

Electronic supplementary information (ESI) for the paper:

**Probing Intermediates Folding Patterns
Determined Carbon Skeleton Construction
Mechanism of Cyathane Diterpene**

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This file contains the following supplementary materials:

QM/MM MD Simulations

Amino acid sequence of EriG
Key active-site residues of EriG
Ligand RMSD curves for each system

DFT Calculations

Optimized geometry structures
Natural bond orbital (NBO) analysis
Assessment of dispersion correction effects
Energy profiles
Cartesian (XYZ) oordinates of optimized geometries

QM/MM MD Simulations

Amino acid sequence of EriG

>sp|A0A1V0QSF1|ERIG_HERER Diterpene cyclase eriG OS=Hericium erinaceus OX=91752

GN=eriG PE=1 SV=1

MSVFAPIARELDIFFGFSWRDWSTTIIPGSIFAVGAMRDLPPATLVKNYLFLVTWLTPYIYF
FNLSNQITGVDEDKINKPDRPIPSGKVTLQGAQRRWIAAFSTFLGIALYQPEFLPETLCWIA
TVAFLCLTSYGDHWFGKNCVAMTTGTWALLSASWKAIPATPTSDAWVYAVSVWAGLI
THIQDLRDMEGDKAVGRKTLPLVFGDMGSRLIITFFALPAACWVLSLAGIFQLAPVTLGA
LHAILGYRVLRQGGPRYDHKTYMFYTYIFCLILAFCALDGLGLKINAESLRALLATTGVSL
KEL

Key active-site residues of EriG

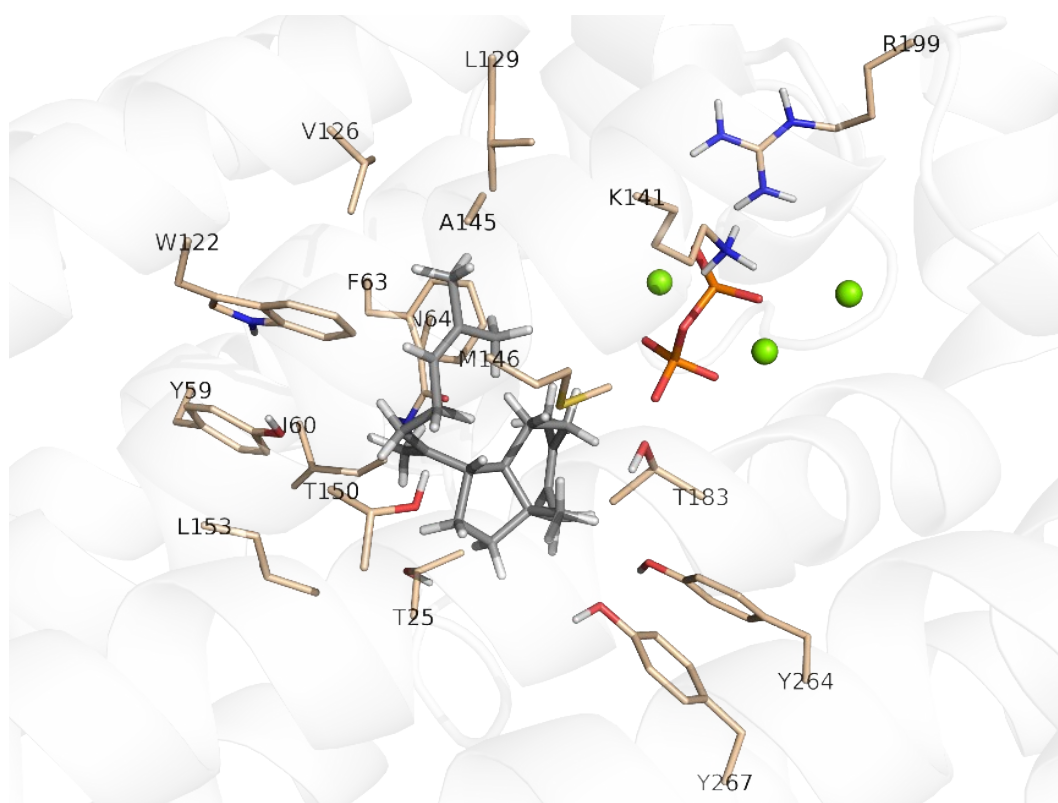


Figure S1. Key residues located within the active site of EriG.

Ligand RMSD curves for each system

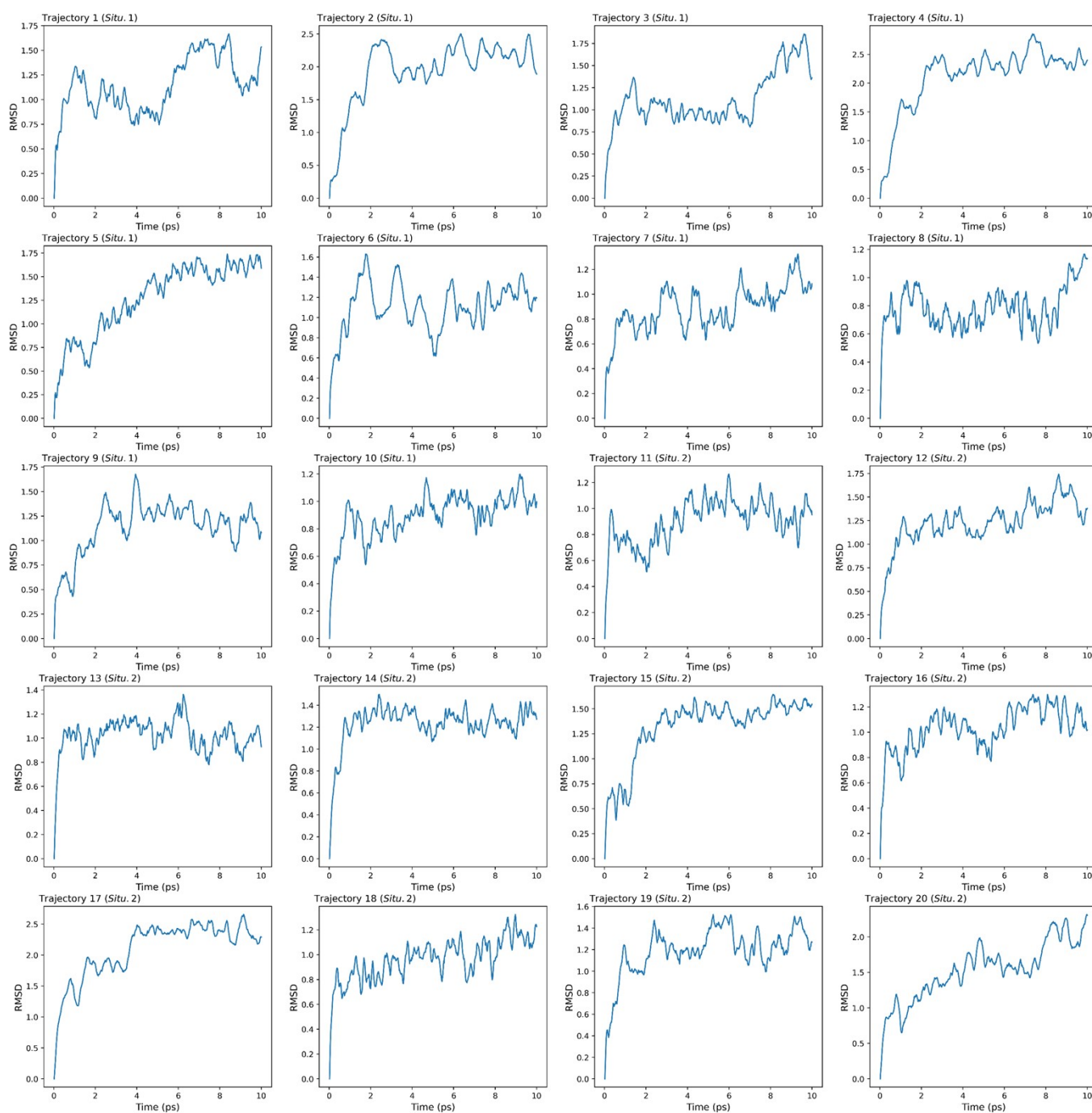


Figure S2. Ligand RMSD curves during the QM/MM simulations for *Situ. 1* and *Situ. 2*.

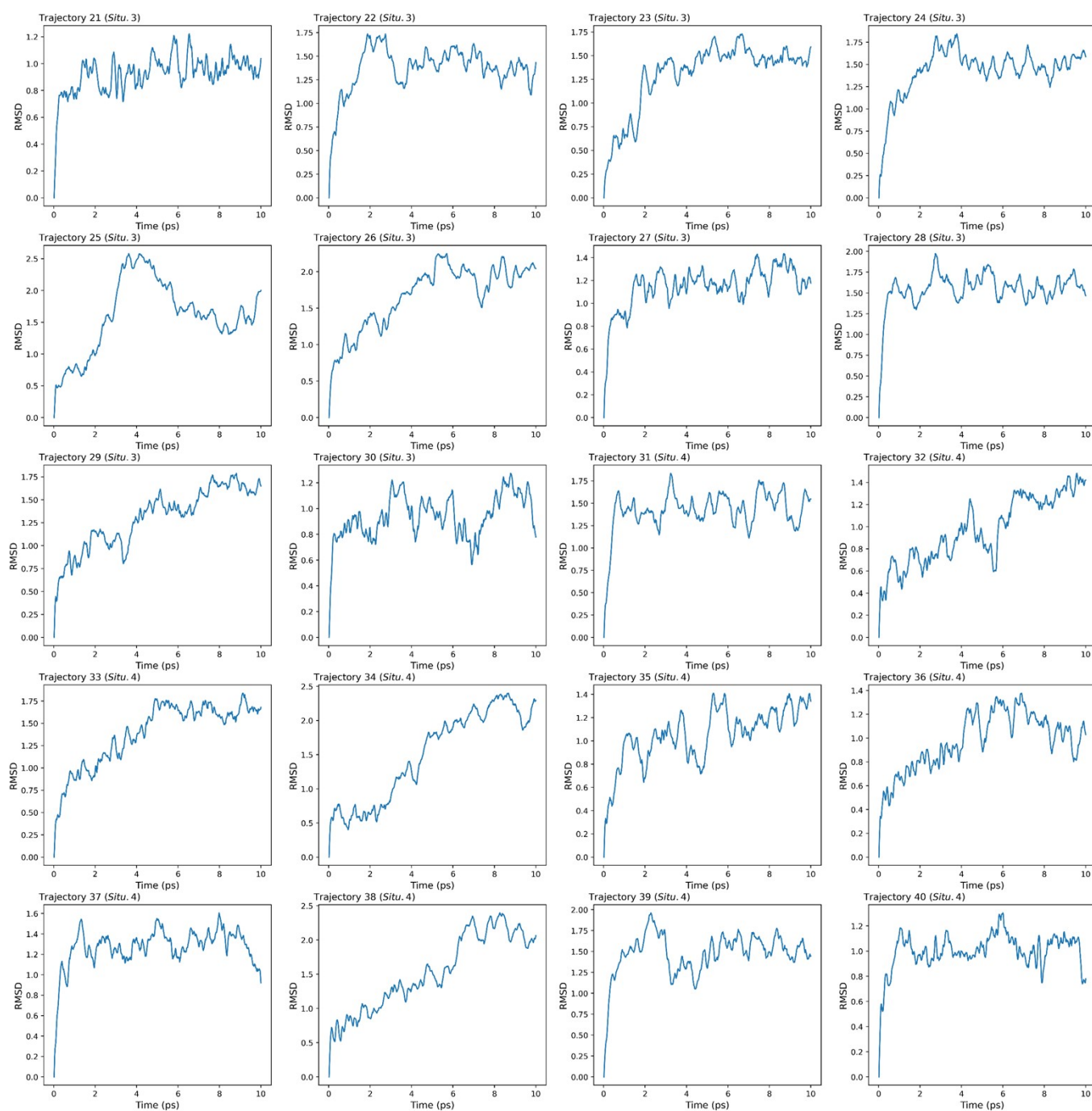
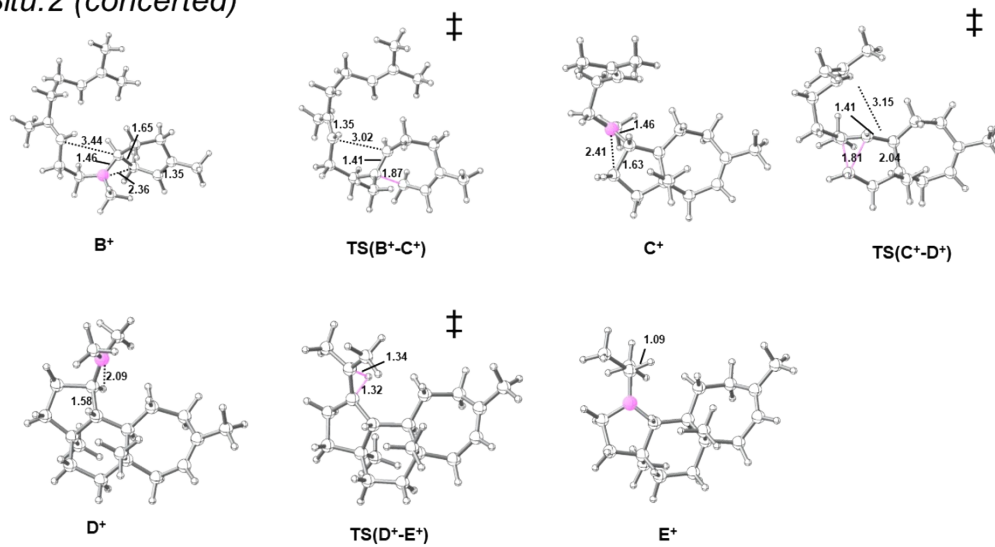


Figure S3. Ligand RMSD curves during the QM/MM simulations for *Situ. 3* and *Situ. 4*.

DFT Calculations

Optimized geometry structures

Situ.2 (concerted)



Situ.4 (stepwise)

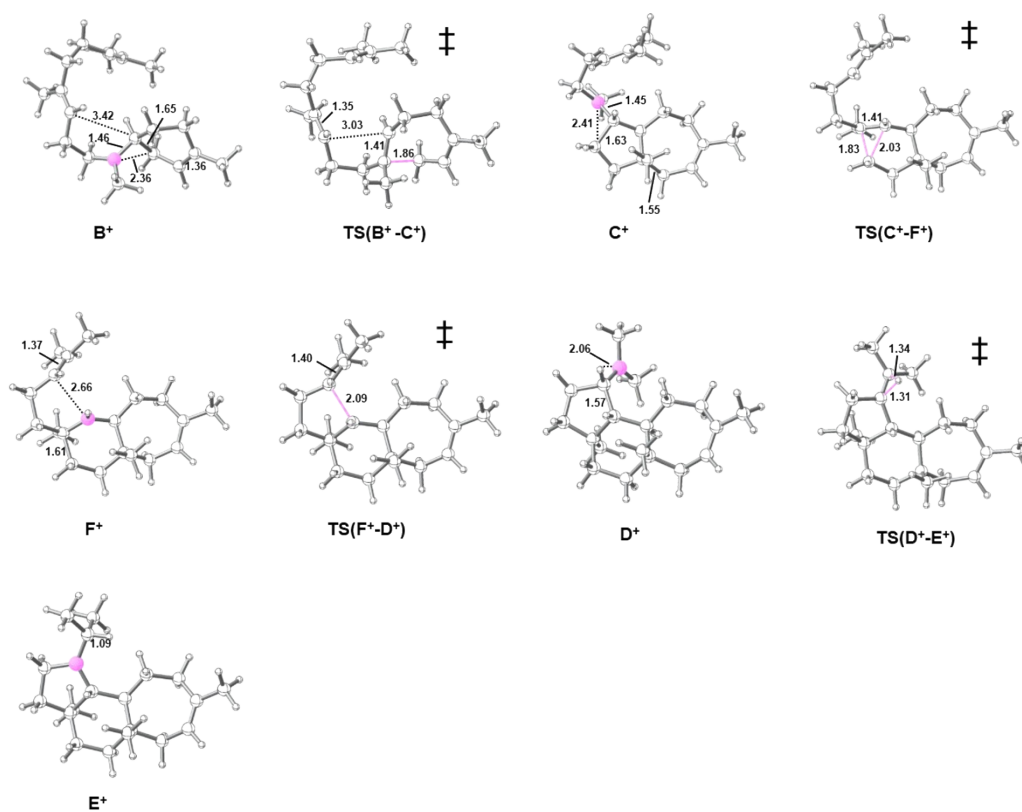


Figure S4. Representative structures for pathways in *Situ. 2* and *Situ. 4*.

Natural bond orbital (NBO) analysis

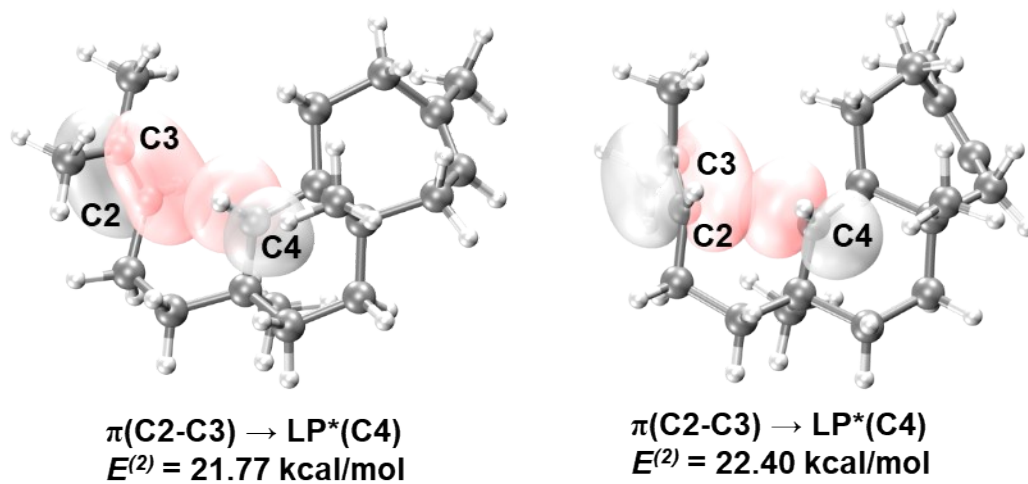


Figure S5. NBO analysis of the stable intermediate F^+ in the H-up conformation vs. the unstable shoulder-peak structures in the H-down conformation in boat-like conformations.

Assessment of dispersion correction effects

Given that hydrogen-hydrogen repulsions are related to dispersion interactions, we compared the optimized structures involved in the key steps featuring potential H3–H4 repulsion (i.e., C⁺, F⁺, D⁺, and the transition states connecting them) using both standard B3LYP/6-31+G(d,p) and dispersion-corrected B3LYP-D3/6-31+G(d,p) functionals. To quantify the geometric influence of dispersion corrections, we analyzed (1) the root-mean-square deviation (RMSD) and (2) the H3–H4 distance differences between the two sets of structures. As shown in Table S1 and S2, no significant differences were observed between the two methods: all RMSD values were below 0.1 Å, and the differences in H3–H4 distances were within 0.2 Å, indicating that the inclusion of dispersion corrections has a negligible effect on the optimized geometries.

Table S1. Comparative geometric parameters between **B3LYP/6-31+G(d,p)** and **B3LYP-D3/6-31+G(d,p)** optimized structures for *Situ. 3*.

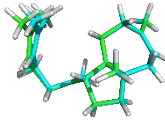
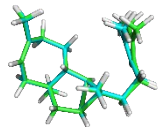
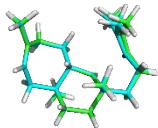
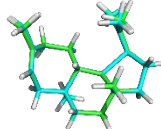
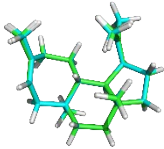
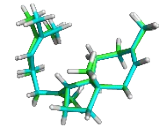
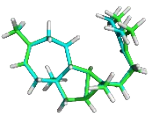
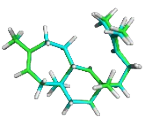
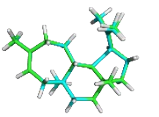
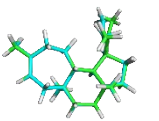
	RMSD	H3-H4 distance (B3LYP/B3LYP-D3)	Structure superposition
C ⁺	0.034	2.93/2.73	
TS(C ⁺ -F ⁺)	0.038	2.71/2.74	
<i>Situ. 3</i> F ⁺	0.048	2.27/2.25	
TS(F ⁺ -D ⁺)	0.030	2.10/2.12	
D ⁺	0.020	2.12/2.13	

Table S2. Comparative geometric parameters between **B3LYP/6-31+G(d,p)** and **B3LYP-D3/6-31+G(d,p)** optimized structures for *Situ. 4*.

		RMSD	H3-H4 distance (B3LYP/B3LYP-D3)	Structure superposition
	C ⁺	0.076	2.91/2.71	
	TS(C ⁺ -F ⁺)	0.051	2.71/2.77	
<i>Situ. 4</i>	F ⁺	0.040	2.29/2.27	
	TS(F ⁺ -D ⁺)	0.019	2.10/2.12	
	D ⁺	0.055	2.16/2.13	

Single-point energy calculations at the mPW1PW91/6-31+G(d,p) level were performed on the optimized structures. As shown in Table S3, the relative energies exhibit only minor differences between B3LYP- and B3LYP-D3-optimized geometries, confirming that the mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p) methodology used in this study is appropriate.

Table S3. Relative energies (kcal/mol) computed at the mPW1PW91/6-31+G(d,p) level for structures optimized with **B3LYP/6-31+G(d,p)** and **B3LYP-D3/6-31+G(d,p)**.

	Functional	Barrier (TS _{C-F} - C ⁺)	Barrier (TS _{D-F} - D ⁺)	ΔE [F ⁺ - C ⁺]	ΔE [D ⁺ - F ⁺]
<i>Situ. 3</i>	B3LYP	5.27	-1.06	1.53	-7.03
	B3LYP-D3	5.30	-1.04	0.83	-6.92
<i>Situ. 4</i>	B3LYP	5.16	-0.92	1.79	-7.63
	B3LYP-D3	5.19	-0.97	1.10	-7.5

Energy profiles

Table S4. Single-point electronic energies (Hartree) calculated at the mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p) level of theory.

mPW1PW91/6-31+G(d,p)		
<i>Situ.1</i>	B ⁺	-781.5769070
	TS(B ⁺ -C ⁺)	-781.5548245
	C ⁺	-781.5986661
	TS(C ⁺ -D ⁺)	-781.5884948
	D ⁺	-781.6165573
	TS(D ⁺ -E ⁺)	-781.5926090
<i>Situ.2</i>	E ⁺	-781.6178537
	B ⁺	-781.5812079
	TS(B ⁺ -C ⁺)	-781.5685568
	C ⁺	-781.6030192
	TS(C ⁺ -D ⁺)	-781.5930162
	D ⁺	-781.6216070
<i>Situ.3</i>	TS(D ⁺ -E ⁺)	-781.5961912
	E ⁺	-781.6113830
	B ⁺	-781.5776711
	TS(B ⁺ -C ⁺)	-781.5550047
	C ⁺	-781.597994
	TS(C ⁺ -F ⁺)	-781.5895898
<i>Situ.4</i>	F ⁺	-781.5955559
	TS(F ⁺ -D ⁺)	-781.5972528
	D ⁺	-781.6067608
	TS(D ⁺ -E ⁺)	-781.5956142
	E ⁺	-781.6178537
	B ⁺	-781.5819291
<i>Situ.4</i>	TS(B ⁺ -C ⁺)	-781.5691645
	C ⁺	-781.6023601
	TS(C ⁺ -F ⁺)	-781.5940898
	F ⁺	-781.5995061
	TS(F ⁺ -D ⁺)	-781.6009780
	D ⁺	-781.6116738
<i>Situ.4</i>	TS(D ⁺ -E ⁺)	-781.6006132
	E ⁺	-781.6206958

XYZ coordinates of optimized geometries

Situ.1

Situ.1 B⁺

C	1.40107700	-2.13534900	-0.62538000
C	2.62432000	-1.70526300	-0.24220100
C	0.61755400	-3.25894700	-0.03391900
C	-0.60919100	-2.80877600	0.92848900
C	-1.65311500	-2.17428500	0.12766500
C	-1.71248600	-0.72175600	0.03319500
C	-2.74327500	-0.31663400	1.23449000
C	-2.90992500	1.17313900	1.19685500
C	-3.23752600	1.77965600	0.04247300
C	-3.36437100	0.89575700	-1.17843200
C	-2.17407400	-0.08884300	-1.31036500
C	2.67212800	1.38054700	0.43841100
C	3.78665400	0.62105600	-0.23072800
C	3.32214900	-0.62158800	-1.03713500
C	2.29722300	2.65759700	0.23720700
C	2.93032700	3.60118000	-0.75676300
C	1.18685900	3.27504500	1.05590700
C	-3.47950800	3.25392900	-0.09301200
C	3.40188700	-2.26907700	0.91990000
C	-2.63560200	-3.03134000	-0.57661400
H	0.95009400	-1.64357700	-1.48742400
H	2.13131200	0.82404200	1.20680000
H	-0.75468100	-0.30246100	0.35409100
H	1.22652700	-3.88968800	0.61596300
H	0.19973800	-3.90626300	-0.81180500
H	-0.96939600	-3.72473700	1.40466000
H	-0.18820300	-2.12777600	1.67092100
H	-3.69212100	-0.83234900	1.04681500
H	-2.35183000	-0.66266000	2.19321500

H	-2.74222000	1.73000400	2.11502100
H	-4.30280300	0.32531400	-1.11191100
H	-3.43567800	1.49258300	-2.09236600
H	-1.31067300	0.45009600	-1.71244000
H	-2.42421400	-0.85658900	-2.04830800
H	4.34265600	1.26442500	-0.91725400
H	4.51294600	0.30181100	0.52904900
H	4.21492900	-1.06964800	-1.49731000
H	2.67412100	-0.29398000	-1.85724800
H	3.38674900	4.45331300	-0.23697600
H	3.70058900	3.13595000	-1.37380900
H	2.16912200	4.01990900	-1.42741400
H	0.38181500	3.65242500	0.41151000
H	1.55710300	4.13770500	1.62468200
H	0.75626200	2.56345400	1.76710700
H	-4.49305300	3.44575500	-0.46689700
H	-3.36221200	3.77548900	0.86009400
H	-2.78885200	3.69860700	-0.82084100
H	2.92432000	-3.12565700	1.39876700
H	4.39979100	-2.58287300	0.59083600
H	3.55747000	-1.50388600	1.68921200
H	-2.19316900	-3.31312800	-1.54775000
H	-2.83620000	-3.96278800	-0.04185400
H	-3.56686400	-2.50912200	-0.80739900

Situ.1 TS(B⁺-C⁺)

C	0.43029535	-2.57314748	-0.47175411
C	1.58426935	-2.33881148	0.19899889
C	-0.79768065	-3.29279748	0.03251989
C	-1.89223765	-2.34914148	0.61072489
C	-2.15367365	-1.17997348	-0.33237811
C	-1.17603465	-0.16706848	-0.30896611
C	-3.25339265	0.03991852	0.54007989

C	-2.85117065	1.33514652	1.15557789
C	-2.33251765	2.35514652	0.43921789
C	-2.01755865	2.11864652	-1.01734911
C	-0.97612665	0.94163152	-1.26866011
C	2.76573435	0.63312252	0.45926889
C	3.55592635	-0.62085548	0.19005789
C	2.77725535	-1.75131848	-0.52854311
C	2.96874835	1.86542552	-0.04465911
C	4.03652935	2.22654152	-1.04894911
C	2.13226335	3.03743252	0.41580889
C	-2.01871865	3.69783352	1.03367389
C	1.80963235	-2.73640848	1.63534389
C	-2.86139865	-1.54123248	-1.62813111
H	0.41414635	-2.29588348	-1.52673011
H	1.96918435	0.52912452	1.20008589
H	-0.61522965	-0.09197748	0.61852289
H	-0.54470965	-4.01375548	0.81529389
H	-1.22656765	-3.87874548	-0.78770011
H	-2.81613665	-2.91229148	0.78125389
H	-1.55567965	-1.96650748	1.58082389
H	-3.93207565	0.17932452	-0.30054011
H	-3.65777465	-0.65794248	1.27034489
H	-3.01740165	1.43948952	2.22444489
H	-2.93650765	1.85588852	-1.55576111
H	-1.61265965	3.01416252	-1.49322311
H	0.03617735	1.32920452	-1.12871411
H	-1.08866465	0.61142652	-2.30436411
H	4.43792135	-0.39868548	-0.41578511
H	3.94351935	-1.00513548	1.14299789
H	3.48632835	-2.57674748	-0.69431211
H	2.46711335	-1.40586548	-1.52108011
H	4.74742435	2.93868252	-0.61086111
H	4.60378035	1.36843152	-1.41207011

H	3.59308435	2.72829752	-1.91846111
H	1.63306735	3.52937252	-0.43062811
H	2.76365735	3.80423652	0.88245589
H	1.37587135	2.73937152	1.14893589
H	-2.58733965	4.48447152	0.52238189
H	-2.26242365	3.73831852	2.09790089
H	-0.95781265	3.94678852	0.90885489
H	0.97002535	-3.28230548	2.06882389
H	2.70280335	-3.36776148	1.71926289
H	1.99733435	-1.85746848	2.26368789
H	-2.24678965	-2.24443248	-2.19889011
H	-3.81500465	-2.03477048	-1.41907511
H	-3.05553265	-0.67534448	-2.26470411

Situ.1 C⁺

C	0.21546700	-0.99961200	-0.06789100
C	0.93457600	-1.30695800	1.15835600
C	-0.23680900	-2.48256600	-0.58315500
C	-1.72004800	-2.29278900	-0.97205800
C	-1.93153300	-0.78235700	-1.22186000
C	-1.10110900	-0.19810400	-0.03869300
C	-3.44857600	-0.37705000	-1.16333800
C	-3.94128200	0.25203600	0.12439500
C	-3.44111200	1.39949600	0.61818700
C	-2.28917200	2.08208600	-0.10203400
C	-0.93565500	1.32678900	0.02005800
C	3.15408000	0.84331000	0.48228200
C	3.19863700	-0.25162900	1.49843800
C	2.36895400	-1.58467800	1.10299600
C	4.09883000	1.12249400	-0.44208100
C	5.36500000	0.33069900	-0.64627600
C	3.94683100	2.31287900	-1.35480500
C	-3.97169400	2.05389500	1.86702500

C	0.25059400	-1.33436400	2.47288500
C	-1.36286000	-0.39315000	-2.60215700
H	0.92127300	-0.61299000	-0.81062400
H	2.28547000	1.49954500	0.52479000
H	-1.65234300	-0.49087300	0.86117500
H	-0.11169200	-3.26358900	0.17301800
H	0.41091900	-2.74249600	-1.42232000
H	-1.96171100	-2.90556100	-1.84777400
H	-2.36698200	-2.62583700	-0.15279800
H	-3.63940500	0.32836700	-1.98309800
H	-4.05280700	-1.26001000	-1.39710000
H	-4.76630500	-0.23376600	0.64200100
H	-2.54051400	2.17276000	-1.16633800
H	-2.15565500	3.10386800	0.26705500
H	-0.45722100	1.59488200	0.97242900
H	-0.26066700	1.67532800	-0.77097600
H	4.21257300	-0.62519900	1.65333300
H	2.83429300	0.09486400	2.47044600
H	2.64810900	-2.34381500	1.83939300
H	2.69550100	-1.87747400	0.10325500
H	6.24066700	0.96521400	-0.46187800
H	5.45033300	-0.55036500	-0.00728200
H	5.43981800	-0.00018200	-1.68922400
H	3.96881500	2.00289100	-2.40703300
H	4.78425900	3.00844200	-1.21950400
H	3.01796300	2.85928500	-1.17271400
H	-4.36544200	3.05375000	1.64347400
H	-4.77455500	1.46871000	2.32370200
H	-3.18057400	2.19428500	2.61609100
H	-0.00978400	-0.30068600	2.74905200
H	-0.71001400	-1.85788600	2.40975200
H	0.86226000	-1.76941700	3.26372800
H	-0.33156000	-0.72954300	-2.75656800

H	-1.97011700	-0.84509100	-3.39355900
H	-1.38363700	0.69004800	-2.75554900

***Situ.1* TS(C⁺-D⁺)**

C	0.42995088	-0.54370589	-0.17695157
C	1.03519788	-1.44279489	0.72244843
C	0.07055588	-2.54602589	-0.35121257
C	-1.44150112	-2.37465089	-0.36149557
C	-1.86361712	-0.99204589	-0.91678857
C	-0.94409612	0.00795011	-0.08998157
C	-3.39072912	-0.72140389	-0.65178557
C	-3.74761212	0.18913711	0.50554743
C	-3.36287512	1.47675811	0.56292243
C	-2.47900512	2.03409011	-0.54167857
C	-1.02364612	1.49475511	-0.50811357
C	3.16922188	0.72016211	0.75395043
C	3.44617188	-0.70681689	1.16018143
C	2.50819388	-1.75919389	0.49946843
C	3.76335388	1.41780111	-0.23657157
C	4.82800588	0.86274611	-1.14986057
C	3.41718888	2.86650111	-0.47982557
C	-3.76017512	2.40441411	1.67984043
C	0.55118788	-1.60308089	2.15352343
C	-1.60114012	-0.91864289	-2.43352257
H	1.00182088	-0.31633789	-1.07606357
H	2.44017488	1.25330111	1.36608443
H	-1.29448612	-0.05869389	0.94124943
H	0.40235688	-3.41241489	0.22712843
H	0.53092888	-2.60604489	-1.33724857
H	-1.86129712	-3.18039689	-0.97688157
H	-1.84349012	-2.51424689	0.64761443
H	-3.81817312	-0.29748789	-1.56948657
H	-3.88524912	-1.69008989	-0.52188157

H	-4.37918612	-0.21665189	1.29303843
H	-2.92599412	1.78873911	-1.51327857
H	-2.44082712	3.12645611	-0.49162357
H	-0.43679312	2.07562911	0.21220043
H	-0.55512812	1.64948511	-1.48670657
H	4.46958288	-0.99850989	0.90786243
H	3.37120788	-0.79421789	2.24996943
H	2.73565488	-2.75098089	0.90618843
H	2.71872788	-1.78869289	-0.57550857
H	5.75734588	1.43527811	-1.03974757
H	5.05916088	-0.18868589	-0.96847157
H	4.52690788	0.96814811	-2.19980157
H	3.07661288	3.02473111	-1.51097457
H	4.30390488	3.49905911	-0.34796157
H	2.64177688	3.22646011	0.20196343
H	-4.33617012	3.25334411	1.29001043
H	-4.36987812	1.89787011	2.43271343
H	-2.88007512	2.83021911	2.17971943
H	0.98903088	-0.80617089	2.76296643
H	-0.53127112	-1.54506389	2.26257343
H	0.89179388	-2.55708089	2.56492343
H	-0.57126612	-1.15960789	-2.71702857
H	-2.25557612	-1.62682189	-2.95238657
H	-1.82454512	0.07555111	-2.82923657

Situ.1 D⁺

C	-0.97297700	-0.32859300	0.12189200
C	-1.38884700	-1.63651800	-0.61176900
C	-0.66506800	-2.79954900	0.09441500
C	0.85606300	-2.56428900	0.14098100
C	1.30209900	-1.22203100	0.78940000
C	0.53078900	-0.03264500	0.09100700

C	2.86244000	-1.07572600	0.58439800
C	3.33771500	-0.20672600	-0.55600900
C	3.14958000	1.12544200	-0.56212100
C	2.38940200	1.75250500	0.59211700
C	0.88070800	1.36807800	0.62966700
C	-1.95106000	0.74138100	-0.50601500
C	-3.31300000	-0.11158400	-0.68124200
C	-2.91472500	-1.58897900	-0.42777200
C	-2.26062900	1.91741900	0.28233700
C	-2.65858900	1.83390500	1.70511500
C	-2.29583600	3.25432500	-0.35024900
C	3.64727400	2.02788700	-1.65925000
C	-1.06000300	-1.64368100	-2.12318300
C	1.04133500	-1.27340800	2.31065500
H	-1.28641900	-0.44870600	1.16632600
H	-1.58825600	1.04164800	-1.49118500
H	0.84836600	-0.04377700	-0.95701000
H	-0.87701600	-3.74382100	-0.42100900
H	-1.06141400	-2.90863400	1.11204400
H	1.32688300	-3.38551200	0.69403700
H	1.26545800	-2.61704200	-0.87507800
H	3.28606100	-0.67578800	1.51496200
H	3.28146100	-2.08183700	0.48210200
H	3.87539600	-0.67716500	-1.37695100
H	2.85127700	1.43547500	1.53566800
H	2.47514500	2.84373100	0.56587600
H	0.33419800	2.09917800	0.01384000
H	0.51675000	1.49080600	1.65792900
H	-4.10754100	0.21802600	-0.00633600
H	-3.66496500	0.07143100	-1.69908200
H	-3.45519800	-2.25162100	-1.11176300
H	-3.18353700	-1.88305500	0.59298800
H	-3.50995000	2.49444500	1.90956000

H	-2.86156500	0.82357800	2.05741000
H	-1.82660100	2.24828600	2.29675500
H	-2.16383600	4.07078600	0.36453600
H	-3.31694200	3.36462100	-0.76057200
H	-1.60913700	3.34599300	-1.19401500
H	4.34366600	2.77766100	-1.26186500
H	4.16437000	1.46685100	-2.44239200
H	2.82412900	2.58597500	-2.12653000
H	-1.59364200	-0.86747800	-2.68079200
H	0.00459800	-1.51894100	-2.32988400
H	-1.36382700	-2.60532600	-2.54914200
H	-0.00166500	-1.48038700	2.56936500
H	1.64308200	-2.07179000	2.75795200
H	1.33063800	-0.34088900	2.80600000

***Situ. I* TS(D⁺-E⁺)**

C	0.95850109	0.37652166	0.23089486
C	1.04997309	1.74222366	-0.54014714
C	0.27131909	2.77490966	0.29091786
C	-1.18447891	2.32149166	0.52543686
C	-1.37489091	0.86928766	1.05977486
C	-0.52013591	-0.13466834	0.19158586
C	-2.89910891	0.51773966	0.94373186
C	-3.35575891	0.01652666	-0.40428214
C	-3.05040391	-1.22101734	-0.83046314
C	-2.23649791	-2.12851834	0.07893586
C	-0.79815891	-1.62854734	0.45589486
C	2.21926309	-0.37782834	-0.22507214
C	3.10246109	0.56366466	-1.04590714
C	2.57141609	1.95357366	-0.62410214
C	2.74273909	-1.59687334	0.27047286
C	2.15935009	-2.35691534	1.43027786
C	4.07219409	-2.12256534	-0.22584514

C	-3.50618991	-1.77689334	-2.15360114
C	0.49314109	1.68499366	-1.98657314
C	-1.01056791	0.81445866	2.55913686
H	1.20965209	0.59760766	1.28090386
H	1.92313309	-1.52897534	-0.79055414
H	-0.84488991	0.01456166	-0.83943214
H	0.27283309	3.74988766	-0.21105814
H	0.78463409	2.92195966	1.25050786
H	-1.66202291	3.01176266	1.23049786
H	-1.74613791	2.42058566	-0.41030814
H	-3.13249091	-0.24229434	1.70134386
H	-3.46815891	1.40783766	1.23266086
H	-3.95542791	0.67240466	-1.03231414
H	-2.80208791	-2.27479634	1.00786386
H	-2.14767791	-3.12244734	-0.37047414
H	-0.08611491	-2.21406834	-0.14211914
H	-0.61620391	-1.89612334	1.50038186
H	4.16096809	0.41883266	-0.82321814
H	2.96809009	0.41419166	-2.12165014
H	2.86734609	2.72879266	-1.33555514
H	2.98193909	2.22610466	0.35619886
H	2.98787909	-2.51926634	2.13001286
H	1.36692809	-1.82064634	1.94390086
H	1.80293409	-3.34838234	1.13624086
H	4.09639709	-3.21336834	-0.16584414
H	4.85779909	-1.74138134	0.43911686
H	4.31267109	-1.81603734	-1.24391314
H	-4.12341591	-2.67310734	-2.00918214
H	-4.09516891	-1.04848334	-2.71761014
H	-2.65436291	-2.08397234	-2.77560114
H	0.84449709	0.81508466	-2.55213614
H	-0.59579891	1.66696766	-2.02740514
H	0.81880109	2.57942166	-2.52757514

H	-0.01967891	1.22191966	2.78639086
H	-1.72952691	1.40963266	3.13187286
H	-1.05488891	-0.20580934	2.95534986

Situ. I E⁺

C	-0.92798600	-0.37442100	0.15855700
C	-1.27955500	-1.67340100	-0.65542400
C	-0.42992700	-2.84141800	-0.13341600
C	1.06113800	-2.48534900	-0.06348700
C	1.40169300	-1.20101400	0.74311000
C	0.57635900	0.01287800	0.16030200
C	2.95165500	-0.96590600	0.58825700
C	3.39161600	-0.05100900	-0.52933000
C	3.16612100	1.27316200	-0.47114600
C	2.40950900	1.81124400	0.72950400
C	0.90959500	1.39889500	0.76128600
C	-2.12845500	0.46236500	0.12427100
C	-3.29289000	-0.36809800	-0.29160400
C	-2.78923700	-1.81882000	-0.37064100
C	-2.28704800	1.89406400	0.47092900
C	-3.60346500	2.25876100	1.18059800
C	-2.16313300	2.66276000	-0.89485000
C	3.62475600	2.24556300	-1.52404400
C	-1.04853500	-1.44926100	-2.16723200
C	1.11428600	-1.41938700	2.24314100
H	-1.19757200	-0.64603700	1.23296900
H	-1.44434100	2.20619700	1.08778200
H	0.85055700	0.07326200	-0.89909600
H	-0.57381800	-3.71805400	-0.77565700
H	-0.79025500	-3.13052000	0.86206500
H	1.60308100	-3.32623200	0.38366700
H	1.46469800	-2.37544000	-1.07772200
H	3.33336400	-0.56437600	1.53552200

H	3.42415600	-1.94683700	0.47694400
H	3.93108100	-0.47561900	-1.37354000
H	2.89805400	1.46184000	1.64708300
H	2.45957600	2.90437400	0.75992500
H	0.36638300	2.14766100	0.17793600
H	0.55018900	1.47807000	1.79501800
H	-4.17588100	-0.20109100	0.33230200
H	-3.57234800	0.01451700	-1.28972000
H	-3.31599600	-2.40241100	-1.12878200
H	-2.94976500	-2.31190600	0.59592800
H	-4.47753800	2.10434300	0.54210800
H	-3.73703700	1.68682600	2.10395100
H	-3.57564600	3.31799100	1.44969600
H	-2.14389700	3.73090400	-0.66303300
H	-3.02691100	2.46459000	-1.53449300
H	-1.25017800	2.41534200	-1.44168100
H	4.31441900	2.98445900	-1.09599000
H	4.13806900	1.73996100	-2.34647300
H	2.78331100	2.81369300	-1.94321500
H	-1.60844400	-0.59125500	-2.55670400
H	0.00284800	-1.28897600	-2.41288400
H	-1.38141600	-2.33481700	-2.71737600
H	0.07731300	-1.70435500	2.45962100
H	1.74244300	-2.22968200	2.62796400
H	1.34251400	-0.52606400	2.83320100

Situ.2

Situ.2 B⁺

C	1.53085600	-2.00578300	-0.74797400
C	2.76617300	-1.64221600	-0.34170200
C	0.69417200	-3.12234400	-0.20834500
C	-0.45046900	-2.66424400	0.83169900

C	-1.46270400	-1.87999300	0.11894700
C	-1.39199100	-0.42548200	0.12623700
C	-2.40349000	-0.13282600	1.39532200
C	-3.75784900	0.31648400	0.96377900
C	-3.91088900	1.19420500	-0.04870500
C	-2.67422000	1.59674700	-0.81931600
C	-1.81708900	0.35250200	-1.13873800
C	2.81566600	1.38173300	0.52378200
C	3.94313600	0.66678900	-0.17322400
C	3.49675000	-0.52704100	-1.06044900
C	2.40339800	2.65194400	0.35477900
C	1.28643400	3.22119000	1.19975900
C	2.99948400	3.63403600	-0.62464900
C	-5.23670400	1.75988300	-0.46203800
C	3.52281300	-2.30340600	0.78304000
C	-2.55785900	-2.57828500	-0.59023100
H	1.09853800	-1.45039600	-1.58049300
H	2.29980400	0.79404300	1.28618200
H	-0.40205600	-0.10601900	0.45989800
H	1.28512500	-3.84158500	0.36238200
H	0.20892500	-3.67864300	-1.01691300
H	-0.87806700	-3.58001000	1.24936900
H	0.04591500	-2.08257900	1.61171000
H	-2.46397700	-0.98701200	2.07785600
H	-1.86034400	0.64602900	1.94297900
H	-4.61651300	-0.05070800	1.52026300
H	-2.94327400	2.10115300	-1.75211200
H	-2.08140200	2.31631000	-0.23659400
H	-0.90910300	0.64398100	-1.67582300
H	-2.39311800	-0.28574600	-1.81412700
H	4.50831400	1.35249200	-0.80960200
H	4.65649000	0.30514000	0.57948300
H	4.39950900	-0.95443200	-1.52005400

H	2.87329600	-0.14913700	-1.87804700
H	0.46279300	3.59093300	0.57377000
H	0.88797500	2.48396700	1.90446200
H	1.63807600	4.08247200	1.78203000
H	3.43786100	4.48738400	-0.09154000
H	2.22060900	4.04566300	-1.27931700
H	3.77535000	3.20232300	-1.25870200
H	-6.05431400	1.38766600	0.16007000
H	-5.22227200	2.85492300	-0.39243400
H	-5.45627600	1.51946400	-1.51022400
H	3.69676100	-1.59754000	1.60369400
H	3.01797700	-3.17641400	1.20072600
H	4.51271200	-2.62355900	0.43650000
H	-2.68966000	-3.60936500	-0.25918900
H	-3.49688100	-2.01519600	-0.49993800
H	-2.33247700	-2.58895800	-1.66810600

***Situ.2* TS(B⁺-C⁺)**

C	1.23480755	-2.20431269	-0.71704840
C	2.42859155	-1.83669869	-0.20212040
C	0.27535155	-3.23845369	-0.18267840
C	-0.88122845	-2.64934369	0.67722560
C	-1.60936645	-1.52375969	-0.04888740
C	-0.97419245	-0.26674669	-0.02410340
C	-2.71641045	-0.70303869	1.20930760
C	-3.79208745	0.12779231	0.64873260
C	-3.60578445	1.36103331	0.12405860
C	-2.21710945	1.92320531	-0.02258340
C	-1.27958345	0.93427331	-0.82623540
C	2.77922555	1.23280231	0.50479160
C	3.83688955	0.35414831	-0.11101440
C	3.29819255	-0.83917369	-0.94194840
C	2.52646155	2.53205531	0.25638260

C	1.48146355	3.28403031	1.04962960
C	3.25552055	3.37712231	-0.76053140
C	-4.74329945	2.17455331	-0.42363840
C	3.01945755	-2.42108169	1.05693460
C	-2.46843845	-1.95452169	-1.22339540
H	0.94740255	-1.74373269	-1.66379040
H	2.18876255	0.75851131	1.29250960
H	-0.21798145	-0.13102169	0.74694760
H	0.78870155	-3.97648269	0.43990560
H	-0.15420545	-3.79901369	-1.02090140
H	-1.58940245	-3.44653069	0.92881460
H	-0.46332245	-2.27080269	1.61726760
H	-3.05745245	-1.66758669	1.58602160
H	-2.09926545	-0.23548469	1.97725360
H	-4.78588345	-0.31255469	0.63160060
H	-2.23970645	2.86776531	-0.57114340
H	-1.75437445	2.12921031	0.94958460
H	-0.33247145	1.45420731	-1.00721240
H	-1.74325045	0.69621931	-1.78504240
H	4.49501155	0.93584931	-0.76147140
H	4.48086955	-0.03243769	0.69029460
H	4.17051555	-1.38394069	-1.33234840
H	2.75406455	-0.45582369	-1.81250340
H	0.72343155	3.73212731	0.39219860
H	0.97968855	2.64328831	1.78243060
H	1.93679055	4.11848831	1.59802660
H	3.80134855	4.18843231	-0.26209140
H	2.54446155	3.85847131	-1.44419540
H	3.97001855	2.81481631	-1.36329140
H	-5.70398945	1.66833531	-0.30517040
H	-4.79882245	3.14426031	0.08609260
H	-4.59230745	2.39143531	-1.48914240
H	3.13415455	-1.65504269	1.83328560

H	2.42361355	-3.23261769	1.47833360
H	4.02566655	-2.81033569	0.85909860
H	-3.13244745	-2.77264869	-0.93129540
H	-3.07631845	-1.14581569	-1.62854940
H	-1.81895245	-2.32748269	-2.02205940

Situ.2 C⁺

C	0.34858900	-1.11145500	-0.15335300
C	1.29968600	-1.63951600	0.81317900
C	0.01400200	-2.41408600	-1.07512500
C	-1.52394600	-2.36619900	-1.22596400
C	-1.95841300	-0.91367100	-0.92959700
C	-1.03801900	-0.59261400	0.28694500
C	-3.45488300	-0.83629200	-0.53911100
C	-4.00993800	0.55613900	-0.32389700
C	-3.55979000	1.47992100	0.54176600
C	-2.38236400	1.25068400	1.47980200
C	-1.04423000	0.84457900	0.82345400
C	3.10176600	0.95344300	0.52263100
C	3.44239100	-0.35560000	1.15703900
C	2.72445200	-1.64727400	0.48933800
C	3.83132400	1.61160500	-0.40502900
C	3.39563700	2.96770100	-0.89878300
C	5.11496000	1.10369400	-1.00972900
C	-4.23297700	2.82522100	0.66877800
C	0.86147900	-2.16142700	2.12916700
C	-1.68080300	-0.02482700	-2.15990200
H	0.86266400	-0.39445900	-0.80296400
H	2.19160400	1.43505100	0.87781900
H	-1.39724800	-1.24015000	1.10033100
H	0.34835900	-3.35660100	-0.63093700
H	0.55352300	-2.29388000	-2.01629900
H	-1.81518600	-2.70042000	-2.22765800

H	-1.99095000	-3.04923200	-0.50704900
H	-4.03756900	-1.32408500	-1.32871400
H	-3.60660600	-1.44779400	0.36452700
H	-4.86969300	0.82081900	-0.93638900
H	-2.20926500	2.16773600	2.05254500
H	-2.65317900	0.48417800	2.22284900
H	-0.25832100	0.94287700	1.58594800
H	-0.78668500	1.55228800	0.02652000
H	4.50485200	-0.58986200	1.06762000
H	3.20487300	-0.35285100	2.22510300
H	3.21869000	-2.52307600	0.91933000
H	2.90636100	-1.58895100	-0.58541600
H	3.26295100	2.96200400	-1.98785400
H	2.46172400	3.29720200	-0.43655500
H	4.16634200	3.71848800	-0.68488100
H	5.03321900	1.07759000	-2.10313900
H	5.40675900	0.10788600	-0.67049300
H	5.93819800	1.79132200	-0.77991600
H	-5.08155400	2.92330900	-0.01300500
H	-4.59870700	2.98340000	1.69183800
H	-3.52907600	3.64173900	0.45957300
H	-0.00637000	-2.82251200	2.02044000
H	1.65501200	-2.67744000	2.67024400
H	0.49915700	-1.31834700	2.73746500
H	-2.32209600	-0.33878500	-2.99034600
H	-1.90024100	1.02572400	-1.95983200
H	-0.64508800	-0.09334000	-2.51035200

***Situ.2* TS(C⁺-D⁺)**

C	-0.53995823	-0.56075430	0.09691055
C	-1.37939523	-1.55750830	-0.43718845
C	-0.32900223	-2.49856430	0.70349055
C	1.16576277	-2.52964030	0.41901055

C	1.80304677	-1.12349630	0.53859555
C	0.83613877	-0.21976830	-0.34310345
C	3.22475477	-1.12491630	-0.07813145
C	4.04152577	0.13820170	0.09603155
C	3.71001377	1.37716870	-0.30262745
C	2.40642377	1.71200570	-1.01451645
C	1.10168977	1.30255470	-0.30153645
C	-3.28038323	0.79917270	-0.67081645
C	-3.75643123	-0.63305530	-0.64712945
C	-2.80540823	-1.61740630	0.09481155
C	-3.59970023	1.78079870	0.19832855
C	-3.08823723	3.18699470	0.00160555
C	-4.50167423	1.59986670	1.39386055
C	4.64909277	2.54076170	-0.09843845
C	-1.19317123	-2.10321330	-1.84276945
C	1.86128577	-0.68910430	2.01559755
H	-0.90672923	-0.06011030	0.99224055
H	-2.64753823	1.07344170	-1.51619645
H	0.97547077	-0.55120530	-1.37803045
H	-0.84027923	-3.42435330	0.42630655
H	-0.59229823	-2.26785330	1.73571455
H	1.62364577	-3.22177830	1.13649055
H	1.35127977	-2.94905330	-0.57585045
H	3.77517277	-1.95664530	0.37712055
H	3.13756777	-1.37657730	-1.14650045
H	5.00651577	0.00759070	0.58126155
H	2.36317377	2.79391570	-1.17562945
H	2.41437277	1.26618070	-2.02109945
H	0.27091277	1.80804370	-0.80764245
H	1.10219877	1.66343070	0.73274855
H	-4.73320023	-0.71725930	-0.16232945
H	-3.90266223	-0.98272830	-1.67529545
H	-3.19178623	-2.63781930	-0.00654845

H	-2.80899323	-1.36939630	1.16216255
H	-2.53331223	3.53378070	0.88256755
H	-2.43952123	3.27233870	-0.87455745
H	-3.92555523	3.88386770	-0.12887045
H	-3.98719523	1.90579670	2.31357255
H	-4.85402923	0.57532970	1.52828655
H	-5.38151923	2.24925670	1.30580355
H	5.57746777	2.23624470	0.39105055
H	4.90699477	3.00463770	-1.05936845
H	4.18043877	3.32492670	0.51052155
H	-0.15057223	-2.21488130	-2.13853645
H	-1.68737023	-3.07340530	-1.94183045
H	-1.66789923	-1.41731430	-2.55151645
H	2.49976377	-1.38321130	2.57228355
H	2.29676677	0.30498470	2.12467255
H	0.88264677	-0.68184130	2.50659355

Situ.2 D⁺

C	-1.08242400	-0.21218200	0.11612200
C	-1.85685300	-1.52017700	-0.21582700
C	-1.10906000	-2.67634600	0.47519800
C	0.37417800	-2.70332300	0.06468600
C	1.15801800	-1.38118200	0.30934000
C	0.37545500	-0.18174100	-0.36709700
C	2.54896800	-1.54894600	-0.38167400
C	3.62360400	-0.54224100	-0.04205400
C	3.57388700	0.77572700	-0.29438300
C	2.36237100	1.41553900	-0.94870300
C	1.03287500	1.19995200	-0.19225700
C	-2.05686700	0.90766800	-0.40961100
C	-3.50501600	0.29533500	-0.03625300
C	-3.24086600	-1.18063300	0.36351000
C	-1.96306600	2.22508100	0.19098200

C	-2.05621600	3.43934200	-0.65003900
C	-1.89575000	2.42200900	1.65647100
C	4.71308200	1.70087200	0.05131100
C	-1.99690200	-1.80362200	-1.72994100
C	1.36349000	-1.18446600	1.82654600
H	-1.08075200	-0.12932800	1.21003900
H	-1.97701000	0.99185000	-1.49546000
H	0.37254800	-0.38853000	-1.44693000
H	-1.57874400	-3.63439100	0.22287700
H	-1.19776800	-2.56666500	1.56355000
H	0.88033400	-3.50730400	0.61138100
H	0.45373300	-2.97113700	-0.99612600
H	2.92124300	-2.54558500	-0.12034000
H	2.38486800	-1.56923200	-1.46985700
H	4.51949200	-0.93624400	0.43418700
H	2.53571900	2.49306300	-1.04236800
H	2.24677700	1.03859600	-1.97607500
H	0.32622600	1.95328900	-0.58146600
H	1.17630200	1.43326900	0.87015700
H	-4.00376900	0.84997100	0.76322400
H	-4.12673600	0.39626600	-0.92875400
H	-4.03958900	-1.82714200	-0.01462700
H	-3.22953800	-1.27905700	1.45472700
H	-1.60634900	4.31903400	-0.18211200
H	-1.67908100	3.28903800	-1.66339900
H	-3.13644400	3.65814800	-0.74161700
H	-0.86816600	2.74303200	1.89117800
H	-2.11375700	1.52802000	2.23944300
H	-2.53601200	3.25553100	1.96834200
H	5.54770200	1.16455500	0.51000500
H	5.08783000	2.21073200	-0.84601000
H	4.39061300	2.48874100	0.74557900
H	-1.03564100	-1.89760500	-2.23891100

H	-2.53041400	-2.74960600	-1.86752800
H	-2.57205300	-1.03620900	-2.25766000
H	1.92268700	-2.03565500	2.22977500
H	1.94481800	-0.28794300	2.05249100
H	0.42347900	-1.13149600	2.38430800

***Situ.2* TS(D⁺-E⁺)**

C	1.04204099	-0.25785724	-0.34200738
C	1.78543399	-1.54908524	0.14073462
C	0.89758199	-2.77525924	-0.10305038
C	-0.48118701	-2.58148824	0.54081462
C	-1.26494101	-1.36606324	-0.02041338
C	-0.41239601	-0.04022224	0.13398662
C	-2.56346701	-1.24257724	0.83327762
C	-3.66587801	-0.31256424	0.37278962
C	-3.58164601	0.99046076	0.06185362
C	-2.28402601	1.78328676	0.08641862
C	-1.07215801	1.14247776	-0.61712538
C	2.20370599	0.76463276	-0.21457138
C	3.40608999	0.03034576	-0.84708838
C	3.06362099	-1.48460624	-0.73155638
C	2.26497099	2.14503176	0.12680662
C	1.20742299	2.89442676	0.87784662
C	3.49873799	2.93782776	-0.18142938
C	-4.80968001	1.78608576	-0.31138938
C	2.17808499	-1.48348224	1.63705962
C	-1.64589601	-1.66944724	-1.48946738
H	0.98146399	-0.35394824	-1.43970638
H	2.48329099	0.89005076	0.95256462
H	-0.40129001	0.18587476	1.21138062
H	1.38275799	-3.67194724	0.29962262
H	0.78840499	-2.94278324	-1.18119238
H	-1.08433401	-3.48245524	0.38436462

H	-0.37528901	-2.48078324	1.62844062
H	-2.99326001	-2.24797124	0.90544462
H	-2.26775901	-0.98154324	1.86196062
H	-4.65529501	-0.76469424	0.32901362
H	-2.46892501	2.75605876	-0.38370538
H	-2.02337001	2.00804676	1.13418962
H	-0.33344101	1.92895376	-0.79561138
H	-1.36922001	0.81696576	-1.61798038
H	3.51733899	0.34946876	-1.88907638
H	4.34436199	0.27273476	-0.34237538
H	3.89315999	-2.05258224	-0.30169038
H	2.86184299	-1.90399024	-1.72196038
H	0.82544399	3.68999476	0.22492262
H	0.37561299	2.28304176	1.21357862
H	1.66619199	3.40059576	1.73425362
H	3.62646299	3.78504076	0.49357762
H	3.35235599	3.33456176	-1.19831238
H	4.41122099	2.34256176	-0.21374338
H	-5.71629501	1.17689476	-0.27538438
H	-4.94624001	2.63705776	0.36931862
H	-4.71917101	2.20577376	-1.32211238
H	1.33338499	-1.25366224	2.29164062
H	2.58525999	-2.44954324	1.95133562
H	2.97056099	-0.75125824	1.84719962
H	-2.06370601	-2.67966624	-1.55496138
H	-2.40791101	-0.98595424	-1.86700338
H	-0.79236401	-1.63081424	-2.17419938

Situ.2 E⁺

C	1.14116400	-0.14982600	-0.19059900
C	1.94077500	-1.47321600	0.17798100
C	1.16496400	-2.70250700	-0.30726400
C	-0.28560700	-2.68936100	0.17967000

C	-1.08723100	-1.41680900	-0.20342800
C	-0.33804800	-0.12255700	0.31686500
C	-2.46772500	-1.56758700	0.51724600
C	-3.60702400	-0.67956300	0.07765900
C	-3.62513900	0.65313000	0.21422900
C	-2.43076400	1.38133600	0.80104400
C	-1.09891400	1.18993800	0.03898700
C	2.17965100	0.89916400	-0.22069200
C	3.50433100	0.25244400	-0.41807800
C	3.27240100	-1.25141700	-0.56522600
C	2.19562600	2.39152300	-0.14240400
C	1.81450600	2.89731800	1.27877600
C	1.42534300	3.09532000	-1.29400800
C	-4.80501700	1.49759700	-0.19151800
C	2.19210300	-1.54642400	1.70166200
C	-1.30537700	-1.38368300	-1.73033700
H	1.09354000	-0.18563900	-1.32056900
H	3.24538100	2.67315700	-0.28270900
H	-0.26886200	-0.22188400	1.40953200
H	1.67064300	-3.61056200	0.04185200
H	1.19250000	-2.73904000	-1.40338900
H	-0.80613200	-3.56103600	-0.23173100
H	-0.31408600	-2.81391400	1.26938900
H	-2.77895700	-2.60916700	0.38548400
H	-2.29669900	-1.44744100	1.59830000
H	-4.47507600	-1.17418600	-0.35358900
H	-2.64501600	2.45519500	0.82535900
H	-2.28851700	1.08183300	1.85093400
H	-0.46033900	2.01754500	0.33861300
H	-1.27847500	1.30887400	-1.03603400
H	4.07204000	0.75077300	-1.21563000
H	4.06951100	0.49876000	0.50043400
H	4.09423600	-1.84722000	-0.16165500

H	3.16540600	-1.50977600	-1.62583700
H	0.77892300	2.69769200	1.55178300
H	2.46495400	2.45963300	2.04155500
H	1.97042400	3.97984900	1.29183700
H	1.64225500	4.16483300	-1.22531900
H	0.34806800	2.95614800	-1.23936600
H	1.77658400	2.74821300	-2.27041300
H	-5.61711600	0.89051200	-0.59984600
H	-5.19780500	2.05767200	0.66723900
H	-4.52153600	2.24297600	-0.94672300
H	1.26836300	-1.62960900	2.27673800
H	2.79627700	-2.43124900	1.92488700
H	2.73442500	-0.67482100	2.08536400
H	-1.78456500	-2.31346900	-2.05488400
H	-1.95825900	-0.56328600	-2.03396100
H	-0.37219900	-1.30028200	-2.30103000

Situ.3

Situ.3 B⁺

C	1.27872700	-2.12808700	-0.70133500
C	2.50223400	-1.56106900	-0.60343400
C	0.66243400	-3.09415900	0.25362000
C	-0.39816500	-2.44651700	1.30206600
C	-1.59856000	-2.03228300	0.58250300
C	-1.73036300	-0.65347700	0.12863100
C	-2.54498900	0.06588100	1.34576800
C	-2.76512600	1.49627300	0.95196000
C	-3.30908700	1.78447500	-0.24335300
C	-3.62229600	0.61381300	-1.14858300
C	-2.44644100	-0.39372500	-1.22779800
C	2.42104100	1.58601400	-0.67262200
C	3.50110100	0.73169500	-1.28340600
C	3.01316900	-0.67351300	-1.71835000

C	2.48128100	2.34384300	0.43782300
C	1.30569300	3.19586500	0.85838700
C	3.69009400	2.47229800	1.33371100
C	-3.61755400	3.17550500	-0.71323600
C	3.45094800	-1.77642600	0.54688500
C	-2.66054100	-3.03304700	0.32408700
H	0.68778400	-1.88977600	-1.58568900
H	1.49234500	1.61870500	-1.24725300
H	-0.74664300	-0.17569900	0.15086200
H	1.40355200	-3.55532400	0.90895700
H	0.14873000	-3.90449800	-0.27301000
H	-0.61456300	-3.22748700	2.03550400
H	0.11278000	-1.60373200	1.77209600
H	-3.49438600	-0.46714700	1.47308800
H	-1.97863500	-0.02169300	2.27513300
H	-2.45764600	2.27165600	1.64862200
H	-4.51732400	0.09812900	-0.77003700
H	-3.87063900	0.95123500	-2.15906100
H	-1.68722900	0.00032600	-1.91053200
H	-2.80283300	-1.32553600	-1.67642200
H	3.88189800	1.22549200	-2.18852600
H	4.36109500	0.63658400	-0.61496400
H	3.85747000	-1.18713500	-2.20021700
H	2.23697000	-0.56659600	-2.48512900
H	0.44923800	3.07314300	0.18856200
H	0.98624300	2.95301400	1.88089300
H	1.57856500	4.25902900	0.86630000
H	3.42459700	2.26158500	2.37767500
H	4.06873700	3.50236900	1.31452100
H	4.51542700	1.81532900	1.05330300
H	-4.68645300	3.27846100	-0.93836900
H	-3.35192600	3.92662000	0.03477700
H	-3.07930800	3.40374800	-1.64204000

H	4.44068600	-2.06658400	0.17483600
H	3.58736400	-0.84332400	1.10565300
H	3.12326500	-2.54092600	1.25365400
H	-2.73646200	-3.77374600	1.12408800
H	-3.63370000	-2.58055800	0.12213000
H	-2.38059100	-3.58581400	-0.58935600

Situ.3 TS(B⁺-C⁺)

C	-0.97724877	-2.44980044	0.42630116
C	-2.12903177	-1.82085944	0.08828716
C	-0.07880977	-3.25450444	-0.48277184
C	1.05480423	-2.42610344	-1.15181184
C	1.80296623	-1.59270644	-0.11664584
C	1.13613723	-0.42887144	0.31334816
C	2.95841323	-0.46064344	-1.02467484
C	2.83751723	1.01622956	-1.19171684
C	2.80559023	1.87679956	-0.15309284
C	2.73671323	1.30883456	1.24250916
C	1.45133023	0.40899056	1.49339816
C	-2.55810377	1.29672156	0.81800616
C	-3.58651277	0.19738956	0.86699016
C	-3.00810477	-1.20767344	1.15945416
C	-2.40861477	2.26534456	-0.10512484
C	-1.37809877	3.35644156	0.07585116
C	-3.25258077	2.41527156	-1.34831584
C	2.78706123	3.36865256	-0.32293084
C	-2.67072877	-1.77857944	-1.31698584
C	2.65122823	-2.39340844	0.85967016
H	-0.71476977	-2.46028544	1.48496916
H	-1.90591177	1.33839856	1.69396716
H	0.42273823	-0.00955544	-0.39158384
H	-0.65033977	-3.72722644	-1.28726884
H	0.36535523	-4.07529344	0.09028516

H	1.74949523	-3.09715944	-1.66868784
H	0.61427723	-1.76315644	-1.90482384
H	3.83292323	-0.73205144	-0.43391884
H	2.94222123	-0.98329544	-1.97851584
H	2.80137223	1.38426656	-2.21370884
H	3.61679723	0.68295456	1.43462216
H	2.73131323	2.09540356	2.00014516
H	0.59842723	1.06283556	1.68717416
H	1.63970223	-0.19959244	2.38212516
H	-4.29390577	0.42043856	1.67794716
H	-4.18616577	0.17101156	-0.04659984
H	-3.86037777	-1.88889944	1.30222316
H	-2.46835977	-1.19280644	2.11395116
H	-0.80302077	3.22939256	0.99877416
H	-0.68164177	3.39264456	-0.77276284
H	-1.86001477	4.34144056	0.11951516
H	-2.61967777	2.49353256	-2.24164184
H	-3.83470277	3.34454356	-1.30145084
H	-3.95616077	1.59523356	-1.50118084
H	3.65382323	3.82079256	0.17479316
H	2.80977523	3.65820556	-1.37616984
H	1.89485023	3.80802556	0.13984116
H	-3.70987677	-2.12904044	-1.33715584
H	-2.68350377	-0.74967844	-1.69583284
H	-2.09734477	-2.38604944	-2.01935684
H	3.35723923	-3.03080644	0.31951416
H	3.21699623	-1.76473444	1.55042416
H	2.00755323	-3.04797444	1.45554616

Situ.3 C⁺

C	-0.30367300	-1.19999900	0.03869100
C	-1.09036500	-1.44053800	-1.15895000
C	0.31734400	-2.68543500	0.33316500

C	1.80491300	-2.39928700	0.63303600
C	1.90460500	-0.91502500	1.05259800
C	0.93042000	-0.27848700	0.01476800
C	3.37084000	-0.36282800	0.93579600
C	3.69918200	0.45413600	-0.29760400
C	3.06337400	1.59838000	-0.60899600
C	1.92219600	2.08076100	0.27228700
C	0.63235600	1.22017300	0.15892200
C	-3.60606500	-0.01347500	0.31266000
C	-3.48369700	-0.68367100	-1.01807200
C	-2.46596100	-1.93044100	-1.03135300
C	-3.50767100	1.30425100	0.58710700
C	-3.77284100	1.81337600	1.98212300
C	-3.18784400	2.37766600	-0.42183200
C	3.42957700	2.44002900	-1.80351900
C	-0.53618400	-1.20262700	-2.51260700
C	1.42166300	-0.74730600	2.50812300
H	-0.97853100	-0.97438400	0.87180500
H	-3.88452000	-0.67835400	1.13100600
H	1.42819300	-0.41021300	-0.95197500
H	0.19802300	-3.38189900	-0.50238100
H	-0.23343300	-3.10141600	1.17868700
H	2.17153900	-3.08393400	1.40616000
H	2.40732400	-2.57036100	-0.26608800
H	3.56718600	0.25864100	1.81967700
H	4.06617000	-1.20510600	1.01622700
H	4.51627100	0.11145000	-0.92966600
H	2.25443600	2.07197400	1.31812700
H	1.67210700	3.12129200	0.04185400
H	0.05169300	1.55102100	-0.71293500
H	-0.00066600	1.40641300	1.03467700
H	-4.43639300	-1.15426200	-1.28796100
H	-3.23675300	0.00721300	-1.82711800

H	-2.73547300	-2.55955200	-1.88310700
H	-2.62147500	-2.47523800	-0.09639300
H	-4.00336800	1.00576100	2.68131600
H	-2.90828200	2.36978700	2.36556200
H	-4.61618200	2.51493000	1.98110500
H	-2.35858100	3.00104800	-0.06679900
H	-4.04779200	3.04863600	-0.54037300
H	-2.92977800	1.99736200	-1.41237800
H	3.75428700	3.44005300	-1.48846300
H	4.23809000	1.99011400	-2.38615400
H	2.56931500	2.59058600	-2.46988100
H	-0.34409900	-0.12694900	-2.63735400
H	0.44981500	-1.67371200	-2.61281400
H	-1.19283600	-1.55036800	-3.31028300
H	2.12907000	-1.22966800	3.19094400
H	1.36229600	0.30726200	2.79371600
H	0.43933200	-1.19603300	2.69321200

***Situ.3* TS(C⁺-F⁺)**

C	0.43964846	-0.80869043	-0.36901070
C	1.16747046	-1.51393643	0.60568730
C	-0.08227354	-2.72478743	0.02790230
C	-1.55077454	-2.39509743	0.25266930
C	-1.98528554	-1.14055543	-0.54442070
C	-0.84988454	-0.09457843	-0.17719870
C	-3.40355154	-0.64142643	-0.08148770
C	-3.45164954	0.54968757	0.85399530
C	-2.97368454	1.76059957	0.51551030
C	-2.29691954	1.93830157	-0.83446470
C	-0.90705554	1.25304057	-0.93200870
C	3.43868746	0.19824957	-0.62009470
C	3.64233946	-0.95682543	0.32281930
C	2.53801246	-2.04538643	0.20945530

C	3.38079246	1.51535157	-0.33373570
C	3.25699246	2.53652257	-1.43958470
C	3.49306346	2.10692157	1.05017130
C	-3.06952754	2.96271957	1.41657230
C	0.96906746	-1.27862043	2.09193830
C	-2.03599954	-1.45395143	-2.05259270
H	0.82375846	-0.86974243	-1.38641970
H	3.39736746	-0.08126543	-1.67496770
H	-0.98383554	0.12327957	0.88356830
H	0.31090046	-3.45450443	0.74040430
H	0.16409146	-3.07086143	-0.97552570
H	-2.13669054	-3.27102843	-0.05335970
H	-1.74512554	-2.24957543	1.32062630
H	-3.98145754	-0.39667743	-0.98191270
H	-3.92560854	-1.48844643	0.37655430
H	-3.93615954	0.41623857	1.81898930
H	-2.94957054	1.52921057	-1.61597370
H	-2.17301654	3.00022457	-1.06739870
H	-0.14389054	1.90968057	-0.49998470
H	-0.64051154	1.12031657	-1.98679670
H	4.58885246	-1.45817543	0.08171230
H	3.73378246	-0.62574743	1.36040230
H	2.80000246	-2.89537743	0.84844130
H	2.51077946	-2.41189143	-0.82358770
H	3.16953446	2.07105457	-2.42497870
H	2.38736546	3.18732157	-1.28291370
H	4.13495846	3.19442557	-1.45314270
H	2.64227746	2.76722657	1.25974730
H	4.39042346	2.73457557	1.11725530
H	3.55368346	1.36304157	1.84689430
H	-3.65260854	3.75921857	0.93694730
H	-3.54657054	2.72037957	2.36993030
H	-2.07856554	3.38694557	1.62602330

H	1.56555946	-0.41021643	2.38832430
H	-0.06434154	-1.07882443	2.37303530
H	1.32712246	-2.13771943	2.66548730
H	-2.82754454	-2.18485743	-2.24832470
H	-2.27056854	-0.56083243	-2.63760770
H	-1.10414954	-1.86951643	-2.45044070

Situ.3 F⁺

C	0.66382800	-0.61022200	-0.44526300
C	1.30169600	-1.54706000	0.49369800
C	0.36843000	-2.82826500	0.24220600
C	-1.11895300	-2.50773100	0.40514600
C	-1.62821800	-1.35413600	-0.48900000
C	-0.65546600	-0.04688600	-0.21040000
C	-3.10385100	-0.97204800	-0.07527400
C	-3.30990100	0.18619700	0.87070200
C	-3.05438800	1.45448300	0.50109800
C	-2.47348000	1.70274500	-0.88093700
C	-1.00997100	1.20894400	-1.03079800
C	3.03586400	0.54923700	-0.67102000
C	3.62616200	-0.57870200	0.12838000
C	2.74759000	-1.85053900	0.06175300
C	2.73220500	1.81668800	-0.26357500
C	2.35975700	2.86977300	-1.27613800
C	2.86098100	2.32016100	1.14811100
C	-3.30489100	2.64173400	1.39014300
C	1.22737800	-1.14996800	1.98308600
C	-1.63114000	-1.76336100	-1.97307900
H	0.98879100	-0.66984500	-1.48182400
H	2.99000800	0.37007800	-1.74635300
H	-0.81000800	0.16414500	0.84919900
H	0.69789900	-3.57822300	0.97033000
H	0.57813800	-3.23569200	-0.75152000

H	-1.69611200	-3.40767300	0.16066900
H	-1.34637700	-2.28078100	1.45232900
H	-3.65452600	-0.76669600	-1.00117200
H	-3.55232100	-1.87824900	0.34542900
H	-3.71952300	-0.01997500	1.85703000
H	-3.10158500	1.20250800	-1.62852800
H	-2.50261800	2.76845800	-1.12727800
H	-0.33672200	1.99767900	-0.68117000
H	-0.77884900	1.05628700	-2.09102500
H	4.61128600	-0.82508200	-0.28821700
H	3.79673100	-0.29124200	1.16798900
H	3.17196400	-2.63579300	0.69562300
H	2.74606700	-2.23952800	-0.96467100
H	2.13747800	2.44816100	-2.25943700
H	1.50748300	3.47198500	-0.94371900
H	3.19938800	3.56807500	-1.39319600
H	3.20007800	1.56706400	1.85956700
H	1.90731800	2.73099900	1.50172800
H	3.57629800	3.15197800	1.17340100
H	-4.02796300	3.32459600	0.92599300
H	-3.69672700	2.34433700	2.36639900
H	-2.38770900	3.22402500	1.55016600
H	1.70352100	-0.18429200	2.16171700
H	0.20584400	-1.08686500	2.35921400
H	1.75284100	-1.90171000	2.57940000
H	-2.37874600	-2.54940100	-2.12295800
H	-1.90967400	-0.92879900	-2.62239200
H	-0.67344900	-2.15680200	-2.32575500

***Situ.3* TS(F⁺-D⁺)**

C	0.91733310	-0.47242934	-0.45022723
C	1.55980710	-1.45469934	0.50391177
C	0.78091810	-2.78229234	0.19904777

C	-0.73494390	-2.60154834	0.34324577
C	-1.33966390	-1.45285734	-0.50610123
C	-0.51200990	-0.09525034	-0.21250123
C	-2.85093090	-1.26686334	-0.07936323
C	-3.19096890	-0.14763234	0.87594277
C	-3.07928490	1.14300366	0.51641277
C	-2.52088190	1.45682066	-0.86005523
C	-1.00893690	1.13558966	-0.99330623
C	2.55760610	0.80020066	-0.65018023
C	3.55598110	-0.07809934	0.09349477
C	3.04154210	-1.53021334	0.11151177
C	2.13918910	2.06926866	-0.24170923
C	1.77322110	3.09363066	-1.27174823
C	2.12718410	2.54533966	1.17242177
C	-3.46758590	2.29114166	1.40822177
C	1.41617310	-1.10931234	2.00136577
C	-1.31761090	-1.83109834	-2.00184723
H	1.10983510	-0.71858734	-1.49300523
H	2.62751710	0.70833766	-1.73385923
H	-0.66634490	0.10747966	0.84965477
H	1.14439310	-3.54978734	0.89262177
H	1.03581810	-3.12785334	-0.80917923
H	-1.23188990	-3.53564834	0.05625177
H	-0.99212790	-2.43937934	1.39608277
H	-3.43698890	-1.12378934	-0.99578523
H	-3.18639790	-2.22187234	0.33739977
H	-3.57881590	-0.40566834	1.85920477
H	-3.07805690	0.88665766	-1.61365923
H	-2.67137090	2.51224766	-1.10946023
H	-0.45136790	1.99037866	-0.59938823
H	-0.74665490	1.05785166	-2.05534323
H	4.51988110	-0.00956234	-0.42307723
H	3.72213310	0.28121566	1.11088877

H	3.62093610	-2.15169434	0.80058077
H	3.14135410	-1.97532034	-0.88661723
H	1.47995410	2.65404766	-2.22677523
H	1.00711010	3.79259166	-0.92678623
H	2.68108610	3.69081666	-1.45381223
H	2.57125710	1.85247166	1.88432977
H	1.09380710	2.75301166	1.48142177
H	2.65168310	3.50725166	1.23512977
H	-4.26123990	2.89102766	0.94453377
H	-3.82807390	1.94606966	2.38102077
H	-2.62376190	2.97383566	1.57844577
H	1.86720310	-0.14801534	2.25322077
H	0.37884910	-1.07659134	2.33602777
H	1.92631510	-1.87587834	2.59276777
H	-1.97413990	-2.69234534	-2.16393123
H	-1.69234490	-1.01970934	-2.63280623
H	-0.32753490	-2.11274834	-2.37240823

Situ.3 D⁺

C	1.03054600	-0.41232800	-0.47514300
C	1.66231600	-1.42275900	0.51858400
C	0.95395400	-2.76751500	0.23475000
C	-0.57521800	-2.62590000	0.37552200
C	-1.23493800	-1.51604000	-0.49714200
C	-0.46237900	-0.15387200	-0.26151900
C	-2.74973900	-1.38454300	-0.06340000
C	-3.12581300	-0.23967300	0.84860800
C	-3.04941400	1.04529600	0.45637200
C	-2.50169100	1.35014100	-0.92519100
C	-0.98814200	1.03755700	-1.07786400
C	2.09585700	0.78284100	-0.68885500
C	3.41597500	0.17967700	-0.01511300
C	3.14511100	-1.33518000	0.11462900

C	1.78263000	2.11218400	-0.18550100
C	1.98851900	3.28013500	-1.07618400
C	1.42844800	2.38433000	1.22405900
C	-3.47399300	2.20087600	1.32269800
C	1.52871300	-1.09165400	2.02435000
C	-1.21987100	-1.95134800	-1.97948000
H	1.12624200	-0.88445300	-1.45940700
H	2.28413800	0.87021400	-1.76130400
H	-0.63274200	0.09561100	0.79096900
H	1.31563800	-3.53961100	0.92380300
H	1.21243200	-3.10976900	-0.77522000
H	-1.04647900	-3.58271000	0.12184400
H	-0.82645400	-2.44129500	1.42703200
H	-3.35259600	-1.29829200	-0.97686600
H	-3.05056400	-2.33229100	0.39411800
H	-3.51024500	-0.47464700	1.83938700
H	-3.04933700	0.75336400	-1.66628300
H	-2.67853400	2.39681500	-1.19422900
H	-0.42696000	1.92900300	-0.73787900
H	-0.74606900	0.92725100	-2.14239200
H	4.27820100	0.42190900	-0.64121000
H	3.58925300	0.62493000	0.96755300
H	3.82554700	-1.79096800	0.84139600
H	3.31056100	-1.83009900	-0.84973700
H	1.54026800	4.20260300	-0.70426100
H	3.08101000	3.43581300	-1.13373400
H	1.66955200	3.07454900	-2.10205900
H	0.65925000	3.16034200	1.29160900
H	2.32151000	2.82703100	1.69938100
H	1.14022100	1.50206800	1.78903900
H	-4.27823900	2.77349800	0.84288300
H	-3.83331300	1.86591300	2.29948200
H	-2.64863100	2.90827400	1.48720500

H	2.14577300	-0.24429800	2.33420100
H	0.50135400	-0.88885100	2.33494900
H	1.87441900	-1.95240300	2.60598600
H	-1.82604400	-2.85572300	-2.09778400
H	-1.65268000	-1.18843500	-2.63435600
H	-0.22171700	-2.18869500	-2.35919700

***Situ.3* TS(D⁺-E⁺)**

C	0.95223884	-0.37511336	-0.46812799
C	1.65920484	-1.41945336	0.47211901
C	0.84510484	-2.72083436	0.47100701
C	-0.63598216	-2.45954836	0.77999601
C	-1.33660316	-1.48767336	-0.20778199
C	-0.55178216	-0.11949336	-0.24589099
C	-2.82024216	-1.27345936	0.30751701
C	-3.17299516	0.05676964	0.93712101
C	-3.12948516	1.21140064	0.25031801
C	-2.63249316	1.17627764	-1.18370999
C	-1.11511816	0.85826164	-1.30693599
C	2.05472084	0.68342964	-0.46457699
C	3.36168284	-0.08182436	-0.72359999
C	3.04627984	-1.52277436	-0.21471199
C	2.07522984	2.03788064	-0.05299099
C	3.37154484	2.82201564	-0.08123799
C	0.92614384	2.78113864	0.57737601
C	-3.55290416	2.53636464	0.82777501
C	1.82592984	-0.89031436	1.91437001
C	-1.41374416	-2.15282536	-1.60150499
H	1.04394384	-0.81546436	-1.47412399
H	1.80635984	1.65166364	-1.31085499
H	-0.69527116	0.32340064	0.74460001
H	1.26603784	-3.41562736	1.20768301
H	0.94269584	-3.21120836	-0.50476199

H	-1.17694916	-3.41251236	0.76835501
H	-0.74105216	-2.06945436	1.80038401
H	-3.49739616	-1.43281336	-0.54206999
H	-3.05099016	-2.07671836	1.01375601
H	-3.52043716	0.05806664	1.96870301
H	-3.19937716	0.41589164	-1.73529499
H	-2.83307616	2.12644564	-1.68923899
H	-0.56936616	1.80733464	-1.25633199
H	-0.91856516	0.46156564	-2.31034599
H	3.62411484	-0.07541536	-1.78640099
H	4.19309884	0.37030364	-0.18168299
H	3.82527384	-1.87901636	0.46453001
H	2.99906084	-2.22189936	-1.05463099
H	3.16898284	3.88684164	-0.21641499
H	3.86099284	2.70311064	0.89383301
H	4.06867684	2.49337164	-0.85165699
H	0.67117584	3.67765164	0.00415501
H	1.30026684	3.13181564	1.54746401
H	0.03952884	2.18172264	0.75067501
H	-4.39543516	2.95480864	0.26208001
H	-3.86116516	2.44393264	1.87288101
H	-2.74687516	3.28136964	0.77313001
H	2.47425184	-0.00774136	1.97163901
H	0.87142284	-0.62712636	2.37676201
H	2.29212784	-1.66237936	2.53434001
H	-1.93106016	-3.11470636	-1.51939299
H	-1.97975816	-1.54660736	-2.31396999
H	-0.43467216	-2.35496136	-2.04740199

Situ.3 E⁺

C	0.92799800	-0.37442400	-0.15888500
C	1.27981700	-1.67320200	0.65541500
C	0.42996100	-2.84140300	0.13419900

C	-1.06111400	-2.48529500	0.06441600
C	-1.40171200	-1.20133600	-0.74272300
C	-0.57633000	0.01280600	-0.16047500
C	-2.95161100	-0.96612900	-0.58792800
C	-3.39149400	-0.05100600	0.52950000
C	-3.16610000	1.27317000	0.47093100
C	-2.40963700	1.81103300	-0.72992100
C	-0.90972100	1.39861400	-0.76189600
C	2.12842600	0.46241800	-0.12480900
C	3.29310300	-0.36812900	0.29028500
C	2.78938400	-1.81877900	0.37008300
C	2.28681800	1.89428200	-0.47082400
C	3.60342400	2.25962000	-1.17980800
C	2.16209400	2.66237500	0.89523000
C	-3.62474800	2.24579600	1.52361800
C	1.04941700	-1.44846500	2.16723200
C	-1.11442900	-1.42040500	-2.24268500
H	1.19743500	-0.64641100	-1.23322600
H	1.44422800	2.20646900	-1.08785800
H	-0.85039300	0.07355600	0.89894500
H	0.57394400	-3.71771800	0.77685700
H	0.79001600	-3.13106200	-0.86121900
H	-1.60317100	-3.32637500	-0.38222800
H	-1.46447500	-2.37487300	1.07867400
H	-3.33328700	-0.56469600	-1.53526100
H	-3.42418600	-1.94700400	-0.47647000
H	-3.93078400	-0.47543900	1.37391200
H	-2.89834800	1.46155600	-1.64738200
H	-2.45962600	2.90416000	-0.76047000
H	-0.36643700	2.14759800	-0.17891700
H	-0.55047800	1.47744600	-1.79571500
H	4.17536800	-0.20139800	-0.33476000
H	3.57393700	0.01478400	1.28787100

H	3.31638300	-2.40211600	1.12825500
H	2.94948400	-2.31229800	-0.59632800
H	3.57557100	3.31900700	-1.44824300
H	4.47729500	2.10493000	-0.54107400
H	3.73740800	1.68828500	-2.10346000
H	2.14293500	3.73060600	0.66382100
H	3.02555200	2.46403700	1.53526200
H	1.24888000	2.41461700	1.44146500
H	-4.31466100	2.98439400	1.09544300
H	-4.13780800	1.74033300	2.34629100
H	-2.78335700	2.81425400	1.94245000
H	1.60955400	-0.59034900	2.55614700
H	-0.00186000	-1.28800700	2.41323700
H	1.38244900	-2.33383500	2.71758000
H	-1.74262200	-2.23088100	-2.62706600
H	-1.34274100	-0.52735100	-2.83312300
H	-0.07747900	-1.70546300	-2.45913300

Situ.4

Situ.4 B⁺

C	-1.54903600	-2.03444700	0.71412900
C	-2.75637700	-1.46396000	0.51579300
C	-0.84833700	-2.99071100	-0.19916100
C	0.19074100	-2.30800800	-1.22815000
C	1.33185600	-1.78074100	-0.47583100
C	1.34666200	-0.38252700	-0.06939200
C	2.20216900	0.23577300	-1.33593700
C	3.62316000	0.52509200	-0.98925400
C	3.95392200	1.07854900	0.19518900
C	2.85233900	1.26519000	1.21353500
C	1.97740700	-0.00502800	1.28897800
C	-2.49684900	1.68765500	0.70807600

C	-3.69943900	0.87302700	1.10763000
C	-3.35377800	-0.56370500	1.57634000
C	-2.32765400	2.45475100	-0.38471500
C	-1.07045900	3.27489900	-0.56756700
C	-3.34578400	2.63121500	-1.48584400
C	5.35081300	1.48487200	0.55908300
C	-3.60522400	-1.68035800	-0.71135400
C	2.46434700	-2.67520500	-0.14723700
H	-1.03149000	-1.80043400	1.64440400
H	-1.68927600	1.68582100	1.44429800
H	0.34247600	0.03838600	-0.16089700
H	-1.54523300	-3.51537000	-0.85658200
H	-0.30934300	-3.75567100	0.36831300
H	0.49990200	-3.08923400	-1.92788600
H	-0.35712400	-1.51976300	-1.74939200
H	2.12946500	-0.39530700	-2.22797100
H	1.63550700	1.14460200	-1.56887000
H	4.38135000	0.31728300	-1.74013200
H	3.26822100	1.47892900	2.20262500
H	2.23004900	2.13069900	0.94445600
H	1.16632200	0.13343800	2.01090600
H	2.60171100	-0.81800300	1.66924100
H	-4.19793800	1.36925900	1.95214000
H	-4.44214300	0.83580600	0.30613300
H	-4.28011000	-1.03028900	1.93970700
H	-2.67517200	-0.50889100	2.43566200
H	-1.30673900	4.34553000	-0.61695800
H	-0.36263100	3.12925500	0.25479100
H	-0.56828200	3.03062900	-1.51410500
H	-3.69487000	3.67135800	-1.51772500
H	-4.22474200	1.99396800	-1.37410300
H	-2.89823900	2.42676900	-2.46707800
H	6.05915500	1.29110300	-0.25008800

H	5.38623900	2.55516900	0.79860900
H	5.69196900	0.95534700	1.45791900
H	-3.67835400	-0.75608400	-1.29656100
H	-3.22874500	-2.46164000	-1.37454800
H	-4.62836100	-1.95002900	-0.42433600
H	2.49267900	-3.57105800	-0.76915600
H	3.41634200	-2.12999800	-0.20304100
H	2.37452300	-2.98957900	0.90436200

***Situ.4* TS(B⁺-C⁺)**

C	1.32815655	-2.19033948	-0.66370240
C	2.50616755	-1.59756148	-0.36920740
C	0.51679555	-3.09661548	0.23022460
C	-0.54178345	-2.35642448	1.09716660
C	-1.48054845	-1.50837148	0.24536960
C	-0.96871645	-0.26712848	-0.18569340
C	-2.44161645	-0.44110048	1.42018760
C	-3.67189345	0.14746052	0.86867460
C	-3.69855445	1.19286352	0.01022060
C	-2.41694445	1.76327752	-0.53553140
C	-1.52727145	0.63947752	-1.20776640
C	2.57703955	1.58951652	-0.72316240
C	3.70321655	0.62426452	-0.98740440
C	3.24383655	-0.79059748	-1.41822040
C	2.40251655	2.40961352	0.33053060
C	1.25846855	3.39808152	0.36381960
C	3.32147255	2.49093552	1.52613760
C	-4.98647645	1.76192052	-0.51290940
C	3.20682955	-1.74371148	0.95848560
C	-2.46902545	-2.29089448	-0.60166440
H	0.94090155	-2.04900548	-1.67382340
H	1.85664355	1.67054752	-1.54146540
H	-0.11283745	0.12014752	0.36587160

H	1.15973455	-3.64961648	0.92148260
H	0.01397955	-3.85406748	-0.38106640
H	-1.12411845	-3.09048048	1.66514460
H	-0.02115845	-1.71784248	1.82001360
H	-2.62250545	-1.27640448	2.09724060
H	-1.75784845	0.25272452	1.91051260
H	-4.60656045	-0.32928548	1.15329460
H	-2.62501045	2.51347052	-1.30214240
H	-1.82362445	2.25648452	0.24292360
H	-0.68756845	1.14135052	-1.69957740
H	-2.11635045	0.11657152	-1.96290440
H	4.31447055	1.02295052	-1.80916740
H	4.37550855	0.55221652	-0.12843540
H	4.14321455	-1.35605048	-1.70239740
H	2.62964555	-0.71554348	-2.32369540
H	1.63574255	4.42699652	0.42116860
H	0.62827155	3.32871152	-0.52872440
H	0.63057155	3.25606152	1.25477960
H	3.80646955	3.47474352	1.56573460
H	4.10955155	1.73627552	1.52284760
H	2.75552755	2.38930552	2.46113060
H	-5.85880445	1.26043052	-0.08773440
H	-5.05454745	2.83126352	-0.27819840
H	-5.03558745	1.67971252	-1.60650940
H	3.22420455	-0.78894948	1.49768560
H	2.74333555	-2.48484248	1.61225760
H	4.25334555	-2.03527748	0.80877360
H	-2.99280245	-3.03070448	0.00979060
H	-3.21229445	-1.65850348	-1.08661240
H	-1.92241545	-2.83410948	-1.37924940

Situ.4 C⁺

C	0.52312300	-1.24582500	-0.14247300
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C	1.56509400	-1.63004100	0.79694600
C	0.10256000	-2.66999000	-0.81906700
C	-1.44179500	-2.62377200	-0.82808900
C	-1.84721700	-1.13689500	-0.71759000
C	-0.81394200	-0.64565200	0.34144500
C	-3.29940300	-0.98216500	-0.20349900
C	-3.83510500	0.43329500	-0.15105400
C	-3.30613100	1.47234300	0.51659300
C	-2.04232400	1.37417700	1.36049400
C	-0.77349100	0.85678800	0.64757200
C	3.47469300	0.57291700	-0.64241700
C	3.72506300	-0.38787100	0.47393400
C	2.94025400	-1.78755700	0.31825800
C	3.12368800	1.87358500	-0.55153800
C	3.02504500	2.72370300	-1.79349100
C	2.85351500	2.60922400	0.73585700
C	-3.96845500	2.82893500	0.50210100
C	1.27162900	-1.86924500	2.22929500
C	-1.69049800	-0.45110100	-2.09077600
H	0.97470500	-0.64494100	-0.94119500
H	3.68291900	0.17668800	-1.63682800
H	-1.09292300	-1.15681300	1.27500100
H	0.47860300	-3.53745000	-0.26827900
H	0.54841800	-2.70328900	-1.81480200
H	-1.82858100	-3.10203600	-1.73450300
H	-1.83693000	-3.18248700	0.02813600
H	-3.95389300	-1.57728400	-0.85037300
H	-3.36260000	-1.44709300	0.79319200
H	-4.75114700	0.61181000	-0.71085900
H	-1.81769600	2.36562600	1.76769100
H	-2.23781300	0.73305300	2.23448400
H	0.08466500	1.06369900	1.30207300
H	-0.59864100	1.42879400	-0.27129500

H	4.77390100	-0.70673800	0.46527000
H	3.53687900	0.03894500	1.46148200
H	3.47841300	-2.52988600	0.91218400
H	2.97943400	-2.05188400	-0.74164800
H	3.73364500	3.55965700	-1.74376000
H	3.23331600	2.15487500	-2.70300200
H	2.02640900	3.16951400	-1.88251800
H	1.88904400	3.12821500	0.68450100
H	3.61276900	3.38640800	0.88886900
H	2.85300700	1.97268500	1.62309300
H	-4.87983100	2.83215200	-0.10114900
H	-4.23329500	3.14477700	1.51973000
H	-3.29139900	3.59637100	0.10371800
H	0.45191300	-2.59416500	2.32690300
H	2.13676200	-2.22460000	2.78933300
H	0.88440600	-0.94790000	2.68629100
H	-2.40574200	-0.88250600	-2.79915600
H	-1.89447300	0.61994700	-2.03556000
H	-0.69206200	-0.58326700	-2.52203600

***Situ.4* TS(C⁺-F⁺)**

C	0.56640835	-0.69827890	-0.35807170
C	1.50918235	-1.52866590	0.27339030
C	0.26507935	-2.70142190	-0.37652770
C	-1.15240465	-2.60485990	0.16891630
C	-1.81647665	-1.25721090	-0.20554270
C	-0.71292065	-0.19527390	0.21019630
C	-3.09981065	-1.03936490	0.63490530
C	-3.94490165	0.16686510	0.28228730
C	-3.55508865	1.45211110	0.26349030
C	-2.14408965	1.91137410	0.60519230
C	-0.99104465	1.27003610	-0.19323670
C	3.39605335	0.67626810	-0.80563070

C	3.84797335	-0.64679390	-0.24854270
C	2.81644035	-1.78990590	-0.46256670
C	3.31075735	1.86639310	-0.17576770
C	2.91672535	3.11057210	-0.93586570
C	3.64425135	2.10398410	1.27685330
C	-4.52763165	2.55727110	-0.06927570
C	1.57722935	-1.67315090	1.78297030
C	-2.15149865	-1.22941290	-1.70932670
H	0.75545335	-0.47239290	-1.40665370
H	3.17423935	0.66487810	-1.87485470
H	-0.65620465	-0.23016990	1.30382230
H	0.83649335	-3.53096090	0.04807530
H	0.33621635	-2.76805590	-1.46194470
H	-1.72269165	-3.44611890	-0.24407970
H	-1.14755965	-2.73888990	1.25617930
H	-3.71858465	-1.93753090	0.52380730
H	-2.81482465	-1.00528990	1.69800230
H	-4.98340165	-0.04630790	0.03773530
H	-2.08251665	2.99376110	0.45306130
H	-1.95951965	1.75553010	1.67936330
H	-0.08350665	1.85426210	-0.00186170
H	-1.18616665	1.34111210	-1.26887870
H	4.76351135	-0.96321690	-0.76531770
H	4.11037035	-0.57561590	0.81004730
H	3.24743635	-2.73583190	-0.11759870
H	2.62375035	-1.89369890	-1.53699470
H	3.73412535	3.84237210	-0.92212070
H	2.67219235	2.89804210	-1.98005170
H	2.05491135	3.60454210	-0.46909470
H	2.80963435	2.59731610	1.79046630
H	4.49913135	2.78685410	1.35795530
H	3.89720635	1.19620810	1.82806230
H	-5.52903165	2.17230210	-0.27711870

H	-4.60294065	3.27131110	0.76114830
H	-4.19125265	3.13000310	-0.94347370
H	0.60309735	-1.67278590	2.27071130
H	2.10168535	-2.59307590	2.05467330
H	2.14981935	-0.83263090	2.18711430
H	-2.86950965	-2.02471390	-1.93582770
H	-2.61566265	-0.28584490	-1.99917070
H	-1.27959365	-1.38502590	-2.35327370

Situ.4 F⁺

C	0.73632400	-0.46630000	-0.38942400
C	1.60575800	-1.52439100	0.14543300
C	0.67950400	-2.79196000	-0.19618400
C	-0.74184900	-2.64423600	0.35006900
C	-1.48157000	-1.37031700	-0.12027700
C	-0.51230700	-0.07276400	0.24491200
C	-2.78347700	-1.20995400	0.72351700
C	-3.80653300	-0.20696900	0.24599400
C	-3.62965800	1.12218200	0.19738700
C	-2.31383400	1.76926200	0.59709200
C	-1.07238900	1.29753800	-0.18467300
C	2.96197800	0.91379900	-0.85070600
C	3.75207500	-0.31070500	-0.48128000
C	2.92134000	-1.60446600	-0.64931100
C	2.73527900	2.03622600	-0.10667600
C	2.12005500	3.25702700	-0.74214900
C	3.17326800	2.22529300	1.31998600
C	-4.72512300	2.05821800	-0.24393600
C	1.86218900	-1.47470900	1.66564600
C	-1.82085300	-1.45195400	-1.61792300
H	0.80592000	-0.28281300	-1.45977200
H	2.67267400	0.97049700	-1.90129400
H	-0.42516500	-0.10375800	1.33529400

H	1.19117000	-3.65272000	0.24932000
H	0.67278000	-2.95009200	-1.27881700
H	-1.32661800	-3.51497000	0.03055600
H	-0.73186800	-2.67611500	1.44520100
H	-3.25176800	-2.20141000	0.73763800
H	-2.49663000	-1.00270800	1.76455600
H	-4.76945600	-0.61159400	-0.05814700
H	-2.39497800	2.85293300	0.46429900
H	-2.13825100	1.61637600	1.67334500
H	-0.27399200	2.02547400	-0.01253900
H	-1.27531500	1.31028400	-1.26119200
H	4.62284300	-0.37877700	-1.14605400
H	4.14742800	-0.24496000	0.53455900
H	3.50376100	-2.47230300	-0.32354500
H	2.69467100	-1.75693700	-1.71239100
H	2.89675900	4.02242000	-0.87353800
H	1.68849300	3.04863000	-1.72414200
H	1.35468700	3.70888100	-0.10181400
H	2.31771100	2.48420800	1.95589400
H	3.86244800	3.07719100	1.37944800
H	3.67619700	1.35887200	1.74974600
H	-5.64105900	1.52144000	-0.50315000
H	-4.96429800	2.77672300	0.55084200
H	-4.41437800	2.64950100	-1.11533200
H	0.95293000	-1.58482300	2.25751500
H	2.53497500	-2.29200600	1.94151800
H	2.33451800	-0.53534600	1.95881200
H	-2.53561600	-2.26747300	-1.77178700
H	-2.29876700	-0.54050500	-1.97977900
H	-0.95288100	-1.65904400	-2.25023400

***Situ.4* TS(F⁺-D⁺)**

C	0.95302628	-0.34058388	-0.42755279
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C	1.81718028	-1.44688588	0.13759621
C	0.99497528	-2.73576488	-0.21380979
C	-0.44062372	-2.66266388	0.31910621
C	-1.24043572	-1.41040088	-0.12670979
C	-0.37462172	-0.08348988	0.22020321
C	-2.55248072	-1.37643588	0.72090621
C	-3.66198472	-0.46789188	0.24870221
C	-3.59265372	0.87070612	0.20818921
C	-2.33004572	1.60255012	0.62666921
C	-1.05383672	1.24289012	-0.16279579
C	2.48675328	1.02528512	-0.78998679
C	3.64171128	0.07953712	-0.48274479
C	3.15410328	-1.37521488	-0.61230079
C	2.19742828	2.19239812	-0.07683779
C	1.60861228	3.37007312	-0.79162279
C	2.53558828	2.41450812	1.35921121
C	-4.75059872	1.72547912	-0.23800679
C	2.05079128	-1.38628388	1.66212221
C	-1.59416572	-1.51750588	-1.62357479
H	0.87139728	-0.39172588	-1.51187479
H	2.28496928	1.12373312	-1.85651779
H	-0.25672372	-0.08947288	1.30987821
H	1.52123828	-3.59578188	0.21705221
H	0.99759328	-2.88078688	-1.29992879
H	-0.98659172	-3.55248888	-0.01480679
H	-0.43404672	-2.71275288	1.41413021
H	-2.93336072	-2.40374988	0.74078221
H	-2.28246472	-1.14041188	1.76104821
H	-4.58550772	-0.95030088	-0.06472879
H	-2.49189272	2.68070812	0.52060221
H	-2.14257072	1.43411312	1.69858221
H	-0.32519772	2.03051612	0.04554021
H	-1.25446172	1.28505712	-1.23985379

H	4.44958928	0.28830312	-1.19304179
H	4.04962828	0.25914312	0.51384321
H	3.88913828	-2.08152688	-0.21534579
H	3.00284028	-1.62654788	-1.66978479
H	2.45406728	4.01959312	-1.07016979
H	1.09462528	3.09710712	-1.71515179
H	0.95294028	3.97223712	-0.15716779
H	1.61166228	2.55596312	1.93604921
H	3.09062628	3.35609512	1.45943921
H	3.11315228	1.61263612	1.81464721
H	-5.61973572	1.12217112	-0.51213279
H	-5.05396572	2.41732412	0.55870621
H	-4.47756772	2.34555312	-1.10232179
H	1.13216528	-1.48980188	2.24065121
H	2.71234928	-2.20805688	1.95294921
H	2.52717528	-0.45572088	1.97572921
H	-2.25289572	-2.37976688	-1.77188079
H	-2.13488772	-0.64077588	-1.98406079
H	-0.72205372	-1.67030988	-2.26604979

Situ.4 D⁺

C	1.00320700	-0.29865700	-0.49021200
C	1.81431000	-1.47263700	0.12422200
C	0.99325600	-2.75192300	-0.13801200
C	-0.44001100	-2.61430300	0.41254800
C	-1.24539600	-1.38124000	-0.09583400
C	-0.38513300	-0.07358700	0.14028000
C	-2.54837200	-1.31200500	0.76129400
C	-3.65174400	-0.40424900	0.26868700
C	-3.56868200	0.92910800	0.13883100
C	-2.29322100	1.68244500	0.47536100
C	-1.04426300	1.24180900	-0.31745200
C	2.00946800	0.87913000	-0.76703600

C	3.47004600	0.15314200	-0.66946600
C	3.12954900	-1.35356700	-0.67041000
C	2.11801800	2.06677900	0.05896500
C	2.53526200	3.33595200	-0.58210000
C	1.92237200	2.09317400	1.52325300
C	-4.73071700	1.76266400	-0.33858900
C	2.12783400	-1.36351300	1.63465900
C	-1.62794500	-1.59634500	-1.57650300
H	0.80668200	-0.61707400	-1.52142800
H	1.92061500	1.20893300	-1.80653600
H	-0.27216800	0.00087300	1.23162300
H	1.47964900	-3.62059400	0.32089400
H	0.96450300	-2.94859800	-1.21712500
H	-1.00469300	-3.51904100	0.15966000
H	-0.40569900	-2.58475100	1.50905800
H	-2.94789800	-2.32980000	0.82893100
H	-2.26561700	-1.03566100	1.78901400
H	-4.59329900	-0.88492100	0.00984300
H	-2.45478400	2.75076900	0.29431300
H	-2.08000900	1.58752300	1.55149600
H	-0.29883400	2.04780900	-0.19877300
H	-1.27332300	1.21288100	-1.38983300
H	4.08165900	0.47869300	-1.51271100
H	3.99452900	0.43144300	0.24794500
H	3.95539800	-1.92951900	-0.23945500
H	2.98421500	-1.69646100	-1.70121200
H	1.60540700	3.85160600	-0.87928000
H	3.05850800	4.00716700	0.10382400
H	3.10719800	3.17799200	-1.49983700
H	1.49453100	3.05164900	1.83688900
H	2.92576900	2.06771600	1.98235100
H	1.34719600	1.25787900	1.91236200
H	-5.61061300	1.14965800	-0.54998800

H	-5.01043800	2.51149300	0.41427300
H	-4.47435200	2.31795000	-1.25094200
H	1.23324900	-1.25295000	2.25187800
H	2.62935900	-2.28065400	1.96024300
H	2.80204600	-0.53705200	1.87568500
H	-2.25815400	-2.48833600	-1.66019500
H	-2.20350900	-0.76078600	-1.97996900
H	-0.76414700	-1.75890200	-2.22792700

***Situ.4* TS(D⁺-E⁺)**

C	0.99135462	-0.25907604	-0.44396457
C	1.78605062	-1.48634604	0.13659543
C	0.89731862	-2.73536504	0.06574043
C	-0.47430438	-2.48686104	0.70770543
C	-1.27949738	-1.32760204	0.06088243
C	-0.42469338	0.00060996	0.11397743
C	-2.56795238	-1.14912104	0.92330343
C	-3.68987638	-0.29527604	0.37443643
C	-3.61864438	0.99604596	0.01828443
C	-2.32867638	1.79665396	0.09589743
C	-1.10682038	1.18193896	-0.61886357
C	2.14686762	0.74376896	-0.47298657
C	3.33663362	-0.00981404	-1.08966557
C	3.00748762	-1.50806804	-0.81696057
C	2.32815662	2.01102496	0.13208643
C	3.65285862	2.73442896	-0.00044357
C	1.34921262	2.69394196	1.05123643
C	-4.83027938	1.75349196	-0.46634257
C	2.25880362	-1.24250004	1.58775043
C	-1.67897238	-1.73334804	-1.37577457
H	0.85654862	-0.50514404	-1.50978157
H	1.82529862	1.84519396	-1.10128157
H	-0.34350338	0.25166496	1.18089243

H	1.40168862	-3.57076904	0.56596343
H	0.77074262	-3.03415704	-0.98154957
H	-1.07160038	-3.40282704	0.64028643
H	-0.35324838	-2.28879904	1.78055643
H	-2.97132538	-2.15083104	1.10750643
H	-2.26317938	-0.77190504	1.91231643
H	-4.65706838	-0.78733504	0.28965143
H	-2.50752638	2.78706896	-0.33677557
H	-2.07554838	1.97618896	1.15343043
H	-0.38263338	1.99308496	-0.76642357
H	-1.39402238	0.87208596	-1.62906057
H	3.43121262	0.19909996	-2.16023157
H	4.27193462	0.29418096	-0.61770057
H	3.86752362	-2.02872704	-0.38752057
H	2.74714162	-2.01840804	-1.74892757
H	4.18783562	2.50935696	-0.92274857
H	3.50597362	3.81441296	0.07052543
H	4.28808962	2.43396196	0.84265743
H	1.07719362	3.68427896	0.67361643
H	1.89106862	2.85959996	1.99081843
H	0.45553362	2.12061996	1.26831343
H	-5.72526738	1.12624596	-0.47480057
H	-5.03086438	2.62214696	0.17480143
H	-4.67598738	2.14340696	-1.48134057
H	1.42995362	-1.04139704	2.27086543
H	2.78071062	-2.13145904	1.95531843
H	2.96388362	-0.40675904	1.67131743
H	-2.17084238	-2.71179104	-1.35300957
H	-2.38756438	-1.03171004	-1.81880757
H	-0.82530538	-1.82287104	-2.05520757

Situ.4 E⁺

C	1.03008100	-0.27164500	-0.09915900
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C	1.71000700	-1.64270600	0.25181800
C	0.86799900	-2.78277500	-0.34187700
C	-0.61472600	-2.66326000	0.03480700
C	-1.28443300	-1.29910800	-0.29818300
C	-0.45152200	-0.13562800	0.37181100
C	-2.71681400	-1.37554700	0.32126400
C	-3.72285100	-0.33513900	-0.10829400
C	-3.62183700	0.96942000	0.18025800
C	-2.42528500	1.48932100	0.95384100
C	-1.05430600	1.28330500	0.26972700
C	2.10468400	0.71718700	-0.18682600
C	3.41533600	0.01244300	-0.24141600
C	3.09667900	-1.48299800	-0.40640700
C	2.01823400	2.19455900	-0.29091500
C	3.01093400	2.83747000	-1.27886300
C	2.26107400	2.73451900	1.16367800
C	-4.66356300	1.97880500	-0.22625800
C	1.87158900	-1.80309100	1.78080100
C	-1.39947500	-1.12346700	-1.82570400
H	1.00359200	-0.26263800	-1.24084000
H	1.00334300	2.47307200	-0.57339700
H	-0.41831700	-0.36942100	1.44531400
H	1.26067700	-3.74831200	-0.00252000
H	0.97642700	-2.77654700	-1.43392400
H	-1.17245400	-3.45449600	-0.47830600
H	-0.73946100	-2.86022900	1.10709400
H	-3.11656400	-2.36457200	0.07366400
H	-2.61253400	-1.36556400	1.41715300
H	-4.58703100	-0.68573800	-0.66895400
H	-2.54737000	2.56405000	1.12512700
H	-2.39580000	1.02933500	1.95344100
H	-0.36863200	1.96844200	0.77481900
H	-1.12309400	1.60804700	-0.77639200

H	4.10473900	0.43981100	-0.97401800
H	3.87650300	0.21050100	0.74352700
H	3.86125800	-2.12338300	0.03853900
H	3.04370100	-1.72494000	-1.47496900
H	2.90935000	2.41948500	-2.28506800
H	2.79542900	3.90736900	-1.34263000
H	4.04971900	2.72931300	-0.95585200
H	2.08083600	3.81254600	1.14333800
H	3.29432900	2.56426000	1.47660000
H	1.58762500	2.29058800	1.90094100
H	-5.48458800	1.51433900	-0.77855900
H	-5.08633100	2.47944800	0.65463000
H	-4.23077900	2.76803500	-0.85563200
H	0.91489000	-1.88235100	2.30014700
H	2.43149600	-2.71996500	1.98906600
H	2.42159400	-0.97163700	2.23634500
H	-1.99804000	-1.93721900	-2.24859600
H	-1.89370200	-0.18673000	-2.09274300
H	-0.43163800	-1.15487900	-2.34195900