

Unexpected and delayed fragmentation dynamics of the organometallic ferrocene induced by ion-collision

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I. GEOMETRIES

We present in this section the optimized geometries at the M06L/SDD level of theory: cartesian coordinates are given in Å, absolute energy E in atomic units, relative energies ΔE in eV including the ZPE correction, charge q , and spin multiplicity s .

Fe(C₅H₅)
E=-186.602196170 a.u.; $\Delta E=0.0$ eV
 $q = 0$ $s = 1$
Fe -0.00000100 0.00011700 0.00016800
C -1.62869300 -0.36668800 1.16746300
C -1.62838800 -1.22373000 0.01202300
C -1.62911500 0.99706600 0.70942500
H -1.61711400 -0.69095000 2.19892900
C -1.62877700 -0.38967100 -1.16012800
H -1.61731400 -2.30491600 0.02267100
C -1.62903900 0.98291100 -0.72908500
H -1.61782200 1.87805300 1.33626800
H -1.61717600 -0.73427800 -2.18497000
H -1.61757800 1.85134600 -1.37319000
C 1.62913000 0.99619000 0.71064100
C 1.62870300 -0.36812200 1.16700300
C 1.62904200 0.98379800 -0.72788500
H 1.61784500 1.87640700 1.33856400
C 1.62837600 -1.22375000 0.01051900
H 1.61710900 -0.69364900 2.19807100
C 1.62877000 -0.38825700 -1.16060300
H 1.61760100 1.85302000 -1.37092800
H 1.61728500 -2.30494700 0.01984300
H 1.61713800 -0.73161700 -2.18586400

[Fe(C₅H₅)²⁺]
E=-185.914852455 a.u.; $\Delta E=18.69$ eV
 $q = 2$ $s = 3$

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Fe 0.00348000 -0.00230500 -0.24532900
C 1.44302100 0.03447100 1.31069300
C 1.63039500 1.18407400 0.45253100
C 1.63430900 -1.15587500 0.51023700
H 1.23973800 0.06037500 2.37368900
C 1.96219500 0.69945400 -0.85748500
H 1.58349900 2.22223700 0.75466400
C 1.96522800 -0.73670100 -0.82144600
H 1.58833900 -2.17795100 0.86323900
H 2.16464400 1.31202700 -1.72819200
H 2.16871700 -1.39153100 -1.66056500
C -1.59119600 -0.68387400 1.06916200
C -1.60991700 0.76089200 1.00997600
C -1.76421100 -1.18758000 -0.26167000
H -1.48240000 -1.28073500 1.96618300
C -1.79545800 1.14826300 -0.35586600
H -1.51409400 1.43200100 1.85448100
C -1.88949900 -0.05470500 -1.14910300
H -1.81876000 -2.23109100 -0.54495100
H -1.86967800 2.16386300 -0.72391600
H -2.05968600 -0.09977700 -2.21826200

Green path in Fig.4

$E=-185.842663617$ a.u.; $\Delta E=20.50$ eV

$q = 2$ $s = 3$

Fe 0.40544400 -0.01681200 -0.06278200
C 2.31735000 -0.94344700 0.89549900
C 2.25265300 0.48180100 1.24808200
C 2.31581500 -1.04916400 -0.49678300
H 2.36995100 -1.75752900 1.60702200
C 2.22612000 1.25575400 0.05790700
H 2.24496700 0.86930600 2.26086700
C 2.26476000 0.33380300 -1.04887600
H 2.40998900 -1.95238500 -1.08545800
H 2.24507700 2.33488100 -0.00958800
H 2.34292100 0.59248800 -2.09959800
C -2.34786600 -1.18313100 -0.25097700
C -3.39424600 -0.63654900 0.56034000
C -1.53171700 -0.08687800 -0.80325100
H -2.21569200 -2.23829400 -0.47049500
C -3.30679200 0.76169300 0.50923300
H -4.13433400 -1.21413500 1.09825600
C -2.22763100 1.12626800 -0.35907400
H -1.23671100 -0.15823600 -1.86062200
H -3.96874200 1.46070400 1.00388400

H -2.00963300 2.13940100 -0.68451900

E=-185.843058710 a.u.; $\Delta E=20.49$ eV

$q = 2$ $s = 3$

Fe -0.41476300 -0.01521100 -0.37062100

C -1.93694500 -1.15410300 0.75393900

C -2.58048200 -0.79526300 -0.44094100

C -1.56544100 0.09132500 1.43558200

H -1.80180400 -2.15291600 1.14630700

C -2.62797400 0.68024400 -0.52604900

H -2.99994300 -1.47046100 -1.17730600

C -2.01126900 1.21646100 0.61381800

H -1.12176400 0.16465500 2.42304700

H -3.07981400 1.23785500 -1.33806300

H -1.92813000 2.26226400 0.87678700

C 2.21551600 -1.15933300 -0.35200500

C 1.54316900 -0.01200100 -0.96820900

C 3.11445700 -0.68375700 0.65532000

H 2.09498800 -2.19765700 -0.64594300

C 2.20493700 1.15670800 -0.38297100

H 1.33047600 -0.02671100 -2.04932600

C 3.10845300 0.71608300 0.63629600

H 3.71962500 -1.31113700 1.29651300

H 2.07502200 2.18570800 -0.70438400

H 3.70866100 1.36567700 1.25982800

E=-185.809008550 a.u.; $\Delta E=21.40$ eV

$q = 2$ $s = 3$

Fe -0.99494700 -0.36386100 0.53028300

C -2.82051200 0.98923400 0.65297200

C -3.30607900 -0.34513900 0.45528100

C -1.92751200 1.30543400 -0.42029700

H -3.09381700 1.64793900 1.46671100

C -2.72333600 -0.87673800 -0.74182600

H -3.99601400 -0.86708400 1.10611000

C -1.86725500 0.13783100 -1.30886700

H -1.46590300 2.26661600 -0.60537200

H -2.93001500 -1.84696900 -1.17418200

H -1.38735700 0.09988300 -2.27825800

C 3.17356600 -1.18395200 -0.21253500

C 2.30548800 -0.21812200 -0.82654200

C 4.17028800 -0.47300700 0.54127700

H 3.12604100 -2.25960800 -0.33562000

C 2.76999800 1.08247700 -0.45346900

H 1.55965900 -0.43368300 -1.58370400

C 3.92327100 0.91929100 0.39581100

H 4.98313500 -0.92259500 1.09742300

H 2.37187100 2.03129800 -0.79349100
H 4.51351700 1.72073400 0.82220900



E=-30.9306874373 a.u.

$q = 1 \quad s = 3$

C -1.09144100 -0.54284400 -0.00036800
C 0.17915800 -1.20599200 0.00044200
C -0.85376100 0.87014600 -0.00002100
H -2.06086100 -1.02486600 -0.00035100
C 1.20215200 -0.20216100 -0.00032400
H 0.33821000 -2.27678900 0.00082900
C 0.56390600 1.08080900 -0.00008800
H -1.61190200 1.64292200 0.00103000
H 2.26981400 -0.38162200 -0.00032800
H 1.06465800 2.04061200 0.00098100



E=-154.952136264 a.u.

$q = 1 \quad s = 3$

Fe 0.98414300 -0.24844600 -0.01520300
C -0.83421300 -0.12349600 -1.15452900
C -1.15717900 -0.97333000 -0.05791600
C -0.40586300 1.18470500 -0.63867400
H -0.93150900 -0.37689500 -2.20311400
C -0.83495700 -0.26536000 1.13145000
H -1.51730900 -1.99022000 -0.12120100
C -0.40260800 1.09713000 0.77602800
H -0.20068800 2.05938700 -1.23973700
H -0.93356600 -0.64234400 2.14194800
H -0.19572000 1.89176800 1.47922800

Orange path in Fig.4

E=-185.833806584 a.u. ; $\Delta E=20.79$ eV

$q = 2 \quad s = 3$

Fe 0.00001300 -1.33532100 -0.00055200
C -1.52001100 0.86458800 -1.15432500
C -1.38924000 1.68755400 -0.00093600
C -1.79316400 -0.48787100 -0.73184000
H -1.51641300 1.20327800 -2.18442600
C -1.51542200 0.86582200 1.15401600
H -1.28373600 2.76455100 -0.00163000
C -1.79030100 -0.48721900 0.73390500
H -2.26876500 -1.23671500 -1.36358300
H -1.50870400 1.20560700 2.18374200
H -2.26393400 -1.23523500 1.36815600

C 1.79317600 -0.48784100 -0.73184000
C 1.52000000 0.86461200 -1.15432500
C 1.79031300 -0.48718900 0.73390500
H 2.26879000 -1.23667700 -1.36358300
C 1.38919200 1.68757200 -0.00093600
H 1.51639100 1.20330200 -2.18442700
C 1.51541200 0.86584600 1.15401600
H 2.26396000 -1.23519700 1.36815500
H 1.28365000 2.76456500 -0.00163100
H 1.50868300 1.20563100 2.18374200

E=-185.825679471 a.u.; $\Delta E=21.01$ eV

$q = 2$ $s = 3$

Fe -0.00000300 -1.46326600 -0.06879000
C -1.72535600 0.75758700 -1.15654400
C -1.34266300 1.71591200 -0.20886800
C -1.85691200 -0.51935600 -0.49871500
H -1.95823600 0.94682200 -2.19718000
C -1.12056200 1.06233700 1.06966600
H -1.26680400 2.78224900 -0.38209600
C -1.49529300 -0.34288400 0.89792800
H -2.44539500 -1.34533200 -0.90075000
H -1.16177500 1.56929900 2.02817600
H -1.82247100 -0.97206700 1.72528800
C 1.85690900 -0.51936400 -0.49870800
C 1.72536200 0.75757700 -1.15654300
C 1.49528800 -0.34288600 0.89793300
H 2.44539100 -1.34534500 -0.90073700
C 1.34267300 1.71590700 -0.20887200
H 1.95824600 0.94680700 -2.19718000
C 1.12056300 1.06233800 1.06966400
H 1.82246100 -0.97206700 1.72529600
H 1.26682000 2.78224400 -0.38210300
H 1.16177300 1.56930300 2.02817200

E=-185.846673115 a.u.; $\Delta E=20.52$ eV

$q = 2$ $s = 3$

Fe -0.00061700 -1.49049900 0.16175700
C 1.97425800 0.72256500 1.05610300
C 1.32763000 1.69421400 0.31249600
C 1.99754000 -0.50897100 0.30147100
H 2.44510400 0.86558200 2.02079900
C 0.80518100 1.12174700 -0.98413700
H 1.24130400 2.73981400 0.58831800
C 1.32987900 -0.30793900 -0.94404200
H 2.64762700 -1.34965600 0.54427900
H 1.17328700 1.66722700 -1.86166400

H 1.50591800 -0.89449700 -1.84689900
C -1.99794300 -0.50762700 0.30138100
C -1.97358800 0.72377900 1.05621800
C -1.33018900 -0.30691900 -0.94416300
H -2.64894500 -1.34766900 0.54398100
C -1.32617000 1.69501600 0.31275000
H -2.44424100 0.86706600 2.02097000
C -0.80430400 1.12239700 -0.98404000
H -1.50669200 -0.89321100 -1.84710100
H -1.23889600 2.74046800 0.58883700
H -1.17217900 1.66827200 -1.86142400

E=-185.823335181 a.u. ; $\Delta E=21.13$ eV

q =2 s=3

Fe 2.36009000 -0.91561400 -0.43441000
C -3.76184800 -0.35481200 0.37761200
C -2.56050400 -0.66267600 1.03740800
C -3.46992700 0.06447900 -0.94474600
H -4.75239400 -0.43529000 0.80791000
C -1.38804600 -0.46998200 0.10636200
H -2.47566800 -0.99804500 2.06727000
C -2.08057400 0.02675400 -1.14322800
H -4.20290300 0.35198000 -1.68824700
H -0.94936900 -1.45959700 -0.10407900
H -1.57237100 0.28359500 -2.06807200
C 2.10103200 0.82799900 0.64090900
C 1.45308200 1.88626700 -0.14687400
C 1.11029200 -0.13556900 1.03462000
H 3.07019700 0.95518100 1.12688600
C 0.11006500 1.67899300 -0.16345300
H 1.97865900 2.72421700 -0.58567900
C -0.25332100 0.46496600 0.66901000
H 1.22340200 -0.77766000 1.90885200
H -0.62512800 2.33922200 -0.61088200
H -0.61827500 0.86385100 1.63498700

E=-185.826130616 a.u. ; $\Delta E=21.07$ eV

q =2 s=3

Fe 2.27130400 -0.99107200 -0.00477300
C -3.67047200 -0.08784800 -0.03481900
C -2.77894600 0.39432100 0.93401300
C -2.97075400 -0.95008500 -0.92040500
H -4.72412300 0.15441200 -0.09570900
C -1.41014200 -0.20476000 0.72837000
H -3.02973500 1.08053000 1.73791300
C -1.63077500 -1.03054700 -0.51883900
H -3.40669100 -1.46710500 -1.76612400

H -1.19151000 -0.85742300 1.59069600
H -0.86826000 -1.61525500 -1.02550600
C 2.03267300 1.06188800 -0.00256800
C 1.20566300 1.58580200 -1.09592100
C 1.17694500 0.46790500 0.98918400
H 3.05673600 1.39614100 0.17866400
C -0.11176600 1.45319200 -0.76873500
H 1.60263400 2.05205700 -1.98834000
C -0.26051300 0.84266100 0.60632800
H 1.46140400 0.36967800 2.03820500
H -0.94864900 1.80377000 -1.36360700
H -0.49720000 1.65590400 1.31824500

Fe⁺

E=-123.557125 a.u.

q =1 s =4

Fe 0.000000 0.000000 0.000000

C₁₀H₁₀⁺

E=-62.2659527058 a.u.

q =1 s =2

C 1.33052600 1.17444400 0.28065500
C 2.01648800 0.72047700 -0.82611900
C 0.79938200 0.00024600 1.06654200
H 1.22196000 2.20821100 0.58443600
C 2.01666500 -0.72039500 -0.82587800
H 2.50656500 1.34033300 -1.56552500
C 1.33082600 -1.17414900 0.28107100
H 1.16181100 0.00044200 2.10102400
H 2.50680500 -1.34041000 -1.56510900
H 1.22285100 -2.20782300 0.58537000
C -0.79895600 -0.00006200 1.06641700
C -1.33074700 1.17417200 0.28095200
C -1.33023600 -1.17443700 0.28077600
H -1.16166100 -0.00007500 2.10083600
C -2.01709600 0.72030900 -0.82560800
H -1.22230700 2.20784600 0.58512200
C -2.01675300 -0.72060500 -0.82569400
H -1.22159200 -2.20812200 0.58480100
H -2.50786600 1.33997300 -1.56467400
H -2.50716500 -1.34038200 -1.56496200

Blue path in Fig.4

E=-185.213898739 a.u.; ΔE=23.77 eV

q =2 s =4

Fe 0.01839800 -0.00472900 -0.25421800

C -1.93684400 0.71687900 -0.86804200
C -1.60360600 1.17616800 0.44747100
C -1.93699000 -0.72040100 -0.86216700
H -2.13788200 1.34614800 -1.72725600
C -1.41630300 0.00707100 1.28816000
H -1.55888300 2.20769500 0.77154000
C -1.60468500 -1.16927300 0.45809300
H -2.13916100 -1.35664500 -1.71596900
H -1.23162500 0.01181500 2.35527900
H -1.56301600 -2.19793200 0.79148400
C 2.00439200 -0.71795700 -0.77667500
C 2.00524200 0.71932300 -0.77786500
C 1.59963400 -1.18140200 0.52732100
H 2.25383000 -1.35392200 -1.61872200
C 1.59977800 1.18479400 0.52384600
H 2.25369900 1.35359700 -1.62146800
C 1.38266100 0.00279700 1.31702900
H 1.54394900 -2.20927400 0.85910400
H 1.54107300 2.21347800 0.85266600

E=-185.204601346 a.u.; $\Delta E=24.01$ eV

$q=2$ $s=4$

Fe -0.02447100 -0.00012700 -0.47569600
C 1.46545400 1.17880200 0.48792900
C 1.11834200 0.00008600 1.31589800
C 2.03326900 0.71935100 -0.73289600
H 1.38500000 2.21151300 0.80201800
C 1.46543400 -1.17870900 0.48803200
H 1.08012000 0.00012700 2.40423300
C 2.03325700 -0.71934900 -0.73284500
H 2.40635300 1.35135200 -1.52998500
H 1.38501800 -2.21139100 0.80222600
H 2.40636700 -1.35140900 -1.52987600
C -1.00104200 0.00016100 1.29817100
C -1.41773200 1.18582200 0.55401200
C -1.41775900 -1.18564400 0.55426400
C -2.15402000 0.71501800 -0.58626400
H -1.28673100 2.21772700 0.84909200
C -2.15401800 -0.71503500 -0.58613600
H -1.28680800 -2.21749300 0.84956300
H -2.64007800 1.34745700 -1.32021500
H -2.64010600 -1.34760100 -1.31995800

E=-185.232767608 a.u.; $\Delta E=23.28$ eV

$q=2$ $s=4$

Fe 0.21311400 -0.91942700 0.00158400
C -1.97274700 -0.66461600 -0.73259400

C -1.50364100 0.56738400 -1.18339100
C -1.97269600 -0.66197600 0.73506900
H -2.38694700 -1.44837000 -1.35766700
C -1.06493400 1.43187200 -0.00257000
H -1.46738800 0.88808500 -2.21922700
C -1.50359000 0.57165500 1.18139400
H -2.38684700 -1.44347600 1.36298800
H -1.43122800 2.46243900 -0.00442900
H -1.46730700 0.89609700 2.21606300
C 2.25891100 -0.12608800 0.70403300
C 2.25893400 -0.12864300 -0.70347700
C 1.15446800 0.70742800 1.15949300
H 2.98560600 -0.60601500 1.34767500
C 1.15449600 0.70321900 -1.16200900
H 2.98566200 -0.61088300 -1.34535100
C 0.47773400 1.24622200 -0.00225600
H 0.95292000 0.94825000 2.19573300
H 0.95296000 0.94024400 -2.19912700

E=-185.230814220 a.u.; $\Delta E=23.32$ eV

$q=2$ $s=4$

H -2.67314800 -0.03154000 -1.88169200
H -1.85153000 2.24688700 -0.78373000
H -2.31240900 -2.03782300 -0.10452000
H -1.41762800 1.63404500 1.81119500
H -1.22412700 -1.05507600 2.11336200
H 3.16234300 -1.06561100 0.52074100
H 2.89463500 0.65752200 -1.53599900
H 1.14847900 -0.60148200 2.26154600
H 0.69775000 2.15788000 -1.14354100
C -2.17872700 0.07211200 -0.92358800
C -1.75701700 1.25716900 -0.34935500
C -1.95250300 -1.02033400 0.02198600
C -1.09330100 0.98157700 0.99350500
C -1.37306700 -0.51300600 1.18625700
C 2.34762500 -0.36811300 0.37508500
C 2.21140600 0.55265400 -0.70093600
C 1.26298000 -0.14230100 1.28711100
C 1.03035200 1.36638100 -0.48529100
C 0.42164900 0.94794900 0.72957100
Fe 0.30997100 -0.79651200 -0.54090100

E=-185.248870273 a.u.; $\Delta E=22.84$ eV

$q=2$ $s=4$

H -3.65248300 0.24446200 -1.35927300
H -2.33716900 2.32812300 -0.35885800
H -2.68280100 -1.99616400 -0.30948300

H -1.25619800 1.24137900 1.86361000
H -1.04076500 -1.33319600 1.68551400
H 3.56492000 0.23997200 0.51621200
H 2.61816300 0.33443800 -2.01767600
H 1.56988700 0.82330600 2.21636600
H 0.00216400 0.99873200 -1.93567500
C -2.83458000 0.20163900 -0.65224700
C -2.17024400 1.28418900 -0.11247000
C -2.29208300 -1.00268100 -0.10586000
C -1.12500200 0.82447700 0.85774200
C -1.23658200 -0.72029800 0.79822000
C 2.54037000 0.46619100 0.24637000
C 2.02221800 0.49116100 -1.12704000
C 1.50339300 0.76058600 1.13766500
C 0.65404800 0.81054200 -1.09163800
C 0.28715500 0.94075000 0.34482500
Fe 0.73546600 -1.04693800 -0.07977500

E=-185.236867781 a.u.; $\Delta E=23.16$ eV

$q=2$ $s=4$

H -3.93266700 -0.53909000 1.32153700
H -2.30665500 -2.31728300 0.17555800
H -3.25313600 1.92049100 0.52245400
H -1.40333800 -0.87407900 -1.91318800
H -1.31654100 1.73633100 -1.30538100
H 3.42206400 -1.14186000 -0.47449700
H 2.48022500 -0.77486900 2.03907300
H 1.35316700 -1.07365000 -2.19386300
H -0.20517000 -0.44307900 1.89227000
C -3.11256600 -0.30872100 0.65284600
C -2.28602000 -1.24162200 0.03646800
C -2.74839500 1.00931400 0.22387400
C -1.31508200 -0.53246500 -0.87413700
C -1.70539900 0.92362800 -0.69605900
C 2.38532600 -0.96854000 -0.21232100
C 1.88662200 -0.74738400 1.13398800
C 1.29378200 -0.93391600 -1.12154200
C 0.47572900 -0.55561700 1.05622700
C 0.09489200 -0.67862700 -0.36804000
Fe 1.35956600 1.06580000 0.03647000

E=-185.238715321 a.u.; $\Delta E= 23.12$ eV

$q=2$ $s=4$

H 4.22861500 -1.00044300 -0.91984000
H 2.22052300 -2.20968000 0.35823000
H 3.88252400 1.64985300 -0.79050900
H 1.43212500 -0.14554400 1.92918300

H 1.66606200 2.18110400 0.57211900
H -3.02154700 -1.78298000 0.29741100
H -2.22383500 -0.89303500 -2.15777000
H -1.05112600 -1.23190400 2.06863400
H 0.24025400 0.17884800 -1.89048600
C 3.39233100 -0.50176900 -0.44510600
C 2.35926000 -1.13991500 0.24286500
C 3.20800900 0.91227400 -0.37372200
C 1.42307100 -0.09845000 0.83030700
C 2.05035000 1.19080400 0.34860000
C -2.10600700 -1.24516900 0.08328600
C -1.67893400 -0.77125000 -1.23020700
C -1.04754900 -0.97374500 1.01664200
C -0.36425600 -0.22679100 -1.08737700
C 0.04356800 -0.37617400 0.29687300
Fe -1.96356400 0.87057300 0.09384800

$C_{10}H_3^+$

E=-61.6545828702 a.u.

q =1 s =1

C 1.78370400 0.13565700 -1.13740900
C 0.87283600 -0.93574600 -0.74271500
C 2.33342900 0.73966700 0.00041000
H 1.95186500 0.44284300 -2.16353100
C 0.87260000 -0.93584100 0.74286100
H 0.68143200 -1.80459700 -1.35766000
C 1.78335300 0.13551700 1.13797800
H 3.00903900 1.58340800 0.00056600
H 0.68104800 -1.80478900 1.35762500
H 1.95117900 0.44258200 2.16419100
C -2.68277900 -0.14029700 -0.00044500
C -2.11503800 1.21736400 -0.00027100
C -1.67018400 -1.06907600 -0.00031100
H -3.74293000 -0.36219900 -0.00064100
C -0.76450600 1.13094800 -0.00003900
H -2.70041100 2.12576800 -0.00032600
C -0.41465400 -0.34837400 -0.00005700
H -1.76958200 -2.14573100 -0.00037600
H -0.05420300 1.94381100 0.00013100

Fe^+

E=-123.557125 a.u.

q =1 s =4

Fe 0.000000 0.000000 0.000000

H

E=-0.501565819087 a.u.

$q=0$ $s=2$

H 0.000000 0.000000 0.000000

Black path in Fig.5

E=-185.785620501 a.u.; $\Delta E= 20.06\text{eV}$

$q=2$ $s=3$

Fe -0.00144700 -0.00019300 -0.06733500

C -1.71797200 1.22568000 -0.12192900

C -1.67626400 0.58153300 1.16155500

C -1.77789900 0.19867800 -1.13072300

H -1.72058100 2.29404300 -0.29676900

C -1.70694100 -0.83555400 0.95707700

H -1.61719700 1.08340300 2.11978300

C -1.76258800 -1.08115200 -0.45586800

H -1.83579200 0.35489000 -2.20009400

H -1.68694500 -1.58995300 1.73381700

H -1.81036900 -2.05204400 -0.93280500

C 1.41046300 0.18532300 -1.32514700

C 1.71744600 1.21384800 -0.35304300

C 1.56853300 -1.20760700 -0.47253500

H 2.40455900 -0.76856800 -1.26926500

C 1.95337300 0.63872300 0.93382100

H 1.76400300 2.26769500 -0.59424600

C 1.83508500 -0.77583200 0.88533700

H 1.37513100 -2.20775500 -0.84393900

H 2.15922800 1.20777200 1.83311400

H 1.94616100 -1.44630300 1.72983800

E=-185.805595768 a.u.; $\Delta E= 21.60\text{eV}$

$q=2$ $s=3$

Fe -0.02117500 -0.14344500 0.01022900

C -1.52379500 1.24204000 -0.31667400

C -1.65367500 0.75762100 1.04370500

C -1.68482400 0.12265100 -1.21267500

H -1.36670000 2.27419900 -0.60450400

C -1.88898500 -0.64159600 0.98392800

H -1.59039100 1.36068400 1.94039000

C -1.89310600 -1.04307000 -0.40347700

H -1.66969900 0.15657700 -2.29388500

H -2.01330900 -1.30297800 1.83326300

H -2.04279500 -2.05161900 -0.77033100

C 1.54428600 -0.12649000 -1.27208100

C 1.62149700 1.13327400 -0.66736700

C 1.79544200 -1.22439800 -0.26765500

H 2.64202300 -1.89149300 -0.50232200

C 1.82435300 0.92920000 0.75904700

H 1.54412200 2.09175200 -1.16498100

C 1.88559700 -0.44144200 1.02847600
H 0.95675700 -1.98452400 -0.25563500
H 1.89893400 1.72030300 1.49568900
H 2.03085700 -0.89008800 2.00500600

E=-185.791282075 a.u.; $\Delta E=21.94$ eV

$q=2$ $s=3$

Fe -0.14746900 -0.14912900 -0.00416200
C -1.67674600 1.26697300 -0.22945700
C -1.81483200 0.75943700 1.12353300
C -1.85206600 0.15741300 -1.14048700
H -1.52883800 2.30387900 -0.50471100
C -2.06013400 -0.63427100 1.05332700
H -1.73874900 1.35209900 2.02693400
C -2.06046700 -1.02703300 -0.33266000
H -1.85894900 0.20571300 -2.22129500
H -2.19536800 -1.30092500 1.89634100
H -2.22354400 -2.02982900 -0.70941600
C 1.27752800 -0.09312000 -1.15648100
C 1.66481100 1.14268900 -0.59760800
C 1.85319900 -1.23083700 -0.30979200
H 2.49986700 -1.88689800 -0.91791000
C 2.46787000 0.87978000 0.58901100
H 1.46649900 2.12368700 -1.01272400
C 2.57343700 -0.48573100 0.78946300
H 1.09966000 -1.97433100 0.05299000
H 2.93680800 1.64819400 1.19176200
H 3.14120100 -0.97603000 1.57314700

E=-185.841958065 a.u.; $\Delta E=20.57$ eV

$q=2$ $s=3$

Fe 0.50672500 -0.25581200 0.00004700
C -2.37500700 -1.22463900 -0.00002700
C -3.69982600 -0.53548300 -0.00002900
C -1.37854200 -0.05675700 -0.00000600
H -2.26646600 -1.88716700 0.87217900
C -3.52943000 0.85574400 -0.00001400
H -4.65177900 -1.05925600 -0.00005900
C -2.14761800 1.14467600 0.00002900
H -2.26647600 -1.88717400 -0.87223100
H -4.32682000 1.58795600 -0.00003100
H -1.74121200 2.14999500 0.00009200
C 1.85548600 1.32896900 -0.00016800
C 2.17285100 0.52500100 1.18315500
C 2.17294900 0.52481900 -1.18326800
H 1.54645900 2.36823600 -0.00021000
C 2.66257200 -0.71805700 0.72743500

H 2.09381500 0.85517400 2.21034400
C 2.66262500 -0.71817600 -0.72728300
H 2.09392600 0.85475200 -2.21053300
H 2.98363000 -1.54388700 1.35031300
H 2.98370900 -1.54411300 -1.35001000

Orange path in Fig.5

-185.844207145 a.u.; $\Delta E=20.56$ eV

$q=2$ $s=3$

Fe -0.30351600 -1.31389200 -0.41855600
C -1.16479800 1.53622700 -0.54506300
C -2.59260300 1.07291900 -0.58334600
C -0.51617000 0.56780000 0.43333200
H -0.68817400 1.61299600 -1.53243100
C -2.79399500 0.03927800 0.31954000
H -3.35635900 1.53164100 -1.20172700
C -1.55241400 -0.26134900 0.99082800
H -1.11381300 2.56141800 -0.13557900
H -3.73828900 -0.45082800 0.52085700
H -1.47373600 -0.84101000 1.90939000
C 2.84739600 0.89141200 -0.42815100
C 1.82971000 1.55187400 0.22858900
C 2.67868300 -0.51619400 -0.25620800
H 3.65900900 1.35544100 -0.97252900
C 0.92454800 0.57965900 0.91627700
H 1.68124300 2.62698600 0.24714600
C 1.51683100 -0.79844900 0.50081200
H 3.38759600 -1.26389700 -0.59975200
H 0.97446900 0.71172500 2.01064200
H 1.49634700 -1.66233300 1.17678400

$E=-185.847985784$ a.u.; $\Delta E=20.56$ eV

$q=2$ $s=3$

Fe 2.87465700 -0.64199600 -0.12866800
C -2.81378000 0.97785900 0.29904800
C -3.77842900 0.03158300 0.65093200
C -1.84727500 0.37381200 -0.70314700
H -2.74576900 1.99504200 0.67046800
C -3.51467400 -1.18909800 -0.03581500
H -4.61417500 0.20729600 1.31676400
C -2.37468000 -1.03761400 -0.82658800
H -1.93680500 0.89231800 -1.67038400
H -4.12129100 -2.08391200 0.02675200
H -1.92910900 -1.79907000 -1.45790700
C -0.42815400 0.45783300 -0.19678100
C 0.07062200 -0.19625500 0.90513900

C 0.62784700 1.35240500 -0.79595400
H 0.33666700 2.41474700 -0.73753100
C 1.45527700 0.22208400 1.13951800
H -0.46958000 -0.87907800 1.55221200
C 1.83609900 1.12987800 0.09638600
H 0.78896100 1.17524600 -1.86887000
H 1.93659900 0.15004700 2.11559900
H 2.61630000 1.88432900 0.20184200

E=-185.802053269 a.u.; $\Delta E=21.72$ eV

$q=2$ $s=3$

Fe 4.48627100 -0.50131400 -0.09141900
C -3.47781500 0.79482000 0.21424600
C -4.28947900 -0.25040800 0.62901500
C -2.46130400 0.27716500 -0.78535100
H -3.53027000 1.82700300 0.54058800
C -3.88339100 -1.45937700 -0.02685700
H -5.12468700 -0.16302500 1.31241700
C -2.80691600 -1.19337300 -0.85815400
H -2.57517200 0.76439300 -1.76263100
H -4.36709300 -2.42096300 0.08889500
H -2.27510300 -1.90688400 -1.47656200
C -1.08496800 0.48764600 -0.22655300
C -0.59351000 -0.07545000 0.94394100
C -0.03483300 1.39406900 -0.81257900
H -0.39048200 2.43260600 -0.89814900
C 0.73908600 0.41772400 1.18483000
H -1.12939200 -0.75441500 1.59798500
C 1.09535800 1.28147700 0.17142900
H 0.23871400 1.10798600 -1.83881500
H 1.31681400 0.19228000 2.07339900
H 1.98025100 1.90942200 0.13596200

Fe⁺

E=-123.557125 a.u.

$q=1$ $s=4$

Fe 0.000000 0.000000 0.000000

C₁₀H₁₀⁺

E=-62.2659527058 a.u.

$q=1$ $s=2$

C 1.33052600 1.17444400 0.28065500
C 2.01648800 0.72047700 -0.82611900
C 0.79938200 0.00024600 1.06654200
H 1.22196000 2.20821100 0.58443600
C 2.01666500 -0.72039500 -0.82587800
H 2.50656500 1.34033300 -1.56552500

C 1.33082600 -1.17414900 0.28107100
 H 1.16181100 0.00044200 2.10102400
 H 2.50680500 -1.34041000 -1.56510900
 H 1.22285100 -2.20782300 0.58537000
 C -0.79895600 -0.00006200 1.06641700
 C -1.33074700 1.17417200 0.28095200
 C -1.33023600 -1.17443700 0.28077600
 H -1.16166100 -0.00007500 2.10083600
 C -2.01709600 0.72030900 -0.82560800
 H -1.22230700 2.20784600 0.58512200
 C -2.01675300 -0.72060500 -0.82569400
 H -1.22159200 -2.20812200 0.58480100
 H -2.50786600 1.33997300 -1.56467400
 H -2.50716500 -1.34038200 -1.56496200

Blue path in Fig.5

E=-185.199676432 a.u.; $\Delta E=24.05$ eV

$q=2$ $s=4$

Fe -0.48094700 -0.27159900 -0.00016500
 C 2.34069000 -1.18118800 -0.00019600
 C 3.66926800 -0.65192900 0.00024800
 C 1.38657800 -0.06611700 -0.00043800
 H 2.10568900 -2.24030000 -0.00035600
 C 3.59149900 0.76415600 0.00031300
 H 4.57887700 -1.24087900 0.00059200
 C 2.21381800 1.14068700 -0.00030000
 H 4.43333100 1.44586800 0.00076800
 H 1.85416400 2.16334900 -0.00060500
 C -1.80550300 1.33071600 0.00013400
 C -2.13468700 0.53084200 -1.18235700
 C -2.13428400 0.53076100 1.18268400
 H -1.48244200 2.36557000 0.00012200
 C -2.64217300 -0.70665500 -0.72603900
 H -2.04964000 0.85838500 -2.21001500
 C -2.64191800 -0.70670600 0.72645200
 H -2.04889000 0.85825100 2.21033000
 H -2.97332700 -1.52798100 -1.34963400
 H -2.97286000 -1.52808000 1.35009800

E=-185.187942701 a.u.; $\Delta E=24.38$ eV

$q=2$ $s=4$

Fe -0.69000200 -0.35210600 -0.84674200
 C 1.98242400 -1.14352400 0.19724200
 C 3.32165500 -0.62487900 0.16224800
 C 1.07496800 -0.04398700 -0.09259900
 H 1.71851800 -2.17852500 0.38844100

C 3.25894200 0.77268000 0.00864600
H 4.22280900 -1.22222700 0.22367800
C 1.88186100 1.16576500 -0.03416300
H 4.10277400 1.44346400 -0.09153500
H 1.52446300 2.18862700 -0.07713300
C -0.73818300 0.33933300 1.23198800
C -1.36577600 1.37253000 0.39173000
C -1.58918100 -0.85786000 1.10990600
H -0.05426400 0.51569400 2.05379400
C -2.53407400 0.82806000 -0.18978400
H -1.01519800 2.39057700 0.28104800
C -2.69051400 -0.53309000 0.28164300
H -1.43722000 -1.78872300 1.64205000
H -3.22584000 1.35278300 -0.83598400
H -3.50871400 -1.19708700 0.02980900

E=-185.219415857 a.u.; $\Delta E=23.58$ eV

q =2 s =4

Fe -0.61899300 -0.00079300 -1.04990500
C 1.76113000 -1.15838900 0.27823600
C 3.08228600 -0.69841700 -0.04934700
C 0.89219800 0.00012900 0.41347000
H 1.48088200 -2.19618700 0.43023500
C 3.08236900 0.69839600 -0.05017500
H 3.93098900 -1.33926700 -0.24822900
C 1.76155700 1.15887200 0.27684600
H 3.93122800 1.33877200 -0.24988000
H 1.48097600 2.19679300 0.42740000
C -0.47113200 0.00068400 1.15974600
C -1.32569100 1.20023200 0.71440000
C -1.32593700 -1.19929700 0.71527300
H -0.33670600 0.00094100 2.25591900
C -2.52516100 0.73477500 0.20034100
H -1.06718300 2.23404500 0.90760900
C -2.52533300 -0.73402900 0.20088100
H -1.06745000 -2.23290400 0.90955500
H -3.34816100 1.34839900 -0.14705300
H -3.34848000 -1.34771100 -0.14607700

E=-185.218502064 a.u.; $\Delta E=23.60$ eV

q =2 s =4

Fe 0.51082800 -0.41814000 0.93306100
C -1.54551200 -1.01985600 -0.50569300
C -2.90340500 -0.77459000 -0.03026200
C -0.86771700 0.22834700 -0.51514000
H -1.19757800 -1.96255000 -0.91443500
C -3.07412600 0.60190200 0.18604100

H -3.65526900 -1.54295400 0.10421500
C -1.85718100 1.25643200 -0.10394000
H -3.98345600 1.08429100 0.51592100
H -1.67289100 2.32473700 -0.05177800
C 0.53011100 0.49938200 -1.10178200
C 1.32793400 1.40069000 -0.13256100
C 1.37172200 -0.78307100 -1.12594400
H 0.47529700 0.95220200 -2.10825300
C 2.49282700 0.74780900 0.23368900
H 1.05886100 2.42346400 0.10168700
C 2.51646200 -0.59242300 -0.36757900
H 1.14806700 -1.64107000 -1.74807400
H 3.27599400 1.15179000 0.86490600
H 3.32274500 -1.30601500 -0.24476500

E=-185.230237423 a.u.; $\Delta E=23.31$ eV

$q = 2$ $s = 4$

Fe -0.46388200 -1.07905900 -0.46812200
C 1.19314900 -0.66934200 0.77225100
C 2.56762100 -0.82884300 0.33907800
C 0.83848400 0.69687400 0.39081700
H 0.85114600 -1.13824100 1.69821200
C 3.00027000 0.35582500 -0.34897600
H 3.18768200 -1.69666200 0.54125600
C 1.96131900 1.27439700 -0.34352000
H 3.97321600 0.49165200 -0.80127000
H 1.97183200 2.25806500 -0.79821500
C -0.53416700 1.31920600 0.59435400
C -1.14849000 1.26469400 -0.80801700
C -1.44455700 0.39851100 1.38803200
H -0.48809100 2.33769200 1.00700600
C -2.21799000 0.38011400 -0.80429200
H -0.79391800 1.85108700 -1.64893700
C -2.41247800 -0.14014500 0.56809500
H -1.34083900 0.22565900 2.45371500
H -2.88388300 0.19403900 -1.64103700
H -3.23518400 -0.77551000 0.87351400

E=-185.220927650 a.u.; $\Delta E=23.55$ eV

$q = 2$ $s = 4$

Fe 0.55963600 -1.30013800 -0.37933100
C -2.02325900 1.39501800 -0.11003400
C -3.04122400 0.48457200 -0.39173500
C -0.93165300 0.68137400 0.49243500
H -2.04652800 2.45817100 -0.31585200
C -2.62221500 -0.82528000 0.00683300
H -3.99873500 0.72003000 -0.83729600

C -1.26762400 -0.74580900 0.54958300
H -3.23547800 -1.71946700 -0.02714300
H -1.04100600 -1.33067000 1.45124100
C 0.46613400 1.18017700 0.75931300
C 1.42845000 0.06222600 1.18404400
C 1.07581500 1.64533100 -0.55719300
H 0.48671100 1.99412600 1.50613000
C 2.49801300 0.02868100 0.27958800
H 1.43368600 -0.38733200 2.17350600
C 2.23672500 0.94558500 -0.81843100
H 0.63903300 2.41735300 -1.18159500
H 3.40736800 -0.55399400 0.39724200
H 2.88942700 1.09412500 -1.67003800

E=-185.227936913 a.u.; $\Delta E=23.36$ eV

$q=2$ $s=4$

Fe -0.10350500 -1.59620300 -0.34910400
C -1.43097800 1.73771400 -0.30778500
C -2.71093600 1.20933400 -0.48861700
C -0.65263700 0.79492800 0.42807300
H -1.09008600 2.69747600 -0.67308200
C -2.77751000 -0.09607700 0.12144500
H -3.53533700 1.69793700 -0.99244300
C -1.49304600 -0.41256400 0.67982800
H -3.66915400 -0.70956300 0.19199400
H -1.42266000 -0.97103300 1.62146900
C 0.80047900 0.83901300 0.81049900
C 1.47104100 -0.55549400 0.63711700
C 1.67937200 1.73795200 -0.01613300
H 0.88611500 1.14078300 1.87466400
C 2.64242300 -0.33118300 -0.12355000
H 1.50555700 -1.26514700 1.47583900
C 2.73658100 1.03511500 -0.54086500
H 1.48868900 2.79669200 -0.15768600
H 3.40607000 -1.08011000 -0.31505700
H 3.53320600 1.44181500 -1.14905300

$C_{10}H_9^+$

E=-61.6545828702 a.u.

$q=1$ $s=1$

C 1.78370400 0.13565700 -1.13740900
C 0.87283600 -0.93574600 -0.74271500
C 2.33342900 0.73966700 0.00041000
H 1.95186500 0.44284300 -2.16353100
C 0.87260000 -0.93584100 0.74286100
H 0.68143200 -1.80459700 -1.35766000
C 1.78335300 0.13551700 1.13797800

H 3.00903900 1.58340800 0.00056600
H 0.68104800 -1.80478900 1.35762500
H 1.95117900 0.44258200 2.16419100
C -2.68277900 -0.14029700 -0.00044500
C -2.11503800 1.21736400 -0.00027100
C -1.67018400 -1.06907600 -0.00031100
H -3.74293000 -0.36219900 -0.00064100
C -0.76450600 1.13094800 -0.00003900
H -2.70041100 2.12576800 -0.00032600
C -0.41465400 -0.34837400 -0.00005700
H -1.76958200 -2.14573100 -0.00037600
H -0.05420300 1.94381100 0.00013100

Fe⁺

E=-123.557125 a.u.

q =1 s =4

Fe 0.000000 0.000000 0.000000

H

E=-0.501565819087 a.u.

q =0 s =2

H 0.000000 0.000000 0.000000

Green path in Fig.5

E=-185.763524379 a.u.; $\Delta E=22.68$ eV

q =2 s =3

Fe 1.35027800 -0.48508200 -0.63877900
C -2.94660800 1.13469600 -0.00738100
C -4.35397300 0.95163300 -0.02946600
C -2.35584500 -0.13579600 0.05024800
H -2.43802200 2.08925700 -0.02955700
C -4.64704100 -0.42555100 0.03755600
H -5.08615100 1.74774900 -0.08462200
C -3.37417700 -1.22819100 0.11026000
H -3.29826900 -1.96004900 -0.70591400
H -5.63987100 -0.86497400 0.03628400
H -3.31418300 -1.82360900 1.03326200
C 3.02376000 -0.73753600 0.84646300
C 3.56465600 0.03974600 -0.22875700
C 1.87537300 -0.04917000 1.36692000
H 3.42481600 -1.67126200 1.21773300
C 2.76340100 1.21281300 -0.39687900
H 4.43094600 -0.22273500 -0.82201200
C 1.70925600 1.18054700 0.58865600
H 1.30739300 -0.32799200 2.24428700
H 2.93974300 2.00627700 -1.11086300
H 1.01355000 1.98032600 0.80393300

E=-30.8776216164 a.u.

q =1 s =3

C 1.14338500 -0.58169700 -0.00002800
C 0.88194300 0.80996700 -0.00012300
C -0.09569500 -1.23937700 -0.00008800
H 2.11709400 -1.05277600 0.00018700
C -0.51274400 1.02406000 0.00021800
H 1.63558000 1.58699700 0.00013300
C -1.24108800 -0.29531800 -0.00017000
H -1.90204700 -0.41575000 -0.87045700
H -1.00558200 1.99083900 -0.00083700
H -1.89985800 -0.41512100 0.87211900

E=-154.952136264 a.u.

q =1 s =3

Fe 0.98414300 -0.24844600 -0.01520300
C -0.83421300 -0.12349600 -1.15452900
C -1.15717900 -0.97333000 -0.05791600
C -0.40586300 1.18470500 -0.63867400
H -0.93150900 -0.37689500 -2.20311400
C -0.83495700 -0.26536000 1.13145000
H -1.51730900 -1.99022000 -0.12120100
C -0.40260800 1.09713000 0.77602800
H -0.20068800 2.05938700 -1.23973700
H -0.93356600 -0.64234400 2.14194800
H -0.19572000 1.89176800 1.47922800

II. MOLECULAR DYNAMICS SIMULATIONS

Table S1 summarises the results obtained with the molecular dynamics simulations. At the lowest excitation energy considered, $E_{exc} = 10$ eV, 100% of the trajectories do not undergo fragmentation within the propagation time. Increasing E_{exc} up to 20 eV reflects a variety of processes that have been grouped in five categories (see Figure S1): (a) intact doubly-charged ferrocene with the same atomic connectivity; (b) still keeping the $[\text{Fe}(\text{C}_5\text{H}_5)_2]^{2+}$ stoichiometry we observe isomerization, where one of the cyclopentadienyl rings undergoes fragmentation but remains bonded to the Fe atom forming a complex, (c) H migration, where one the H atoms in one of the cyclopentadienyl rings forms a new bond with other C atom, and the C atom where the migrated H was originally bonded is now directly linked to the Fe atom; (d) fragmentation is also observed, mainly populating the channel $\text{FeC}_5\text{H}_5^+/\text{C}_5\text{H}_5^+$, i.e. the loss of one of the cyclopentadienyl rings, with a 30% of probability; and (e) H migration from one ring to other, subsequently followed by the lost of the C_5H_4^+ moiety.

TABLE S1. Populated channels in the MD simulations

Channel	10 eV	20 eV
$[\text{Fe}(\text{C}_5\text{H}_5)_2]^{2+}$: $[\text{Fe}(\text{Cp})_2]^{2+}$	100%	50%
$[\text{FeC}_{10}\text{H}_{10}]^{2+}$: isomerization	–	10%
$[\text{FeC}_{10}\text{H}_{10}]^{2+}$: H migration	–	8%
$[\text{Fe}(\text{Cp})]^+ / [\text{Cp}]^+$	–	30%
$[\text{Fe}(\text{Cp} + \text{H})]^+ / [\text{C}_5\text{H}_4]^+$	–	2%

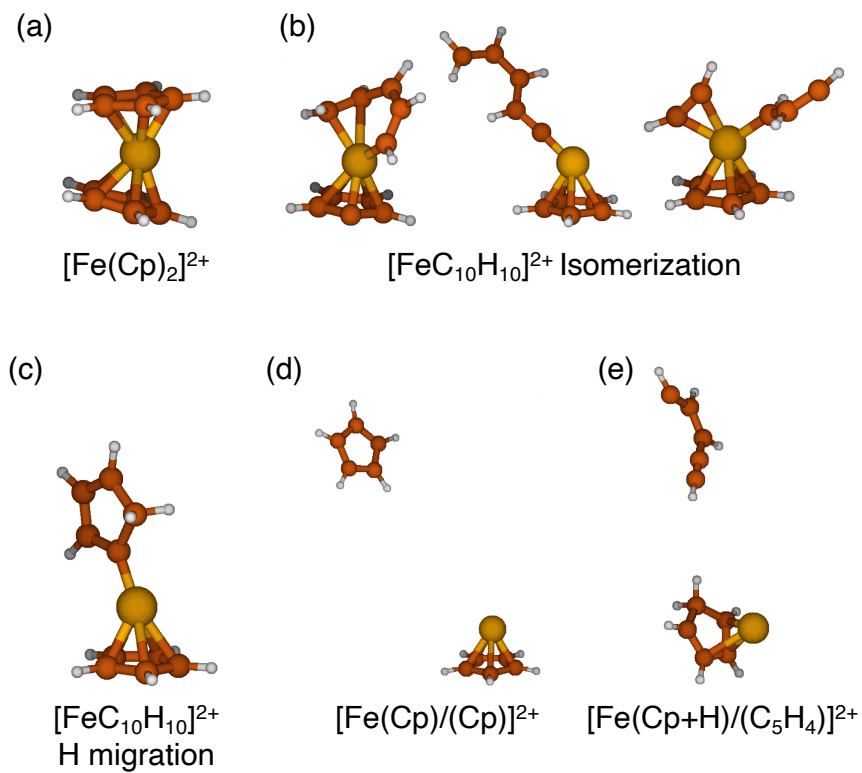


FIG. S1. Channels identified in the molecular dynamics. The structures shown in the figure correspond to that obtained after geometry optimisation from the last step of some selected trajectories.