

Experimental and Theoretical Investigations into the Mechanisms of Haliranium Ion π -Ligand Exchange Reactions with Cyclic Alkenes in the Gas Phase

SUPPORTING INFORMATION

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Experimental

A known flow of helium ($500\text{--}1200\text{ cm}^3\text{ min}^{-1}$; 99.999%, Coregas) is passed through a copper tube ($\sim 3\text{ m}$), and a measured flow of neutral reagent ($1\text{--}10\text{ }\mu\text{L hr}^{-1}$) is injected *via* a septum downstream from a gas tight syringe using a syringe drive (Pump 11 Elite, Harvard Apparatus). The helium pressure regulator that controls the flow of helium into the ion trap under normal operating conditions is bypassed, and instead the helium pressure is controlled manually by matching the pressure in the vacuum chamber surrounding the ion trap ($2 \times 10^{-5}\text{ Torr}$), measured using an ion gauge, to that under normal operating conditions. The injection port and subsequent, coiled copper tubing is heated to about $20\text{--}30^\circ\text{C}$ above the boiling point of the corresponding neutral to ensure efficient vaporisation of the reagent into the helium flow. This is achieved by applying a variable voltage ($0\text{--}260\text{V}$) to heating tape wrapped around the copper tubing (Powertech Variac SRV – 5).

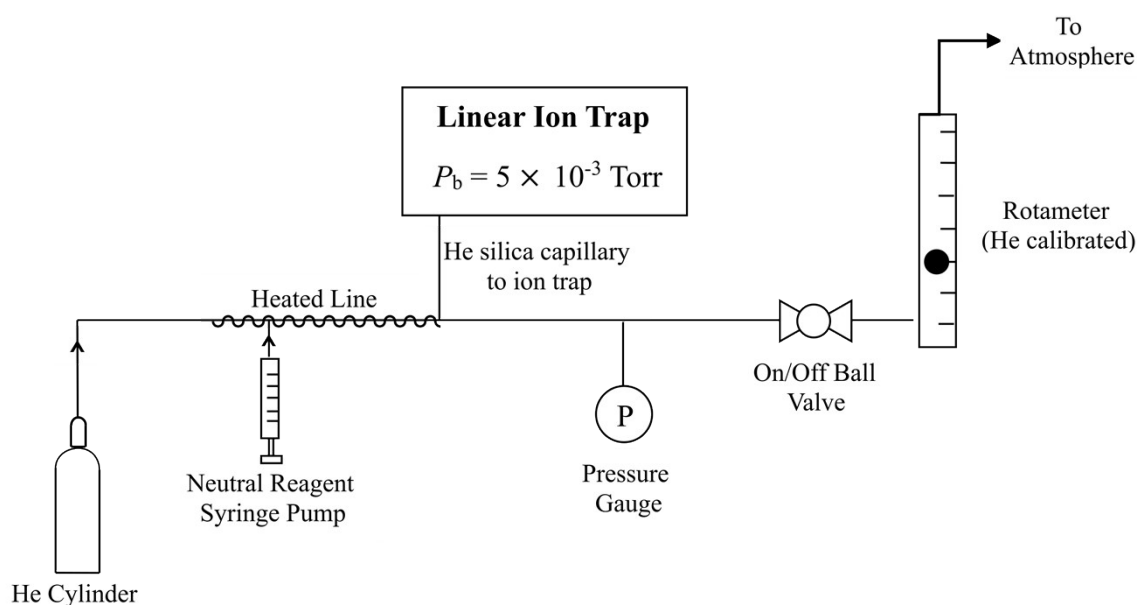


Figure S1. Schematic of apparatus utilized to add neutral reagents to the ion trap for ion-molecule reactions *via* the helium gas line.

The composition of this external mixture is calculated using the known molar flow rates of helium and neutral reagent. A small fraction of this mixture is carried through a silica capillary into the ion trap, whilst the remainder exits through a flowmeter (P single flow tube rotameter, He calibrated, Aalborg) allowing variation of the helium flowrate. The restriction capillary maintains the pressure of the ion trap at $P_b = 5 \times 10^{-3}\text{ Torr}$ in the region where IMR occur.¹ This mixture of helium and neutral reagent effuse out of the ion trap into the vacuum manifold and since the lighter helium atoms effuse more rapidly and are lost at greater rate, then the steady-state solution of the differential equations describing the molar flow of neutral reagents about the ion trap (i.e. the “flux” of neutral reagents) allows the equilibrium pressure of neutral reagents, P_n (Torr), to be calculated (Eq. S1).² Once an appropriate flow of this mixture was established, the reagent pressure was allowed to equilibrate (typically $1\text{--}2$ hours) prior to kinetic measurements.

$$P_n = P_b \times \frac{\text{molar flow rate of neutral}}{\text{molar flow rate of helium}} \times \sqrt{\frac{\text{molar mass of neutral}}{\text{molar mass of helium}}}$$

Eq. S1

Theoretical Collision Rates – Average Dipole Orientation (ADO) Theory

The ADO rate, k_{ADO} , is dependent on the charge of the ion (q), the reduced mass of the reactants (μ), the polarizability (α) and permanent dipole moment (μ_{D}) of the neutral, and can be calculated according to the following equation S2:

$$k_{\text{ADO}} = (2\pi q / \mu^{1/2}) [\alpha^{1/2} + C\mu_{\text{D}}(2/\pi kT)^{1/2}], \quad \text{Eq. S2}$$

where C has been parametrized to have a value between 0 and 1 with the expression $f(\mu_{\text{D}}/\alpha^{1/2})$. Experimental data has been used for the polarizability and permanent dipole moment where available, but the polarizability has not been measured for *cis*-cyclooctene (**Table S1**). Instead, this quantity has been calculated from the atomic hybrid polarisabilities (ahp) using the additivity method discussed by Miller,³ with comparison included for cyclohexene.

Table S1. Experimental permanent dipole moments (μ) and comparison of experimental and calculated polarizabilities (α) for cyclohexene and *cis*-cyclooctene

Neutral	μ_{D} (D)		α (amu Å ²)	
	Experimental ^{4, 5}	Experimental ⁶	Experimental ⁶	Calculated ³
Cyclohexene	0.331	10.73	10.73	10.82
<i>cis</i> -Cyclooctene	0.43			14.49 [#]

[#]calculated from (2 CTR × 1.352 ahp) + (6 CTE × 1.061 ahp) + (14 H × 0.387 ahp). See SI reference 3 for further information.

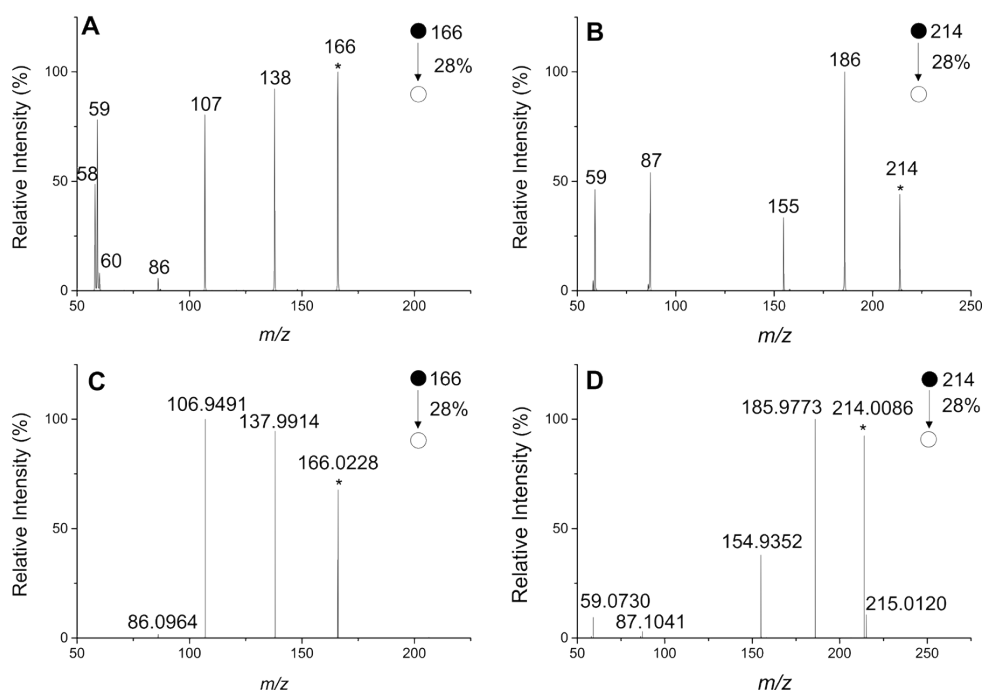


Figure S2. MS² of (A) CID of (2-bromoethyl)trimethylammonium ion, ⁷⁹BrCH₂CH₂NMe₃⁺ **10.Br** (*m/z* 166, *), to give the bromiranium ion, *c*-C₂H₄Br⁺ **6.Br** (*m/z* 107), and (B) CID of (2-iodoethyl)trimethylammonium ion, ICH₂CH₂NMe₃⁺ **10.I** (*m/z* 214, *) to give the iodiranium ion, *c*-C₂H₄I⁺ **6.I** (*m/z* 155), at an NCE of 28% and *t* = 10 ms. High-resolution MS² spectra of (A) and (B) are provided in (C) and (D) respectively

Table S2. HRMS experiments confirming assignments of key ion formulae for the MS² CID of the (2-bromoethyl)trimethylammonium ion **10.Br**, *m/z* 166, (Figure S2C), and MS² CID of the (2-iodoethyl)trimethylammonium ion **10.I**, *m/z* 214, (Figure S2D).

Ion	Molecular Formula	Exact mass – calculated (<i>m/z</i>)	Exact mass – experimental (<i>m/z</i>)	Mass error (ppm)
BrCH ₂ CH ₂ NMe ₃ ⁺	C5 H13 ⁷⁹ Br1 N1	166.0226	166.0228	1.2
BrNMe ₃ ⁺	C3 H9 ⁷⁹ Br1 N1	137.9913	137.9914	0.7
<i>c</i> -BrCH ₂ CH ₂ ⁺	C2 H4 ⁷⁹ Br1	106.9491	106.9491	0
CH ₂ CHNMe ₃ ⁺	C5 H12 N1	86.0964	86.0964	0
ICH ₂ CH ₂ NMe ₃ ⁺	C5 H13 I1 N1	214.0088	214.0086	-0.9
	Isotope	215.0121	215.0120	-0.5
INMe ₃ ⁺	C3 H9 I1 N1	185.9774	185.9773	-0.5
<i>c</i> -ICH ₂ CH ₂ ⁺	C2 H4 I1	154.9352	154.9352	0
CH ₃ CHNMe ₃ ⁺	C5 H13 N1	87.1043	87.1041	-2.3
N(CH ₃) ₃ ⁺	C3 H9 N1	59.0730	59.0730	0

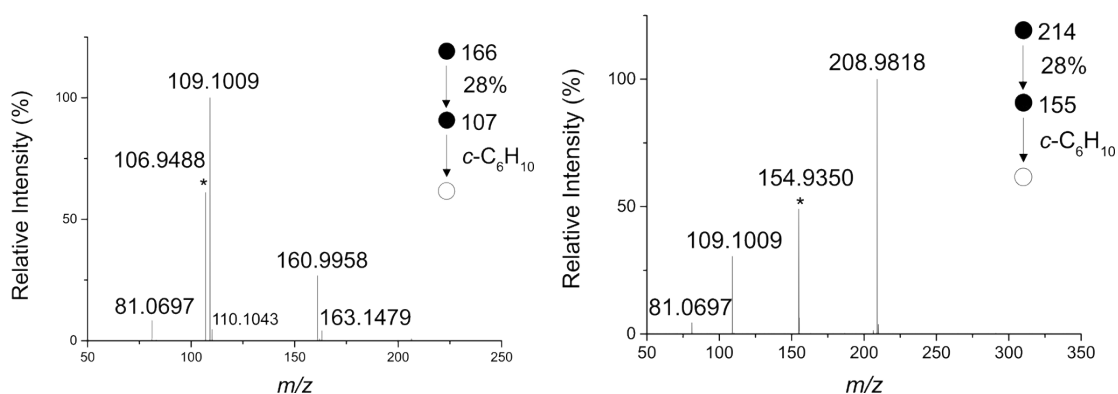


Figure S3. High-resolution MS³ IMR of cyclohexene with (A) bromiranium ion **6.Br**, *m/z* 107 (*), and (B) iodiranium ion **6.I**, *m/z* 155 (*) shown in Figure 1A and B.

Table S3. HRMS experiments confirming assignments of key ion formulae for the MS³ IMR of cyclohexene with bromiranium ion **6.Br**, m/z 107 (**Figure S3A**), and iodiranium ion **6.I**, m/z 155 (**Figure S3B**).

Ion	Molecular Formula	Exact mass – calculated (m/z)	Exact mass – experimental (m/z)	Mass error (ppm)
$C_{12}H_{19}^+$	C12 H19	163.1481	163.1479	-1.2
$c-C_6H_{10}Br^+$	C6 H10 ⁷⁹ Br1	160.9960	160.9958	-1.2
$c-C_6H_{10}CHCH_2^+$	C8 H13	109.1012	109.1009	-2.7
	Isotope	110.1046	110.1043	-2.7
$c-CH_2CH_2Br^+$	C2 H4 ⁷⁹ Br1	106.9491	106.9488	-2.8
$c-C_6H_9^+$	C6 H9	81.0699	81.0697	-2.5
$c-C_6H_{10}I^+$	C6 H10 I1	208.9822	208.9818	-1.9
$c-CH_2CH_2I^+$	C2 H4 I1	154.9352	154.9350	-1.3
$c-C_6H_{10}CHCH_2^+$	C8 H13	109.1012	109.1009	-2.7
$c-C_6H_9^+$	C6 H9	81.0699	81.0697	-2.5

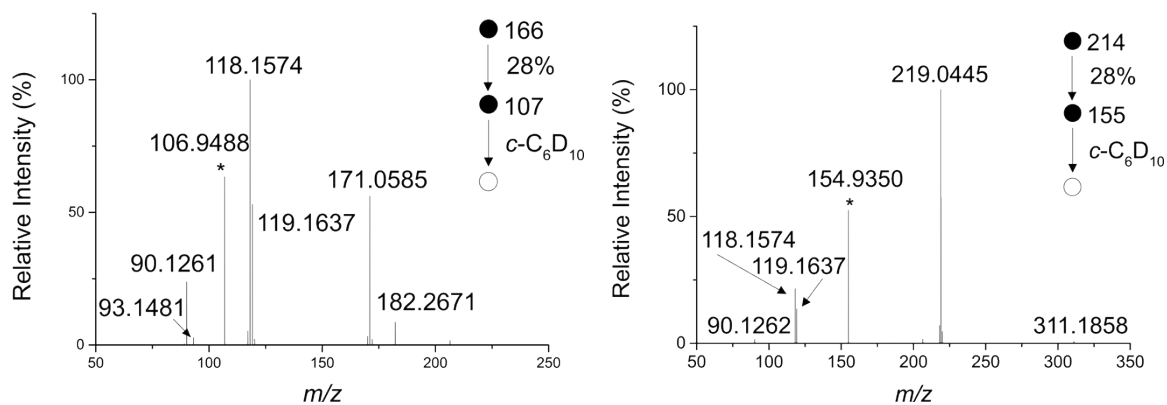


Figure S4. High-resolution MS³ IMR of cyclohexene- d_{10} with (A) bromiranium ion **6.Br**, m/z 107 (*), and (B) iodiranium ion **6.I**, m/z 155 (*) shown in **Figure 1C** and **D**.

Table S4. HRMS experiments confirming assignments of key ion formulae for the MS³ IMR of cyclohexene-d₁₀ with bromiranium ion **6.Br**, *m/z* 107 (**Figure S4A**), and iodiranium ion **6.I**, *m/z* 155 (**Figure S4B**).

Ion	Molecular Formula	Exact mass – calculated (<i>m/z</i>)	Exact mass – experimental (<i>m/z</i>)	Mass error (ppm)
C ₁₂ D ₁₉ ⁺	C12 D19	182.2674	182.2671	-1.6
<i>c</i> -C ₆ D ₁₀ Br ⁺	C6 D10 ⁷⁹ Br1	171.0588	171.0585	-1.8
<i>c</i> -C ₆ D ₁₀ CHCH ₂ ⁺	C8 H3 D10	119.1639	119.1637	-1.7
<i>c</i> -C ₆ D ₉ HCHCH ₂ ⁺	C8 H4 D9	118.1577	118.1574	-2.5
<i>c</i> -CH ₂ CH ₂ Br ⁺	C2 H4 ⁷⁹ Br1	106.9491	106.9488	-2.8
<i>c</i> -CHD ₁₀ ⁺	C6 H D10	93.1483	93.1481	-2.1
<i>c</i> -C ₆ D ₉ ⁺	C6 D9	90.1264	90.1261	-3.3
C ₁₂ D ₂₀ I ⁺	C12 D20 I1	311.1860	311.1858	-0.6
<i>c</i> -C ₆ D ₁₀ I ⁺	C6 D10 I1	219.0449	219.0445	-1.8
<i>c</i> -CH ₂ CH ₂ I ⁺	C2 H4 I1	154.9352	154.9350	-1.3
<i>c</i> -C ₆ D ₁₀ CHCH ₂ ⁺	C8 H3 D10	119.1639	119.1637	-1.7
<i>c</i> -C ₆ D ₉ HCHCH ₂ ⁺	C8 H4 D9	118.1577	118.1574	-2.5
<i>c</i> -C ₆ D ₉ ⁺	C6 D9	90.1264	90.1262	-2.2

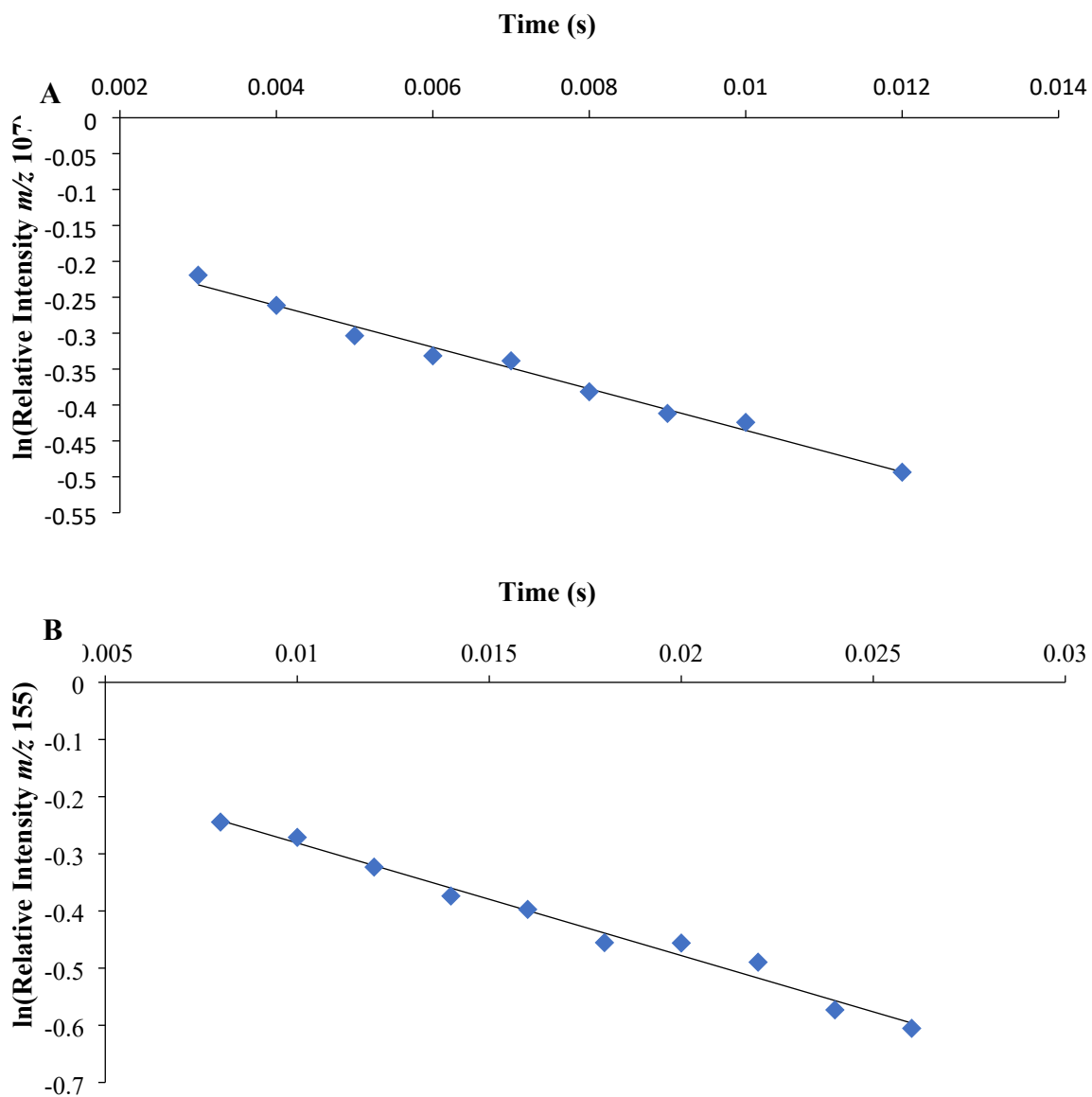


Figure S5. Early onset of the reaction of (A) bromiranium ion **6.Br** (m/z 107) with c -C₆H₁₀ (conc. ca 1.97×10^{10} molecule cm^{-3}) and (B) iodonium ion **6.I** (m/z 155) with c -C₆H₁₀ (conc. ca 1.74×10^{10} molecule cm^{-3}) in the ion trap mass spectrometer.

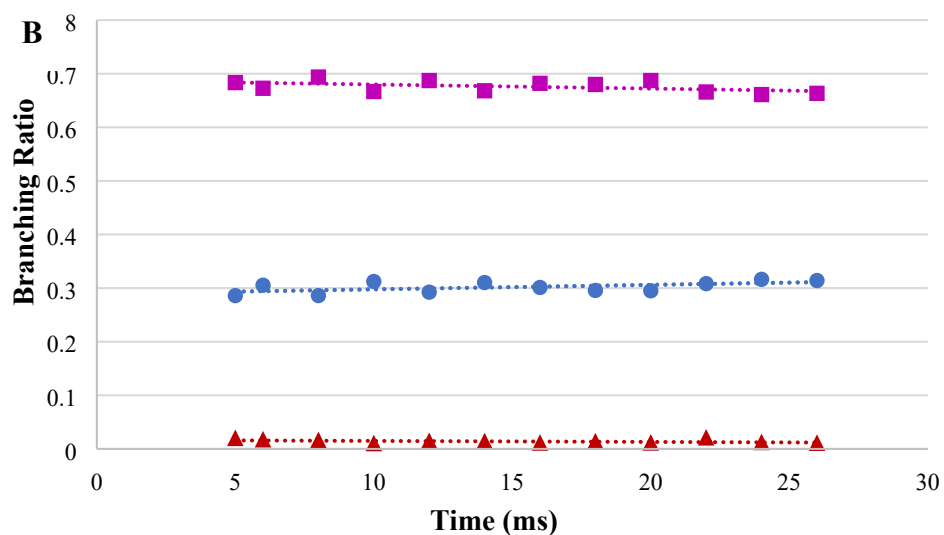
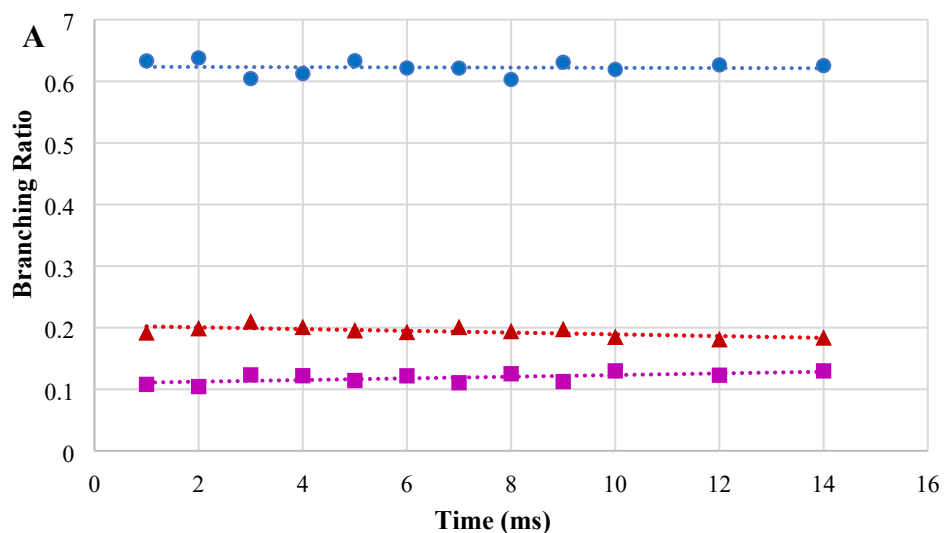


Figure S6. Branching ratio plot of π -ligand exchange (Br: m/z 161; I: m/z 209, pink squares), addition-elimination (m/z 109, blue circles), and hydride transfer (m/z 81, red triangles) products from reaction of (A) bromiranium ion **6.Br** (m/z 107) with c -C₆H₁₀ (conc. *ca* 1.97×10^{10} molecule cm⁻³) and (B) iodiranium ion **6.I** (m/z 155) with c -C₆H₁₀ (conc. *ca* 1.74×10^{10} molecule cm⁻³) in the ion trap mass spectrometer

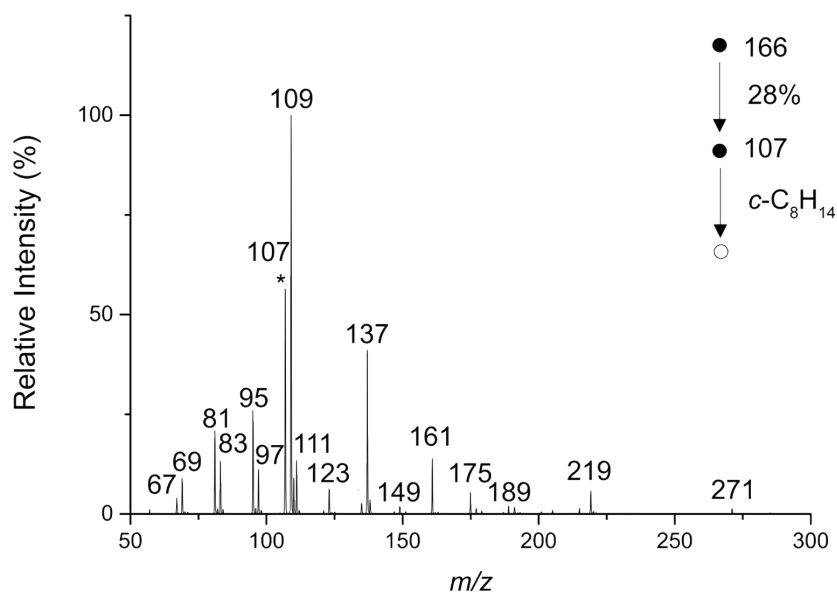


Figure S7. MS³ IMR of *cis*-cyclooctene with bromiranium ion **6.Br**, *m/z* 107 (*), at *t* = 25 ms. [*cis*-cyclooctene] = 3.20×10^{10} molecule cm⁻³.

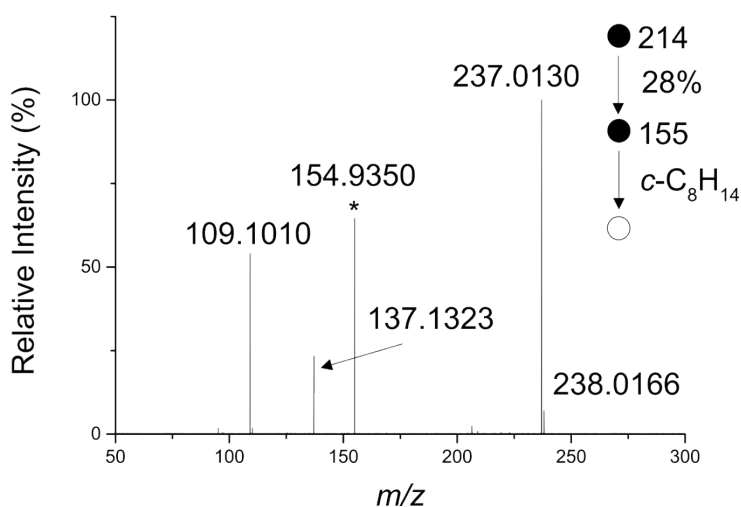


Figure S8. High-resolution MS³ IMR of *cis*-cyclooctene iodiranium ion **6.I**, *m/z* 155 (*) shown in **Figure 6**.

Table S5. HRMS experiments confirming assignments of key ion formulae for the MS³ IMR of *cis*-cyclooctene with iodiranium ion **6.I**, *m/z* 155 (**Figure S8**)

Ion	Molecular Formula	Exact mass – calculated (<i>m/z</i>)	Exact mass – experimental (<i>m/z</i>)	Mass error (ppm)
<i>c</i> -C ₈ H ₁₄ I ⁺	C8 H14 I1	237.0135	237.0130	-2.1
	Isotope	238.0169	238.0166	-1.3
<i>c</i> -CH ₂ CH ₂ I ⁺	C2 H4 I1	154.9352	154.9350	-1.3
<i>c</i> -C ₈ H ₁₄ CHCH ₂ ⁺	C10 H17	137.1325	137.1323	-1.5

$c\text{-C}_8\text{H}_{13}^+$

C8 H13

109.1012

109.1010

-1.8

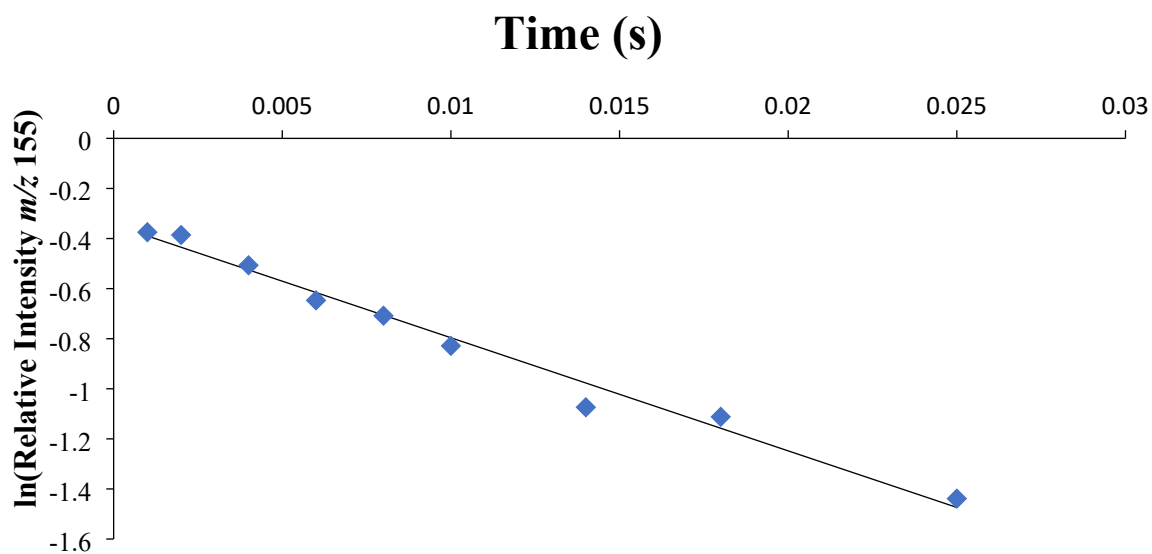


Figure S9. Early onset of the reaction of iodiranium ion **6.I** (m/z 155) with $c\text{-C}_8\text{H}_{14}$ (conc. *ca* 3.20×10^{10} molecule cm^{-3}) in the ion trap mass spectrometer

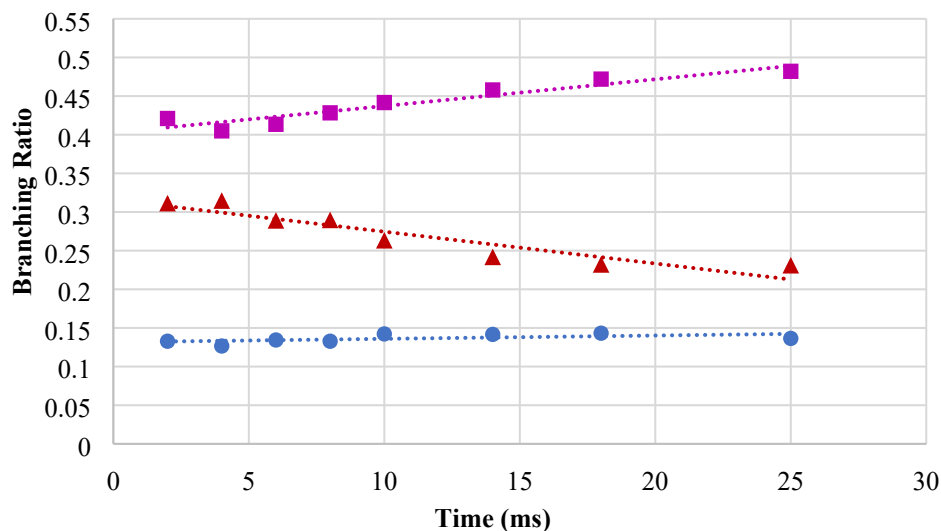


Figure S10. Branching ratio plot of π -ligand exchange (m/z 237, pink squares), addition-elimination (m/z 137, blue circles), and hydride transfer (m/z 109, red triangles) products from reaction of iodiranium ion **6.I** (m/z 155) with $c\text{-C}_8\text{H}_{14}$ (conc. *ca* 3.20×10^{10} molecule cm^{-3}) in the ion trap mass spectrometer

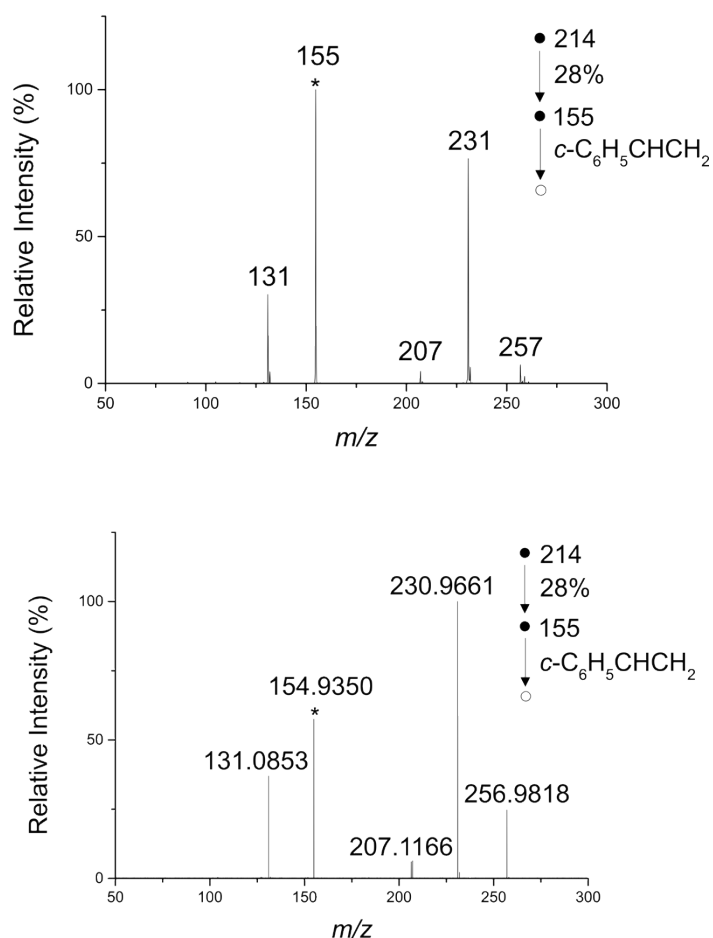


Figure S11. LTQ (top) and Orbitrap HRMS (bottom) MS³ IMR of styrene with iodonium ion **6.I**, m/z 155 (*). [styrene] *ca.* 10^{10} molecule cm^{-3} . Major products included: π -ligand exchange (m/z 231), addition-elimination of HI (m/z 131), and addition-elimination of H₂ (m/z 257). The latter peak arises due to the feasibility of benzylic stabilization of the charge in the initial addition adduct with subsequent elimination of H₂ introducing additional allylic stabilization. m/z 207 is styrene addition to a styryl cation followed by H₂ elimination.

Table S6. HRMS experiments confirming assignments of key ion formulae for the MS³ IMR of styrene with iodonium ion **6.I**, m/z 155 (**Figure S11**)

Ion	Molecular Formula	Exact mass – calculated (m/z)	Exact mass – experimental (m/z)	Mass error (ppm)
$\text{C}_{10}\text{H}_{10}\text{I}^+$	C10 H10 I1	256.9822	256.9818	-1.6
$c\text{-C}_6\text{H}_5\text{CHCH}_2\text{I}^+$	C8 H8 I1	230.9665	230.9661	-1.7
$\text{C}_{16}\text{H}_{15}^+$	C16 H15	207.1168	207.1166	-1.0
$c\text{-CH}_2\text{CH}_2\text{I}^+$	C2 H4 I1	154.9352	154.9350	-1.3
$\text{C}_{10}\text{H}_{11}^+$	C10 H11	131.0855	131.0853	-1.5

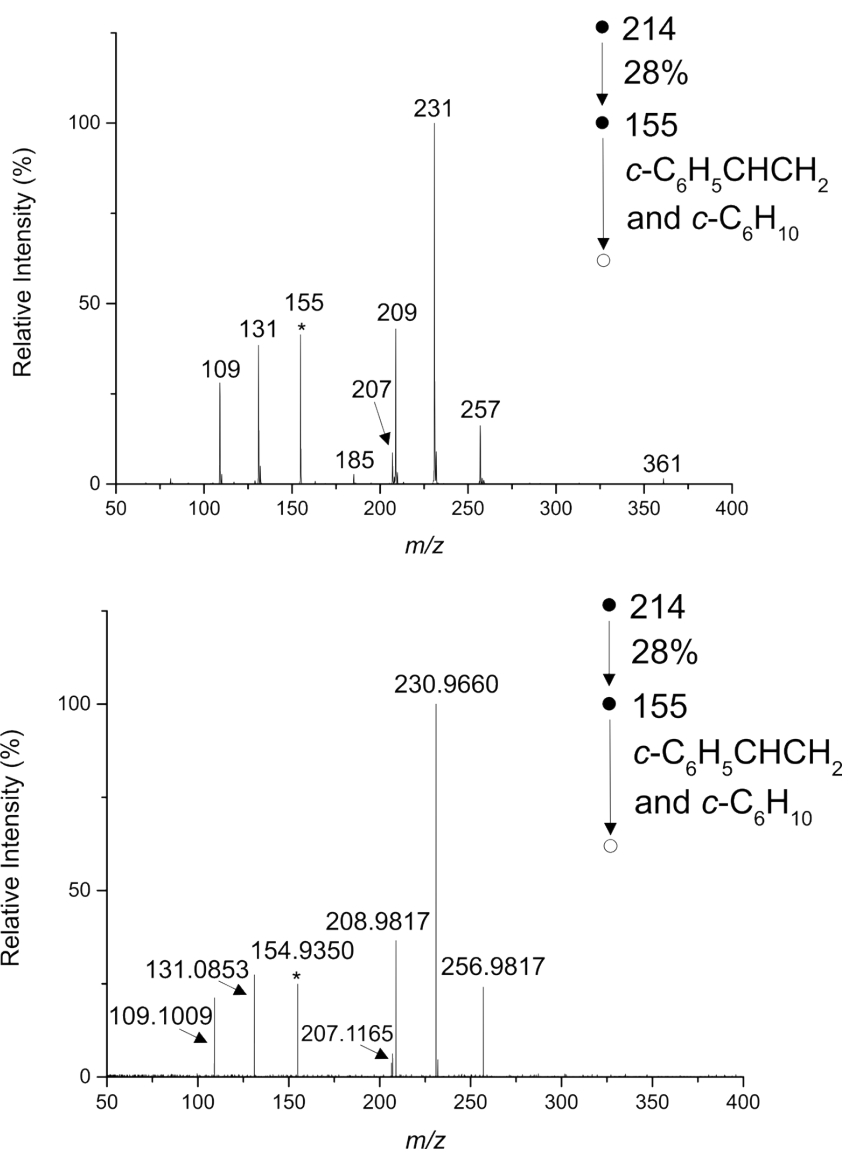


Figure S12. LTQ (top) and Orbitrap HRMS (bottom) MS³ IMR of 50:50 cyclohexene:styrene mixture with iodiranium ion **6.I**, m/z 155 (*) at $t = 15$ ms. [cyclohexene and styrene] *ca.* 10^{10} molecule cm^{-3} . π -Ligand exchange products are at m/z 209 (**12.I**) and m/z 231 (**37.I**). Other products present in the IMR between **6.I** and cyclohexene include m/z 109 (see **Figure 1B** and **Table S3**), whilst products present in the IMR between **6.I** and styrene include m/z 131, m/z 207 and m/z 257 (see **Figure S11** and **Table S6**).

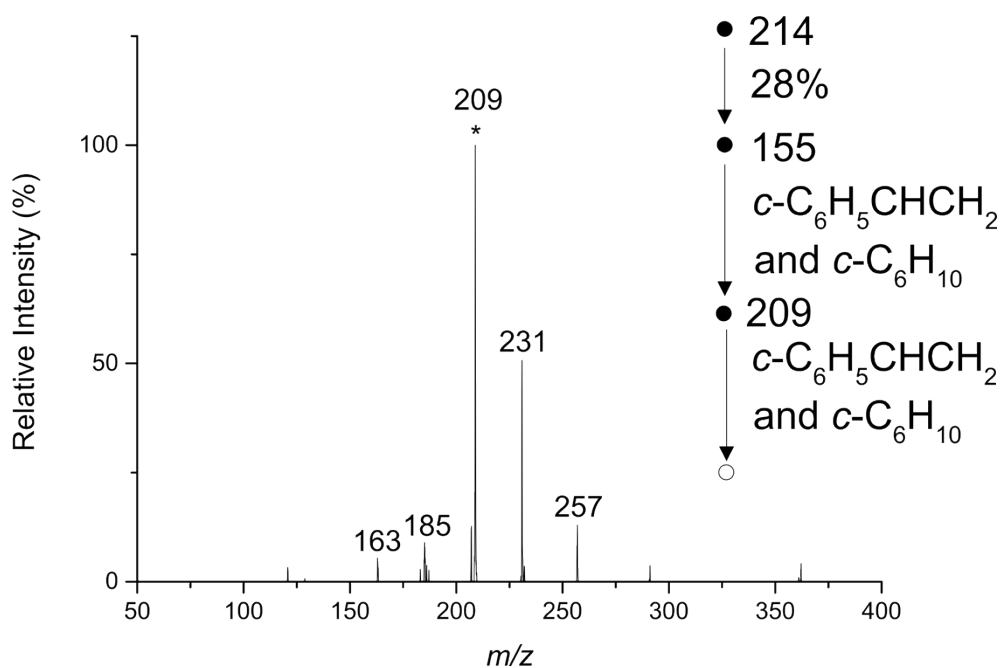


Figure S13. MS⁴ IMR of 50:50 cyclohexene:styrene mixture with cyclohexyl iodonium ion **12.I**, m/z 209 (*). [cyclohexene and styrene] *ca.* 10^{10} molecule cm^{-3} . π -Ligand exchange products are at m/z 209 (**12.I**) and m/z 231 (**37.I**). HRMS was not possible for this IMR due to the low signal, however, the high-resolution data present in **Figure S12** may be used to support the assignment of m/z 231 as the ion **37.I**.

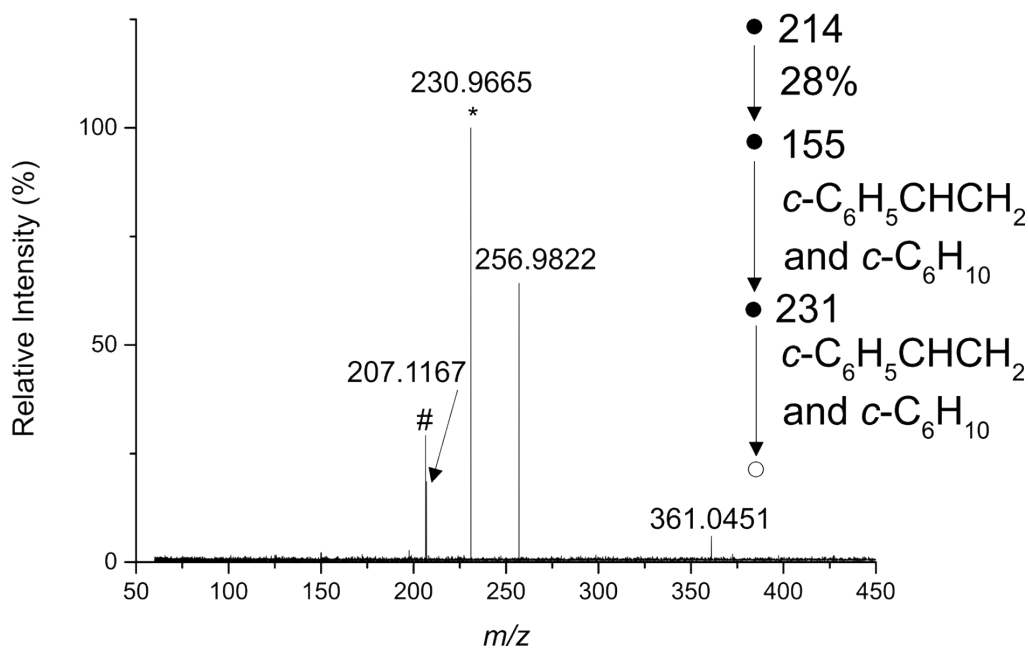
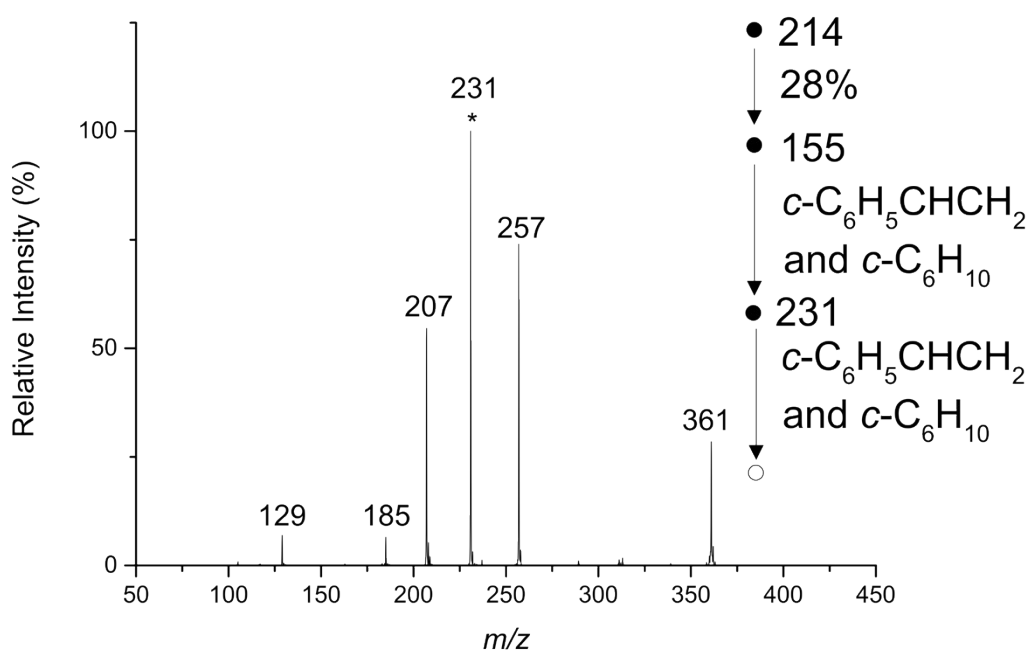


Figure S14. LTQ (top) and Orbitrap HRMS (bottom) MS^4 IMR of 50:50 cyclohexene:styrene mixture with benzylic ion **37.I**, m/z 231 (*). [cyclohexene and styrene] *ca.* 10^{10} molecule cm^{-3} . π -Ligand exchange product is **not** observed at m/z 209 (**12.I**). Note that m/z 257 may be produced by addition of styrene to m/z 231 followed by elimination of benzene, with further addition of styrene to m/z 257 giving m/z 361. # is noise present in the Orbitrap.

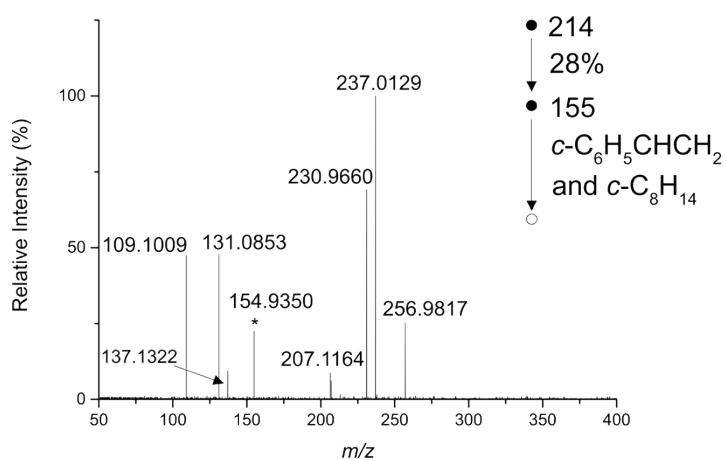
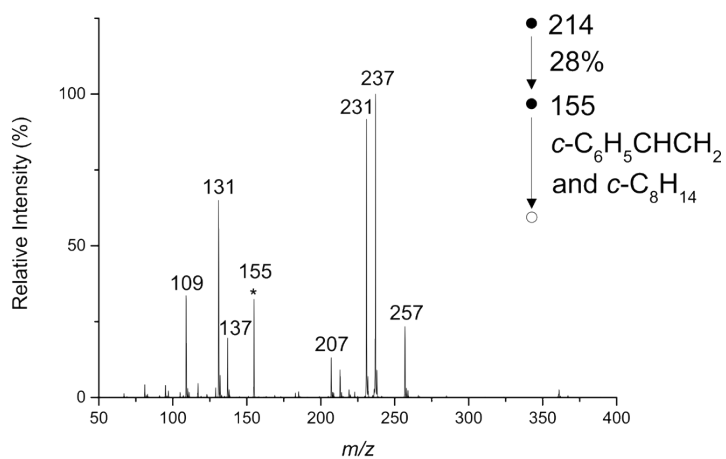


Figure S15. LTQ (top) and Orbitrap HRMS (bottom) MS³ IMR of 50:50 *cis*-cyclooctene: styrene mixture with iodonium ion **6.I**, m/z 155 (*) at $t = 20$ ms. [*cis*-cyclooctene and styrene] *ca.* 10^{10} molecule cm^{-3} . π -Ligand exchange products are at m/z 237 (**17.I**) and m/z 231 (**37.I**). Other products present in the IMR between **6.I** and *cis*-cyclooctene include m/z 109 and m/z 137 (see **Figure 6** and **Table S5**), whilst products present in the IMR between **6.I** and styrene include m/z 131, m/z 207 and m/z 257 (see **Figure S11** and **Table S6**).

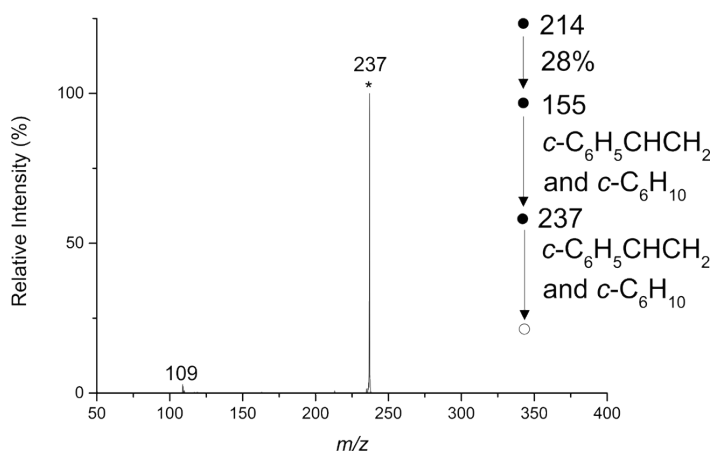


Figure S16. MS⁴ IMR of 50:50 *cis*-cyclooctene:styrene mixture with cyclooctyl iodonium ion **17.I**, *m/z* 237 (*). [*cis*-cyclooctene and styrene] *ca.* 10¹⁰ molecule cm⁻³. π -Ligand exchange product is **not** observed at *m/z* 231 (**37.I**). HRMS was not possible for this IMR due to the low signal, however, the high-resolution data present in **Figure S15** may be used to support the assignment of *m/z* 237 as the ion **17.I**.

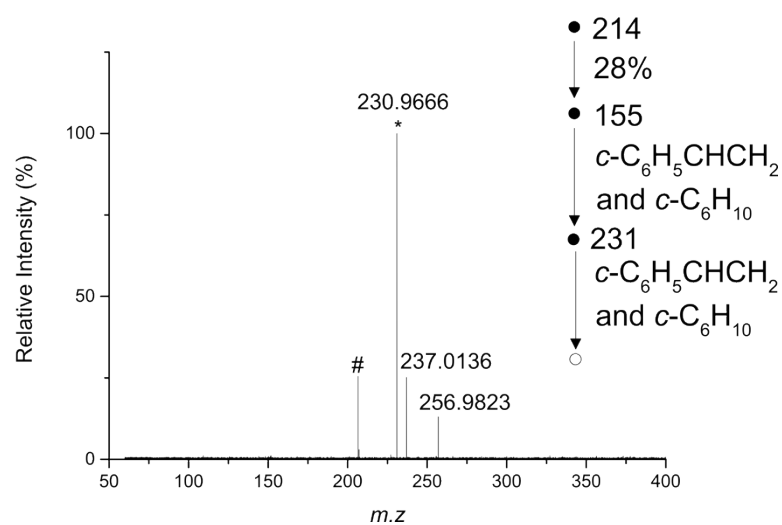
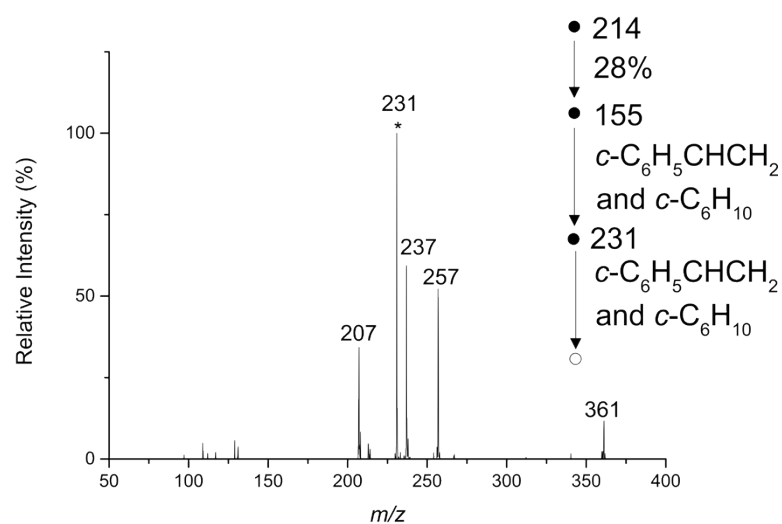


Figure S17. LTQ (top) and Orbitrap HRMS (bottom) MS⁴ IMR of 50:50 *cis*-cyclooctene:styrene mixture with benzylic ion **37.I**, *m/z* 231 (*). [*cis*-cyclooctene and styrene] *ca.* 10¹⁰ molecule cm⁻³. π -Ligand exchange product is observed at *m/z* 237 (**17.I**). Note that *m/z* 257 may be produced by addition of styrene to *m/z* 231 followed by elimination of benzene, with further addition of styrene to *m/z* 257 giving *m/z* 361. # is noise present in the Orbitrap.

Thermochemical Data and Optimized Cartesian Coordinates for Structures Calculated at M06-2X-D3/def2-TZVP

Figure 3

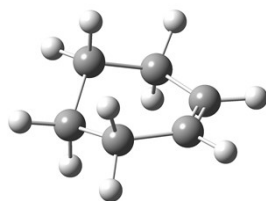
Bromiranium Ion 6.Br



Zero-point correction=	0.055189 (Hartree/Particle)
Thermal correction to Energy=	0.058729
Thermal correction to Enthalpy=	0.059673
Thermal correction to Gibbs Free Energy=	0.028585
Sum of electronic and zero-point Energies=	-2652.404056
Sum of electronic and thermal Energies=	-2652.400516
Sum of electronic and thermal Enthalpies=	-2652.399572
Sum of electronic and thermal Free Energies=	-2652.430660

C	-2.14349000	0.65689000	0.28017200
H	-1.67484700	0.55824500	-0.69126100
H	-3.08975300	0.15474600	0.43935100
C	-1.34707700	1.06033800	1.42112700
H	-0.29029000	1.25889300	1.29178600
H	-1.70605000	0.85567300	2.42227500
Br	-2.38451300	2.61376400	0.67712500

Cyclohexene

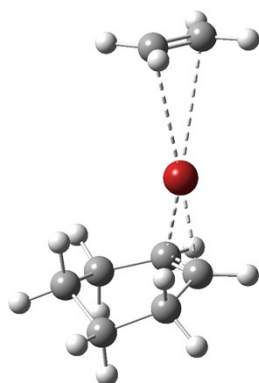


Zero-point correction=	0.147369
(Hartree/Particle)	
Thermal correction to Energy=	0.152825
Thermal correction to Enthalpy=	0.153769
Thermal correction to Gibbs Free Energy=	0.119452
Sum of electronic and zero-point Energies=	-234.466759
Sum of electronic and thermal Energies=	-234.461303
Sum of electronic and thermal Enthalpies=	-234.460358
Sum of electronic and thermal Free Energies=	-234.494675

C	-0.12529000	-0.65215800	1.29651100
C	0.12529000	0.65215800	1.29651100
C	0.25861000	1.47078700	0.04227900

C	-0.25861000	0.71771800	-1.18101200
C	0.25861000	-0.71771800	-1.18101200
C	-0.25861000	-1.47078700	0.04227900
H	-0.27916500	2.41426600	0.16408200
H	0.23623800	1.17126400	2.24270300
H	-0.23623800	-1.17126400	2.24270300
H	-1.35256100	0.70079200	-1.15576800
H	0.03295800	1.23625300	-2.09567600
H	-0.03295800	-1.23625300	-2.09567600
H	1.35256100	-0.70079200	-1.15576800
H	-1.31033300	-1.74335400	-0.10200100
H	0.27916500	-2.41426600	0.16408200
H	1.31033300	1.74335400	-0.10200100

21.Br

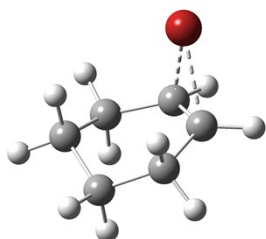


Zero-point correction=	0.202016
(Hartree/Particle)	
Thermal correction to Energy=	0.213690
Thermal correction to Enthalpy=	0.214634
Thermal correction to Gibbs Free Energy=	0.161291
Sum of electronic and zero-point Energies=	-2886.905804
Sum of electronic and thermal Energies=	-2886.894130
Sum of electronic and thermal Enthalpies=	-2886.893186
Sum of electronic and thermal Free Energies=	-2886.946529

C	2.00527900	-0.78361600	0.47454000
H	1.95690200	-1.15587100	1.49174600
C	1.98881200	0.64747400	0.29968900
H	1.95363200	1.26142400	1.19336600
C	-2.93575200	-0.29584400	-0.79835600
C	-3.07200000	0.06780600	0.47239000
H	-3.17832200	-0.66458800	1.26379100
H	-2.92688700	-1.33898900	-1.09156400
C	2.51948900	-1.70966600	-0.59401900
H	3.20321700	-2.39972100	-0.09373100
H	1.69847200	-2.32869000	-0.95987400
C	2.45145700	1.27643100	-0.97259800

H	1.86386600	2.17107900	-1.17970000
H	3.46676200	1.62956800	-0.74353700
C	2.48934200	0.30043100	-2.14319900
H	1.47292800	0.07189900	-2.47399400
H	2.99255600	0.77646300	-2.98308100
C	3.22194300	-0.97562200	-1.74095900
H	3.31277500	-1.65256600	-2.58845000
H	4.23895700	-0.71907600	-1.43394100
H	-2.87196000	0.43682300	-1.59413700
H	-3.12394900	1.11089400	0.76126500
Br	0.03315800	-0.10741100	0.17659700

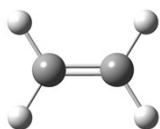
Product 12.Br



Zero-point correction=	0.149468
(Hartree/Particle)	
Thermal correction to Energy=	0.156270
Thermal correction to Enthalpy=	0.157214
Thermal correction to Gibbs Free Energy=	0.117612
Sum of electronic and zero-point Energies=	-2808.376112
Sum of electronic and thermal Energies=	-2808.369309
Sum of electronic and thermal Enthalpies=	-2808.368365
Sum of electronic and thermal Free Energies=	-2808.407967

C	-4.97747300	-1.60076800	-0.01626400
C	-3.45372000	-1.62973200	0.01581000
C	-2.84285700	-0.27605100	0.15230300
C	-3.62140800	0.84924000	0.64932200
C	-5.05465400	0.69233700	1.07870100
C	-5.51330800	-0.76886000	1.14471300
H	-1.76234600	-0.20194200	0.21908300
H	-3.10536700	-2.16495500	0.91110300
H	-3.01356600	-2.15231000	-0.83378200
H	-5.32611700	-1.20127300	-0.97200900
H	-5.34920500	-2.62183900	0.04908800
H	-3.06381600	1.69674000	1.03286800
H	-5.12679600	1.17055100	2.05875700
H	-5.69351100	1.28454300	0.42126400
H	-5.17125000	-1.20996100	2.08415100
H	-6.60118200	-0.79305800	1.16658100
Br	-3.32380500	1.01147200	-1.39701000

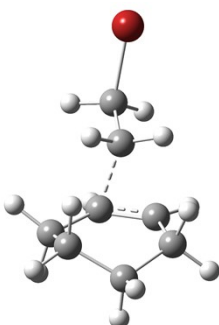
Ethene



Zero-point correction= 0.051412
 (Hartree/Particle)
 Thermal correction to Energy= 0.054446
 Thermal correction to Enthalpy= 0.055391
 Thermal correction to Gibbs Free Energy= 0.029899
 Sum of electronic and zero-point Energies= -78.520570
 Sum of electronic and thermal Energies= -78.517535
 Sum of electronic and thermal Enthalpies= -78.516591
 Sum of electronic and thermal Free Energies= -78.542083

C	0.00000000	0.66100900	0.00000000
H	0.92229300	1.22855200	0.00000000
H	-0.92225200	1.22859300	0.00000000
C	0.00000000	-0.66100900	0.00000000
H	-0.92229300	-1.22855200	0.00000000
H	0.92225200	-1.22859300	0.00000000

22.Br

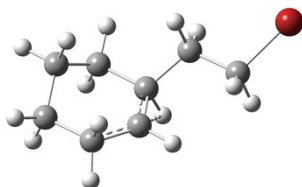


Zero-point correction= 0.206104
 (Hartree/Particle)
 Thermal correction to Energy= 0.215870
 Thermal correction to Enthalpy= 0.216814
 Thermal correction to Gibbs Free Energy= 0.169209
 Sum of electronic and zero-point Energies= -2886.923459
 Sum of electronic and thermal Energies= -2886.913693
 Sum of electronic and thermal Enthalpies= -2886.912749
 Sum of electronic and thermal Free Energies= -2886.960354

C	-1.19761700	-0.62872100	0.25847600
H	-1.02114700	-0.87415100	1.30346800
C	-0.63807800	0.73303200	-0.09812400
H	0.44947200	0.70845200	0.02799200
H	-0.80488900	1.05729900	-1.12287000
C	-1.60950100	1.89034100	0.73405600
C	-2.27338600	2.86955300	-0.20309100

C	-0.31573500	2.10927400	1.21188700
C	-1.26859000	3.75441600	-0.93669700
H	-2.93159200	3.48437200	0.41766900
H	-2.92214800	2.32858100	-0.89392900
C	0.54664400	3.23371000	0.73824900
H	0.03366000	1.50312500	2.04320000
C	-0.25326400	4.33660300	0.04077200
H	-0.75160900	3.18746600	-1.71693700
H	-1.80481400	4.55254500	-1.44758800
H	1.07196400	3.60910100	1.62042000
H	1.33468400	2.84030900	0.08812300
H	-0.77580600	4.93050700	0.79432100
H	0.43595200	5.00804700	-0.46804400
H	-2.26637200	1.28219100	1.34755300
H	-2.25858900	-0.69658700	0.03689500
Br	-0.29708600	-1.95975900	-0.81395300

TS23.Br

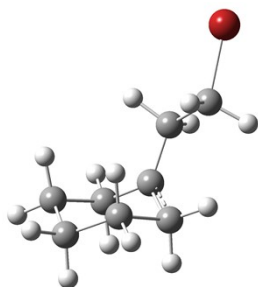


Zero-point correction=	0.203399
(Hartree/Particle)	
Thermal correction to Energy=	0.212597
Thermal correction to Enthalpy=	0.213541
Thermal correction to Gibbs Free Energy=	0.167594
Sum of electronic and zero-point Energies=	-2886.917946
Sum of electronic and thermal Energies=	-2886.908748
Sum of electronic and thermal Enthalpies=	-2886.907804
Sum of electronic and thermal Free Energies=	-2886.953751

C	1.27874900	0.60554500	0.30904900
H	1.08494600	1.44915500	-0.34992500
C	0.27097900	-0.51457400	0.14683800
H	0.18601800	-0.80514500	-0.90233400
H	0.60098000	-1.39334100	0.69885800
C	-1.17339100	-0.19901200	0.65401700
C	-2.16276800	-1.35763800	0.46761900
C	-1.66874200	1.10554200	0.32141500
C	-3.19552300	-1.05604600	-0.61478800
H	-2.67326500	-1.55603000	1.41172100
H	-1.59921500	-2.25709900	0.22234600
C	-2.98172900	1.39343800	-0.18752100
H	-0.99171100	1.94881500	0.45570800
C	-3.95254900	0.22761500	-0.29079700
H	-2.69824200	-0.95688900	-1.58598200
H	-3.89017900	-1.88927500	-0.70334200
H	-3.37678900	2.33477900	0.20934200
H	-2.63990700	1.71690100	-1.20830100

H	-4.48381200	0.12253100	0.65770700
H	-4.70086300	0.45232600	-1.04893000
H	-1.01982200	0.02790900	1.74312700
H	1.34099100	0.95621300	1.33832900
Br	3.03916300	-0.03943100	-0.16495200

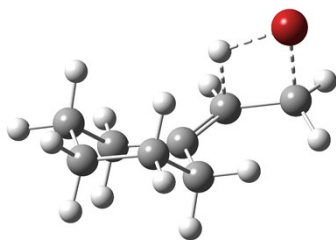
24.Br



Zero-point correction=	0.205528
(Hartree/Particle)	
Thermal correction to Energy=	0.215198
Thermal correction to Enthalpy=	0.216142
Thermal correction to Gibbs Free Energy=	0.168939
Sum of electronic and zero-point Energies=	-2886.941704
Sum of electronic and thermal Energies=	-2886.932034
Sum of electronic and thermal Enthalpies=	-2886.931090
Sum of electronic and thermal Free Energies=	-2886.978294

C	0.12815200	-0.31836700	0.28173700
H	0.90238500	0.26143300	0.77851900
C	-0.72033000	0.53706000	-0.64139500
H	-0.15095300	0.89771300	-1.50825900
H	-1.51064600	-0.07592100	-1.11234700
C	-1.46032700	1.66501500	-0.06397000
C	-2.02939500	2.66215600	-0.95810000
C	-1.47485900	1.95526500	1.35261600
C	-0.99058300	3.85614500	-0.87533500
H	-2.98599600	3.03527200	-0.59183000
H	-2.10801900	2.31723900	-1.98715500
C	-0.37870000	3.11536900	1.43142100
H	-1.17461200	1.12677500	1.98718600
C	-0.79680600	4.28945900	0.56604700
H	-0.04507600	3.53283000	-1.31591100
H	-1.39222800	4.65053000	-1.50234600
H	-0.30847800	3.36792400	2.48852100
H	0.59178100	2.72407500	1.11918200
H	-1.71630200	4.73281900	0.95487300
H	-0.02562100	5.06103400	0.61187400
H	-2.41684000	2.39200400	1.68148000
H	-0.47248100	-0.83468600	1.02551500
Br	1.02278200	-1.68071800	-0.75534900

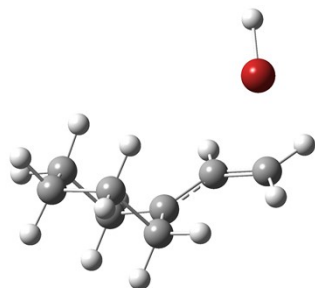
TS25.Br



Zero-point correction= 0.200079
 (Hartree/Particle)
 Thermal correction to Energy= 0.209364
 Thermal correction to Enthalpy= 0.210308
 Thermal correction to Gibbs Free Energy= 0.164361
 Sum of electronic and zero-point Energies= -2886.897206
 Sum of electronic and thermal Energies= -2886.887921
 Sum of electronic and thermal Enthalpies= -2886.886977
 Sum of electronic and thermal Free Energies= -2886.932924

C	-1.06267200	-0.84817300	0.31888400
H	-0.92760700	-0.81839000	1.39383200
C	-1.64658500	0.36426200	-0.33723500
H	-0.03750600	0.49313400	-0.87822900
H	-2.26498500	0.17656700	-1.20849800
C	-1.48906200	1.63647600	0.11114800
C	-2.09011000	2.78079500	-0.64242200
C	-0.68017700	2.01987400	1.31048900
C	-1.01725000	3.81787900	-1.00981300
H	-2.82189400	3.25414200	0.02207200
H	-2.62577800	2.42927800	-1.52365800
C	0.38458500	3.06767400	0.93402500
H	-0.21987400	1.16200700	1.80049600
C	-0.23934400	4.26239300	0.22260200
H	-0.33139100	3.38053500	-1.74298300
H	-1.49754300	4.66623500	-1.49609600
H	0.90524300	3.37745400	1.83956400
H	1.13405800	2.60449000	0.28304800
H	-0.91057100	4.78544300	0.91015200
H	0.53830700	4.97188800	-0.06039600
H	-1.37096100	2.46929400	2.03228400
H	-1.46003900	-1.79456700	-0.02858700
Br	0.83653400	-0.77153000	-0.44036500

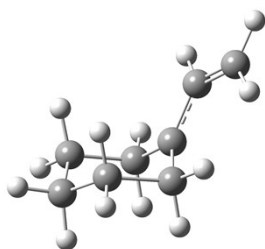
26.Br



Zero-point correction=			0.200790
(Hartree/Particle)			
Thermal correction to Energy=			0.211919
Thermal correction to Enthalpy=			0.212864
Thermal correction to Gibbs Free Energy=			0.160960
Sum of electronic and zero-point Energies=			-2886.934503
Sum of electronic and thermal Energies=			-2886.923373
Sum of electronic and thermal Enthalpies=			-2886.922429
Sum of electronic and thermal Free Energies=			-2886.974332

C	-1.34476000	-0.59087600	0.18985900
H	-0.96572700	-0.61489900	1.20205400
C	-1.77974700	0.54319500	-0.39922200
H	2.10186500	-0.99982600	-1.42108300
H	-2.22422500	0.49764300	-1.38655000
C	-1.74538400	1.80604800	0.24392300
C	-2.35060600	2.96293100	-0.42034200
C	-0.94478100	2.10110900	1.43448400
C	-1.13512000	3.78756600	-0.98493100
H	-2.86650600	3.59838800	0.30149400
H	-3.02514800	2.67944400	-1.22495700
C	0.28166700	2.92924200	0.89731500
H	-0.58459700	1.22288200	1.96168400
C	-0.18706500	4.16181000	0.14194400
H	-0.62047100	3.19101100	-1.74155000
H	-1.55211700	4.66186500	-1.48286400
H	0.88882600	3.18666900	1.76422300
H	0.88245600	2.28320300	0.25314300
H	-0.68095100	4.85446300	0.82810400
H	0.67860900	4.68404600	-0.26960200
H	-1.50384200	2.74265900	2.11763300
H	-1.41209700	-1.54357200	-0.32101700
Br	1.92049900	-0.80604000	-0.02163000

Product 14



Zero-point correction=			0.192773
(Hartree/Particle)			
Thermal correction to Energy=			0.200687
Thermal correction to Enthalpy=			0.201631
Thermal correction to Gibbs Free Energy=			0.160455
Sum of electronic and zero-point Energies=			-312.145159
Sum of electronic and thermal Energies=			-312.137246
Sum of electronic and thermal Enthalpies=			-312.136301

Sum of electronic and thermal Free Energies= -312.177477

C	-1.12651400	-0.61453900	0.45182400
H	-0.31293200	-0.58124800	1.16470100
C	-1.80441400	0.48318000	0.06886600
H	-2.64430800	0.38562200	-0.60916300
C	-1.52566600	1.78613600	0.57572900
C	-2.39106700	2.89648000	0.18511100
C	-0.29900500	2.14894900	1.28459600
C	-1.55619800	3.66632300	-0.91306800
H	-2.54643900	3.58831100	1.01393000
H	-3.34317000	2.56879300	-0.22537300
C	0.55745900	2.93430000	0.21836200
H	0.27281500	1.30526400	1.65822000
C	-0.22340700	4.11264400	-0.33777800
H	-1.40972200	3.01200900	-1.77517600
H	-2.17245500	4.50422500	-1.23616600
H	1.47025100	3.24731300	0.72329000
H	0.83940500	2.24461900	-0.58007000
H	-0.38645000	4.85593600	0.44644400
H	0.36401700	4.59800600	-1.11962800
H	-0.52183500	2.83949900	2.09930800
H	-1.39872200	-1.59135200	0.07083100

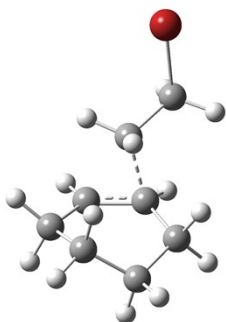
HBr



Zero-point correction=	0.006101
(Hartree/Particle)	
Thermal correction to Energy=	0.008462
Thermal correction to Enthalpy=	0.009406
Thermal correction to Gibbs Free Energy=	-0.013121
Sum of electronic and zero-point Energies=	-2574.784514
Sum of electronic and thermal Energies=	-2574.782153
Sum of electronic and thermal Enthalpies=	-2574.781209
Sum of electronic and thermal Free Energies=	-2574.803736

Br	-5.39404400	0.60327200	0.00000000
H	-6.81546200	0.60327200	0.00000000

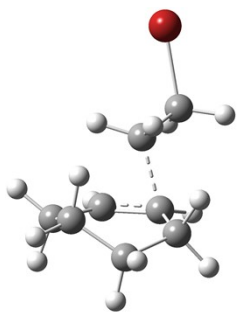
TS27.Br



Zero-point correction=	0.206244
(Hartree/Particle)	
Thermal correction to Energy=	0.215094
Thermal correction to Enthalpy=	0.216038
Thermal correction to Gibbs Free Energy=	0.171073
Sum of electronic and zero-point Energies=	-2886.922446
Sum of electronic and thermal Energies=	-2886.913597
Sum of electronic and thermal Enthalpies=	-2886.912653
Sum of electronic and thermal Free Energies=	-2886.957617

C	-0.04973500	0.03993200	0.72536800
H	0.63447000	0.19520300	1.55481500
C	-0.51558800	1.36319300	0.13327500
H	0.29071000	1.98688600	-0.23549900
H	-1.17799500	1.13824600	-0.70942600
C	-2.05848400	2.52257300	0.48748000
C	-1.98612300	3.74116300	-0.34809500
C	-1.12139600	2.22568000	1.48192900
C	-0.73622400	4.58625800	-0.11092800
H	-2.88881500	4.29556000	-0.04534900
H	-2.15620800	3.49366600	-1.39883700
C	-0.13821400	3.27513800	1.97592000
H	-1.40883600	1.45915600	2.19398300
C	-0.41887200	4.65712800	1.38023000
H	0.11047400	4.17638400	-0.66609500
H	-0.90728400	5.58383600	-0.51202400
H	-0.21990900	3.30873100	3.06227700
H	0.88212500	2.95169300	1.75878400
H	-1.26955800	5.10397300	1.90196700
H	0.43514900	5.30794000	1.55855400
H	-2.91665800	1.86722600	0.36726800
H	-0.88661100	-0.57722300	1.04059300
Br	0.90700500	-0.92418100	-0.64698700

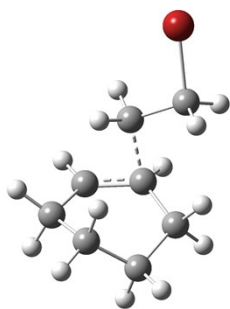
28.Br



Zero-point correction=	0.206089
(Hartree/Particle)	
Thermal correction to Energy=	0.215826
Thermal correction to Enthalpy=	0.216770
Thermal correction to Gibbs Free Energy=	0.169405
Sum of electronic and zero-point Energies=	-2886.922903
Sum of electronic and thermal Energies=	-2886.913166
Sum of electronic and thermal Enthalpies=	-2886.912221
Sum of electronic and thermal Free Energies=	-2886.959587

C	-0.45510700	-0.82429900	0.65232000
H	0.12800900	-0.99553200	1.55221400
C	-0.48629800	0.64168000	0.27808000
H	0.48358100	1.12428500	0.20107000
H	-0.93475100	0.74822700	-0.71821500
C	-2.04435400	1.68416500	0.60376500
C	-2.11042000	2.91885100	-0.22160400
C	-1.11704000	1.51470300	1.63457700
C	-0.89156300	3.81965300	-0.04213500
H	-3.01545000	3.42512600	0.14469200
H	-2.31837500	2.67203400	-1.26408200
C	-0.24606300	2.65879200	2.11844600
H	-1.31935000	0.72534000	2.35052900
C	-0.58234900	3.99122900	1.44227100
H	-0.03220200	3.39663600	-0.57001900
H	-1.09191800	4.78401200	-0.50556300
H	-0.39702200	2.73331500	3.19598000
H	0.80549100	2.39911100	1.98365700
H	-1.45325000	4.43303100	1.93309800
H	0.24290500	4.68628100	1.58539500
H	-2.82189900	0.93567600	0.47526900
H	-1.45691900	-1.22873100	0.78011500
Br	0.38972000	-1.80914500	-0.77965600

TS29.Br



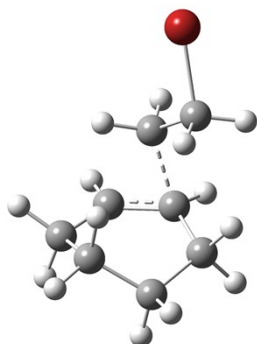
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Zero-point correction=                0.205937
(Hartree/Particle)
Thermal correction to Energy=         0.214927
Thermal correction to Enthalpy=       0.215871
Thermal correction to Gibbs Free Energy= 0.170543
Sum of electronic and zero-point Energies= -2886.918867
Sum of electronic and thermal Energies= -2886.909877
Sum of electronic and thermal Enthalpies= -2886.908933
Sum of electronic and thermal Free Energies= -2886.954261

```

C	0.43274300	0.28203100	0.92905000
H	1.19300200	0.88344100	1.41276800
C	-0.65031800	1.13652900	0.26808200
H	-0.17018000	1.90604600	-0.33550300
H	-1.28229800	0.51470100	-0.35785800
C	-2.10230200	2.56667900	0.55981000
C	-1.63888800	3.94749100	0.38195100
C	-1.61714900	1.71173300	1.55930600
C	-0.50321000	4.33531000	1.31940600
H	-2.54686300	4.53881300	0.59819200
H	-1.44213700	4.14567700	-0.67587100
C	-0.88770100	2.30043600	2.76245600
H	-2.22060100	0.83092300	1.76073200
C	-0.80797200	3.82828900	2.72491100
H	0.43723300	3.90768400	0.95742000
H	-0.37895000	5.41648400	1.30863000
H	-1.43385700	1.97469300	3.64825800
H	0.10775400	1.87040300	2.85687100
H	-1.75995600	4.25252400	3.05541500
H	-0.05254900	4.16832600	3.43068300
H	-2.84592600	2.18553900	-0.13582200
H	0.01665300	-0.44109000	1.62427100
Br	1.31384100	-0.69757200	-0.48300500

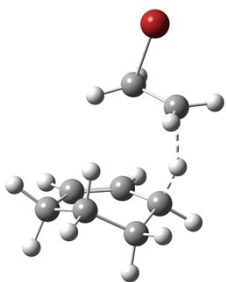
30.Br



Zero-point correction=	0.206569
(Hartree/Particle)	
Thermal correction to Energy=	0.216205
Thermal correction to Enthalpy=	0.217149
Thermal correction to Gibbs Free Energy=	0.170271
Sum of electronic and zero-point Energies=	-2886.918835
Sum of electronic and thermal Energies=	-2886.909199
Sum of electronic and thermal Enthalpies=	-2886.908255
Sum of electronic and thermal Free Energies=	-2886.955133

C	-0.91493400	0.37955200	0.28318100
H	-0.92073800	-0.51420600	0.89734200
C	0.43806600	0.61231500	-0.37856100
H	1.23328900	0.72325100	0.35230600
H	0.42819900	1.45588900	-1.06002000
C	-2.41679500	1.42752000	0.99906600
C	-3.11768000	2.26644600	0.00275300
C	-1.11385900	1.68427500	1.43082300
C	-2.18857400	3.24370500	-0.70653000
H	-3.86366700	2.81005200	0.60400700
H	-3.70166500	1.64232700	-0.67658700
C	-0.44488100	3.01176300	1.12625900
H	-0.79044200	1.19080600	2.34093300
C	-1.32338600	3.97260000	0.31679100
H	-1.56745700	2.70207400	-1.42678300
H	-2.78182300	3.95124900	-1.28287400
H	-0.20675300	3.45165300	2.09611700
H	0.51810600	2.85207000	0.64338400
H	-1.97971000	4.51961800	0.99790300
H	-0.69431900	4.71497100	-0.17084200
H	-2.96356600	0.60511900	1.45291700
H	-1.65607100	0.25954300	-0.51157100
Br	0.83080800	-0.96568700	-1.42363300

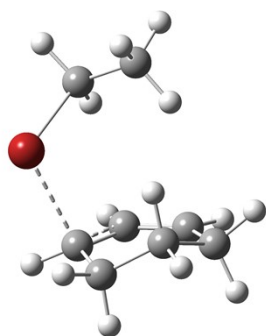
TS31.Br



Zero-point correction=	0.201588
(Hartree/Particle)	
Thermal correction to Energy=	0.211515
Thermal correction to Enthalpy=	0.212459
Thermal correction to Gibbs Free Energy=	0.164350
Sum of electronic and zero-point Energies=	-2886.880486
Sum of electronic and thermal Energies=	-2886.870559
Sum of electronic and thermal Enthalpies=	-2886.869615
Sum of electronic and thermal Free Energies=	-2886.917725

C	-0.29888100	-0.02873200	-0.26996400
H	-0.26187400	-0.59447100	0.65200300
C	0.69449500	1.00962600	-0.47231500
H	1.63170000	0.97823300	0.07018400
H	0.58707700	1.71377800	-1.28847000
C	-2.77775900	1.69384600	1.34609000
C	-3.33825800	2.45106900	0.18041000
C	-1.52834300	1.83580200	1.79395900
C	-2.25491900	3.13184500	-0.65256800
H	-4.04014200	3.19734800	0.56876000
H	-3.94276700	1.78279800	-0.43706400
C	-0.57415400	2.79959100	1.18353600
H	-1.19871100	1.27761000	2.66335200
C	-1.21987200	3.80398600	0.24368300
H	-1.76262400	2.38902000	-1.29204800
H	-2.70060700	3.85964000	-1.32945300
H	0.06188000	3.27365500	1.93364500
H	0.20393800	2.20339300	0.58570500
H	-1.71214000	4.56190100	0.86014700
H	-0.46190400	4.32533000	-0.34254100
H	-3.45164400	1.02704700	1.87383600
H	-1.28635200	0.12609100	-0.68444800
Br	0.82881000	-0.93910000	-1.62445800

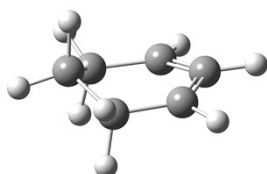
32.Br



Zero-point correction=	0.203758
(Hartree/Particle)	
Thermal correction to Energy=	0.214439
Thermal correction to Enthalpy=	0.215383
Thermal correction to Gibbs Free Energy=	0.166408
Sum of electronic and zero-point Energies=	-2886.934123
Sum of electronic and thermal Energies=	-2886.923442
Sum of electronic and thermal Enthalpies=	-2886.922498
Sum of electronic and thermal Free Energies=	-2886.971473

C	0.21341500	-0.10536400	0.22353900
H	0.55806600	-1.12895200	0.10487500
C	0.99572500	0.90294800	-0.57265300
H	0.98356200	0.67369500	-1.63664900
H	0.62094800	1.91336300	-0.41623400
C	-2.73181800	1.44654100	0.79000900
C	-3.21651500	2.38069300	-0.27003800
C	-1.76197800	1.93187900	1.74145600
C	-2.11048200	3.29778800	-0.76918900
H	-4.00253500	2.96502900	0.23163300
H	-3.71133300	1.84279800	-1.07765600
C	-1.20667100	3.14556300	1.57546000
H	-1.57574200	1.35135000	2.63579800
C	-1.44291400	4.02368700	0.39546100
H	-1.37192400	2.69877900	-1.30801100
H	-2.51253700	4.01524200	-1.48200000
H	-0.58405800	3.54248600	2.37131500
H	2.03155700	0.86889700	-0.22822900
H	-2.06092500	4.86250100	0.74205900
H	-0.49752000	4.47907700	0.09106200
H	-3.45907500	0.73861900	1.17379300
H	0.12283500	0.13717800	1.27901900
Br	-1.66483000	-0.22909100	-0.39773900

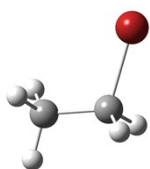
Product 15 (2-cyclohexenium ion)



Zero-point correction=			0.134172
(Hartree/Particle)			
Thermal correction to Energy=			0.139725
Thermal correction to Enthalpy=			0.140669
Thermal correction to Gibbs Free Energy=			0.105564
Sum of electronic and zero-point Energies=			-233.581498
Sum of electronic and thermal Energies=			-233.575944
Sum of electronic and thermal Enthalpies=			-233.575000
Sum of electronic and thermal Free Energies=			-233.610106

C	-3.83135900	-0.88153900	-0.09932200
C	-2.31356500	-0.99284400	-0.04875400
C	-1.66199800	0.23029100	0.43477900
C	-2.31434200	1.21337600	1.15213100
C	-3.59767300	0.94424800	1.58539400
C	-4.36638700	-0.23536100	1.17129800
H	-0.59205500	0.33285300	0.27059100
H	-1.97570600	-1.78507000	0.64534000
H	-1.87750800	-1.28169100	-1.00863600
H	-4.11078200	-0.26180800	-0.95388600
H	-4.28170400	-1.85998000	-0.24940100
H	-1.78742500	2.09344300	1.49308600
H	-4.04432000	1.60622500	2.32330300
H	-4.32120000	-0.91981600	2.03915400
H	-5.42516500	0.02729500	1.09994800

2-Bromoethane

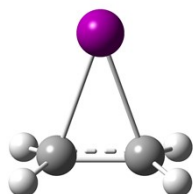


Zero-point correction=			0.066532
(Hartree/Particle)			
Thermal correction to Energy=			0.070645
Thermal correction to Enthalpy=			0.071590
Thermal correction to Gibbs Free Energy=			0.039168
Sum of electronic and zero-point Energies=			-2653.337027
Sum of electronic and thermal Energies=			-2653.332914
Sum of electronic and thermal Enthalpies=			-2653.331970
Sum of electronic and thermal Free Energies=			-2653.364391

C	-1.70396000	0.34096100	0.00018000
H	-1.34392400	-0.69019500	-0.00472600
H	-1.34909500	0.83518900	-0.90298100
H	-2.79267800	0.32708200	-0.02012500
C	-1.19508500	1.04402500	1.23681700
H	-1.55883600	0.58782700	2.15247000
H	-0.11104300	1.09746200	1.26689300
Br	-1.80900100	2.89816000	1.30032400

Figure 4

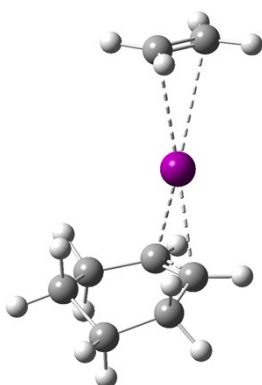
Iodiranium Ion 6.I



Zero-point correction=			0.054543
(Hartree/Particle)			
Thermal correction to Energy=			0.058191
Thermal correction to Enthalpy=			0.059135
Thermal correction to Gibbs Free Energy=			0.027089
Sum of electronic and zero-point Energies=			-375.855440
Sum of electronic and thermal Energies=			-375.851793
Sum of electronic and thermal Enthalpies=			-375.850848
Sum of electronic and thermal Free Energies=			-375.882894

C	0.91381700	-0.71656200	-0.00021700
H	1.07328100	-1.25344900	-0.92740800
H	1.07325900	-1.25402700	0.92664300
C	0.91253100	0.71784100	0.00023300
H	1.07102000	1.25558700	-0.92662800
H	1.07101000	1.25500900	0.92743100
I	-1.18274600	-0.00126800	-0.00001100

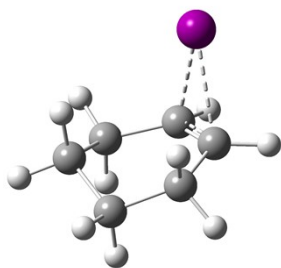
21.I



Zero-point correction=			0.201987
(Hartree/Particle)			
Thermal correction to Energy=			0.213544
Thermal correction to Enthalpy=			0.214488
Thermal correction to Gibbs Free Energy=			0.161760
Sum of electronic and zero-point Energies=			-610.358044
Sum of electronic and thermal Energies=			-610.346487
Sum of electronic and thermal Enthalpies=			-610.345542
Sum of electronic and thermal Free Energies=			-610.398270

C	2.05624400	-0.75145200	0.46778200
H	1.96221300	-1.11896500	1.48426100
C	2.04339400	0.64332400	0.27651800
H	1.96472200	1.27604200	1.15502000
C	-3.00837700	-0.23242400	-0.78338100
C	-3.13828300	0.01946900	0.52330800
H	-3.23319700	-0.78126400	1.24707100
H	-2.99449100	-1.24646800	-1.16492100
C	2.55914700	-1.70410400	-0.58360700
H	3.22799700	-2.40126500	-0.07319400
H	1.73430800	-2.31491900	-0.95548800
C	2.49307800	1.26863000	-1.00505600
H	1.88411100	2.14450800	-1.23045800
H	3.49916200	1.65371200	-0.78936900
C	2.55126700	0.27615900	-2.16081700
H	1.53901900	0.03412500	-2.49674600
H	3.05890700	0.74020900	-3.00490700
C	3.28216300	-0.99178800	-1.73002800
H	3.38915400	-1.68030700	-2.56644900
H	4.29277000	-0.72733800	-1.40853800
H	-2.97128200	0.56828500	-1.51241000
H	-3.21006600	1.03309500	0.89936600
I	-0.22128400	-0.08863100	0.15428500

Product 12.I

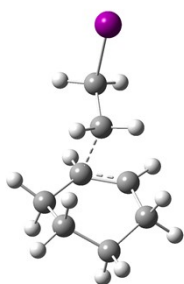


Zero-point correction=	0.149028
(Hartree/Particle)	
Thermal correction to Energy=	0.155967
Thermal correction to Enthalpy=	0.156912
Thermal correction to Gibbs Free Energy=	0.116339
Sum of electronic and zero-point Energies=	-531.823252
Sum of electronic and thermal Energies=	-531.816313
Sum of electronic and thermal Enthalpies=	-531.815369
Sum of electronic and thermal Free Energies=	-531.855942

C	-4.98093400	-1.60539400	-0.00869200
C	-3.45772300	-1.63272500	0.02234600
C	-2.84828400	-0.27687300	0.17014800
C	-3.61857800	0.83701800	0.66260200
C	-5.05671000	0.68507500	1.08767700
C	-5.51429100	-0.77619900	1.15549600

H	-1.76755900	-0.20614900	0.24483700
H	-3.11166400	-2.17534000	0.91417700
H	-3.01881100	-2.15320300	-0.82883400
H	-5.33221600	-1.20183000	-0.96240400
H	-5.35320100	-2.62656900	0.05324300
H	-3.06059600	1.68082000	1.05502400
H	-5.13015900	1.16297800	2.06784900
H	-5.70042400	1.27309000	0.43238600
H	-5.16706500	-1.21808700	2.09269500
H	-6.60208200	-0.80199800	1.18206800
I	-3.28008100	1.11952300	-1.57593700

22.I

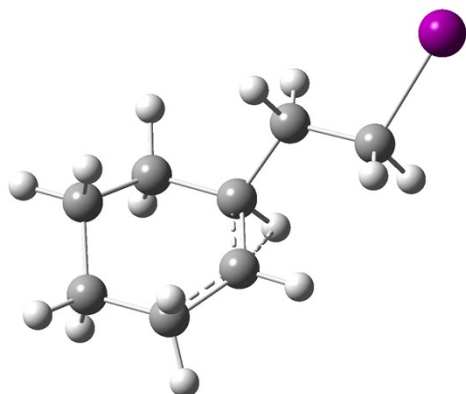


Zero-point correction=	0.205389
(Hartree/Particle)	
Thermal correction to Energy=	0.215376
Thermal correction to Enthalpy=	0.216321
Thermal correction to Gibbs Free Energy=	0.167429
Sum of electronic and zero-point Energies=	-610.362125
Sum of electronic and thermal Energies=	-610.352137
Sum of electronic and thermal Enthalpies=	-610.351193
Sum of electronic and thermal Free Energies=	-610.400084

C	-1.14630000	-0.64056000	0.30028400
H	-0.86943700	-0.87746700	1.32465500
C	-0.65673800	0.72392000	-0.11929400
H	0.43495000	0.75957900	-0.07484300
H	-0.91533900	1.02939100	-1.13118300
C	-1.64010800	1.90929500	0.72215200
C	-2.27988100	2.90054100	-0.21569100
C	-0.34636700	2.09756700	1.20156900
C	-1.25252600	3.76460400	-0.94234100
H	-2.92809100	3.52805500	0.40350700
H	-2.93763800	2.37446600	-0.90946200
C	0.53220500	3.22362900	0.75867700
H	-0.00557400	1.47057700	2.02069800
C	-0.24125100	4.33539600	0.04622400
H	-0.73458600	3.18231600	-1.71085800
H	-1.76820900	4.56792000	-1.46596500
H	1.02906300	3.59250700	1.66008800
H	1.34052200	2.83339900	0.13250900
H	-0.76614200	4.93962600	0.78983900

H	0.46383300	4.99541900	-0.45574400
H	-2.30643200	1.28793600	1.31070100
H	-2.21854800	-0.74785500	0.17158700
I	-0.22695900	-2.10627900	-0.94849800

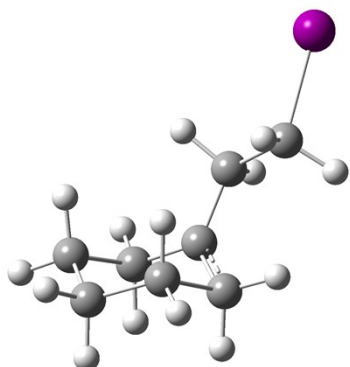
TS23.I



Zero-point correction=	0.202737
(Hartree/Particle)	
Thermal correction to Energy=	0.212107
Thermal correction to Enthalpy=	0.213052
Thermal correction to Gibbs Free Energy=	0.165989
Sum of electronic and zero-point Energies=	-610.356154
Sum of electronic and thermal Energies=	-610.346784
Sum of electronic and thermal Enthalpies=	-610.345840
Sum of electronic and thermal Free Energies=	-610.392902

C	0.70729000	0.64403400	0.37053400
H	0.52222400	1.48585700	-0.29238600
C	-0.28492500	-0.48550000	0.19016500
H	-0.34699000	-0.78477400	-0.85824600
H	0.03135900	-1.36113500	0.75511000
C	-1.74899400	-0.18152200	0.66056800
C	-2.71865800	-1.35564700	0.47144000
C	-2.25133200	1.11114200	0.30357700
C	-3.74767400	-1.07499000	-0.62015400
H	-3.23293400	-1.55881100	1.41249900
H	-2.13919100	-2.24714800	0.23393000
C	-3.56452100	1.38123900	-0.21940900
H	-1.58140600	1.96100200	0.43144700
C	-4.52134500	0.20262000	-0.31199300
H	-3.24482300	-0.97780400	-1.58867300
H	-4.43176000	-1.91717900	-0.70638900
H	-3.97206500	2.31722300	0.17841600
H	-3.23316500	1.70721800	-1.24065800
H	-5.05366600	0.10031000	0.63622200
H	-5.27042800	0.40949600	-1.07438600
H	-1.61630200	0.06399800	1.74897100
H	0.75349400	0.99438600	1.40016500
I	2.67163400	-0.03096000	-0.11517700

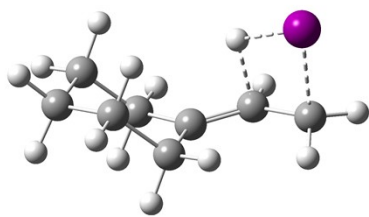
24.I



Zero-point correction=	0.204984
(Hartree/Particle)	
Thermal correction to Energy=	0.214766
Thermal correction to Enthalpy=	0.215711
Thermal correction to Gibbs Free Energy=	0.167664
Sum of electronic and zero-point Energies=	-610.379666
Sum of electronic and thermal Energies=	-610.369883
Sum of electronic and thermal Enthalpies=	-610.368939
Sum of electronic and thermal Free Energies=	-610.416985

C	0.13048800	-0.31046800	0.27862600
H	0.89887900	0.27741400	0.77388500
C	-0.72981400	0.53509900	-0.64158500
H	-0.17742900	0.89408200	-1.51988100
H	-1.52848400	-0.07844400	-1.09827600
C	-1.46692500	1.66643900	-0.06382300
C	-2.03154900	2.66639100	-0.95810500
C	-1.48138500	1.95660000	1.35270200
C	-0.98666900	3.85440800	-0.87498000
H	-2.98656100	3.04406600	-0.59243500
H	-2.11139100	2.32157600	-1.98716700
C	-0.38096500	3.11164900	1.43298900
H	-1.18405100	1.12589600	1.98574600
C	-0.79201100	4.28759000	0.56648100
H	-0.04225200	3.52565200	-1.31395000
H	-1.38263800	4.65096100	-1.50286800
H	-0.31076600	3.36477700	2.48994100
H	0.58813800	2.71589600	1.12223000
H	-1.70975600	4.73576100	0.95395100
H	-0.01704400	5.05529900	0.61272500
H	-2.42214800	2.39655300	1.68078500
H	-0.46042900	-0.83651300	1.02273100
I	1.14949500	-1.80886600	-0.84303900

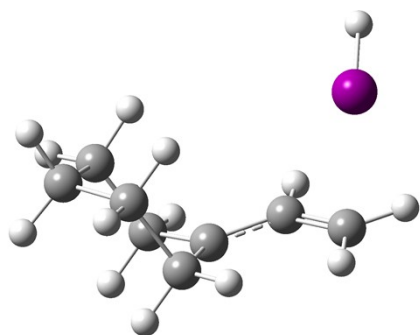
TS25.I



Zero-point correction=	0.199437
(Hartree/Particle)	
Thermal correction to Energy=	0.208848
Thermal correction to Enthalpy=	0.209792
Thermal correction to Gibbs Free Energy=	0.162989
Sum of electronic and zero-point Energies=	-610.336450
Sum of electronic and thermal Energies=	-610.327038
Sum of electronic and thermal Enthalpies=	-610.326094
Sum of electronic and thermal Free Energies=	-610.372897

C	-1.09237200	-0.85747300	0.34185500
H	-0.95421500	-0.80810800	1.41562900
C	-1.64282400	0.36318300	-0.33003500
H	-0.01837900	0.53392300	-0.94613200
H	-2.25602800	0.17669600	-1.20584900
C	-1.48514300	1.63658300	0.11066000
C	-2.08635000	2.77994500	-0.64619600
C	-0.67642800	2.02138600	1.31022700
C	-1.01888400	3.82347100	-1.00753200
H	-2.82557300	3.24966900	0.01271800
H	-2.61530000	2.42588300	-1.53067100
C	0.38133600	3.07679100	0.93802000
H	-0.20924800	1.16299800	1.79327700
C	-0.24875600	4.26990900	0.22921600
H	-0.32649500	3.39150300	-1.73794200
H	-1.50075900	4.67068300	-1.49445400
H	0.90054400	3.38778400	1.84411500
H	1.13342800	2.62070600	0.28501000
H	-0.92695100	4.78472000	0.91627300
H	0.52429100	4.98683100	-0.04780000
H	-1.36648600	2.46102100	2.03884200
H	-1.54246200	-1.79084600	0.02465400
I	0.95843100	-0.88009800	-0.50357200

26.I



Zero-point correction=	0.199409
(Hartree/Particle)	
Thermal correction to Energy=	0.210958
Thermal correction to Enthalpy=	0.211902
Thermal correction to Gibbs Free Energy=	0.158214
Sum of electronic and zero-point Energies=	-610.369761
Sum of electronic and thermal Energies=	-610.358213
Sum of electronic and thermal Enthalpies=	-610.357268
Sum of electronic and thermal Free Energies=	-610.410957

C	-1.28179600	-0.60040600	0.23010300
H	-0.91678300	-0.60877400	1.24743500
C	-1.72700200	0.52388000	-0.37642700
H	1.84406700	-0.88992100	-1.75946500
H	-2.16348400	0.45920400	-1.36625400
C	-1.71498700	1.79110700	0.25077700
C	-2.33093900	2.93504100	-0.42986900
C	-0.93270600	2.10991400	1.44947800
C	-1.13083100	3.79044300	-0.97402600
H	-2.87717500	3.55637800	0.28242100
H	-2.98582500	2.63339800	-1.24415900
C	0.27943800	2.96472800	0.92837400
H	-0.56066700	1.24133400	1.98436900
C	-0.20738100	4.18639200	0.16611800
H	-0.59020600	3.20866600	-1.72415500
H	-1.56002900	4.65611000	-1.47668300
H	0.87130300	3.23728600	1.80122800
H	0.90326300	2.33296200	0.29147700
H	-0.72761000	4.86613200	0.84581900
H	0.65102900	4.72997700	-0.23252700
H	-1.51671400	2.73848200	2.12416400
H	-1.34260000	-1.56084000	-0.26658400
I	2.04451000	-0.95013200	-0.16440000

HI

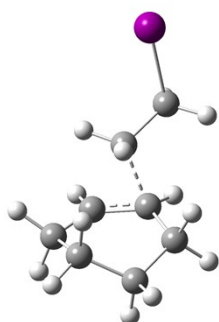


Zero-point correction=	0.005379
(Hartree/Particle)	
Thermal correction to Energy=	0.007739

Thermal correction to Enthalpy=			0.008684
Thermal correction to Gibbs Free Energy=			-0.014745
Sum of electronic and zero-point Energies=			-298.218594
Sum of electronic and thermal Energies=			-298.216233
Sum of electronic and thermal Enthalpies=			-298.215289
Sum of electronic and thermal Free Energies=			-298.238717

I	-5.39656500	0.60327200	0.00000000
H	-7.00294100	0.60327200	0.00000000

TS27.I

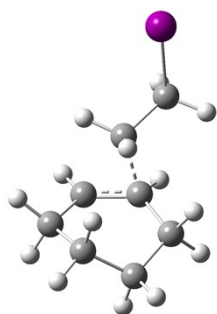


Zero-point correction=			0.205690
(Hartree/Particle)			
Thermal correction to Energy=			0.214679
Thermal correction to Enthalpy=			0.215623
Thermal correction to Gibbs Free Energy=			0.169781
Sum of electronic and zero-point Energies=			-610.360851
Sum of electronic and thermal Energies=			-610.351862
Sum of electronic and thermal Enthalpies=			-610.350917
Sum of electronic and thermal Free Energies=			-610.396760

C	-0.06125700	0.03331900	0.71325500
H	0.60836300	0.17049200	1.55697800
C	-0.50699300	1.36018600	0.12573700
H	0.30204300	1.99193500	-0.22258600
H	-1.16465600	1.15847100	-0.72521100
C	-2.05350900	2.51870300	0.49621700
C	-1.98878200	3.73650600	-0.34348900
C	-1.11803200	2.23226600	1.49121000
C	-0.74002800	4.58538900	-0.11218500
H	-2.89156200	4.29089100	-0.04295800
H	-2.15715800	3.48434300	-1.39336600
C	-0.13546000	3.28333600	1.97847900
H	-1.39349700	1.45961600	2.20051600
C	-0.41887600	4.66256100	1.37789000
H	0.10631400	4.17578900	-0.66826500
H	-0.91394300	5.58131700	-0.51621500
H	-0.21601300	3.32068300	3.06493000
H	0.88507700	2.95957500	1.76243600
H	-1.26929100	5.10983100	1.89968500

H	0.43435400	5.31560600	1.55183400
H	-2.90776600	1.85803600	0.37792900
H	-0.90509400	-0.58697400	1.00119400
I	1.02236100	-1.03532600	-0.78085500

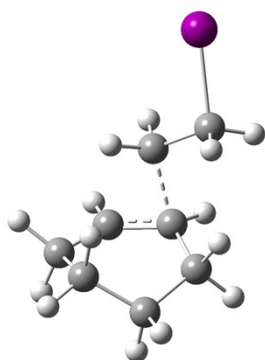
28.I



Zero-point correction=			0.205791
(Hartree/Particle)			
Thermal correction to Energy=			0.215677
Thermal correction to Enthalpy=			0.216621
Thermal correction to Gibbs Free Energy=			0.167509
Sum of electronic and zero-point Energies=			-610.360762
Sum of electronic and thermal Energies=			-610.350877
Sum of electronic and thermal Enthalpies=			-610.349933
Sum of electronic and thermal Free Energies=			-610.399045

C	-0.22120500	-0.71705800	0.79550100
H	0.45212200	-0.56102400	1.63303300
C	-0.68628100	0.59738600	0.19220300
H	0.11634900	1.22601000	-0.17590500
H	-1.35849100	0.37749600	-0.64193600
C	-2.20898200	1.80542000	0.55971400
C	-2.09286300	3.02514300	-0.26933000
C	-1.28998900	1.47320100	1.55579800
C	-0.82578800	3.83808400	-0.01013700
H	-2.98635000	3.60194600	0.01738900
H	-2.24993300	2.78411500	-1.32386500
C	-0.27723100	2.48623300	2.06298400
H	-1.59931100	0.70367300	2.25464100
C	-0.51874900	3.88259000	1.48410900
H	0.01646300	3.41610200	-0.56287400
H	-0.96979800	4.84445800	-0.39976200
H	-0.35838500	2.50856400	3.14973600
H	0.73392000	2.13691500	1.84214600
H	-1.36224300	4.34315800	2.00561300
H	0.34971500	4.50968200	1.67716500
H	-3.08356200	1.17519000	0.42535600
H	-1.05556000	-1.34383000	1.09604000
I	0.86594900	-1.79069100	-0.69253400

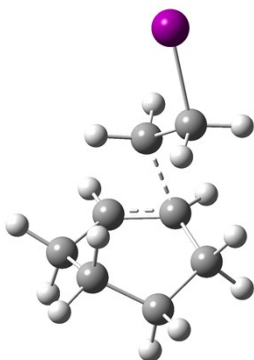
TS29.I



Zero-point correction=	0.205407
(Hartree/Particle)	
Thermal correction to Energy=	0.214530
Thermal correction to Enthalpy=	0.215474
Thermal correction to Gibbs Free Energy=	0.169327
Sum of electronic and zero-point Energies=	-610.357501
Sum of electronic and thermal Energies=	-610.348378
Sum of electronic and thermal Enthalpies=	-610.347434
Sum of electronic and thermal Free Energies=	-610.393581

C	0.42440500	0.27610100	0.92495000
H	1.17723400	0.86511000	1.43387700
C	-0.64018100	1.13722300	0.25628400
H	-0.16033700	1.91680900	-0.33330500
H	-1.28291000	0.53175400	-0.37448500
C	-2.10836800	2.56359900	0.56734000
C	-1.64591900	3.94556400	0.38383200
C	-1.62052800	1.71465600	1.56574800
C	-0.50429100	4.33327900	1.31439200
H	-2.54962800	4.54196800	0.60060400
H	-1.44994500	4.13806900	-0.67521600
C	-0.88834000	2.30357100	2.76485300
H	-2.21059000	0.82416800	1.76295700
C	-0.80227000	3.83112000	2.72306300
H	0.43329500	3.90221000	0.94919000
H	-0.37712200	5.41409600	1.30012900
H	-1.43536300	1.98227800	3.65193000
H	0.10478100	1.86819800	2.85961200
H	-1.75016200	4.26043900	3.05846000
H	-0.04071800	4.16964200	3.42301100
H	-2.85330900	2.18037300	-0.12544900
H	-0.00084000	-0.46415500	1.59549600
I	1.44906100	-0.78208500	-0.61925400

30.I



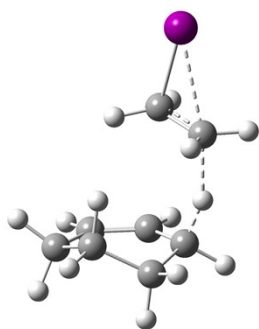
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Zero-point correction=                0.205944
(Hartree/Particle)
Thermal correction to Energy=         0.215765
Thermal correction to Enthalpy=       0.216709
Thermal correction to Gibbs Free Energy= 0.168792
Sum of electronic and zero-point Energies= -610.357584
Sum of electronic and thermal Energies= -610.347763
Sum of electronic and thermal Enthalpies= -610.346819
Sum of electronic and thermal Free Energies= -610.394736

```

C	-0.91317600	0.37584300	0.25555300
H	-0.92594600	-0.51515500	0.87326700
C	0.44072700	0.62906900	-0.38212900
H	1.23111900	0.73367400	0.35430000
H	0.43513700	1.47715300	-1.05740200
C	-2.41458200	1.42407000	1.00018600
C	-3.11979100	2.26604300	0.00707000
C	-1.11988300	1.68960400	1.43803500
C	-2.19162200	3.24828900	-0.69701100
H	-3.87132900	2.80506200	0.60427200
H	-3.69566200	1.64089100	-0.67829600
C	-0.45573500	3.01830400	1.14309800
H	-0.78264500	1.17735600	2.33254900
C	-1.33213900	3.97840800	0.33031500
H	-1.56558900	2.71023900	-1.41569100
H	-2.78480800	3.95513200	-1.27431600
H	-0.22629100	3.45498600	2.11684300
H	0.51185900	2.86242800	0.66754900
H	-1.99242100	4.52388400	1.00874900
H	-0.70220300	4.72206300	-0.15428800
H	-2.95641600	0.59394100	1.44530400
H	-1.65588800	0.26777500	-0.53760400
I	0.91353900	-1.08712100	-1.56177600

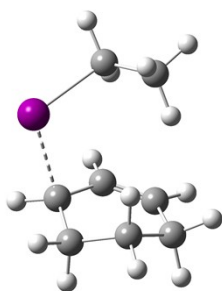
TS31.I



Zero-point correction=	0.200691
(Hartree/Particle)	
Thermal correction to Energy=	0.210730
Thermal correction to Enthalpy=	0.211674
Thermal correction to Gibbs Free Energy=	0.162628
Sum of electronic and zero-point Energies=	-610.329245
Sum of electronic and thermal Energies=	-610.319206
Sum of electronic and thermal Enthalpies=	-610.318262
Sum of electronic and thermal Free Energies=	-610.367309

C	-0.25697100	-0.02676000	-0.27713600
H	-0.21767300	-0.59208100	0.64532800
C	0.69336700	1.04683200	-0.44513900
H	1.63825400	1.02284900	0.08555000
H	0.59383100	1.73686300	-1.27519900
C	-2.79981900	1.70772700	1.35357100
C	-3.35577900	2.47147000	0.19120300
C	-1.54681900	1.83721800	1.79885700
C	-2.26786900	3.13448100	-0.64976200
H	-4.04412500	3.22807500	0.58452700
H	-3.97408500	1.81126200	-0.42096000
C	-0.59065400	2.78709500	1.18305800
H	-1.21838800	1.27420900	2.66515400
C	-1.21889300	3.79527100	0.23855600
H	-1.78883600	2.38186000	-1.28712900
H	-2.70674400	3.86638800	-1.32657800
H	0.07739300	3.24271500	1.91611500
H	0.17036400	2.16035800	0.56666400
H	-1.69377100	4.56653800	0.85276000
H	-0.45267600	4.29861000	-0.35269500
H	-3.47886000	1.04840300	1.88402700
H	-1.24701500	0.10884000	-0.69338000
I	0.94882300	-1.08228500	-1.75481400

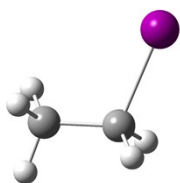
32.I



Zero-point correction= 0.203438
 (Hartree/Particle)
 Thermal correction to Energy= 0.214082
 Thermal correction to Enthalpy= 0.215026
 Thermal correction to Gibbs Free Energy= 0.165922
 Sum of electronic and zero-point Energies= -610.374732
 Sum of electronic and thermal Energies= -610.364089
 Sum of electronic and thermal Enthalpies= -610.363144
 Sum of electronic and thermal Free Energies= -610.412248

C	0.16679400	-0.09430500	-0.15311300
H	0.53166300	-1.06549700	-0.47715500
C	0.98029900	1.06995600	-0.65317800
H	1.04347700	1.08730800	-1.73968100
H	0.58087900	2.01940800	-0.30009700
C	-2.86826300	1.44269100	0.59480700
C	-3.23186800	2.66246100	-0.20176800
C	-1.91272400	1.61887400	1.67666600
C	-2.02807500	3.55972300	-0.44656500
H	-3.96900900	3.18411100	0.42494700
H	-3.74831200	2.40085200	-1.12437600
C	-1.24947200	2.77601100	1.81851600
H	-1.82049900	0.83117600	2.41412700
C	-1.34752400	3.92520800	0.87041400
H	-1.32306500	3.03843500	-1.10031300
H	-2.33463500	4.46011500	-0.97594000
H	-0.63722400	2.91586200	2.70372900
H	1.99260300	0.96247600	-0.25612300
H	-1.89850600	4.72230300	1.38479700
H	-0.35037800	4.33745800	0.69800600
H	-3.69147700	0.77115900	0.81822000
H	0.00649300	-0.09597700	0.92198000
I	-1.84962100	-0.09439000	-0.94643000

2-Iodoethane

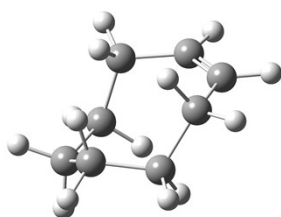


Zero-point correction=			0.066004
(Hartree/Particle)			
Thermal correction to Energy=			0.070218
Thermal correction to Enthalpy=			0.071162
Thermal correction to Gibbs Free Energy=			0.037809
Sum of electronic and zero-point Energies=			-376.773188
Sum of electronic and thermal Energies=			-376.768975
Sum of electronic and thermal Enthalpies=			-376.768031
Sum of electronic and thermal Free Energies=			-376.801384

C	-1.70414400	0.33752200	-0.00210200
H	-1.34179100	-0.69347700	-0.00373900
H	-1.35069000	0.82638000	-0.90880500
H	-2.79276600	0.31825900	-0.02651600
C	-1.19684100	1.04476100	1.23435000
H	-1.56174500	0.59543300	2.15254200
H	-0.11354100	1.10474400	1.26709600
I	-1.86514900	3.08612500	1.31585400

Figure 7

cis-Cyclooctene

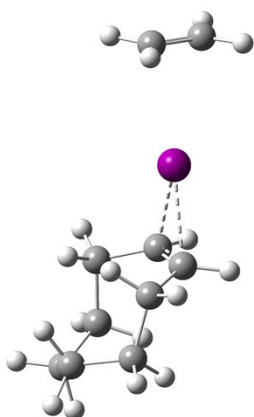


Zero-point correction=			0.205486
(Hartree/Particle)			
Thermal correction to Energy=			0.213337
Thermal correction to Enthalpy=			0.214281
Thermal correction to Gibbs Free Energy=			0.173596
Sum of electronic and zero-point Energies=			-313.004886
Sum of electronic and thermal Energies=			-312.997035
Sum of electronic and thermal Enthalpies=			-312.996091
Sum of electronic and thermal Free Energies=			-313.036776

C	-1.94670700	0.02275200	-0.20511800
C	-1.27792700	1.29987800	0.23751700
C	1.00800400	-1.32016000	-0.46296800
C	0.09697800	1.63006900	-0.39235800
C	1.96732200	-0.18130200	-0.10756300
C	1.32164500	1.11793700	0.38550200
H	-1.16177800	1.29448400	1.32662000
H	0.12245000	1.27389100	-1.42557400
H	0.56298800	-1.12127900	-1.43945200
H	2.57609900	0.03439800	-0.99000600
H	-2.90347000	0.13205100	-0.70548100

H	-1.95917700	2.12224300	0.01715500
H	1.59085700	-2.23580800	-0.57856000
H	0.16845200	2.71774100	-0.44645600
H	2.66349000	-0.52232300	0.66415100
H	2.09736000	1.88672200	0.36829100
H	1.04561200	1.01510300	1.43807100
C	-1.47398700	-1.20706900	-0.03842600
H	-2.06028400	-2.03765100	-0.41903700
C	-0.13565300	-1.53941600	0.55773100
H	0.03733000	-0.92206600	1.44316000
H	-0.13798600	-2.57363700	0.90121900

33.I

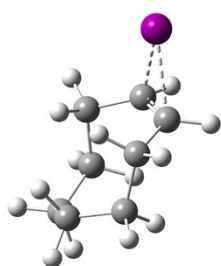


Zero-point correction=	0.260211
(Hartree/Particle)	
Thermal correction to Energy=	0.274280
Thermal correction to Enthalpy=	0.275225
Thermal correction to Gibbs Free Energy=	0.216904
Sum of electronic and zero-point Energies=	-688.905782
Sum of electronic and thermal Energies=	-688.891713
Sum of electronic and thermal Enthalpies=	-688.890769
Sum of electronic and thermal Free Energies=	-688.949090

C	-1.10917100	-0.59934500	-0.55100100
H	-0.49692800	-1.43434400	-0.87952900
C	-1.10126300	-0.32210100	0.84132300
H	-0.50190600	-0.98734100	1.45627900
C	-2.21704300	-0.19612100	-1.45805100
H	-2.61519500	0.78243500	-1.19249000
H	-1.86380800	-0.15130100	-2.48553800
C	-2.14695100	0.48902500	1.54128300
H	-1.77473100	0.72148400	2.53757200
H	-2.31008800	1.43790500	1.03009400
C	-3.50155900	-0.26893200	1.64104800
H	-3.92163200	-0.00531500	2.61077000
H	-3.33876300	-1.35009700	1.67544700
C	-3.29842000	-1.30524300	-1.28146700
H	-2.89693200	-2.11122800	-0.65918200

H	-3.49463800	-1.76228900	-2.25048800
C	-4.51741900	0.10337200	0.54786500
H	-4.32659800	1.13100400	0.22816900
H	-5.50917700	0.13062400	1.00085400
C	-4.61445900	-0.81678800	-0.67379400
H	-5.18994400	-0.29434700	-1.44062800
H	-5.19420300	-1.70375600	-0.41064100
C	3.20776800	2.51152400	-0.56608000
H	3.52972700	1.99387300	-1.46198400
H	3.68556100	2.22555800	0.36350300
C	2.30921900	3.49399200	-0.61430100
H	1.86723500	3.81204500	-1.55113300
H	2.02306100	4.04390400	0.27451200
I	0.54765700	0.99589100	-0.14555300

Product 17.I

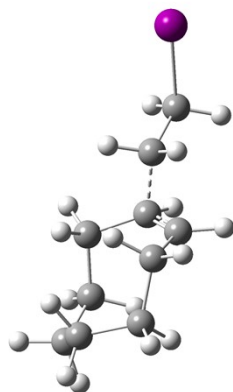


Zero-point correction=	0.207352
(Hartree/Particle)	
Thermal correction to Energy=	0.216725
Thermal correction to Enthalpy=	0.217669
Thermal correction to Gibbs Free Energy=	0.171792
Sum of electronic and zero-point Energies=	-610.373142
Sum of electronic and thermal Energies=	-610.363769
Sum of electronic and thermal Enthalpies=	-610.362825
Sum of electronic and thermal Free Energies=	-610.408702

C	-1.39383500	-0.61297900	-1.29067300
H	-1.21485100	-1.45899300	-1.94816500
C	-0.78217600	-0.68869600	0.01339900
H	-0.22930600	-1.60106900	0.21942900
C	-2.61919000	0.18187200	-1.56025800
H	-2.62398500	1.11660700	-1.00160200
H	-2.69380000	0.41445500	-2.61966900
C	-1.24455800	0.10035300	1.19703800
H	-0.47689900	0.02357500	1.96514600
H	-1.34903200	1.15613400	0.94818500
C	-2.60236800	-0.43065600	1.74266000
H	-2.53894400	-0.34511500	2.82650000
H	-2.71247300	-1.50009400	1.53984500
C	-3.78109600	-0.75411200	-1.10226200
H	-3.37794100	-1.73363900	-0.82386300
H	-4.43100300	-0.94589100	-1.95489300

C	-3.83045700	0.35686900	1.25610900
H	-3.52776500	1.38682700	1.05107900
H	-4.53481900	0.43196300	2.08523700
C	-4.60756500	-0.21110400	0.06360400
H	-5.27701500	0.56876600	-0.30426700
H	-5.24820300	-1.02595800	0.40638800
I	0.61887200	0.44893400	-1.36255800

34.I

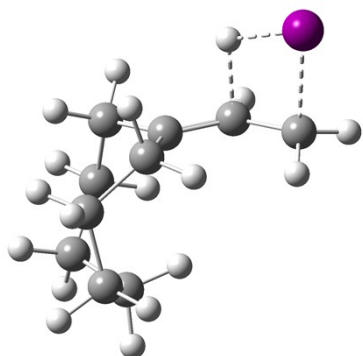


Zero-point correction=	0.263703
(Hartree/Particle)	
Thermal correction to Energy=	0.276084
Thermal correction to Enthalpy=	0.277029
Thermal correction to Gibbs Free Energy=	0.222740
Sum of electronic and zero-point Energies=	-688.908710
Sum of electronic and thermal Energies=	-688.896329
Sum of electronic and thermal Enthalpies=	-688.895385
Sum of electronic and thermal Free Energies=	-688.949674

C	0.35145000	1.86938500	-0.13981400
H	-0.32076900	1.11441700	-0.54250100
C	1.79676900	1.44344600	0.01565900
H	1.89152600	0.58855400	0.67844700
H	2.42147900	2.25860700	0.37081300
C	-0.27544300	2.08432900	1.41504400
C	-0.59984300	3.30828400	0.81486200
H	0.14439200	4.09930900	0.87743800
H	0.58972800	2.11603800	2.07184200
H	0.30785300	2.70715900	-0.84961200
C	-1.90411800	3.64039700	0.20463700
H	-1.78530900	4.48932400	-0.46528300
H	-2.29030100	2.79929400	-0.37282500
C	-1.32539400	1.08588200	1.83141500
H	-2.06538700	0.95147500	1.04139600
H	-0.84601900	0.11946900	1.98566500
C	-2.93567300	3.98257200	1.33222100
H	-3.54535600	4.78822700	0.92647100
H	-2.43001800	4.40581800	2.20487100

C	-1.99192300	1.59788200	3.12910700
H	-1.92187500	0.83432400	3.90268900
H	-1.42049000	2.44850200	3.51144500
C	-3.46184700	2.00432200	2.97908900
H	-4.08347300	1.10683800	2.98959500
H	-3.73600100	2.57029100	3.87143300
C	-3.84602600	2.81161800	1.73441100
H	-4.84335400	3.21482600	1.91555000
H	-3.96450500	2.14671500	0.87535500
I	2.56281700	0.85082000	-1.88413400

TS35.I

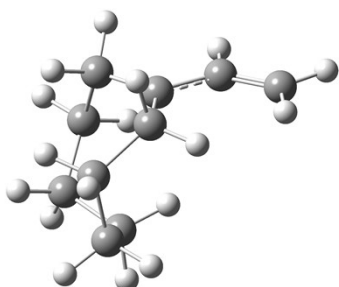


Zero-point correction=	0.257490
(Hartree/Particle)	
Thermal correction to Energy=	0.269213
Thermal correction to Enthalpy=	0.270158
Thermal correction to Gibbs Free Energy=	0.218208
Sum of electronic and zero-point Energies=	-688.885475
Sum of electronic and thermal Energies=	-688.873752
Sum of electronic and thermal Enthalpies=	-688.872807
Sum of electronic and thermal Free Energies=	-688.924757

C	-0.05364100	0.06509300	-0.34589400
H	-0.09560800	-0.32606700	-1.35551600
H	-0.62351300	-0.53155500	0.35699000
C	-0.46823000	2.23814900	0.89467400
H	1.48057200	1.44067700	0.34286100
C	-1.99540100	4.17207500	0.26842600
H	-1.93908500	5.24985100	0.10833400
H	-2.14182900	3.71785300	-0.71623100
C	-0.58117700	1.58360800	2.23942300
H	-0.69844900	0.50153800	2.15084100
H	0.39132100	1.74796200	2.72585100
C	-3.20523000	3.85775700	1.14562500
H	-4.06845300	4.32141000	0.66692600
H	-3.10180400	4.35830400	2.11278600
C	-1.66594100	2.13446400	3.17105600
H	-1.49582000	1.70262200	4.15797000
H	-1.53604600	3.21075400	3.29167200
C	-3.09102600	1.82141100	2.72914600

H	-3.24739100	0.73902300	2.75136200
H	-3.77000200	2.24161000	3.47480200
C	-3.48335700	2.35898700	1.35183300
H	-4.54744100	2.16375400	1.21494500
H	-2.98542700	1.78335400	0.56403000
I	2.07686300	-0.21431900	0.27354000
C	-0.61459400	3.73069400	0.79992000
H	-0.42462600	4.19075200	1.76986300
H	0.13808300	4.11142700	0.10677500
C	-0.16469800	1.54944800	-0.23849100
H	-0.06757900	2.09096800	-1.17476500

Product 18

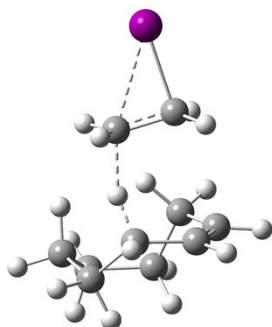


Zero-point correction=	0.250520
(Hartree/Particle)	
Thermal correction to Energy=	0.260570
Thermal correction to Enthalpy=	0.261514
Thermal correction to Gibbs Free Energy=	0.215727
Sum of electronic and zero-point Energies=	-390.699784
Sum of electronic and thermal Energies=	-390.689734
Sum of electronic and thermal Enthalpies=	-390.688790
Sum of electronic and thermal Free Energies=	-390.734578

C	-0.15441700	0.17895000	-0.40768900
H	0.06850600	-0.28369100	-1.36129500
H	-0.23406600	-0.48361300	0.44387900
C	-0.55009900	2.20994200	0.90812600
C	-1.99303400	4.15229500	0.24688500
H	-1.87805200	5.22258600	0.07708300
H	-2.14249200	3.68452100	-0.72886500
C	-0.64420300	1.54785400	2.21752500
H	-0.75623400	0.46888600	2.13379100
H	0.35756900	1.73173300	2.64578400
C	-3.19157800	3.87540900	1.14564600
H	-4.05320700	4.34318500	0.66718300
H	-3.06579600	4.39140800	2.10123900
C	-1.68077300	2.12625100	3.19595900
H	-1.49749600	1.66664700	4.16669800
H	-1.51496200	3.19497700	3.33236100
C	-3.11692800	1.85592400	2.75915100
H	-3.31250500	0.78110600	2.79455200
H	-3.78093500	2.31182800	3.49740100

C	-3.47368700	2.38232800	1.37129400
H	-4.53000700	2.17444100	1.19653600
H	-2.95451000	1.79411000	0.60164400
C	-0.61652900	3.67395700	0.82777600
H	-0.45426800	4.14254700	1.79558700
H	0.14744900	4.01358500	0.12318000
C	-0.30726000	1.51077700	-0.31807800
H	-0.20744800	2.11730300	-1.21099900

TS36.I

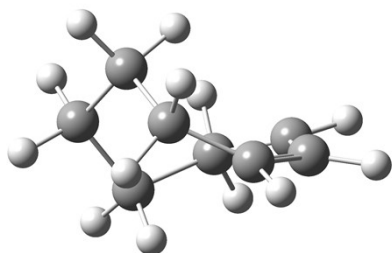


Zero-point correction=	0.258827
(Hartree/Particle)	
Thermal correction to Energy=	0.271290
Thermal correction to Enthalpy=	0.272234
Thermal correction to Gibbs Free Energy=	0.217953
Sum of electronic and zero-point Energies=	-688.868773
Sum of electronic and thermal Energies=	-688.856309
Sum of electronic and thermal Enthalpies=	-688.855365
Sum of electronic and thermal Free Energies=	-688.909646

C	-0.46919700	2.33914700	-1.17588900
H	-1.30625500	1.65358200	-1.24668800
C	0.79730700	1.87794000	-0.65404400
H	0.77587900	1.05751900	0.05193200
H	1.55896100	2.62374300	-0.46631400
C	0.04433200	2.24758400	2.52227100
C	-0.07744500	3.41315500	1.88237000
H	0.68653400	4.16750600	2.03509900
H	0.89126200	2.12848200	3.19065600
H	-0.51133100	3.24439000	-1.76891500
C	-1.17694000	3.78687700	0.95375600
H	-0.94678600	4.74285900	0.48399900
H	-1.13854800	3.04183400	0.05710900
C	-0.94233700	1.12214700	2.46832600
H	-1.27154700	0.95214300	1.43748800
H	-0.46535600	0.20066800	2.79778800
C	-2.65271500	3.76768000	1.39624600
H	-3.16749300	4.50013200	0.77510300
H	-2.68952000	4.15119800	2.41952600
C	-2.17897700	1.43661900	3.35100500
H	-2.30526600	0.65535600	4.09978100

H	-1.98828300	2.35622500	3.90682400
C	-3.48189700	1.57999700	2.56431300
H	-3.84955800	0.59041000	2.28282100
H	-4.23381400	2.00432300	3.23280600
C	-3.40857400	2.43224400	1.29500100
H	-4.43212200	2.64822400	0.98700500
H	-2.98903900	1.84428300	0.47249900
I	1.16628900	1.03667400	-2.62863600

Product 19

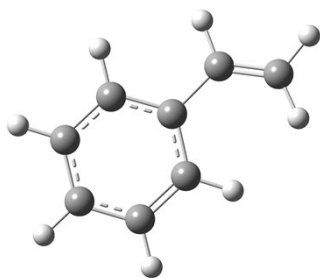


Zero-point correction=	0.191741
(Hartree/Particle)	
Thermal correction to Energy=	0.199477
Thermal correction to Enthalpy=	0.200421
Thermal correction to Gibbs Free Energy=	0.160196
Sum of electronic and zero-point Energies=	-312.130724
Sum of electronic and thermal Energies=	-312.122989
Sum of electronic and thermal Enthalpies=	-312.122044
Sum of electronic and thermal Free Energies=	-312.162270

C	-0.79061500	2.51814100	0.74542300
C	-0.19139300	3.51421400	1.49061800
H	0.70742000	3.21244200	2.02241000
H	-0.16667500	1.64419400	0.56541900
C	-0.55742800	4.83413500	1.66628400
H	-0.07405500	5.33444600	2.50385700
C	-2.18776800	2.33805100	0.33905900
H	-2.18657900	2.05982800	-0.72685400
H	-2.44697300	1.37852400	0.81872200
C	-1.31454500	5.73962600	0.79681700
H	-0.57997400	6.53943800	0.60001700
H	-2.04910100	6.26432400	1.42834500
C	-3.22715300	3.39664000	0.66936000
H	-4.20433700	2.91520400	0.69116400
H	-3.05436200	3.76614800	1.68566000
C	-3.26218500	4.54762900	-0.32800700
H	-3.60260300	4.17833900	-1.29719700
H	-4.00187700	5.27988100	0.00103000
C	-1.91362000	5.23381600	-0.50516200
H	-2.03282000	6.08478300	-1.17505900
H	-1.19761200	4.56622500	-0.99585300

Scheme 5

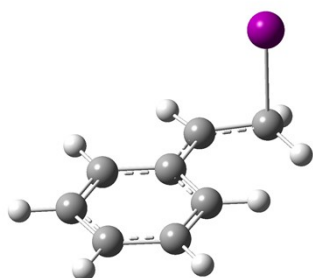
Styrene



Zero-point correction=	0.134278
(Hartree/Particle)	
Thermal correction to Energy=	0.141050
Thermal correction to Enthalpy=	0.141994
Thermal correction to Gibbs Free Energy=	0.102425
Sum of electronic and zero-point Energies=	-309.482896
Sum of electronic and thermal Energies=	-309.476124
Sum of electronic and thermal Enthalpies=	-309.475180
Sum of electronic and thermal Free Energies=	-309.514749

C	2.24803500	0.26278300	0.03030000
C	1.77051900	-1.03877200	0.03735900
C	0.40407100	-1.27599400	0.00121700
C	-0.50944900	-0.22292500	-0.03654400
C	-0.01345700	1.08290900	-0.05162300
C	1.34900600	1.32259300	-0.01665100
H	3.31289800	0.45346500	0.05583100
H	2.46136200	-1.87131100	0.06925800
H	0.03330600	-2.29431400	0.00647300
H	-0.69864900	1.91912100	-0.10243900
H	1.71498700	2.34117200	-0.03134800
C	-1.94868900	-0.52845900	-0.06030300
H	-2.18911700	-1.57860400	-0.19734200
C	-2.94655500	0.33641100	0.08125000
H	-2.78039900	1.39427700	0.24042000
H	-3.97527100	0.00492800	0.04911000

37.I

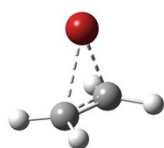


Zero-point correction=			0.136751
(Hartree/Particle)			
Thermal correction to Energy=			0.144957
Thermal correction to Enthalpy=			0.145901
Thermal correction to Gibbs Free Energy=			0.101056
Sum of electronic and zero-point Energies=			-606.841880
Sum of electronic and thermal Energies=			-606.833674
Sum of electronic and thermal Enthalpies=			-606.832730
Sum of electronic and thermal Free Energies=			-606.877576

C	-2.96589500	-0.96597200	0.00914100
C	-1.60142500	-0.96682800	0.19117100
C	-0.89845500	0.25497400	0.30956200
C	-1.60446100	1.47887100	0.22470800
C	-2.96392600	1.46901200	0.03639500
C	-3.64167400	0.24939500	-0.06906700
H	-3.50833300	-1.89714700	-0.07504800
H	-1.05527300	-1.90044600	0.25152300
H	-1.08056700	2.42257800	0.30026600
H	-3.51273900	2.39804500	-0.02985600
H	-4.71463500	0.25231400	-0.21554800
C	0.48619600	0.19110200	0.53974100
H	0.92541800	-0.79896200	0.62840100
C	1.39943400	1.29785200	0.72037800
H	2.27076300	1.08889600	1.32978800
H	0.98282300	2.28536700	0.86657900
I	2.07137100	1.13909200	-1.34113500

Figure 8

38.Br

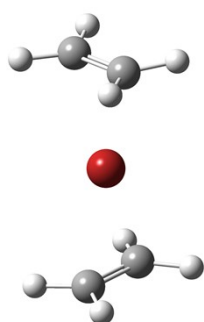


Zero-point correction=			0.107728
(Hartree/Particle)			
Thermal correction to Energy=			0.116038
Thermal correction to Enthalpy=			0.116982
Thermal correction to Gibbs Free Energy=			0.071628
Sum of electronic and zero-point Energies=			-2730.936592
Sum of electronic and thermal Energies=			-2730.928283
Sum of electronic and thermal Enthalpies=			-2730.927339
Sum of electronic and thermal Free Energies=			-2730.972693

C	2.40132100	-0.59465800	0.10803700
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H	2.45129400	-1.20862300	-0.78367400
H	2.40976500	-1.11286200	1.05988200
C	2.39381500	0.73413700	0.03888400
H	2.43749700	1.25267100	-0.91182300
H	2.39570500	1.34853800	0.93169100
C	-2.49145100	0.01468900	-0.75446800
H	-2.63227400	0.92821700	-1.31795900
C	-2.52611600	0.04715400	0.67632700
H	-2.69311800	0.98507600	1.19038300
H	-2.67864900	-0.86877800	1.23281200
H	-2.61792100	-0.92565500	-1.27566500
Br	-0.58499100	0.04683900	0.00708700

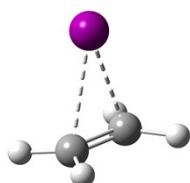
TS39.Br



Zero-point correction=	0.107811
(Hartree/Particle)	
Thermal correction to Energy=	0.115006
Thermal correction to Enthalpy=	0.115950
Thermal correction to Gibbs Free Energy=	0.075269
Sum of electronic and zero-point Energies=	-2730.930074
Sum of electronic and thermal Energies=	-2730.922879
Sum of electronic and thermal Enthalpies=	-2730.921935
Sum of electronic and thermal Free Energies=	-2730.962616

C	1.99990500	-0.61536400	0.09018300
H	2.07969900	-1.20758200	-0.81297100
H	2.03730500	-1.13868700	1.03753500
C	1.99054300	0.74886300	0.03912300
H	2.06274300	1.27301000	-0.90578500
H	2.02022600	1.34202800	0.94467100
C	-2.60759200	0.00617200	-0.72251500
H	-2.65556700	0.91038300	-1.31653100
C	-2.63909500	0.05703900	0.64136700
H	-2.71289000	1.00287800	1.16360600
H	-2.70056400	-0.84804100	1.23282200
H	-2.64336100	-0.94052000	-1.24714400
Br	-0.31397600	0.04906600	0.01215400

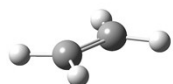
38.I



Zero-point correction=	0.107580
(Hartree/Particle)	
Thermal correction to Energy=	0.115740
Thermal correction to Enthalpy=	0.116684
Thermal correction to Gibbs Free Energy=	0.072758
Sum of electronic and zero-point Energies=	-454.394023
Sum of electronic and thermal Energies=	-454.385863
Sum of electronic and thermal Enthalpies=	-454.384919
Sum of electronic and thermal Free Energies=	-454.428845

C	2.42017700	-0.60013100	0.10511200
H	2.48592500	-1.20499000	-0.79162200
H	2.44265900	-1.12100200	1.05511800
C	2.41035100	0.74422200	0.04375200
H	2.46786400	1.26572200	-0.90445100
H	2.42462500	1.34988000	0.94224600
C	-2.55996500	0.00929700	-0.73118100
H	-2.64663400	0.91744300	-1.31484700
C	-2.59206900	0.05177000	0.65074100
H	-2.70444800	0.99383200	1.17304200
H	-2.69042400	-0.85792000	1.23014100
H	-2.63280500	-0.93430900	-1.25769200
I	-0.26727900	0.04973000	0.01285500

TS39.I



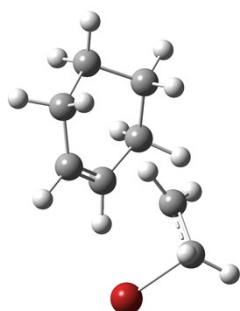
Zero-point correction=	0.107567
(Hartree/Particle)	
Thermal correction to Energy=	0.114838
Thermal correction to Enthalpy=	0.115783
Thermal correction to Gibbs Free Energy=	0.074355
Sum of electronic and zero-point Energies=	-454.393952

Sum of electronic and thermal Energies=	-454.386680
Sum of electronic and thermal Enthalpies=	-454.385736
Sum of electronic and thermal Free Energies=	-454.427164

C	2.16603700	-0.61238300	0.09350400
H	2.25180700	-1.20513400	-0.80922500
H	2.20946100	-1.13711800	1.04028600
C	2.15669700	0.74833700	0.04323600
H	2.23486900	1.27400700	-0.90080500
H	2.19241200	1.34208500	0.94867200
C	-2.77376900	0.00469800	-0.72443200
H	-2.82765100	0.90803900	-1.32000000
C	-2.80534600	0.05604700	0.63585000
H	-2.88511900	1.00162500	1.15851100
H	-2.87281100	-0.84824900	1.22858300
H	-2.81541900	-0.94181400	-1.24980400
I	-0.31379100	0.04910200	0.01213700

Footnote 91

TS40.Br

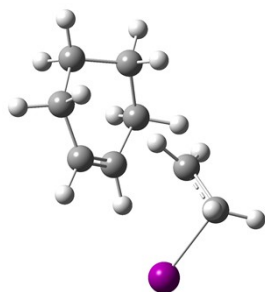


Zero-point correction=	0.202396
(Hartree/Particle)	
Thermal correction to Energy=	0.212584
Thermal correction to Enthalpy=	0.213528
Thermal correction to Gibbs Free Energy=	0.164678
Sum of electronic and zero-point Energies=	-2886.865940
Sum of electronic and thermal Energies=	-2886.855752
Sum of electronic and thermal Enthalpies=	-2886.854808
Sum of electronic and thermal Free Energies=	-2886.903658

C	-1.48539100	-0.41478300	-0.51211300
H	-2.36755600	-0.73684000	0.02904600
C	0.64079700	2.18551200	1.46786900
C	-0.21391600	3.35469400	1.84881700
C	1.38805500	2.15708700	0.34546300
C	-0.40664600	4.33503500	0.69194000
H	0.26399100	3.85732700	2.69737100
H	-1.17477200	3.00514700	2.24266700
C	1.47800100	3.30905000	-0.60601700
H	2.00475300	1.28719400	0.14324200

C	0.92034200	4.60007300	-0.01075800
H	-1.12123300	3.92784700	-0.03316200
H	-0.84417400	5.26149100	1.06142900
H	2.52052400	3.42938500	-0.90903900
H	0.94793500	3.06247100	-1.53871700
H	1.63640900	4.99920200	0.71173900
H	0.80284200	5.35074200	-0.79104500
H	0.69801900	1.35560400	2.16467300
H	-1.42019600	-0.77269000	-1.53316100
Br	0.07935400	-1.12873100	0.45172500
C	-1.06558600	0.95074500	-0.28971700
H	-0.51554800	1.48298600	-1.05325400
H	-1.48467800	1.52219500	0.52778700

TS40.I



Zero-point correction=	0.201952
(Hartree/Particle)	
Thermal correction to Energy=	0.212260
Thermal correction to Enthalpy=	0.213204
Thermal correction to Gibbs Free Energy=	0.163350
Sum of electronic and zero-point Energies=	-610.313905
Sum of electronic and thermal Energies=	-610.303597
Sum of electronic and thermal Enthalpies=	-610.302652
Sum of electronic and thermal Free Energies=	-610.352506

C	-1.47174900	-0.39396700	-0.50723700
H	-2.35320200	-0.71649300	0.03492100
C	0.63306500	2.18810400	1.46331800
C	-0.21594900	3.36037600	1.84782500
C	1.37928100	2.15913200	0.34028200
C	-0.40723100	4.34286500	0.69269500
H	0.26689000	3.86005500	2.69533900
H	-1.17716300	3.01420500	2.24315000
C	1.47356200	3.31300400	-0.60882200
H	1.99290300	1.28757600	0.13610000
C	0.91983100	4.60473400	-0.01114000
H	-1.12404800	3.93853800	-0.03149500
H	-0.84087100	5.27031000	1.06431800
H	2.51702700	3.43089500	-0.90957600
H	0.94397700	3.06985700	-1.54225800
H	1.63767600	5.00116300	0.71111400

H	0.80365200	5.35664500	-0.79046400
H	0.68877500	1.35734800	2.15916600
H	-1.39591500	-0.75291700	-1.52724800
C	-1.06502400	0.95957500	-0.29013900
H	-0.52432300	1.49739100	-1.05643800
H	-1.49345700	1.53439200	0.52024300
I	0.19554100	-1.34854800	0.53591200

Thermochemical Data and Optimized Cartesian Coordinates for Structures Calculated at ω B97X-D3/def2-TZVP

Figure 3

Bromiranium Ion 6.Br

Electronic energy	...	-2652.50426923 Eh	
Zero point energy	...	0.05526118 Eh	34.68 kcal/mol
Thermal vibrational correction	...	0.00069555 Eh	0.44 kcal/mol
Thermal rotational correction	...	0.00141627 Eh	0.89 kcal/mol
Thermal translational correction	...	0.00141627 Eh	0.89 kcal/mol
Total Enthalpy	...	-2652.44453575 Eh	
Final Gibbs free energy	...	-2652.47561691 Eh	

C	-2.14566	0.66212	0.27984
H	-1.67455	0.55615	-0.69032
H	-3.08928	0.15308	0.43745
C	-1.34915	1.06545	1.42097
H	-0.29018	1.25651	1.29260
H	-1.70302	0.85410	2.42327
Br	-2.38419	2.61113	0.67676

Cyclohexene

Electronic energy	...	-234.66872462 Eh	
Zero point energy	...	0.14749906 Eh	92.56 kcal/mol
Thermal vibrational correction	...	0.00262547 Eh	1.65 kcal/mol
Thermal rotational correction	...	0.00141627 Eh	0.89 kcal/mol
Thermal translational correction	...	0.00141627 Eh	0.89 kcal/mol
Total Enthalpy	...	-234.51482334 Eh	
Final Gibbs free energy	...	-234.54916540 Eh	

C	0.66114	1.29859	0.05633
C	-0.66114	1.29859	-0.05633
C	-1.48959	0.04563	-0.10776
C	-0.69179	-1.18343	0.32090
C	0.69179	-1.18343	-0.32090
C	1.48959	0.04563	0.10776
H	-2.37240	0.16468	0.52692
H	-1.18958	2.24567	-0.11167

H	1.18958	2.24567	0.11167
H	-0.58064	-1.17691	1.41055
H	-1.23675	-2.09545	0.06671
H	1.23675	-2.09545	-0.06671
H	0.58064	-1.17691	-1.41055
H	1.87413	-0.08972	1.12611
H	2.37240	0.16468	-0.52692
H	-1.87413	-0.08971	-1.12611

21 ω .Br

Electronic energy	...	-2887.19235791 Eh	
Zero point energy	...	0.20352413 Eh	127.71 kcal/mol
Thermal vibrational correction	...	0.00820686 Eh	5.15 kcal/mol
Thermal rotational correction	...	0.00141627 Eh	0.89 kcal/mol
Thermal translational correction	...	0.00141627 Eh	0.89 kcal/mol
Total Enthalpy	...	-2886.97685016 Eh	
Final Gibbs free energy	...	-2887.02643281 Eh	

C	2.25167	-0.73464	0.52598
H	2.09090	-1.14771	1.51833
C	2.22599	0.59502	0.36273
H	2.07044	1.23146	1.23027
C	-2.43005	-0.29689	-0.83289
C	-2.62343	0.09153	0.52436
H	-2.86943	-0.65265	1.27157
H	-2.52933	-1.33675	-1.11828
C	2.58831	-1.69651	-0.57744
H	3.28104	-2.44562	-0.18652
H	1.69167	-2.26183	-0.86347
C	2.49103	1.26822	-0.95195
H	1.78852	2.09432	-1.09750
H	3.47883	1.73926	-0.89871
C	2.43685	0.28903	-2.12145
H	1.39209	0.04561	-2.35529
H	2.84724	0.75541	-3.01790
C	3.19149	-0.99410	-1.79194
H	3.19853	-1.66819	-2.64938
H	4.23572	-0.74682	-1.57992
H	-2.48045	0.44455	-1.62050
H	-2.82066	1.12801	0.76840
Br	-0.60879	-0.08211	0.11374

TS21 ω .Br

Electronic energy	...	-2887.19019747 Eh	
Zero point energy	...	0.20303655 Eh	127.41 kcal/mol
Thermal vibrational correction	...	0.00748965 Eh	4.70 kcal/mol
Thermal rotational correction	...	0.00141627 Eh	0.89 kcal/mol
Thermal translational correction	...	0.00141627 Eh	0.89 kcal/mol
Total Enthalpy	...	-2886.97589451 Eh	

Final Gibbs free energy ... -2887.02326453 Eh

C	2.00666	-0.75039	0.49717
H	1.81092	-1.15864	1.48428
C	1.98489	0.60170	0.33325
H	1.80558	1.23073	1.20060
C	-2.55665	-0.29842	-0.82922
C	-2.73234	0.07859	0.48474
H	-2.90749	-0.66039	1.25676
H	-2.58901	-1.34192	-1.11702
C	2.44579	-1.69720	-0.57681
H	3.10149	-2.44139	-0.11806
H	1.57982	-2.26523	-0.93575
C	2.36560	1.27019	-0.94888
H	1.68754	2.10375	-1.14801
H	3.34744	1.73078	-0.78510
C	2.42315	0.29704	-2.12300
H	1.40647	0.05731	-2.45374
H	2.91677	0.77375	-2.96998
C	3.14941	-0.98555	-1.73175
H	3.22644	-1.65919	-2.58536
H	4.17322	-0.74164	-1.43387
H	-2.54271	0.43929	-1.62182
H	-2.86117	1.12045	0.75083
Br	-0.48114	-0.08499	0.11297

21.Br

Electronic energy	...	-2887.20663017 Eh	
Zero point energy	...	0.20266535 Eh	127.17 kcal/mol
Thermal vibrational correction	...	0.00871423 Eh	5.47 kcal/mol
Thermal rotational correction	...	0.00141627 Eh	0.89 kcal/mol
Thermal translational correction	...	0.00141627 Eh	0.89 kcal/mol
Total Enthalpy	...	-2886.99147383 Eh	
Final Gibbs free energy	...	-2887.04156519 Eh	

C	2.01605	-0.77195	0.47877
H	1.99042	-1.13409	1.50083
C	1.99735	0.66024	0.29232
H	1.98249	1.27936	1.18344
C	-2.97718	-0.27402	-0.80084
C	-3.12493	0.03807	0.48096
H	-3.23881	-0.72553	1.24246
H	-2.96392	-1.30512	-1.13662
C	2.53243	-1.70578	-0.58147
H	3.22484	-2.38284	-0.07466
H	1.71674	-2.34095	-0.93209
C	2.46804	1.27740	-0.98270
H	1.88611	2.17374	-1.20105
H	3.48178	1.63076	-0.74819
C	2.50990	0.29708	-2.14908
H	1.49499	0.08013	-2.49457

H	3.02505	0.76702	-2.98624
C	3.22497	-0.98729	-1.74368
H	3.29249	-1.67048	-2.58950
H	4.25286	-0.74760	-1.45755
H	-2.90944	0.48940	-1.56802
H	-3.18426	1.06894	0.81221
Br	0.06270	-0.09784	0.19752

Bromiranium Ion 12.Br

Electronic energy	...	-2808.60528663 Eh	
Zero point energy	...	0.14981689 Eh	94.01 kcal/mol
Thermal vibrational correction	...	0.00396593 Eh	2.49 kcal/mol
Thermal rotational correction	...	0.00141627 Eh	0.89 kcal/mol
Thermal translational correction	...	0.00141627 Eh	0.89 kcal/mol
Total Enthalpy	...	-2808.44772707 Eh	
Final Gibbs free energy	...	-2808.48722630 Eh	

C	-4.97760	-1.60750	-0.01116
C	-3.45381	-1.62710	0.00992
C	-2.84457	-0.27285	0.14453
C	-3.62142	0.85095	0.64495
C	-5.05269	0.69348	1.07594
C	-5.51580	-0.76609	1.14141
H	-1.76416	-0.20360	0.22387
H	-3.09476	-2.16312	0.90022
H	-3.01673	-2.14919	-0.84228
H	-5.33816	-1.22564	-0.97075
H	-5.34381	-2.63048	0.06720
H	-3.06277	1.69168	1.04276
H	-5.12321	1.16932	2.05763
H	-5.69303	1.29178	0.42480
H	-5.18328	-1.20375	2.08688
H	-6.60468	-0.78861	1.15847
Br	-3.30990	1.02484	-1.38971

Ethene

Electronic energy	...	-78.59191383 Eh	
Zero point energy	...	0.05139738 Eh	32.25 kcal/mol
Thermal vibrational correction	...	0.00019779 Eh	0.12 kcal/mol
Thermal rotational correction	...	0.00141627 Eh	0.89 kcal/mol
Thermal translational correction	...	0.00141627 Eh	0.89 kcal/mol
Total Enthalpy	...	-78.53654191 Eh	
Final Gibbs free energy	...	-78.56137707 Eh	

C	0.00001	0.66096	0.00000
H	0.92299	1.22952	-0.00000
H	-0.92295	1.22956	-0.00000
C	-0.00001	-0.66096	-0.00000
H	-0.92299	-1.22952	-0.00000

H	0.92295	-1.22956	0.00000
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22.Br

Electronic energy	...	-2887.23072259 Eh	
Zero point energy	...	0.20622154 Eh	129.41 kcal/mol
Thermal vibrational correction	...	0.00696310 Eh	4.37 kcal/mol
Thermal rotational correction	...	0.00141627 Eh	0.89 kcal/mol
Thermal translational correction	...	0.00141627 Eh	0.89 kcal/mol
Total Enthalpy	...	-2887.01376120 Eh	
Final Gibbs free energy	...	-2887.06028008 Eh	

C	-1.17752	-0.66578	0.26308
H	-0.95852	-0.87354	1.30919
C	-0.71557	0.71755	-0.14481
H	0.37956	0.75659	-0.08097
H	-0.93683	0.99382	-1.17492
C	-1.59829	1.86296	0.69769
C	-2.26639	2.88812	-0.19358
C	-0.31612	2.12011	1.21369
C	-1.25816	3.76017	-0.93633
H	-2.89524	3.50865	0.45099
H	-2.94366	2.37892	-0.88148
C	0.53106	3.25636	0.78389
H	0.05286	1.47893	2.01081
C	-0.23200	4.34600	0.02777
H	-0.75274	3.18529	-1.71964
H	-1.78731	4.56197	-1.45041
H	0.99335	3.63995	1.70049
H	1.37999	2.86883	0.20862
H	-0.74148	4.98891	0.75002
H	0.47984	4.97839	-0.50133
H	-2.26229	1.28415	1.33389
H	-2.24270	-0.79377	0.08679
Br	-0.24970	-1.98287	-0.79161

24.Br

Electronic energy	...	-2887.25008081 Eh	
Zero point energy	...	0.20615523 Eh	129.36 kcal/mol
Thermal vibrational correction	...	0.00684771 Eh	4.30 kcal/mol
Thermal rotational correction	...	0.00141627 Eh	0.89 kcal/mol
Thermal translational correction	...	0.00141627 Eh	0.89 kcal/mol
Total Enthalpy	...	-2887.03330111 Eh	
Final Gibbs free energy	...	-2887.07962898 Eh	

C	0.13519	-0.34207	0.25889
H	0.93464	0.23600	0.71810
C	-0.73357	0.51482	-0.64343
H	-0.19240	0.85120	-1.53717
H	-1.55307	-0.08749	-1.07796

C	-1.43831	1.66119	-0.06718
C	-2.00115	2.66141	-0.96457
C	-1.44914	1.96253	1.35132
C	-0.98417	3.86388	-0.87000
H	-2.96899	3.01692	-0.60749
H	-2.07445	2.31524	-1.99429
C	-0.39563	3.14349	1.45592
H	-1.14461	1.13417	1.98539
C	-0.80955	4.30669	0.57186
H	-0.02828	3.55676	-1.30196
H	-1.38370	4.65515	-1.50332
H	-0.35681	3.41182	2.51124
H	0.59561	2.77558	1.17987
H	-1.73642	4.74950	0.94604
H	-0.04632	5.08585	0.62289
H	-2.41124	2.36235	1.67350
H	-0.44240	-0.83303	1.03859
Br	0.97163	-1.73155	-0.77925

TS25.Br

Electronic energy	...	-2887.19806622 Eh	
Zero point energy	...	0.20065052 Eh	125.91 kcal/mol
Thermal vibrational correction	...	0.00644369 Eh	4.04 kcal/mol
Thermal rotational correction	...	0.00141627 Eh	0.89 kcal/mol
Thermal translational correction	...	0.00141627 Eh	0.89 kcal/mol
Total Enthalpy	...	-2886.98719527 Eh	
Final Gibbs free energy	...	-2887.03231669 Eh	

C	-1.05498	-0.85884	0.32583
H	-0.88827	-0.81675	1.39679
C	-1.63510	0.35922	-0.33057
H	-0.07236	0.44187	-0.92549
H	-2.27390	0.17005	-1.18753
C	-1.47163	1.63502	0.10711
C	-2.07256	2.77334	-0.65523
C	-0.67083	2.02644	1.30877
C	-1.01397	3.82811	-1.00540
H	-2.82755	3.22934	-0.00415
H	-2.58955	2.41506	-1.54593
C	0.38150	3.08918	0.95149
H	-0.20397	1.17162	1.79895
C	-0.24361	4.27644	0.23048
H	-0.31979	3.41074	-1.74355
H	-1.50326	4.67465	-1.48769
H	0.88386	3.40755	1.86527
H	1.15182	2.63671	0.31645
H	-0.91687	4.80654	0.91170
H	0.53355	4.98814	-0.05169
H	-1.37580	2.45393	2.03072
H	-1.50102	-1.79764	0.01628
Br	0.78967	-0.83353	-0.51231

26.Br

Electronic energy	...	-2887.23921222 Eh	
Zero point energy	...	0.20045264 Eh	125.79 kcal/mol
Thermal vibrational correction	...	0.00886640 Eh	5.56 kcal/mol
Thermal rotational correction	...	0.00141627 Eh	0.89 kcal/mol
Thermal translational correction	...	0.00141627 Eh	0.89 kcal/mol
Total Enthalpy	...	-2887.02611642 Eh	
Final Gibbs free energy	...	-2887.07704605 Eh	

C	-1.35547	-0.60806	0.27892
H	-0.89329	-0.58562	1.25692
C	-1.83506	0.49662	-0.32882
H	1.98642	-1.04362	-1.69203
H	-2.32737	0.40703	-1.29028
C	-1.74230	1.79124	0.23652
C	-2.29068	2.93787	-0.49886
C	-0.97529	2.11985	1.44549
C	-1.06586	3.77775	-0.99150
H	-2.87262	3.56858	0.17858
H	-2.91572	2.63369	-1.33636
C	0.25684	2.96104	0.97854
H	-0.64528	1.25142	2.00892
C	-0.18176	4.17734	0.17884
H	-0.49923	3.19044	-1.71896
H	-1.46296	4.64541	-1.51787
H	0.81409	3.24231	1.87185
H	0.91040	2.32282	0.37758
H	-0.71699	4.87788	0.82647
H	0.69886	4.70405	-0.19383
H	-1.58716	2.75161	2.09477
H	-1.44532	-1.58205	-0.18745
Br	1.97653	-0.69866	-0.31531

Product 14

Electronic energy	...	-312.41132431 Eh	
Zero point energy	...	0.19320148 Eh	121.24 kcal/mol
Thermal vibrational correction	...	0.00511275 Eh	3.21 kcal/mol
Thermal rotational correction	...	0.00141627 Eh	0.89 kcal/mol
Thermal translational correction	...	0.00141627 Eh	0.89 kcal/mol
Total Enthalpy	...	-312.20923334 Eh	
Final Gibbs free energy	...	-312.25011695 Eh	

C	-1.15787	-0.64786	0.50257
H	-0.29318	-0.59784	1.15259
C	-1.84742	0.44289	0.11937
H	-2.72734	0.32736	-0.50325
C	-1.51595	1.76103	0.53710
C	-2.37190	2.87680	0.12354
C	-0.27599	2.12816	1.22917

C	-1.54425	3.70591	-0.91737
H	-2.57055	3.53011	0.97708
H	-3.31342	2.54081	-0.30648
C	0.57228	2.96689	0.21475
H	0.30081	1.27911	1.58536
C	-0.21952	4.14946	-0.31878
H	-1.38166	3.09798	-1.81116
H	-2.16276	4.55269	-1.21372
H	1.47241	3.28613	0.73942
H	0.88914	2.31410	-0.60275
H	-0.39625	4.87306	0.48205
H	0.36834	4.66368	-1.08170
H	-0.51782	2.77625	2.07569
H	-1.46547	-1.63627	0.18131

HBr

Electronic energy	...	-2574.82066682 Eh	
Zero point energy	...	0.00614723 Eh	3.86
kcal/mol			
Thermal vibrational correction	...	0.00000003 Eh	0.00
kcal/mol			
Thermal rotational correction	...	0.00094418 Eh	0.59
kcal/mol			
Thermal translational correction	...	0.00141627 Eh	0.89
kcal/mol			
Total Enthalpy	...	-2574.81121490 Eh	
Final Gibbs free energy	...	-2574.83375306 Eh	

Br	-5.39628	0.60327	0.00000
H	-6.81323	0.60327	0.00000

30.Br

Electronic energy	...	-2887.22582111 Eh	
Zero point energy	...	0.20694304 Eh	129.86 kcal/mol
Thermal vibrational correction	...	0.00671764 Eh	4.22 kcal/mol
Thermal rotational correction	...	0.00141627 Eh	0.89 kcal/mol
Thermal translational correction	...	0.00141627 Eh	0.89 kcal/mol
Total Enthalpy	...	-2887.00838368 Eh	
Final Gibbs free energy	...	-2887.05424209 Eh	

C	-0.83495	0.35004	0.44461
H	-0.68873	-0.46707	1.14563
C	0.36132	0.58094	-0.46335
H	1.25561	0.81375	0.10819
H	0.18304	1.35792	-1.20034
C	-2.41853	1.43696	0.93380
C	-3.04666	2.24574	-0.12564
C	-1.12492	1.67725	1.44031
C	-2.14680	3.33112	-0.70430

H	-3.89921	2.69735	0.40915
H	-3.51632	1.60539	-0.87678
C	-0.42834	2.99648	1.11894
H	-0.93233	1.29155	2.43510
C	-1.34539	3.99447	0.41025
H	-1.47830	2.90463	-1.45725
H	-2.76386	4.06113	-1.22712
H	-0.08102	3.41065	2.06551
H	0.47192	2.82494	0.52928
H	-2.03692	4.43437	1.13565
H	-0.74895	4.81622	0.01591
H	-3.01692	0.65660	1.39800
H	-1.66590	0.02739	-0.20109
Br	0.70430	-1.05095	-1.42809

TS31.Br

Electronic energy	...	-2887.17992610 Eh	
Zero point energy	...	0.20174162 Eh	126.59 kcal/mol
Thermal vibrational correction	...	0.00725148 Eh	4.55 kcal/mol
Thermal rotational correction	...	0.00141627 Eh	0.89 kcal/mol
Thermal translational correction	...	0.00141627 Eh	0.89 kcal/mol
Total Enthalpy	...	-2886.96715625 Eh	
Final Gibbs free energy	...	-2887.01460569 Eh	

C	-0.21926	-0.10002	-0.27176
H	-0.17726	-0.61752	0.67868
C	0.71620	0.98845	-0.48591
H	1.65054	1.01597	0.06162
H	0.58966	1.65836	-1.32779
C	-2.80594	1.71215	1.33700
C	-3.37243	2.49631	0.19390
C	-1.54997	1.82700	1.76911
C	-2.29443	3.18591	-0.63772
H	-4.06866	3.23683	0.60390
H	-3.98729	1.84394	-0.43124
C	-0.58890	2.78741	1.16360
H	-1.21946	1.25189	2.62790
C	-1.23199	3.81992	0.25315
H	-1.82589	2.45302	-1.30727
H	-2.74151	3.93731	-1.28877
H	0.06156	3.23976	1.91576
H	0.18251	2.20172	0.54356
H	-1.69518	4.57827	0.89200
H	-0.47509	4.33996	-0.33710
H	-3.48166	1.04667	1.86526
H	-1.21137	0.00150	-0.69323
Br	0.94275	-1.02549	-1.56266

32.Br

Electronic energy	...	-2887.23897873 Eh	
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Zero point energy	...	0.20296869 Eh	127.36 kcal/mol
Thermal vibrational correction	...	0.00848085 Eh	5.32 kcal/mol
Thermal rotational correction	...	0.00141627 Eh	0.89 kcal/mol
Thermal translational correction	...	0.00141627 Eh	0.89 kcal/mol
Total Enthalpy	...	-2887.02375244 Eh	
Final Gibbs free energy	...	-2887.07343740 Eh	

C	0.34392	-0.18887	0.16766
H	0.70811	-1.20653	0.28067
C	1.20605	0.64426	-0.74888
H	1.29196	0.19601	-1.73796
H	0.81386	1.65545	-0.86171
C	-2.88658	1.62099	0.89709
C	-3.28752	2.46440	-0.24001
C	-1.91425	2.02592	1.81828
C	-2.18638	3.40965	-0.69167
H	-4.16655	3.01593	0.14019
H	-3.67717	1.85238	-1.05380
C	-1.32105	3.24183	1.65611
H	-1.72077	1.42378	2.69608
C	-1.55458	4.12642	0.49604
H	-1.42404	2.82506	-1.21260
H	-2.57508	4.13134	-1.40813
H	-0.67376	3.61226	2.44677
H	2.20782	0.71587	-0.32011
H	-2.19517	4.94249	0.86730
H	-0.61836	4.62100	0.22503
H	-3.51332	0.77205	1.14862
H	0.23174	0.25433	1.15544
Br	-1.47364	-0.40128	-0.52334

Cyclohexenium Ion 15

Electronic energy	...	-233.77035858 Eh	
Zero point energy	...	0.13483417 Eh	84.61 kcal/mol
Thermal vibrational correction	...	0.00264373 Eh	1.66 kcal/mol
Thermal rotational correction	...	0.00141627 Eh	0.89 kcal/mol
Thermal translational correction	...	0.00141627 Eh	0.89 kcal/mol
Total Enthalpy	...	-233.62910393 Eh	
Final Gibbs free energy	...	-233.66406878 Eh	

C	-3.82995	-0.88871	-0.09247
C	-2.31083	-0.98879	-0.05419
C	-1.66012	0.23062	0.43727
C	-2.30974	1.20602	1.16439
C	-3.59676	0.94583	1.58634
C	-4.36898	-0.23023	1.17063
H	-0.59110	0.33787	0.26706
H	-1.96058	-1.78754	0.62498
H	-1.88281	-1.26516	-1.02166
H	-4.12232	-0.28671	-0.95626
H	-4.27400	-1.87313	-0.22836

H	-1.78040	2.08320	1.51150
H	-4.04686	1.61495	2.31641
H	-4.34161	-0.90857	2.04303
H	-5.42513	0.03997	1.08635

Bromoethane

Electronic energy	...	-2653.45318145 Eh	
Zero point energy	...	0.06649846 Eh	41.73 kcal/mol
Thermal vibrational correction	...	0.00130183 Eh	0.82 kcal/mol
Thermal rotational correction	...	0.00141627 Eh	0.89 kcal/mol
Thermal translational correction	...	0.00141627 Eh	0.89 kcal/mol
Total Enthalpy	...	-2653.38160442 Eh	
Final Gibbs free energy	...	-2653.41409937 Eh	

C	-1.70454	0.34204	0.00021
H	-1.33928	-0.68816	-0.00427
H	-1.35248	0.83288	-0.90722
H	-2.79419	0.31876	-0.02229
C	-1.19820	1.04969	1.23591
H	-1.56136	0.58966	2.15171
H	-0.11249	1.09615	1.26842
Br	-1.80108	2.89948	1.30638

Table S7: Comparison of M06-2X-D3 and ω B97X-D3 relative enthalpies (ΔH^0) for key species involved in the addition pathways from **Figure 3** (in kJ mol⁻¹)

		22.Br	24.Br	TS25.Br	26.Br	Products
Addition-Elimination	M06-2X-D3	-138.2	-186.1	-69.3	-167.2	-154.5
	ω B97X-D3	-142.5	-193.5	-71.4	-179.9	-163.9
	Absolute Difference	4.3	7.4	2.1	12.7	9.4
		28.Br	30.Br	TS31.Br	32.Br	Products
Hydride Transfer	M06-2X-D3	-136.8	-126.1	-25.4	-166.2	-125.3
	ω B97X-D3	-140.4	-127.7	-20.9	-172.7	-136.5
	Absolute Difference	3.6	1.6	4.5	6.5	11.2

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