Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Fragmentation dynamics and absolute dissociative electron attachment cross sections in the low energy electron collision with ethanol

Anirban Paul[1†], **Soumya Ghosh**[1] and **Dhananjay Nandi**[1,2*]
[1] Indian Institute of Science Education and Research Kolkata, Mohanpur 741246, India
[2] Center for Atomic, Molecular and Optical Sciences & Technologies,
Joint initiative of IIT Tirupati & IISER Tirupati, Yerpedu, 517619, Andhra Pradesh, India
email: [†]anirban.paul1995@gmail.com,[*]dhananjay@iiserkol.ac.in

Quantum chemical calculations are performed using the GAUSSIAN 16 software.[1] We have obtained the threshold energies for each dissociation pathway using the density functional theory (DFT) B3LYP/aug-cc-pVTZ method. Threshold energies for different dissociation channels are calculated as the differences between the total energies of the products and the targets.

In Tables I, II, and III we have listed the optimized structures and their electronic energy for different neutrals, anions and cations respectively. Table IV and Table V are the calculated threshold energies of different three and many body dissociation channels producing H^- ions as discussed in the main text.

For the reaction given below:

$$e^- + C_2H_5OH \rightarrow C_2H_5OH^- \rightarrow CH_3CH_2O + H^-$$

The threshold is calculated by the following way:

$$\begin{aligned} E_{Th} &= E(CH_3CH_2O) + E(H^-) - E(C_2H_5OH) \\ &= [-154.436628 + (-0.535667) - (-155.110261)] \\ &= 0.137966\,H = 3.75\,eV \end{aligned}$$

From Table II, we can see that the $CH_2CH_2OH^-$ dissociates during the time of geometry optimization, which suggests that it is unstable to dissociation and spontaneously dissociates to produce more stable C_2H_4 and OH^- fragments. Since the $CH_2CH_2OH^-$ is unstable, in Table II, we have mentioned the final optimization energy value. We, therefore, have also calculated the combined energy of C_2H_4 and OH^- fragments [-78.624065 +(-75.836271) = -154.460336]. This suggests that the combined energy of these fragments is less than the final optimized energy value (-154.454494 H) of $CH_2CH_2OH^-$. This again means that the $CH_2CH_2OH^-$ spontaneously dissociates to produce a C_2H_4 and an OH^- fragment.

In Tables VI and VII, we have listed the positions of different atoms in the optimized structures of neutrals in Cartesian coordinates. The coordinates of the atoms are copied from the output files of the optimized structures. On the other hand, the Cartesian coordinates of the atoms in the optimized structures of different anions and cations are listed in Tables VIII and IX, respectively.

[1] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, *Gaussian˜16 Revision C.01*, 2016, Gaussian Inc. Wallingford CT.

TABLE I. Different optimized structures with their electronic energies.

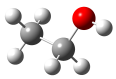
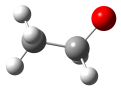
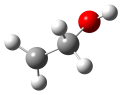
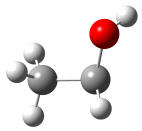
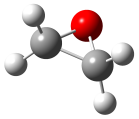
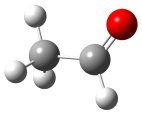
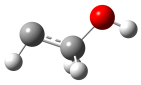
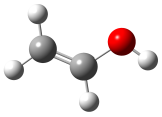
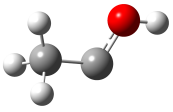
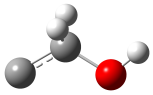
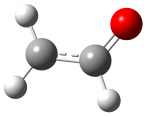
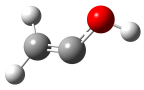
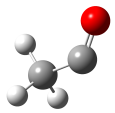
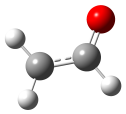
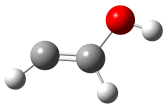
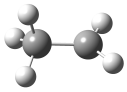
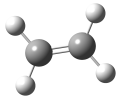
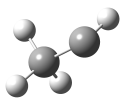
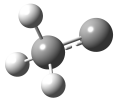
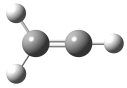
Species	Energy (H)	Optimized Structure	Species	Energy (H)	Optimized Structure
C_2H_5OH	-155.110261		CH_3CH_2O	-154.436628	
CH_2CH_2OH	-154.434668		CH_3CHOH	-154.450633	
CH_2CH_2O	-153.852563		CH_3CHO	-153.89642	
$CHCH_2OH$	-153.79717		CH_2CHOH	-153.879496	
CH_3COH	-153.815297		CCH_2OH	-153.101394	
CH_2CHO	-153.236837		CH_2COH	-153.198424	
CH_3CO	-153.245884		$CHCH_2O$	-153.236802	
CHCHOH	-153.186805		H_2	-1.180024	
H	-0.50226		OH	-75.768599	
CH_3CH_3	-79.864711		CH_3CH_2	-79.193142	
O	-75.09418		CH_2CH_2	-78.624065	
CH_3CH	-78.501298		CH_3C	-77.858186	
CH_2CH	-77.930594		H_2O	-76.466197	

TABLE II. Different optimized structures of anions with their electronic energies.

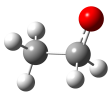
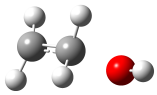
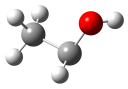
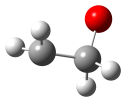
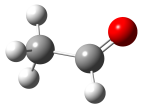
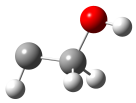
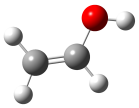
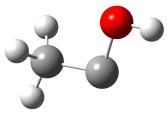
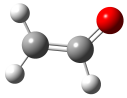
Species	Energy (H)	Optimized Structure	Species	Energy (H)	Optimized Structure
$CH_3CH_2O^-$	-154.496837		$CH_2CH_2OH^-$	-154.454494	
CH_3CHOH^-	-154.439724		$CH_2CH_2O^-$	-153.83133	
CH_3CHO^-	-153.881431		$CHCH_2OH^-$	-153.781624	
CH_2CHOH^-	-153.867569		CH_3COH^-	-153.79943	
CH_2CHO^-	-153.303989		$CH_3CH_2^-$	-79.184061	
H^-	-0.535667		OH^-	-75.836271	
O^-	-75.155815				

TABLE III. Different optimized structures of cations with their electronic energies.

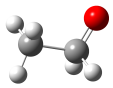
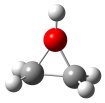
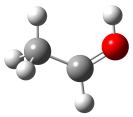
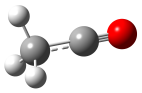
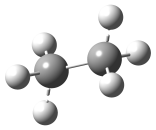
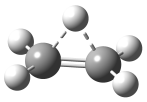
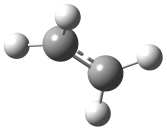
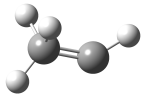
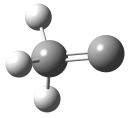
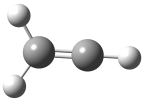
Species	Energy (H)	Optimized Structure	Species	Energy (H)	Optimized Structure
$CH_3CH_2O^+$	-154.065289		$CH_2CH_2OH^+$	-154.132279	
CH_3CHOH^+	-154.202729		CH_3CO^+	-152.985149	
H_2^+	-0.610293		$CH_3CH_3^+$	-79.440269	
$CH_3CH_2^+$	-78.892614		$CH_2CH_2^+$	-78.24378	
CH_3CH^+	-78.193475		CH_3C^+	-77.540745	
CH_2CH^+	-77.616958		H^+	0	

TABLE IV. Different three-body dissociation channels producing H^- ions and their calculated threshold values.

Ch. no.	Dissociative products	Threshold energy
A.1	$H^- + CH_2CH_2O + H$	5.98 eV
A.2	$H^- + CH_3CHO + H$	4.79 eV
A.3	$H^- + CHCH_2OH + H$	7.49 eV
A.4	$H^- + CH_2CHOH + H$	5.25 eV
A.5	$H^- + CH_3COH + H$	6.99 eV

TABLE V. Different many-body dissociation channels producing H^- ions and their calculated threshold values.

Ch. no.	Dissociative products	Threshold energy
B.1	$H^- + CH_2CHO + H_2$	4.29 eV
B.2	$H^- + CH_3CO + H_2$	4.05 eV
B.3	$H^- + CH_2COH + H_2$	5.34 eV
B.4	$H^- + CHCH_2O + H_2$	4.29 eV
B.5	$H^- + CHCHOH + H_2$	5.65 eV
B.6	$H^- + CHCH_2 + H_2O$	4.84 eV

TABLE VI. Positions of different atoms in the optimized structures of neutrals in Cartesian coordinates.

Species	Atoms and their coordinates	Species	Atoms and their coordinates
C_2H_5OH	C 1.17743300 -0.39742000 0.00000000	CH_3CH_2O	C 1.04308400 -0.60036400 0.00000000
	H 1.15400100 -1.03570800 0.88357500		H 0.93235200 -1.22963000 0.88320000
	H 2.11572000 0.15922200 0.00000000		H 2.05127100 -0.18168800 0.00000000
	H 1.15400100 -1.03570800 -0.88357500		H 0.93235200 -1.22963000 -0.88320000
	C 0.00000000 0.55409200 0.00000000		C 0.00000000 0.50738200 0.00000000
	H 0.03392100 1.19907400 0.88538100		H 0.12492200 1.18965500 0.86272600
	H 0.03392100 1.19907400 -0.88538100		H 0.12492200 1.18965500 -0.86272600
	O -1.19980400 -0.22410700 0.00000000		O -1.30304000 0.10244100 0.00000000
	H -1.95772900 0.36686400 0.00000000		
CH_2CH_2OH	C -1.26380800 -0.23901200 0.00000000	CH_3CHOH	C 1.20839900 -0.18004800 0.01877500
	H -1.69080400 -0.59274600 0.92709000		H 1.37495800 -0.58395900 1.02951100
	H -1.69080400 -0.59274600 -0.92709000		H 2.03108000 0.49931600 -0.20270300
	C 0.00000000 0.53538400 0.00000000		H 1.28155100 -1.02212700 -0.67851700
	H 0.05228700 1.17525900 0.88708600		C -0.09051000 0.52510400 -0.10814400
	H 0.05228700 1.17525900 -0.88708600		H -0.20781900 1.56136000 0.17291000
	O 1.11614900 -0.38411400 0.00000000		O -1.25975800 -0.17705600 0.04539300
	H 1.93069300 0.12965200 0.00000000		H -1.10904300 -1.10848300 -0.14813000
CH_2CH_2O	C 0.73141600 0.37358300 0.00001400	CH_3CHO	C -1.16564000 -0.14854200 -0.00003000
	H 1.26638700 0.59041000 -0.91802700		H -1.70067000 0.22501200 0.87710000
	H 1.26635300 0.59039400 0.91807700		H -1.16187700 -1.23580900 -0.00147500
	C -0.73176400 0.37302800 0.00000200		H -1.70209100 0.22736600 -0.87515100
	H -1.26702100 0.58957400 0.91788900		C 0.23247600 0.39613300 -0.00008800
	H -1.26692000 0.58975600 -0.91789600		H 0.30613700 1.50368500 0.00002700
	O 0.00041200 -0.85497500 -0.00001700		O 1.23218600 -0.27572500 0.00002600
$CHCH_2OH$	C 1.27704800 -0.44142100 -0.00000600	CH_2CHOH	C -1.22353600 -0.17985300 0.00003200
	H 2.12375700 0.26707100 -0.00001500		H -2.11997900 0.41959800 0.00010000
	C 0.10720400 0.39346200 -0.00000500		H -1.31875900 -1.25632500 -0.00021200
	H 0.19850400 1.06842000 0.87675600		C -0.03824300 0.41237700 -0.00000500
	H 0.19842700 1.06855200 -0.87666500		H 0.06656100 1.49162800 -0.00017000
	O -1.12241700 -0.30550700 -0.00000400		O 1.13282300 -0.29473700 0.00000900
	H -1.84686300 0.32776700 0.00002600		H 1.88027200 0.30784300 0.00004800
CH_3COH	C -1.16492900 -0.13668700 0.00001900	CCH_2OH	C -1.39886500 -0.37609500 -0.00000100
	H -1.08137400 -1.22832100 -0.00003600		C -0.18918000 0.39217500 0.00000000
	H -1.73990400 0.20258300 -0.86664400		H -0.29660700 1.05954400 -0.88002900
	H -1.73838000 0.20287500 0.86750900		H -0.29660900 1.05954000 0.88003200
	C 0.12503400 0.60581500 -0.00017000		O 1.04402800 -0.31661400 0.00000000
	O 1.10661500 -0.27448900 -0.00003800		H 1.76926500 0.31735000 -0.00000400
	H 1.94611000 0.20401300 0.00037900		
CH_2CHO	C -1.16501400 -0.17159100 0.00012900	CH_2COH	C 1.24106800 -0.10210500 -0.01615600
	H -1.26771500 -1.24781000 0.00079500		H 1.39882100 -1.16966900 -0.14771100
	H -2.05143600 0.44753000 -0.00169800		H 2.10566800 0.53730900 0.07373100
	C 0.13121600 0.40606700 0.00016500		C 0.02935000 0.40436500 0.00935500
	H 0.18820100 1.50760300 0.00070700		O -1.16546900 -0.18347400 0.07389400
	O 1.16671700 -0.26427200 -0.00019700		H -1.80324800 0.28659600 -0.47635900
CH_3CO	C 1.16675000 -0.09752200 0.00001900	$CHCH_2O$	C 1.16135200 -0.17187200 -0.00062300
	H 1.18500000 -1.18964100 0.00103500		H 2.05645500 0.43499600 -0.01342900
	H 1.68223000 0.29455200 0.87644000		C -0.12883900 0.40899300 0.00316600
	H 1.68149400 0.29282600 -0.87767700		H 1.25496600 -1.24859000 0.01147000
	C -0.24467900 0.42687000 0.00003000		H -0.18795000 1.51161200 0.00463100
	O -1.26014400 -0.17172800 -0.00001100		O -1.16481900 -0.26509300 -0.00224100

TABLE VII. Positions of different atoms in the optimized structures of neutrals in Cartesian coordinates.

Species	Atoms and their coordinates	Species	Atoms and their coordinates
CHCHOH	C 1.26061900 -0.27547500 0.00004300 H 2.30400600 -0.02664200 -0.00019500 C 0.11379900 0.35080000 0.00006800 H 0.07695700 1.44131600 -0.00022100 O -1.10302400 -0.28051900 -0.00006400 H -1.80327400 0.37753500 0.00026100	H_2	H 0.00000000 0.00000000 0.37143200 H 0.00000000 0.00000000 -0.37143200
OH	O 0.00000000 0.00000000 0.10836800 H 0.00000000 0.00000000 -0.86694100	CH_3CH_3	C 0.00000000 0.00000000 0.76357800 H 0.50786800 0.88018600 1.16108900 H -1.01619700 -0.00026700 1.16108900 H 0.50832900 -0.87991900 1.16108900 C 0.00000000 0.00000000 -0.76357800 H 1.01619700 -0.00026700 -1.16108900 H -0.50832900 -0.87991900 -1.16108900 H -0.50786800 0.88018600 -1.16108900
CH_3CH_2	C -0.00911100 -0.69144100 0.00000000 H -0.50272000 -1.09865800 0.88457200 H -0.50272000 -1.09865800 -0.88457200 H 1.01156100 -1.10210100 0.00000000 C -0.00911100 0.79211500 0.00000000 H 0.05160500 1.34768700 0.92437200 H 0.05160500 1.34768700 -0.92437200	CH_2CH_2	C 0.00000000 -0.66235600 -0.00001900 H 0.92059600 -1.23177900 -0.00011100 H -0.92069400 -1.23155000 0.00022400 C 0.00000000 0.66235600 -0.00001900 H 0.92069400 1.23155000 0.00022400 H -0.92059600 1.23177900 -0.00011100
CH_3CH	C -0.86048000 0.19954200 -0.00018500 H -1.30212200 -0.81543700 -0.00014100 C 0.59078300 -0.00312300 -0.00023200 H 0.86441900 -0.63131500 0.86456900 H 0.86643700 -0.63818100 -0.85923700 H 1.18945300 0.90642300 -0.00268300	CH_3C	C 0.50059800 0.01359000 -0.00000400 H 1.00602400 0.98891500 -0.00015700 H 0.82829200 -0.57737400 -0.87102600 H 0.82843100 -0.57711500 0.87114900 C -0.94438900 0.01400500 0.00000900
CH_2CH	C -0.59497200 0.00028400 0.00021400 H -1.18305300 -0.92117000 -0.00033100 H -1.18847700 0.91758500 -0.00033300 C 0.69691500 0.00024500 -0.00016700 H 1.75987300 0.00041100 0.00038300	H_2O	O 0.00000000 0.00000000 0.11697300 H 0.00000000 0.76339900 -0.46789400 H 0.00000000 -0.76339900 -0.46789400

TABLE VIII. Positions of different atoms of the optimized structures of different anions in Cartesian coordinates.

Species	Atoms and their coordinates	Species	Atoms and their coordinates
$CH_3CH_2O^-$	C 0.99467500 -0.66841100 0.00000000	$CH_2CH_2OH^-$	C -1.35098500 0.05069000 0.00000000
	H 0.82159500 -1.29029100 0.88426600		H -1.72703200 -0.40170700 0.91553500
	H 2.04360700 -0.33157600 0.00000000		H -1.72703200 -0.40170700 -0.91553500
	H 0.82159500 -1.29029100 -0.88426600		C 0.00000000 0.52777500 0.00000000
	C 0.00000000 0.53011700 0.00000000		H 0.25160400 1.10800100 0.89574600
	H 0.31392600 1.16440200 0.88805600		H 0.25160400 1.10800100 -0.89574600
	H 0.31392600 1.16440200 -0.88805600		O 1.13444800 -0.59543700 0.00000000
	O -1.28533700 0.17664000 0.00000000		H 1.98118500 -0.11987800 0.00000000
CH_3CHOH^-	C 1.20476100 -0.21337700 0.00511400	$CH_2CH_2O^-$	C 1.18640000 -0.12888400 0.00007100
	H 1.24641900 -0.75686600 0.98541100		H 1.45288100 -0.66002200 -0.91208200
	H 2.07947500 0.44749500 -0.03892500		H 1.45223900 -0.66150700 0.91155400
	H 1.34300900 -0.97705500 -0.76779300		C -0.16066600 0.55413000 0.00009900
	C -0.05533900 0.60545800 -0.19930100		H -0.23826200 1.22938300 -0.88731100
	H -0.06908900 1.38623800 0.57653800		H -0.23830700 1.22890400 0.88786000
	O -1.22537900 -0.26400400 0.13747300		O -1.07286900 -0.46103000 -0.00013000
	H -1.69331400 -0.34027400 -0.68989400		
CH_3CHO^-	O 1.24036800 -0.27077100 -0.00004200	$CHCH_2OH^-$	O 1.13490400 -0.33791000 0.00000800
	C 0.22705300 0.39139900 0.00015200		H 1.84568300 0.31386800 -0.00004700
	H 0.29223600 1.49647400 -0.00019000		C -0.12541100 0.43514300 0.00000000
	C -1.16512600 -0.15085000 0.00004000		H -0.07533700 1.10542100 0.89108300
	H -1.70658800 0.23356000 0.87290300		H -0.07532400 1.10544800 -0.89106300
	H -1.70531300 0.23169200 -0.87463000		C -1.30345500 -0.44025200 -0.00001200
	H -1.17484000 -1.23885100 0.00109600		H -2.20105500 0.20919900 0.00003000
CH_2CHOH^-	C 1.22918200 -0.17463700 0.00010600	CH_3COH^-	C 1.17581000 -0.13721700 -0.00000400
	H 2.11410600 0.44661500 -0.00015700		H 1.25762700 -0.81061200 -0.88554800
	H 1.34792500 -1.24876100 0.00030600		H 1.25767000 -0.81056700 0.88556600
	C 0.03021500 0.40170200 -0.00002100		H 2.05398700 0.51302800 -0.00003800
	H -0.07701300 1.48179200 -0.00033800		C -0.07937200 0.67889500 0.00000600
	O -1.13142500 -0.29515100 -0.00024800		O -1.15043200 -0.29728300 0.00000800
	H -1.89000300 0.31917000 0.00165700		H -1.94444800 0.23634300 -0.00006200
CH_2CHO^-	C 1.17928700 -0.16989800 0.00001500	$CH_3CH_2^-$	C -0.05540600 -0.68638600 0.00000000
	H 1.35232800 -1.24153800 -0.00010100		H -0.58518600 -1.08596600 0.87264700
	H 2.03551500 0.49473800 0.00006800		H -0.58518600 -1.08596600 -0.87264700
	C -0.09751600 0.35431500 -0.00001800		H 0.94221400 -1.21226900 0.00000000
	H -0.10969500 1.47755000 -0.00005400		C -0.05540600 0.83548400 0.00000000
	O -1.22109600 -0.22965600 0.00001300		H 0.44651300 1.24480900 0.88771300
			H 0.44651300 1.24480900 -0.88771300
OH^-	O 0.00000000 0.00000000 0.10727800		
	H 0.00000000 0.00000000 -0.85822800		

TABLE IX. Positions of different atoms of the optimized structures of different cations in Cartesian coordinates.

Species	Atoms and their coordinates	Species	Atoms and their coordinates
$CH_3CH_2O^+$	C 0.98671600 -0.76051900 0.00000000	$CH_2CH_2OH^+$	C -0.74599200 0.46551900 0.00000000
	H 0.77168800 -1.32072600 0.90501500		H -1.27586800 0.63550600 0.92719600
	H 1.98053900 -0.31701800 0.00000000		H -1.27586800 0.63550600 -0.92719600
	H 0.77168800 -1.32072600 -0.90501500		C 0.74624200 0.46655100 0.00000000
	C 0.00000000 0.55357100 0.00000000		H 1.27438400 0.63590800 0.92808500
	H 0.23215300 1.16767600 0.91166100		H 1.27438400 0.63590800 -0.92808500
	H 0.23215300 1.16767600 -0.91166100		O 0.00000000 -0.79579000 0.00000000
	O -1.23856500 0.23310100 0.00000000		H 0.00146400 -1.76892400 0.00000000
CH_3CHOH^+	C 1.19399900 -0.18242300 -0.00000600	CH_3CO^+	C -1.20965800 0.00041200 0.00003000
	H 1.75287500 0.19708400 0.86712300		H -1.55439500 -0.47311700 -0.92654000
	H 1.75374300 0.19774900 -0.86616900		H -1.55654200 1.03826500 0.05499500
	H 1.16718700 -1.27004200 -0.00049500		H -1.55446900 -0.56868000 0.87124800
	C -0.10982700 0.44997600 -0.00013000		C 0.21559000 0.00025700 0.00003300
	H -0.21125600 1.53460000 0.00005100		O 1.32872700 -0.00006100 -0.00001000
	O -1.22400500 -0.14296200 0.00004700		
	H -1.17554600 -1.12101500 -0.00006900		
H_2^+	H 0.00000000 0.00000000 0.55766900	$CH_3CH_3^+$	C 0.00000000 0.72422400 0.00000000
	H 0.00000000 0.00000000 -0.55766900		H -0.35494300 1.14486100 -0.95719100
			H -0.35494200 1.14486000 0.95719100
			H 0.99805200 1.27920500 0.00000100
			C 0.00000000 -0.72422400 0.00000000
			H 0.35494300 -1.14486100 -0.95719100
			H 0.35494200 -1.14486000 0.95719100
			H -0.99805200 -1.27920500 0.00000100
$CH_3CH_2^+$	C -0.06417600 -0.68799600 0.00000000	$CH_2CH_2^+$	C 0.00000000 -0.69380100 0.00001200
	H -0.07442700 -1.24371700 0.93233700		H 0.90270900 -1.25672400 -0.23105500
	H -0.07442700 -1.24371700 -0.93233700		H -0.90253700 -1.25700200 0.23098400
	H 1.06028500 -0.00339000 0.00000000		C 0.00000000 0.69380100 0.00001200
	C -0.06417600 0.68881500 0.00000000		H 0.90253700 1.25700200 0.23098400
	H -0.07066000 1.24295500 0.93308900		H -0.90270900 1.25672400 -0.23105500
	H -0.07066000 1.24295500 -0.93308900		
CH_3CH^+	C -0.78371300 0.15511500 -0.00011100	CH_3C^+	C 0.00000000 0.00000000 -0.47103600
	H -1.67963000 -0.46651400 -0.00058100		H 0.00000000 1.05891800 -0.82465500
	C 0.58765000 -0.00339700 -0.00040300		H -0.91705000 -0.52945900 -0.82465500
	H 0.83049300 -0.67035200 0.86277800		H 0.91705000 -0.52945900 -0.82465500
	H 0.83280300 -0.67881000 -0.85596700		C 0.00000000 0.00000000 0.88336300
	H 1.19271200 0.90536600 -0.00314800		
CH_2CH^+	C -0.57903300 -0.00003200 0.00008500		
	H -1.15473300 -0.93783900 -0.00017100		
	H -1.15385900 0.93835900 -0.00017000		
	C 0.67176400 -0.00003700 -0.00003100		
	H 1.75221100 -0.00010500 0.00001600		