438	-11.631085053
C	-11.948712428	2.647505331	-10.728841317
H	-8.677336802	3.659851795	-10.904009514
H	-10.634081858	0.426547717	-12.989226792
H	-10.831650905	4.226790171	-9.762623173
H	-12.784526317	0.994051083	-11.843601975
H	-12.882461647	2.892066275	-10.232580341
Br	-5.276103993	0.852550072	-12.830568123
Br	-7.906069041	-1.011304212	-13.875860313
Br	-8.168118768	2.415350882	-13.940662549

3i

B	-5.175191181	-1.309932915	-12.917838167
O	-5.280817739	-1.167959646	-11.609843327
C	-6.097411951	-1.879353954	-10.670693262
H	-6.461272601	-1.149453798	-9.945577487
H	-6.934992092	-2.372021650	-11.169177080
H	-5.473153428	-2.620645007	-10.165440618
C	-11.778392938	4.490650862	-12.016371750
C	-11.498456389	5.436780534	-11.035517502
C	-12.960074115	4.509823696	-12.749911874
C	-12.442394906	6.436386106	-10.785536032
C	-13.891259141	5.518018942	-12.487050846
C	-13.635897476	6.479557462	-11.508032966
H	-10.568372481	5.398557960	-10.479262909
H	-13.151809412	3.759970989	-13.509274503
H	-12.237455737	7.182002643	-10.022206885
H	-14.819017105	5.544804758	-13.051950796
H	-14.363681637	7.261248169	-11.310341169
Br	-3.928868416	-0.169620342	-13.881515080
Br	-6.253232893	-2.670923514	-13.991587511
Br	-10.458941722	3.081423751	-12.381701763

TS 2i →4i

B	-7.449990597	1.062649217	-13.050578342
O	-8.141730263	1.165018666	-11.792099422
C	-7.872604461	-0.861333553	-10.846542029
H	-7.373937900	-0.140014971	-10.217052902
H	-8.949015486	-0.955589471	-10.786168932
H	-7.296832602	-1.713542686	-11.178537264
C	-9.384962486	1.686617264	-11.505461794
C	-9.462551747	2.529502735	-10.391052464
C	-10.531392178	1.339281007	-12.230764017
C	-10.699376619	3.043506083	-10.007493960
C	-11.760231068	1.865024888	-11.835779439
C	-11.849942891	2.713012067	-10.728073013
H	-8.551634562	2.782897033	-9.858045858
H	-10.454373290	0.684124326	-13.090341522
H	-10.762744962	3.706094391	-9.149258350
H	-12.652963399	1.610426785	-12.399685665
H	-12.813170300	3.116460319	-10.429640206
Br	-5.450220968	1.055033898	-12.668214078
Br	-7.997650683	-0.984216889	-13.664732643
Br	-7.995502903	2.383452976	-14.462433485

4i

B	-7.460885071	1.228720181	-12.960708239
O	-8.104042228	1.535147808	-11.795597096
C	-7.447587615	-1.877672354	-11.040335725
H	-7.050879526	-0.920827199	-10.717953401
H	-8.455644113	-2.159999040	-10.760341906
H	-6.765128004	-2.634270368	-11.408906742
C	-9.396668456	1.892428350	-11.477796159
C	-9.564238346	2.472242710	-10.216102431
C	-10.497475181	1.672663036	-12.309275151
C	-10.837338673	2.839337090	-9.786982186
C	-11.768217433	2.046126045	-11.864673066

C	-11.946669592	2.627682958	-10.609630485
H	-8.688027080	2.633875098	-9.596115846
H	-10.372109780	1.226001946	-13.286905089
H	-10.960524721	3.294413469	-8.807924201
H	-12.623407598	1.878475981	-12.513751813
H	-12.939424936	2.916065565	-10.276466838
Br	-5.454056924	1.087829678	-12.623227580
Br	-8.102779184	-0.836159656	-13.543466097
Br	-7.921154192	2.238456174	-14.673500252

2i+2i

B	-7.265858495	-0.114065990	-11.758728924
O	-8.619929595	0.714310110	-11.625734602
C	-9.155820931	1.025497925	-10.279433322
H	-9.750535866	1.930338812	-10.390214966
H	-9.754344438	0.181886675	-9.939338493
H	-8.301037447	1.193430036	-9.631592032
C	-9.640067731	0.733898883	-12.643657255
C	-9.757077259	1.894937492	-13.393472856
C	-10.476076819	-0.362977096	-12.795691617
C	-10.768244737	1.954133143	-14.353747886
C	-11.480133531	-0.285257955	-13.763052370
C	-11.627293937	0.868044557	-14.536609336
H	-9.066686252	2.716934686	-13.236718218
H	-10.332427017	-1.256086979	-12.197517639
H	-10.878475934	2.848249815	-14.959640350
H	-12.143821106	-1.131605761	-13.911084459
H	-12.411211848	0.919963313	-15.286274587
Br	-5.836371517	1.046350859	-10.877306324
Br	-7.561874737	-1.876240426	-10.744178597
Br	-6.892514531	-0.407376547	-13.709533127
B	-7.407502471	0.738587891	-5.419475950
O	-6.317383231	-0.350043077	-5.820830099
C	-5.943898974	-0.520106148	-7.246352534
H	-4.934505664	-0.927218066	-7.250411791
H	-6.656096917	-1.195225684	-7.718525431
H	-5.971201413	0.467618910	-7.696383549
C	-6.060442697	-1.534343683	-5.040453218
C	-4.881984807	-1.561670247	-4.309426083
C	-6.952501928	-2.595842495	-5.091557608
C	-4.588197154	-2.716809416	-3.583333424
C	-6.641999657	-3.742031333	-4.356878860
C	-5.465206744	-3.803482257	-3.607754915
H	-4.226655772	-0.697500168	-4.299653516
H	-7.867215470	-2.522369745	-5.668860200
H	-3.675201215	-2.762226847	-2.997537147
H	-7.325927474	-4.585102867	-4.371663120
H	-5.232102828	-4.699092578	-3.039608241
Br	-6.652459911	2.528556521	-6.025934300
Br	-9.124776029	0.246673332	-6.445222462
Br	-7.664189382	0.663703175	-3.427465498

Bimolecular attack on methyl (TS)

B	-7.197542968	-0.060405587	-11.670925564
O	-8.416930567	0.595771423	-11.293378079
C	-8.805256508	0.567158386	-9.131230922

H	-9.733781341	1.079187239	-9.343980876
H	-8.736065743	-0.500051851	-9.277130037
H	-7.901139331	1.154141228	-9.049069322
C	-9.611125197	0.619365973	-12.008915936
C	-10.193925311	1.869993348	-12.218077004
C	-10.242938000	-0.551040478	-12.431984334
C	-11.425495063	1.950477045	-12.868685737
C	-11.471354603	-0.454400772	-13.087118657
C	-12.067197760	0.789691895	-13.304963479
H	-9.668563356	2.760368934	-11.886466097
H	-9.772543259	-1.513060857	-12.262786835
H	-11.877628952	2.923477541	-13.040526596
H	-11.963005526	-1.361090513	-13.428897255
H	-13.023949443	0.854350501	-13.815354469
Br	-5.649274587	1.015597565	-10.751410135
Br	-7.170873029	-2.051074009	-10.823310401
Br	-6.895274331	-0.176486770	-13.668967518
B	-7.328931668	0.790532454	-5.700963153
O	-6.397837210	-0.381587885	-6.027778878
C	-5.801829022	-0.582730375	-7.390277771
H	-4.807150437	-0.988596234	-7.219663604
H	-6.433780060	-1.279516263	-7.939853244
H	-5.753511101	0.388608334	-7.871135870
C	-6.283584470	-1.568025881	-5.198973896
C	-5.208006510	-1.623287580	-4.326029268
C	-7.201307964	-2.593939892	-5.361618194
C	-5.055583309	-2.778882081	-3.558299212
C	-7.030111897	-3.741214509	-4.583514235
C	-5.963623510	-3.832687447	-3.686984725
H	-4.523344744	-0.786214377	-4.241667041
H	-8.024441776	-2.502837811	-6.061285846
H	-4.227463981	-2.850326288	-2.860222025
H	-7.733506426	-4.561754248	-4.683912431
H	-5.838467233	-4.728976039	-3.087348515
Br	-6.551645815	2.498936609	-6.370949509
Br	-9.207284142	0.366669523	-6.803087179
Br	-7.839896036	0.789455657	-3.782461051

Phenoxydibromoborane

B	-7.974078958	-1.394087215	-12.013132971
O	-9.016619585	-0.566445614	-11.932082569
C	-9.579793811	0.219041076	-12.940499911
C	-9.133437917	1.526754548	-13.104745622
C	-10.621281770	-0.303783904	-13.700934046
C	-9.744306220	2.327119585	-14.071076031
C	-11.222398857	0.508742634	-14.663270303
C	-10.786365699	1.821833547	-14.851110920
H	-8.327785439	1.904050509	-12.483223676
H	-10.951176801	-1.324270545	-13.534977226
H	-9.402809884	3.348705504	-14.210885533
H	-12.034297050	0.110962336	-15.265241492
H	-11.258663518	2.449976676	-15.600582663
Br	-7.461960913	-2.335010481	-10.384242360
Br	-6.966587328	-1.690822181	-13.661077507

CH_3Br

C	-11.103006575	0.490596223	-9.124643443

H	-12.127601052	0.250235671	-9.399633045
H	-10.386243555	-0.107963529	-9.682445644
H	-10.899899070	1.554764065	-9.221840324
Br	-10.885049188	0.021352150	-7.187787559

j

1j

O	-0.540879056	-0.442974694	-1.097351540
C	-0.802502155	-1.591088352	-0.320328163
H	-1.832157740	-1.621280819	0.067296121
H	-0.654291845	-2.456233134	-0.972897143
H	-0.110034063	-1.670392450	0.534103973
C	-0.551188163	0.787819773	-0.372806097
C	-1.974515870	1.230824972	-0.017788746
H	-2.567234345	1.362302770	-0.930231812
H	-2.483267459	0.498692394	0.618249312
H	-1.956923823	2.183432623	0.524124391
C	0.164044865	1.806736204	-1.254672417
H	1.176575380	1.464157331	-1.489309230
H	-0.379124259	1.938630908	-2.197241418
H	0.228797535	2.778480516	-0.753057434
H	0.024375715	0.653072109	0.560337277

pre-reactional complex (1j+BBr_3)

O	0.970148139	-0.501189059	-1.988329207
C	0.188947792	-1.668566016	-1.795258235
H	-0.801360275	-1.590683035	-2.264343638
H	0.734370799	-2.485854751	-2.272404094
H	0.059795271	-1.910755989	-0.731703115
C	0.446262270	0.726427819	-1.450726286
B	3.446326033	-0.476010299	-3.402364778
Br	3.125830151	-2.199585611	-4.221515628
Br	4.460451451	-0.362945346	-1.760602684
Br	2.988867295	1.140023811	-4.364950995
C	-0.844211183	1.160433487	-2.151983525
H	-0.714690627	1.137608477	-3.238798862
H	-1.693025443	0.518803722	-1.889425850
H	-1.103904753	2.183618117	-1.857872181
C	0.307545928	0.684432761	0.073662757
H	-0.515985282	0.036930650	0.395438443
H	1.233622742	0.324858022	0.533801861
H	0.102160322	1.690403797	0.456471282
H	1.229960553	1.449303186	-1.702647877

TS pre-reactional complex →2j

O	1.157584210	-0.508834543	-2.107504146
C	0.379919566	-1.682637865	-1.905540941
H	-0.611223920	-1.599196584	-2.368431455
H	0.920607280	-2.500290175	-2.383759472
H	0.264075592	-1.913697031	-0.839816592
C	0.636504329	0.719027078	-1.547370657
B	3.294530197	-0.475447908	-3.320342323
Br	3.095429134	-2.197652174	-4.206221761

Br	4.390609626	-0.355367745	-1.716256625
Br	2.930006011	1.143654882	-4.341407518
C	-0.662144658	1.149331377	-2.232730507
H	-0.543881748	1.138347329	-3.320714814
H	-1.505100753	0.502187505	-1.965351588
H	-0.921695852	2.168837758	-1.926110834
C	0.516634264	0.653775399	-0.023302964
H	-0.301575462	0.000980285	0.300549027
H	1.449502576	0.294761231	0.422641403
H	0.311920798	1.655368215	0.370643320
H	1.414036772	1.445922717	-1.799623042

2j

O	0.121186873	-0.648319643	-2.035119005
C	0.483267172	-1.646916782	-1.026146933
H	-0.366213519	-2.308834002	-0.852272697
H	1.333704264	-2.197285188	-1.415404732
H	0.761159231	-1.108369427	-0.122831438
C	-0.583057697	0.589504724	-1.480142207
B	-0.163171763	-1.113738380	-3.516706723
Br	-2.050265812	-1.908563584	-3.538169878
Br	1.245178599	-2.487110716	-4.036199796
Br	-0.000529611	0.532866268	-4.709311198
C	0.497299943	1.531155179	-0.979979755
H	1.035930074	1.124621387	-0.117110713
H	1.211983395	1.757997007	-1.774678850
H	0.024567053	2.466998898	-0.661970570
C	-1.649495623	0.222313409	-0.460149971
H	-2.336956494	-0.529311470	-0.854603525
H	-1.233052744	-0.122196087	0.491297471
H	-2.228005750	1.129910887	-0.255019056
H	-1.053016488	0.998901288	-2.370302510

2j+2j

O	-1.429829872	-1.260613236	-2.354610105
C	-1.315265362	-1.135716198	-0.892694814
H	-0.973073191	-2.081150951	-0.470651552
H	-0.611782477	-0.333132418	-0.698405906
H	-2.301493252	-0.872467830	-0.517675354
C	-2.769558367	-1.820534503	-2.847057010
B	-0.162889775	-1.424453139	-3.243740879
Br	0.318925774	-3.435498018	-3.258479071
Br	1.356183420	-0.314805644	-2.467632572
Br	-0.630659528	-0.760440517	-5.112699437
O	1.572062257	-5.034643519	0.706498981
C	1.227429088	-6.135183558	-0.209354716
H	0.205880380	-6.435226384	-0.000510003
H	1.307128559	-5.740200461	-1.222289146
H	1.914079128	-6.963874257	-0.031447435
C	3.041531405	-4.604789927	0.499953706
B	0.685057511	-4.896209488	1.985311055
Br	0.812213683	-6.654965103	3.020683594
Br	-1.240394606	-4.575724156	1.293870749
Br	1.241625926	-3.313116914	3.121572312
C	3.100346292	-3.126233148	0.169422624

H	4.110343092	-2.914601036	-0.201679176
H	2.395448655	-2.872558977	-0.626490961
H	2.912737330	-2.493603566	1.036459620
C	3.922181187	-5.089056929	1.637283793
H	3.735695493	-4.548010517	2.565484975
H	3.793116197	-6.159424577	1.817871108
H	4.963097572	-4.915586333	1.339768491
C	-3.215090631	-3.009133834	-2.012114629
H	-2.428063600	-3.761438581	-1.929815392
H	-3.552014485	-2.727673782	-1.010484915
H	-4.066197109	-3.466500231	-2.529136576
C	-3.745971741	-0.660283568	-2.900601590
H	-4.683437770	-1.015947699	-3.342455654
H	-3.979387535	-0.267790648	-1.905099984
H	-3.355232076	0.147663897	-3.523405119
H	-2.518611046	-2.148873262	-3.852448095
H	3.281815877	-5.169252936	-0.401958186

TS 2j → 3j

O	0.528608224	-0.741262923	-2.172622021
C	0.837965237	-1.737195664	-1.190779656
H	-0.001458118	-2.428809348	-1.062565562
H	1.727576482	-2.296733292	-1.490302280
H	1.037679997	-1.219555285	-0.249013003
C	-0.821798655	1.297317808	-1.350131291
B	0.171660620	-1.119276959	-3.464229437
Br	-1.997102827	-1.920814114	-3.225586592
Br	1.214504051	-2.624986001	-4.322325055
Br	0.031616194	0.530497330	-4.668697507
C	-0.134732875	1.307127110	-0.048553245
H	-0.600815276	0.647987390	0.689151237
H	0.933432066	1.100008368	-0.151835362
H	-0.218015562	2.341337451	0.332402360
C	-2.167413599	0.903146481	-1.555405746
H	-2.095196038	-0.148354154	-2.075631522
H	-2.764341472	0.745635488	-0.654755967
H	-2.679711002	1.460232345	-2.345594454
H	-0.279353984	1.695477526	-2.204897721

Alkene+HBr + methoxydibromoborane

O	0.825131448	-1.258258963	-2.685019055
C	0.741251232	-2.504181652	-1.970534313
H	-0.197262468	-2.999454140	-2.227859744
H	1.590027124	-3.147984128	-2.210794845
H	0.745304282	-2.255189205	-0.908789565
C	-2.248867242	1.550851877	-1.970986549
B	1.242048531	-1.080951241	-3.930430865
Br	-3.354219039	-2.125922033	-1.880845442
Br	1.895104497	-2.538842221	-5.067570930
Br	1.202649419	0.739014373	-4.645811437
C	-1.117978207	1.490946916	-0.989504820
H	-1.473820874	1.335680742	0.034165990
H	-0.422771865	0.684179403	-1.253367719
H	-0.537095673	2.422291997	-1.016933442
C	-3.551641354	1.462219531	-1.665671874
H	-3.268171425	-0.631032477	-1.911026270
H	-3.891270114	1.368678336	-0.635713032

H	-4.322664754	1.536773397	-2.428153883
H	-1.963443821	1.666077386	-3.017220344

Reactant of the halohydrogenation step

C	0.168766555	2.109823681	-1.378965187
Br	-4.250555805	-2.214172486	-2.392808137
C	0.208159381	2.311496462	0.105823323
H	-0.782554270	2.204427249	0.558268860
H	0.886916614	1.591905673	0.581991965
H	0.591904408	3.311603112	0.346167135
C	-0.930150985	1.835174433	-2.097814545
H	-2.810375694	-2.126549597	-2.109803412
H	-1.912752579	1.767533117	-1.634576514
H	-0.893148807	1.730691891	-3.179067267
H	1.124001359	2.191892899	-1.899409038
Br	-0.295367329	-1.651295290	-1.620890673
H	-0.388789047	-0.154644339	-1.738436204

TS of the halohydrogenation step

C	-1.125619367	1.138873873	-1.768174976
Br	-3.658898072	-1.542493086	-2.253534854
C	-0.703212087	1.600937883	-0.373766596
H	-1.404784156	1.243782086	0.386678787
H	0.288099712	1.211331267	-0.128412014
H	-0.666931585	2.694531161	-0.326598321
C	-2.477636728	1.157036701	-2.131853867
H	-2.115319151	-1.898239784	-1.957535872
H	-3.266486894	1.242373713	-1.391017291
H	-2.789516303	1.143575422	-3.170638991
H	-0.445995881	1.416150065	-2.581940273
Br	-0.225303647	-1.919573370	-1.599138007
H	-0.866470361	-0.066121037	-1.764518777

Product of the halohydrogenation step

C	-2.075122160	1.626192253	-1.780646543
Br	-3.453862251	-1.008575141	-1.952293446
C	-2.974418941	2.192578172	-0.680090361
H	-3.382777755	1.396627026	-0.049893279
H	-2.408466727	2.874836164	-0.037422572
H	-3.815146956	2.753688223	-1.105339487
C	-2.773965808	0.732304308	-2.786267214
H	-1.184491531	-2.110865982	-1.761191374
H	-3.676914343	1.176821061	-3.205232009
H	-2.117016526	0.389227265	-3.584724768
H	-1.653784031	2.453677060	-2.373032259
Br	0.209610859	-2.592300822	-1.720090781
H	-1.219156387	1.096431557	-1.346761606

4j

O	-1.946159506	1.303355215	-2.279900038
C	3.008313204	-6.737355436	-1.346758141

H	1.933188086	-6.572785219	-1.359743192
H	3.253286371	-7.796933624	-1.324798248
H	3.487428360	-6.197447551	-0.533008265
C	-1.889508103	2.551740636	-1.527274483
B	-1.942366528	0.986451238	-3.559182746
Br	-2.062095431	-0.921879882	-4.003145255
Br	3.740914012	-5.995610809	-3.059005480
Br	-1.826958423	2.258483312	-5.063052634
C	-3.122079618	3.406640550	-1.800462619
H	-3.120490621	3.805663301	-2.818187874
H	-4.036478893	2.824346663	-1.649692619
H	-3.136069662	4.250510515	-1.101846921
C	-0.561781658	3.266180322	-1.754108305
H	0.276548212	2.580824413	-1.594705938
H	-0.491966251	3.681627246	-2.762726116
H	-0.470170272	4.088964743	-1.036558529
H	-1.927627547	2.200407720	-0.491771879

TS 2j→4j

O	-0.052078520	-0.535651353	-2.164304065
C	0.454697987	-2.337617202	-1.054731933
H	-0.515082967	-2.060320967	-0.669568798
H	0.568085353	-3.372068744	-1.343802845
H	1.329769617	-1.819683554	-0.687507318
C	-0.556259043	0.571285419	-1.358112477
B	-0.332594856	-0.915612997	-3.505103954
Br	-2.106967741	-1.920036499	-3.761114414
Br	1.265700284	-2.395347973	-3.663771379
Br	-0.060421744	0.536477695	-4.896798737
C	-1.980884918	0.999678226	-1.696975963
H	-2.043408880	1.419572612	-2.704160584
H	-2.682807710	0.166036390	-1.624850560
H	-2.286528513	1.773670571	-0.983747282
C	0.457132246	1.713651195	-1.405484853
H	1.462345284	1.350805877	-1.169739514
H	0.479433157	2.172928265	-2.396837535
H	0.182164392	2.477743472	-0.669629361
H	-0.554778727	0.149345573	-0.341752538

Bimolecular attack on methyl (TS)

O	-1.140115197	-1.210841129	-1.952439352
C	-0.452500583	-2.022088393	0.028742542
H	-0.244462097	-2.890082760	-0.580270579
H	0.215620940	-1.175459262	-0.024680586
H	-1.445926393	-1.894605786	0.432334899
C	-2.578242096	-1.108452927	-2.165781179
B	-0.169356419	-1.402971735	-2.957254062
Br	0.203511947	-3.561325191	-3.190294169
Br	1.630763563	-0.556904695	-2.295897285
Br	-0.633396107	-0.669440614	-4.807565811
O	1.655984417	-5.299205983	0.599089450
C	1.349567029	-6.166771579	-0.571921615
H	0.902816314	-7.083754602	-0.195422120
H	0.687164031	-5.625078991	-1.244182931
H	2.299094374	-6.374203555	-1.058790440
C	3.146047130	-4.768676954	0.555372136
B	0.582361104	-5.060994225	1.638383936

Br	1.017447892	-5.930668702	3.393797140
Br	-1.247223725	-5.562515241	0.965550891
Br	0.500113330	-2.886694393	2.003255770
C	3.200383919	-3.637219841	-0.447810157
H	4.255750552	-3.435677724	-0.665887492
H	2.706153036	-3.877360904	-1.392842758
H	2.760963275	-2.719287210	-0.053771485
C	3.711050166	-4.449022789	1.921692842
H	3.234302217	-3.591304746	2.396901949
H	3.689869515	-5.304256826	2.596294228
H	4.760413106	-4.184034293	1.741765214
C	-3.260385537	-2.459745747	-1.972119523
H	-2.832018715	-3.212871811	-2.638020483
H	-3.171016933	-2.818413785	-0.939607271
H	-4.328527528	-2.363561776	-2.198349228
C	-3.105352711	-0.018321619	-1.239311728
H	-4.170978851	0.148682457	-1.431015852
H	-2.998483391	-0.293354128	-0.182415059
H	-2.570848838	0.920920739	-1.407956493
H	-2.714600619	-0.787610179	-3.200907111
H	3.639312329	-5.663901842	0.175681137

Bimolecular attack on methyl (product)

O	-1.231719009	0.598065976	-3.453024813
C	-1.165448534	0.181890702	0.439777207
H	-1.403400685	-0.813588036	0.071383139
H	-0.623975502	0.764373641	-0.302021671
H	-2.049041694	0.702250207	0.802841431
C	-2.507227295	0.253240794	-4.077165761
B	-0.022291411	0.564580701	-3.983870402
Br	-0.606075036	-3.676107182	-1.439678262
Br	1.480010010	1.118869801	-2.851616040
Br	0.355227594	0.001418645	-5.829411223
O	0.816329040	-7.619579860	0.950055301
C	-0.018325302	-7.600279709	-0.219821200
H	-0.503853351	-8.566343001	-0.372189056
H	-0.767029785	-6.813351089	-0.106972929
H	0.629250698	-7.364979404	-1.065405383
C	2.941860645	-3.724447551	-0.145720156
B	0.649997295	-8.340981237	2.049524937
Br	1.960230719	-8.121248840	3.480879058
Br	-0.829542368	-9.608980052	2.294953408
Br	0.054343358	-0.053114193	2.018674043
C	2.582704613	-2.491947920	-0.540662647
H	2.783088600	-2.136957270	-1.548615802
H	0.805682093	-3.335580229	-1.010436215
H	2.148373675	-1.774677385	0.153542917
C	2.757493918	-4.284092274	1.231575122
H	2.264852475	-3.568798641	1.897202046
H	2.168033718	-5.209620498	1.208742311
H	3.729449953	-4.548967547	1.668735492
C	-3.337903607	-0.455904133	-3.017633320
H	-2.820195803	-1.345106446	-2.645699455
H	-3.538641614	0.212898725	-2.173649499
H	-4.296293210	-0.766851141	-3.446922652
C	-3.142983084	1.536744028	-4.595555624
H	-4.111075398	1.311606879	-5.055635555
H	-3.303406111	2.245251891	-3.776099583
H	-2.509019706	2.012190364	-5.350479197
H	-2.299182964	-0.426128805	-4.909085510

H	3.404431015	-4.390571697	-0.876027642

Energy tables (kcal.mol^{-1})

		Zero-point and vibrational contributions to enthalpy at								
	Solution energy	210 K	220 K	230 K	240 K	250 K	260 K	270 K	280 K	298 K
BBr3	-40846.77	5.937	6.087	6.239	6.393	6.548	6.706	6.865	7.026	7.322
1a	-97309.39	51.838	51.964	52.092	52.224	52.357	52.494	52.633	52.775	53.040
Pre-reactional complex (PRC)	-138156.1	58.707	59.023	59.344	59.669	59.999	60.333	60.672	61.015	61.650
TS PRC->2a	-138156.24	58.331	58.627	58.927	59.233	59.542	59.857	60.176	60.499	61.098
2a	-138166.79	59.488	59.788	60.094	60.406	60.724	61.047	61.376	61.711	62.332
TS 2a->3a	-138124.33	56.837	57.145	57.459	57.778	58.103	58.434	58.770	59.111	59.744
3a (=4a)	-138180.32	57.459	57.722	57.990	58.262	58.539	58.820	59.106	59.397	59.937
2a+2a	-276333.66	118.521	119.102	119.695	120.300	120.916	121.544	122.183	122.833	124.041
bimolecular TS	-276311.91	117.544	118.166	118.800	119.446	120.102	120.769	121.448	122.137	123.414
bimolecular product	-276321.22	117.889	118.516	119.153	119.801	120.459	121.127	121.805	122.494	123.768

		Zero-point and vibrational contributions to enthalpy at								
	Solution energy	210 K	220 K	230 K	240 K	250 K	260 K	270 K	280 K	298 K
1b	-242330.73	103.696	103.944	104.202	104.470	104.748	105.036	105.334	105.643	106.229
Pre-reactional complex (PRC)	-283177.39	110.529	110.968	111.418	111.881	112.355	112.841	113.338	113.848	114.804
TS PRC->2b										
2b	-283188.28	111.206	111.632	112.070	112.522	112.986	113.463	113.953	114.456	115.402
TS 2b->3b	-283170.34	108.955	109.395	109.847	110.311	110.787	111.276	111.777	112.290	113.252
3b	-283202.2	110.363	110.788	111.225	111.673	112.134	112.606	113.090	113.587	114.518
TS 2b->4b	-283143.58	108.546	108.981	109.429	109.889	110.361	110.847	111.345	111.856	112.815
4b	-283201.69	109.269	109.654	110.050	110.458	110.878	111.310	111.754	112.210	113.070
2b+2b	-566376.97	222.171	223.001	223.856	224.737	225.645	226.578	227.537	228.522	230.375
bimolecular TS (attack on the methyl)	-566353.16	220.551	221.408	222.290	223.197	224.129	225.086	226.069	227.078	228.972
bimolecular product (attack on the methyl)	-566402.7	220.043	220.874	221.728	222.605	223.506	224.431	225.381	226.354	228.182
bimolecular TS (attack on the alkyl)	-566363.21	220.611	221.474	222.363	223.276	224.214	225.177	226.165	227.178	229.080

		Zero-point and vibrational contributions to enthalpy at								
	Solution energy	210 K	220 K	230 K	240 K	250 K	260 K	270 K	280 K	298 K
1c	-145886.07	73.129	73.312	73.500	73.693	73.892	74.096	74.305	74.521	74.926
Pre-reactional complex (PRC)	-186732.94	79.589	79.942	80.302	80.669	81.043	81.425	81.814	82.211	82.949
TS PRC->2c	-186732.65	79.165	79.499	79.840	80.189	80.545	80.908	81.279	81.657	82.361
2c	-186743.19	80.688	81.046	81.413	81.788	82.171	82.563	82.963	83.372	84.134
TS 2c->3c	-186721.82	78.018	78.370	78.730	79.097	79.472	79.855	80.246	80.643	81.385
3c	-186758.08	80.800	81.159	81.526	81.902	82.286	82.678	83.078	83.487	84.250
TS 2c->4c	-186699.44	78.033	78.400	78.774	79.157	79.548	79.948	80.355	80.771	81.546
4c	-186757.82	79.103	79.440	79.784	80.135	80.494	80.861	81.235	81.616	82.328
2c+2c	-373486.68	162.009	162.746	163.500	164.271	165.059	165.864	166.685	167.523	169.085
bimolecular TS (attack on the methyl)	-373462.6	160.031	160.772	161.529	162.302	163.092	163.898	164.720	165.559	167.121
bimolecular product (attack on the methyl)	-373474.87	159.882	160.604	161.342	162.096	162.866	163.651	164.452	165.268	166.790
bimolecular TS (attack on the alkyl)	-373473.91	159.789	160.518	161.263	162.023	162.799	163.591	164.398	165.221	166.754

		Zero-point and vibrational contributions to enthalpy at								
	Solution energy	210 K	220 K	230 K	240 K	250 K	260 K	270 K	280 K	298 K
1d	-385732.25	46.976	47.124	47.275	47.429	47.587	47.748	47.913	48.081	48.396
Pre-reactional complex (PRC)	-426578.8	53.780	54.117	54.459	54.807	55.160	55.518	55.882	56.251	56.933
TS PRC->2d	-426575.8	53.434	53.749	54.070	54.397	54.729	55.067	55.410	55.759	56.406
2d	-426578.09	53.648	53.955	54.269	54.589	54.915	55.248	55.586	55.930	56.570
TS 2d->3d	-426542.57	51.669	52.002	52.341	52.686	53.037	53.394	53.757	54.125	54.807
3d	-426593.92	53.772	54.114	54.462	54.814	55.172	55.536	55.904	56.278	56.969
TS 2d->4d	-426540.1	51.654	51.984	52.321	52.664	53.014	53.370	53.732	54.100	54.784
4d	-426596.8	51.822	52.083	52.349	52.621	52.898	53.180	53.468	53.761	54.307
2d+2d	-853156.77	109.267	109.954	110.654	111.368	112.094	112.833	113.585	114.349	115.765
bimolecular TS (attack on the methyl)	-853139.12	107.484	108.169	108.866	109.577	110.300	111.036	111.784	112.544	113.953
bimolecular product (attack on the methyl)	-853151.03	107.283	107.951	108.632	109.324	110.029	110.744	111.472	112.210	113.580
bimolecular TS (attack on the alkyl)	-853133.78	106.766	107.436	108.118	108.812	109.519	110.238	110.969	111.711	113.089

		Zero-point and vibrational contributions to enthalpy at								
	Solution energy	210 K	220 K	230 K	240 K	250 K	260 K	270 K	280 K	298 K
1e	-171336.58	105.935	106.177	106.426	106.681	106.944	107.213	107.490	107.775	108.311
Pre-reactional complex (PRC)	-212180.87	112.451	112.861	113.280	113.709	114.146	114.593	115.049	115.515	116.383
TS PRC->2e	-212179.79	112.567	112.978	113.398	113.827	114.265	114.713	115.170	115.636	116.506
2e	-212191.33	113.748	114.161	114.585	115.019	115.464	115.920	116.386	116.862	117.752
TS 2e->3e	-212162.36	110.005	110.414	110.833	111.263	111.702	112.151	112.610	113.079	113.955
3e	-212207.25	111.233	111.591	111.957	112.333	112.718	113.111	113.514	113.927	114.698
TS 2e->4e	-212147.93	110.519	110.924	111.339	111.765	112.200	112.646	113.102	113.567	114.439
4e	-212208.22	112.420	112.836	113.261	113.695	114.138	114.591	115.053	115.524	116.404
2e+2e	-424385.4	227.504	228.332	229.182	230.052	230.944	231.856	232.789	233.742	235.525
bimolecular TS (attack on the methyl)	-424362.11	225.914	226.765	227.637	228.529	229.441	230.374	231.327	232.301	234.120
bimolecular product (attack on the methyl)	-424376.21	225.925	226.783	227.660	228.557	229.474	230.410	231.366	232.342	234.164
bimolecular TS (attack on the alkyl)	-424365.17	225.653	226.509	227.386	228.282	229.199	230.137	231.094	232.071	233.897

		Zero-point and vibrational contributions to enthalpy at								
	Solution energy	210 K	220 K	230 K	240 K	250 K	260 K	270 K	280 K	298 K
1f	-155206.51	51.739	51.907	52.079	52.255	52.435	52.619	52.806	52.998	53.357
Pre-reactional complex (PRC)	-196053.08	58.552	58.909	59.273	59.642	60.017	60.399	60.785	61.178	61.905
TS PRC->2f	-196051.13	58.221	58.557	58.901	59.250	59.606	59.967	60.335	60.709	61.402
2f	-196053.84	58.470	58.799	59.135	59.479	59.829	60.185	60.548	60.918	61.605
TS 2f->3f	-196015.93	56.435	56.789	57.149	57.516	57.890	58.271	58.658	59.051	59.780
3f	-196074.82	58.209	58.552	58.900	59.255	59.615	59.981	60.353	60.731	61.431
TS 2f->4f	-196017.79	56.439	56.789	57.146	57.510	57.882	58.260	58.645	59.037	59.764
4f	-196073.12	57.628	57.950	58.277	58.611	58.951	59.297	59.649	60.007	60.672
2f+2f	-392110.22	118.528	119.237	119.960	120.699	121.451	122.217	122.996	123.789	125.261
bimolecular TS (attack on the methyl)	-392092.29	116.796	117.502	118.222	118.957	119.705	120.467	121.243	122.031	123.495
bimolecular product (attack on the methyl)	-392127.5	117.568	118.272	118.990	119.722	120.467	121.224	121.994	122.777	124.230
bimolecular TS (attack on the alkyl)	-392087.25	116.555	117.264	117.988	118.726	119.478	120.243	121.021	121.812	123.280

	Solution energy	Zero-point and vibrational contributions to enthalpy at								
		210 K	220 K	230 K	240 K	250 K	260 K	270 K	280 K	298 K
1g	-121986.15	69.901	70.064	70.230	70.401	70.576	70.755	70.939	71.127	71.480
Pre-reactional complex (PRC)	-162832.8	76.345	76.678	77.017	77.362	77.713	78.071	78.434	78.804	79.491
TS PRC->2g	-162832.75	76.375	76.709	77.048	77.394	77.746	78.105	78.469	78.840	79.529
2g	-162843.21	76.683	76.983	77.290	77.605	77.927	78.256	78.592	78.935	79.576
TS 2g->3g	-162810.95	74.272	74.602	74.939	75.283	75.634	75.992	76.356	76.727	77.417
3g	-162857.41	77.049	77.405	77.768	78.136	78.511	78.892	79.280	79.673	80.404
TS 2g->4g	-162799.14	74.854	75.201	75.556	75.918	76.287	76.664	77.047	77.438	78.165
4g	-162859.13	76.520	76.855	77.196	77.544	77.898	78.259	78.626	78.999	79.694
2g+2g	-325689.91	155.653	156.348	157.057	157.781	158.520	159.273	160.041	160.824	162.280
bimolecular TS (attack on the methyl)	-325666.53	154.159	154.875	155.606	156.351	157.111	157.885	158.673	159.474	160.966
bimolecular product (attack on the methyl)	-325703.85	154.873	155.587	156.315	157.057	157.812	158.581	159.364	160.160	161.639
bimolecular TS (attack on the alkyl)	-325667.97	153.577	154.275	154.988	155.715	156.456	157.211	157.980	158.764	160.221

		Zero-point and vibrational contributions to enthalpy at								
	Solution energy	210 K	220 K	230 K	240 K	250 K	260 K	270 K	280 K	298 K
1h	-171339.06	105.147	105.397	105.655	105.921	106.194	106.476	106.765	107.063	107.623
Pre-reactional complex (PRC)	-212184.58	111.166	111.565	111.974	112.393	112.822	113.261	113.709	114.167	115.023
TS PRC->2h	-212180.45	112.079	112.493	112.917	113.352	113.798	114.253	114.719	115.195	116.085
2h	-212187.52	112.874	113.299	113.736	114.184	114.643	115.113	115.594	116.086	117.005
TS 2h->3h	-212184.27	110.139	110.574	111.019	111.473	111.938	112.412	112.896	113.390	114.310
3h	-212210.65	111.131	111.519	111.917	112.324	112.740	113.166	113.601	114.045	114.874
TS 2h->4h	-212147.76	110.211	110.644	111.088	111.544	112.010	112.488	112.976	113.475	114.407
4h	-212210.76	111.518	111.945	112.381	112.828	113.285	113.751	114.227	114.713	115.620
2h+2h	-424375.71	226.293	227.164	228.057	228.973	229.911	230.871	231.853	232.856	234.730
bimolecular TS (attack on the methyl)	-424353.64	223.744	224.597	225.471	226.368	227.286	228.226	229.186	230.168	232.003
bimolecular product (attack on the methyl)	-424404.07	220.872	221.778	222.704	223.648	224.613	225.596	226.599	227.621	229.526

		Zero-point and vibrational contributions to enthalpy at								
	Solution energy	210 K	220 K	230 K	240 K	250 K	260 K	270 K	280 K	298 K
1i	-217659.82	85.413	85.625	85.846	86.075	86.313	86.561	86.817	87.082	87.587
Pre-reactional complex (PRC)	-258506.20	91.761	92.143	92.535	92.938	93.352	93.777	94.212	94.658	95.495
TS PRC->2i										
2i	-258505.85	92.396	92.791	93.196	93.613	94.042	94.482	94.933	95.396	96.264
TS 2i->3i	-258469.88	90.505	90.903	91.312	91.731	92.162	92.603	93.055	93.518	94.385
3i	-258522.05	91.309	91.683	92.068	92.463	92.868	93.283	93.709	94.144	94.961
TS 2i->4i	-258469.08	89.927	90.327	90.739	91.163	91.598	92.045	92.504	92.974	93.855
4i	-258482.52	89.627	90.037	90.458	90.891	91.335	91.79	92.256	92.733	93.627
2i+2i	-517018.09	184.347	185.116	185.908	186.723	187.56	188.421	190.119	190.211	191.913
bimolecular TS (attack on the methyl)	-516999.47	183.14	183.923	184.73	185.56	186.413	187.289	188.188	189.109	190.839
Phenoxydibromoborane	-225078.68	65.679	65.938	66.207	66.485	66.772	67.068	67.374	67.689	68.284
CH3Br	-33448.11	24.862	24.952	25.043	25.136	25.23	25.325	25.422	25.521	25.704

Note: the reaction products of the bimolecular attack on the methyl moiety are 2 CH_3Br + 2 Phenoxydobromoborane

		Zero-point and vibrational contributions to enthalpy at								
	Solution energy	210 K	220 K	230 K	240 K	250 K	260 K	270 K	280 K	298 K
1j	-146664.08	87.617	87.822	88.033	88.249	88.471	88.699	88.934	89.174	89.627
Pre-reactional complex (PRC)	-187508.71	94.134	94.51	94.895	95.286	95.686	96.094	96.509	96.932	97.72
TS PRC->2j	-187508.77	93.77	94.127	94.492	94.865	95.246	95.635	96.032	96.436	97.19
2j	-187520.46	94.833	95.195	95.566	95.946	96.335	96.733	97.14	97.556	98.332
TS 2j->3j	-187500.57	91.481	91.871	92.27	92.676	93.091	93.513	93.944	94.383	95.2
3j	-187515.8	90.141	90.531	90.929	91.335	91.749	92.17	92.599	93.035	93.847
TS 2j->4j	-187474.54	92.692	93.08	93.477	93.884	94.299	94.723	95.156	95.598	96.421
4j	-187534.04	93.422	93.762	94.109	94.465	94.829	95.2	95.58	95.968	96.692
2j+2j	-375038.07	191.505	192.309	193.132	193.973	194.832	195.709	196.603	197.515	199.214
bimolecular TS (attack on the methyl)	-375012.97	188.915	189.703	190.509	191.333	192.175	193.033	193.909	194.802	196.467
bimolecular product (attack on the methyl)	-375051.81	185.280	186.085	186.905	187.741	188.593	189.461	190.344	191.243	192.916
Reactant of the halohydrogenation step	-91559.45	62.329	62.594	62.864	63.139	63.420	63.705	63.996	64.292	64.842
TS of the halohydrogenation step	-91541.1	62.304	62.531	62.764	63.004	63.250	63.502	63.761	64.026	64.523
Product of the halohydrogenation step	-91576.32	66.446	66.675	66.909	67.147	67.391	67.640	67.895	68.154	68.639