This supplemental information document includes additional experimental details and computational data as referenced in the text.

Experimental Methods

Sample preparation

Methanol (CH_3OH), acetonitrile (CH_3CN), acrylonitrile (CH_2CHCN), propionitrile (CH_3CH_2CN), buytronitrile ($CH_3CH_2CH_2CN$), and benzonitrile (C_6H_5CN) were purchased from Sigma-Aldrich Chemical (St Louis, MO) and used as received. A sample of uranyl propiolate was prepared as described previously by combining 2–3 mg of $U^{VI}O_3$ (Strem Chemicals, Newburyport MA), corresponding to approximately 7×10^{-6} to 1×10^{-5} mol, with 2–3 mL of propiolic acid ($HO_2C–C\equiv CH$, Sigma Aldrich, St Louis MO) and 400 mL of deionized/distilled H_2O in a glass scintillation vial. *Caution: uranium oxide is radioactive (a- and g-emitter), and proper shielding, waste disposal and personal protective gear should be used when handling the material*.

Mass spectrometry experiments

The formation of $[UH]^+$ from a UO_2^{2+} precursor and its corresponding dissociation mechanism have been thoroughly detailed elsewhere. Methanol (CH_3OH) and propiolic acid were sourced from Sigma-Aldrich Chemical (St. Louis, MO) and used without further purification. Uranyl propiolate was synthesized in-house by reacting solid UO_3 (Strem Chemicals, Newburyport MA) with aqueous propiolic acid. The generation of the $[O=U\equiv CH]^+$ intermediate from uranyl propiolate precursors via preparative tandem ion trap mass spectrometry ($PTMS^n$) was accomplished following an established protocol. In brief, electrospray ionization (ESI) and collision-induced dissociation (CID) experiments were conducted using a ThermoScientific (San Jose, CA) LTQ-XL linear ion trap mass spectrometer, which had been modified to facilitate the study of ion-molecule reactions. The atmospheric pressure ionization stack parameters were optimized to maximize the transmission of $[UO_2(O2C\text{-}C\equiv CH)(CH_3OH)_2]^+$ (*m/z* 403) to the ion trap using the auto-tune feature in the LTQ Tune program. Helium served as the bath/buffer gas in the CID experiments. Target ions were isolated with a width of 1.0 to 1.5 m/z units, chosen empirically to achieve maximum ion intensity while isolating a single isotopic peak. The normalized collision energy (NCE) and activation Q values for CID of $[UO_2(C\equiv CH)]^+$ were set to 20% and 0.35, respectively. For CID of $[O=U\equiv CH]^+$, the NCE was set to 18% and the activation Q to 0.33, while for CID of $[UH]^+$, the settings were 22% and 0.75, respectively.

The linear ion trap was modified to enable the mixing of neutral liquid and gaseous reagents with the helium buffer gas before their introduction into the ion trap. Liquid reagents were introduced into the system via a metered syringe pump, where they were vaporized. The partial pressure of these reagents was controlled through the syringe pump flow rate, helium flow rate, and by adjusting the temperature of the manifold, which was managed by wrapping the manifold tubing with a temperature-controlled water coil. All gas ports were regulated using manually actuated precision needle valves, allowing fine control of the flow rates.

To investigate gas-phase reactions of $[UH]^+$ with background neutrals, ions were isolated using widths of 1–2 *m/z* units, selected empirically to ensure optimal ion isolation efficiency. The ions were then stored in the LIT for periods ranging from 1 ms to 10 s. For ion-molecule reaction (IMR) studies, the goal was to identify the reaction pathways of ions with nitrile neutrals in the LIT rather than to measure rates or rate constants. The specific isolation times were selected to illustrate the general changes in precursor and product ion intensities as isolation time varied, confirming that specific ions were generated by bimolecular reactions within the ion trap. Since the experiments utilized the multi-dimensional tandem mass spectrometry capabilities of the linear ion trap, care was taken to ensure sufficient neutral reagent was present in the ion trap for ion-molecule reaction studies, without compromising the synthesis of reactive species through multiple initial CID steps in series. For both CID and IMR experiments, the displayed mass spectra were generated by accumulating and averaging at least 30 isolation, dissociation, and ejection/detection cycles.

CID Process

Collision-induced dissociation (CID) is often referred to as a slow heating process, meaning that the ions being studied gradually gain energy through multiple collisions with inert gas molecules (in this case He), leading to bond dissociation along the lowest energy pathways. Normalized collision energy (NCE) is the unit used to perform CID, where ions are accelerated using a separate RF frequency voltage. Essentially, the higher the NCE, the more kinetic energy the ions have, and thus, more internal energy is imposed with collisions with helium. The activation Q is a unit that describes how tightly the ions are being held in the trap. In an ion trap mass spectrometer, the activation Q (Qz) is directly related to the ion's secular frequency and the RF voltage applied, which defines the depth of the potential well in which the ions are confined. When the activation Q is set lower, the RF voltage creates a deeper potential well, meaning ions are more tightly trapped, with less motion and lower excitation. This stronger confinement limits the amount of energy transferred to the ions during collision-induced dissociation (CID). In contrast, a higher activation Q creates a shallower potential well, allowing ions to move more freely, absorb more energy during collisions, and undergo more energetic fragmentation. However, the shallow well also increases the likelihood that ions will escape the trap before they dissociate, leading to signal loss.

To balance these effects, the normalized collision energy (NCE) must be adjusted in conjunction with the activation Q. A lower activation Q requires less NCE because the ions are tightly confined and only need a small amount of energy to undergo dissociation. Conversely, at a higher activation Q, the shallow potential well means the ions need more energy to ensure sufficient excitation for fragmentation. Therefore, increasing the NCE at higher activation Q compensates for the shallower well, allowing the ions to gain enough energy to fragment, but this also comes with the trade-off of potentially losing low-energy products and reducing ion trapping efficiency. Optimizing both the activation Q and NCE is crucial to ensure the desired fragmentation while maintaining ion confinement.

Computational methodology

Kohn–Sham DFT calculations were carried out using the Gaussian16[1] quantum chemistry software. For uranium and iodine, the Stuttgart Dresden basis set (SDD-VDZ-MWB)[2] was applied, along with its corresponding small-core quasi-relativistic effective core potential (MWB60). For the other elements in the system, the 6-311+g(d,p) Pople triple-ζ basis set with diffuse functions was utilized. The structures of reactants, intermediates, transition states, and products were optimized using two different density functionals, B3LYP and PBE0 (PBE1PBE). The selection of these density functionals and basis sets was

informed by their successful application in prior computational studies on uranium oxides and related species. All identified transition states were verified through intrinsic reaction coordinate (IRC) calculations. The relative energies obtained with B3LYP and PBE0 were in reasonable agreement, though PBE0 consistently predicted higher energy values than B3LYP. Calculations for singlet states were conducted using the restricted Kohn–Sham formalism, while triplet and quintet states were evaluated using the unrestricted formalism. Although spin–orbit corrections could potentially influence the energies of reaction intermediates and transition states involving different uranium oxidation states, this effect does not significantly impact the key interpretations derived from the computed relative energies. Details of the potential energy surfaces and additional computational specifics are provided in the ESI.

References

1 *Gaussian 16, Revision C.01*, 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, D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

2 M. Dolg, H. Stoll, H. Preuss, *Theor. Chim. Acta*, 1993, **85**, 441–450. DOI: 10.1007/BF01113224.

Figure 1: Generation of $[UH]^+$ (*m/z* 239) from $[UO_2(O_2C\text{-}C{\equiv}CH)(CH_3OH)_2]^+$ (*m/z* 403)

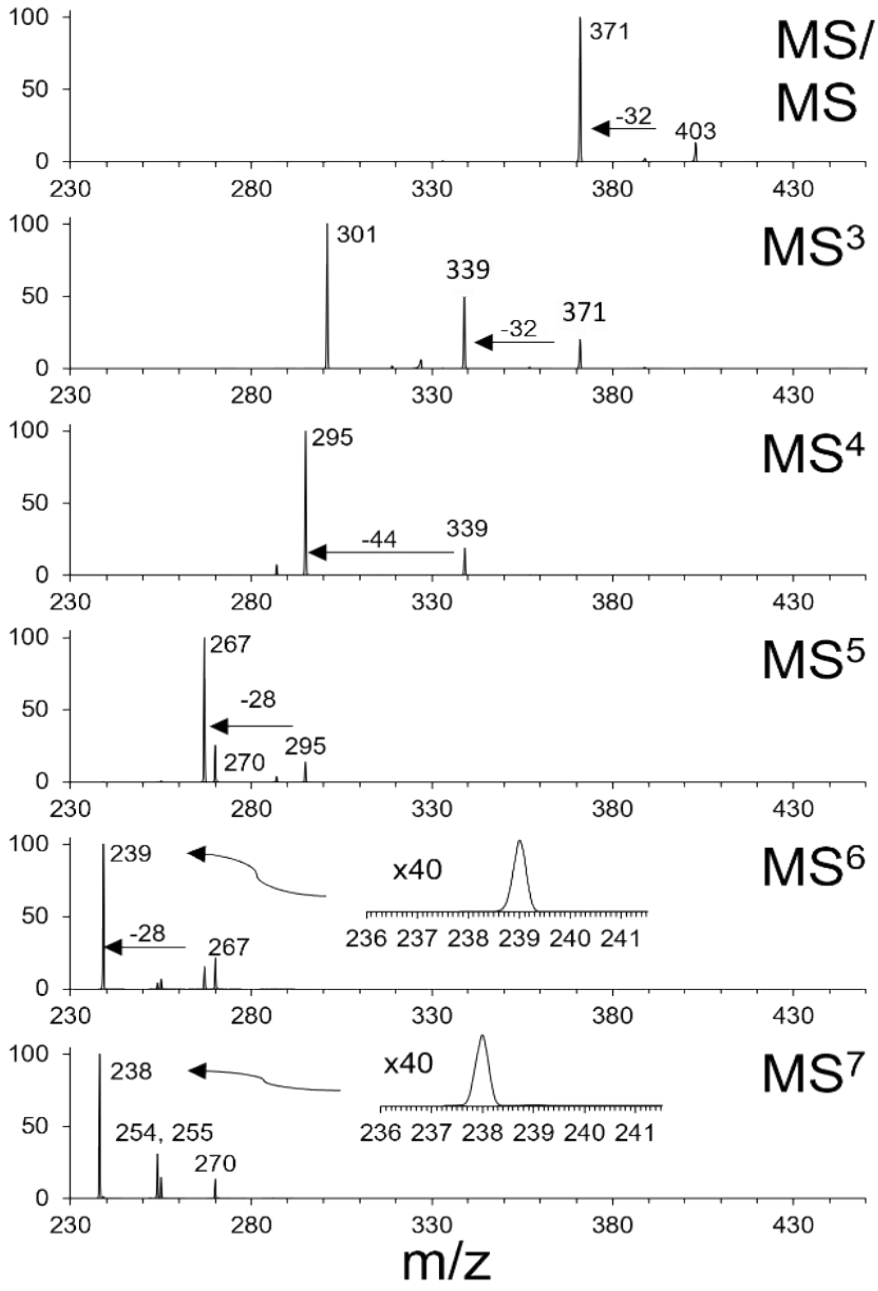

Figure 2: Isolation of $[UH]^+$ and U^+

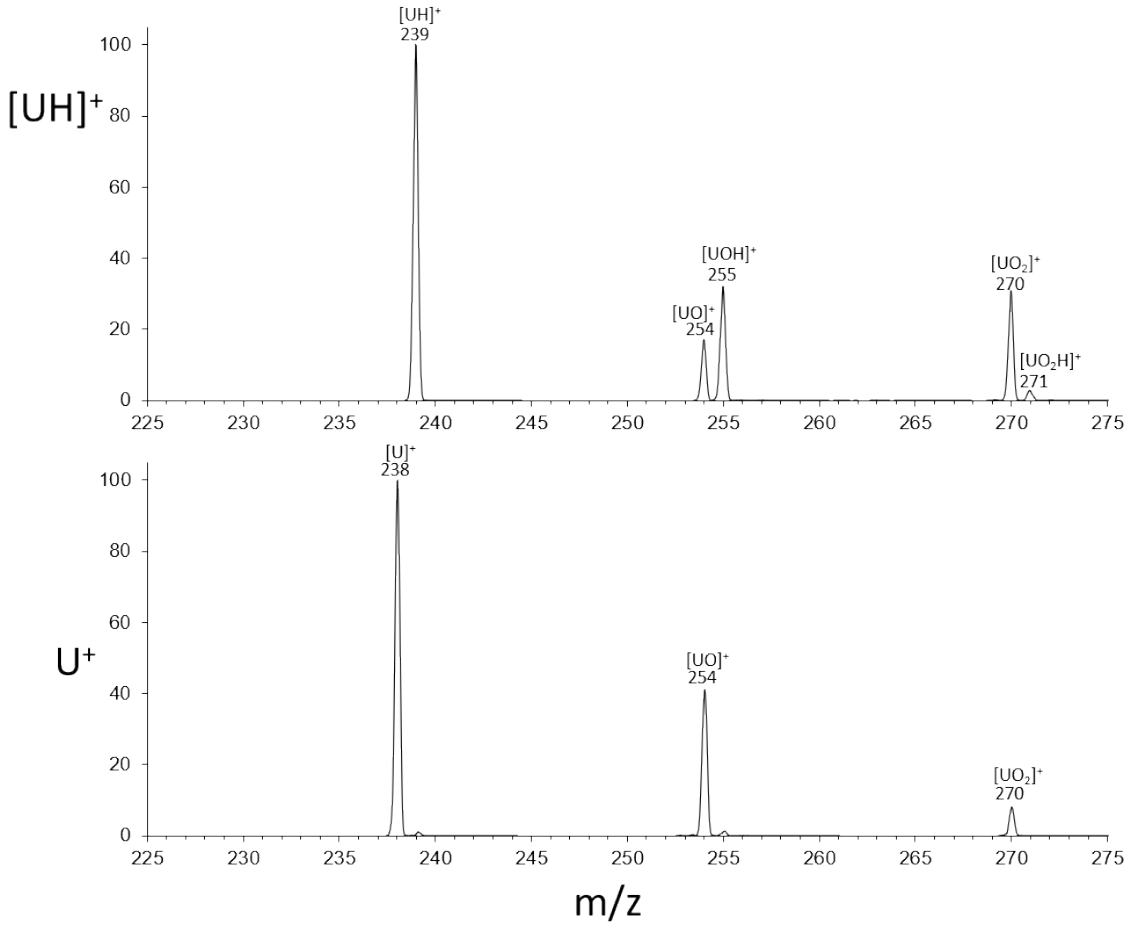

Figure 2: Isolation of $[UH]^+$ (top) (m/z 239) and U^+ (bottom) (m/z 238) for 100ms. Reactions observed are from background O_2 and H_2O.

Table 1.1: $[UH]^+ + CH_3CN$ B3LYP/SDD/6-311+g(d,p) Quintet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-477.20060	.00371	.00608	.00702	-.01919	-477.19689	-477.19453	-477.19358	-477.21980
CH_3CN	-132.79616	.04515	.04876	.04970	.02113	-132.75101	-132.74740	-132.74646	-132.77503
$[UH]^+ + CH_3CN$ (I)	-609.99676	.04886	.05483	.05672	.00194	-609.94791	-609.94193	-609.94004	-609.99483
II	-610.07653	.04979	.05617	.05711	.01601	-610.02674	-610.02037	-610.01942	-610.06053
TSII→III	-610.06089	.05004	.05540	.05634	.01754	-610.01085	-610.00549	-610.00455	-610.04336
III	-610.12038	.05692	.06239	.06333	.02416	-610.06345	-610.05799	-610.05704	-610.09621
TSIII→IV	-610.06935	.04868	.05545	.05639	.01421	-610.02067	-610.01391	-610.01296	-610.05514
IV	-610.07823	.04974	.05653	.05748	.01574	-610.02849	-610.02170	-610.02076	-610.06249
HCN	-93.45449	.01636	.01890	.01985	-.00300	-93.43813	-93.43559	-93.43465	-93.45749
$[UCH_3]^+$	-516.58290	.03202	.03595	.03690	.00328	-516.55087	-516.54694	-516.54600	-516.57961
$[UCH_3]^+ + HCN$ (V)	-610.03739	.04839	.05486	.05675	.00029	-609.98900	-609.98253	-609.98064	-610.03710

Table 1.1.1: $[UH]^+$ + CH_3CN B3LYP/SDD/6-311+g(d,p) Quintet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	0.000000	0.000000	0.021045
	H	0.000000	0.000000	-1.936098
CH_3CN	C	-1.924802	0.984461	-0.000015
	C	-3.381457	0.984487	-0.000000
	H	-3.758144	1.465575	0.904967
	H	-3.758156	1.527530	-0.869198
	H	-3.758174	-0.039776	-0.035766
	N	-0.772097	0.984458	0.000013
II	U	-0.568238	-0.039518	-0.025738
	H	-0.623379	-0.774579	1.845324
	C	2.022213	0.150280	-0.008388
	N	1.349216	1.144560	0.141612
	C	3.368560	-0.448248	-0.044018
	H	4.121056	0.328227	0.123199
	H	3.450121	-1.213064	0.731741
	H	3.540979	-0.929040	-1.009194
TSII→III	U	0.055553	-0.762879	0.280819
	H	-0.978521	0.643931	1.323840
	C	-0.126671	1.665677	0.216727
	N	-0.016144	1.051230	-0.857499
	C	-0.320941	3.039071	0.727440
	H	-0.155408	3.102722	1.801625
	H	0.366294	3.707460	0.201927
	H	-1.344366	3.360535	0.506435
III	U	-0.678000	-0.024231	-0.000002
	H	2.951280	1.603103	-0.000107
	C	2.618267	0.556757	0.000019
	N	1.364021	0.314390	0.000050
	C	3.696885	-0.467715	0.000028
	H	4.339837	-0.313333	-0.874806
	H	4.341327	-0.312081	0.873496
	H	3.304460	-1.483379	0.000965
TSIII→IV	U	0.543628	-0.573200	0.579860
	H	3.008398	2.547484	0.197218
	C	2.208647	1.881180	-0.077110
	N	1.355581	1.301219	-0.623916
	C	2.024583	-2.302497	0.055640
	H	2.733808	-2.124549	-0.762218
	H	2.616443	-2.558822	0.950128
	H	1.439170	-3.198016	-0.215256
IV	U	-0.177735	-0.279305	-0.013947
	H	2.929578	1.105170	-1.087934
	C	2.134024	0.702957	-0.461254
	N	1.876331	0.480388	0.699745
	C	-1.321940	1.772149	0.025076
	H	-0.985848	2.430149	0.838286
	H	-1.195729	2.338005	-0.909951
	H	-2.403193	1.609389	0.161586
UCH_3^+	U	-3.289712	1.030298	-0.450766
	C	-1.044265	0.778059	-0.038123
	H	-0.444203	1.483373	-0.634672
	H	-0.808150	0.957408	1.022779
	H	-0.702269	-0.239348	-0.285902
HCN	C	0.000000	0.000000	-0.498334
	H	0.000000	0.000000	-1.564845

	N	-0.000000	0.000000	0.650693

Table 1.2: $[UH]^+ + CH_3CN$ PBE1PBE/SDD/6-311+g(d,p) Quintet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-477.12109	.00377	.00614	.00708	-.01913	-477.11732	-477.11495	-477.11401	-477.14021
CH_3CN	-132.62746	.04543	.04903	.04997	.02143	-132.58203	-132.57844	-132.57749	-132.60603
$[UH]^+ + CH_3CN$ (**I**)	-609.74855	.04920	.05516	.05705	.00230	-609.69935	-609.69339	-609.69150	-609.74625
II	-609.81206	.05026	.05656	.05751	.01653	-609.76181	-609.75550	-609.75456	-609.79554
TSII→III	-609.80275	.05066	.05592	.05686	.01822	-609.75209	-609.74683	-609.74589	-609.78453
III	-609.85514	.05727	.06273	.06367	.02451	-609.79787	-609.79241	-609.79147	-609.83063
TSIII→IV	-609.79517	.05103	.05685	.05779	.01824	-609.74414	-609.73832	-609.73738	-609.77693
IV	-609.81383	.05013	.05689	.05783	.01619	-609.76370	-609.75694	-609.75600	-609.79764
HCN	-93.33544	.01649	.01903	.01997	-.00287	-93.31895	-93.31641	-93.31547	-93.33831
$[UCH_3]^+$	-516.42679	.03203	.03603	.03698	.00321	-516.39477	-516.39076	-516.38981	-516.42358
$[UCH_3]^+ + HCN$ (**V**)	-609.76223	.04852	.05506	.05695	.00034	-609.71371	-609.70717	-609.70528	-609.76189

Table 1.2.1: $[UH]^+ + CH_3CN$ PBE1PBE/SDD/6-311+g(d,p) Quintet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	-0.282792	0.024095	0.017719
	H	-0.733284	1.219330	1.490648
CH_3CN	C	-1.929495	0.984458	-0.000024
	C	-3.379841	0.984488	-0.000001
	H	-3.755309	1.465863	0.905510
	H	-3.755327	1.527855	-0.869719
	H	-3.755344	-0.040389	-0.035786
	N	-0.777514	0.984461	0.000021
II	U	-0.557163	-0.040143	-0.025084
	H	-0.529416	-0.827794	1.812523
	C	1.969716	0.154018	-0.010191
	N	1.318616	1.165209	0.145250
	C	3.304424	-0.453020	-0.048571
	H	4.065530	0.315802	0.115554
	H	3.378509	-1.218170	0.728444
	H	3.469204	-0.939095	-1.012997
TSII→III	U	0.073614	-0.711486	0.307564
	H	-1.045984	0.615771	1.317784
	C	-0.120056	1.665676	0.210311
	N	-0.003628	1.069056	-0.873754
	C	-0.310464	3.029708	0.726561
	H	-0.125403	3.093072	1.798167
	H	0.354837	3.708754	0.186039
	H	-1.343120	3.337195	0.528643
III	U	-0.672993	-0.024170	0.000006
	H	2.932951	1.602434	0.000180
	C	2.601194	0.554909	0.000058
	N	1.349033	0.313744	-0.000157
	C	3.670733	-0.466768	0.000059
	H	4.315071	-0.311363	-0.873965
	H	4.316262	-0.310510	0.873001

	H	3.276313	-1.482020	0.000678
TSIII→IV	U	0.178550	-0.814864	0.620037
	H	3.145200	1.031107	-0.503672
	C	2.121924	1.034815	-0.171120
	N	1.044491	1.339131	0.155275
	C	2.229931	-1.620852	0.018838
	H	3.261709	-1.552573	-0.324761
	H	2.252683	-2.147733	1.006427
	H	1.695769	-2.296232	-0.696678
IV	U	-0.178467	-0.276721	-0.014009
	H	2.878373	1.088313	-1.104265
	C	2.092776	0.684504	-0.464489
	N	1.859430	0.460182	0.701644
	C	-1.270863	1.772641	0.028577
	H	-0.925598	2.423084	0.845237
	H	-1.122999	2.340518	-0.903292
	H	-2.358289	1.642279	0.155131
HCN	C	0.000000	0.000000	-0.497856
	H	0.000000	0.000000	-1.566083
	N	-0.000000	-0.000000	0.650460

Table 1.3: $[UH]^+ + CH_3CN$ B3LYP/SDD/6-311+g(d,p) Triplet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-132.79616	.04515	.04876	.04970	.02113	-132.75101	-132.74740	-132.74646	-132.77503
CH_3CN	-477.14828	.00361	.00597	.00691	-.01880	-477.14467	-477.14231	-477.14136	-477.16708
$[UH]^+ + CH_3CN$ (**I**)	-609.94443	.04875	.05472	.05661	.00233	-609.89569	-609.88971	-609.88782	-609.94210
II	-610.07751	.04957	.05593	.05688	.01626	-610.02794	-610.02158	-610.02063	-610.06125
TSII→III	-610.05730	.05036	.05551	.05645	.01876	-610.00694	-610.00179	-610.00084	-610.03854
III	-610.08969	.05691	.06237	.06332	.02462	-610.03278	-610.02731	-610.02637	-610.06507
TSIII→IV	-610.04717	.05177	.05682	.05777	.02061	-609.99540	-609.99035	-609.98940	-610.02656
IV	-610.08235	.04978	.05652	.05747	.01634	-610.03257	-610.02582	-610.02488	-610.06601
HCN	-516.57310	.03193	.03590	.03684	.00362	-516.54117	-516.53720	-516.53626	-516.56948
$[UCH_3]^+$	-93.45449	.01636	.01890	.01985	-.00300	-93.43813	-93.43559	-93.43465	-93.45749
$[UCH_3]^+ + HCN$ (**V**)	-610.02759	.04829	.05480	.05669	.00063	-609.97930	-609.97279	-609.97090	-610.02697

Table 1.3.1: $[UH]^+ + CH_3CN$ B3LYP/SDD/6-311+g(d,p) Triplet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	-0.275143	0.003800	-0.007291
	H	-0.722447	1.190578	1.455215
CH_3CN	C	-1.924802	0.984461	-0.000015
	C	-3.381457	0.984487	-0.000000
	H	-3.758144	1.465575	0.904967
	H	-3.758156	1.527530	-0.869198
	H	-3.758174	-0.039776	-0.035766
	N	-0.772097	0.984458	0.000013
II	U	0.225312	-0.439592	-0.150674
	H	0.908112	-0.694200	1.700005
	C	-0.502999	1.818698	0.242628

	N	-1.361116	0.915792	0.220397
	C	-0.469980	3.276482	0.496148
	H	-1.475502	3.671105	0.659929
	H	0.150996	3.468968	1.376256
	H	0.004979	3.790499	-0.343375
TSII→III	U	-0.217406	-0.603487	-0.119396
	H	0.050210	0.772933	1.349212
	C	-0.512080	1.653392	0.134087
	N	-1.475018	0.980181	-0.405200
	C	-0.356478	3.083929	0.490840
	H	-1.144190	3.384491	1.189674
	H	0.617707	3.294870	0.930224
	H	-0.480905	3.678323	-0.419237
III	U	1.164608	-0.927065	-0.839965
	H	0.864224	2.005588	1.830746
	C	0.116093	1.498091	1.207679
	N	0.504749	0.565772	0.424519
	C	-1.285545	1.971340	1.359751
	H	-1.588167	1.867142	2.408695
	H	-1.328244	3.045687	1.144090
	H	-1.978169	1.432261	0.715423
TSIII→IV	U	-0.114660	0.621154	-0.715655
	H	0.924324	1.885626	2.166109
	C	0.622061	1.334762	1.282894
	N	0.907247	0.099620	0.944759
	C	-1.271835	1.773055	1.060366
	H	-2.007749	0.934829	1.005822
	H	-1.356593	2.172627	2.068300
	H	-1.548743	2.586641	0.364213
IV	U	-0.117690	-0.280543	-0.016037
	H	2.682908	1.432992	-0.955026
	C	1.863306	0.885265	-0.484768
	N	1.667919	0.595514	0.714846
	C	-1.549162	1.550665	0.035918
	H	-1.534517	2.076844	1.000744
	H	-1.295110	2.293356	-0.733710
	H	-2.586138	1.222545	-0.147470
UCH_3^+	U	-3.286944	1.029979	-0.450263
	C	-1.045147	0.778165	-0.038280
	H	-0.444776	1.483636	-0.634961
	H	-0.808810	0.957534	1.022921
	H	-0.702923	-0.239524	-0.286102
HCN	C	0.000000	0.000000	-0.498334
	H	0.000000	0.000000	-1.564845
	N	-0.000000	0.000000	0.650693

Table 1.4: $[UH]^+ + CH_3CN$ PBE1PBE/SDD/6-311+g(d,p) Triplet Spin Energies (Hartrees)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-477.06589	.00353	.00589	.00684	-.01891	-477.06236	-477.06000	-477.05905	-477.08480
CH_3CN	-132.62746	.04543	.04903	.04997	.02143	-132.58203	-132.57844	-132.57749	-132.60603
$[UH]^+ + CH_3CN$ (**I**)	-609.69335	.04896	.05492	.05681	.00252	-609.64439	-609.63843	-609.63654	-609.69083
II	-609.81324	.04986	.05621	.05715	.01654	-609.76338	-609.75703	-609.75608	-609.79670
TSII→III	-609.80021	.05071	.05585	.05679	.01914	-609.74950	-609.74436	-609.74342	-609.78107
III	-609.82240	.05726	.06272	.06367	.02497	-609.76514	-609.75968	-609.75873	-609.79743

TSIII→IV	-609.79056	.05182	.05693	.05787	.02059	-609.73874	-609.73363	-609.73269	-609.76997
IV	-609.81882	.05031	.05694	.05789	.01706	-609.76851	-609.76188	-609.76093	-609.80176
HCN	-93.33544	.01649	.01903	.01997	-.00287	-93.31895	-93.31641	-93.31547	-93.33831
$[UCH_3]^+$	-516.41461	.03195	.03599	.03694	.00357	-516.38266	-516.37862	-516.37767	-516.41104
$[UCH_3]^+$ + HCN (**V**)	-609.75005	.04844	.05502	.05691	.00070	-609.70161	-609.69503	-609.69314	-609.74935

Table 1.4.1: $[UH]^+$ + CH_3CN PBE1PBE/SDD/6-311+g(d,p) Triplet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	-0.280565	0.018185	0.010435
	H	-0.735512	1.225240	1.497931
CH_3CN	C	-1.929495	0.984458	-0.000024
	C	-3.379841	0.984488	-0.000001
	H	-3.755309	1.465863	0.905510
	H	-3.755327	1.527855	-0.869719
	H	-3.755344	-0.040389	-0.035786
	N	-0.777514	0.984461	0.000021
II	U	0.167912	-0.396152	-0.155275
	H	0.940615	-0.581615	1.649012
	C	-0.490639	1.795328	0.241322
	N	-1.382393	0.909725	0.263767
	C	-0.463862	3.245275	0.492794
	H	-1.471183	3.653287	0.603240
	H	0.104972	3.420825	1.412889
	H	0.074381	3.761078	-0.306434
TSII→III	U	-0.209963	-0.552652	-0.125537
	H	0.058224	0.741731	1.373162
	C	-0.510912	1.654662	0.128356
	N	-1.490398	0.987307	-0.390255
	C	-0.355797	3.076736	0.485289
	H	-1.150669	3.378227	1.175728
	H	0.616035	3.288298	0.930340
	H	-0.474678	3.670322	-0.426878
III	U	1.152187	-0.911275	-0.827607
	H	0.863860	2.004442	1.829740
	C	0.113257	1.498282	1.207243
	N	0.500845	0.567625	0.425133
	C	-1.281113	1.966719	1.356369
	H	-1.583019	1.864365	2.406058
	H	-1.323398	3.041819	1.142556
	H	-1.973070	1.426839	0.711446
TSIII→IV	U	-0.095780	0.648738	-0.668309
	H	0.935875	1.886363	2.154303
	C	0.638928	1.350686	1.257885
	N	0.871206	0.081607	0.964249
	C	-1.273649	1.767218	1.042754
	H	-2.015489	0.931252	0.996502
	H	-1.332131	2.150120	2.060914
	H	-1.574908	2.592329	0.368509
IV	U	-0.107451	-0.278783	-0.015076
	H	2.611368	1.436597	-0.953193
	C	1.786954	0.882545	-0.497712
	N	1.601634	0.628989	0.723050
	C	-1.544274	1.506944	0.029914
	H	-1.532195	2.044660	0.989124

	H	-1.279171	2.242980	-0.744602
	H	-2.581985	1.183938	-0.158882
UCH_3^+	U	-3.269914	1.028067	-0.447124
	C	-1.051626	0.778898	-0.039478
	H	-0.448351	1.483802	-0.635412
	H	-0.812296	0.957855	1.021974
	H	-0.706412	-0.238832	-0.286646
HCN	C	0.000000	0.000000	-0.497856
	H	0.000000	0.000000	-1.566083
	N	-0.000000	-0.000000	0.650460

Table 1.5: $[UH]^+ + CH_3CN$ B3LYP/SDD/6-311+g(d,p) Singlet Spin Energies (Hartrees)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-516.49451	.03174	.03581	.03675	.00439	-516.46277	-516.45871	-516.45776	-516.49012
CH_3CN	-76.45846	.02129	.02413	.02507	.00299	-76.43718	-76.43434	-76.43340	-76.45547
$[UH]^+ + CH_3CN$ (**I**)	-592.95297	.05303	.05993	.06182	.00738	-592.89995	-592.89305	-592.89116	-592.94559
II	-593.00750	.05582	.06312	.06406	.02281	-592.95168	-592.94438	-592.94344	-592.98469
TSII→III	-592.98456	.04976	.05610	.05704	.01849	-592.93480	-592.92847	-592.92752	-592.96608
III	-593.07282	.05071	.05725	.05819	.01953	-593.02211	-593.01558	-593.01463	-593.05329
TSIII→IV	-593.03595	.05113	.05660	.05755	.02081	-592.98482	-592.97934	-592.97840	-593.01514
IV	-593.05982	.05830	.06443	.06537	.02677	-593.00152	-592.99539	-592.99445	-593.03305
HCN	-40.53393	.04455	.04742	.04836	.02488	-40.48938	-40.48651	-40.48557	-40.50904
$[UCH_3]^+$	-552.50789	.01148	.01463	.01557	-.00833	-552.49641	-552.49326	-552.49232	-552.51622
$[UCH_3]^+ + HCN$ (**V**)	-593.04182	.05603	.06204	.06393	.01656	-592.98579	-592.97977	-592.97789	-593.02526

Table 1.5.1: $[UH]^+ + CH_3CN$ B3LYP/SDD/6-311+g(d,p) Singlet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	-0.274048	0.000897	-0.010869
	H	-0.723542	1.193481	1.458793
CH_3CN	C	-1.924802	0.984461	-0.000015
	C	-3.381457	0.984487	-0.000000
	H	-3.758144	1.465575	0.904967
	H	-3.758156	1.527530	-0.869198
	H	-3.758174	-0.039776	-0.035766
	N	-0.772097	0.984458	0.000013
II	U	-0.514404	-0.038849	-0.025579
	H	-0.632029	-0.697917	1.821330
	C	1.737010	-0.013448	-0.037414
	N	1.118160	1.100545	0.139786
	C	3.179968	-0.336233	-0.031305
	H	3.799725	0.562339	-0.054964
	H	3.398190	-0.898169	0.884808
	H	3.430264	-0.997854	-0.864126
TSII→III	U	0.217858	-0.450641	-0.166068
	H	0.212338	0.702370	1.457191

	C	-0.234443	1.590323	0.264081
	N	-1.189445	0.838772	-0.357769
	C	-0.350661	3.006808	0.685841
	H	-1.243481	3.157972	1.300017
	H	0.532108	3.341096	1.231012
	H	-0.464478	3.621046	-0.212990
III	U	-0.664649	-0.024450	0.004426
	H	2.874182	1.597800	0.161980
	C	2.562991	0.554811	0.026436
	N	1.313227	0.309175	-0.123752
	C	3.644428	-0.460899	0.015226
	H	4.361709	-0.205827	-0.774988
	H	4.207819	-0.399177	0.954278
	H	3.266860	-1.471054	-0.132210
TSIII→IV	U	-0.044710	0.635199	-0.654928
	H	0.947623	1.889528	2.137971
	C	0.629301	1.386468	1.232694
	N	0.819796	0.060014	0.975540
	C	-1.277601	1.776232	1.046108
	H	-1.984782	0.912270	1.000247
	H	-1.344419	2.153645	2.064554
	H	-1.591155	2.594958	0.374620
IV	U	-0.092302	-0.280093	-0.016333
	H	2.523504	1.537060	-0.922094
	C	1.714152	0.938638	-0.502432
	N	1.535746	0.649069	0.733016
	C	-1.589521	1.461690	0.036342
	H	-1.518087	2.061663	0.953300
	H	-1.391196	2.140198	-0.807426
	H	-2.620468	1.084220	-0.055750
UCH_3^+	U	-3.253294	1.047442	-0.437384
	C	-1.044015	0.762871	-0.042847
	H	-0.472086	1.487361	-0.644763
	H	-0.837913	0.958493	1.021838
	H	-0.681292	-0.246377	-0.283530
HCN	C	0.000000	0.000000	-0.498334
	H	0.000000	0.000000	-1.564845
	N	-0.000000	0.000000	0.650693

Table 1.6: $[UH]^+ + CH_3CN$ PBE1PBE/SDD/6-311+g(d,p) Singlet Spin Energies (Hartrees)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-516.32691	.03153	.03580	.03674	.00387	-516.29538	-516.29111	-516.29017	-516.32304
CH_3CN	-76.37202	.02160	.02444	.02538	.00331	-76.35042	-76.34758	-76.34664	-76.36871
$[UH]^+ + CH_3CN$ (**I**)	-592.69893	.05313	.06024	.06212	.00718	-592.64580	-592.63870	-592.63681	-592.69175
II	-592.75618	.05599	.06341	.06435	.02286	-592.70019	-592.69278	-592.69183	-592.73332
TSII→III	-592.73709	.05027	.05662	.05757	.01902	-592.68683	-592.68047	-592.67952	-592.71807
III	-592.82919	.05112	.05760	.05854	.02013	-592.77807	-592.77159	-592.77065	-592.80906
TSIII→IV	-592.79286	.05154	.05690	.05785	.02137	-592.74132	-592.73596	-592.73501	-592.77150
IV	-592.80953	.05847	.06434	.06528	.02737	-592.75106	-592.74519	-592.74424	-592.78216
HCN	-552.31752	.01154	.01470	.01564	-.01097	-552.30598	-552.30282	-552.30188	-552.32849
$[UCH_3]^+$	-40.47076	.04475	.04762	.04856	.02508	-40.42601	-40.42314	-40.42219	-40.44567
$[UCH_3]^+ + HCN$ (**V**)	-592.78828	.05629	.06232	.06421	.01412	-592.73199	-592.72596	-592.72407	-592.77416

Table 1.6.1: $[UH]^+$ + CH_3CN PBE1PBE/SDD/6-311+g(d,p) Singlet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	-0.274832	0.002976	-0.008307
	H	-0.722758	1.191402	1.456231
CH_3CN	C	-1.929495	0.984458	-0.000024
	C	-3.379841	0.984488	-0.000001
	H	-3.755309	1.465863	0.905510
	H	-3.755327	1.527855	-0.869719
	H	-3.755344	-0.040389	-0.035786
	N	-0.777514	0.984461	0.000021
II	U	-0.505820	-0.038360	-0.025164
	H	-0.541070	-0.787240	1.777197
	C	1.695170	-0.020889	-0.044714
	N	1.088284	1.104482	0.153655
	C	3.132564	-0.332788	-0.041180
	H	3.742856	0.556873	-0.212751
	H	3.376082	-0.732851	0.951953
	H	3.373215	-1.116968	-0.761522
TSII→III	U	0.209531	-0.414354	-0.158848
	H	0.222901	0.677667	1.470104
	C	-0.228711	1.593967	0.259240
	N	-1.194417	0.846052	-0.353381
	C	-0.349846	3.001569	0.681710
	H	-1.247195	3.148448	1.290551
	H	0.530588	3.338450	1.229690
	H	-0.463056	3.615948	-0.217752
III	U	-0.654393	-0.025611	0.007019
	H	2.833591	1.584399	0.270785
	C	2.526544	0.555870	0.045716
	N	1.285581	0.336593	-0.197415
	C	3.590790	-0.467911	0.021447
	H	4.357676	-0.163154	-0.702047
	H	4.098142	-0.491315	0.993616
	H	3.211708	-1.457652	-0.229150
TSIII→IV	U	-0.018503	0.636447	-0.616278
	H	0.956860	1.895544	2.126850
	C	0.643573	1.402142	1.212050
	N	0.748516	0.045775	1.016922
	C	-1.266448	1.792608	1.013648
	H	-1.948670	0.905296	0.960134
	H	-1.308791	2.104187	2.057644
	H	-1.652484	2.626314	0.405837
IV	U	-0.088522	-0.279036	-0.016306
	H	2.463081	1.548610	-0.927319
	C	1.661531	0.938539	-0.507784
	N	1.504495	0.651397	0.736408
	C	-1.564385	1.444612	0.039366
	H	-1.472617	2.064772	0.941924
	H	-1.355089	2.105325	-0.818196
	H	-2.605687	1.093905	-0.040629
UCH_3^+	U	-3.229849	1.070378	-0.424760
	C	-1.051291	0.744150	-0.050543
	H	-0.496983	1.487813	-0.650181
	H	-0.863313	0.958928	1.016452

	H	-0.647163	-0.251479	-0.277653
HCN	C	0.000000	0.000000	-0.497856
	H	0.000000	0.000000	-1.566083
	N	-0.000000	-0.000000	0.650460

Table 1.7.1: $[UH]^+ + CH_3CN$ B3LYP/SDD/6-311+g(d,p) Quintet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
Reactants (I)	0	0	0	0
II	-206.981	-205.934	-208.412	-172.501
TSII→III	-165.259	-166.879	-169.361	-127.416
III	-303.369	-304.708	-307.189	-266.192
TSIII→IV	-191.042	-188.973	-191.451	-158.368
IV	-211.584	-209.434	-211.915	-177.657
Products (V)	-107.903	-106.598	-106.601	-111.004

Table 1.7.2: $[UH]^+ + CH_3CN$ PBE1PBE/SDD/6-311+g(d,p) Quintet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
Reactants (I)	0	0	0	0
II	-163.991	-163.083	-165.561	-129.416
TSII→III	-138.482	-140.322	-142.801	-100.507
III	-258.68	-259.988	-262.466	-221.555
TSIII→IV	-117.609	-117.969	-120.447	-80.5661
IV	-168.967	-166.856	-169.334	-134.932
Products (V)	-37.7153	-36.1873	-36.1873	-41.0628

Table 1.7.3: $[UH]^+ + CH_3CN$ B3LYP/SDD/6-311+g(d,p) Triplet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
Reactants (I)	137.1036	137.1062	137.1036	138.4216
II	-210.127	-209.113	-211.592	-174.391
TSII→III	-154.994	-157.155	-159.636	-114.779
III	-222.842	-224.173	-226.654	-184.428
TSIII→IV	-124.696	-127.114	-129.592	-83.3255
IV	-222.277	-220.258	-222.74	-186.888
Products (V)	-82.4381	-81.0256	-81.0282	-84.3888

Table 1.7.4: $[UH]^+ + CH_3CN$ PBE1PBE/SDD/6-311+g(d,p) Triplet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	144.2844	144.2896	144.2896	145.5
II	-168.116	-167.084	-169.563	-132.467
TSII→III	-131.679	-133.835	-136.313	-91.4357
III	-172.742	-174.039	-176.518	-134.381
TSIII→IV	-103.434	-105.661	-108.139	-62.2795
IV	-181.58	-179.818	-182.296	-145.757
Products (V)	-5.93888	-4.3137	-4.3137	-8.14168

Table 1.7.5: $[UH]^+ + CH_3CN$ B3LYP/SDD/6-311+g(d,p) Singlet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	165.1177	165.1203	165.1177	169.1373
II	-88.0383	-87.8492	-90.3303	-48.8474
TSII→III	-32.1309	-34.9375	-37.4186	11.83838
III	-74.3909	-75.4201	-77.9012	-34.2759
TSIII→IV	-80.2878	-83.4489	-9.41242	-35.2552
IV	-109.956	-108.882	-111.363	-70.177
Products (V)	123.409	125.0631	125.0605	123.9577

Table 1.7.6: $[UH]^+ + CH_3CN$ B3LYP/SDD/6-311+g(d,p) Singlet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	267.1394	267.1394	267.1394	271.1564
II	-42.8272	-42.6565	-45.135	-3.24774
TSII→III	-5.74985	-8.6484	-11.1269	38.31918
III	-4.17192	-5.35865	-7.83712	36.57322
TSIII→IV	22.58718	19.34994	16.87146	67.7064
IV	-65.8265	-64.7737	-67.2522	-25.9242
Products (V)	223.2227	225.4333	225.4333	222.8997

Figure 3: $[UH]^+ + CH_3CN$ B3LYP/SDD/6-311+g(d,p) Relative Enthalpy (kJ/mol)

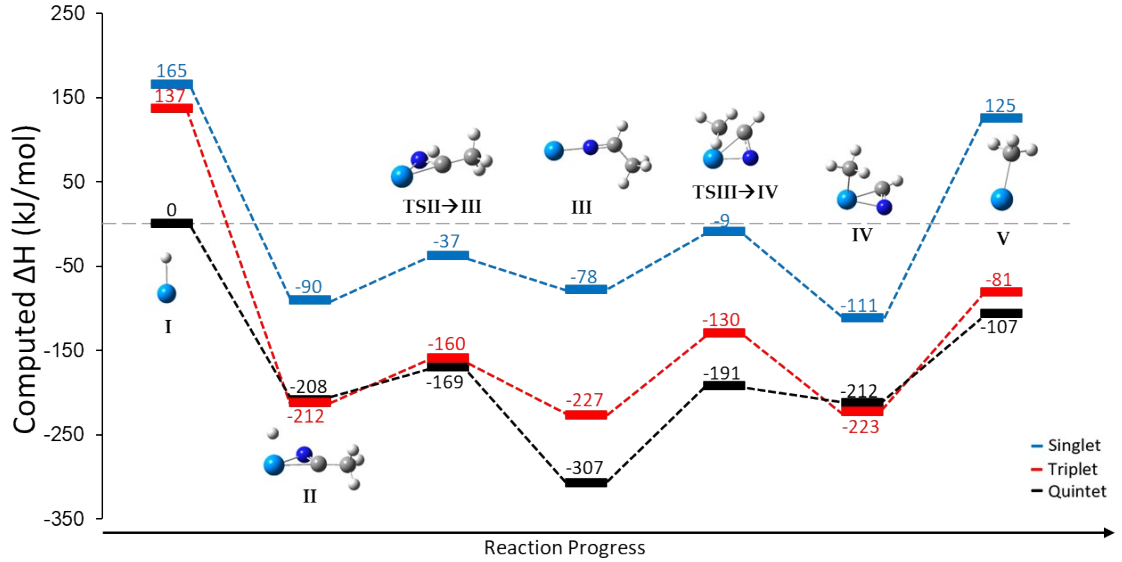

Figure 3.1: $[UH]^+ + CH_3CN$ PBE1PBE/SDD/6-311+g(d,p) Relative Enthalpy (kJ/mol)

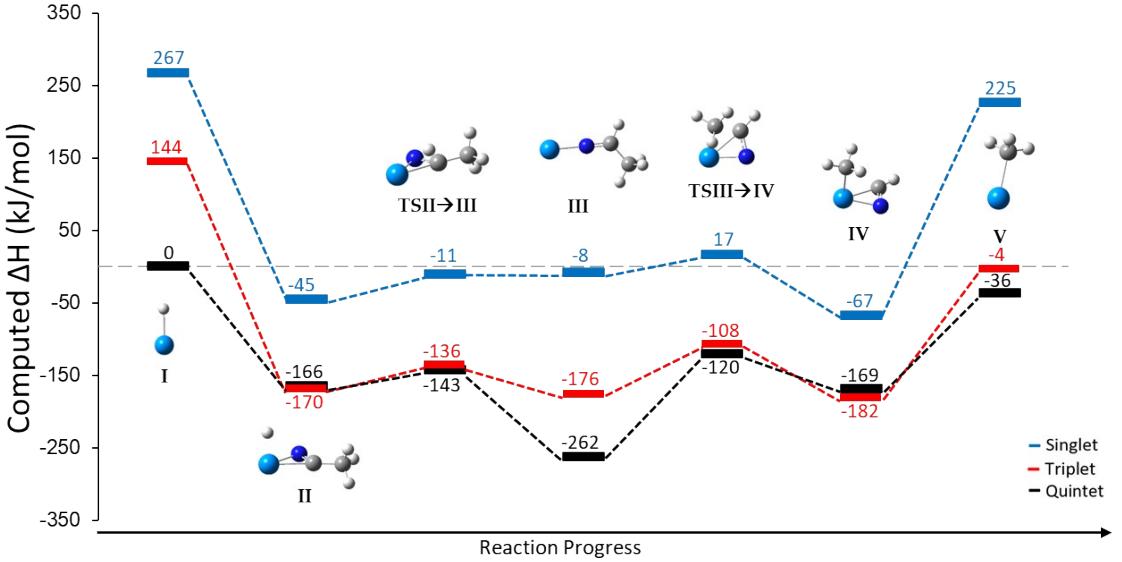

Table 2.1: $[UCH_3]^+ + H_2O$ B3LYP/SDD/6-311+g(d,p) Quintet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UCH_3]^+$	-516.58290	.03202	.03595	.03690	.00328	-516.55087	-516.54694	-516.54600	-516.57961
H_2O	-76.45846	.02129	.02413	.02507	.00299	-76.43718	-76.43434	-76.43340	-76.45547
$[UCH_3]^+ + H_2O$ (**I**)	-593.04136	.05331	.06008	.06197	.00628	-592.98805	-592.98128	-592.97939	-593.03508
II	-593.08696	.05609	.06337	.06431	.02116	-593.03087	-593.02359	-593.02265	-593.06580
TSII→III	-593.04514	.04859	.05496	.05590	.01570	-592.99655	-592.99018	-592.98924	-593.02944
III	-593.07478	.04944	.05685	.05780	.01474	-593.02534	-593.01793	-593.01699	-593.06004
TSIII→IV	-593.07363	.04970	.05609	.05704	.01638	-593.02393	-593.01754	-593.01660	-593.05726
IV	-593.14012	.05774	.06479	.06574	.02198	-593.08239	-593.07533	-593.07439	-593.11815
$[UOH]^+$	-552.59856	.01139	.01459	.01553	-.01207	-552.58717	-552.58397	-552.58303	-552.61063
CH_4	-40.53393	.04455	.04742	.04836	.02488	-40.48938	-40.48651	-40.48557	-40.50904
$[UOH]^+ + CH_4$ (**V**)	-593.13249	.05593	.06200	.06389	.01282	-593.07655	-593.07048	-593.06859	-593.11967

Table 2.1.1: $[UCH_3]^+ + H_2O$ B3LYP/SDD/6-311+g(d,p) Quintet Spin Structure Coordinates

Structure	Coordinates			
$[UCH_3]^+$	U	-3.289712	1.030298	-0.450766
	C	-1.044265	0.778059	-0.038123
	H	-0.444203	1.483373	-0.634672
	H	-0.808150	0.957408	1.022779
	H	-0.702269	-0.239348	-0.285902
H_2O	O	-1.313436	-0.308152	0.000000
	H	-1.631916	-1.215829	0.000000
	H	-0.354171	-0.379700	0.000000
II	U	-3.338670	0.774412	-0.166271
	C	-1.011103	0.734771	-0.057839
	H	-0.500447	1.335336	-0.823166
	H	-0.655571	1.079786	0.925727
	H	-0.666353	-0.305611	-0.183147
	O	-3.865348	3.016401	-1.114914
	H	-4.347517	3.214983	-1.933403
	H	-3.549174	3.863861	-0.764044
TSII→III	U	-3.434974	0.781127	-0.527464
	C	-1.106975	0.900606	-0.231472
	H	-0.561561	0.912178	-1.186444
	H	-0.750778	0.024430	0.334049
	H	-0.795429	1.795903	0.323571
	O	-3.699246	2.770124	-1.309664
	H	-3.680951	3.683451	-1.626090
	H	-3.904270	2.846120	0.106454
III	U	-2.927481	2.276272	0.486089
	C	-0.932131	0.361536	-0.212394
	H	-0.446007	1.108368	-0.835804
	H	-0.476015	0.104332	0.739072
	H	-1.613130	-0.347365	-0.676506
	O	-3.850615	2.189566	-1.305999
	H	-4.232687	2.229301	-2.190792
	H	-1.525572	3.613698	-0.079000
TSIII→IV	U	-3.172978	1.982015	0.496788
	C	-0.916116	0.589719	-0.242155
	H	-0.500928	1.066811	-1.120710

	H	-0.307215	0.595550	0.656462
	H	-1.564634	-0.275221	-0.411147
	O	-3.910521	2.202301	-1.369116
	H	-4.187955	2.356848	-2.279968
	H	-1.443290	3.017684	0.194514
IV	U	-3.731002	1.664271	-0.427065
	C	-0.708604	1.102026	-0.195553
	H	0.374311	0.982645	-0.140127
	H	-1.060959	1.335693	0.816577
	H	-1.125015	0.156879	-0.561760
	O	-5.076850	2.956667	-1.175199
	H	-5.710450	3.587604	-1.539551
	H	-0.895612	1.928156	-0.894381
CH_4	C	-1.155386	-0.323437	0.000000
	H	-0.791856	-1.351694	-0.000000
	H	-0.791837	0.190685	0.890494
	H	-0.791837	0.190685	-0.890494
	H	-2.246013	-0.323423	0.000000
$[UOH]^+$	U	-0.232296	-0.100323	-0.331137
	O	-0.430081	-0.996584	-2.100677
	H	-0.514192	-1.437147	-2.955227

Table 2.2: $[UCH_3]^+ + H_2O$ PBE1PBE/SDD/6-311+g(d,p) Quintet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UCH_3]^+$	-516.42679	.03203	.03603	.03698	.00321	-516.39477	-516.39076	-516.38981	-516.42358
H_2O	-76.37202	.02160	.02444	.02538	.00331	-76.35042	-76.34758	-76.34664	-76.36871
$[UCH_3]^+ + H_2O$ (**I**)	-592.79881	.05362	.06047	.06236	.00652	-592.74519	-592.73834	-592.73645	-592.79229
II	-592.84768	.05652	.06376	.06471	.02195	-592.79115	-592.78391	-592.78297	-592.82573
TSII→III	-592.80708	.04872	.05518	.05613	.01580	-592.75836	-592.75190	-592.75096	-592.79128
III	-592.83241	.04982	.05714	.05809	.01545	-592.78259	-592.77527	-592.77433	-592.81696
TSIII→IV	-592.83177	.04987	.05632	.05727	.01652	-592.78190	-592.77544	-592.77450	-592.81524
IV	-592.89809	.05861	.06522	.06616	.02393	-592.83948	-592.83287	-592.83193	-592.87416
$[UOH]^+$	-552.41689	.01156	.01473	.01567	-.01092	-552.40533	-552.40216	-552.40122	-552.42780
CH_4	-40.47076	.04475	.04762	.04856	.02508	-40.42601	-40.42314	-40.42219	-40.44567
$[UOH]^+ + CH_4$ (**V**)	-592.88764	.05630	.06234	.06423	.01417	-592.83134	-592.82530	-592.82341	-592.87348

Table 2.2.1: $[UCH_3]^+ + H_2O$ PBE1PBE/SDD/6-311+g(d,p) Quintet Spin Structure Coordinates

Structure	Coordinates			
$[UCH_3]^+$	U	-3.272222	1.028329	-0.447550
	C	-1.051155	0.778843	-0.039390
	H	-0.447809	1.483494	-0.635086
	H	-0.811631	0.957714	1.021772
	H	-0.705783	-0.238591	-0.286431
H_2O	O	-1.313077	-0.308700	0.000000
	H	-1.629005	-1.213533	0.000000
	H	-0.357440	-0.381448	0.000000
II	U	-3.405649	0.752138	0.011670
	C	-1.105156	0.786988	-0.144444
	H	-0.670669	1.289778	-1.018643

	H	-0.689293	1.270370	0.756200
	H	-0.729561	-0.250716	-0.152148
	O	-3.753504	2.941224	-1.028813
	H	-3.629017	3.151441	-1.964715
	H	-3.951333	3.772717	-0.576164
TSII→III	U	-3.460408	0.864205	-0.302310
	C	-1.136530	0.902908	-0.216880
	H	-0.645546	1.210015	-1.150081
	H	-0.734903	-0.088306	0.051517
	H	-0.794801	1.604806	0.561031
	O	-3.698853	2.697106	-1.353048
	H	-3.695236	3.548622	-1.803159
	H	-3.767907	2.974583	0.095870
III	U	-2.909570	2.265824	0.500943
	C	-0.970370	0.403455	-0.215883
	H	-0.510147	1.213341	-0.783100
	H	-0.499449	0.084797	0.710584
	H	-1.650443	-0.277793	-0.723920
	O	-3.802251	2.144056	-1.284568
	H	-4.177492	2.162707	-2.170194
	H	-1.483917	3.539320	-0.109197
TSIII→IV	U	-3.146089	1.990025	0.504358
	C	-0.942696	0.562335	-0.256499
	H	-0.594542	1.078844	-1.144111
	H	-0.311351	0.601395	0.627086
	H	-1.585914	-0.311602	-0.396878
	O	-3.843541	2.194950	-1.359160
	H	-4.114952	2.347332	-2.269458
	H	-1.464552	3.072429	0.219330
IV	U	-3.740867	1.207207	-0.591915
	C	-0.857493	1.182405	-0.213158
	H	0.225251	1.181376	-0.075340
	H	-1.303062	1.049330	0.783082
	H	-1.089300	0.349370	-0.891400
	O	-4.807334	2.786640	-1.176353
	H	-5.290841	3.569569	-1.459551
	H	-1.110532	2.158043	-0.652425
CH_4	C	-1.155386	-0.323437	-0.000000
	H	-0.791754	-1.351983	0.000000
	H	-0.791735	0.190830	0.890743
	H	-0.791735	0.190830	-0.890743
	H	-2.246319	-0.323423	-0.000000
$[UOH]^+$	U	-0.234402	-0.104984	-0.341597
	O	-0.426395	-0.995996	-2.095363
	H	-0.515772	-1.433074	-2.950081

Table 2.3: $[UCH_3]^+ + H_2O$ B3LYP/SDD/6-311+g(d,p) Singlet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UCH_3]^+$	-516.49451	.03174	.03581	.03675	.00439	-516.46277	-516.45871	-516.45776	-516.49012
H_2O	-76.45846	.02129	.02413	.02507	.00299	-76.43718	-76.43434	-76.43340	-76.45547
$[UCH_3]^+ + H_2O$ (**I**)	-592.95297	.05303	.05993	.06182	.00738	-592.89995	-592.89305	-592.89116	-592.94559
II	-593.00750	.05582	.06312	.06406	.02281	-592.95168	-592.94438	-592.94344	-592.98469
TSII→III	-592.98456	.04976	.05610	.05704	.01849	-592.93480	-592.92847	-592.92752	-592.96608
III	-593.07282	.05071	.05725	.05819	.01953	-593.02211	-593.01558	-593.01463	-593.05329

TSIII→IV	-593.03595	.05113	.05660	.05755	.02081	-592.98482	-592.97934	-592.97840	-593.01514
IV	-593.05982	.05830	.06443	.06537	.02677	-593.00152	-592.99539	-592.99445	-593.03305
CH_4	-40.53393	.04455	.04742	.04836	.02488	-40.48938	-40.48651	-40.48557	-40.50904
$[UOH]^+$	-552.50789	.01148	.01463	.01557	-.00833	-552.49641	-552.49326	-552.49232	-552.51622
$[UOH]^+ + CH_4$ (**V**)	-593.04182	.05603	.06204	.06393	.01656	-592.98579	-592.97977	-592.97789	-593.02526

Table 2.3.1: $[UCH_3]^+ + H_2O$ B3LYP/SDD/6-311+g(d,p) Singlet Spin Structure Coordinates

Structure	Coordinates			
$[UCH_3]^+$	U	-3.253294	1.047442	-0.437384
	C	-1.044015	0.762871	-0.042847
	H	-0.472086	1.487361	-0.644763
	H	-0.837913	0.958493	1.021838
	H	-0.681292	-0.246377	-0.283530
H_2O	O	-1.313436	-0.308152	0.000000
	H	-1.631916	-1.215829	0.000000
	H	-0.354171	-0.379700	0.000000
II	U	-3.160569	0.651947	-0.890090
	C	-1.036646	0.788296	-0.067015
	H	-0.315708	1.194791	-0.790241
	H	-0.946219	1.351137	0.872005
	H	-0.754375	-0.260107	0.141879
	O	-3.804704	2.962712	-1.100931
	H	-4.712879	3.300985	-1.169353
	H	-3.203084	3.724177	-1.113314
TSII→III	U	-3.396388	0.827527	-0.374106
	C	-1.117903	0.899598	-0.246342
	H	-0.548553	1.093309	-1.162560
	H	-0.783060	-0.064562	0.173624
	H	-0.874158	1.693146	0.480203
	O	-3.736161	2.728880	-1.252540
	H	-3.774074	3.598905	-1.676094
	H	-3.703887	2.937135	-0.059245
III	U	-2.725338	2.089793	0.461273
	C	-1.202658	0.539161	-0.189597
	H	-0.571292	1.108426	-0.894628
	H	-0.579616	0.261173	0.676175
	H	-1.546576	-0.371596	-0.690901
	O	-3.722816	2.147348	-1.246029
	H	-4.090928	2.186736	-2.139259
	H	-1.564415	3.574666	-0.052367
TSIII→IV	U	-2.956166	1.668753	0.433186
	C	-0.987366	0.920107	-0.282029
	H	-0.106007	0.950935	-0.919937
	H	-0.695674	0.552157	0.727806
	H	-1.710685	0.151058	-0.744497
	O	-3.974237	2.275830	-1.178532
	H	-4.372105	2.571756	-2.008166
	H	-1.201398	2.445111	-0.103164
IV	U	-3.591418	1.020416	-0.778183
	C	-1.016168	1.242228	-0.265381
	H	0.034325	1.444457	-0.054772
	H	-1.591455	1.695740	0.568792
	H	-1.141412	0.145678	-0.303434
	O	-4.501291	2.784836	-0.977007

	H	-4.894819	3.662548	-1.062440
	H	-1.231944	1.718037	-1.244634
CH_4	C	-1.155386	-0.323437	0.000000
	H	-0.791856	-1.351694	-0.000000
	H	-0.791837	0.190685	0.890494
	H	-0.791837	0.190685	-0.890494
	H	-2.246013	-0.323423	0.000000
$[UOH]^+$	U	-0.232542	-0.091598	-0.316443
	O	-0.418249	-0.970342	-2.041828
	H	-0.511919	-1.406538	-2.900016

Table 2.4: $[UCH_3]^+ + H_2O$ PBE1PBE/SDD/6-311+g(d,p) Singlet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UCH_3]^+$	-516.32691	.03153	.03580	.03674	.00387	-516.29538	-516.29111	-516.29017	-516.32304
H_2O	-76.37202	.02160	.02444	.02538	.00331	-76.35042	-76.34758	-76.34664	-76.36871
$[UCH_3]^+ + H_2O$ (**I**)	-592.69893	.05313	.06024	.06212	.00718	-592.64580	-592.63870	-592.63681	-592.69175
II	-592.75618	.05599	.06341	.06435	.02286	-592.70019	-592.69278	-592.69183	-592.73332
TSII→III	-592.73709	.05027	.05662	.05757	.01902	-592.68683	-592.68047	-592.67952	-592.71807
III	-592.82919	.05112	.05760	.05854	.02013	-592.77807	-592.77159	-592.77065	-592.80906
TSIII→IV	-592.79286	.05154	.05690	.05785	.02137	-592.74132	-592.73596	-592.73501	-592.77150
IV	-592.80953	.05847	.06434	.06528	.02737	-592.75106	-592.74519	-592.74424	-592.78216
$[UOH]^+$	-552.31752	.01154	.01470	.01564	-.01097	-552.30598	-552.30282	-552.30188	-552.32849
CH_4	-40.47076	.04475	.04762	.04856	.02508	-40.42601	-40.42314	-40.42219	-40.44567
$[UOH]^+ + CH_4$ (**V**)	-592.78828	.05629	.06232	.06421	.01412	-592.73199	-592.72596	-592.72407	-592.77416

Table 2.4.1: $[UCH_3]^+ + H_2O$ PBE1PBE/SDD/6-311+g(d,p) Singlet Spin Structure Coordinates

Structure	Coordinates			
$[UCH_3]^+$	U	-3.229849	1.070378	-0.424760
	C	-1.051291	0.744150	-0.050543
	H	-0.496983	1.487813	-0.650181
	H	-0.863313	0.958928	1.016452
	H	-0.647163	-0.251479	-0.277653
H_2O	O	-1.313077	-0.308700	0.000000
	H	-1.629005	-1.213533	0.000000
	H	-0.357440	-0.381448	0.000000
II	U	-3.146413	0.658233	-0.897347
	C	-1.054426	0.812483	-0.074391
	H	-0.324347	1.195299	-0.802661
	H	-0.943879	1.372075	0.864585
	H	-0.798087	-0.244991	0.135996
	O	-3.787786	2.941504	-1.090531
	H	-4.690672	3.278603	-1.185102
	H	-3.188572	3.700733	-1.067606
TSII→III	U	-3.388260	0.834577	-0.336028
	C	-1.136669	0.895997	-0.272149
	H	-0.539104	1.116876	-1.163083
	H	-0.786164	-0.058543	0.158365
	H	-0.944819	1.694059	0.471660
	O	-3.716732	2.716126	-1.229991

	H	-3.755154	3.573988	-1.672037
	H	-3.667282	2.940857	-0.073797
III	U	-2.699936	2.107530	0.461343
	C	-1.236460	0.538515	-0.172968
	H	-0.607262	1.199269	-0.807339
	H	-0.617363	0.204434	0.674957
	H	-1.529828	-0.328872	-0.771878
	O	-3.699385	2.125780	-1.222563
	H	-4.082208	2.143990	-2.107539
	H	-1.531198	3.545060	-0.129345
TSIII→IV	U	-2.948558	1.620613	0.442167
	C	-1.008816	0.956977	-0.301467
	H	-0.127658	0.981240	-0.942716
	H	-0.712584	0.584494	0.710892
	H	-1.733296	0.164350	-0.751211
	O	-3.933635	2.243570	-1.159594
	H	-4.317793	2.547474	-1.990026
	H	-1.221300	2.436989	-0.083377
IV	U	-3.510306	1.007025	-0.769842
	C	-1.066508	1.257754	-0.275723
	H	-0.018948	1.475404	-0.062969
	H	-1.649652	1.712761	0.563961
	H	-1.175598	0.152446	-0.304575
	O	-4.425626	2.751932	-0.959570
	H	-4.808118	3.632495	-1.038155
	H	-1.279426	1.724123	-1.270186
CH_4	C	-1.155386	-0.323437	-0.000000
	H	-0.791754	-1.351983	0.000000
	H	-0.791735	0.190830	0.890743
	H	-0.791735	0.190830	-0.890743
	H	-2.246319	-0.323423	-0.000000
$[UOH]^+$	U	-0.379865	-0.013097	-0.353081
	O	-0.379789	-0.990924	-2.032415
	H	-0.403056	-1.464458	-2.872792

Table 2.5: $[UCH_3]^+ + H_2O$ B3LYP/SDD/6-311+g(d,p) Triplet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UCH_3]^+$	-516.57310	.03193	.03590	.03684	.00362	-516.54117	-516.53720	-516.53626	-516.56948
H_2O	-76.45846	.02129	.02413	.02507	.00299	-76.43718	-76.43434	-76.43340	-76.45547
$[UCH_3]^+ + H_2O$ (I)	-593.03156	.05321	.06002	.06191	.00662	-592.97835	-592.97154	-592.96965	-593.02495
II	-593.07715	.05596	.06324	.06418	.02167	-593.02119	-593.01392	-593.01297	-593.05548
TSII→III	-593.04529	.04904	.05536	.05630	.01673	-592.99625	-592.98993	-592.98899	-593.02856
III	-593.11485	.05065	.05722	.05817	.01826	-593.06420	-593.05763	-593.05669	-593.09659
TSIII→IV	-593.08637	.05051	.05630	.05724	.01868	-593.03586	-593.03007	-593.02913	-593.06769
IV	-593.13129	.05802	.06487	.06582	.02268	-593.07327	-593.06642	-593.06548	-593.10861
$[UOH]^+$	-552.56987	.01135	.01456	.01551	-.01109	-552.55852	-552.55531	-552.55436	-552.58096
CH_4	-40.53393	.04455	.04742	.04836	.02488	-40.48938	-40.48651	-40.48557	-40.50904
$[UOH]^+ + CH_4$ (V)	-593.10380	.05590	.06198	.06387	.01380	-593.04790	-593.04182	-593.03993	-593.09000

Table 2.5.1: $[UCH_3]^+ + H_2O$ B3LYP/SDD/6-311+g(d,p) Triplet Spin Structure Coordinates

Structure	Coordinates			
$[UCH_3]^+$	U	-3.286944	1.029979	-0.450263
	C	-1.045147	0.778165	-0.038280
	H	-0.444776	1.483636	-0.634961
	H	-0.808810	0.957534	1.022921
	H	-0.702923	-0.239524	-0.286102
H_2O	O	-1.313436	-0.308152	0.000000
	H	-1.631916	-1.215829	0.000000
	H	-0.354171	-0.379700	0.000000
II	U	-3.380145	0.732612	-0.095543
	C	-1.057463	0.765945	-0.138866
	H	-0.562147	1.168046	-1.031003
	H	-0.685551	1.326306	0.734858
	H	-0.716259	-0.277544	-0.019170
	O	-3.804090	2.978936	-1.043022
	H	-3.743314	3.227118	-1.979808
	H	-3.985214	3.792519	-0.544506
TSII→III	U	-3.482317	0.896542	-0.271659
	C	-1.153649	0.864411	-0.157171
	H	-0.662719	0.907786	-1.139231
	H	-0.770246	1.709311	0.433626
	H	-0.817690	-0.061981	0.337470
	O	-3.689075	2.746851	-1.355545
	H	-3.652358	3.570870	-1.862310
	H	-3.706129	3.080148	-0.102239
III	U	-2.718056	2.073979	0.403038
	C	-1.158951	0.516460	-0.161413
	H	-0.485641	1.112348	-0.805635
	H	-0.588616	0.205445	0.727666
	H	-1.477111	-0.371535	-0.717851
	O	-3.790423	2.175648	-1.272803
	H	-4.230550	2.269872	-2.128980
	H	-1.554291	3.553491	-0.119356
TSIII→IV	U	-3.050986	1.766908	0.424933
	C	-0.977684	0.956502	-0.205015
	H	-0.165862	1.034682	-0.924888
	H	-0.565851	0.671472	0.777223
	H	-1.657487	0.114648	-0.569141
	O	-3.982249	2.127681	-1.327902
	H	-4.356794	2.314032	-2.197609
	H	-1.246726	2.549782	-0.052935
IV	U	-3.797484	1.324014	-0.572370
	C	-0.783752	1.164152	-0.223110
	H	0.291290	1.092153	-0.049325
	H	-1.230834	1.543645	0.706397
	H	-1.135846	0.153681	-0.465551
	O	-4.908609	2.904753	-1.100011
	H	-5.437518	3.671223	-1.355404
	H	-0.931429	1.860320	-1.057685
CH_4	C	-1.155386	-0.323437	0.000000
	H	-0.791856	-1.351694	-0.000000
	H	-0.791837	0.190685	0.890494
	H	-0.791837	0.190685	-0.890494
	H	-2.246013	-0.323423	0.000000
$[UOH]^+$	U	-0.233077	-0.100261	-0.331941
	O	-0.427826	-0.997432	-2.099505
	H	-0.515666	-1.436362	-2.955596

Table 2.6: $[UCH_3]^+ + H_2O$ PBE1PBE/SDD/6-311+g(d,p) Triplet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UCH_3]^+$	-516.41461	.03195	.03599	.03694	.00357	-516.38266	-516.37862	-516.37767	-516.41104
H_2O	-76.37202	.02160	.02444	.02538	.00331	-76.35042	-76.34758	-76.34664	-76.36871
$[UCH_3]^+ + H_2O$ (I)	-592.78663	.05355	.06043	.06232	.00688	-592.73308	-592.72620	-592.72431	-592.77975
II	-592.80940	.05624	.06361	.06456	.02181	-592.75316	-592.74579	-592.74484	-592.78760
TSII→III	-592.78500	.04962	.05601	.05695	.01723	-592.73538	-592.72899	-592.72804	-592.76776
III	-592.87494	.05106	.05758	.05852	.01884	-592.82388	-592.81736	-592.81642	-592.85610
TSIII→IV	-592.84836	.05089	.05661	.05755	.01922	-592.79747	-592.79175	-592.79080	-592.82914
IV	-592.88741	.05827	.06497	.06592	.02277	-592.82914	-592.82244	-592.82149	-592.86464
$[UOH]^+$	-552.40278	.01147	.01464	.01559	-.01094	-552.39130	-552.38813	-552.38719	-552.41372
CH_4	-40.47076	.04475	.04762	.04856	.02508	-40.42601	-40.42314	-40.42219	-40.44567
$[UOH]^+ + CH_4$ (V)	-592.87353	.05622	.06226	.06415	.01414	-592.81731	-592.81127	-592.80938	-592.85939

Table 2.6.1: $[UCH_3]^+ + H_2O$ PBE1PBE/SDD/6-311+g(d,p) Triplet Spin Structure Coordinates

Structure	Coordinates			
$[UCH_3]^+$	U	-3.269914	1.028067	-0.447124
	C	-1.051626	0.778898	-0.039478
	H	-0.448351	1.483802	-0.635412
	H	-0.812296	0.957855	1.021974
	H	-0.706412	-0.238832	-0.286646
H_2O	O	-1.313077	-0.308700	0.000000
	H	-1.629005	-1.213533	0.000000
	H	-0.357440	-0.381448	0.000000
II	U	-3.206961	0.660235	-0.735059
	C	-1.026076	0.789835	-0.080097
	H	-0.343518	1.115876	-0.878450
	H	-0.811965	1.381861	0.819771
	H	-0.774708	-0.262820	0.156334
	O	-3.831622	2.976863	-1.072364
	H	-4.603856	3.302097	-1.556548
	H	-3.335476	3.749993	-0.770647
TSII→III	U	-3.449573	0.940461	-0.257353
	C	-1.154808	0.851223	-0.183668
	H	-0.638218	0.821971	-1.152387
	H	-0.775105	1.732878	0.358950
	H	-0.836789	-0.039727	0.384801
	O	-3.645194	2.762677	-1.334079
	H	-3.591840	3.604249	-1.803962
	H	-3.842656	3.040207	-0.129361
III	U	-2.700177	2.082425	0.407562
	C	-1.193391	0.514943	-0.147726
	H	-0.539490	1.185533	-0.747834
	H	-0.607402	0.173777	0.719532
	H	-1.462143	-0.344840	-0.769605
	O	-3.761466	2.159750	-1.252979
	H	-4.207691	2.243727	-2.104190
	H	-1.531879	3.520393	-0.180094

TSIII→IV	U	-3.036689	1.753088	0.439089
	C	-1.006821	0.975118	-0.218306
	H	-0.198601	1.040501	-0.945463
	H	-0.585150	0.693119	0.763668
	H	-1.687190	0.119390	-0.563579
	O	-3.929711	2.108519	-1.311864
	H	-4.292270	2.289718	-2.184920
	H	-1.267206	2.556254	-0.053958
IV	U	-3.744123	0.983565	-0.738033
	C	-0.984877	1.246512	-0.258563
	H	0.075673	1.422286	-0.067871
	H	-1.528291	1.662269	0.606883
	H	-1.114729	0.158682	-0.349284
	O	-4.524138	2.791672	-0.995232
	H	-4.891894	3.672974	-1.118693
	H	-1.221801	1.775979	-1.196265
CH_4	C	-1.155386	-0.323437	-0.000000
	H	-0.791754	-1.351983	0.000000
	H	-0.791735	0.190830	0.890743
	H	-0.791735	0.190830	-0.890743
	H	-2.246319	-0.323423	-0.000000
$[UOH]^+$	U	-0.233077	-0.100261	-0.331941
	O	-0.427826	-0.997432	-2.099505
	H	-0.515666	-1.436362	-2.955596

Table 2.7.1: $[UCH_3]^+ + H_2O$ B3LYP/SDD/6-311+g(d,p) Quintet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
Reactants (**I**)	-107.903	-106.598	-106.601	-111.004
II	-220.335	-217.691	-220.172	-191.646
TSII→*III*	-130.233	-129.973	-132.454	-96.1773
III	-205.818	-202.82	-205.301	-176.533
TSIII→*IV*	-202.116	-201.806	-204.285	-169.216
IV	-355.595	-353.529	-356.01	-329.088
Products (**V**)	-340.27	-340.793	-340.795	-333.084

Table 2.7.2: $[UCH_3]^+ + H_2O$ PBE1PBE/SDD/6-311+g(d,p) Quintet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
Reactants (**I**)	-37.7153	-36.1873	-36.1873	-41.0628
II	-158.404	-155.837	-158.318	-128.854
TSII→*III*	-72.2984	-71.7864	-74.2649	-38.4268
III	-135.922	-133.142	-135.623	-105.842
TSIII→*IV*	-134.103	-133.599	-136.08	-101.334
IV	-285.292	-284.371	-286.852	-256.013
Products (**V**)	-263.915	-264.498	-264.498	-254.225

Table 2.7.3: $[UCH_3]^+ + H_2O$ B3LYP/SDD/6-311+g(d,p) Singlet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	123.409	125.0631	125.0605	123.9577
II	-12.4186	-9.72223	-12.2033	21.30068
TSII→III	31.89458	32.06523	29.58414	70.17174
III	-197.335	-196.639	-199.121	-158.811
TSIII→IV	-99.4198	-101.512	-103.993	-58.6379
IV	-143.263	-143.654	-146.135	-105.653
Products (V)	-101.974	-102.644	-102.644	-85.208

Table 2.7.4: $[UCH_3]^+ + H_2O$ PBE1PBE/SDD/6-311+g(d,p) Singlet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	223.2227	225.4333	225.4333	222.8997
II	80.4322	83.44627	80.9678	113.7682
TSII→III	115.5115	115.7609	113.2798	153.7887
III	-124.047	-123.49	-125.969	-85.0977
TSIII→IV	-27.5756	-29.9281	-32.4092	13.52658
IV	-53.1296	-54.1562	-56.6347	-14.4718
Products (V)	-3.06396	-3.67833	-3.67833	6.532244

Table 2.7.5: $[UCH_3]^+ + H_2O$ B3LYP/SDD/6-311+g(d,p) Triplet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	-82.4381	-81.0256	-81.0282	-84.3888
II	-194.917	-192.281	-194.762	-164.566
TSII→III	-129.432	-129.314	-131.795	-93.8748
III	-307.845	-307.06	-309.541	-272.493
TSIII→IV	-233.425	-234.699	-237.177	-196.613
IV	-331.658	-330.138	-332.619	-304.054
Products (V)	-265.039	-265.54	-265.543	-255.196

Table 2.7.6: $[UCH_3]^+ + H_2O$ PBE1PBE/SDD/6-311+g(d,p) Triplet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	-5.93888	-4.3137	-4.3137	-8.14168
II	-58.6432	-55.7289	-58.21	-28.7414
TSII→III	-11.9749	-11.631	-14.1094	23.32757
III	-244.334	-243.657	-246.138	-208.593
TSIII→IV	-174.976	-176.402	-178.883	-137.82
IV	-258.139	-256.981	-259.462	-231.034
Products (V)	-227.085	-227.668	-227.668	-217.244

Figure 4: $[UCH_3]^+ + H_2O$ B3LYP/SDD/6-311+g(d,p) Relative Enthalpy (kJ/mol)

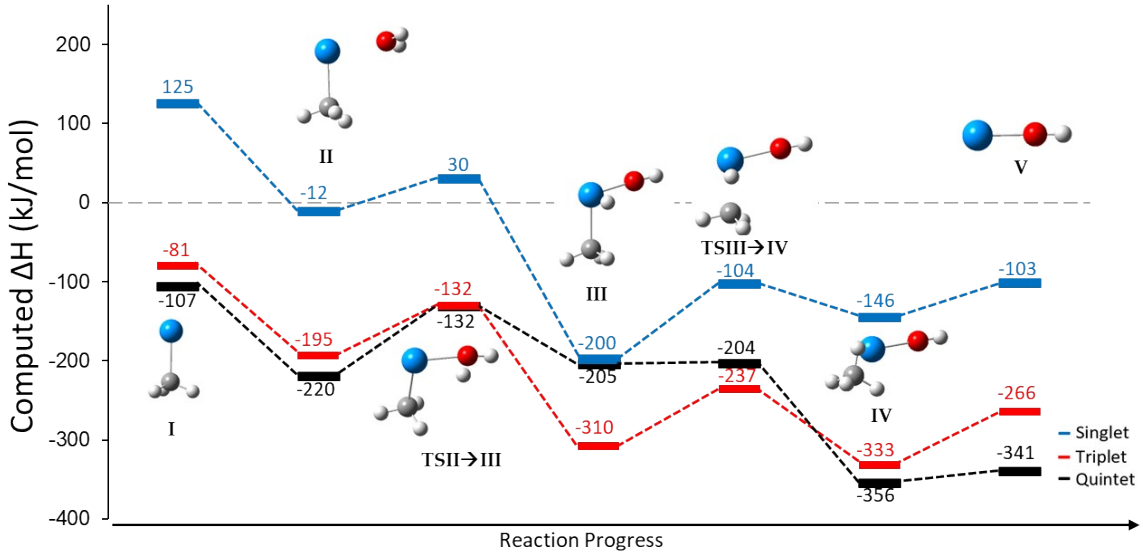

Figure 4.1: $[UCH_3]^+ + H_2O$ PBE1PBE/SDD/6-311+g(d,p) Relative Enthalpy (kJ/mol)

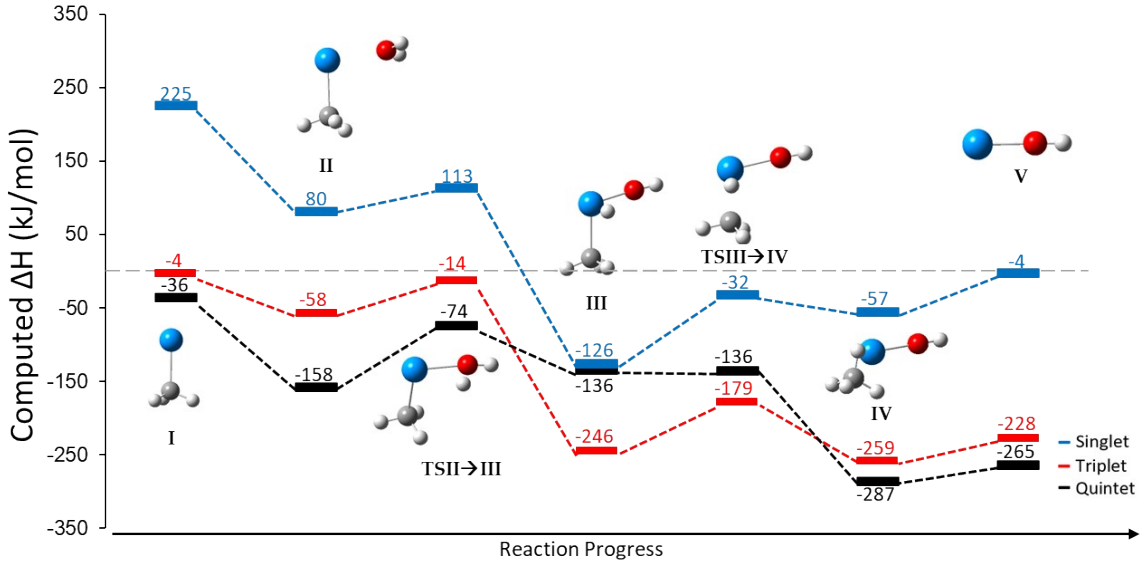

Table 3.1: $[UH]^+ + CH_3CH_2CN$ B3LYP/SDD/6-311+g(d,p) Quintet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-477.20060	.00371	.00608	.00702	-.01919	-477.19689	-477.19453	-477.19358	-477.21980
CH_3CH_2CN	-172.12044	.07406	.07874	.07968	.04736	-172.04639	-172.04171	-172.04076	-172.07308
$[UH]^+ + CH_3CH_2CN$ (I)	-649.32105	.07777	.08482	.08670	.02817	-649.24328	-649.23623	-649.23435	-649.29288
II	-649.40250	.07841	.08606	.08700	.04136	-649.32409	-649.31644	-649.31550	-649.36114
TSII→III	-649.38704	.07825	.08501	.08596	.04317	-649.30879	-649.30203	-649.30108	-649.34387
III	-649.44615	.08549	.09212	.09306	.05053	-649.36066	-649.35404	-649.35309	-649.39562

TSIII→IV	-649.38434	.08085	.08746	.08841	.04664	-649.30349	-649.29687	-649.29593	-649.33769
IV	-649.40417	.07864	.08662	.08756	.04216	-649.32553	-649.31755	-649.31661	-649.36201
$[UCH_2CH_3]^+$	-555.90647	.06094	.06524	.06618	.03012	-555.84553	-555.84123	-555.84029	-555.87635
HCN	-93.45449	.01636	.01890	.01985	-.00300	-93.43813	-93.43559	-93.43465	-93.45749
$[UCH_2CH_3]^+$ + HCN (**V**)	-649.36096	.07731	.08414	.08603	.02712	-649.28366	-649.27682	-649.27493	-649.33384

Table 3.1.1: $[UH]^+$ + CH_3CH_2CN B3LYP/SDD/6-311+g(d,p) Quintet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	0.000000	0.000000	0.021045
	H	0.000000	0.000000	-1.936098
CH_3CH_2CN	C	-1.429488	0.666866	0.304718
	C	-0.038681	0.098523	-0.027641
	C	1.032188	1.075832	0.161780
	N	1.866229	1.857431	0.315500
	H	-1.665097	1.520854	-0.332711
	H	-1.479887	0.992900	1.345047
	H	0.181016	-0.770291	0.600286
	H	-0.002845	-0.246048	-1.065624
	H	-2.188892	-0.101524	0.146757
II	U	0.106883	0.167081	-0.701608
	H	-0.008015	2.168334	-0.524749
	N	2.349297	-0.059321	-0.550389
	C	2.322569	0.030586	0.655418
	C	3.070810	0.101360	1.931704
	C	2.435677	-0.681525	3.088698
	H	3.057644	-0.575390	3.978143
	H	1.440281	-0.301751	3.328582
	H	2.362236	-1.745721	2.856851
	H	4.087655	-0.250082	1.720038
	H	3.143415	1.165903	2.182196
TSII→III	U	0.504458	0.459788	-0.971954
	H	0.959759	1.058656	0.918628
	N	2.624202	0.323159	-0.682316
	C	2.424234	0.183561	0.531334
	C	3.131041	0.052763	1.828998
	C	2.283646	-0.469469	2.990143
	H	2.890655	-0.518825	3.895043
	H	1.436959	0.191043	3.188692
	H	1.904178	-1.472845	2.785240
	H	3.990844	-0.598694	1.635673
	H	3.540919	1.044457	2.059310
III	U	0.407186	0.059497	0.351564
	H	4.190439	0.369506	-0.848101
	N	2.458033	-0.090554	0.137939
	C	3.724367	-0.169051	-0.012226
	C	4.667087	-0.938294	0.853433
	C	4.060898	-1.700428	2.025099
	H	4.843811	-2.219835	2.579520
	H	3.553581	-1.026981	2.720353
	H	3.342246	-2.450267	1.685233
	H	5.223344	-1.607417	0.180178
	H	5.428975	-0.219204	1.189544
TSIII→IV	U	3.086826	-2.292785	-0.169799
	H	4.257100	1.124148	-0.115909
	N	3.093594	-0.292872	-1.294330
	C	3.763000	0.226673	-0.455696
	C	4.477558	-1.048612	1.340951
	C	3.583875	-1.338944	2.553166

	H	4.157982	-1.750676	3.387391
	H	3.070411	-0.437144	2.887194
	H	2.778571	-2.086992	2.375357
	H	5.152545	-1.912115	1.102703
	H	5.148823	-0.216654	1.533992
IV	U	3.002867	-1.157136	-0.241847
	H	3.412548	2.162374	0.341091
	N	4.039983	0.559772	-0.892480
	C	3.389313	1.115658	0.028505
	C	4.602097	-2.132252	1.122647
	C	3.603752	-2.070902	2.291275
	H	4.075301	-1.904817	3.262203
	H	2.902713	-1.192362	2.226512
	H	2.978468	-2.965881	2.378036
	H	4.931517	-3.152887	0.907573
	H	5.483596	-1.510602	1.299476
HCN	C	0.000000	0.000000	-0.498334
	H	0.000000	0.000000	-1.564845
	N	-0.000000	0.000000	0.650693
$[UCH_2CH_3]^+$	U	2.892999	-1.381855	-0.378885
	C	4.583783	-2.057440	1.009661
	C	3.662196	-1.935509	2.247734
	H	4.175821	-2.214062	3.171323
	H	3.297651	-0.907490	2.418575
	H	2.779228	-2.597352	2.199476
	H	4.945241	-3.083850	0.876606
	H	5.451805	-1.392429	1.086801

Table 3.2: $[UH]^+ + CH_3CH_2CN$ PBE1PBE/SDD/6-311+g(d,p) Quintet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-477.12109	.00377	.00614	.00708	-.01913	-477.11732	-477.11495	-477.11401	-477.14021
CH_3CH_2CN	-171.90168	.07452	.07919	.08013	.04785	-171.82716	-171.82249	-171.82155	-171.85383
$[UH]^+ + CH_3CH_2CN$ (**I**)	-649.02276	.07829	.08532	.08721	.02872	-648.94447	-648.93744	-648.93555	-648.99404
II	-649.08825	.07906	.08655	.08749	.04285	-649.00919	-649.00170	-649.00075	-649.04540
TSII→III	-649.07918	.07932	.08580	.08675	.04469	-648.99986	-648.99338	-648.99244	-649.03449
III	-649.13164	.08599	.09261	.09356	.05104	-649.04564	-649.03903	-649.03808	-649.08060
TSIII→IV	-649.07292	.08107	.08735	.08829	.04758	-648.99185	-648.98557	-648.98463	-649.02533
IV	-649.09237	.07948	.08721	.08816	.04361	-649.01289	-649.00516	-649.00422	-649.04876
$[UCH_2CH_3]^+$	-555.70335	.06129	.06628	.06723	.02954	-555.64207	-555.63707	-555.63612	-555.67381
HCN	-93.33544	.01649	.01903	.01997	-.00287	-93.31895	-93.31641	-93.31547	-93.33831
$[UCH_2CH_3]^+ + HCN$ (**V**)	-649.03879	.07778	.08531	.08720	.02668	-648.96101	-648.95348	-648.95159	-649.01211

Table 3.2.1: $[UH]^+ + CH_3CH_2CN$ PBE1PBE/SDD/6-311+g(d,p) Quintet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	-0.282792	0.024095	0.017719
	H	-0.733284	1.219330	1.490648
CH_3CH_2CN	C	-1.423276	0.666142	0.303808
	C	-0.042260	0.099303	-0.026986
	C	1.023045	1.073641	0.162122
	N	1.855821	1.855504	0.315992

	H	-1.657991	1.521138	-0.333377
	H	-1.472810	0.993170	1.344342
	H	0.180748	-0.769399	0.600941
	H	-0.003160	-0.244935	-1.065573
	H	-2.185573	-0.100020	0.146843
II	U	0.499845	-0.014950	-0.923635
	H	-0.531823	1.257157	0.225837
	N	2.542107	0.778711	-0.485609
	C	2.518802	0.213095	0.586871
	C	3.197169	-0.042218	1.870714
	C	2.279283	-0.477301	3.005977
	H	2.865794	-0.622586	3.914437
	H	1.519605	0.279154	3.214133
	H	1.780847	-1.422542	2.776984
	H	3.956080	-0.807082	1.660594
	H	3.740744	0.878033	2.118580
TSII→III	U	0.535063	0.391800	-0.912659
	H	0.903443	1.063782	0.944513
	N	2.654086	0.395473	-0.672303
	C	2.431071	0.187208	0.531188
	C	3.133375	0.041799	1.821526
	C	2.279771	-0.461855	2.973472
	H	2.878779	-0.518719	3.883788
	H	1.440872	0.211753	3.165071
	H	1.886119	-1.461034	2.770692
	H	3.983836	-0.622842	1.625970
	H	3.564479	1.026229	2.047531
III	U	0.393780	-0.162551	0.135203
	H	4.198801	0.367590	-0.852257
	N	2.438633	-0.184318	0.028963
	C	3.711832	-0.193650	-0.042893
	C	4.624941	-0.907537	0.884331
	C	3.974784	-1.687750	2.007634
	H	4.736232	-2.169808	2.623057
	H	3.387209	-1.034835	2.658878
	H	3.317000	-2.470906	1.620778
	H	5.259539	-1.549184	0.254008
	H	5.327212	-0.150075	1.264834
TSIII→IV	U	2.953364	-2.145451	-0.129806
	H	3.960367	1.095169	0.042270
	N	3.532198	-0.496757	-1.354232
	C	3.678401	0.092376	-0.265077
	C	4.479496	-1.019549	1.307386
	C	3.607936	-1.304370	2.512713
	H	4.137420	-1.842784	3.303279
	H	3.199006	-0.380954	2.924812
	H	2.717663	-1.952808	2.304010
	H	5.143135	-1.882879	1.028851
	H	5.161300	-0.187966	1.470816
IV	U	2.838734	-1.242207	-0.246677
	H	3.454295	2.090682	0.696908
	N	4.000815	0.643139	-0.815319
	C	3.474258	1.144631	0.153905
	C	4.494444	-2.271434	1.000547
	C	3.703333	-1.962460	2.262899
	H	4.281097	-1.469684	3.047177
	H	2.866762	-1.204573	2.103508
	H	3.206698	-2.834874	2.694189
	H	4.623448	-3.347534	0.839889
	H	5.478270	-1.794719	0.985968

HCN	C	0.000000	0.000000	-0.497856
	H	0.000000	0.000000	-1.566083
	N	-0.000000	-0.000000	0.650460
$[UCH_2CH_3]^+$	U	2.854953	-1.363659	-0.248048
	C	4.607200	-2.071516	1.006094
	C	3.668381	-1.935105	2.214754
	H	4.151224	-2.176959	3.164985
	H	3.284598	-0.902384	2.355508
	H	2.789568	-2.609488	2.164034
	H	4.957017	-3.102382	0.880047
	H	5.475784	-1.408495	1.093917

Table 3.3: $[UH]^+ + CH_3CH_2CN$ B3LYP/SDD/6-311+g(d,p) Singlet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-477.13768	.00368	.00605	.00699	-.01769	-477.13400	-477.13164	-477.13069	-477.15538
CH_3CH_2CN	-172.12044	.07406	.07874	.07968	.04736	-172.04639	-172.04171	-172.04076	-172.07308
$[UH]^+ + CH_3CH_2CN$ (**I**)	-649.25813	.07774	.08479	.08667	.02967	-649.18039	-649.17334	-649.17146	-649.22846
II	-649.35711	.07857	.08584	.08679	.04401	-649.27854	-649.27127	-649.27032	-649.31310
TSII→III	-649.33619	.07953	.08575	.08669	.04700	-649.25666	-649.25044	-649.24949	-649.28919
III	-649.36013	.08525	.09194	.09288	.05167	-649.27488	-649.26819	-649.26725	-649.30846
TSIII→IV	-649.33196	.08090	.08695	.08790	.04911	-649.25105	-649.24500	-649.24406	-649.28285
IV	-649.36754	.07908	.08686	.08780	.04408	-649.28846	-649.28069	-649.27974	-649.32346
$[UCH_2CH_3]^+$	-555.81767	.06084	.06601	.06695	.03009	-555.75683	-555.75166	-555.75072	-555.78758
HCN	-93.45449	.01636	.01890	.01985	-.00300	-93.43813	-93.43559	-93.43465	-93.45749
$[UCH_2CH_3]^+ + HCN$ (**V**)	-649.27216	.07720	.08491	.08680	.02710	-649.19496	-649.18725	-649.18537	-649.24507

Table 3.3.1: $[UH]^+ + CH_3CH_2CN$ B3LYP/SDD/6-311+g(d,p) Singlet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	-0.274048	0.000897	-0.010869
	H	-0.723542	1.193481	1.458793
CH_3CH_2CN	C	-1.429488	0.666866	0.304718
	C	-0.038681	0.098523	-0.027641
	C	1.032188	1.075832	0.161780
	N	1.866229	1.857431	0.315500
	H	-1.665097	1.520854	-0.332711
	H	-1.479887	0.992900	1.345047
	H	0.181016	-0.770291	0.600286
	H	-0.002845	-0.246048	-1.065624
	H	-2.188892	-0.101524	0.146757
II	U	0.598767	0.072643	-0.907251
	H	-0.329118	1.624950	-0.137970
	N	2.486033	0.586646	-0.514397
	C	2.230856	0.086961	0.644531
	C	3.064623	-0.001726	1.869371
	C	2.359039	-0.579512	3.098234
	H	3.046070	-0.610120	3.945046
	H	1.502050	0.032631	3.388055
	H	2.011494	-1.599397	2.916304
	H	3.946033	-0.600137	1.598824

	H	3.452603	1.006533	2.064135
TSII→III	U	-0.346346	1.002889	0.267431
	H	1.328271	1.848144	0.934467
	N	1.035381	-0.326862	0.243201
	C	1.355495	0.356600	1.381390
	C	2.512537	0.101086	2.282759
	C	2.431603	-1.301361	2.914678
	H	3.296071	-1.455032	3.562123
	H	1.531789	-1.413771	3.523977
	H	2.433739	-2.077866	2.148338
	H	3.433093	0.185713	1.693477
	H	2.544281	0.870320	3.058020
III	U	0.493997	0.195364	0.419777
	H	4.162430	0.367946	-0.848798
	N	2.428387	-0.214112	0.065561
	C	3.708769	-0.203915	-0.030652
	C	4.659229	-0.925029	0.862140
	C	4.060175	-1.712510	2.020849
	H	4.852303	-2.206169	2.585432
	H	3.521115	-1.058620	2.711589
	H	3.371737	-2.483118	1.667526
	H	5.253085	-1.574063	0.199626
	H	5.388739	-0.178802	1.209486
TSIII→IV	U	2.914264	-2.033124	-0.247181
	H	3.811184	1.031537	0.055324
	N	3.726374	-0.658712	-1.310932
	C	3.552630	-0.008016	-0.107982
	C	4.453290	-0.995537	1.271879
	C	3.640208	-1.264535	2.530724
	H	4.216308	-1.789182	3.295949
	H	3.262604	-0.331984	2.951929
	H	2.735818	-1.896596	2.367035
	H	5.069016	-1.874071	0.928666
	H	5.188591	-0.205752	1.409609
IV	U	2.703057	-0.653209	0.299587
	H	4.205174	2.241993	-0.317110
	N	3.616619	0.397616	-1.177042
	C	3.725286	1.265418	-0.240779
	C	4.428573	-1.811747	1.266835
	C	3.594010	-2.406132	2.407142
	H	4.098181	-2.365951	3.374879
	H	2.641273	-1.842225	2.601611
	H	3.289188	-3.437833	2.220192
	H	4.955510	-2.559871	0.667751
	H	5.165285	-1.077094	1.619925
HCN	C	0.000000	0.000000	-0.498334
	H	0.000000	0.000000	-1.564845
	N	-0.000000	0.000000	0.650693
$[UCH_2CH_3]^+$	U	2.877133	-1.366789	-0.279487
	C	4.601124	-2.070055	1.009579
	C	3.662676	-1.935256	2.232318
	H	4.159545	-2.181387	3.173505
	H	3.281012	-0.904941	2.369694
	H	2.786891	-2.608183	2.177613
	H	4.951609	-3.096820	0.867941
	H	5.468735	-1.406557	1.080128

Table 3.4: $[UH]^+ + CH_3CH_2CN$ PBE1PBE/SDD/6-311+g(d,p) Singlet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-477.01929	.00372	.00608	.00703	-.01765	-477.01557	-477.01321	-477.01226	-477.03694
CH_3CH_2CN	-171.90168	.07452	.07919	.08013	.04785	-171.82716	-171.82249	-171.82155	-171.85383
$[UH]^+ + CH_3CH_2CN$ (I)	-648.92096	.07824	.08527	.08716	.03020	-648.84273	-648.83569	-648.83381	-648.89076
II	-649.04193	.07910	.08637	.08731	.04471	-648.96283	-648.95556	-648.95462	-648.99722
TSII→III	-649.02823	.08023	.08640	.08734	.04775	-648.94800	-648.94183	-648.94089	-648.98048
III	-649.03462	.08571	.09239	.09333	.05207	-648.94891	-648.94223	-648.94129	-648.98256
TSIII→IV	-649.02556	.08138	.08737	.08831	.04963	-648.94418	-648.93820	-648.93725	-648.97594
IV	-649.05726	.08048	.08764	.08858	.04719	-648.97678	-648.96962	-648.96868	-649.01008
$[UCH_2CH_3]^+$	-555.60359	.06123	.06602	.06696	.03182	-555.54235	-555.53757	-555.53663	-555.57177
HCN	-93.33544	.01649	.01903	.01997	-.00287	-93.31895	-93.31641	-93.31547	-93.33831
$[UCH_2CH_3]^+ + HCN$ (V)	-648.93903	.07773	.08504	.08693	.02895	-648.86130	-648.85399	-648.85210	-648.91008

Table 3.4.1: $[UH]^+ + CH_3CH_2CN$ PBE1PBE/SDD/6-311+g(d,p) Singlet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	-0.274832	0.002976	-0.008307
	H	-0.722758	1.191402	1.456231
CH_3CH_2CN	C	-1.423276	0.666142	0.303808
	C	-0.042260	0.099303	-0.026986
	C	1.023045	1.073641	0.162122
	N	1.855821	1.855504	0.315992
	H	-1.657991	1.521138	-0.333377
	H	-1.472810	0.993170	1.344342
	H	0.180748	-0.769399	0.600941
	H	-0.003160	-0.244935	-1.065573
	H	-2.185573	-0.100020	0.146843
II	U	0.632750	0.065869	-0.885759
	H	-0.262154	1.571430	-0.023287
	N	2.498777	0.574248	-0.527023
	C	2.219983	0.081878	0.637701
	C	3.048886	0.002983	1.856436
	C	2.345544	-0.566164	3.079324
	H	3.028150	-0.589240	3.930521
	H	1.484493	0.044510	3.361859
	H	2.002515	-1.589141	2.903550
	H	3.934697	-0.591245	1.588656
	H	3.434810	1.014345	2.042905
TSII→III	U	-0.313079	0.984431	0.289687
	H	1.324616	1.868205	0.908122
	N	1.040722	-0.343274	0.262124
	C	1.353112	0.354265	1.395704
	C	2.508282	0.101531	2.287844
	C	2.427588	-1.296307	2.906238
	H	3.293674	-1.458754	3.550073
	H	1.529486	-1.412195	3.518301
	H	2.424762	-2.067194	2.133262
	H	3.425469	0.190070	1.692908

	H	2.541282	0.869082	3.065599
III	U	0.571262	0.198405	0.513233
	H	4.165554	0.378905	-0.844641
	N	2.435160	-0.264122	0.035512
	C	3.716217	-0.212481	-0.037790
	C	4.656102	-0.919439	0.863598
	C	4.042238	-1.707089	2.002228
	H	4.822727	-2.202180	2.582315
	H	3.489705	-1.054224	2.685242
	H	3.359697	-2.476771	1.633942
	H	5.263693	-1.564022	0.207880
	H	5.377610	-0.170012	1.221020
TSIII→IV	U	2.981737	-2.014129	-0.213396
	H	3.829856	1.034640	0.072496
	N	3.744088	-0.649580	-1.294750
	C	3.561979	-0.004028	-0.093428
	C	4.469828	-0.999787	1.282555
	C	3.615532	-1.278517	2.500585
	H	4.115828	-1.902282	3.244702
	H	3.299574	-0.346978	2.972837
	H	2.652787	-1.806765	2.277387
	H	5.116604	-1.868890	0.963855
	H	5.182472	-0.189658	1.432179
IV	U	3.049581	-1.197392	-0.276829
	H	3.322234	1.926366	0.627532
	N	4.002098	0.485663	-0.768723
	C	3.309097	0.908924	0.232893
	C	4.632433	-2.127836	1.062911
	C	3.626773	-1.956007	2.195976
	H	4.085273	-1.755084	3.167467
	H	3.002189	-1.023200	2.069907
	H	2.949203	-2.809635	2.319884
	H	4.908269	-3.173075	0.890270
	H	5.535005	-1.527758	1.201705
HCN	C	0.000000	0.000000	-0.497856
	H	0.000000	0.000000	-1.566083
	N	-0.000000	-0.000000	0.650460
$[UCH_2CH_3]^+$	U	2.827585	-1.387547	-0.137334
	C	4.628725	-2.075961	1.010431
	C	3.674085	-1.932058	2.202154
	H	4.109644	-2.182967	3.171679
	H	3.299304	-0.888206	2.317781
	H	2.781335	-2.593681	2.108924
	H	4.977594	-3.104166	0.875530
	H	5.490453	-1.405402	1.082126

Table 3.5: $[UH]^+$ + CH_3CH_2CN B3LYP/SDD/6-311+g(d,p) Triplet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-477.14828	.00361	.00597	.00691	-.01880	-477.14467	-477.14231	-477.14136	-477.16708
CH_3CH_2CN	-172.12044	.07406	.07874	.07968	.04736	-172.04639	-172.04171	-172.04076	-172.07308
$[UH]^+$ + CH_3CH_2CN (**I**)	-649.26872	.07766	.08471	.08660	.02857	-649.19106	-649.18401	-649.18213	-649.24016
II	-649.40316	.07814	.08570	.08665	.04229	-649.32503	-649.31746	-649.31652	-649.36088
TSII→III	-649.38313	.07880	.08524	.08618	.04486	-649.30433	-649.29790	-649.29695	-649.33827
III	-649.43703	.08539	.09208	.09303	.05073	-649.35164	-649.34494	-649.34400	-649.38630
TSIII→IV	-649.37777	.08053	.08680	.08775	.04751	-649.29724	-649.29097	-649.29003	-649.33027
IV	-649.40933	.07891	.08680	.08775	.04245	-649.33042	-649.32253	-649.32158	-649.36688
$[UCH_2CH_3]^+$	-93.45449	.01636	.01890	.01985	-.00300	-93.43813	-93.43559	-93.43465	-93.45749
HCN	-555.89760	.06115	.06613	.06708	.03009	-555.83645	-555.83146	-555.83052	-555.86751
$[UCH_2CH_3]^+$ + HCN (**V**)	-649.35209	.07751	.08504	.08692	.02709	-649.27458	-649.26706	-649.26517	-649.32500

Table 3.5.1: $[UH]^+$ + CH_3CH_2CN B3LYP/SDD/6-311+g(d,p) Triplet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	-0.275143	0.003800	-0.007291
	H	-0.722447	1.190578	1.455215
CH_3CH_2CN	C	-1.429488	0.666866	0.304718
	C	-0.038681	0.098523	-0.027641
	C	1.032188	1.075832	0.161780
	N	1.866229	1.857431	0.315500
	H	-1.665097	1.520854	-0.332711
	H	-1.479887	0.992900	1.345047
	H	0.181016	-0.770291	0.600286
	H	-0.002845	-0.246048	-1.065624
	H	-2.188892	-0.101524	0.146757
II	U	0.349455	0.098990	-0.822241
	H	-0.188974	1.952749	-0.335943
	N	2.447851	0.237442	-0.559730
	C	2.250597	0.068126	0.658403
	C	3.066322	0.041319	1.901700
	C	2.402172	-0.635402	3.103455
	H	3.065341	-0.586808	3.968100
	H	1.466410	-0.140368	3.372740
	H	2.195905	-1.689382	2.903884
	H	4.028154	-0.422200	1.651983
	H	3.285217	1.095007	2.122533
TSII→III	U	0.640746	0.340191	-1.005174
	H	0.952228	0.958791	0.904491
	N	2.642240	0.542905	-0.655116
	C	2.322435	0.196916	0.548087
	C	3.094807	0.040295	1.809880
	C	2.286871	-0.450433	3.011713
	H	2.933300	-0.541849	3.885664
	H	1.485655	0.248844	3.263313
	H	1.844155	-1.431141	2.821121
	H	3.910387	-0.653374	1.572173

	H	3.578071	1.002449	2.022638
III	U	0.408420	0.061077	0.350912
	H	4.189702	0.369194	-0.848300
	N	2.457331	-0.091177	0.137965
	C	3.723938	-0.169434	-0.012397
	C	4.666829	-0.938246	0.853486
	C	4.061140	-1.700586	2.025264
	H	4.844465	-2.219596	2.579505
	H	3.553548	-1.027467	2.720620
	H	3.342821	-2.450845	1.685587
	H	5.223359	-1.607211	0.180344
	H	5.428411	-0.218736	1.189552
TSIII→IV	U	2.915633	-2.086607	-0.233250
	H	3.873063	1.066924	0.083831
	N	3.677109	-0.559426	-1.329205
	C	3.638559	0.037711	-0.166348
	C	4.470078	-1.009409	1.290208
	C	3.612975	-1.284753	2.517450
	H	4.163851	-1.804909	3.304126
	H	3.208499	-0.357382	2.924719
	H	2.724779	-1.934000	2.325302
	H	5.097699	-1.884183	0.973276
	H	5.188042	-0.209939	1.454913
IV	U	3.002870	-1.157141	-0.241849
	H	3.412537	2.162370	0.341095
	N	4.039986	0.559771	-0.892472
	C	3.389306	1.115654	0.028509
	C	4.602100	-2.132255	1.122646
	C	3.603753	-2.070896	2.291272
	H	4.075302	-1.904822	3.262202
	H	2.902726	-1.192347	2.226511
	H	2.978458	-2.965868	2.378028
	H	4.931516	-3.152892	0.907577
	H	5.483601	-1.510607	1.299474
HCN	C	0.000000	0.000000	-0.498334
	H	0.000000	0.000000	-1.564845
	N	-0.000000	0.000000	0.650693
$[UCH_2CH_3]^+$	U	3.095756	-0.949841	-0.322578
	C	4.538012	-2.139912	1.006418
	C	3.664389	-1.987371	2.261230
	H	4.234844	-1.750027	3.160914
	H	2.938495	-1.129671	2.196152
	H	3.048526	-2.867315	2.457492
	H	4.793714	-3.178042	0.780769
	H	5.474989	-1.567808	1.090894

Table 3.5: $[UH]^+ + CH_3CH_2CN$ PBE1PBE/SDD/6-311+g(d,p) Triplet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-477.06589	.00353	.00589	.00684	-.01891	-477.06236	-477.06000	-477.05905	-477.08480
CH_3CH_2CN	-171.90168	.07452	.07919	.08013	.04785	-171.82716	-171.82249	-171.82155	-171.85383
$[UH]^+ + CH_3CH_2CN$ (I)	-648.96757	.07805	.08508	.08697	.02894	-648.88952	-648.88249	-648.88060	-648.93862
II	-649.08904	.07852	.08611	.08705	.04212	-649.01052	-649.00293	-649.00199	-649.04692
TSII→III	-649.07639	.07930	.08572	.08666	.04541	-648.99709	-648.99067	-648.98972	-649.03098
III	-649.11984	.08588	.09257	.09352	.05116	-649.03396	-649.02727	-649.02632	-649.06868
TSIII→IV	-649.07275	.08086	.08713	.08807	.04779	-648.99189	-648.98562	-648.98467	-649.02496
IV	-649.09929	.08013	.08753	.08848	.04504	-649.01915	-649.01175	-649.01081	-649.05424
$[UCH_2CH_3]^+$	-93.33544	.01649	.01903	.01997	-.00287	-93.31895	-93.31641	-93.31547	-93.33831
HCN	-555.67186	.06176	.06654	.06749	.03110	-555.61010	-555.60532	-555.60438	-555.64077
$[UCH_2CH_3]^+ + HCN$ (V)	-649.00730	.07826	.08557	.08746	.02823	-648.92905	-648.92174	-648.91985	-648.97907

Table 3.6.1: $[UH]^+ + CH_3CH_2CN$ PBE1PBE/SDD/6-311+g(d,p) Triplet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	-0.280565	0.018185	0.010435
	H	-0.735512	1.225240	1.497931
CH_3CH_2CN	C	-1.423276	0.666142	0.303808
	C	-0.042260	0.099303	-0.026986
	C	1.023045	1.073641	0.162122
	N	1.855821	1.855504	0.315992
	H	-1.657991	1.521138	-0.333377
	H	-1.472810	0.993170	1.344342
	H	0.180748	-0.769399	0.600941
	H	-0.003160	-0.244935	-1.065573
	H	-2.185573	-0.100020	0.146843
II	U	0.460061	0.069833	-0.837516
	H	-0.225840	1.786545	-0.146943
	N	2.491036	0.367882	-0.556875
	C	2.256818	0.077607	0.642652
	C	3.064472	0.021631	1.879707
	C	2.369843	-0.598795	3.081928
	H	3.031465	-0.576799	3.949467
	H	1.461527	-0.050304	3.343593
	H	2.105770	-1.643001	2.896047
	H	3.999063	-0.497799	1.630616
	H	3.354235	1.062671	2.082208
TSII→III	U	0.646741	0.283168	-0.946509
	H	0.892028	0.932318	0.929220
	N	2.622197	0.583004	-0.643524
	C	2.318167	0.192769	0.550819
	C	3.096580	0.050708	1.800312
	C	2.304164	-0.449059	2.997208
	H	2.951248	-0.528614	3.872347
	H	1.490732	0.237348	3.247585
	H	1.877431	-1.437850	2.809108
	H	3.922283	-0.630242	1.556008

	H	3.569326	1.020045	2.006215
III	U	0.395966	-0.164183	0.135160
	H	4.198425	0.367402	-0.852746
	N	2.438335	-0.184672	0.028744
	C	3.711910	-0.193767	-0.043238
	C	4.624830	-0.907437	0.884299
	C	3.974512	-1.687236	2.007793
	H	4.735843	-2.169116	2.623511
	H	3.386825	-1.034089	2.658744
	H	3.316706	-2.470534	1.621174
	H	5.259468	-1.549425	0.254361
	H	5.327143	-0.149969	1.264736
TSIII→IV	U	2.938433	-2.047420	-0.193616
	H	3.868525	1.064843	0.081782
	N	3.678043	-0.570474	-1.320464
	C	3.613221	0.036477	-0.158241
	C	4.476140	-1.021189	1.287839
	C	3.615109	-1.288352	2.503508
	H	4.147193	-1.822490	3.294371
	H	3.217732	-0.357195	2.911104
	H	2.714638	-1.924375	2.307491
	H	5.122183	-1.892205	0.992188
	H	5.179070	-0.203595	1.439061
IV	U	3.137924	-1.215892	-0.338424
	H	3.183037	1.997786	0.534949
	N	4.165168	0.549832	-0.644389
	C	3.282698	0.974949	0.162236
	C	4.638813	-2.185871	1.091931
	C	3.619302	-1.953760	2.199336
	H	4.052808	-1.629793	3.148163
	H	2.923883	-1.081279	1.988570
	H	2.981132	-2.820950	2.397224
	H	4.865390	-3.246120	0.939578
	H	5.572001	-1.637936	1.243817
HCN	C	0.000000	0.000000	-0.497856
	H	0.000000	0.000000	-1.566083
	N	-0.000000	-0.000000	0.650460
$[UCH_2CH_3]^+$	U	2.870083	-1.310116	-0.228967
	C	4.610644	-2.068576	1.006147
	C	3.665707	-1.945095	2.212143
	H	4.161800	-2.113676	3.171049
	H	3.225862	-0.926953	2.320006
	H	2.827540	-2.666651	2.182124
	H	4.930538	-3.105636	0.852918
	H	5.496552	-1.433285	1.115870

Table 3.7.1: $[UH]^+ + CH_3CH_2CN$ B3LYP/SDD/6-311+g(d,p) Quintet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	0	0	0	0
II	-212.159	-210.583	-213.065	-179.214
TSII→III	-171.999	-172.742	-175.223	-133.877
III	-308.189	-309.294	-311.776	-269.754
TSIII→IV	-158.068	-159.21	-161.689	-117.662
IV	-215.955	-213.5	-215.982	-181.498

Products (V)	-106.005	-106.564	-106.566	-107.548

Table 3.7.2: $[UH]^+ + CH_3CH_2CN$ PBE1PBE/SDD/6-311+g(d,p) Quintet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	0	0	0	0
II	-169.914	-168.702	-171.18	-134.846
TSII→III	-145.421	-146.873	-149.352	-106.204
III	-265.622	-266.709	-269.185	-227.253
TSIII→IV	-124.383	-126.36	-128.839	-82.1519
IV	-179.639	-177.794	-180.269	-143.67
Products (V)	-43.4205	-42.1051	-42.1051	-47.4428

Table 3.7.3: $[UH]^+ + CH_3CH_2CN$ B3LYP/SDD/6-311+g(d,p) Singlet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	165.1177	165.1203	165.1177	169.1373
II	-92.5699	-91.9739	-94.455	-53.0876
TSII→III	-35.1134	-37.29	-39.7711	9.690721
III	-82.9553	-83.9057	-86.3868	-40.9027
TSIII→IV	-20.4054	-23.0204	-25.5015	26.33114
IV	-118.617	-116.706	-119.187	-80.2904
Products (V)	126.8563	128.5996	128.597	125.5252

Table 3.7.4: $[UH]^+ + CH_3CH_2CN$ PBE1PBE/SDD/6-311+g(d,p) Singlet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	267.1394	267.1394	267.1394	271.1564
II	-48.2016	-47.5714	-50.0499	-8.33596
TSII→III	-9.25489	-11.5233	-14.0018	35.60703
III	-11.652	-12.5761	-15.0546	30.15912
TSIII→IV	0.764021	-1.977	-4.45547	47.53468
IV	-84.8325	-84.4938	-86.9697	-42.0946
Products (V)	218.3707	219.1137	219.1137	220.4501

Table 3.7.5: $[UH]^+ + CH_3CH_2CN$ B3LYP/SDD/6-311+g(d,p) Triplet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	137.1036	137.1062	137.1036	138.4216
II	-214.622	-213.262	-215.743	-178.529
TSII→III	-160.295	-161.896	-164.377	-119.185
III	-284.489	-285.418	-287.899	-245.266
TSIII→IV	-141.667	-143.707	-146.188	-98.1596

IV	-228.77	-226.565	-229.046	-194.287
Products (V)	-82.1729	-80.9205	-80.9205	-84.3258

Table 3.7.6: $[UH]^+ + CH_3CH_2CN$ PBE1PBE/SDD/6-311+g(d,p) Triplet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	144.2844	144.2896	144.2896	145.5
II	-173.404	-171.936	-174.415	-138.818
TSII→*III*	-138.141	-139.742	-142.221	-96.986
III	-234.953	-235.833	-238.311	-195.965
TSIII→*IV*	-124.499	-126.486	-128.965	-81.1778
IV	-196.07	-195.101	-197.579	-158.058
Products (V)	40.49834	41.23611	41.23611	39.30899

Figure 5: $[UH]^+$ + CH_3CH_2CN B3LYP/SDD/6-311+g(d,p) Relative Enthalpy (kJ/mol)

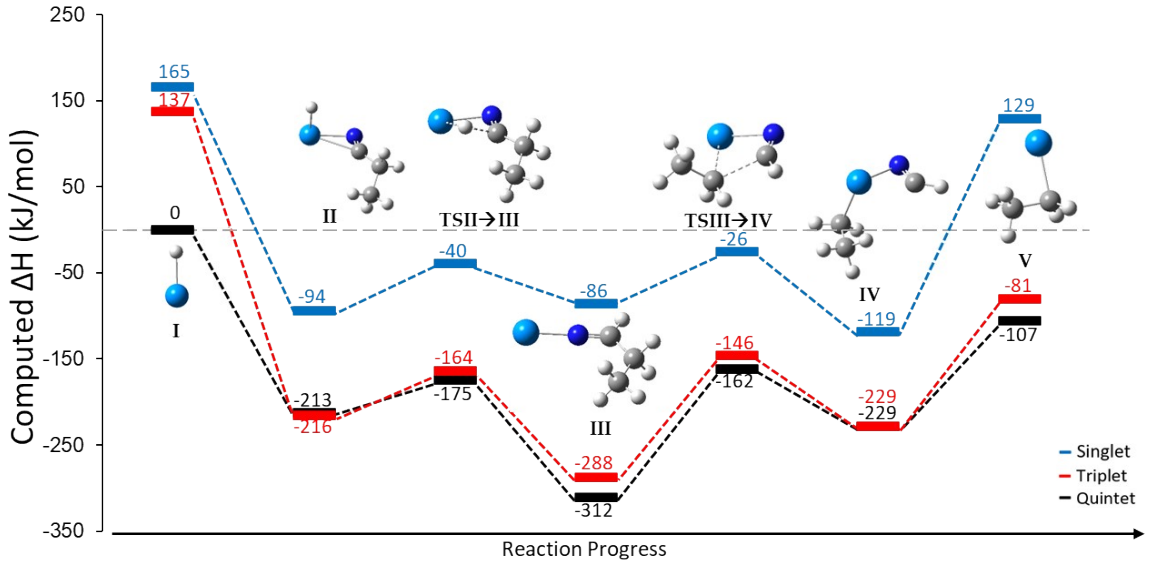

Figure 5.1: $[UH]^+$ + CH_3CH_2CN PBE1PBE/SDD/6-311+g(d,p) Relative Enthalpy (kJ/mol)

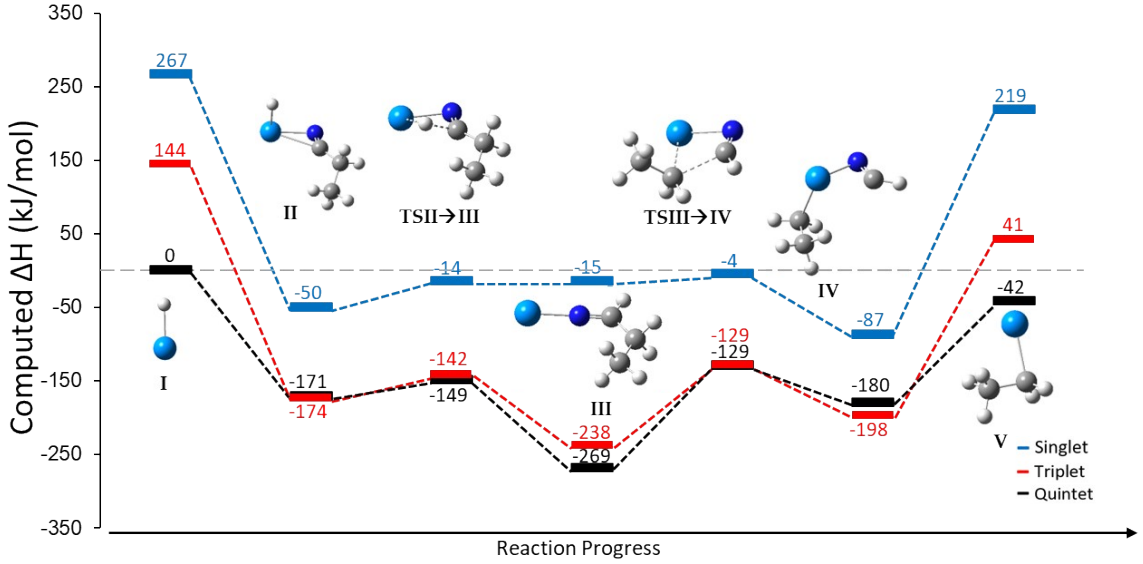

Table 4.1: $[UH]^+$ + $CH_3CH_2CH_2CN$ B3LYP/SDD/6-311+g(d,p) Quintet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-477.20060	.00371	.00608	.00702	-.01919	-477.19689	-477.19453	-477.19358	-477.21980
$CH_3CH_2CH_2CN$	-211.44532	.10244	.10841	.10935	.07343	-211.34289	-211.33691	-211.33597	-211.37189
$[UH]^+$ + CH_3CH_2CN (I)	-688.64592	.10615	.11448	.11637	.05424	-688.53978	-688.53144	-688.52955	-688.59168

II	-688.72780	.10687	.11576	.11671	.06791	-688.62093	-688.61204	-688.61109	-688.65989
TSII→III	-688.70823	.10706	.11439	.11533	.07156	-688.60117	-688.59384	-688.59290	-688.63667
III	-688.76911	.11382	.12176	.12271	.07659	-688.65529	-688.64735	-688.64640	-688.69252
TSIII→IV	-688.70619	.10915	.11707	.11801	.07283	-688.59705	-688.58913	-688.58818	-688.63337
IV	-688.73009	.10737	.11628	.11722	.07002	-688.62272	-688.61381	-688.61286	-688.66007
HCN	-93.45449	.01636	.01890	.01985	-.00300	-93.43813	-93.43559	-93.43465	-93.45749
$[UCH_2CH_2CH_3]^+$	-595.23373	.08963	.09569	.09663	.05581	-595.14409	-595.13804	-595.13710	-595.17792
$[UCH_2CH_2CH_3]^+$ + HCN (V)	-688.68822	.10600	.11459	.11648	.05281	-688.58222	-688.57363	-688.57174	-688.63541

Table 4.1.1: $[UH]^+$ + $CH_3CH_2CH_2CN$ B3LYP/SDD/6-311+g(d,p) Quintet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	0.000000	0.000000	0.021045
	H	0.000000	0.000000	-1.936098
$CH_3CH_2CH_2CN$	C	-2.522854	-0.398896	0.089360
	C	-1.432195	0.652798	0.300119
	C	-0.030160	0.099753	-0.028426
	C	1.031270	1.085065	0.165164
	N	1.856379	1.875364	0.323011
	H	-2.363618	-1.272371	0.728972
	H	-3.507281	0.011013	0.326889
	H	-2.548541	-0.744398	-0.948611
	H	-1.624726	1.527313	-0.327858
	H	-1.441327	1.003630	1.335991
	H	0.191242	-0.769653	0.599702
	H	0.007683	-0.244642	-1.067379
II	U	0.701634	-0.238544	-1.504276
	H	-0.645339	0.937899	-0.578939
	N	2.586599	0.822055	-0.854872
	C	2.593596	0.271429	0.220764
	C	3.207998	0.088633	1.554230
	C	2.227235	0.282107	2.731387
	H	3.629351	-0.921806	1.577571
	H	4.042682	0.798145	1.618761
	C	1.666717	1.700732	2.840821
	H	2.468254	2.437116	2.944722
	H	1.068446	1.975076	1.966734
	H	1.022208	1.788366	3.717424
	H	2.778640	0.026511	3.639580
	H	1.415797	-0.448044	2.648089
TSII→III	U	0.311914	0.003491	-1.052672
	H	0.367137	1.987112	-1.392400
	N	2.529602	-0.361046	-0.862006
	C	2.522411	0.013531	0.290256
	C	3.316299	0.314209	1.506024
	C	2.545152	0.278534	2.836583
	H	4.149670	-0.398907	1.509213
	H	3.750449	1.308432	1.339756
	C	1.510679	1.394084	2.988987
	H	1.974030	2.381862	2.921024
	H	0.735084	1.344123	2.214281
	H	1.007354	1.327505	3.955233
	H	3.286188	0.358861	3.635871
	H	2.076814	-0.703518	2.957502

III	U	-0.162283	0.891662	-1.661051
	H	3.458136	2.452009	-1.158567
	N	1.676537	1.479088	-0.923167
	C	2.818625	1.857012	-0.492611
	C	3.416508	1.545378	0.841696
	C	2.530156	0.850641	1.877259
	H	4.310130	0.941845	0.614597
	H	3.831899	2.484948	1.233151
	C	1.494977	1.775441	2.527026
	H	1.981404	2.601782	3.052402
	H	0.812831	2.213214	1.791459
	H	0.892603	1.232352	3.258540
	H	3.179904	0.440115	2.654435
	H	2.036781	-0.010731	1.413705
TSIII→IV	U	0.155288	3.159255	0.212029
	H	2.734073	0.647536	-0.135981
	N	1.236308	1.769479	-1.252708
	C	1.943003	1.334790	-0.395612
	C	1.738006	2.128455	1.753718
	C	0.876423	1.369704	2.777715
	H	2.780543	1.822726	1.823908
	H	1.774507	3.227466	2.000662
	C	-0.589688	1.827748	2.868112
	H	-0.678729	2.896425	3.115185
	H	-1.172447	1.605646	1.954317
	H	-1.121100	1.293915	3.658218
	H	1.332213	1.486626	3.766913
	H	0.906412	0.299572	2.554831
IV	U	0.520724	2.703742	-0.070773
	H	3.595350	1.211872	-1.092584
	N	1.636596	0.688166	-0.350765
	C	2.575518	1.354473	-0.733154
	C	1.221647	3.226287	2.103506
	C	0.164791	2.213529	2.595022
	H	2.235073	2.927445	2.383435
	H	1.027629	4.227427	2.503375
	C	-1.259902	2.783859	2.635962
	H	-1.316753	3.611315	3.345770
	H	-1.599328	3.207401	1.668508
	H	-1.996541	2.028801	2.914432
	H	0.422689	1.783572	3.566159
	H	0.169251	1.293823	1.947895
HCN	C	0.000000	0.000000	-0.498334
	H	0.000000	0.000000	-1.564845
	N	-0.000000	0.000000	0.650693
$[UCH_2CH_2CH_3]^+$	U	0.795087	2.122141	-0.058600
	C	1.141705	3.209688	1.938936
	C	0.160880	2.269272	2.662182
	H	2.179187	3.052313	2.268914
	H	0.892406	4.265572	2.073982
	C	-1.288592	2.764162	2.659607
	H	-1.358783	3.716423	3.189216
	H	-1.674527	2.948509	1.644133
	H	-1.960475	2.049035	3.136947
	H	0.495659	2.035058	3.675346
	H	0.180534	1.241847	2.189733

Table 4.2: $[UH]^+ + CH_3CH_2CH_2CN$ PBE1PBE/SDD/6-311+g(d,p) Quintet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr

$[UH]^+$	-477.12109	.00377	.00614	.00708	-.01913	-477.11732	-477.11495	-477.11401	-477.14021
$CH_3CH_2CH_2CN$	-211.17680	.10305	.10900	.10995	.07408	-211.07375	-211.06780	-211.06685	-211.10272
$[UH]^+ + CH_3CH_2CN$ (**I**)	-688.29789	.10682	.11514	.11703	.05495	-688.19106	-688.18275	-688.18086	-688.24294
II	-688.36420	.10766	.11636	.11731	.06946	-688.25654	-688.24784	-688.24690	-688.29475
TSII→III	-688.35408	.10823	.11597	.11692	.07131	-688.24585	-688.23810	-688.23716	-688.28276
III	-688.40520	.11449	.12239	.12334	.07734	-688.29071	-688.28281	-688.28186	-688.32785
TSIII→IV	-688.34881	.10973	.11716	.11810	.07443	-688.23908	-688.23165	-688.23071	-688.27439
IV	-688.37001	.10824	.11695	.11790	.07138	-688.26177	-688.25306	-688.25212	-688.29864
HCN	-93.33544	.01649	.01903	.01997	-.00287	-93.31895	-93.31641	-93.31547	-93.33831
$[UCH_2CH_2CH_3]^+$	-594.98208	.09017	.09597	.09691	.05730	-594.89192	-594.88612	-594.88517	-594.92478
$[UCH_2CH_2CH_3]^+ + HCN$ (**V**)	-688.31752	.10666	.11499	.11688	.05443	-688.21086	-688.20253	-688.20064	-688.26309

Table 4.2.1: $[UH]^+ + CH_3CH_2CH_2CN$ PBE1PBE/SDD/6-311+g(d,p) Quintet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	-0.282792	0.024095	0.017719
	H	-0.733284	1.219330	1.490648
$CH_3CH_2CH_2CN$	C	-2.513350	-0.394731	0.089606
	C	-1.430125	0.651711	0.299570
	C	-0.038341	0.099404	-0.027597
	C	1.018885	1.080285	0.165007
	N	1.843719	1.869872	0.322588
	H	-2.352853	-1.268753	0.728890
	H	-3.499479	0.012196	0.326398
	H	-2.537774	-0.740716	-0.948687
	H	-1.621486	1.527527	-0.328203
	H	-1.438102	1.003772	1.335793
	H	0.184209	-0.770412	0.600718
	H	0.000569	-0.245177	-1.067148
II	U	0.523058	-0.232881	-1.225020
	H	-0.420936	1.379779	-0.505095
	N	2.620766	0.481502	-0.936565
	C	2.561734	0.169919	0.233232
	C	3.223640	0.123245	1.549066
	C	2.281593	0.287859	2.742779
	H	3.741247	-0.843695	1.590908
	H	3.997317	0.902395	1.539958
	C	1.588468	1.641147	2.777455
	H	2.315648	2.457527	2.816583
	H	0.956783	1.802401	1.896163
	H	0.948933	1.726982	3.658332
	H	2.879573	0.148455	3.647610
	H	1.545994	-0.524961	2.736589
TSII→III	U	1.169106	-0.113360	-1.806146
	H	1.111702	-0.854742	0.063419
	N	2.048997	1.339388	-0.512471
	C	2.383711	0.370949	0.192692
	C	3.044364	0.068101	1.477041
	C	2.136522	0.377938	2.681780
	H	3.346809	-0.981262	1.493416
	H	3.949001	0.687448	1.517804
	C	1.816982	1.853369	2.855591
	H	2.728268	2.443322	2.990050
	H	1.280088	2.264590	1.995829
	H	1.191768	2.005246	3.738394

	H	2.658109	-0.000642	3.566147
	H	1.217358	-0.212072	2.594108
III	U	-0.184431	0.929913	-1.536918
	H	3.464353	2.439087	-1.156945
	N	1.673238	1.494574	-0.889190
	C	2.825400	1.856134	-0.478931
	C	3.422102	1.536792	0.844076
	C	2.529527	0.848076	1.864368
	H	4.313222	0.930532	0.612593
	H	3.844483	2.472594	1.239444
	C	1.496344	1.773567	2.494799
	H	1.979675	2.598155	3.026838
	H	0.829009	2.217648	1.748045
	H	0.878046	1.236676	3.218127
	H	3.167876	0.433448	2.649595
	H	2.039364	-0.012440	1.392974
TSIII→IV	U	0.266661	3.165134	0.319034
	H	2.762179	0.955197	-0.242090
	N	0.748884	1.469283	-0.836667
	C	1.853626	1.550187	-0.239524
	C	1.837915	2.110878	1.802890
	C	0.906477	1.375117	2.764364
	H	2.848565	1.709198	1.854859
	H	1.949882	3.196267	2.080928
	C	-0.560958	1.813707	2.708380
	H	-0.697203	2.889402	2.919492
	H	-1.069155	1.527651	1.763996
	H	-1.156612	1.302546	3.467781
	H	1.267753	1.500339	3.792062
	H	0.956799	0.304437	2.545804
IV	U	0.492604	2.746296	-0.023203
	H	3.525910	1.245537	-0.996140
	N	1.536719	0.724542	-0.333427
	C	2.496708	1.389577	-0.662884
	C	1.246548	3.218382	2.120083
	C	0.189681	2.199332	2.559755
	H	2.258861	2.903262	2.387342
	H	1.052328	4.205575	2.555196
	C	-1.224937	2.772525	2.597357
	H	-1.287252	3.570936	3.340268
	H	-1.547975	3.249643	1.646861
	H	-1.975376	2.014150	2.827527
	H	0.428315	1.724998	3.515980
	H	0.204608	1.296958	1.882073
HCN	C	0.000000	0.000000	-0.497856
	H	0.000000	0.000000	-1.566083
	N	-0.000000	-0.000000	0.650460
$[UCH_2CH_2CH_3]^+$	U	0.492291	2.165845	0.049288
	C	1.173266	3.193174	1.974840
	C	0.184746	2.278529	2.697675
	H	2.215640	2.971262	2.240000
	H	0.973244	4.252801	2.160999
	C	-1.256308	2.763954	2.590415
	H	-1.356571	3.747544	3.054353
	H	-1.605342	2.914903	1.544797
	H	-1.963662	2.072944	3.052520
	H	0.457480	2.084385	3.738189
	H	0.248295	1.228678	2.277321

Table 4.3: $[UH]^+ + CH_3CH_2CH_2CN$ B3LYP/SDD/6-311+g(d,p) Singlet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-477.13768	.00368	.00605	.00699	-.01769	-477.13400	-477.13164	-477.13069	-477.15538
$CH_3CH_2CH_2CN$	-211.44532	.10244	.10841	.10935	.07343	-211.34289	-211.33691	-211.33597	-211.37189
$[UH]^+ + CH_3CH_2CN$ (**I**)	-688.58300	.10612	.11445	.11634	.05574	-688.47689	-688.46855	-688.46666	-688.52726
II	-688.68196	.10701	.11548	.11642	.07082	-688.57496	-688.56649	-688.56554	-688.61115
TSII→III	-688.65972	.10759	.11515	.11610	.07231	-688.55213	-688.54457	-688.54362	-688.58741
III	-688.68554	.11307	.12037	.12132	.07948	-688.57247	-688.56517	-688.56422	-688.60606
TSIII→IV	-688.66041	.10979	.11688	.11783	.07655	-688.55062	-688.54353	-688.54259	-688.58386
IV	-688.69530	.10802	.11657	.11752	.07263	-688.58728	-688.57873	-688.57779	-688.62267
HCN	-93.45449	.01636	.01890	.01985	-.00300	-93.43813	-93.43559	-93.43465	-93.45749
$[UCH_2CH_2CH_3]^+$	-595.14973	.08955	.09539	.09633	.05801	-595.06018	-595.05434	-595.05339	-595.09172
$[UCH_2CH_2CH_3]^+ + HCN$ (**V**)	-688.60422	.10591	.11429	.11618	.05501	-688.49831	-688.48993	-688.48804	-688.54921

Table 4.3.1: $[UH]^+ + CH_3CH_2CH_2CN$ B3LYP/SDD/6-311+g(d,p) Singlet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	-0.274048	0.000897	-0.010869
	H	-0.723542	1.193481	1.458793
$CH_3CH_2CH_2CN$	C	-2.522854	-0.398896	0.089360
	C	-1.432195	0.652798	0.300119
	C	-0.030160	0.099753	-0.028426
	C	1.031270	1.085065	0.165164
	N	1.856379	1.875364	0.323011
	H	-2.363618	-1.272371	0.728972
	H	-3.507281	0.011013	0.326889
	H	-2.548541	-0.744398	-0.948611
	H	-1.624726	1.527313	-0.327858
	H	-1.441327	1.003630	1.335991
	H	0.191242	-0.769653	0.599702
	H	0.007683	-0.244642	-1.067379
II	U	0.689192	-0.137116	-1.288731
	H	-0.041196	1.669922	-1.028204
	N	2.623888	0.238145	-0.978948
	C	2.309336	0.084436	0.260381
	C	3.126504	0.191122	1.494428
	C	2.327353	0.271117	2.803056
	H	3.774434	-0.698301	1.490642
	H	3.803327	1.047549	1.381155
	C	1.519683	1.563424	2.941311
	H	2.170392	2.442019	2.918247
	H	0.787851	1.676697	2.133068
	H	0.970841	1.582651	3.884805
	H	3.033702	0.189236	3.633217
	H	1.668511	-0.601225	2.877570
TSII→III	U	0.865048	-0.034092	-1.440366
	H	1.171747	1.250929	0.041753
	N	2.751013	0.058591	-1.118106
	C	2.269297	0.149139	0.158755
	C	3.079964	0.297591	1.397667
	C	2.303008	0.325091	2.724276
	H	3.771602	-0.554392	1.383050
	H	3.713695	1.187987	1.292881

	C	1.516736	1.614105	2.979848
	H	2.173947	2.488218	2.959620
	H	0.726592	1.775658	2.240614
	H	1.039816	1.583959	3.961813
	H	3.031394	0.187921	3.528203
	H	1.636685	-0.543394	2.770650
III	U	0.413995	2.321219	-0.487688
	H	3.363068	2.368554	-1.220987
	N	1.683251	1.074958	-0.970239
	C	2.724694	1.910250	-0.461687
	C	3.472567	1.526517	0.804121
	C	2.632904	0.859293	1.908102
	H	4.297990	0.851756	0.544610
	H	3.945301	2.436467	1.192284
	C	1.299647	1.561379	2.232879
	H	1.348394	2.655109	2.084123
	H	0.448304	1.117355	1.670923
	H	0.991346	1.424068	3.271601
	H	3.233691	0.826704	2.819463
	H	2.423056	-0.178872	1.641370
TSIII→IV	U	0.129704	2.129152	-0.151820
	H	3.312959	1.975283	-0.077028
	N	1.509425	0.896846	-0.645485
	C	2.230326	1.930298	-0.072337
	C	1.718681	2.068017	1.811070
	C	0.579440	1.229122	2.376760
	H	2.688463	1.640349	2.048635
	H	1.703611	3.108155	2.147423
	C	-0.544951	2.048092	3.025589
	H	-0.952843	2.836877	2.365723
	H	-1.383031	1.419534	3.330908
	H	-0.170538	2.578469	3.903092
	H	0.940537	0.462161	3.065328
	H	0.153033	0.546985	1.573449
IV	U	0.557642	2.333777	-0.067173
	H	3.556452	1.341903	-1.056629
	N	1.731814	0.693011	-0.201740
	C	2.545395	1.552778	-0.705240
	C	1.200287	3.161774	1.983706
	C	0.159806	2.225782	2.625717
	H	2.223020	2.929194	2.285874
	H	0.989691	4.216965	2.190582
	C	-1.264403	2.794874	2.657317
	H	-1.296358	3.701216	3.264997
	H	-1.647221	3.089658	1.661362
	H	-1.980285	2.077110	3.060551
	H	0.468722	1.909571	3.625145
	H	0.152179	1.234098	2.092319
HCN	C	0.000000	0.000000	-0.498334
	H	0.000000	0.000000	-1.564845
	N	-0.000000	0.000000	0.650693
$[UCH_2CH_2CH_3]^+$	U	-0.152646	3.691684	0.411097
	C	1.336762	3.026067	1.974070
	C	0.214523	2.422637	2.871291
	H	2.053425	2.269356	1.638086
	H	1.875462	3.839274	2.471907
	C	-1.276758	2.535371	2.359825
	H	-1.668511	3.582683	2.276645
	H	-1.496280	1.968587	1.417925
	H	-1.937157	2.073929	3.095138
	H	0.222943	2.907127	3.847315

	H	0.391316	1.357303	3.017097

Table 4.4: $[UH]^+$ + $CH_3CH_2CH_2CN$ PBE1PBE/SDD/6-311+g(d,p) Singlet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-477.01929	.00372	.00608	.00703	-.01765	-477.01557	-477.01321	-477.01226	-477.03694
$CH_3CH_2CH_2CN$	-211.17680	.10305	.10900	.10995	.07408	-211.07375	-211.06780	-211.06685	-211.10272
$[UH]^+$ + CH_3CH_2CN (**I**)	-688.19608	.10677	.11508	.11697	.05643	-688.08932	-688.08100	-688.07911	-688.13966
II	-688.31743	.10766	.11611	.11706	.07156	-688.20976	-688.20132	-688.20037	-688.24587
TSII→III	-688.30247	.10842	.11593	.11688	.07303	-688.19405	-688.18654	-688.18560	-688.22944
III	-688.32778	.11385	.12095	.12189	.08062	-688.21393	-688.20683	-688.20589	-688.24716
TSIII→IV	-688.30094	.11006	.11730	.11824	.07655	-688.19088	-688.18365	-688.18270	-688.22439
IV	-688.33464	.10890	.11725	.11819	.07403	-688.22575	-688.21740	-688.21645	-688.26061
HCN	-93.33544	.01649	.01903	.01997	-.00287	-93.31895	-93.31641	-93.31547	-93.33831
$[UCH_2CH_2CH_3]^+$	-594.89042	.08956	.09523	.09618	.05841	-594.80085	-594.79518	-594.79424	-594.83201
$[UCH_2CH_2CH_3]^+$ + HCN (**V**)	-688.22585	.10606	.11426	.11615	.05554	-688.11980	-688.11160	-688.10971	-688.17031

Table 4.4.1: $[UH]^+$ + $CH_3CH_2CH_2CN$ PBE1PBE/SDD/6-311+g(d,p) Singlet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	-0.274832	0.002976	-0.008307
	H	-0.722758	1.191402	1.456231
$CH_3CH_2CH_2CN$	C	-2.513350	-0.394731	0.089606
	C	-1.430125	0.651711	0.299570
	C	-0.038341	0.099404	-0.027597
	C	1.018885	1.080285	0.165007
	N	1.843719	1.869872	0.322588
	H	-2.352853	-1.268753	0.728890
	H	-3.499479	0.012196	0.326398
	H	-2.537774	-0.740716	-0.948687
	H	-1.621486	1.527527	-0.328203
	H	-1.438102	1.003772	1.335793
	H	0.184209	-0.770412	0.600718
	H	0.000569	-0.245177	-1.067148
II	U	0.679491	-0.116559	-1.211868
	H	0.045338	1.708041	-0.914956
	N	2.610168	0.183768	-0.973609
	C	2.289453	0.078919	0.276107
	C	3.121942	0.197395	1.488699
	C	2.337821	0.278842	2.795074
	H	3.786291	-0.680154	1.478192
	H	3.785006	1.063380	1.358136
	C	1.502970	1.545613	2.906453
	H	2.132006	2.439994	2.868333
	H	0.773789	1.626940	2.090439
	H	0.946828	1.571681	3.845936
	H	3.050355	0.231299	3.623525
	H	1.702359	-0.609486	2.891533
TSII→III	U	0.876219	0.027761	-1.393851
	H	1.189801	1.319933	0.041056
	N	2.746932	0.044570	-1.096610
	C	2.261183	0.151884	0.178849

	C	3.076301	0.279598	1.407511
	C	2.304798	0.321774	2.725533
	H	3.753315	-0.584808	1.387403
	H	3.727339	1.157820	1.298241
	C	1.513870	1.602274	2.953370
	H	2.163549	2.481859	2.910090
	H	0.719713	1.740708	2.212692
	H	1.039042	1.592934	3.937152
	H	3.033638	0.202452	3.532874
	H	1.644844	-0.551449	2.786346
III	U	0.457514	2.305626	-0.448615
	H	3.326434	2.385668	-1.194917
	N	1.677585	1.040716	-0.929721
	C	2.696089	1.939443	-0.417655
	C	3.473536	1.528709	0.813413
	C	2.634024	0.854764	1.899515
	H	4.292081	0.854534	0.532646
	H	3.951460	2.431726	1.213748
	C	1.308667	1.563018	2.201494
	H	1.360251	2.652089	2.003815
	H	0.452572	1.086211	1.671781
	H	1.005478	1.484214	3.248619
	H	3.222481	0.806974	2.818907
	H	2.420039	-0.178936	1.615846
TSIII→IV	U	0.214535	2.858441	0.200720
	H	2.905358	1.254326	-0.312434
	N	0.751513	1.173049	-0.509083
	C	1.951229	1.750717	-0.165702
	C	1.854394	2.127993	1.776875
	C	0.861235	1.344876	2.647074
	H	2.838769	1.666656	1.850946
	H	1.996978	3.171544	2.125311
	C	-0.579673	1.884021	2.732020
	H	-0.632717	2.963208	2.950587
	H	-1.225783	1.632122	1.866146
	H	-1.112717	1.398582	3.552805
	H	1.257657	1.341183	3.667968
	H	0.834036	0.302624	2.318074
IV	U	0.519100	2.361156	-0.031125
	H	3.470548	1.299990	-0.936344
	N	1.609123	0.693340	-0.135174
	C	2.457439	1.543835	-0.611619
	C	1.216088	3.203301	1.969810
	C	0.205111	2.239437	2.591724
	H	2.245968	2.986481	2.260181
	H	0.979881	4.250528	2.192036
	C	-1.226498	2.765727	2.617274
	H	-1.285993	3.665771	3.233376
	H	-1.615506	3.068402	1.623593
	H	-1.929481	2.026072	3.004720
	H	0.513633	1.910063	3.587930
	H	0.237330	1.247606	2.050404
HCN	C	0.000000	0.000000	-0.497856
	H	0.000000	0.000000	-1.566083
	N	-0.000000	-0.000000	0.650460
$[UCH_2CH_2CH_3]^+$	U	-0.213106	3.702483	0.535776
	C	1.343447	3.067303	2.002448
	C	0.226989	2.417179	2.850027
	H	2.073286	2.336229	1.637967
	H	1.855580	3.877168	2.533408
	C	-1.263973	2.517085	2.327015
	H	-1.691420	3.567670	2.290116

	H	-1.472155	1.965060	1.357529
	H	-1.909777	2.009950	3.046187
	H	0.202001	2.866029	3.843510
	H	0.412208	1.347862	2.956416

Table 4.5: $[UH]^+$ + $CH_3CH_2CH_2CN$ B3LYP/SDD/6-311+g(d,p) Triplet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-477.14828	.00361	.00597	.00691	-.01880	-477.14467	-477.14231	-477.14136	-477.16708
$CH_3CH_2CH_2CN$	-211.44532	.10244	.10841	.10935	.07343	-211.34289	-211.33691	-211.33597	-211.37189
$[UH]^+$ + CH_3CH_2CN (**I**)	-688.59360	.10604	.11438	.11626	.05464	-688.48756	-688.47922	-688.47733	-688.53896
II	-688.72812	.10663	.11538	.11633	.06910	-688.62149	-688.61274	-688.61180	-688.65903
TSII→III	-688.70572	.10716	.11493	.11587	.07081	-688.59856	-688.59079	-688.58985	-688.63491
III	-688.75999	.11373	.12173	.12267	.07680	-688.64626	-688.63827	-688.63732	-688.68319
TSIII→IV	-688.70207	.10913	.11656	.11750	.07446	-688.59294	-688.58551	-688.58456	-688.62761
IV	-688.73621	.10748	.11629	.11723	.07074	-688.62873	-688.61992	-688.61898	-688.66547
HCN	-93.45449	.01636	.01890	.01985	-.00300	-93.43813	-93.43559	-93.43465	-93.45749
$[UCH_2CH_2CH_3]^+$	-595.22444	.08961	.09566	.09661	.05626	-595.13483	-595.12878	-595.12783	-595.16818
$[UCH_2CH_2CH_3]^+$ + HCN (**V**)	-688.67893	.10598	.11457	.11646	.05326	-688.57296	-688.56437	-688.56248	-688.62567

Table 4.5.1: $[UH]^+$ + $CH_3CH_2CH_2CN$ B3LYP/SDD/6-311+g(d,p) Triplet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	-0.275143	0.003800	-0.007291
	H	-0.722447	1.190578	1.455215
$CH_3CH_2CH_2CN$	C	-2.522854	-0.398896	0.089360
	C	-1.432195	0.652798	0.300119
	C	-0.030160	0.099753	-0.028426
	C	1.031270	1.085065	0.165164
	N	1.856379	1.875364	0.323011
	H	-2.363618	-1.272371	0.728972
	H	-3.507281	0.011013	0.326889
	H	-2.548541	-0.744398	-0.948611
	H	-1.624726	1.527313	-0.327858
	H	-1.441327	1.003630	1.335991
	H	0.191242	-0.769653	0.599702
	H	0.007683	-0.244642	-1.067379
II	U	0.658068	-0.159646	-1.369540
	H	-0.319802	1.499306	-0.860609
	N	2.650619	0.430674	-0.949709
	C	2.435302	0.131135	0.239356
	C	3.175996	0.154072	1.528557
	C	2.297286	0.265649	2.784396
	H	3.746542	-0.785183	1.545759
	H	3.912211	0.965436	1.478037
	C	1.562044	1.603098	2.893992
	H	2.264924	2.440440	2.918264
	H	0.882185	1.767399	2.050756
	H	0.966707	1.644970	3.808062
	H	2.946555	0.128973	3.652900
	H	1.585181	-0.566650	2.801774

TSII→III	U	0.797343	-0.144970	-1.512347
	H	0.999379	0.980617	0.159295
	N	2.773274	0.159664	-1.112105
	C	2.379905	0.153853	0.120549
	C	3.104706	0.312732	1.410431
	C	2.252214	0.326464	2.690067
	H	3.807175	-0.530753	1.428937
	H	3.729925	1.212786	1.342514
	C	1.577235	1.669645	2.984891
	H	2.320293	2.464279	3.096309
	H	0.884865	1.970937	2.193859
	H	1.008505	1.617863	3.915827
	H	2.909060	0.069272	3.525095
	H	1.506665	-0.475079	2.637335
III	U	-0.226950	0.915506	-1.609691
	H	3.423841	2.423692	-1.187188
	N	1.625258	1.494920	-0.905154
	C	2.787175	1.845226	-0.504296
	C	3.410533	1.520777	0.815090
	C	2.534274	0.848960	1.873984
	H	4.284060	0.896318	0.567324
	H	3.857514	2.451045	1.194002
	C	1.536862	1.798744	2.546293
	H	2.054853	2.615124	3.056862
	H	0.846732	2.249788	1.826390
	H	0.940714	1.271369	3.294208
	H	3.193488	0.425174	2.635935
	H	2.009856	-0.001886	1.425116
TSIII→IV	U	0.223276	3.125176	0.233103
	H	2.788691	1.103610	-0.275739
	N	0.679820	1.373576	-0.659629
	C	1.864354	1.655666	-0.149001
	C	1.866062	2.093704	1.794057
	C	0.905304	1.347872	2.734475
	H	2.868195	1.679288	1.869811
	H	1.989613	3.166554	2.076853
	C	-0.562854	1.819843	2.694428
	H	-0.669717	2.907439	2.861095
	H	-1.094506	1.508180	1.775061
	H	-1.149120	1.358202	3.491184
	H	1.270691	1.447747	3.762069
	H	0.935004	0.282485	2.493541
IV	U	0.600676	2.630279	-0.067341
	H	3.559738	1.207601	-0.944353
	N	1.552793	0.768582	-0.422867
	C	2.544969	1.499891	-0.663752
	C	1.230562	3.202906	2.092771
	C	0.173918	2.199096	2.589998
	H	2.244357	2.930251	2.394986
	H	1.018414	4.221007	2.438900
	C	-1.252337	2.766250	2.618761
	H	-1.314610	3.600647	3.319852
	H	-1.590434	3.176015	1.645383
	H	-1.987492	2.011461	2.901608
	H	0.433372	1.774862	3.562978
	H	0.182817	1.272865	1.949862
HCN	C	0.000000	0.000000	-0.498334
	H	0.000000	0.000000	-1.564845
	N	-0.000000	0.000000	0.650693
$[UCH_2CH_2CH_3]^+$	U	0.839797	2.099447	-0.055278
	C	1.133302	3.214047	1.932820
	C	0.157877	2.271494	2.656764

	H	2.171628	3.064912	2.266994
	H	0.877784	4.269671	2.056501
	C	-1.291288	2.765831	2.669915
	H	-1.357411	3.710951	3.212775
	H	-1.681942	2.961143	1.659340
	H	-1.959184	2.044790	3.144033
	H	0.501536	2.024887	3.663942
	H	0.170982	1.246847	2.172591

Table 4.6: $[UH]^+ + CH_3CH_2CH_2CN$ PBE1PBE/SDD/6-311+g(d,p) Triplet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-477.06589	.00353	.00589	.00684	-.01891	-477.06236	-477.06000	-477.05905	-477.08480
$CH_3CH_2CH_2CN$	-211.17680	.10305	.10900	.10995	.07408	-211.07375	-211.06780	-211.06685	-211.10272
$[UH]^+ + CH_3CH_2CN$ (I)	-688.24269	.10658	.11490	.11678	.05517	-688.13611	-688.12779	-688.12591	-688.18752
II	-688.36466	.10709	.11587	.11682	.06918	-688.25757	-688.24879	-688.24785	-688.29548
TSII→III	-688.34937	.10795	.11567	.11661	.07143	-688.24142	-688.23370	-688.23276	-688.27794
III	-688.39343	.11436	.12235	.12330	.07734	-688.27906	-688.27107	-688.27013	-688.31609
TSIII→IV	-688.34343	.10971	.11712	.11807	.07500	-688.23371	-688.22630	-688.22536	-688.26843
IV	-688.37748	.10855	.11707	.11801	.07244	-688.26893	-688.26041	-688.25947	-688.30504
HCN	-93.33544	.01649	.01903	.01997	-.00287	-93.31895	-93.31641	-93.31547	-93.33831
$[UCH_2CH_2CH_3]^+$	-594.97030	.09013	.09593	.09688	.05772	-594.88018	-594.87437	-594.87343	-594.91258
$[UCH_2CH_2CH_3]^+ + HCN$ (V)	-688.30574	.10662	.11496	.11685	.05485	-688.19912	-688.19078	-688.18889	-688.25089

Table 4.6.1: $[UH]^+ + CH_3CH_2CH_2CN$ B3LYP/SDD/6-311+g(d,p) Triplet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	-0.280565	0.018185	0.010435
	H	-0.735512	1.225240	1.497931
$CH_3CH_2CH_2CN$	C	-2.513350	-0.394731	0.089606
	C	-1.430125	0.651711	0.299570
	C	-0.038341	0.099404	-0.027597
	C	1.018885	1.080285	0.165007
	N	1.843719	1.869872	0.322588
	H	-2.352853	-1.268753	0.728890
	H	-3.499479	0.012196	0.326398
	H	-2.537774	-0.740716	-0.948687
	H	-1.621486	1.527527	-0.328203
	H	-1.438102	1.003772	1.335793
	H	0.184209	-0.770412	0.600718
	H	0.000569	-0.245177	-1.067148
II	U	0.617889	-0.132557	-1.242898
	H	-0.150717	1.638345	-0.823381
	N	2.630661	0.278362	-0.956264
	C	2.383594	0.101438	0.261688
	C	3.162398	0.172970	1.516011
	C	2.322638	0.274870	2.785787
	H	3.778196	-0.738772	1.523045
	H	3.866044	1.010782	1.424458
	C	1.531257	1.571333	2.869508
	H	2.194277	2.441582	2.862968
	H	0.839336	1.683364	2.025446
	H	0.939481	1.613447	3.786317

	H	2.996717	0.194983	3.643302
	H	1.652044	-0.590472	2.846007
TSII→III	U	0.686045	0.337244	-1.337764
	H	1.560791	1.599181	-0.066565
	N	2.560086	-0.318645	-0.978277
	C	2.309228	0.164792	0.197391
	C	3.122893	0.262771	1.432180
	C	2.339170	0.322999	2.743315
	H	3.803612	-0.595793	1.423301
	H	3.758974	1.152436	1.322629
	C	1.450034	1.547607	2.899676
	H	2.022081	2.474759	2.796012
	H	0.644153	1.573415	2.157438
	H	0.978233	1.558942	3.884790
	H	3.069434	0.300035	3.557860
	H	1.745812	-0.592431	2.848671
III	U	-0.249233	0.970453	-1.478394
	H	3.426676	2.428752	-1.180621
	N	1.625272	1.516496	-0.872329
	C	2.794153	1.854630	-0.489453
	C	3.416622	1.517844	0.817164
	C	2.536047	0.841827	1.856191
	H	4.290226	0.895876	0.561828
	H	3.866138	2.443672	1.206006
	C	1.536265	1.784043	2.515033
	H	2.047889	2.597591	3.037485
	H	0.858817	2.243083	1.786540
	H	0.926054	1.256059	3.251651
	H	3.185150	0.411713	2.624082
	H	2.018134	-0.007282	1.393692
TSIII→IV	U	0.232403	3.020918	0.267818
	H	2.855511	1.131677	-0.275972
	N	0.744710	1.321349	-0.685598
	C	1.907542	1.652344	-0.175093
	C	1.851278	2.100468	1.770418
	C	0.881432	1.364363	2.702183
	H	2.846996	1.669527	1.861467
	H	1.984124	3.177060	2.049577
	C	-0.577628	1.848749	2.726954
	H	-0.678793	2.922656	2.955702
	H	-1.159396	1.580111	1.821328
	H	-1.132554	1.336542	3.516106
	H	1.268157	1.441252	3.724594
	H	0.891032	0.302326	2.441824
IV	U	0.601025	2.675160	-0.025034
	H	3.474567	1.164976	-0.802173
	N	1.437493	0.801394	-0.371968
	C	2.467928	1.511931	-0.554882
	C	1.252553	3.219164	2.107028
	C	0.204868	2.198831	2.547658
	H	2.267137	2.945158	2.406685
	H	1.024104	4.226344	2.476345
	C	-1.218391	2.750921	2.561376
	H	-1.302138	3.558622	3.291989
	H	-1.539900	3.204790	1.599771
	H	-1.958237	1.982906	2.793725
	H	0.445455	1.733490	3.507500
	H	0.240277	1.288025	1.878767
HCN	C	0.000000	0.000000	-0.497856
	H	0.000000	0.000000	-1.566083
	N	-0.000000	-0.000000	0.650460

$[UCH_2CH_2CH_3]^+$	U	0.502834	2.176129	0.041740
	C	1.163109	3.207397	1.969234
	C	0.188562	2.279257	2.693473
	H	2.209504	2.992337	2.226578
	H	0.954904	4.264196	2.161831
	C	-1.256778	2.753085	2.601432
	H	-1.362213	3.731689	3.074679
	H	-1.611818	2.907751	1.558558
	H	-1.955201	2.052073	3.062151
	H	0.473908	2.077180	3.729015
	H	0.256268	1.232924	2.261707

Table 4.7.1: $[UH]^+ + CH_3CH_2CH_2CN$ B3LYP/SDD/6-311+g(d,p) Quintet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	0	0	0	0
II	-213.062	-211.594	-214.075	-179.075
TSII→III	-161.182	-163.826	-166.307	-118.119
III	-303.269	-304.309	-306.79	-264.745
TSIII→IV	-150.365	-151.447	-153.928	-109.439
IV	-217.756	-216.249	-218.728	-179.54
Products (V)	-111.442	-110.765	-110.767	-114.81

Table 4.7.2: $[UH]^+ + CH_3CH_2CH_2CN$ PBE1PBE/SDD/6-311+g(d,p) Quintet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	0	0	0	0
II	-171.92	-170.899	-173.378	-136.025
TSII→III	-143.835	-145.324	-147.803	-104.566
III	-261.613	-262.697	-265.176	-222.952
TSIII→IV	-126.077	-128.392	-130.871	-82.572
IV	-185.641	-184.599	-187.075	-146.243
Products (V)	-51.9875	-51.9271	-51.9271	-52.9117

Table 4.7.3: $[UH]^+ + CH_3CH_2CH_2CN$ B3LYP/SDD/6-311+g(d,p) Singlet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	165.1177	165.1203	165.1177	169.1373
II	-92.3651	-92.0107	-94.4918	-51.1027
TSII→III	-32.4354	-34.4544	-36.9355	11.22926
III	-85.8434	-88.5424	-91.0235	-37.7547
TSIII→IV	-28.4683	-31.7318	-34.2129	20.54454
IV	-124.722	-124.155	-126.636	-81.3669

Products (V)	108.8821	109.0003	108.9976	111.5129

Table 4.7.4: $[UH]^+ + CH_3CH_2CH_2CN$ PBE1PBE/SDD/6-311+g(d,p) Singlet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	267.1394	267.1394	267.1394	271.1564
II	-49.0995	-48.7424	-51.2183	-7.70322
TSII→III	-7.85025	-9.95065	-12.4265	35.43113
III	-60.0399	-63.2247	-65.7031	-11.0927
TSIII→IV	0.477841	-2.36032	-4.83617	48.68465
IV	-91.0655	-90.9605	-93.4389	-46.4031
Products (V)	187.1036	186.8148	186.8148	190.6691

Table 4.7.5: $[UH]^+ + CH_3CH_2CH_2CN$ B3LYP/SDD/6-311+g(d,p) Triplet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	137.1036	137.1062	137.1036	138.4216
II	-214.543	-213.445	-215.926	-176.812
TSII→III	-154.335	-155.823	-158.302	-113.495
III	-279.579	-280.464	-282.942	-240.262
TSIII→IV	-139.566	-141.948	-144.429	-94.3158
IV	-233.541	-232.294	-234.775	-193.72
Products (V)	-87.1115	-86.442	-86.4446	-89.2355

Table 4.7.6: $[UH]^+ + CH_3CH_2CH_2CN$ PBE1PBE/SDD/6-311+g(d,p) Triplet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	144.2844	144.2896	144.2896	145.5
II	-174.619	-173.385	-175.864	-137.954
TSII→III	-132.218	-133.767	-136.245	-91.903
III	-231.041	-231.892	-234.371	-192.063
TSIII→IV	-111.98	-114.348	-116.827	-66.924
IV	-204.432	-203.902	-206.377	-163.041
Products (V)	-21.1589	-21.088	-21.088	-20.8806

Figure 6: $[UH]^+ + CH_3CH_2CH_2CN$ B3LYP/SDD/6-311+g(d,p) Relative Enthalpy (kJ/mol)

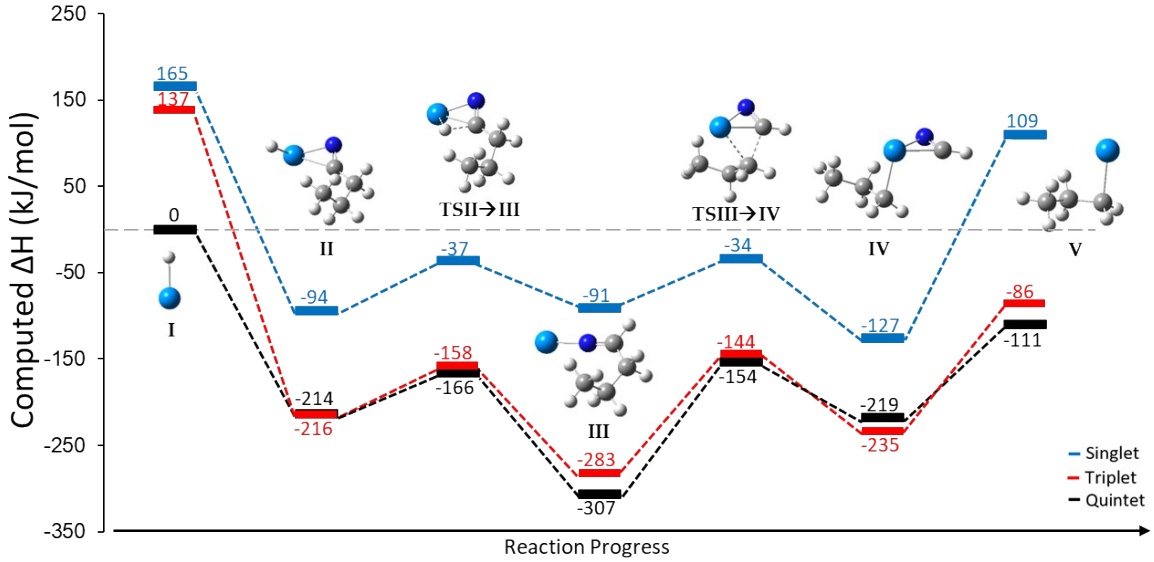

Figure 6.1: $[UH]^+$ + $CH_3CH_2CH_2CN$ PBE1PBE/SDD/6-311+g(d,p) Relative Enthalpy (kJ/mol)

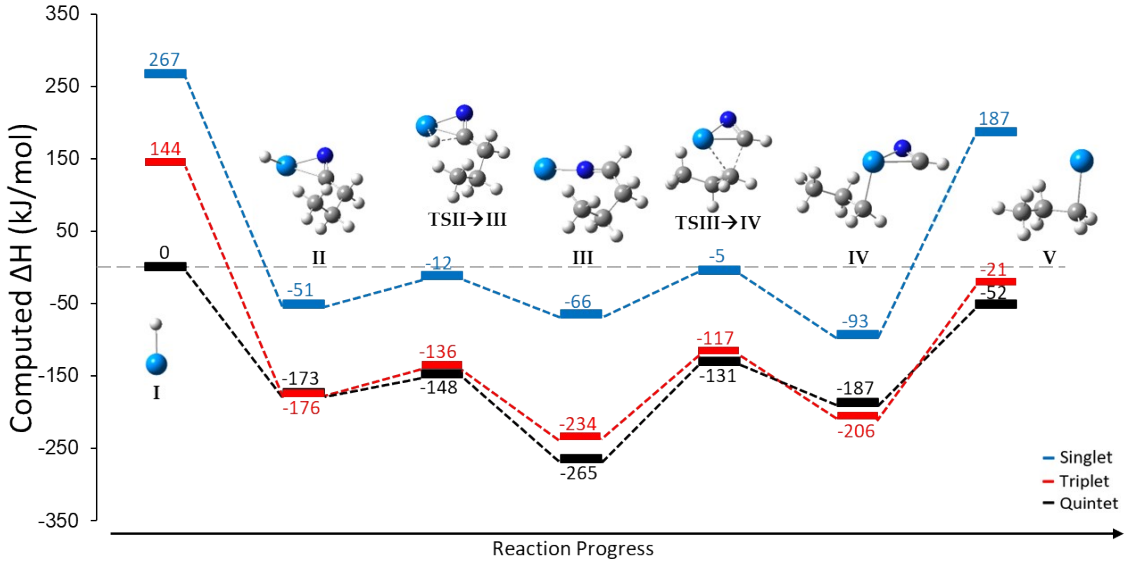

Table 5.1: $[UH]^+$ + C_6H_5CN B3LYP/SDD/6-311+g(d,p) Quintet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-477.20060	.00371	.00608	.00702	-.01919	-477.19689	-477.19453	-477.19358	-477.21980
C_6H_5CN	-324.57776	.09886	.10496	.10590	.06860	-324.47890	-324.47280	-324.47186	-324.50916
$[UH]^+$ + C_6H_5CN (I)	-801.77836	.10257	.11103	.11292	.04941	-801.67579	-801.66733	-801.66544	-801.72896
II	-801.86635	.10353	.11261	.11355	.06445	-801.76282	-801.75375	-801.75280	-801.80190
TSII→III	-801.85081	.10357	.11171	.11265	.06592	-801.74725	-801.73911	-801.73816	-801.78489
III	-801.91353	.11094	.11908	.12003	.07285	-801.80259	-801.79445	-801.79350	-801.84068

TSIII→IV	-801.84755	.10620	.11449	.11543	.06848	-801.74135	-801.73306	-801.73211	-801.77906
IV	-801.86884	.10528	.11479	.11574	.06504	-801.76356	-801.75405	-801.75311	-801.80381
HCN	-93.45449	.01636	.01890	.01985	-.00300	-93.43813	-93.43559	-93.43465	-93.45749
$[UC_6H_5]^+$	-708.37166	.08839	.09467	.09561	.05346	-708.28328	-708.27700	-708.27605	-708.31820
$[UC_6H_5]^+$ + HCN (**V**)	-801.82616	.10475	.11357	.11546	.05046	-801.72141	-801.71259	-801.71070	-801.77570

Table 5.1.1: $[UH]^+$ + C_6H_5CN B3LYP/SDD/6-311+g(d,p) Quintet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	0.000000	0.000000	0.021045
	H	0.000000	0.000000	-1.936098
C_6H_5CN	C	-1.055947	0.491891	2.538959
	C	0.012079	0.288629	3.426226
	C	0.319458	1.263129	4.368751
	C	-0.429975	2.438154	4.432931
	C	-1.491221	2.640988	3.551891
	C	-1.808457	1.673241	2.604426
	H	0.587893	-0.626722	3.368545
	H	1.144135	1.106670	5.054186
	H	-0.185961	3.194753	5.169870
	H	-2.073506	3.553624	3.601569
	H	-2.631243	1.823115	1.916425
	C	-1.376868	-0.508430	1.566180
	N	-1.635176	-1.316419	0.781279
II	U	-2.161000	0.071976	0.284512
	H	-1.953291	1.233563	-1.350101
	N	-0.059596	-0.655525	0.467581
	C	0.306835	0.353496	1.047764
	C	1.396404	1.081126	1.633971
	C	2.681723	0.499558	1.616329
	C	3.747021	1.188163	2.176632
	C	3.544926	2.446199	2.750213
	C	2.274604	3.024654	2.767325
	C	1.199042	2.346237	2.211267
	H	2.824803	-0.475110	1.166468
	H	4.736707	0.747894	2.166587
	H	4.383005	2.978444	3.184638
	H	2.127872	4.001401	3.211320
	H	0.210333	2.789784	2.215313
TSII→III	U	-1.920295	-0.021046	0.108650
	H	-0.807405	1.663138	0.346390
	N	0.132766	-0.588367	0.173019
	C	0.351120	0.441724	0.849237
	C	1.434916	1.140088	1.492092
	C	2.679840	0.488207	1.600764
	C	3.731508	1.122737	2.246377
	C	3.556756	2.401650	2.779748
	C	2.325595	3.051657	2.671500
	C	1.264134	2.423561	2.035250
	H	2.803453	-0.501706	1.178919
	H	4.690122	0.625184	2.330484
	H	4.383011	2.893827	3.279195
	H	2.198110	4.045214	3.083468
	H	0.306736	2.922228	1.940711
III	U	-0.533681	-1.994178	-0.715044
	H	-0.724554	1.549973	0.973809
	N	-0.066181	-0.267046	0.288058

	C	0.119589	0.853103	0.905402
	C	1.339090	1.312495	1.535283
	C	2.523154	0.548654	1.542594
	C	3.660154	1.038228	2.161270
	C	3.633866	2.294262	2.781032
	C	2.468901	3.061364	2.781542
	C	1.325904	2.574335	2.161775
	H	2.534692	-0.421533	1.060910
	H	4.571641	0.452876	2.168011
	H	4.527378	2.672427	3.264116
	H	2.455939	4.031520	3.262669
	H	0.415685	3.164470	2.157591
TSIII→IV	U	-2.345103	0.146893	0.533457
	H	1.720067	-0.480215	-0.697515
	N	-0.436376	-0.292396	-1.189171
	C	0.677659	-0.376053	-0.930850
	C	-0.752861	0.876134	2.032819
	C	0.462679	0.625012	2.700737
	C	0.908099	1.468337	3.710494
	C	0.150777	2.586074	4.087646
	C	-1.060801	2.856650	3.464800
	C	-1.493462	1.994424	2.451555
	H	1.059100	-0.246421	2.446218
	H	1.842578	1.260023	4.219220
	H	0.508459	3.238370	4.875644
	H	-1.654743	3.713835	3.758691
	H	-2.460037	2.253632	1.981759
IV	U	-1.709006	0.158950	0.254847
	H	1.212738	0.849383	-1.670631
	N	0.070574	-0.810951	-0.882743
	C	0.413505	0.317847	-1.154078
	C	-0.792363	0.696005	2.294640
	C	0.136544	0.391132	3.308042
	C	0.280074	1.228689	4.407130
	C	-0.491474	2.393541	4.521519
	C	-1.414009	2.728795	3.537584
	C	-1.551495	1.871652	2.441289
	H	0.748502	-0.501744	3.236710
	H	0.996154	0.984623	5.183581
	H	-0.366899	3.039014	5.382998
	H	-2.010788	3.629158	3.621783
	H	-2.303630	2.175058	1.685821
HCN	C	0.000000	0.000000	-0.498334
	H	0.000000	0.000000	-1.564845
	N	-0.000000	0.000000	0.650693
$[UC_6H_5]^+$	U	-1.619128	0.164753	0.203762
	C	-0.720398	0.738416	2.200776
	C	0.231964	0.440728	3.195893
	C	0.332274	1.239782	4.326384
	C	-0.510507	2.349084	4.492019
	C	-1.460134	2.668979	3.528984
	C	-1.551571	1.857277	2.394241
	H	0.891660	-0.413299	3.085424
	H	1.066132	1.008227	5.089724
	H	-0.420171	2.963139	5.380370
	H	-2.111780	3.524959	3.655734
	H	-2.318279	2.145734	1.652696

Table 5.2: $[UH]^+ + C_6H_5CN$ PBE1PBE/SDD/6-311+g(d,p) Quintet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-477.12109	.00377	.00614	.00708	-.01913	-477.11732	-477.11495	-477.11401	-477.14021
C_6H_5CN	-324.18042	.09961	.10570	.10664	.06936	-324.08081	-324.07472	-324.07378	-324.11106
$[UH]^+ + C_6H_5CN$ (**I**)	-801.30151	.10339	.11183	.11372	.05023	-801.19812	-801.18967	-801.18779	-801.25127
II	-801.37328	.10443	.11345	.11439	.06550	-801.26885	-801.25983	-801.25889	-801.30778
TSII→III	-801.36438	.10466	.11271	.11365	.06712	-801.25972	-801.25167	-801.25073	-801.29726
III	-801.41999	.11173	.11986	.12080	.07365	-801.30826	-801.30013	-801.29918	-801.34634
TSIII→IV	-801.36248	.10680	.11501	.11596	.06946	-801.25568	-801.24747	-801.24652	-801.29302
IV	-801.37767	.10623	.11563	.11657	.06640	-801.27144	-801.26204	-801.26110	-801.31127
HCN	-93.33544	.01649	.01903	.01997	-.00287	-93.31895	-93.31641	-93.31547	-93.33831
$[UC_6H_5]^+$	-707.99054	.08892	.09514	.09609	.05417	-707.90162	-707.89539	-707.89445	-707.93636
$[UC_6H_5]^+ + HCN$ (**V**)	-801.32597	.10541	.11417	.11606	.05131	-801.22056	-801.21181	-801.20992	-801.27467

Table 5.2.1: $[UH]^+ + C_6H_5CN$ PBE1PBE/SDD/6-311+g(d,p) Quintet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	-0.282792	0.024095	0.017719
	H	-0.733284	1.219330	1.490648
C_6H_5CN	C	-1.054586	0.494902	2.542305
	C	0.009974	0.290792	3.425682
	C	0.316578	1.262988	4.365902
	C	-0.430932	2.434561	4.429598
	C	-1.489871	2.637178	3.550649
	C	-1.806101	1.672161	2.605991
	H	0.585621	-0.625896	3.366956
	H	1.142065	1.105662	5.051529
	H	-0.187126	3.192135	5.166963
	H	-2.072462	3.550623	3.600568
	H	-2.629208	1.819719	1.916153
	C	-1.374792	-0.502883	1.571847
	N	-1.633949	-1.309317	0.787096
II	U	-2.109168	0.083336	0.323645
	H	-1.876672	1.300821	-1.250590
	N	-0.033680	-0.672473	0.449949
	C	0.308515	0.343663	1.036120
	C	1.392365	1.073867	1.623614
	C	2.672943	0.494450	1.615839
	C	3.731564	1.185718	2.177528
	C	3.524091	2.443223	2.741246
	C	2.256544	3.019440	2.747770
	C	1.188305	2.337559	2.190455
	H	2.818121	-0.483511	1.170770
	H	4.722995	0.746787	2.175830
	H	4.359658	2.979621	3.178159
	H	2.106298	3.999615	3.185436
	H	0.197506	2.779745	2.184049
TSII→III	U	-1.890774	0.011156	0.179734
	H	-0.828082	1.711085	0.304723
	N	0.148916	-0.591354	0.166350
	C	0.362964	0.434065	0.847310
	C	1.441831	1.131113	1.492084
	C	2.683381	0.484313	1.602049
	C	3.728557	1.121954	2.248028
	C	3.546675	2.397381	2.778131

	C	2.317104	3.042018	2.667066
	C	1.262346	2.410156	2.030487
	H	2.809498	-0.506460	1.179543
	H	4.690141	0.628536	2.335314
	H	4.370768	2.893805	3.279373
	H	2.185646	4.036771	3.077486
	H	0.301395	2.903558	1.928126
III	U	-0.498466	-1.979809	-0.696154
	H	-0.723523	1.553588	0.976231
	N	-0.057092	-0.260404	0.294252
	C	0.123022	0.857903	0.909033
	C	1.338983	1.314835	1.536509
	C	2.516486	0.549654	1.540910
	C	3.652149	1.035652	2.157239
	C	3.627229	2.288275	2.775723
	C	2.467053	3.056185	2.778315
	C	1.325617	2.572319	2.160769
	H	2.522698	-0.421165	1.057157
	H	4.563844	0.448813	2.163216
	H	4.522658	2.665208	3.258731
	H	2.456705	4.026907	3.260577
	H	0.414213	3.162990	2.156510
TSIII→IV	U	-2.117364	-0.329609	0.744662
	H	0.875757	0.864929	-0.387435
	N	-0.498797	-0.793511	-0.618050
	C	-0.032406	0.288199	-0.233235
	C	-0.429529	0.836456	1.799083
	C	0.598967	0.480759	2.681691
	C	0.857939	1.279774	3.790798
	C	0.110709	2.432853	4.022812
	C	-0.902882	2.807174	3.144018
	C	-1.156233	2.018546	2.027683
	H	1.190030	-0.415095	2.510838
	H	1.650093	1.003774	4.479121
	H	0.332183	3.054185	4.883550
	H	-1.460806	3.722784	3.308944
	H	-1.891625	2.373080	1.291022
IV	U	-1.714336	-0.019095	0.355632
	H	0.949783	1.231086	-1.571172
	N	0.133116	-0.645826	-0.870200
	C	0.269333	0.539950	-1.072058
	C	-0.790872	0.541031	2.360694
	C	0.091906	0.275931	3.419582
	C	0.260509	1.198188	4.439597
	C	-0.438456	2.409558	4.428231
	C	-1.313879	2.708355	3.396571
	C	-1.475044	1.764747	2.381764
	H	0.649138	-0.655572	3.445607
	H	0.942591	0.983748	5.255847
	H	-0.293884	3.122175	5.233116
	H	-1.857868	3.646351	3.383505
	H	-2.193610	2.050525	1.581775
HCN	C	0.000000	0.000000	-0.497856
	H	0.000000	0.000000	-1.566083
	N	-0.000000	-0.000000	0.650460
$[UC_6H_5]^+$	U	-1.619128	0.164753	0.203762
	C	-0.720398	0.738416	2.200776
	C	0.231964	0.440728	3.195893
	C	0.332274	1.239782	4.326384
	C	-0.510507	2.349084	4.492019
	C	-1.460134	2.668979	3.528984
	C	-1.551571	1.857277	2.394241

	H	0.891660	-0.413299	3.085424
	H	1.066132	1.008227	5.089724
	H	-0.420171	2.963139	5.380370
	H	-2.111780	3.524959	3.655734
	H	-2.318279	2.145734	1.652696

Table 5.3: $[UH]^+ + C_6H_5CN$ B3LYP/SDD/6-311+g(d,p) Singlet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-477.13768	.00368	.00605	.00699	-.01769	-477.13400	-477.13164	-477.13069	-477.15538
C_6H_5CN	-324.57776	.09886	.10496	.10590	.06860	-324.47890	-324.47280	-324.47186	-324.50916
$[UH]^+ + C_6H_5CN$ (**I**)	-801.71544	.10254	.11100	.11289	.05091	-801.61290	-801.60444	-801.60255	-801.66453
II	-801.82619	.10409	.11273	.11368	.06780	-801.72211	-801.71346	-801.71251	-801.75839
TSII→III	-801.80007	.10421	.11204	.11298	.06860	-801.69586	-801.68803	-801.68709	-801.73147
III	-801.84095	.10912	.11673	.11767	.07458	-801.73183	-801.72422	-801.72327	-801.76637
TSIII→IV	-801.80312	.10674	.11465	.11560	.07098	-801.69638	-801.68847	-801.68753	-801.73215
IV	-801.83312	.10601	.11520	.11614	.06759	-801.72711	-801.71792	-801.71698	-801.76554
HCN	-93.45449	.01636	.01890	.01985	-.00300	-93.43813	-93.43559	-93.43465	-93.45749
$[UC_6H_5]^+$	-708.28231	.08817	.09449	.09543	.05469	-708.19414	-708.18782	-708.18687	-708.22762
$[UC_6H_5]^+ + HCN$ (**V**)	-801.73680	.10453	.11339	.11528	.05169	-801.63227	-801.62341	-801.62152	-801.68511

Table 5.3.1: $[UH]^+ + C_6H_5CN$ B3LYP/SDD/6-311+g(d,p) Singlet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	-0.274048	0.000897	-0.010869
	H	-0.723542	1.193481	1.458793
C_6H_5CN	C	-1.055947	0.491891	2.538959
	C	0.012079	0.288629	3.426226
	C	0.319458	1.263129	4.368751
	C	-0.429975	2.438154	4.432931
	C	-1.491221	2.640988	3.551891
	C	-1.808457	1.673241	2.604426
	H	0.587893	-0.626722	3.368545
	H	1.144135	1.106670	5.054186
	H	-0.185961	3.194753	5.169870
	H	-2.073506	3.553624	3.601569
	H	-2.631243	1.823115	1.916425
	C	-1.376868	-0.508430	1.566180
	N	-1.635176	-1.316419	0.781279
II	U	-1.875737	-0.054241	0.284638
	H	-1.749140	0.992459	-1.380597
	N	0.004096	-0.621870	0.487262
	C	0.145578	0.528386	1.088992
	C	1.306058	1.159497	1.646991
	C	2.570481	0.533482	1.578588
	C	3.679705	1.160895	2.120954
	C	3.544991	2.411700	2.733656
	C	2.300314	3.041191	2.806394
	C	1.184158	2.420251	2.265559
	H	2.658000	-0.434220	1.099472
	H	4.651405	0.684856	2.070241
	H	4.417057	2.898070	3.155346
	H	2.208764	4.010396	3.280913

	H	0.213657	2.901010	2.311409
TSII→III	U	-1.683399	-0.115523	0.157663
	H	-0.522149	1.500729	-0.017333
	N	0.148035	-0.651452	0.288568
	C	0.199054	0.563001	0.932059
	C	1.353382	1.195793	1.536348
	C	2.592081	0.530373	1.565171
	C	3.683952	1.127407	2.182191
	C	3.555338	2.389762	2.763644
	C	2.329618	3.059522	2.734551
	C	1.231474	2.465511	2.129504
	H	2.680123	-0.447339	1.107679
	H	4.637049	0.612999	2.207158
	H	4.411150	2.853885	3.239673
	H	2.235873	4.040127	3.185154
	H	0.278785	2.983302	2.103772
III	U	0.571713	-1.128519	1.708943
	H	-0.636895	1.538437	0.148099
	N	0.189449	-0.438934	-0.015559
	C	0.193025	0.885177	0.403967
	C	1.307099	1.379698	1.147908
	C	2.390578	0.464454	1.459428
	C	3.410302	0.849600	2.381296
	C	3.341069	2.064916	3.015503
	C	2.303706	2.980704	2.684529
	C	1.321470	2.659084	1.782640
	H	2.647760	-0.267142	0.663007
	H	4.252137	0.188022	2.552304
	H	4.102670	2.353149	3.729196
	H	2.303357	3.962198	3.144316
	H	0.554138	3.380105	1.523438
TSIII→IV	U	-1.745840	-0.758795	0.865263
	H	0.483989	1.035523	-0.600596
	N	-0.115213	-0.996837	-0.135460
	C	-0.244354	0.366842	-0.154746
	C	-0.439734	0.977928	1.691972
	C	0.500025	0.481966	2.614487
	C	0.748546	1.190727	3.793211
	C	0.084449	2.391860	4.035230
	C	-0.827880	2.902091	3.104161
	C	-1.082550	2.207687	1.925302
	H	1.060269	-0.424154	2.394937
	H	1.481780	0.822129	4.501137
	H	0.294296	2.949421	4.940228
	H	-1.319188	3.849807	3.291320
	H	-1.752560	2.628102	1.179057
IV	U	-1.532845	0.354223	0.109314
	H	1.374388	0.409884	-1.471300
	N	-0.131019	-0.865212	-0.694364
	C	0.414402	0.262848	-0.975105
	C	-0.741960	0.878834	2.160327
	C	0.251847	0.555217	3.102190
	C	0.341092	1.269809	4.290617
	C	-0.547587	2.319633	4.556410
	C	-1.535730	2.666138	3.638951
	C	-1.624519	1.938063	2.450916
	H	0.951113	-0.249111	2.903097
	H	1.106052	1.019160	5.016369
	H	-0.463965	2.871403	5.485355
	H	-2.219254	3.481072	3.844090
	H	-2.423588	2.239191	1.751625

HCN	C	0.000000	0.000000	-0.498334
	H	0.000000	0.000000	-1.564845
	N	-0.000000	0.000000	0.650693
$[UC_6H_5]^+$	U	-1.554512	0.302139	0.191644
	C	-0.746247	0.700624	2.226813
	C	0.219383	0.416980	3.213079
	C	0.337385	1.241671	4.322684
	C	-0.498988	2.358857	4.474649
	C	-1.460413	2.662566	3.518692
	C	-1.568008	1.828731	2.401074
	H	0.872158	-0.443104	3.110202
	H	1.080296	1.024529	5.081472
	H	-0.394804	2.990519	5.348993
	H	-2.112367	3.519184	3.639569
	H	-2.363821	2.085082	1.677137

Table 5.4: $[UH]^+ + C_6H_5CN$ PBE1PBE/SDD/6-311+g(d,p) Singlet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-477.01929	.00372	.00608	.00703	-.01765	-477.01557	-477.01321	-477.01226	-477.03694
C_6H_5CN	-324.18042	.09961	.10570	.10664	.06936	-324.08081	-324.07472	-324.07378	-324.11106
$[UH]^+ + C_6H_5CN$ (I)	-801.19970	.10333	.11178	.11367	.05171	-801.09638	-801.08793	-801.08604	-801.14800
II	-801.33219	.10488	.11353	.11448	.06858	-801.22732	-801.21866	-801.21772	-801.26361
TSII→III	-801.31370	.10522	.11299	.11393	.06969	-801.20848	-801.20071	-801.19977	-801.24401
III	-801.35882	.11007	.11759	.11854	.07566	-801.24875	-801.24123	-801.24028	-801.28316
TSIII→IV	-801.31774	.10755	.11537	.11632	.07193	-801.21019	-801.20237	-801.20142	-801.24582
IV	-801.34073	.10695	.11601	.11695	.06900	-801.23378	-801.22473	-801.22378	-801.27173
HCN	-93.33544	.01649	.01903	.01997	-.00287	-93.31895	-93.31641	-93.31547	-93.33831
$[UC_6H_5]^+$	-707.88915	.08865	.09497	.09591	.05517	-707.80050	-707.79419	-707.79324	-707.83399
$[UC_6H_5]^+ + HCN$ (V)	-801.22459	.10514	.11399	.11588	.05230	-801.11945	-801.11060	-801.10871	-801.17229

Table 5.4.1: $[UH]^+ + C_6H_5CN$ PBE1PBE/SDD/6-311+g(d,p) Singlet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	-0.274832	0.002976	-0.008307
	H	-0.722758	1.191402	1.456231
C_6H_5CN	C	-1.054586	0.494902	2.542305
	C	0.009974	0.290792	3.425682
	C	0.316578	1.262988	4.365902
	C	-0.430932	2.434561	4.429598
	C	-1.489871	2.637178	3.550649
	C	-1.806101	1.672161	2.605991
	H	0.585621	-0.625896	3.366956
	H	1.142065	1.105662	5.051529
	H	-0.187126	3.192135	5.166963
	H	-2.072462	3.550623	3.600568
	H	-2.629208	1.819719	1.916153
	C	-1.374792	-0.502883	1.571847
	N	-1.633949	-1.309317	0.787096
II	U	-1.835443	-0.051177	0.303710
	H	-1.699763	1.008512	-1.338054
	N	0.021724	-0.622712	0.483895
	C	0.142641	0.533140	1.087980

	C	1.301664	1.161468	1.644202
	C	2.559570	0.534407	1.575680
	C	3.666974	1.158994	2.116883
	C	3.532828	2.406892	2.727123
	C	2.292541	3.037094	2.799297
	C	1.178737	2.418306	2.259566
	H	2.643300	-0.434715	1.095668
	H	4.639228	0.681752	2.066935
	H	4.406145	2.892960	3.149452
	H	2.202341	4.007582	3.273728
	H	0.206899	2.899360	2.303754
TSII→III	U	-1.643221	-0.096402	0.161753
	H	-0.514095	1.502823	-0.047073
	N	0.157858	-0.653153	0.307907
	C	0.196857	0.567066	0.945129
	C	1.351223	1.195185	1.544978
	C	2.585348	0.531525	1.565975
	C	3.677206	1.128448	2.175439
	C	3.549211	2.387179	2.756262
	C	2.326030	3.054208	2.734928
	C	1.228263	2.460132	2.136848
	H	2.669337	-0.447364	1.106885
	H	4.632221	0.615321	2.195644
	H	4.407760	2.852699	3.228478
	H	2.233688	4.035203	3.187328
	H	0.272681	2.975225	2.115321
III	U	0.583925	-1.069476	1.730702
	H	-0.631103	1.506554	0.137002
	N	0.231049	-0.460783	-0.006586
	C	0.207763	0.867906	0.404831
	C	1.310410	1.377312	1.143204
	C	2.388540	0.468693	1.466009
	C	3.405406	0.855881	2.385862
	C	3.330086	2.068355	3.014330
	C	2.292556	2.978264	2.677748
	C	1.318447	2.655789	1.774225
	H	2.636233	-0.271991	0.669729
	H	4.247105	0.193856	2.562087
	H	4.089426	2.361521	3.729996
	H	2.288316	3.962044	3.135247
	H	0.553418	3.377027	1.504632
TSIII→IV	U	-1.561934	-0.855204	0.965410
	H	0.338090	1.096212	-0.674259
	N	0.015128	-0.968696	-0.102384
	C	-0.291991	0.363971	-0.176915
	C	-0.458944	1.004845	1.684315
	C	0.453168	0.474961	2.609548
	C	0.710070	1.162765	3.795442
	C	0.079822	2.378111	4.035058
	C	-0.804227	2.918049	3.099165
	C	-1.073443	2.240437	1.916902
	H	1.011617	-0.434693	2.374679
	H	1.429938	0.770971	4.506245
	H	0.295410	2.925023	4.946384
	H	-1.273836	3.877167	3.290560
	H	-1.742832	2.670379	1.175354
IV	U	-1.572313	0.198915	0.211243
	H	1.214139	0.768110	-1.395625
	N	-0.099184	-0.760636	-0.741603
	C	0.293409	0.455899	-0.900287
	C	-0.736898	0.726739	2.218306
	C	0.222737	0.434649	3.198862

	C	0.327676	1.238388	4.322254
	C	-0.508238	2.347765	4.483423
	C	-1.459641	2.666328	3.525416
	C	-1.563784	1.845183	2.404084
	H	0.884927	-0.416838	3.078965
	H	1.068169	1.012260	5.082255
	H	-0.409872	2.970064	5.366464
	H	-2.104109	3.529471	3.648397
	H	-2.338592	2.134854	1.666338
HCN	C	0.000000	0.000000	-0.497856
	H	0.000000	0.000000	-1.566083
	N	-0.000000	-0.000000	0.650460
$[UC_6H_5]^+$	U	-1.493511	0.334631	0.195316
	C	-0.762557	0.688760	2.235264
	C	0.205872	0.412357	3.216288
	C	0.335323	1.242371	4.315082
	C	-0.493957	2.360883	4.463929
	C	-1.458908	2.659582	3.516314
	C	-1.577791	1.821726	2.406455
	H	0.854499	-0.451825	3.112492
	H	1.084407	1.028518	5.070200
	H	-0.381873	2.999367	5.333719
	H	-2.110946	3.517123	3.638867
	H	-2.390497	2.074285	1.702080

Table 5.5: $[UH]^+ + C_6H_5CN$ B3LYP/SDD/6-311+g(d,p) Triplet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-477.14828	.00361	.00597	.00691	-.01880	-477.14467	-477.14231	-477.14136	-477.16708
C_6H_5CN	-324.57776	.09886	.10496	.10590	.06860	-324.47890	-324.47280	-324.47186	-324.50916
$[UH]^+ + C_6H_5CN$ (**I**)	-801.72604	.10247	.11093	.11282	.04980	-801.62357	-801.61511	-801.61322	-801.67623
II	-801.87043	.10352	.11245	.11339	.06565	-801.76691	-801.75798	-801.75704	-801.80477
TSII→III	-801.84724	.10379	.11181	.11275	.06683	-801.74345	-801.73544	-801.73449	-801.78041
III	-801.90450	.11200	.11989	.12084	.07475	-801.79250	-801.78461	-801.78366	-801.82975
TSIII→IV	-801.84766	.10627	.11448	.11543	.06904	-801.74138	-801.73317	-801.73223	-801.77861
IV	-801.87471	.10560	.11496	.11590	.06606	-801.76911	-801.75975	-801.75881	-801.80864
HCN	-93.45449	.01636	.01890	.01985	-.00300	-93.43813	-93.43559	-93.43465	-93.45749
$[UC_6H_5]^+$	-708.34263	.08844	.09472	.09566	.05397	-708.25419	-708.24791	-708.24697	-708.28866
$[UC_6H_5]^+ + HCN$ (**V**)	-801.79712	.10480	.11362	.11551	.05097	-801.69232	-801.68350	-801.68161	-801.74615

Table 5.5.1: $[UH]^+ + C_6H_5CN$ B3LYP/SDD/6-311+g(d,p) Triplet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	-0.275143	0.003800	-0.007291
	H	-0.722447	1.190578	1.455215
C_6H_5CN	C	-1.055947	0.491891	2.538959
	C	0.012079	0.288629	3.426226
	C	0.319458	1.263129	4.368751
	C	-0.429975	2.438154	4.432931
	C	-1.491221	2.640988	3.551891
	C	-1.808457	1.673241	2.604426
	H	0.587893	-0.626722	3.368545
	H	1.144135	1.106670	5.054186

	H	-0.185961	3.194753	5.169870
	H	-2.073506	3.553624	3.601569
	H	-2.631243	1.823115	1.916425
	C	-1.376868	-0.508430	1.566180
	N	-1.635176	-1.316419	0.781279
II	U	-1.957922	-0.034743	0.271601
	H	-1.863374	1.034622	-1.401667
	N	-0.003607	-0.619505	0.485170
	C	0.186323	0.492273	1.078664
	C	1.332643	1.145064	1.645742
	C	2.601080	0.526617	1.589936
	C	3.701066	1.165676	2.138183
	C	3.552139	2.418507	2.742650
	C	2.302471	3.038906	2.801573
	C	1.194889	2.406783	2.255181
	H	2.699869	-0.442881	1.116715
	H	4.676441	0.696166	2.097654
	H	4.417100	2.913702	3.168596
	H	2.199640	4.010073	3.269651
	H	0.220629	2.880601	2.290170
TSII→III	U	-1.816812	-0.089749	0.146724
	H	-0.679466	1.593235	0.196032
	N	0.153210	-0.601178	0.201709
	C	0.280153	0.496025	0.885199
	C	1.397663	1.168148	1.505939
	C	2.640434	0.510030	1.578976
	C	3.709266	1.124152	2.217548
	C	3.554573	2.393850	2.777517
	C	2.325797	3.054517	2.703667
	C	1.249247	2.444556	2.076386
	H	2.748139	-0.472874	1.136711
	H	4.665669	0.618506	2.274851
	H	4.393542	2.871377	3.269963
	H	2.213602	4.041692	3.135186
	H	0.295350	2.955809	2.009394
III	U	-0.514472	-1.964913	-0.766253
	H	-0.730371	1.540646	0.992564
	N	-0.073277	-0.278568	0.310311
	C	0.114583	0.845107	0.921754
	C	1.336724	1.308936	1.541828
	C	2.519891	0.543430	1.552156
	C	3.658723	1.036019	2.164848
	C	3.635463	2.296951	2.774799
	C	2.471522	3.065746	2.772277
	C	1.326440	2.575529	2.159207
	H	2.528624	-0.430778	1.078578
	H	4.569296	0.449294	2.174649
	H	4.530630	2.677597	3.252882
	H	2.461047	4.039464	3.246210
	H	0.416753	3.166491	2.153207
TSIII→IV	U	-1.900067	-0.665159	0.849358
	H	0.596587	1.014096	-0.549810
	N	-0.225786	-0.963878	-0.269897
	C	-0.159218	0.335554	-0.166056
	C	-0.432525	0.947157	1.713085
	C	0.530339	0.484888	2.628153
	C	0.782067	1.213914	3.792426
	C	0.092482	2.401919	4.034756
	C	-0.847936	2.879043	3.116146
	C	-1.099535	2.165182	1.946900
	H	1.094221	-0.421086	2.421085
	H	1.530370	0.867479	4.495930

	H	0.303801	2.973025	4.930954
	H	-1.357935	3.817533	3.300014
	H	-1.780830	2.574631	1.202459
IV	U	-1.594873	0.112349	0.241092
	H	1.217858	0.685486	-1.567088
	N	-0.052303	-0.846119	-0.836250
	C	0.332299	0.334172	-1.033049
	C	-0.724523	0.743662	2.249957
	C	0.243083	0.484165	3.238326
	C	0.333319	1.298203	4.360420
	C	-0.528782	2.392141	4.517804
	C	-1.488802	2.682022	3.554679
	C	-1.574598	1.851764	2.433377
	H	0.924180	-0.352521	3.127858
	H	1.077920	1.091007	5.120395
	H	-0.444467	3.021041	5.396238
	H	-2.151350	3.531101	3.671169
	H	-2.350532	2.122681	1.693563
HCN	C	0.000000	0.000000	-0.498334
	H	0.000000	0.000000	-1.564845
	N	-0.000000	0.000000	0.650693
$[UC_6H_5]^+$	U	-1.599832	0.160642	0.200300
	C	-0.726892	0.739230	2.203111
	C	0.228239	0.439889	3.195314
	C	0.332273	1.239555	4.325011
	C	-0.508815	2.350024	4.491386
	C	-1.460661	2.670744	3.530437
	C	-1.556742	1.858795	2.396433
	H	0.886492	-0.415021	3.083011
	H	1.067602	1.007795	5.086866
	H	-0.415569	2.964619	5.379105
	H	-2.110862	3.527567	3.658923
	H	-2.325173	2.143939	1.656110

Table 5.6: $[UH]^+ + C_6H_5CN$ PBE1PBE/SDD/6-311+g(d,p) Triplet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-477.06589	.00353	.00589	.00684	-.01891	-477.06236	-477.06000	-477.05905	-477.08480
C_6H_5CN	-324.18042	.09961	.10570	.10664	.06936	-324.08081	-324.07472	-324.07378	-324.11106
$[UH]^+ + C_6H_5CN$ (**I**)	-801.24631	.10314	.11159	.11348	.05045	-801.14317	-801.13472	-801.13283	-801.19586
II	-801.37840	.10454	.11333	.11428	.06697	-801.27386	-801.26507	-801.26412	-801.31143
TSII→III	-801.36183	.10463	.11262	.11357	.06770	-801.25720	-801.24921	-801.24826	-801.29413
III	-801.38817	.11156	.11972	.12066	.07391	-801.27662	-801.26846	-801.26751	-801.31427
TSIII→IV	-801.36326	.10689	.11515	.11610	.06932	-801.25637	-801.24811	-801.24717	-801.29395
IV	-801.38462	.10661	.11584	.11679	.06736	-801.27801	-801.26878	-801.26783	-801.31726
HCN	-93.33544	.01649	.01903	.01997	-.00287	-93.31895	-93.31641	-93.31547	-93.33831
$[UC_6H_5]^+$	-707.95895	.08894	.09517	.09612	.05462	-707.87002	-707.86378	-707.86284	-707.90434
$[UC_6H_5]^+ + HCN$ (**V**)	-801.29439	.10543	.11420	.11609	.05175	-801.18896	-801.18019	-801.17830	-801.24264

Table 5.6.1: $[UH]^+ + C_6H_5CN$ PBE1PBE/SDD/6-311+g(d,p) Triplet Spin Structure Coordinates

Structure	Coordinates

$[UH]^+$	U	-0.280565	0.018185	0.010435
	H	-0.735512	1.225240	1.497931
C_6H_5CN	C	-1.054586	0.494902	2.542305
	C	0.009974	0.290792	3.425682
	C	0.316578	1.262988	4.365902
	C	-0.430932	2.434561	4.429598
	C	-1.489871	2.637178	3.550649
	C	-1.806101	1.672161	2.605991
	H	0.585621	-0.625896	3.366956
	H	1.142065	1.105662	5.051529
	H	-0.187126	3.192135	5.166963
	H	-2.072462	3.550623	3.600568
	H	-2.629208	1.819719	1.916153
	C	-1.374792	-0.502883	1.571847
	N	-1.633949	-1.309317	0.787096
II	U	-1.899106	-0.030137	0.295560
	H	-1.810442	0.994433	-1.385820
	N	0.018191	-0.607537	0.480773
	C	0.170252	0.519187	1.081513
	C	1.321355	1.157248	1.644718
	C	2.581029	0.532811	1.582346
	C	3.683608	1.161165	2.128950
	C	3.542354	2.409086	2.737508
	C	2.300067	3.035876	2.802890
	C	1.190680	2.413441	2.257900
	H	2.669982	-0.436228	1.103102
	H	4.657549	0.686824	2.084183
	H	4.412104	2.898072	3.163824
	H	2.204759	4.006480	3.276029
	H	0.217004	2.891141	2.296343
TSII→III	U	-1.778660	-0.061164	0.180258
	H	-0.673500	1.607529	0.145967
	N	0.159265	-0.606547	0.224467
	C	0.276683	0.497755	0.900646
	C	1.395807	1.165593	1.514679
	C	2.632198	0.506358	1.585650
	C	3.701400	1.120220	2.216544
	C	3.549485	2.389824	2.768519
	C	2.325299	3.051419	2.695530
	C	1.248703	2.440874	2.076195
	H	2.733977	-0.480195	1.146736
	H	4.658233	0.613368	2.274600
	H	4.391496	2.869022	3.256577
	H	2.216578	4.042026	3.122525
	H	0.293404	2.952015	2.006912
III	U	-0.488273	-1.970244	-0.689831
	H	-0.726517	1.551110	0.975169
	N	-0.055797	-0.262653	0.293656
	C	0.121991	0.858752	0.909710
	C	1.337144	1.314752	1.536247
	C	2.514863	0.549103	1.540589
	C	3.650912	1.034689	2.156527
	C	3.627175	2.287358	2.774921
	C	2.467138	3.055739	2.777675
	C	1.325229	2.572648	2.160786
	H	2.520904	-0.421916	1.057081
	H	4.562196	0.447187	2.162190
	H	4.522940	2.663891	3.257566
	H	2.457391	4.026558	3.259785
	H	0.414280	3.163978	2.156948

TSIII→IV	U	-1.779672	-0.683571	0.869879
	H	0.524814	1.039983	-0.630374
	N	-0.135223	-0.970423	-0.212393
	C	-0.201417	0.345599	-0.214157
	C	-0.448186	0.974962	1.711969
	C	0.512828	0.491554	2.610409
	C	0.770915	1.197265	3.784209
	C	0.088758	2.380984	4.045619
	C	-0.849115	2.876924	3.139748
	C	-1.111479	2.185117	1.963222
	H	1.079081	-0.409661	2.376558
	H	1.524143	0.839000	4.478119
	H	0.306293	2.938147	4.950343
	H	-1.353951	3.815776	3.341792
	H	-1.801754	2.602642	1.230561
IV	U	-1.452819	-0.319587	0.476012
	H	0.390437	1.454136	-1.680242
	N	0.141378	-0.475328	-0.854872
	C	-0.130138	0.743932	-1.032990
	C	-0.601992	0.435637	2.422035
	C	0.178012	0.249219	3.572925
	C	0.233013	1.237465	4.542415
	C	-0.475804	2.433010	4.383484
	C	-1.244924	2.654845	3.251944
	C	-1.295515	1.647343	2.289126
	H	0.741091	-0.668627	3.710765
	H	0.832391	1.087308	5.434290
	H	-0.419751	3.197012	5.151414
	H	-1.784712	3.585746	3.119428
	H	-1.892240	1.889041	1.382756
HCN	C	0.000000	0.000000	-0.497856
	H	0.000000	0.000000	-1.566083
	N	-0.000000	-0.000000	0.650460
$[UC_6H_5]^+$	U	-1.643435	0.264475	0.230490
	C	-0.711583	0.716108	2.210422
	C	0.237063	0.431794	3.206567
	C	0.331768	1.240582	4.325633
	C	-0.510965	2.347792	4.478836
	C	-1.457088	2.656676	3.515178
	C	-1.542798	1.832008	2.393092
	H	0.898705	-0.422517	3.102595
	H	1.065165	1.018001	5.093590
	H	-0.422974	2.971185	5.362173
	H	-2.112075	3.512725	3.632063
	H	-2.321721	2.118950	1.655367

Table 5.7.1: $[UH]^+ + C_6H_5CN$ B3LYP/SDD/6-311+g(d,p) Quintet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	0	0	0	0
II	-228.492	-226.877	-229.358	-191.52
TSII→III	-187.6	-188.44	-190.921	-146.855
III	-332.919	-333.74	-336.222	-293.339

TSIII →*IV*	-172.112	-172.564	-175.045	-131.561
IV	-230.438	-227.681	-230.162	-196.519
Products (V)	-119.757	-118.817	-118.82	-122.716

Table 5.7.2: $[UH]^+ + C_6H_5CN$ PBE1PBE/SDD/6-311+g(d,p) Quintet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	0	0	0	0
II	-185.686	-184.2	-186.678	-148.349
TSII →*III*	-161.72	-162.776	-165.254	-120.739
III	-289.173	-290	-292.478	-249.601
TSIII →*IV*	-151.119	-151.733	-154.211	-109.604
IV	-192.496	-190.007	-192.486	-157.509
Products (V)	-58.9136	-58.1076	-58.1076	-61.4183

Table 5.7.3: $[UH]^+ + C_6H_5CN$ B3LYP/SDD/6-311+g(d,p) Singlet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	165.1177	165.1203	165.1177	169.1373
II	-121.595	-121.101	-123.58	-77.2868
TSII →*III*	-52.6964	-54.3452	-56.8263	-6.61364
III	-147.117	-149.346	-151.827	-98.2305
TSIII →*IV*	-54.0617	-55.4952	-57.9763	-8.3806
IV	-134.728	-132.827	-135.308	-96.0408
Products (V)	114.2618	115.3172	115.3172	115.1124

Table 5.7.4: $[UH]^+ + C_6H_5CN$ PBE1PBE/SDD/6-311+g(d,p) Singlet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	267.1394	267.1394	267.1394	271.1564
II	-76.6489	-76.108	-78.5865	-32.3882
TSII →*III*	-27.2002	-28.975	-31.4535	19.06901
III	-132.924	-135.358	-137.834	-83.722
TSIII →*IV*	-31.6898	-33.3281	-35.8066	14.32998
IV	-93.6253	-92.029	-94.5049	-53.6967
Products (V)	206.556	207.6088	207.6088	207.3725

Table 5.7.5: $[UH]^+ + C_6H_5CN$ B3LYP/SDD/6-311+g(d,p) Triplet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	137.1036	137.1062	137.1036	138.4216
II	-239.217	-237.996	-240.477	-199.063
TSII →*III*	-177.641	-178.807	-181.288	-135.098

III	-306.412	-307.903	-310.384	-264.645
TSIII→IV	-172.209	-172.863	-175.341	-130.38
IV	-245.009	-242.646	-245.127	-209.218
Products (V)	-43.389	-42.4543	-42.457	-45.1534

Table 5.7.6: $[UH]^+ + C_6H_5CN$ PBE1PBE/SDD/6-311+g(d,p) Triplet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	144.2844	144.2896	144.2896	145.5
II	-198.85	-197.95	-200.428	-157.947
TSII→III	-155.109	-156.304	-158.78	-112.516
III	-206.086	-206.847	-209.326	-165.383
TSIII→IV	-152.925	-153.426	-155.905	-112.041
IV	-209.743	-207.685	-210.163	-173.238
Products (V)	24.04958	24.89237	24.89237	22.66857

Figure 7: $[UH]^+ + C_6H_5CN$ B3LYP/SDD/6-311+g(d,p) Relative Enthalpy (kJ/mol)

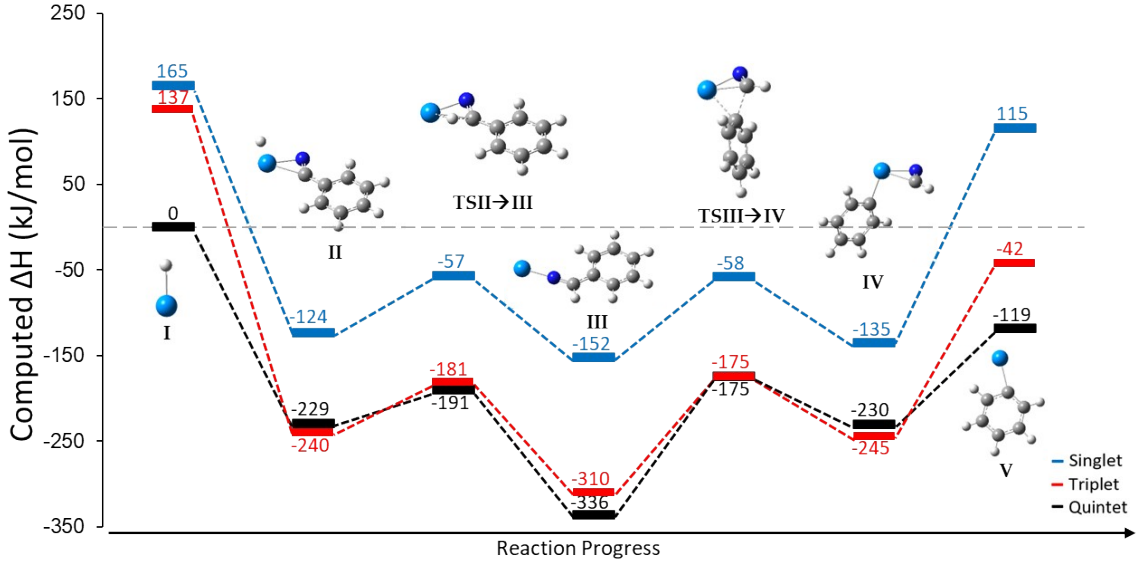

Figure 7.1: $[UH]^+ + C_6H_5CN$ PBE1PBE/SDD/6-311+g(d,p) Relative Enthalpy (kJ/mol)

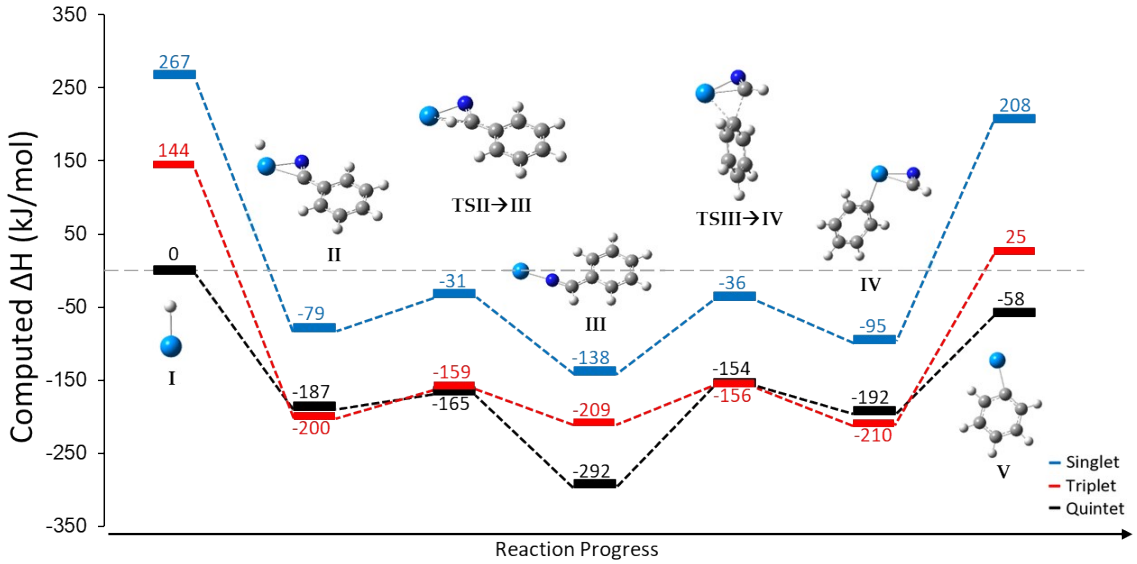

Table 6.1: $[UH]^+ + C_2H_3CN$ B3LYP/SDD/6-311+g(d,p) Quintet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-477.20060	.00371	.00608	.00702	-.01919	-477.19689	-477.19453	-477.19358	-477.21980
C_2H_3CN	-170.88287	.05058	.05473	.05567	.02471	-170.83229	-170.82814	-170.82720	-170.85817
$[UH]^+ + C_2H_3CN$ (**I**)	-648.08348	.05429	.06080	.06269	.00551	-648.02919	-648.02267	-648.02078	-648.07796
II	-648.16677	.05538	.06230	.06324	.02034	-648.11139	-648.10447	-648.10353	-648.14643
TSII→III	-648.15255	.05501	.06107	.06202	.02122	-648.09753	-648.09147	-648.09053	-648.13133
III	-648.21084	.06270	.06880	.06975	.02827	-648.14814	-648.14204	-648.14109	-648.18256
TSIII→IV	-648.15045	.05654	.06279	.06374	.02286	-648.09391	-648.08766	-648.08672	-648.12760
IV	-648.17534	.05672	.06385	.06480	.02137	-648.11862	-648.11148	-648.11054	-648.15397
HCN	-93.45449	.01636	.01890	.01985	-.00300	-93.43813	-93.43559	-93.43465	-93.45749
$[UC_2H_3]^+$	-554.67847	.03960	.04362	.04456	.00945	-554.63887	-554.63486	-554.63391	-554.66902
$[UC_2H_3]^+ + HCN$ (**V**)	-648.13297	.05597	.06252	.06441	.00646	-648.07700	-648.07045	-648.06856	-648.12651

Table 6.1.1: $[UH]^+ + C_2H_3CN$ B3LYP/SDD/6-311+g(d,p) Quintet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	0.000000	0.000000	0.021045
	H	0.000000	0.000000	-1.936098
C_2H_3CN	C	1.084518	0.344036	-0.019635
	H	0.914276	-0.640466	0.397992
	H	0.427223	0.673058	-0.815343
	C	2.073373	1.114763	0.439465
	C	2.345993	2.419922	-0.071050
	N	2.586238	3.478529	-0.467545
	H	2.726683	0.776254	1.237052
II	U	0.328596	0.474488	-1.044486
	H	-0.500736	1.953478	0.037776
	N	2.468256	0.771001	-0.444646

	C	2.314441	0.156416	0.596532
	C	2.943156	-0.283650	1.814540
	C	2.298785	-0.964866	2.767501
	H	1.251877	-1.230915	2.676129
	H	2.809061	-1.268692	3.673221
	H	3.992055	-0.012891	1.914891
TSII→III	U	0.519747	0.760629	-0.953046
	H	0.598198	0.420945	1.052096
	N	2.539198	1.063530	-0.319995
	C	2.317221	0.283901	0.627361
	C	2.966191	-0.317259	1.761937
	C	2.323286	-0.829180	2.817620
	H	1.241589	-0.814642	2.887996
	H	2.872706	-1.253360	3.648454
	H	4.051801	-0.324370	1.702367
III	U	0.328298	0.106377	0.461080
	H	4.086742	0.533617	-0.594059
	N	2.366265	-0.133046	0.292574
	C	3.639487	-0.184473	0.102805
	C	4.579968	-1.110036	0.722572
	C	4.234396	-2.062818	1.600420
	H	4.975362	-2.724937	2.031555
	H	3.204733	-2.204626	1.909625
	H	5.617400	-0.988853	0.429706
TSIII→IV	U	3.123265	-1.398476	-0.024159
	H	3.818421	2.036951	0.322202
	N	3.020309	0.566623	-1.046417
	C	3.481406	1.065945	-0.027919
	C	4.494811	-0.203913	1.398979
	C	3.875528	-0.431317	2.587815
	H	4.414824	-0.584109	3.518539
	H	2.786218	-0.439715	2.686153
	H	5.568579	-0.004969	1.373239
IV	U	2.852345	-1.431073	-0.115824
	H	3.184140	2.063363	0.507516
	N	3.625729	0.571820	-0.998037
	C	3.224673	1.089765	0.019298
	C	4.626753	-2.111165	1.192893
	C	3.828698	-2.461728	2.209620
	H	4.120275	-2.835155	3.188739
	H	2.716871	-2.394189	2.143375
	H	5.705476	-2.189714	1.303802
HCN	C	0.000000	0.000000	-0.498334
	H	0.000000	0.000000	-1.564845
	N	-0.000000	0.000000	0.650693
$[UC_2H_3]^+$	U	3.350310	-0.852024	0.087605
	C	4.551117	-2.507507	1.091832
	C	3.978540	-2.299097	2.283509
	H	4.167664	-2.827835	3.214952
	H	3.205216	-1.512596	2.439854
	H	5.304103	-3.280937	0.964502

Table 6.2: $[UH]^+ + C_2H_3CN$ PBE1PBE/SDD/6-311+g(d,p) Quintet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-477.12109	.00377	.00614	.00708	-.01913	-477.11732	-477.11495	-477.11401	-477.14021
C_2H_3CN	-170.66582	.05092	.05506	.05600	.02505	-170.61491	-170.61077	-170.60982	-170.64078

$[UH]^+ + C_2H_3CN$ (**I**)	-647.78691	.05469	.06119	.06308	.00592	-647.73223	-647.72572	-647.72383	-647.78099
II	-647.85404	.05581	.06273	.06368	.02070	-647.79823	-647.79131	-647.79037	-647.83334
TSII→III	-647.84618	.05603	.06188	.06282	.02247	-647.79015	-647.78430	-647.78336	-647.82371
III	-647.89744	.06308	.06919	.07013	.02863	-647.83436	-647.82825	-647.82731	-647.86881
TSIII→IV	-647.84490	.05689	.06296	.06390	.02358	-647.78802	-647.78195	-647.78100	-647.82132
IV	-647.86523	.05727	.06430	.06524	.02207	-647.80796	-647.80093	-647.79999	-647.84316
HCN	-93.33544	.01649	.01903	.01997	-.00287	-93.31895	-93.31641	-93.31547	-93.33831
$[UC_2H_3]^+$	-554.47741	.03982	.04378	.04472	.00977	-554.43759	-554.43363	-554.43269	-554.46764
$[UC_2H_3]^+ + HCN$ (**V**)	-647.81285	.05632	.06281	.06469	.00690	-647.75653	-647.75004	-647.74816	-647.80594

Table 6.2.1: $[UH]^+ + C_2H_3CN$ PBE1PBE/SDD/6-311+g(d,p) Quintet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	-0.282792	0.024095	0.017719
	H	-0.733284	1.219330	1.490648
C_2H_3CN	C	1.086352	0.346666	-0.019481
	H	0.914460	-0.638959	0.397278
	H	0.431026	0.680535	-0.816207
	C	2.074126	1.113793	0.440727
	C	2.343110	2.415483	-0.071108
	N	2.580985	3.473049	-0.469180
	H	2.728243	0.775529	1.238906
II	U	0.370273	0.455008	-1.018539
	H	-0.453536	1.858359	0.143937
	N	2.493059	0.791861	-0.455660
	C	2.319008	0.167635	0.578266
	C	2.936280	-0.279980	1.795351
	C	2.269143	-0.938626	2.745249
	H	1.215023	-1.176815	2.645589
	H	2.764883	-1.250037	3.657769
	H	3.991358	-0.033038	1.899494
TSII→III	U	0.538456	0.698568	-0.908284
	H	0.559041	0.466605	1.088914
	N	2.557278	1.067003	-0.319420
	C	2.325122	0.285731	0.623094
	C	2.976377	-0.317581	1.753072
	C	2.319418	-0.828281	2.796869
	H	1.235213	-0.808835	2.847670
	H	2.855673	-1.252486	3.637821
	H	4.063360	-0.320531	1.705055
III	U	0.353496	0.077047	0.481766
	H	4.082949	0.536366	-0.596730
	N	2.373316	-0.140521	0.297511
	C	3.642745	-0.185086	0.102352
	C	4.581617	-1.106568	0.719225
	C	4.225982	-2.054034	1.595017
	H	4.960371	-2.721432	2.031895
	H	3.191191	-2.185318	1.896510
	H	5.620984	-0.989247	0.428732
TSIII→IV	U	3.064579	-1.324181	0.072478
	H	3.841932	2.025206	0.298776
	N	3.008003	0.552743	-1.040502
	C	3.475520	1.049408	-0.013286
	C	4.538381	-0.208483	1.388759

	C	3.888058	-0.451670	2.557814
	H	4.377074	-0.568108	3.520838
	H	2.788938	-0.509892	2.608768
	H	5.600876	0.041998	1.394788
IV	U	2.889574	-1.467483	-0.162560
	H	3.122940	1.950908	0.629034
	N	3.684908	0.554033	-0.925745
	C	3.213302	1.004943	0.093477
	C	4.642501	-2.147776	1.132919
	C	3.822544	-2.374706	2.164399
	H	4.081170	-2.689973	3.173725
	H	2.712676	-2.249824	2.087266
	H	5.715344	-2.278198	1.258866
HCN	C	0.000000	0.000000	-0.497856
	H	0.000000	0.000000	-1.566083
	N	-0.000000	-0.000000	0.650460
$[UC_2H_3]^+$	U	3.328212	-0.852125	0.158389
	C	4.556924	-2.507581	1.077347
	C	3.985713	-2.301507	2.267099
	H	4.167634	-2.824811	3.204207
	H	3.207254	-1.513679	2.430146
	H	5.311214	-3.280294	0.945067

Table 6.3: $[UH]^+ + C_2H_3CN$ B3LYP/SDD/6-311+g(d,p) Singlet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-477.13768	.00368	.00605	.00699	-.01769	-477.13400	-477.13164	-477.13069	-477.15538
C_2H_3CN	-170.88287	.05058	.05473	.05567	.02471	-170.83229	-170.82814	-170.82720	-170.85817
$[UH]^+ + C_2H_3CN$ (**I**)	-648.02056	.05426	.06077	.06266	.00701	-647.96630	-647.95978	-647.95789	-648.01354
II	-648.12609	.05603	.06249	.06343	.02362	-648.07006	-648.06360	-648.06265	-648.10247
TSII→III	-648.10095	.05601	.06171	.06266	.02399	-648.04495	-648.03924	-648.03829	-648.07696
III	-648.12605	.06250	.06861	.06955	.02965	-648.06354	-648.05744	-648.05650	-648.09640
TSIII→IV	-648.09964	.05754	.06326	.06420	.02581	-648.04210	-648.03638	-648.03544	-648.07383
IV	-648.13635	.05745	.06397	.06491	.02524	-648.07890	-648.07238	-648.07144	-648.11111
HCN	-93.45449	.01636	.01890	.01985	-.00300	-93.43813	-93.43559	-93.43465	-93.45749
$[UC_2H_3]^+$	-554.58948	.03906	.04321	.04416	.01034	-554.55042	-554.54627	-554.54532	-554.57914
$[UC_2H_3]^+ + HCN$ (**V**)	-648.04397	.05542	.06211	.06400	.00734	-647.98855	-647.98186	-647.97997	-648.03663

Table 6.3.1: $[UH]^+ + C_2H_3CN$ B3LYP/SDD/6-311+g(d,p) Singlet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	-0.274048	0.000897	-0.010869
	H	-0.723542	1.193481	1.458793
C_2H_3CN	C	1.084518	0.344036	-0.019635
	H	0.914276	-0.640466	0.397992
	H	0.427223	0.673058	-0.815343
	C	2.073373	1.114763	0.439465
	C	2.345993	2.419922	-0.071050
	N	2.586238	3.478529	-0.467545
	H	2.726683	0.776254	1.237052

II	U	0.536899	0.494706	-0.977318
	H	-0.328407	1.985356	-0.031239
	N	2.417948	0.778867	-0.424546
	C	2.072134	0.089634	0.622319
	C	2.842180	-0.261008	1.786216
	C	2.313886	-0.991486	2.780712
	H	1.288753	-1.343774	2.744291
	H	2.893636	-1.251869	3.658423
	H	3.868463	0.093941	1.832600
TSII→III	U	0.700672	0.680664	-0.924083
	H	0.766759	0.829244	1.063751
	N	2.525018	0.951864	-0.400910
	C	2.086191	0.169296	0.632694
	C	2.866271	-0.297918	1.761368
	C	2.331768	-0.905991	2.826859
	H	1.263223	-1.068059	2.921688
	H	2.952791	-1.238897	3.649214
	H	3.937245	-0.130009	1.694209
III	U	0.379235	0.004103	0.321961
	H	4.062205	0.580915	-0.537280
	N	2.366102	-0.058270	0.416658
	C	3.633647	-0.153414	0.150800
	C	4.562752	-1.123875	0.696296
	C	4.237032	-2.063544	1.599509
	H	4.982319	-2.743923	1.992984
	H	3.224011	-2.171574	1.970628
	H	5.585347	-1.039211	0.344722
TSIII→IV	U	3.085074	-1.219187	-0.090065
	H	3.578484	1.932719	0.427201
	N	3.361566	0.405019	-1.093051
	C	3.380872	0.895449	0.178753
	C	4.455296	-0.121527	1.366031
	C	3.888241	-0.364071	2.572539
	H	4.471236	-0.641046	3.444673
	H	2.820936	-0.216774	2.739285
	H	5.541659	-0.063560	1.243066
IV	U	3.072060	-1.387462	-0.313742
	H	2.785056	1.758861	0.655081
	N	3.941870	0.427241	-0.522008
	C	2.988611	0.758344	0.271201
	C	4.656951	-2.275523	1.026050
	C	3.859903	-2.156972	2.092909
	H	4.043599	-2.494499	3.109844
	H	2.898703	-1.590615	2.046742
	H	5.638209	-2.737452	1.085305
HCN	C	0.000000	0.000000	-0.498334
	H	0.000000	0.000000	-1.564845
	N	-0.000000	0.000000	0.650693
$[UC_2H_3]^+$	U	3.322525	-0.907163	0.161934
	C	4.533955	-2.545733	1.071754
	C	3.998156	-2.270800	2.270159
	H	4.190777	-2.759984	3.221317
	H	3.250096	-1.453857	2.414850
	H	5.261441	-3.342459	0.942241

Table 6.4: $[UH]^+ + C_2H_3CN$ PBE1PBE/SDD/6-311+g(d,p) Singlet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr

$[UH]^+$	-477.01929	.00372	.00608	.00703	-.01765	-477.01557	-477.01321	-477.01226	-477.03694
C_2H_3CN	-170.66582	.05092	.05506	.05600	.02505	-170.61491	-170.61077	-170.60982	-170.64078
$[UH]^+ + C_2H_3CN$ (**I**)	-647.68511	.05463	.06114	.06303	.00740	-647.63048	-647.62397	-647.62209	-647.67771
II	-647.81238	.05643	.06290	.06385	.02399	-647.75595	-647.74948	-647.74853	-647.78839
TSII→III	-647.79387	.05643	.06206	.06300	.02465	-647.73744	-647.73181	-647.73087	-647.76922
III	-647.80182	.06273	.06888	.06982	.02963	-647.73909	-647.73294	-647.73200	-647.77219
TSIII→IV	-647.79397	.05779	.06353	.06447	.02589	-647.73618	-647.73044	-647.72950	-647.76808
IV	-647.82757	.05817	.06444	.06538	.02643	-647.76940	-647.76314	-647.76219	-647.80115
HCN	-93.33544	.01649	.01903	.01997	-.00287	-93.31895	-93.31641	-93.31547	-93.33831
$[UC_2H_3]^+$	-554.37884	.03919	.04331	.04426	.01052	-554.33965	-554.33553	-554.33458	-554.36832
$[UC_2H_3]^+ + HCN$ (**V**)	-647.71428	.05568	.06234	.06423	.00766	-647.65860	-647.65194	-647.65005	-647.70662

Table 6.4.1: $[UH]^+ + C_2H_3CN$ PBE1PBE/SDD/6-311+g(d,p) Singlet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	-0.274832	0.002976	-0.008307
	H	-0.722758	1.191402	1.456231
C_2H_3CN	C	1.086352	0.346666	-0.019481
	H	0.914460	-0.638959	0.397278
	H	0.431026	0.680535	-0.816207
	C	2.074126	1.113793	0.440727
	C	2.343110	2.415483	-0.071108
	N	2.580985	3.473049	-0.469180
	H	2.728243	0.775529	1.238906
II	U	0.565155	0.483198	-0.957638
	H	-0.291026	1.936125	0.029185
	N	2.425951	0.782632	-0.431865
	C	2.064909	0.091432	0.614309
	C	2.835062	-0.254417	1.774991
	C	2.298876	-0.978273	2.766917
	H	1.270357	-1.323539	2.723932
	H	2.873007	-1.239862	3.649361
	H	3.863201	0.097072	1.822266
TSII→III	U	0.700672	0.680664	-0.924083
	H	0.766759	0.829244	1.063751
	N	2.525018	0.951864	-0.400910
	C	2.086191	0.169296	0.632694
	C	2.866271	-0.297918	1.761368
	C	2.331768	-0.905991	2.826859
	H	1.263223	-1.068059	2.921688
	H	2.952791	-1.238897	3.649214
	H	3.938116	-0.130331	1.692912
III	U	0.431231	-0.077548	0.258478
	H	4.054543	0.612780	-0.501666
	N	2.374581	-0.027115	0.480247
	C	3.633048	-0.136498	0.174793
	C	4.550971	-1.131689	0.678332
	C	4.229714	-2.054419	1.597193
	H	4.968934	-2.752976	1.972512
	H	3.225447	-2.126219	2.003595
	H	5.564182	-1.075111	0.292794
TSIII→IV	U	3.085074	-1.219187	-0.090065
	H	3.578484	1.932719	0.427201

	N	3.361566	0.405019	-1.093051
	C	3.380872	0.895449	0.178753
	C	4.455296	-0.121527	1.366031
	C	3.888241	-0.364071	2.572539
	H	4.471236	-0.641046	3.444673
	H	2.820936	-0.216774	2.739285
	H	5.543038	-0.061101	1.245555
IV	U	3.081461	-1.403305	-0.297073
	H	2.759304	1.678787	0.708227
	N	3.966872	0.378356	-0.449905
	C	2.975679	0.683410	0.316452
	C	4.670273	-2.272419	0.998285
	C	3.858395	-2.104933	2.045656
	H	4.000495	-2.423887	3.075750
	H	2.942915	-1.456716	1.977406
	H	5.629567	-2.777371	1.076583
HCN	C	0.000000	0.000000	-0.497856
	H	0.000000	0.000000	-1.566083
	N	-0.000000	-0.000000	0.650460
$[UC_2H_3]^+$	U	3.359061	-0.880159	0.238854
	C	4.606685	-2.487049	1.077758
	C	3.958407	-2.305099	2.238611
	H	4.097069	-2.830724	3.180558
	H	3.148587	-1.538948	2.370254
	H	5.387142	-3.238017	0.976220

Table 6.5: $[UH]^+ + C_2H_3CN$ B3LYP/SDD/6-311+g(d,p) Triplet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-477.14828	.00361	.00597	.00691	-.01880	-477.14467	-477.14231	-477.14136	-477.16708
C_2H_3CN	-170.88287	.05058	.05473	.05567	.02471	-170.83229	-170.82814	-170.82720	-170.85817
$[UH]^+ + C_2H_3CN$ (**I**)	-648.03115	.05419	.06070	.06259	.00591	-647.97697	-647.97045	-647.96856	-648.02524
II	-648.17053	.05539	.06219	.06314	.02136	-648.11514	-648.10834	-648.10740	-648.14917
TSII→III	-648.14864	.05551	.06136	.06230	.02245	-648.09313	-648.08729	-648.08634	-648.12620
III	-648.17570	.06228	.06838	.06933	.02844	-648.11342	-648.10731	-648.10637	-648.14726
TSIII→IV	-648.14498	.05747	.06347	.06442	.02431	-648.08751	-648.08151	-648.08057	-648.12067
IV	-648.17961	.05683	.06389	.06484	.02194	-648.12279	-648.11572	-648.11478	-648.15768
HCN	-93.45449	.01636	.01890	.01985	-.00300	-93.43813	-93.43559	-93.43465	-93.45749
$[UC_2H_3]^+$	-554.64803	.03958	.04359	.04453	.00993	-554.60845	-554.60444	-554.60349	-554.63810
$[UC_2H_3]^+ + HCN$ (**V**)	-648.10252	.05595	.06249	.06438	.00693	-648.04658	-648.04003	-648.03814	-648.09559

Table 6.5.1: $[UH]^+ + C_2H_3CN$ B3LYP/SDD/6-311+g(d,p) Triplet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	-0.275143	0.003800	-0.007291
	H	-0.722447	1.190578	1.455215
C_2H_3CN	C	1.084518	0.344036	-0.019635
	H	0.914276	-0.640466	0.397992
	H	0.427223	0.673058	-0.815343
	C	2.073373	1.114763	0.439465
	C	2.345993	2.419922	-0.071050
	N	2.586238	3.478529	-0.467545

	H	2.726683	0.776254	1.237052
II	U	0.473656	0.504383	-1.007441
	H	-0.423137	1.984461	-0.035440
	N	2.438875	0.775090	-0.417395
	C	2.143139	0.109601	0.619074
	C	2.880165	-0.272470	1.797347
	C	2.316959	-0.987135	2.781625
	H	1.282297	-1.308126	2.731953
	H	2.877690	-1.264639	3.666269
	H	3.915846	0.053203	1.855464
TSII→III	U	0.620246	0.710623	-0.969191
	H	0.657580	0.519785	1.053003
	N	2.519849	1.090307	-0.305235
	C	2.219701	0.246388	0.625043
	C	2.922155	-0.319520	1.750054
	C	2.326315	-0.849891	2.825579
	H	1.247358	-0.864828	2.933965
	H	2.910955	-1.254326	3.642087
	H	4.005779	-0.288345	1.669484
III	U	0.383216	0.144823	0.515653
	H	4.068802	0.522052	-0.609584
	N	2.345540	-0.184408	0.244999
	C	3.633081	-0.199734	0.088340
	C	4.575321	-1.094020	0.733207
	C	4.231810	-2.063750	1.597423
	H	4.978840	-2.713166	2.037203
	H	3.199576	-2.232852	1.882691
	H	5.616463	-0.947738	0.466345
TSIII→IV	U	3.115461	-1.317354	-0.245737
	H	3.518985	1.910127	0.515707
	N	3.397034	0.501929	-1.109010
	C	3.386117	0.902610	0.132881
	C	4.411102	-0.181207	1.373387
	C	3.899912	-0.316731	2.610825
	H	4.519242	-0.534964	3.475957
	H	2.836923	-0.178619	2.808300
	H	5.498589	-0.178768	1.226122
IV	U	2.995989	-1.365841	-0.251639
	H	3.180680	1.913340	0.659454
	N	3.640753	0.553625	-0.906568
	C	3.186062	0.923373	0.198002
	C	4.644001	-2.166540	1.130166
	C	3.798480	-2.347768	2.151070
	H	4.025161	-2.713047	3.150136
	H	2.711503	-2.110289	2.071993
	H	5.702333	-2.384929	1.248768
HCN	C	0.000000	0.000000	-0.498334
	H	0.000000	0.000000	-1.564845
	N	-0.000000	0.000000	0.650693
$[UC_2H_3]^+$	U	3.353285	-0.847099	0.103208
	C	4.543881	-2.511123	1.085943
	C	3.979833	-2.298936	2.281948
	H	4.181270	-2.820615	3.214732
	H	3.198499	-1.521334	2.441128
	H	5.300181	-3.280889	0.955296

Table 6.6: $[UH]^+ + C_2H_3CN$ PBE1PBE/SDD/6-311+g(d,p) Triplet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UH]^+$	-477.06589	.00353	.00589	.00684	-.01891	-477.06236	-477.06000	-477.05905	-477.08480
C_2H_3CN	-170.66582	.05092	.05506	.05600	.02505	-170.61491	-170.61077	-170.60982	-170.64078
$[UH]^+ + C_2H_3CN$ (**I**)	-647.73171	.05444	.06095	.06284	.00614	-647.67727	-647.67076	-647.66888	-647.72557
II	-647.85863	.05597	.06266	.06361	.02214	-647.80266	-647.79596	-647.79502	-647.83648
TSII→III	-647.84316	.05597	.06180	.06275	.02291	-647.78719	-647.78136	-647.78042	-647.82025
III	-647.86579	.06296	.06907	.07001	.02893	-647.80283	-647.79672	-647.79578	-647.83686
TSIII→IV	-647.84118	.05775	.06354	.06449	.02526	-647.78344	-647.77764	-647.77670	-647.81592
IV	-647.87064	.05756	.06441	.06536	.02315	-647.81308	-647.80623	-647.80528	-647.84749
HCN	-93.33544	.01649	.01903	.01997	-.00287	-93.31895	-93.31641	-93.31547	-93.33831
$[UC_2H_3]^+$	-554.44537	.03981	.04377	.04471	.01025	-554.40556	-554.40161	-554.40066	-554.43512
$[UC_2H_3]^+ + HCN$ (**V**)	-647.78081	.05630	.06279	.06468	.00738	-647.72451	-647.71802	-647.71613	-647.77343

Table 6.6.1: $[UH]^+ + C_2H_3CN$ PBE1PBE/SDD/6-311+g(d,p) Triplet Spin Structure Coordinates

Structure	Coordinates			
$[UH]^+$	U	-0.280565	0.018185	0.010435
	H	-0.735512	1.225240	1.497931
C_2H_3CN	C	1.086352	0.346666	-0.019481
	H	0.914460	-0.638959	0.397278
	H	0.431026	0.680535	-0.816207
	C	2.074126	1.113793	0.440727
	C	2.343110	2.415483	-0.071108
	N	2.580985	3.473049	-0.469180
	H	2.728243	0.775529	1.238906
II	U	0.506039	0.485647	-0.967246
	H	-0.375285	1.967303	-0.019136
	N	2.431554	0.781775	-0.414073
	C	2.110834	0.103390	0.620909
	C	2.866726	-0.265489	1.785499
	C	2.311594	-0.981840	2.771127
	H	1.276484	-1.305747	2.722006
	H	2.876287	-1.257387	3.655381
	H	3.901258	0.066717	1.836990
TSII→III	U	0.637883	0.686561	-0.925362
	H	0.641031	0.563990	1.072981
	N	2.529377	1.077287	-0.309593
	C	2.219562	0.234863	0.619780
	C	2.926830	-0.324297	1.741877
	C	2.322702	-0.849483	2.811821
	H	1.241099	-0.864102	2.906213
	H	2.899890	-1.247406	3.638315
	H	4.011564	-0.287220	1.668759
III	U	0.383216	0.144823	0.515653
	H	4.068802	0.522052	-0.609584
	N	2.345540	-0.184408	0.244999
	C	3.633081	-0.199734	0.088340
	C	4.575321	-1.094020	0.733207
	C	4.231810	-2.063750	1.597423
	H	4.978840	-2.713166	2.037203
	H	3.199576	-2.232852	1.882691
	H	5.616463	-0.947738	0.466345

TSIII→IV	U	2.863244	-1.183431	0.110326
	H	3.852134	1.967503	0.271767
	N	3.259105	0.399713	-1.075131
	C	3.459937	0.970013	0.081507
	C	4.445584	-0.056957	1.390650
	C	3.909153	-0.459307	2.554884
	H	4.470527	-0.637050	3.467794
	H	2.817106	-0.569125	2.681583
	H	5.506573	0.175664	1.305052
IV	U	3.040594	-1.418503	-0.283934
	H	2.959674	1.772905	0.730696
	N	3.745308	0.487889	-0.754761
	C	3.074145	0.789765	0.267158
	C	4.662621	-2.273050	1.049975
	C	3.850673	-2.188958	2.106699
	H	4.055722	-2.460153	3.140695
	H	2.816194	-1.765989	2.035548
	H	5.680030	-2.641983	1.159305
HCN	C	0.000000	0.000000	-0.497856
	H	0.000000	0.000000	-1.566083
	N	-0.000000	-0.000000	0.650460
$[UC_2H_3]^+$	U	3.356122	-0.852170	0.158197
	C	4.550935	-2.519726	1.075873
	C	3.982028	-2.294217	2.265011
	H	4.168878	-2.803877	3.208207
	H	3.196985	-1.512650	2.418091
	H	5.302004	-3.297355	0.956875

Table 6.7.1: $[UH]^+ + C_2H_3CN$ B3LYP/SDD/6-311+g(d,p) Quintet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	0	0	0	0
II	-215.84	-214.761	-217.242	-179.744
TSII→III	-179.445	-180.637	-183.118	-140.099
III	-312.316	-313.388	-315.869	-274.625
TSIII→IV	-169.941	-170.631	-173.11	-130.311
IV	-234.798	-233.176	-235.657	-199.546
Products (V)	-125.546	-125.439	-125.441	-127.46

Table 6.7.2: $[UH]^+ + C_2H_3CN$ PBE1PBE/SDD/6-311+g(d,p) Quintet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	0	0	0	0
II	-173.291	-172.207	-174.685	-137.45
TSII→III	-152.069	-153.802	-156.28	-112.164
III	-268.153	-269.2	-271.676	-230.571
TSIII→IV	-146.474	-147.621	-150.1	-105.892
IV	-198.834	-197.466	-199.945	-163.233
Products (V)	-63.8154	-63.8574	-63.8574	-65.5141

Table 6.7.3: $[UH]^+ + C_2H_3CN$ B3LYP/SDD/6-311+g(d,p) Singlet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	165.1177	165.1203	165.1177	169.1373
II	-107.315	-107.449	-109.93	-64.33
TSII→III	-41.3779	-43.494	-45.9751	2.630751
III	-90.2096	-91.2834	-93.7645	-48.3906
TSIII→IV	-33.9005	-35.9904	-38.4715	10.84594
IV	-130.514	-130.506	-132.987	-87.0196
Products (V)	106.6846	107.1598	107.1572	108.5145

Table 6.7.4: $[UH]^+ + C_2H_3CN$ PBE1PBE/SDD/6-311+g(d,p) Singlet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	267.1394	267.1394	267.1394	271.1564
II	-62.29	-62.3688	-64.8472	-19.4129
TSII→III	-13.6946	-15.9972	-18.4756	30.89689
III	-18.0109	-18.9509	-21.4293	23.10965
TSIII→IV	-10.3891	-12.395	-14.8735	33.89783
IV	-97.6003	-98.2383	-100.717	-52.9248
Products (V)	193.3051	193.712	193.712	195.2558

Table 6.7.5: $[UH]^+ + C_2H_3CN$ B3LYP/SDD/6-311+g(d,p) Triplet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	137.1036	137.1062	137.1036	138.4216
II	-225.685	-224.921	-227.402	-186.962
TSII→III	-167.895	-169.652	-172.13	-126.641
III	-221.149	-222.225	-224.703	-181.924
TSIII→IV	-153.122	-154.477	-156.958	-112.114
IV	-245.752	-244.3	-246.781	-209.294
Products (V)	-45.6653	-45.5708	-45.5734	-46.2744

Table 6.7.6: $[UH]^+ + C_2H_3CN$ PBE1PBE/SDD/6-311+g(d,p) Triplet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
Reactants (I)	144.2844	144.2896	144.2896	145.5
II	-184.911	-184.423	-186.901	-145.697
TSII→III	-144.311	-146.078	-148.556	-103.072
III	-185.373	-186.413	-188.892	-146.687
TSIII→IV	-134.449	-136.316	-138.794	-91.7166
IV	-212.274	-211.363	-213.842	-174.58

Products (V)	20.26624	20.2216	20.2216	19.85928

Figure 8: $[UH]^+ + C_2H_3CN$ B3LYP/SDD/6-311+g(d,p) Relative Enthalpy (kJ/mol)

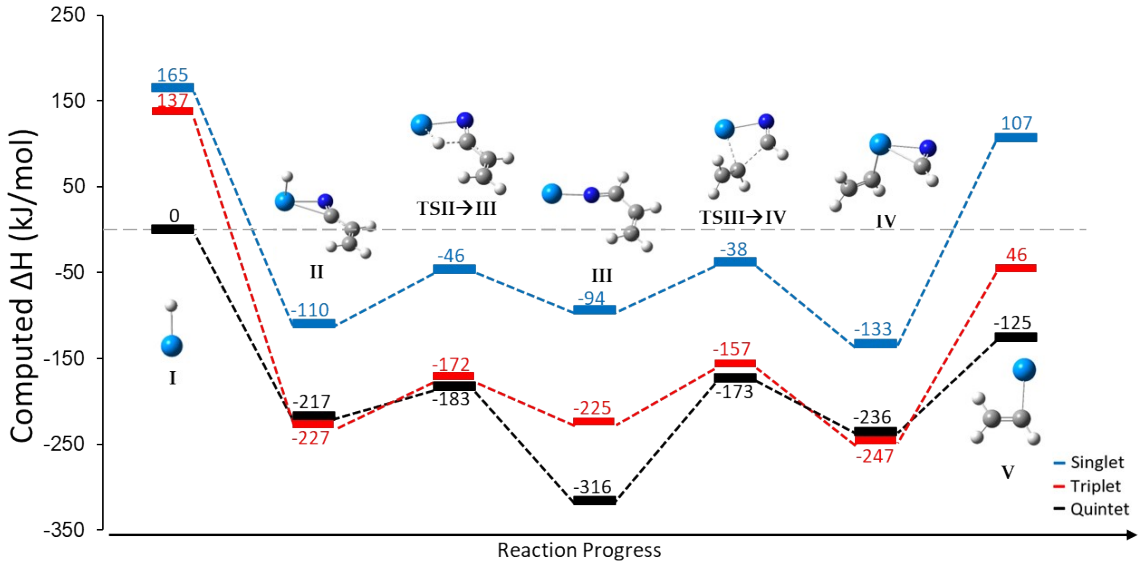

Figure 8.1: $[UH]^+ + C_2H_3CN$ PBE1PBE/SDD/6-311+g(d,p) Relative Enthalpy (kJ/mol)

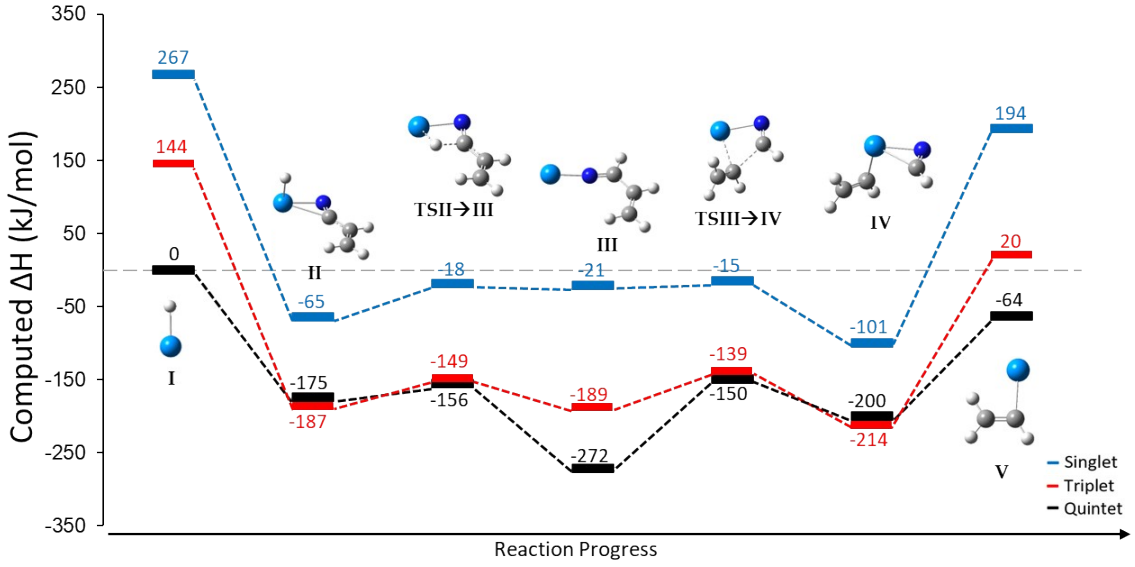

Table 7.1: $[UCH_3]^+$ Rearrangement B3LYP/SDD/6-311+g(d,p) Quintet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UHC_3]^+$ (V)	-516.58290	.03202	.03595	.03690	.00328	-516.55087	-516.54694	-516.54600	-516.57961
TSV→VI	-516.51239	.02468	.02869	.02963	-.00426	-516.48772	-516.48371	-516.48276	-516.51665
VI	-516.52012	.02520	.02974	.03068	-.00426	-516.49492	-516.49039	-516.48944	-516.52438

TSVI→VII	-516.42836	.01992	.02413	.02507	-.00919	-516.40844	-516.40423	-516.40329	-516.43755
VII	-516.42859	.02041	.02518	.02612	-.00917	-516.40818	-516.40341	-516.40247	-516.43776

Table 7.1.1: $[UCH_3]^+$ Rearrangement B3LYP/SDD/6-311+g(d,p) Quintet Spin Structure Coordinates

Structure	Coordinates			
$[UHC_3]^+$ (V)	U	-3.289712	1.030298	-0.450766
	C	-1.044265	0.778059	-0.038123
	H	-0.444203	1.483373	-0.634672
	H	-0.808150	0.957408	1.022779
	H	-0.702269	-0.239348	-0.285902
TSV→VI	U	-0.270334	0.121000	-0.299332
	C	1.897852	-0.236839	0.115856
	H	0.831139	1.637730	0.436111
	H	2.352926	-0.507480	1.075369
	H	2.688380	0.018767	-0.601536
VI	U	-0.360956	-0.059712	-0.003691
	C	1.936823	0.159322	0.001362
	H	-0.689602	1.911264	-0.002921
	H	2.439713	1.133729	0.003762
	H	2.682963	-0.643922	0.001805
TSVI→VII	U	0.205380	0.064804	-0.090929
	C	-2.014593	-0.145062	0.021440
	H	0.889730	-1.038180	1.356320
	H	-3.102041	-0.157464	0.133984
	H	-0.085697	1.685220	0.936006
VII	U	-2.327016	2.255848	1.004581
	C	-0.580505	1.427792	-0.127237
	H	-3.847275	2.228291	-0.208158
	H	0.311548	1.095721	-0.665642
	H	-1.860619	4.134110	0.837157

Table 7.2: $[UCH_3]^+$ Rearrangement PBE1PBE/SDD/6-311+g(d,p) Quintet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UHC_3]^+$ (V)	-516.42679	.03203	.03603	.03698	.00321	-516.39477	-516.39076	-516.38981	-516.42358
TSV→VI	-516.35731	.02482	.02883	.02978	-.00412	-516.33249	-516.32847	-516.32753	-516.36142
VI	-516.36320	.02537	.02989	.03084	-.00404	-516.33783	-516.33331	-516.33237	-516.36724
TSVI→VII	-516.27018	.02017	.02436	.02531	-.00890	-516.25001	-516.24582	-516.24488	-516.27908
VII	-516.27025	.02062	.02538	.02633	-.00895	-516.24963	-516.24487	-516.24393	-516.27920

Table 7.2.1: $[UCH_3]^+$ Rearrangement PBE1PBE/SDD/6-311+g(d,p) Quintet Spin Structure Coordinates

Structure	Coordinates			
$[UHC_3]^+$ (V)	U	-3.272222	1.028329	-0.447550
	C	-1.051155	0.778843	-0.039390
	H	-0.447809	1.483494	-0.635086
	H	-0.811631	0.957714	1.021772
	H	-0.705783	-0.238591	-0.286431
TSV→VI	U	-0.255715	0.116932	-0.264047
	C	1.911064	-0.232481	0.079102
	H	0.787449	1.663299	0.445181
	H	2.312891	-0.504888	1.065426
	H	2.744274	-0.009684	-0.599194
VI	U	-0.354574	-0.049095	-0.001753
	C	1.926607	0.124405	0.000408
	H	-0.654472	1.920795	-0.000459
	H	2.367873	1.132546	0.002029
	H	2.723507	-0.627970	0.000093
TSVI→VII	U	0.11293900	0.00087500	-0.03581900
	C	-2.01208700	-0.11950900	0.04316800
	H	1.00988800	-1.01860600	1.34383100
	H	-3.10708500	-0.10849500	0.07112600
	H	-0.11087600	1.65505300	0.93451500
VII	U	-2.329997	2.271675	0.997244
	C	-0.601322	1.439833	-0.115291
	H	-3.830475	2.194294	-0.218679
	H	0.288627	1.105388	-0.657367
	H	-1.830700	4.130573	0.834793

Table 7.3: $[UCH_3]^+$ Rearrangement B3LYP/SDD/6-311+g(d,p) Singlet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UHC_3]^+$ (V)	-516.49451	.03174	.03581	.03675	.00439	-516.46277	-516.45871	-516.45776	-516.49012
TSV→VI	-516.46033	.02608	.02953	.03047	-.00060	-516.43425	-516.43080	-516.42985	-516.46093
VI	-516.47867	.02669	.03049	.03143	-.00026	-516.45197	-516.44818	-516.44723	-516.47892
TSVI→VII	-516.41699	.02100	.02497	.02592	-.00602	-516.39599	-516.39202	-516.39108	-516.42301
VII	-516.42432	.02073	.02569	.02663	-.00813	-516.40360	-516.39863	-516.39769	-516.43245

Table 7.3.1: $[UCH_3]^+$ Rearrangement B3LYP/SDD/6-311+g(d,p) Singlet Spin Structure Coordinates

Structure	Coordinates			
$[UHC_3]^+$ (V)	U	-3.253294	1.047442	-0.437384
	C	-1.044015	0.762871	-0.042847
	H	-0.472086	1.487361	-0.644763
	H	-0.837913	0.958493	1.021838
	H	-0.681292	-0.246377	-0.283530
TSV→VI	U	-0.168782	-0.022172	0.032049
	C	1.850745	-0.068118	-0.099086
	H	1.073854	1.473243	0.301303
	H	1.886670	-0.492567	0.948918
	H	2.857476	0.142792	-0.456716

VI	U	-0.166444	-0.021079	-0.027568
	C	1.813022	-0.058423	0.001394
	H	-0.236947	1.932740	-0.002501
	H	1.762938	1.079559	0.016929
	H	2.836373	-0.432115	0.012063
TSVI→VII	U	-0.047424	-0.238844	0.037183
	C	-1.894364	-0.034593	0.097617
	H	1.235936	-0.926968	1.301565
	H	-2.954917	0.204687	-0.024664
	H	-0.476124	1.363200	0.966775
VII	U	-2.054204	2.503468	0.302377
	C	-0.587527	1.477407	-0.196833
	H	-3.918081	2.067617	0.038586
	H	0.276786	0.872319	-0.490534
	H	-2.020841	4.220952	1.187105

Table 7.4: $[UCH_3]^+$ Rearrangement PBE1PBE/SDD/6-311+g(d,p) Singlet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UHC_3]^+$ (V)	-516.32691	.03153	.03580	.03674	.00387	-516.29538	-516.29111	-516.29017	-516.32304
TSV→VI	-516.30114	.02642	.02982	.03076	-.00018	-516.27472	-516.27132	-516.27038	-516.30132
VI	-516.32105	.02727	.03094	.03189	.00043	-516.29378	-516.29011	-516.28917	-516.32062
TSVI→VII	-516.25868	.02134	.02529	.02624	-.00558	-516.23735	-516.23339	-516.23245	-516.26426
VII	-516.26538	.02112	.02602	.02697	-.00735	-516.24427	-516.23936	-516.23842	-516.27273

Table 7.4.1: $[UCH_3]^+$ Rearrangement PBE1PBE/SDD/6-311+g(d,p) Singlet Spin Structure Coordinates

Structure	Coordinates			
$[UHC_3]^+$ (V)	U	-3.229849	1.070378	-0.424760
	C	-1.051291	0.744150	-0.050543
	H	-0.496983	1.487813	-0.650181
	H	-0.863313	0.958928	1.016452
	H	-0.647163	-0.251479	-0.277653
TSV→VI	U	-0.144523	-0.029693	0.077337
	C	1.841721	-0.046066	-0.113663
	H	1.094027	1.456999	0.264581
	H	1.844518	-0.514780	0.926735
	H	2.864219	0.166717	-0.428522
VI	U	-0.158534	-0.021627	0.000116
	C	1.797320	-0.074316	0.000214
	H	-0.162265	1.919575	0.000483
	H	1.691996	1.071263	-0.000749
	H	2.840425	-0.394214	0.000252
TSVI→VII	U	-0.101902	-0.334237	0.129433
	C	-1.902672	-0.031357	0.168578
	H	1.347701	-0.836122	1.269504
	H	-2.937510	0.251984	-0.052234
	H	-0.512837	1.359050	0.841539
VII	U	-2.040602	2.495685	0.296486
	C	-0.594519	1.482386	-0.193966
	H	-3.896870	2.089663	0.051561
	H	0.270053	0.875880	-0.488449

	H	-2.041928	4.198148	1.175068

Table 7.5: $[UCH_3]^+$ Rearrangement B3LYP/SDD/6-311+g(d,p) Triplet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UHC_3]^+$ (**V**)	-516.57310	.03193	.03590	.03684	.00362	-516.54117	-516.53720	-516.53626	-516.56948
TSV→VI	-516.51350	.02494	.02873	.02967	-.00313	-516.48856	-516.48477	-516.48383	-516.51663
VI	-516.52597	.02557	.02981	.03075	-.00284	-516.50039	-516.49616	-516.49522	-516.52881
TSVI→VII	-516.42111	.01974	.02395	.02490	-.00877	-516.40137	-516.39716	-516.39621	-516.42988
VII	-516.42605	.02051	.02526	.02620	-.00864	-516.40554	-516.40079	-516.39985	-516.43469

Table 7.5.1: $[UCH_3]^+$ Rearrangement B3LYP/SDD/6-311+g(d,p) Triplet Spin Structure Coordinates

Structure	Coordinates			
$[UHC_3]^+$ (**V**)	U	-3.286944	1.029979	-0.450263
	C	-1.045147	0.778165	-0.038280
	H	-0.444776	1.483636	-0.634961
	H	-0.808810	0.957534	1.022921
	H	-0.702923	-0.239524	-0.286102
TSV→VI	U	-2.563740	1.268775	0.189545
	C	-0.734651	2.171245	-0.286428
	H	-0.914745	0.947585	1.258744
	H	-0.424200	1.389429	-1.025181
	H	0.075297	2.883902	-0.136682
VI	U	0.161329	-0.021252	-0.020066
	C	-1.835552	-0.048355	0.005404
	H	0.283091	1.940099	-0.003920
	H	-1.817234	1.081224	0.016156
	H	-2.840510	-0.466992	0.014839
TSVI→VII	U	0.157816	0.003898	-0.029103
	C	-1.982450	-0.104373	0.036424
	H	1.016990	-1.083713	1.346163
	H	-3.073257	-0.077069	0.110456
	H	-0.226320	1.670574	0.892882
VII	U	-2.130011	2.569408	0.315691
	C	-0.546502	1.418840	-0.184247
	H	-3.973610	2.127795	-0.174596
	H	0.313004	0.795850	-0.456746
	H	-1.966748	4.229872	1.340599

Table 7.6: $[UCH_3]^+$ Rearrangement PBE1PBE/SDD/6-311+g(d,p) Triplet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UHC_3]^+$ (**V**)	-516.41461	.03195	.03599	.03694	.00357	-516.38266	-516.37862	-516.37767	-516.41104
TSV→VI	-516.35900	.02535	.02900	.02994	-.00254	-516.33365	-516.33001	-516.32906	-516.36154
VI	-516.37218	.02676	.03059	.03153	-.00122	-516.34542	-516.34159	-516.34065	-516.37340
TSVI→VII	-516.25938	.01977	.02406	.02501	-.00879	-516.23961	-516.23532	-516.23438	-516.26818
VII	-516.26592	.02106	.02571	.02666	-.00790	-516.24485	-516.24021	-516.23926	-516.27382

Table 7.6.1: $[UCH_3]^+$ Rearrangement PBE1PBE/SDD/6-311+g(d,p) Triplet Spin Structure Coordinates

Structure	Coordinates			
$[UHC_3]^+$ (**V**)	U	-3.269914	1.028067	-0.447124
	C	-1.051626	0.778898	-0.039478
	H	-0.448351	1.483802	-0.635412
	H	-0.812296	0.957855	1.021974
	H	-0.706412	-0.238832	-0.286646
TSV→VI	U	-2.527167	1.246578	0.154748
	C	-0.742572	2.195570	-0.262811
	H	-0.915747	0.957866	1.258289
	H	-0.479470	1.386325	-1.002061
	H	0.102918	2.874597	-0.148167
VI	U	0.152170	-0.020985	-0.020714
	C	-1.819269	-0.065765	0.005418
	H	0.207035	1.928960	-0.003322
	H	-1.741639	1.070773	0.014811
	H	-2.847173	-0.428261	0.016218
TSVI→VII	U	0.112940	0.000875	-0.035819
	C	-2.012086	-0.119509	0.043169
	H	1.009889	-1.018607	1.343831
	H	-3.107084	-0.108494	0.071126
	H	-0.110878	1.655054	0.934514
VII	U	-2.125105	2.565744	0.314828
	C	-0.567568	1.435260	-0.177545
	H	-3.948111	2.121109	-0.175708
	H	0.292197	0.809831	-0.450549
	H	-1.955281	4.209820	1.329676

Table 7.7.1: $[UCH_3]^+$ Rearrangement B3LYP/SDD/6-311+g(d,p) Quintet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
$[UHC_3]^+$ (**V**)	-107.903	-106.598	-106.601	-111.004
TSV→VI	57.916	59.423	59.420	54.303
VI	38.991	41.890	41.887	33.998
TSVI→VII	266.063	268.092	268.090	261.988
VII	266.743	270.245	270.243	261.434

Table 7.7.2: $[UCH_3]^+$ Rearrangement PBE1PBE/SDD/6-311+g(d,p) Quintet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
$[UHC_3]^+$ (**V**)	-37.715	-36.187	-36.187	-41.063
TSV→VI	125.790	127.342	127.345	122.136
VI	111.762	114.635	114.635	106.853
TSVI→VII	342.355	344.350	344.350	338.327
VII	343.331	346.839	346.842	338.007

Table 7.7.3: $[UCH_3]^+$ Rearrangement B3LYP/SDD/6-311+g(d,p) Singlet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
$[UHC_3]^+$ (V)	123.409	125.063	125.060	123.958
TSV→VI	198.294	198.338	198.336	200.609
VI	151.759	152.710	152.707	153.363
TSVI→VII	298.732	300.147	300.145	300.145
VII	278.776	282.782	282.782	275.360

Table 7.7.4: $[UCH_3]^+$ Rearrangement PBE1PBE/SDD/6-311+g(d,p) Singlet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
$[UHC_3]^+$ (V)	223.223	225.433	225.433	222.900
TSV→VI	277.481	277.400	277.400	279.944
VI	227.421	228.056	228.056	229.261
TSVI→VII	375.596	376.980	376.980	377.229
VII	357.417	361.308	361.308	354.991

Table 7.7.5: $[UCH_3]^+$ Rearrangement B3LYP/SDD/6-311+g(d,p) Triplet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
$[UHC_3]^+$ (V)	-82.438	-81.026	-81.028	-84.389
TSV→VI	55.700	56.622	56.619	54.364
VI	24.630	26.722	26.720	22.377
TSVI→VII	284.630	286.663	286.663	282.115
VII	273.672	277.124	277.122	269.492

Table 7.7.6: $[UCH_3]^+$ Rearrangement PBE1PBE/SDD/6-311+g(d,p) Triplet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
$[UHC_3]^+$ (V)	-5.939	-4.314	-4.314	-8.142
TSV→VI	122.747	123.317	123.317	121.818
VI	91.850	92.893	92.893	90.687
TSVI→VII	369.642	371.915	371.915	366.953
VII	355.887	359.090	359.090	352.145

Figure 9.1: $[UCH_3]^+$ Rearrangement B3LYP/SDD/6-311+g(d,p) Relative Enthalpy (kJ/mol)

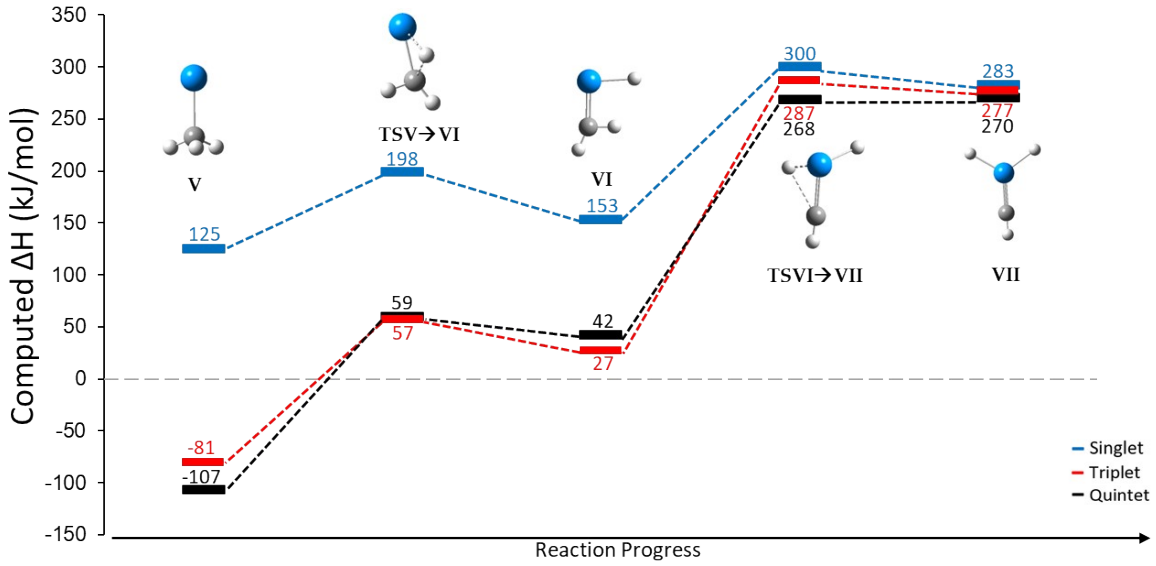

Figure 9.2: $[UCH_3]^+$ Rearrangement PBE1PBE/SDD/6-311+g(d,p) Relative Enthalpy (kJ/mol)

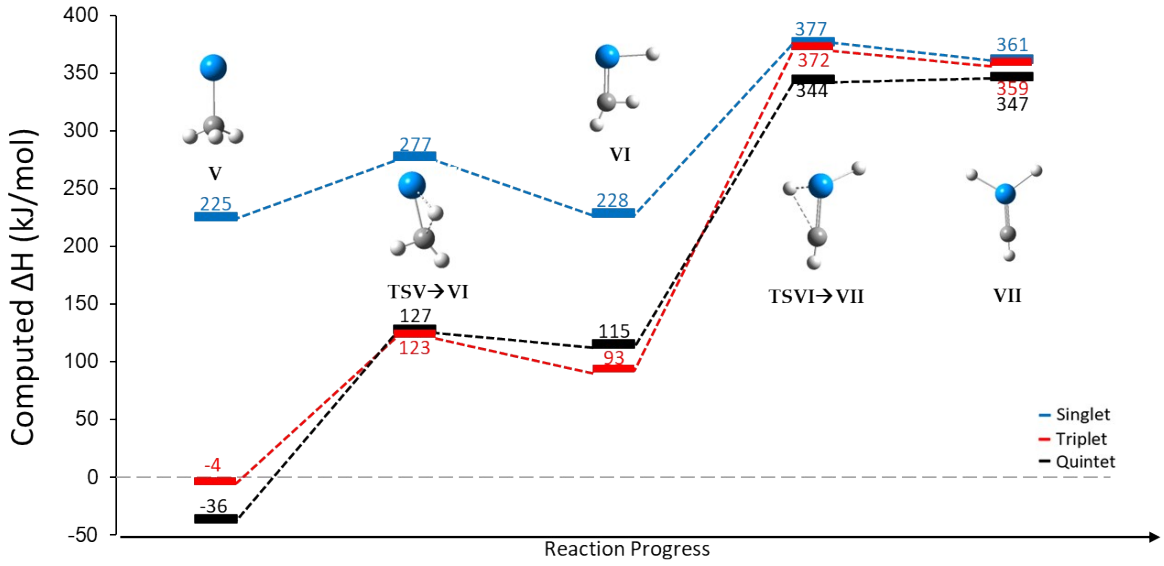

Table 8.1: $[UCH_3]^+$ Dissociation B3LYP/SDD/6-311+g(d,p) Quintet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UHC_3]^+$ (**V**)	-516.58290	.03202	.03595	.03690	.00328	-516.55087	-516.54694	-516.54600	-516.57961
TSV→VI	-516.51239	.02468	.02869	.02963	-.00426	-516.48772	-516.48371	-516.48276	-516.51665
VI	-516.52012	.02520	.02974	.03068	-.00426	-516.49492	-516.49039	-516.48944	-516.52438
TSVI→VII	-516.42836	.01992	.02413	.02507	-.00919	-516.40844	-516.40423	-516.40329	-516.43755
VII	-516.42859	.02041	.02518	.02612	-.00917	-516.40818	-516.40341	-516.40247	-516.43776
H (2)	-.50216	.00000	.00142	.00236	-.01065	-.50216	-.50074	-.49980	-.51281
$[UCH_2]^+$ (4)	-515.93826	.02094	.02420	.02515	-.00645	-515.91732	-515.91406	-515.91311	-515.94470
H + $[UCH_2]^+$ (**VIII**)	-516.44041	.02094	.02562	.02751	-.01710	-516.41947	-516.41480	-516.41291	-516.45751
H-UCH_2^+ BDE	.07971	-.00426	-.00412	-.00318	-.01284	.07545	.07559	.07653	.06687
TSVI →*IX*	-516.47684	.02373	.02709	.02804	-.00471	-516.45312	-516.44975	-516.44881	-516.48156
IX	-516.47739	.02569	.02962	.03056	-.00325	-516.45170	-516.44777	-516.44683	-516.48064
$[UCH]^+$	-1.17957	.01007	.01243	.01337	-.00142	-1.16950	-1.16714	-1.16620	-1.18099
H_2	-515.27769	.01001	.01316	.01410	-.01365	-515.26768	-515.26454	-515.26359	-515.29134
H_2 + $[UCH]^+$ (**X**)	-516.45726	.02008	.02558	.02747	-.01507	-516.43719	-516.43168	-516.42979	-516.47233
^4I $5f^3 7s^2$ U^+ (4)	-476.62730	.00000	.00142	.00236	-.01905	-476.62730	-476.62588	-476.62494	-476.64635
CH_3 (2)	-39.85517	.02963	.03268	.03362	.01154	-39.82554	-39.82249	-39.82155	-39.84363
U^+ + CH_3 (**XI**)	-516.48246	.02963	.03409	.03598	-.00751	-516.45283	-516.44837	-516.44648	-516.48997
U^+-CH_3 BDE	.10043	-.00239	-.00186	-.00092	-.01079	.09804	.09857	.09951	.08964

Table 8.1.1: $[UCH_3]^+$ Dissociation B3LYP/SDD/6-311+g(d,p) Quintet Spin Structure Coordinates

Structure	Coordinates			
$[UHC_3]^+$ (**V**)	U	-3.289712	1.030298	-0.450766
	C	-1.044265	0.778059	-0.038123
	H	-0.444203	1.483373	-0.634672
	H	-0.808150	0.957408	1.022779
	H	-0.702269	-0.239348	-0.285902
TSV→VI	U	-0.270334	0.121000	-0.299332
	C	1.897852	-0.236839	0.115856
	H	0.831139	1.637730	0.436111
	H	2.352926	-0.507480	1.075369
	H	2.688380	0.018767	-0.601536
VI	U	-0.360956	-0.059712	-0.003691
	C	1.936823	0.159322	0.001362
	H	-0.689602	1.911264	-0.002921
	H	2.439713	1.133729	0.003762
	H	2.682963	-0.643922	0.001805
TSVI→VII	U	0.205380	0.064804	-0.090929
	C	-2.014593	-0.145062	0.021440
	H	0.889730	-1.038180	1.356320
	H	-3.102041	-0.157464	0.133984
	H	-0.085697	1.685220	0.936006
VII	U	-2.327016	2.255848	1.004581
	C	-0.580505	1.427792	-0.127237
	H	-3.847275	2.228291	-0.208158

	H	0.311548	1.095721	-0.665642
	H	-1.860619	4.134110	0.837157
$[UCH_2]^+$ (**VIII**)	U	-0.048167	-0.534393	-0.307877
	C	1.680058	0.434748	0.076897
	H	2.396246	1.219843	0.320945
	H	2.214029	-0.550173	-0.089784
TSVI→*IX*	U	-0.310566	-0.126750	0.061681
	C	1.794779	-0.297302	0.006525
	H	1.196640	1.342078	-0.024393
	H	2.886442	-0.306775	-0.024232
	H	0.441646	1.889430	-0.019263
IX	U	-0.160180	0.150355	-0.032018
	H	1.456954	1.468263	-0.969784
	C	-0.172413	-0.660772	-1.953259
	H	-0.159226	-1.070737	-2.965810
	H	1.225682	0.972729	-1.574198
$[UCH]^+$ (**X**)	U	-0.003076	0.000898	0.290262
	C	0.008610	-0.002512	-1.773316
	H	-0.005534	0.001615	-2.864596

Table 8.2: $[UCH_3]^+$ Dissociation PBE1PBE/SDD/6-311+g(d,p) Quintet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UHC_3]^+$ (**V**)	-516.58290	.03202	.03595	.03690	.00328	-516.55087	-516.54694	-516.54600	-516.57961
TSV→VI	-516.51239	.02468	.02869	.02963	-.00426	-516.48772	-516.48371	-516.48276	-516.51665
VI	-516.52012	.02520	.02974	.03068	-.00426	-516.49492	-516.49039	-516.48944	-516.52438
TSVI→VII	-516.42836	.01992	.02413	.02507	-.00919	-516.40844	-516.40423	-516.40329	-516.43755
VII	-516.42859	.02041	.02518	.02612	-.00917	-516.40818	-516.40341	-516.40247	-516.43776
H (2)	-.50104	.00000	.00142	.00236	-.01065	-.50104	-.49962	-.49868	-.51169
$[UCH_2]^+$ (4)	-515.78116	.02113	.02437	.02532	-.00624	-515.76004	-515.75679	-515.75585	-515.78740
H + $[UCH_2]^+$ (**VIII**)	-516.28220	.02113	.02579	.02768	-.01689	-516.26107	-516.25641	-516.25452	-516.29909
H-UCH_2^+ BDE	.08100	-.00424	-.00410	-.00316	-.01285	.07676	.07690	.07785	.06815
TSVI →*IX*	-516.32471	.02389	.02727	.02821	-.00456	-516.30082	-516.29744	-516.29650	-516.32926
IX	-516.32328	.02598	.02994	.03089	-.00295	-516.29730	-516.29334	-516.29240	-516.32623
$[UCH]^+$	-1.16816	.01005	.01241	.01336	-.00144	-1.15811	-1.15575	-1.15480	-1.16960
H_2	-515.13071	.01009	.01324	.01418	-.01348	-515.12062	-515.11747	-515.11653	-515.14419
H_2 + $[UCH]^+$ (**X**)	-516.29887	.02014	.02565	.02754	-.01492	-516.27872	-516.27322	-516.27133	-516.31379
$^4I\ 5f^37s^2\ U^+$ (4)	-476.51684	.00000	.00142	.00236	-.01905	-476.51685	-476.51543	-476.51448	-476.53589
CH_3 (2)	-39.79550	.02974	.03280	.03374	.01165	-39.76575	-39.76270	-39.76176	-39.78385
U^+ + CH_3 (**XI**)	-516.31234	.02974	.03421	.03610	-.00740	-516.28260	-516.27813	-516.27624	-516.31974
U^+-CH_3 BDE	.11445	-.00228	-.00182	-.00088	-.01061	.11217	.11263	.11357	.10384

Table 8.2.1: $[UCH_3]^+$ Rearrangement PBE1PBE/SDD/6-311+g(d,p) Quintet Spin Structure Coordinates

Structure	Coordinates			
$[UHC_3]^+$ (**V**)	U	-3.272222	1.028329	-0.447550
	C	-1.051155	0.778843	-0.039390
	H	-0.447809	1.483494	-0.635086
	H	-0.811631	0.957714	1.021772
	H	-0.705783	-0.238591	-0.286431

TSV→VI	U	-0.255715	0.116932	-0.264047
	C	1.911064	-0.232481	0.079102
	H	0.787449	1.663299	0.445181
	H	2.312891	-0.504888	1.065426
	H	2.744274	-0.009684	-0.599194
VI	U	-0.354574	-0.049095	-0.001753
	C	1.926607	0.124405	0.000408
	H	-0.654472	1.920795	-0.000459
	H	2.367873	1.132546	0.002029
	H	2.723507	-0.627970	0.000093
TSVI→VII	U	0.11293900	0.00087500	-0.03581900
	C	-2.01208700	-0.11950900	0.04316800
	H	1.00988800	-1.01860600	1.34383100
	H	-3.10708500	-0.10849500	0.07112600
	H	-0.11087600	1.65505300	0.93451500
VII	U	-2.329997	2.271675	0.997244
	C	-0.601322	1.439833	-0.115291
	H	-3.830475	2.194294	-0.218679
	H	0.288627	1.105388	-0.657367
	H	-1.830700	4.130573	0.834793
$[UCH_2]^+$ (VIII)	U	-0.048167	-0.534393	-0.307877
	C	1.680058	0.434748	0.076897
	H	2.396246	1.219843	0.320945
	H	2.214029	-0.550173	-0.089784
TSVI →*IX*	U	-0.310566	-0.126750	0.061681
	C	1.794779	-0.297302	0.006525
	H	0.441646	1.889430	-0.019263
	H	1.196640	1.342078	-0.024393
	H	2.886442	-0.306775	-0.024232
IX	U	-0.160180	0.150355	-0.032018
	H	1.456954	1.468263	-0.969784
	C	-0.172413	-0.660772	-1.953259
	H	-0.159226	-1.070737	-2.965810
	H	1.225682	0.972729	-1.574198
$[UCH]^+$ (X)	U	-0.002836	0.000828	0.279490
	C	0.007984	-0.002329	-1.767013
	H	-0.005148	0.001502	-2.860127

Table 8.3: $[UCH_3]^+$ Dissociation B3LYP/SDD/6-311+g(d,p) Singlet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UHC_3]^+$ (V)	-516.58290	.03202	.03595	.03690	.00328	-516.55087	-516.54694	-516.54600	-516.57961
TSV→VI	-516.51239	.02468	.02869	.02963	-.00426	-516.48772	-516.48371	-516.48276	-516.51665
VI	-516.52012	.02520	.02974	.03068	-.00426	-516.49492	-516.49039	-516.48944	-516.52438
TSVI→VII	-516.42836	.01992	.02413	.02507	-.00919	-516.40844	-516.40423	-516.40329	-516.43755
VII	-516.42859	.02041	.02518	.02612	-.00917	-516.40818	-516.40341	-516.40247	-516.43776
H (2)	-.50216	.00000	.00142	.00236	-.01065	-.50216	-.50074	-.49980	-.51281
$[UCH_2]^+$ (2)	-515.91385	.02081	.02408	.02503	-.00590	-515.89304	-515.88977	-515.88883	-515.91975
H + $[UCH_2]^+$ (VIII)	-516.41601	.02081	.02550	.02739	-.01656	-516.39520	-516.39051	-516.38862	-516.43256
H-UCH_2^+ BDE	.06266	-.00588	-.00499	-.00405	-.01630	.05678	.05767	.05861	.04636
TSVI →*IX*	-516.42995	.02335	.02674	.02769	-.00358	-516.40661	-516.40321	-516.40227	-516.43353
IX	-516.44701	.02577	.02966	.03060	-.00139	-516.42125	-516.41736	-516.41641	-516.44841
$[UCH]^+$	-1.17957	.01007	.01243	.01337	-.00142	-1.16950	-1.16714	-1.16620	-1.18099
H_2	-515.23631	.01202	.01474	.01569	-.01194	-515.22429	-515.22157	-515.22063	-515.24825

H_2 + $[UCH]^+$ (**X**)	-516.41588	.02209	.02717	.02906	-.01336	-516.39380	-516.38872	-516.38683	-516.42924
$5f^37s^2$ U^+ (2)	-476.56467	.00000	.00142	.00236	-.01839	-476.56467	-476.56325	-476.56231	-476.58306
CH_3 (2)	-39.85517	.02963	.03268	.03362	.01154	-39.82554	-39.82249	-39.82155	-39.84363
U^+ + CH_3 (**XI**)	-516.41984	.02963	.03409	.03598	-.00685	-516.39020	-516.38574	-516.38386	-516.42669
U^+-CH_3 BDE	.07467	-.00211	-.00171	-.00077	-.01124	.07257	.07296	.07391	.06343

Table 8.3.1: $[UCH_3]^+$ Dissociation B3LYP/SDD/6-311+g(d,p) Singlet Spin Structure Coordinates

Structure	Coordinates			
$[UHC_3]^+$ (**V**)	U	-3.253294	1.047442	-0.437384
	C	-1.044015	0.762871	-0.042847
	H	-0.472086	1.487361	-0.644763
	H	-0.837913	0.958493	1.021838
	H	-0.681292	-0.246377	-0.283530
TSV→VI	U	-0.168782	-0.022172	0.032049
	C	1.850745	-0.068118	-0.099086
	H	1.073854	1.473243	0.301303
	H	1.886670	-0.492567	0.948918
	H	2.857476	0.142792	-0.456716
VI	U	-0.166444	-0.021079	-0.027568
	C	1.813022	-0.058423	0.001394
	H	-0.236947	1.932740	-0.002501
	H	1.762938	1.079559	0.016929
	H	2.836373	-0.432115	0.012063
TSVI→VII	U	-0.047424	-0.238844	0.037183
	C	-1.894364	-0.034593	0.097617
	H	1.235936	-0.926968	1.301565
	H	-2.954917	0.204687	-0.024664
	H	-0.476124	1.363200	0.966775
VII	U	-2.054204	2.503468	0.302377
	C	-0.587527	1.477407	-0.196833
	H	-3.918081	2.067617	0.038586
	H	0.276786	0.872319	-0.490534
	H	-2.020841	4.220952	1.187105
$[UCH_2]^+$ (**VIII**)	U	-0.038234	-0.529051	-0.305513
	C	1.681708	0.432800	0.075898
	H	2.389871	1.222269	0.320892
	H	2.208820	-0.555992	-0.091097
TSVI→*IX*	U	-0.204757	-0.127640	0.032447
	C	1.716342	-0.162842	0.049762
	H	0.413581	1.848992	0.001060
	H	1.292447	1.255696	-0.041738
	H	2.791327	-0.313525	-0.041213
IX	U	-2.063659	0.725809	0.197760
	C	-1.530068	2.364932	-0.630669
	H	-1.636237	2.577024	0.785642
	H	-1.184307	3.275558	-1.135105
	H	-1.889596	2.176341	1.565273
$[UCH]^+$ (**X**)	U	-0.000000	0.000000	0.143174
	C	0.000000	-0.000000	-1.725919
	H	0.000000	-0.000000	-2.816462

Table 8.4: $[UCH_3]^+$ Dissociation PBE1PBE/SDD/6-311+g(d,p) Singlet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UHC_3]^+$ (**V**)	-516.58290	.03202	.03595	.03690	.00328	-516.55087	-516.54694	-516.54600	-516.57961
TSV→VI	-516.51239	.02468	.02869	.02963	-.00426	-516.48772	-516.48371	-516.48276	-516.51665
VI	-516.52012	.02520	.02974	.03068	-.00426	-516.49492	-516.49039	-516.48944	-516.52438
TSVI→VII	-516.42836	.01992	.02413	.02507	-.00919	-516.40844	-516.40423	-516.40329	-516.43755
VII	-516.42859	.02041	.02518	.02612	-.00917	-516.40818	-516.40341	-516.40247	-516.43776
H (2)	-.50104	.00000	.00142	.00236	-.01065	-.50104	-.49962	-.49868	-.51169
$[UCH_2]^+$ (2)	-515.76260	.02120	.02441	.02536	-.00548	-515.74140	-515.73818	-515.73724	-515.76807
H + $[UCH_2]^+$ (**VIII**)	-516.26363	.02120	.02583	.02772	-.01613	-516.24243	-516.23781	-516.23592	-516.27977
H-UCH_2^+ BDE	.05742	-.00607	-.00511	-.00417	-.01656	.05135	.05231	.05325	.04085
TSVI →*IX*	-516.26923	.02344	.02684	.02778	-.00349	-516.24579	-516.24239	-516.24144	-516.27271
IX	-516.29268	.02654	.03013	.03107	-.00022	-516.26614	-516.26256	-516.26161	-516.29290
$[UCH]^+$	-1.16816	.01005	.01241	.01336	-.00144	-1.15811	-1.15575	-1.15480	-1.16960
H_2	-515.09093	.01233	.01501	.01595	-.01158	-515.07860	-515.07592	-515.07498	-515.10251
H_2 + $[UCH]^+$ (**X**)	-516.25908	.02238	.02742	.02931	-.01302	-516.23670	-516.23167	-516.22978	-516.27211
$5f^37s^2$ U^+ (2)	-476.44907	.00000	.00142	.00236	-.01839	-476.44907	-476.44765	-476.44671	-476.46746
CH_3 (2)	-39.79550	.02974	.03280	.03374	.01165	-39.76575	-39.76270	-39.76176	-39.78385
U^+ + CH_3 (**XI**)	-516.24456	.02974	.03421	.03610	-.00675	-516.21482	-516.21035	-516.20846	-516.25131
U^+-CH_3 BDE	.08235	-.00179	-.00159	-.00064	-.01062	.08056	.08076	.08171	.07173

Table 8.4.1: $[UCH_3]^+$ Dissociation PBE1PBE/SDD/6-311+g(d,p) Singlet Spin Structure Coordinates

Structure	Coordinates			
$[UHC_3]^+$ (**V**)	U	-3.229849	1.070378	-0.424760
	C	-1.051291	0.744150	-0.050543
	H	-0.496983	1.487813	-0.650181
	H	-0.863313	0.958928	1.016452
	H	-0.647163	-0.251479	-0.277653
TSV→VI	U	-0.144523	-0.029693	0.077337
	C	1.841721	-0.046066	-0.113663
	H	1.094027	1.456999	0.264581
	H	1.844518	-0.514780	0.926735
	H	2.864219	0.166717	-0.428522
VI	U	-0.158534	-0.021627	0.000116
	C	1.797320	-0.074316	0.000214
	H	-0.162265	1.919575	0.000483
	H	1.691996	1.071263	-0.000749
	H	2.840425	-0.394214	0.000252
TSVI→VII	U	-0.101902	-0.334237	0.129433
	C	-1.902672	-0.031357	0.168578
	H	1.347701	-0.836122	1.269504
	H	-2.937510	0.251984	-0.052234
	H	-0.512837	1.359050	0.841539
VII	U	-2.040602	2.495685	0.296486
	C	-0.594519	1.482386	-0.193966
	H	-3.896870	2.089663	0.051561
	H	0.270053	0.875880	-0.488449

	H	-2.041928	4.198148	1.175068
$[UCH_2]^+$ (**VIII**)	U	-0.031581	-0.542943	-0.308088
	C	1.673282	0.446644	0.078745
	H	2.407315	1.216184	0.320893
	H	2.193149	-0.549859	-0.091370
TSVI→*IX*	U	-0.180368	-0.086920	0.017698
	C	1.722862	-0.193159	0.051252
	H	0.339339	1.879686	0.033596
	H	1.321782	1.221277	-0.088804
	H	2.805327	-0.320204	-0.013424
IX	U	-2.063659	0.725809	0.197760
	C	-1.530068	2.364932	-0.630669
	H	-1.636237	2.577024	0.785642
	H	-1.184307	3.275558	-1.135105
	H	-1.889596	2.176341	1.565273
$[UCH]^+$ (**X**)	U	-0.000000	0.000000	0.141080
	C	0.000000	-0.000000	-1.698121
	H	0.000000	-0.000000	-2.790609

Table 8.5: $[UCH_3]^+$ Dissociation B3LYP/SDD/6-311+g(d,p) Triplet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UHC_3]^+$ (**V**)	-516.58290	.03202	.03595	.03690	.00328	-516.55087	-516.54694	-516.54600	-516.57961
TSV→VI	-516.51239	.02468	.02869	.02963	-.00426	-516.48772	-516.48371	-516.48276	-516.51665
VI	-516.52012	.02520	.02974	.03068	-.00426	-516.49492	-516.49039	-516.48944	-516.52438
TSVI→VII	-516.42836	.01992	.02413	.02507	-.00919	-516.40844	-516.40423	-516.40329	-516.43755
VII	-516.42859	.02041	.02518	.02612	-.00917	-516.40818	-516.40341	-516.40247	-516.43776
H (2)	-.50216	.00000	.00142	.00236	-.01065	-.50216	-.50074	-.49980	-.51281
$[UCH_2]^+$ (2)	-515.91385	.02081	.02408	.02503	-.00590	-515.89304	-515.88977	-515.88883	-515.91975
H + $[UCH_2]^+$ (**VIII**)	-516.41601	.02081	.02550	.02739	-.01656	-516.39520	-516.39051	-516.38862	-516.43256
H-UCH_2^+ BDE	.10996	-.00476	-.00431	-.00336	-.01371	.10520	.10565	.10660	.09625
TSVI→*IX*	-516.48409	.02297	.02675	.02770	-.00542	-516.46112	-516.45734	-516.45639	-516.48951
IX	-516.49099	.02654	.03028	.03123	-.00138	-516.46445	-516.46071	-516.45977	-516.49237
$[UCH]^+$	-1.17957	.01007	.01243	.01337	-.00142	-1.16950	-1.16714	-1.16620	-1.18099
H_2	-515.23631	.01202	.01474	.01569	-.01194	-515.22429	-515.22157	-515.22063	-515.24825
H_2 + $[UCH]^+$ (**X**)	-516.41588	.02209	.02717	.02906	-.01336	-516.39380	-516.38872	-516.38683	-516.42924
$5f^37s^2$ U^+ (2)	-476.56467	.00000	.00142	.00236	-.01839	-476.56467	-476.56325	-476.56231	-476.58306
CH_3 (2)	-39.85517	.02963	.03268	.03362	.01154	-39.82554	-39.82249	-39.82155	-39.84363
U^+ + CH_3 (**XI**)	-516.41984	.02963	.03409	.03598	-.00685	-516.39020	-516.38574	-516.38386	-516.42669
U^+-CH_3 BDE	.15326	-.00229	-.00181	-.00086	-.01048	.15097	.15146	.15240	.14279

Table 8.5.1: $[UCH_3]^+$ Rearrangement B3LYP/SDD/6-311+g(d,p) Triplet Spin Structure Coordinates

Structure	Coordinates			
$[UHC_3]^+$ (**V**)	U	-3.253294	1.047442	-0.437384
	C	-1.044015	0.762871	-0.042847
	H	-0.472086	1.487361	-0.644763
	H	-0.837913	0.958493	1.021838
	H	-0.681292	-0.246377	-0.283530
TSV→VI	U	-0.168782	-0.022172	0.032049
	C	1.850745	-0.068118	-0.099086

	H	1.073854	1.473243	0.301303
	H	1.886670	-0.492567	0.948918
	H	2.857476	0.142792	-0.456716
VI	U	-0.166444	-0.021079	-0.027568
	C	1.813022	-0.058423	0.001394
	H	-0.236947	1.932740	-0.002501
	H	1.762938	1.079559	0.016929
	H	2.836373	-0.432115	0.012063
TSVI→VII	U	-0.047424	-0.238844	0.037183
	C	-1.894364	-0.034593	0.097617
	H	1.235936	-0.926968	1.301565
	H	-2.954917	0.204687	-0.024664
	H	-0.476124	1.363200	0.966775
VII	U	-2.054204	2.503468	0.302377
	C	-0.587527	1.477407	-0.196833
	H	-3.918081	2.067617	0.038586
	H	0.276786	0.872319	-0.490534
	H	-2.020841	4.220952	1.187105
$[UCH_2]^+$ (**VIII**)	U	-0.038234	-0.529051	-0.305513
	C	1.681708	0.432800	0.075898
	H	2.389871	1.222269	0.320892
	H	2.208820	-0.555992	-0.091097
TSVI →*IX*	U	-0.205463	-0.138446	0.051410
	C	1.715021	-0.215597	0.048744
	H	0.479251	1.841256	-0.055552
	H	1.222110	1.291901	0.012727
	H	2.798021	-0.278433	-0.057010
IX	U	-2.063659	0.725809	0.197760
	C	-1.530068	2.359832	-0.632369
	H	-1.763737	2.602524	0.817942
	H	-1.153707	3.270458	-1.113005
	H	-1.792696	2.183141	1.570373
$[UCH]^+$ (**X**)	U	-0.000000	0.000000	0.143174
	C	0.000000	-0.000000	-1.725919
	H	0.000000	-0.000000	-2.816462

Table 8.6: $[UCH_3]^+$ Dissociation PBE1PBE/SDD/6-311+g(d,p) Triplet Spin Energies (Hartree)

Structure	E0	E_ZPE	E_tot	H_corr	G_corr	E0+E_ZPE	E0+E_tot	E0+H_corr	E0+G_corr
$[UHC_3]^+$ (**V**)	-516.58290	.03202	.03595	.03690	.00328	-516.55087	-516.54694	-516.54600	-516.57961
TSV→VI	-516.51239	.02468	.02869	.02963	-.00426	-516.48772	-516.48371	-516.48276	-516.51665
VI	-516.52012	.02520	.02974	.03068	-.00426	-516.49492	-516.49039	-516.48944	-516.52438
TSVI→VII	-516.42836	.01992	.02413	.02507	-.00919	-516.40844	-516.40423	-516.40329	-516.43755
VII	-516.42859	.02041	.02518	.02612	-.00917	-516.40818	-516.40341	-516.40247	-516.43776
H (2)	-.50104	.00000	.00142	.00236	-.01065	-.50104	-.49962	-.49868	-.51169
$[UCH_2]^+$ (2)	-515.76260	.02120	.02441	.02536	-.00548	-515.74140	-515.73818	-515.73724	-515.76807
H + $[UCH_2]^+$ (**VIII**)	-516.26363	.02120	.02583	.02772	-.01613	-516.24243	-516.23781	-516.23592	-516.27977
H-UCH_2^+ BDE	.10855	-.00556	-.00476	-.00381	-.01491	.10298	.10379	.10473	.09363
TSVI →*IX*	-516.32935	.02299	.02689	.02783	-.00566	-516.30637	-516.30246	-516.30152	-516.33501
IX	-516.34030	.02663	.03044	.03138	-.00137	-516.31367	-516.30986	-516.30892	-516.34167
$[UCH]^+$	-1.16816	.01005	.01241	.01336	-.00144	-1.15811	-1.15575	-1.15480	-1.16960
H_2	-515.09093	.01233	.01501	.01595	-.01158	-515.07860	-515.07592	-515.07498	-515.10251
H_2 + $[UCH]^+$ (**X**)	-516.25908	.02238	.02742	.02931	-.01302	-516.23670	-516.23167	-516.22978	-516.27211

$5f^3 7s^2$ U^+ (2)	-476.44907	.00000	.00142	.00236	-.01839	-476.44907	-476.44765	-476.44671	-476.46746
CH_3 (2)	-39.79550	.02974	.03280	.03374	.01165	-39.76575	-39.76270	-39.76176	-39.78385
$U^+ + CH_3$ (**XI**)	-516.24456	.02974	.03421	.03610	-.00675	-516.21482	-516.21035	-516.20846	-516.25131
U^+-CH_3 BDE	.17005	-.00220	-.00178	-.00084	-.01032	.16785	.16827	.16921	.15973

Table 8.6.1: $[UCH_3]^+$ Rearrangement PBE1PBE/SDD/6-311+g(d,p) Triplet Spin Structure Coordinates

Structure	Coordinates			
$[UHC_3]^+$ (**V**)	U	-3.229849	1.070378	-0.424760
	C	-1.051291	0.744150	-0.050543
	H	-0.496983	1.487813	-0.650181
	H	-0.863313	0.958928	1.016452
	H	-0.647163	-0.251479	-0.277653
TSV→VI	U	-0.144523	-0.029693	0.077337
	C	1.841721	-0.046066	-0.113663
	H	1.094027	1.456999	0.264581
	H	1.844518	-0.514780	0.926735
	H	2.864219	0.166717	-0.428522
VI	U	-0.158534	-0.021627	0.000116
	C	1.797320	-0.074316	0.000214
	H	-0.162265	1.919575	0.000483
	H	1.691996	1.071263	-0.000749
	H	2.840425	-0.394214	0.000252
TSVI→VII	U	-0.101902	-0.334237	0.129433
	C	-1.902672	-0.031357	0.168578
	H	1.347701	-0.836122	1.269504
	H	-2.937510	0.251984	-0.052234
	H	-0.512837	1.359050	0.841539
VII	U	-2.040602	2.495685	0.296486
	C	-0.594519	1.482386	-0.193966
	H	-3.896870	2.089663	0.051561
	H	0.270053	0.875880	-0.488449
	H	-2.041928	4.198148	1.175068
$[UCH_2]^+$ (**VIII**)	U	-0.031581	-0.542943	-0.308088
	C	1.673282	0.446644	0.078745
	H	2.407315	1.216184	0.320893
	H	2.193149	-0.549859	-0.091370
TSVI →*IX*	U	-0.191086	-0.128977	0.045031
	C	1.715911	-0.223046	0.063751
	H	0.464833	1.843538	-0.056356
	H	1.221157	1.294533	0.015973
	H	2.798125	-0.285366	-0.068080
IX	U	-2.063659	0.725809	0.197760
	C	-1.530068	2.359832	-0.632369
	H	-1.763737	2.602524	0.817942
	H	-1.153707	3.270458	-1.113005
	H	-1.792696	2.183141	1.570373
$[UCH]^+$ (**X**)	U	-0.000000	0.000000	0.143174
	C	0.000000	-0.000000	-1.725919
	H	0.000000	-0.000000	-2.816462

Table 8.7.1: $[UCH_3]^+$ Rearrangement B3LYP/SDD/6-311+g(d,p) Quintet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r

$[UHC_3]^+$ (V)	-107.903	-106.598	-106.601	-111.004
TSV→VI	57.916	59.423	59.420	54.303
VI	38.991	41.890	41.887	33.998
TSVI→VII	266.063	268.092	268.090	261.988
VII	266.743	270.245	270.243	261.434
$[UCH_2]^+$ (VIII)	237.088	240.349	242.827	209.565
TSVI →*IX*	148.761	148.574	148.572	146.445
IX	152.468	153.770	153.768	148.850
$[UCH]^+$ (X)	190.585	196.025	198.504	170.665
$U^+ + CH_3$ (XI)	149.504	152.195	154.673	124.346

Table 8.7.2: $[UCH_3]^+$ Rearrangement PBE1PBE/SDD/6-311+g(d,p) Quintet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
$[UHC_3]^+$ (V)	-37.715	-36.187	-36.187	-41.063
TSV→VI	125.790	127.342	127.345	122.136
VI	111.762	114.635	114.635	106.853
TSVI→VII	342.355	344.350	344.350	338.327
VII	343.331	346.839	346.842	338.007
$[UCH_2]^+$ (VIII)	313.298	316.541	319.019	285.786
TSVI →*IX*	208.950	208.814	208.817	206.569
IX	218.184	219.584	219.586	214.537
$U^+ + CH_3$ (XI)	266.961	272.411	274.890	247.201
$[UCH_2]^+$ (VIII)	256.787	259.522818	262.0039	231.5691

Table 8.7.3: $[UCH_3]^+$ Rearrangement B3LYP/SDD/6-311+g(d,p) Singlet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
$[UHC_3]^+$ (V)	123.409	125.063	125.060	123.958
TSV→VI	198.294	198.338	198.336	200.609
VI	151.759	152.710	152.707	153.363
TSVI→VII	298.732	300.147	300.145	300.145
VII	278.776	282.782	282.782	275.360
$[UCH_2]^+$ (VIII)	300.825	304.112	306.590	275.071
TSVI →*IX*	270.865	270.760	270.760	272.527
IX	232.428	233.628	233.625	233.473
$[UCH]^+$ (X)	304.503	308.822	311.300	283.790
$U^+ + CH_3$ (XI)	313.934	316.625	319.103	290.496

Table 8.7.4: $[UCH_3]^+$ Rearrangement PBE1PBE/SDD/6-311+g(d,p) Singlet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
$[UHC_3]^+$ (V)	223.223	225.433	225.433	222.900

TSV→VI	277.481	277.400	277.400	279.944
VI	227.421	228.056	228.056	229.261
TSVI→VII	375.596	376.980	376.980	377.229
VII	357.417	361.308	361.308	354.991
$[UCH_2]^+$ (VIII)	362.235	365.391	367.869	336.526
TSVI →*IX*	353.426	353.358	353.358	355.041
IX	299.990	300.410	300.410	302.032
$[UCH]^+$ (X)	377.284	381.506	383.985	356.632
$U^+ + CH_3$ (XI)	434.741	437.477	439.955	411.240

Table 8.7.5: $[UCH_3]^+$ Rearrangement B3LYP/SDD/6-311+g(d,p) Triplet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
$[UHC_3]^+$ (V)	-82.438	-81.026	-81.028	-84.389
TSV→VI	55.700	56.622	56.619	54.364
VI	24.630	26.722	26.720	22.377
TSVI→VII	284.630	286.663	286.663	282.115
VII	273.672	277.124	277.122	269.492
$[UCH_2]^+$ (VIII)	300.825	304.112	306.590	275.071
TSVI →*IX*	127.733	128.655	128.655	125.565
IX	118.990	119.796	119.796	118.042
$[UCH]^+$ (X)	304.503	308.822	311.300	283.790
$U^+ + CH_3$ (XI)	313.934	316.625	319.103	290.496

Table 8.7.6: $[UCH_3]^+$ Rearrangement PBE1PBE/SDD/6-311+g(d,p) Triplet Spin Relative Energies (kJ/mol)

Structure	E0+E_ZPE	E0+E_tot	E0+H_cor r	E0+G_cor r
$[UHC_3]^+$ (V)	-5.939	-4.314	-4.314	-8.142
TSV→VI	122.747	123.317	123.317	121.818
VI	91.850	92.893	92.893	90.687
TSVI→VII	369.642	371.915	371.915	366.953
VII	355.887	359.090	359.090	352.145
$[UCH_2]^+$ (VIII)	362.235	365.391	367.869	336.526
TSVI →*IX*	194.382	195.631	195.631	191.478
IX	175.213	176.210	176.213	174.002
$[UCH]^+$ (X)	377.284	381.506	383.985	356.632
$U^+ + CH_3$ (XI)	434.741	437.477	439.955	411.240

Figure 10.1 Dissociation of $[UCH_3]^+$ B3LYP/SDD/6-311+g(d,p) Quintet Spin Relative Enthalpy (kJ/mol)

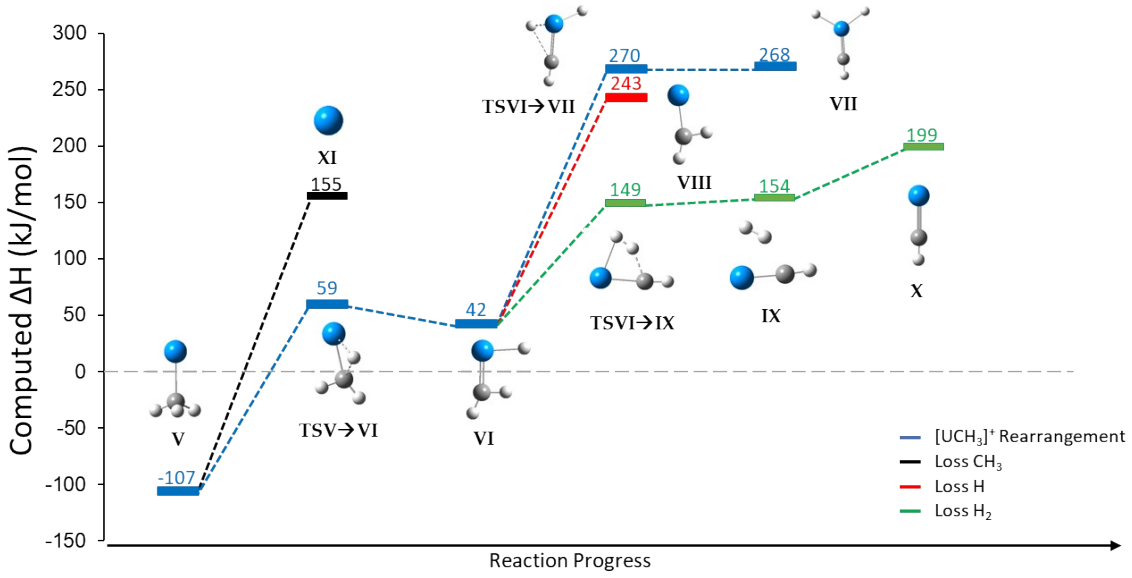

Figure 10.2 Dissociation of $[UCH_3]^+$ PBE0/SDD/6-311+g(d,p) Quintet Spin Relative Enthalpy (kJ/mol)

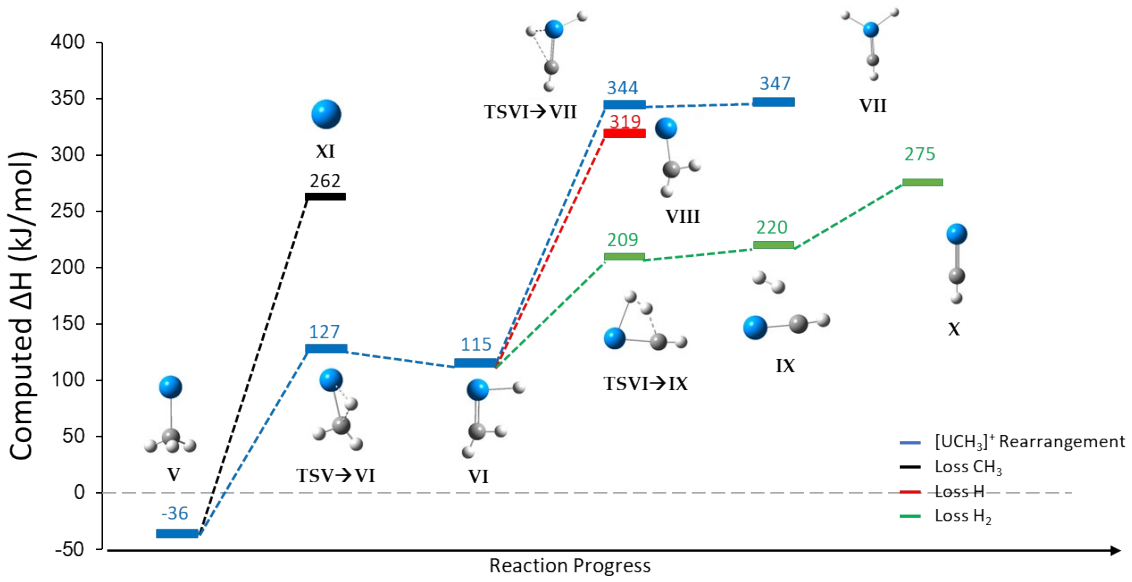

Figure 11.1 CID Mass Spectra of the Dissociation of $[UCH_3]^+$

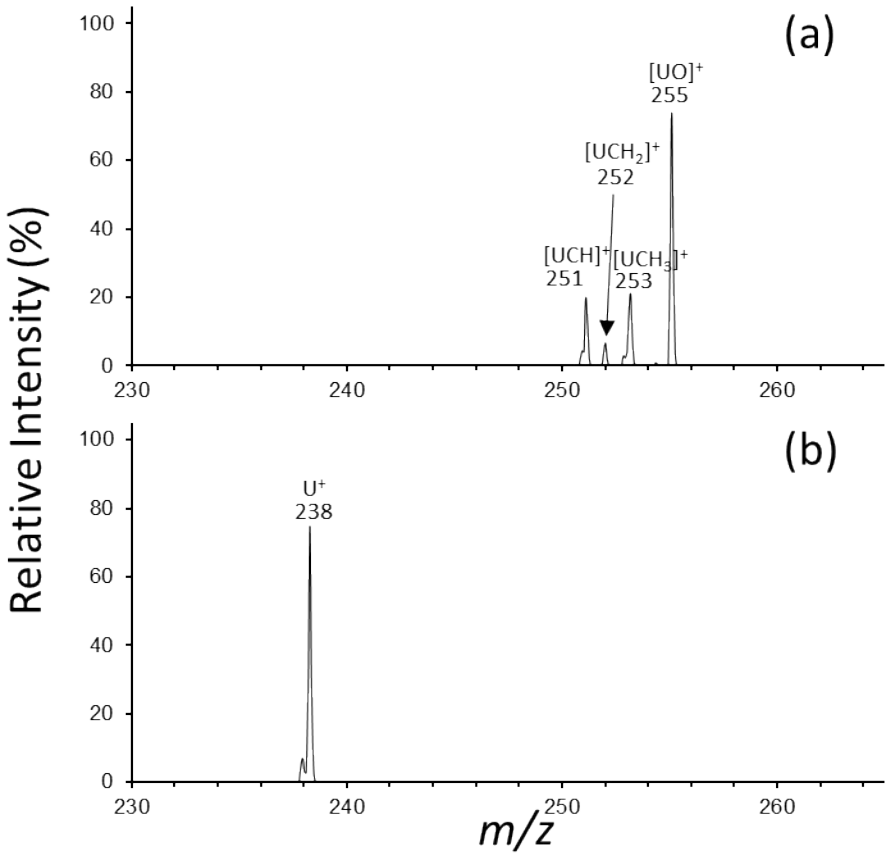

Figure 11.1 : (a) CID of *m/z* 253 ($[UCH_3]^+$) at 10 NCE and a 0.30 q_z to produce $[UCH_2]^+$ and $[UCH]^+$. (b) CID of *m/z* 253 ($[UCH_3]^+$) at 25 NCE and a 0.7 q_z to produce U^+ at *m/z* 238. Note that CID is a slow heating process, and harsher conditions are required to access higher energy channels shown in Figures 10.1 and 10.2.