Electronic Supplementary Material (ESI) for Dalton Transactions.

Atomic Level Mechanism of the White Phosphorous Demolition by Di-iodine

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Supporting Information

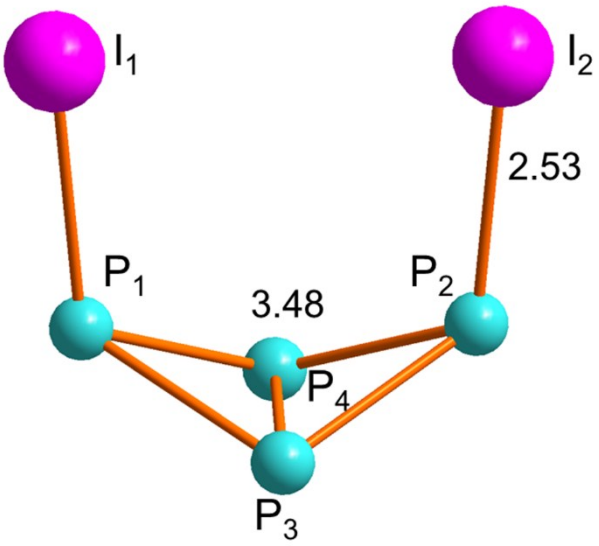

Fig. S1 Optimized structure of isomer of **2**, with two iodide groups in the same orientation.

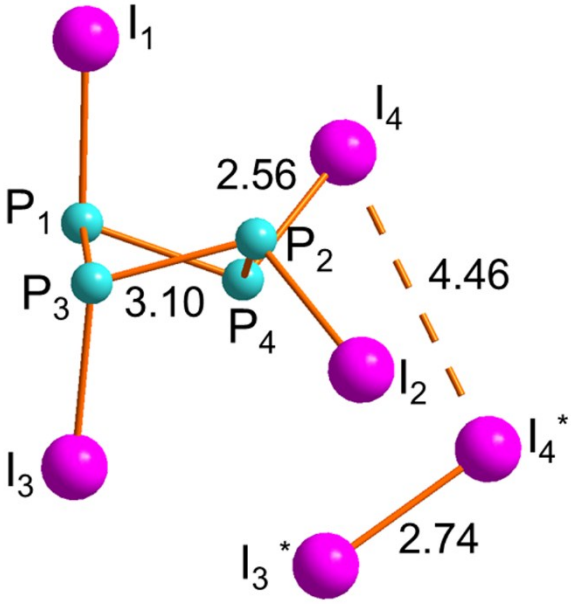

Fig. S2 Optimized structure of compound **3**·$\mathbf{I_2}$.

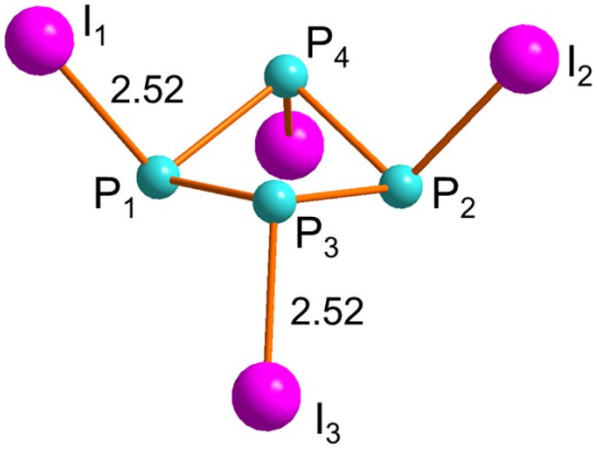

Fig. S3 Optimized structure of isomer of **3**, namely **3'**, with pairs of trans-diagonal P-I linkages equally oriented at the same side of the ring.

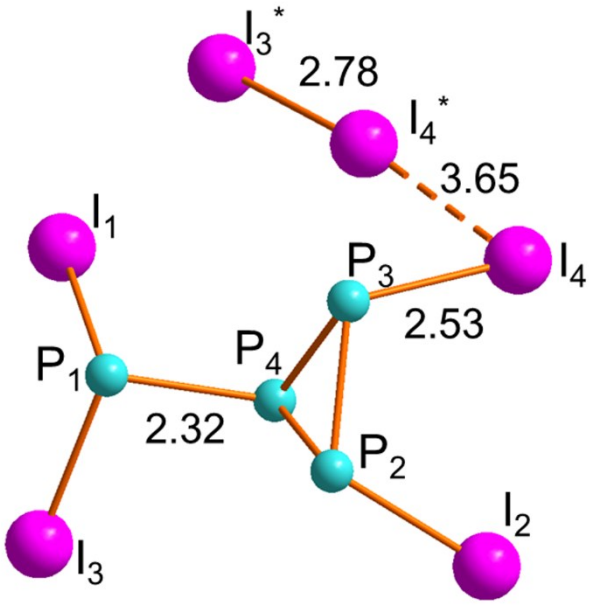

Fig. S4 Optimized structure of compound **4**·$\mathbf{I_2}$.

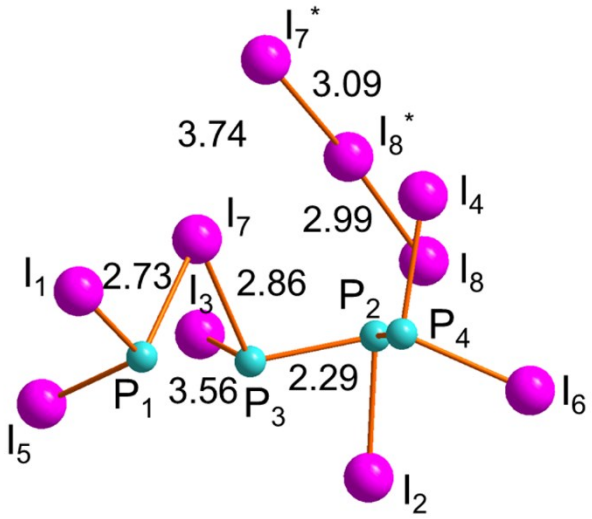

Fig. S5 Optimized structure of compound **5**·**2I$_2$**‡ adduct.

Unique mode of chain-breaking in **P$_4$I$_6$, 5** *(step **IVa**)*

As it has been lately noticed for P_4 derivatives with numerous I-substituents, the P-P bond to be cleaved is definitely less strained and allows the formation of exergonic derivatives. Thus, the formation of the adduct **5**·**2I$_2$**, involving a non-terminal P atom, is exergonic by -4.4 kcal mol^{-1} and reaches the Transition State, **(5-9)$_{TS}$** with a barrier of +3.9 kcal mol^{-1}, which by itself lies lower in energy than the separated reactants. At this point, the I_3 grouping is already charged -0.63, although the corresponding electron density is far from accumulating at the most remote I atom, as indicated by the still scarce activation of the external I_2 unit (I-I distance of 2.89 Å). Yet, **(5-9)$_{TS}$** appears as in other cases an early transition state, as indicated by the still relatively short P_2-P_3 bond (2.35 Å) and the I_8-P_2-P_3 angle of 133.2°, which is still far from the linearity, which favours the P-P σ^* population. Yet these effects may be attained along the downhill pathway, which corresponds to a net energy gain of -10.4 kcal mol^{-1} at the intermediate **9**·**I$_2$**·**9** with another -4.4 kcal mol^{-1} to be added for the complete disaggregation of the two diphosphine molecules.

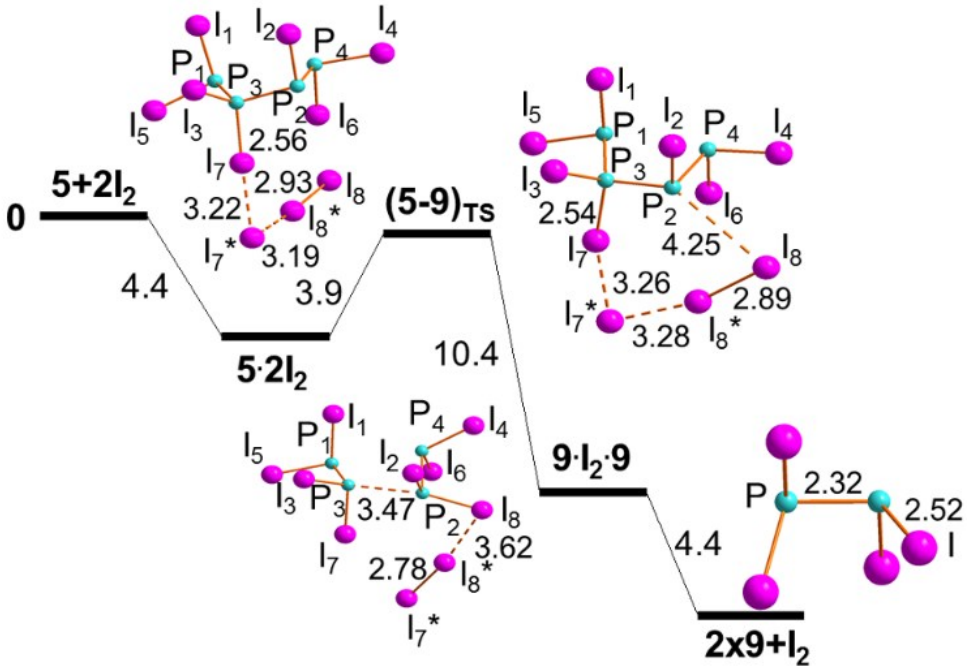

Fig. S6 Step ***IVa*** for breaking the four-membered chain **5** into two equal diphosphine parts, **9**. All the reported free energy values are given in kcal mol^{-1}.

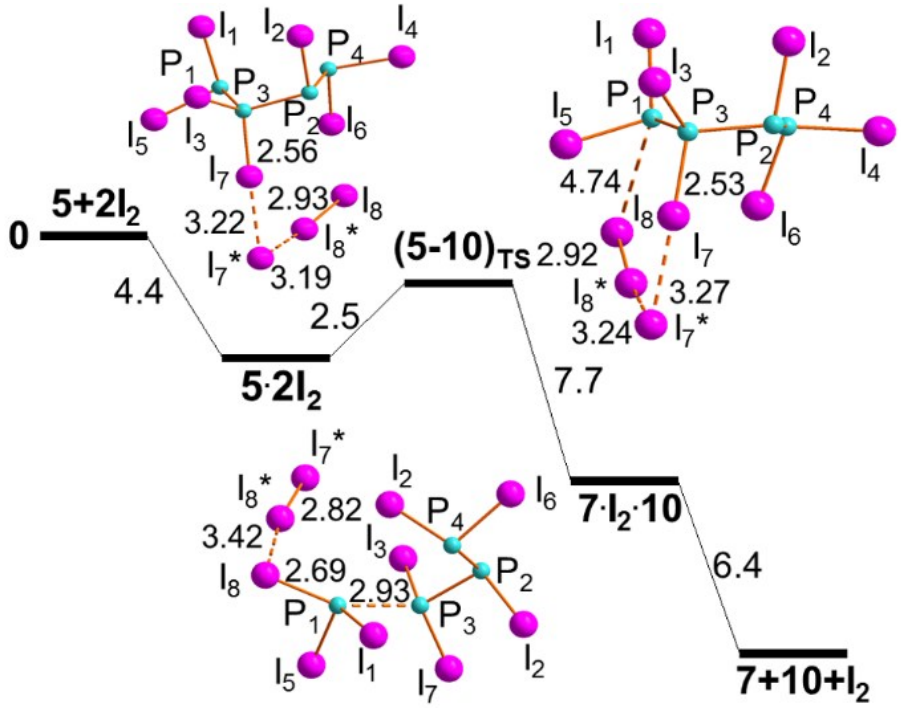

Fig. S7 Step ***IVa bis*** for lateral breaking the four-membered chain **5** into a linear chain $\mathbf{P_3I_5}$, **10** and $\mathbf{PI_3}$, **7**. All the reported free energy values are given in kcal mol^{-1}.

Opening of the three-membered ring $\mathbf{(PI)_3}$, **6**, *in step* ***IVb***

Fig. S8 illustrates some details on the profile determined by using our standard technique starting from compound **6**. Thus, the aggregate **6·2I$_2$**, now very slightly exergonic (-0.6 kcal mol^{-1}), eventually transforms into the three membered chain **I$_5$P$_3$**, **10**, upon the P_3 ring opening thanks to two newly formed P-I linkages. In this case, the transition state **(6-10)$_{TS}$** at +3.1 kcal mol^{-1} is slightly disfavoured with respect to the separate reactants, while the second I_2 molecule is only slightly perturbed with the $I_{8'}$-I_8 distance being 2.88 Å and I_8 is still as far as 4.52 Å from the P_2 atom. However, the reduction of the latter distance is highly stabilizing for the system with an overall free energy gain of -20.9 kcal mol^{-1} after **(6-10)$_{TS}$**, while along the way there is evidence for the adduct **10·I$_2$·7**, which involves the I_8-I_7' as subproduct. The final disaggregation of the **10·I$_2$·7** adduct, affords a further stabilization of the system of -2.0 kcal mol^{-1}.

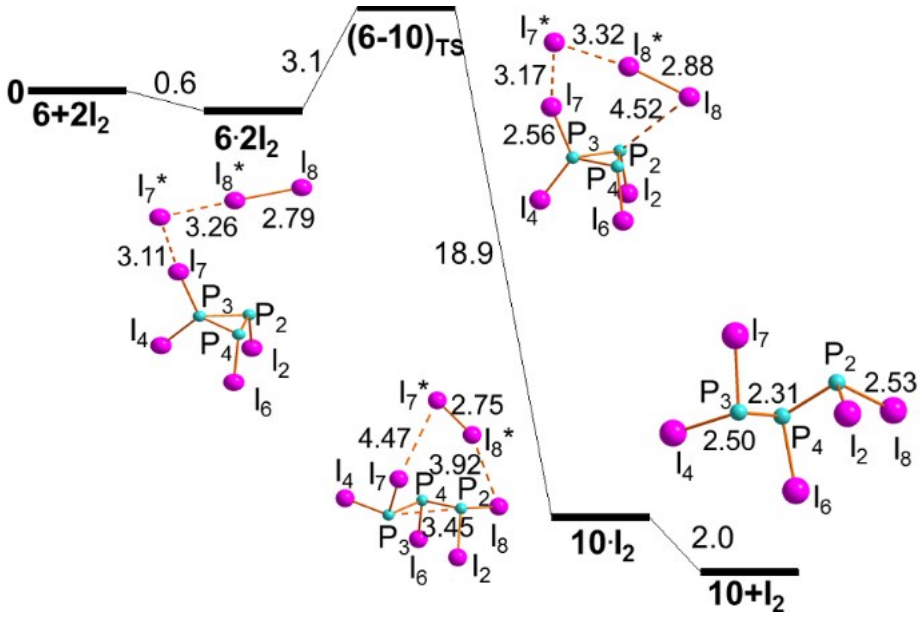

Fig. S8 Step ***IVb*** for the opening of the P_3 ring in **6**. All the reported free energy values are given in kcal mol^{-1}.

*Evolution of the dendrimer **P(PI$_2$)$_3$**, **8**, to separate the phosphine, **7**, from the three-membered chain **P$_3$I$_5$**, **10** (step **IVc**).*

Fig. S9 shows that from **(8·2I$_2$)$_{centr}$** the transition state **(8-10)$_{TS}$** is reached at +4.3 kcal mol^{-1}, although starting from the separate reactants there is still an exergonic balance of -3.2 kcal mol^{-1}, hence the process should proceed smoothly. The TS geometry is consistent with other observed ones, since the

I_3 grouping with -0.73 charge is already quite isolated. The still scarce starching of the second $\mathbf{I_2}$ molecule to 2.95 Å distance excludes a prevailing iodidic character at the terminal I_8 atom, hence with scarce possibilities of a nucleophilic attack on the remote P_4 atom, or better the P_4-P_3 σ^* level. This and similar processes are more likely concerted, with the electron density delocalized from the P_3 lone pair being drifted from one to the other end of the I_3 grouping and then to the P_4-P_3 linkage to be broken. At $\mathbf{(8\text{-}10)_{TS}}$, however, the latter distance is still scarcely elongates (2.35 Å), also because the I_8-P_1 distance is still as large as 4.27 Å and moreover the I_8-P_1-P_4 angle is far from linearity (125.9°). Certainly, in the following descent toward the aggregate $\mathbf{10{\cdot}I_2{\cdot}7}$ with an energy gain of -10.6 kcal mol^{-1}, all the previous parameters are more deeply affected. In particular, the $P_1\cdots P_4$ splitting is practically effective at the 3.20 Å distance, while the new I_7-P_4 bond is already formed (2.48 Å) as well as the new I_7^*-I_8^* one of 2.79 Å) All the trends become somewhat more pronounced with the final separation of the three molecular components. The further free energy gain of -3.4 kcal mol^{-1} seems to indicate how their larger inner stabilities overcome the cementing effects, first of all the dispersion ones.

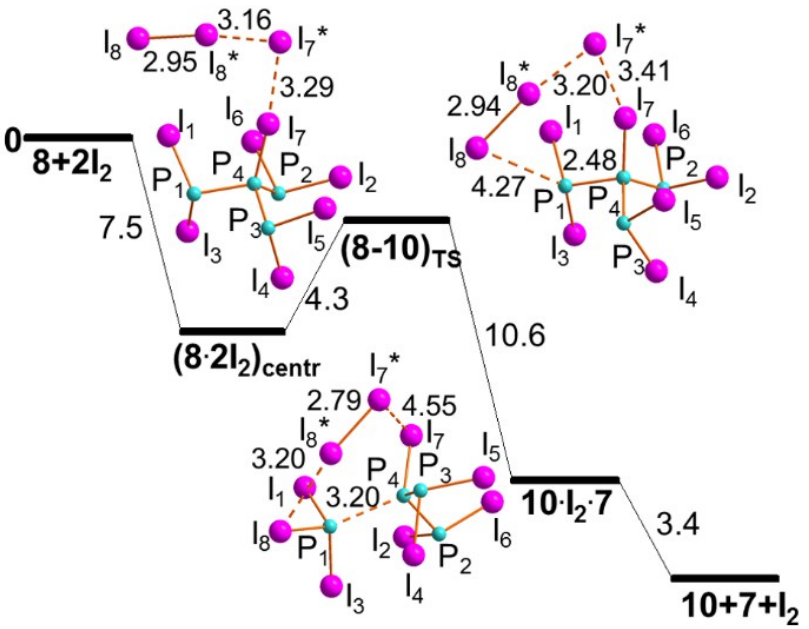

Fig. S9 Step ***IVc*** for the demolition of the dendrimer **8** into the three-membered chain **10** and the phosphine **7**. All the reported free energy values are given in kcal mol^{-1}.

*Mechanistic details of step **V** for the splitting of the three-membered chain* $\mathbf{P_3I_5}$, **10**, *in the diphosphine* **9** *and the phosphine* **7**.

Fig. S10 illustrates the evolution of the intermediate **10** in step *V* through the standard mechanism. In theory, the two $\mathbf{I_2}$ molecules may alternatively anchor at one lateral or the central P atom of the chain. The latter species $\mathbf{(10{\cdot}2I_2)_{centr}}$, which is favoured by about -3.0 kcal mol^{-1}, was chosen as the starting point of the process, although it is clear that even by starting from $\mathbf{(10{\cdot}2I_2)_{later}}$ the same P-P cleavage could occur without major differences. In our analysis, we found a barrier of +2.3 kcal mol^{-1} at $\mathbf{(10\text{-}9/7)_{TS}}$, which does not represent an obstacle for the process, since it is already -3.0 kcal mol^{-1} lower than the separated reactants. Then, the reactivity proceeds smoothly toward the aggregate $\mathbf{(9{\cdot}I_2{\cdot}7)}$, lower by -7.3 kcal mol^{-1} below. As in other cases, the *in situ* formed I_2 molecule, I_9*-I_{10}* diatomic, temporarily holds together the already formed products $\mathbf{P_2I_4}$, **9**, and $\mathbf{PI_3}$, **7**, thanks to a possible contribution of the dispersion forces. The separation of the species is stabilizing by -4.0 kcal mol^{-1} possibly because of an extra-stabilization of the products, but also thanks to a favorable entropy.

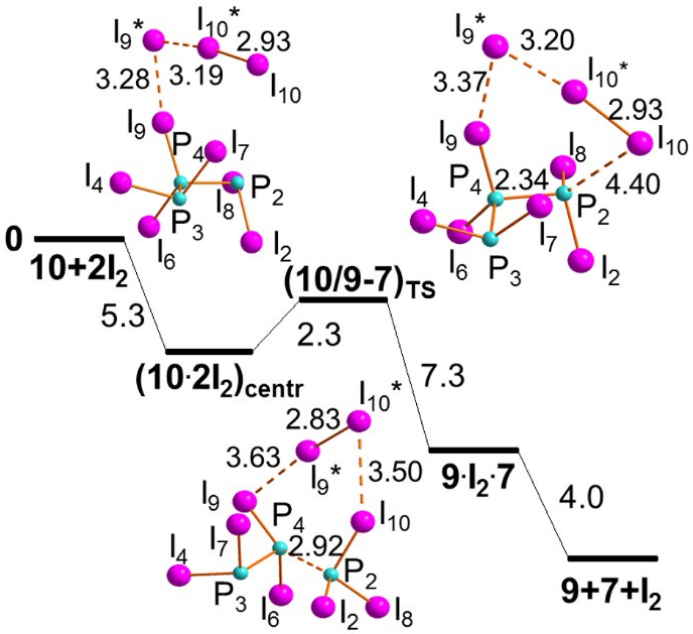

Fig. S10: Profile of step V allowing the $\mathbf{P_3I_5}$, **10**, dissociation into the diphosphine $\mathbf{P_2I_4}$, **9**, and the phosphine $\mathbf{PI_3}$, **7**. Free energies in kcal mol^{-1}.

LIST OF CARTESIAN COORDINATES AND ENERGY PARAMETERS FOR THE OPTIMIZED GEOMETRIES

1st P-P cleavage

P_4, 1

CARTESIAN COORDINATES

P -1.599386 1.297811 0.033438 P -3.174366 -0.254783 -0.007417
P -1.290782 -0.620024 1.089884 P -1.288466 -0.563703 -1.119705

ENERGY AND THERMAL PARAMETERS
HF=-1365.3664665
Zero-point vibrational energy 15914.5 (Joules/Mol)
Zero-point correction= 0.006062 (Hartree/Particle)
Thermal correction to Energy= 0.010547
Thermal correction to Enthalpy= 0.011491
Thermal correction to Gibbs Free Energy= -0.022716
Sum of electronic and zero-point Energies= -1365.360405
Sum of electronic and thermal Energies= -1365.355920
Sum of electronic and thermal Enthalpies= -1365.354975
Sum of electronic and thermal Free Energies= -1365.389183

1˙I_2

CARTESIAN COORDINATES

P -0.709897 -1.239151 -0.408496 P -0.913507 0.959276 -0.667699
P 0.270304 0.140514 0.990571 I 1.116576 0.592153 4.076306
P 1.038181 -0.029839 -1.059257 I 1.848145 0.983947 6.741275

ENERGY AND THERMAL PARAMETERS
HF=-1388.2854234
Zero-point vibrational energy 17482.1 (Joules/Mol)
Zero-point correction= 0.006659 (Hartree/Particle)
Thermal correction to Energy= 0.014390
Thermal correction to Enthalpy= 0.015334
Thermal correction to Gibbs Free Energy= -0.033172
Sum of electronic and zero-point Energies= -1388.278765
Sum of electronic and thermal Energies= -1388.271034
Sum of electronic and thermal Enthalpies= -1388.270090
Sum of electronic and thermal Free Energies= -1388.318595

1˙$(I_2)_{br}$

CARTESIAN COORDINATES

P 1.082623 1.126314 0.000152 P 2.615176 0.002686 -1.114390
P 2.614751 0.002320 1.114859 I -2.381033 -0.000428 -0.000243
P 1.086796 -1.126942 -0.000257 I -5.172013 -0.004751 0.000079

ENERGY AND THERMAL PARAMETERS

HF=-1388.2878722
Zero-point vibrational energy 17579.9 (Joules/Mol)
Zero-point correction= 0.006696 (Hartree/Particle)
Thermal correction to Energy= 0.015285
Thermal correction to Enthalpy= 0.016229
Thermal correction to Gibbs Free Energy= -0.034375
Sum of electronic and zero-point Energies= -1388.281176
Sum of electronic and thermal Energies= -1388.272587
Sum of electronic and thermal Enthalpies= -1388.271643
Sum of electronic and thermal Free Energies= -1388.322247

1˙2I_2
CARTESIAN COORDINATES

P -2.723643 -1.176182 -0.027792	I 0.564578 0.135758 0.065358
P -4.270307 -0.071983 1.076729	I 3.394849 0.135754 0.069667
P -2.728594 1.102920 0.036253	I 3.736288 -2.671103 -1.951760
P -4.201020 -0.008682 -1.161449	I 3.970247 -4.945382 -3.593107

ENERGY AND THERMAL PARAMETERS
HF=-1411.2107447
Zero-point vibrational energy 19311.4 (Joules/Mol)
Zero-point correction= 0.007355 (Hartree/Particle)
Thermal correction to Energy= 0.021909
Thermal correction to Enthalpy= 0.022853
Thermal correction to Gibbs Free Energy= -0.049691
Sum of electronic and zero-point Energies= -1411.203389
Sum of electronic and thermal Energies= -1411.188836
Sum of electronic and thermal Enthalpies= -1411.187892
Sum of electronic and thermal Free Energies= -1411.260436

$(1\text{-}2)_{TS}$
Imaginary Frequency at -54.2 cm^{-1}
CARTESIAN COORDINATES

P 2.179556 -1.413482 -0.108259	I 1.994651 1.450729 0.146337
P 3.936917 -1.819871 -1.356375	I -1.041402 3.065480 0.396714
P 4.383187 -0.084545 -0.073440	I -1.648744 -0.079577 0.144589
P 4.019677 -2.016897 0.921794	I -1.697541 -3.014739 -0.108263

ENERGY AND THERMAL PARAMETERS
HF=-1411.1991742
****** 1 imaginary frequencies (negative Signs) ******
Zero-point vibrational energy 18664.6 (Joules/Mol)
Zero-point correction= 0.007109 (Hartree/Particle)
Thermal correction to Energy= 0.020734
Thermal correction to Enthalpy= 0.021678
Thermal correction to Gibbs Free Energy= -0.045235
Sum of electronic and zero-point Energies= -1411.192065
Sum of electronic and thermal Energies= -1411.178440
Sum of electronic and thermal Enthalpies= -1411.177496
Sum of electronic and thermal Free Energies= -1411.244409

2·I_2

CARTESIAN COORDINATES

P 1.826790 0.792344 1.045913	I 1.348346 4.295253 1.689512
P 0.824808 1.305305 -0.890344	I -3.643868 -2.544996 -1.611156
P 1.705327 3.339789 -0.675665	I -1.083103 -2.278615 -0.502848
P 3.060654 1.577860 -0.654249	I 2.166346 -1.769739 0.876338

ENERGY AND THERMAL PARAMETERS

HF=-1411.2324505

Zero-point vibrational energy 20384.1 (Joules/Mol)

Zero-point correction= 0.007764 (Hartree/Particle)

Thermal correction to Energy= 0.021721

Thermal correction to Enthalpy= 0.022665

Thermal correction to Gibbs Free Energy= -0.044321

Sum of electronic and zero-point Energies= -1411.224687

Sum of electronic and thermal Energies= -1411.210729

Sum of electronic and thermal Enthalpies= -1411.209785

Sum of electronic and thermal Free Energies= -1411.276772

2

CARTESIAN COORDINATES

P 1.876685 0.942881 -0.326379	P 2.713170 1.006704 1.756749
P 1.171742 -0.550492 1.195483	I 4.513478 -1.522344 -0.728935
P 3.297197 -1.124374 1.507706	I 0.053028 2.731125 -0.279324

ENERGY AND THERMAL PARAMETERS

HF=-1388.3089248

Zero-point vibrational energy 18489.3 (Joules/Mol)

Zero-point correction= 0.007042 (Hartree/Particle)

Thermal correction to Energy= 0.015991

Thermal correction to Enthalpy= 0.016935

Thermal correction to Gibbs Free Energy= -0.031858

Sum of electronic and zero-point Energies= -1388.301883

Sum of electronic and thermal Energies= -1388.292934

Sum of electronic and thermal Enthalpies= -1388.291990

Sum of electronic and thermal Free Energies= -1388.340783

2 with two up iodide ligands

CARTESIAN COORDINATES

P 1.958245 0.925575 0.971685	P 0.401502 -0.519408 1.699671
P 0.012031 0.770210 -0.137201	I 3.991475 -0.069032 -0.157673
P -0.274837 -1.455016 -0.226140	I 1.455685 -2.772429 -1.517843

ENERGY AND THERMAL PARAMETERS

HF=-1388.287936

Zero-point vibrational energy 17678.1 (Joules/Mol)

Zero-point correction= 0.006733 (Hartree/Particle)

Thermal correction to Energy= 0.015843

Thermal correction to Enthalpy= 0.016787

Thermal correction to Gibbs Free Energy= -0.033314

Sum of electronic and zero-point Energies= -1388.281203

Sum of electronic and thermal Energies= -1388.272093

Sum of electronic and thermal Enthalpies= -1388.271149
Sum of electronic and thermal Free Energies= -1388.321250

2nd P-P cleavage

Pathway IIa

$(2{\cdot}2I_2)_{hinge}$

CARTESIAN COORDINATES

P 2.372291 1.021526 -0.083338
P 0.746969 1.154244 -1.609172
P -0.695866 -0.072158 -0.350293
P 0.344708 1.731585 0.506024
I 2.651942 -1.325684 0.812032
I -2.924802 0.814449 -1.060507
I -0.639147 4.194667 0.820119
I -1.744730 7.029953 0.959067
I 0.059885 7.821139 -1.672827
I 1.680150 8.405176 -3.974607

ENERGY AND THERMAL PARAMETERS
HF=-1434.1612597
Zero-point vibrational energy 22922.7 (Joules/Mol)
Zero-point correction= 0.008731 (Hartree/Particle)
Thermal correction to Energy= 0.027465
Thermal correction to Enthalpy= 0.028409
Thermal correction to Gibbs Free Energy= -0.054456
Sum of electronic and zero-point Energies= -1434.152529
Sum of electronic and thermal Energies= -1434.133795
Sum of electronic and thermal Enthalpies= -1434.132851
Sum of electronic and thermal Free Energies= -1434.215716

$(2\text{-}3)_{TS}$

Imaginary Frequency at -52.9 cm^{-1}

CARTESIAN COORDINATES

P -2.874408 -0.675138 -1.620519
P -1.311358 0.559099 -0.688534
P -2.079310 0.437339 1.398442
P -1.883485 -1.550306 0.226921
I -5.221642 -0.254451 -0.770588
I -0.042625 0.702186 2.766672
I 0.332503 -2.682425 0.136396
I 4.058208 -1.643689 -0.356435
I 2.445854 0.869468 -0.690141
I 0.605163 3.348117 -0.930616

ENERGY AND THERMAL PARAMETERS
HF=-1434.1557162
****** 1 imaginary frequencies (negative Signs) ******
Zero-point vibrational energy 21949.6 (Joules/Mol)
Zero-point correction= 0.008360 (Hartree/Particle)
Thermal correction to Energy= 0.026314
Thermal correction to Enthalpy= 0.027258
Thermal correction to Gibbs Free Energy= -0.050138
Sum of electronic and zero-point Energies= -1434.147356
Sum of electronic and thermal Energies= -1434.129402
Sum of electronic and thermal Enthalpies= -1434.128458
Sum of electronic and thermal Free Energies= -1434.205854

$3{\cdot}I_2$

CARTESIAN COORDINATES

P -2.468003 -0.544139 -1.296836
P -0.612160 0.559248 -0.506295
P -1.152686 -0.352305 1.484271
P -1.912510 -2.147433 0.275172
I -4.529096 0.378619 -0.133466
I 1.000667 -0.957873 2.591739

I 0.040582 -3.202543 -0.961665 I 3.180338 1.982836 -0.007955
I 3.207034 -0.489343 -1.187104 I -1.160367 2.988934 -0.291861

ENERGY AND THERMAL PARAMETERS
HF=-1434.1821209
Zero-point vibrational energy 23515.3 (Joules/Mol)
Zero-point correction= 0.008957 (Hartree/Particle)
Thermal correction to Energy= 0.027406
Thermal correction to Enthalpy= 0.028351
Thermal correction to Gibbs Free Energy= -0.051791
Sum of electronic and zero-point Energies= -1434.173164
Sum of electronic and thermal Energies= -1434.154714
Sum of electronic and thermal Enthalpies= -1434.153770
Sum of electronic and thermal Free Energies= -1434.233912

3
CARTESIAN COORDINATES
P 1.513937 -1.066789 0.984182 I 3.435152 0.514109 0.471887
P -0.150992 0.124394 2.029931 I -2.704866 1.772678 -0.227499
P -0.272201 1.302168 0.111194 I -1.590609 -2.352537 -0.480423
P 0.266192 -0.678174 -0.926405 I 0.873288 1.677851 3.701132

ENERGY AND THERMAL PARAMETERS
HF=-1411.2595125
Zero-point vibrational energy 21552.1 (Joules/Mol)
Zero-point correction= 0.008209 (Hartree/Particle)
Thermal correction to Energy= 0.021655
Thermal correction to Enthalpy= 0.022600
Thermal correction to Gibbs Free Energy= -0.039934
Sum of electronic and zero-point Energies= -1411.251304
Sum of electronic and thermal Energies= -1411.237857
Sum of electronic and thermal Enthalpies= -1411.236913
Sum of electronic and thermal Free Energies= -1411.299447

3'
CARTESIAN COORDINATES
P -0.466977 -1.817359 -1.009375 I -2.737978 -2.864247 -0.666608
P -0.937738 0.415199 -0.709156 I -0.002297 1.633769 2.702025
P 0.900819 0.431234 0.674909 I 2.566324 -2.912133 0.887958
P 0.340218 -1.750750 1.144733 I 0.009228 1.420988 -2.821486

ENERGY AND THERMAL PARAMETERS
HF=-1411.258885
Zero-point vibrational energy 21535.8 (Joules/Mol)
Zero-point correction= 0.008203 (Hartree/Particle)
Thermal correction to Energy= 0.021657
Thermal correction to Enthalpy= 0.022601
Thermal correction to Gibbs Free Energy= -0.040415
Sum of electronic and zero-point Energies= -1411.250682

Sum of electronic and thermal Energies= -1411.237228
Sum of electronic and thermal Enthalpies= -1411.236284
Sum of electronic and thermal Free Energies= -1411.299300

Pathway IIb

$(2{\cdot}2I_2)_{periph}$

CARTESIAN COORDINATES

P -3.256889 1.865396 -0.630474
P -2.767697 1.112487 1.377307
P -4.298654 -0.495064 0.945240
P -2.569484 -0.218827 -0.485831
I -5.651064 2.252905 -1.162409
I -3.426959 -2.385752 2.389261
I -1.534890 3.573267 -1.668898
I 0.584946 5.462023 -2.795293
I 2.945749 3.732679 -1.308702
I 4.960541 2.172787 0.020798

ENERGY AND THERMAL PARAMETERS
HF=-1434.1628068
Zero-point vibrational energy 23434.7 (Joules/Mol)
Zero-point correction= 0.008926 (Hartree/Particle)
Thermal correction to Energy= 0.027575
Thermal correction to Enthalpy= 0.028519
Thermal correction to Gibbs Free Energy= -0.054983
Sum of electronic and zero-point Energies= -1434.153881
Sum of electronic and thermal Energies= -1434.135232
Sum of electronic and thermal Enthalpies= -1434.134288
Sum of electronic and thermal Free Energies= -1434.217790

$(2\text{-}4)_{TS}^{\ddagger}$

CARTESIAN COORDINATES

P 1.4029 -1.7276 0.0286
P 2.0300 -0.1617 1.4470
P 1.6714 0.3091 -0.7702
I 3.0820 -3.4537 -0.6165
P 3.7752 0.1494 0.0423
I 4.2837 2.5960 0.4735
I -1.1705 -2.1961 0.2000
I -4.2072 -1.7459 0.3651
I -3.0036 1.4107 -0.1125
I -1.4976 3.7940 -0.5212

ENERGY AND THERMAL PARAMETERS
HF=-1434.1612818800

$4{\cdot}I_2$

CARTESIAN COORDINATES

P 0.613623 -2.392437 1.153096
P 1.407418 0.919180 1.722226
P 3.221856 -0.129568 0.859581
P 1.181965 -0.475817 -0.022675
I 1.525441 -4.055970 -0.518630
I 4.340595 1.271956 -0.891316
I -1.869716 -2.300479 0.731636
I -4.615566 0.527981 -0.732970
I -2.240893 1.883476 -0.222019
I 1.061977 3.179579 0.637771

ENERGY AND THERMAL PARAMETERS
HF=-1434.1818644
Zero-point vibrational energy 23228.8 (Joules/Mol)
Zero-point correction= 0.008847 (Hartree/Particle)
Thermal correction to Energy= 0.027405
Thermal correction to Enthalpy= 0.028349
Thermal correction to Gibbs Free Energy= -0.052867

Sum of electronic and zero-point Energies= -1434.173017
Sum of electronic and thermal Energies= -1434.154459
Sum of electronic and thermal Enthalpies= -1434.153515
Sum of electronic and thermal Free Energies= -1434.234731

4
CARTESIAN COORDINATES
P 0.655814 -2.408679 1.125409 I 1.472479 -4.092945 -0.572299
P 1.339875 0.927028 1.675435 I 4.376314 1.291399 -0.819334
P 3.208835 -0.100941 0.904199 I -1.845970 -2.270827 0.798873
P 1.214099 -0.503160 -0.058443 I 0.995654 3.150425 0.575360

ENERGY AND THERMAL PARAMETERS
HF=-1411.2562282
Zero-point vibrational energy 21331.4 (Joules/Mol)
Zero-point correction= 0.008125 (Hartree/Particle)
Thermal correction to Energy= 0.021686
Thermal correction to Enthalpy= 0.022630
Thermal correction to Gibbs Free Energy= -0.041613
Sum of electronic and zero-point Energies= -1411.248104
Sum of electronic and thermal Energies= -1411.234542
Sum of electronic and thermal Enthalpies= -1411.233598
Sum of electronic and thermal Free Energies= -1411.297842

3rd P-P cleavage

Pathway IIIa

3'2I_2
CARTESIAN COORDINATES

P	-4.2138	-0.8613	0.2503	I -4.8758	2.4520 -1.1499
P	-2.8847	0.3551	1.7400	I -1.5172	-1.1775 3.0785
P	-1.6352	0.8639	-0.0742	I 0.2837	-0.7133 -0.7050
P	-3.4033	0.4587	-1.4888	I 2.7205	-2.6274 -1.4369
I	-3.1328	-3.0438	-0.2627	I 4.6095	-0.2542 -0.3405
I	-0.8832	3.1941	0.0230	I 6.2303	1.9391 0.672

ENERGY AND THERMAL PARAMETERS
HF=-1457.1211879
Zero-point vibrational energy 26581.2 (Joules/Mol)
Zero-point correction= 0.010124 (Hartree/Particle)
Thermal correction to Energy= 0.033217
Thermal correction to Enthalpy= 0.034161
Thermal correction to Gibbs Free Energy= -0.059486
Sum of electronic and zero-point Energies= -1457.111064
Sum of electronic and thermal Energies= -1457.087971
Sum of electronic and thermal Enthalpies= -1457.087027
Sum of electronic and thermal Free Energies= -1457.184091

$(3\text{-}5)_{TS}$
Imaginary Frequency at -8.5 cm^{-1}
CARTESIAN COORDINATES
P 1.350273 1.149272 2.044473 P 2.947486 -0.415461 1.347999

P 1.907353 -0.335584 -0.660334
P 0.949107 1.717537 -0.183502
I -0.759264 -0.003959 2.639629
I 3.541731 -0.348490 -2.493841
I 2.840231 3.312938 -0.509087
I 2.407013 -2.617756 2.281697
I -0.122567 -1.789134 -1.054280
I -3.260892 -2.722860 -1.322882
I -3.469586 0.408718 -0.531441
I -3.134784 3.184777 0.270969

ENERGY AND THERMAL PARAMETERS
HF=-1457.1238444
Zero-point vibrational energy 26391.7 (Joules/Mol)
Zero-point correction= 0.010052 (Hartree/Particle)
Thermal correction to Energy= 0.032250
Thermal correction to Enthalpy= 0.033194
Thermal correction to Gibbs Free Energy= -0.056302
Sum of electronic and zero-point Energies= -1457.113792
Sum of electronic and thermal Energies= -1457.091594
Sum of electronic and thermal Enthalpies= -1457.090650
Sum of electronic and thermal Free Energies= -1457.180146

5·I_2
CARTESIAN COORDINATES
P -0.838973 0.700531 0.790873
P -1.690190 -1.374624 0.291457
P 1.743096 -1.360463 -0.398868
P 0.969904 0.817023 -0.622309
I -2.284149 2.513949 -0.065032
I 2.659857 -1.623905 1.901680
I 2.461833 2.330335 0.661835
I -1.969078 -1.252344 -2.201085
I 3.742714 -1.058259 -1.892396
I -3.971910 -1.156538 1.260355
I -0.493163 0.755238 3.475436
I -0.078242 0.674358 6.437554

ENERGY AND THERMAL PARAMETERS
HF=-1457.1438013
Zero-point vibrational energy 26610.1 (Joules/Mol)
Zero-point correction= 0.010135 (Hartree/Particle)
Thermal correction to Energy= 0.033151
Thermal correction to Enthalpy= 0.034096
Thermal correction to Gibbs Free Energy= -0.058936
Sum of electronic and zero-point Energies= -1457.133666
Sum of electronic and thermal Energies= -1457.110650
Sum of electronic and thermal Enthalpies= -1457.109706
Sum of electronic and thermal Free Energies= -1457.202737

5
CARTESIAN COORDINATES
P 0.659666 1.842727 1.324936
P 2.515182 0.870614 0.403031
P 1.756675 -0.589065 -1.184351
P -0.657290 1.922111 -0.582660
I -0.739726 0.155587 2.570739
I 4.002254 -1.259583 -2.121087
I 0.883358 3.352955 -2.002373
I 3.461547 -0.401218 2.318262
I 0.899458 -2.640688 -0.050446
I -2.423623 3.509859 0.271648

ENERGY AND THERMAL PARAMETERS
HF=-1434.2081414
Zero-point vibrational energy 23785.8 (Joules/Mol)
Zero-point correction= 0.009060 (Hartree/Particle)
Thermal correction to Energy= 0.027325
Thermal correction to Enthalpy= 0.028270
Thermal correction to Gibbs Free Energy= -0.049824

Sum of electronic and zero-point Energies= -1434.199082
Sum of electronic and thermal Energies= -1434.180816
Sum of electronic and thermal Enthalpies= -1434.179872
Sum of electronic and thermal Free Energies= -1434.257965

Pathway IIIb

$(4^{\cdot}2I_2)_a$
CARTESIAN COORDINATES

P -2.377548 -0.447584 -0.706199	I -2.518918 -2.038295 1.190506
P 0.682115 0.182298 1.097905	I 2.472522 1.922929 1.002863
P 0.932648 -1.323000 -0.587300	I -2.636248 -1.627419 -3.001930
P -0.325260 0.511149 -0.882681	I -2.335182 -2.923989 -5.846417
I -3.951183 1.407913 -0.312159	I 0.771343 -2.008873 -5.952034
I 2.857283 -0.843316 -2.096533	I 3.544827 -1.181011 -6.082922

ENERGY AND THERMAL PARAMETERS
HF=-1457.1200611
Zero-point vibrational energy 26373.8 (Joules/Mol)
Zero-point correction= 0.010045 (Hartree/Particle)
Thermal correction to Energy= 0.033247
Thermal correction to Enthalpy= 0.034191
Thermal correction to Gibbs Free Energy= -0.060541
Sum of electronic and zero-point Energies= -1457.110016
Sum of electronic and thermal Energies= -1457.086814
Sum of electronic and thermal Enthalpies= -1457.085870
Sum of electronic and thermal Free Energies= -1457.1825800

$(4\text{-}6)_{TS}$ Imaginary Frequency at -38.1 cm^{-1}
CARTESIAN COORDINATES

P 0.261985 -2.261952 -0.066513	I -0.584109 -3.956091 1.608409
P -2.934580 -0.914543 0.192294	I -4.487154 0.798768 -0.729003
P -1.575746 -0.055189 1.781879	I 2.583359 -1.625748 0.502714
P -0.859758 -0.155715 -0.377472	I 4.687116 1.721866 0.444341
I 0.232212 -3.318922 -2.302100	I 2.002570 2.357797 -0.602264
I -2.049448 2.318287 2.288899	I -0.937747 2.660542 -1.622683

ENERGY AND THERMAL PARAMETERS
HF=-1457.1163303
Zero-point vibrational energy 25300.3 (Joules/Mol)
Zero-point correction= 0.009636 (Hartree/Particle)
Thermal correction to Energy= 0.032106
Thermal correction to Enthalpy= 0.033051
Thermal correction to Gibbs Free Energy= -0.057780
Sum of electronic and zero-point Energies= -1457.106694
Sum of electronic and thermal Energies= -1457.084224
Sum of electronic and thermal Enthalpies= -1457.083280
Sum of electronic and thermal Free Energies= -1457.174110

$(6\text{-}7\text{-}I_2)$
CARTESIAN COORDINATES

P 2.339447 -1.388423 -0.100477	P -1.371423 -2.789250 -0.098345

P -0.829440 -0.943215 1.117009
P -0.921777 -0.818557 -1.160490
I 3.721412 -1.963147 -2.127523
I -2.832319 0.097984 2.156930
I 3.486563 -2.540687 1.823827
I -3.824610 -3.208038 -0.035601
I 2.722701 1.066037 0.281528
I 0.968080 4.782346 0.466703
I -0.979072 3.129766 -0.624045

ENERGY AND THERMAL PARAMETERS
HF=-1457.1210906
Zero-point vibrational energy 24938.2 (Joules/Mol)
Zero-point correction= 0.009498 (Hartree/Particle)
Thermal correction to Energy= 0.033022
Thermal correction to Enthalpy= 0.033966
Thermal correction to Gibbs Free Energy= -0.063821
Sum of electronic and zero-point Energies= -1457.111592
Sum of electronic and thermal Energies= -1457.088068
Sum of electronic and thermal Enthalpies= -1457.087124
Sum of electronic and thermal Free Energies= -1457.184912

6

CARTESIAN COORDINATES
P -0.951811 0.424787 -1.196509
P -0.977247 -1.278555 0.320538
P -1.008697 0.886378 1.035697
I -3.242030 -2.306813 0.474832
I -3.197105 0.732012 -2.233152
I -3.296411 1.560592 1.753194

ENERGY AND THERMAL PARAMETERS
HF=-1058.4331516
Zero-point vibrational energy 15567.0 (Joules/Mol)
Zero-point correction= 0.005929 (Hartree/Particle)
Thermal correction to Energy= 0.015476
Thermal correction to Enthalpy= 0.016421
Thermal correction to Gibbs Free Energy= -0.034569
Sum of electronic and zero-point Energies= -1058.427222
Sum of electronic and thermal Energies= -1058.417675
Sum of electronic and thermal Enthalpies= -1058.416731
Sum of electronic and thermal Free Energies= -1058.467721

6 Isomer with one iodide in the opposite sense than the other two

CARTESIAN COORDINATES
P -1.476346 -2.595051 -0.316918
P -0.686264 -0.917508 0.962662
P -0.922816 -0.635063 -1.280731
I -2.743412 -0.185374 2.191721
I 0.635456 -3.952685 -0.712080
I -3.168817 0.323681 -1.8423

ENERGY AND THERMAL PARAMETERS
HF=-1058.4386252
Zero-point vibrational energy 15662.0 (Joules/Mol)
Zero-point correction= 0.005965 (Hartree/Particle)
Thermal correction to Energy= 0.015562
Thermal correction to Enthalpy= 0.016507
Thermal correction to Gibbs Free Energy= -0.035343

Sum of electronic and zero-point Energies= -1058.432660
Sum of electronic and thermal Energies= -1058.423063
Sum of electronic and thermal Enthalpies= -1058.422119
Sum of electronic and thermal Free Energies= -1058.473968

7

CARTESIAN COORDINATES

P	-1.234467	0.572044	0.000000	I	-0.185711	-1.728942	0.000000
I	-0.185369	1.722135	1.993213	I	-0.185369	1.722135	-1.993213

ENERGY AND THERMAL PARAMETERS
HF=-375.752298
Zero-point vibrational energy 6340.2 (Joules/Mol)
Zero-point correction= 0.002415 (Hartree/Particle)
Thermal correction to Energy= 0.008921
Thermal correction to Enthalpy= 0.009865
Thermal correction to Gibbs Free Energy= -0.034345
Sum of electronic and zero-point Energies= -375.749883
Sum of electronic and thermal Energies= -375.743377
Sum of electronic and thermal Enthalpies= -375.742433
Sum of electronic and thermal Free Energies= -375.786643

$(4{\cdot}2I_2)_b$

CARTESIAN COORDINATES

P	-0.916536	2.314617	-1.530125	I	-2.501189	4.056581	-0.623635
P	-2.816894	0.814994	1.474261	I	-2.385740	-1.258536	2.754495
P	-3.992499	0.353268	-0.489134	I	-0.203208	-1.493333	-0.774893
P	-1.763848	0.476198	-0.465667	I	2.239841	-3.572452	-0.965922
I	1.231476	2.542465	-0.266197	I	3.815759	-0.941449	0.003429
I	-4.437874	-2.074093	-0.699752	I	4.926113	1.620141	0.858541

ENERGY AND THERMAL PARAMETERS
HF=-1457.1213863
Zero-point vibrational energy 26461.5 (Joules/Mol)
Zero-point correction= 0.010079 (Hartree/Particle)
Thermal correction to Energy= 0.033212
Thermal correction to Enthalpy= 0.034156
Thermal correction to Gibbs Free Energy= -0.059028
Sum of electronic and zero-point Energies= -1457.111308
Sum of electronic and thermal Energies= -1457.088175
Sum of electronic and thermal Enthalpies= -1457.087230
Sum of electronic and thermal Free Energies= -1457.180414

Pathway IIIc

$(4{\cdot}2I_2)_c$

CARTESIAN COORDINATES

P	0.726045	1.548694	-1.750064	P	2.205854	-1.159896	-0.111186
P	1.965453	0.354948	1.510142	P	2.663058	0.938612	-0.592295

I 1.677428 3.639617 -2.795577
I 4.206242 -2.566513 -0.135995
I -0.883311 2.350362 0.002136
I 4.079832 0.389358 2.831484
I -0.073911 -2.215689 -0.794573
I -2.984157 -3.166592 -1.370764
I -3.841365 -0.631388 0.471287
I -4.288569 1.733390 2.071105

ENERGY AND THERMAL PARAMETERS
HF=-1457.1161827
Zero-point vibrational energy 26284.8 (Joules/Mol)
Zero-point correction= 0.010011 (Hartree/Particle)
Thermal correction to Energy= 0.033214
Thermal correction to Enthalpy= 0.034158
Thermal correction to Gibbs Free Energy= -0.059687
Sum of electronic and zero-point Energies= -1457.106171
Sum of electronic and thermal Energies= -1457.082969
Sum of electronic and thermal Enthalpies= -1457.082025
Sum of electronic and thermal Free Energies= -1457.176838

$(4\text{-}8)_{TS}$
Imaginary Frequency at -24.7 cm^{-1}
CARTESIAN COORDINATES
P -0.686357 0.896954 1.514409
P 1.150706 -1.488366 -0.520802
P 1.996914 0.590107 -0.750822
P 1.442669 -0.046713 1.281516
I 0.127489 2.986728 2.702749
I 4.390848 1.039452 -1.037321
I -1.478358 -0.660459 3.316397
I 3.131720 -2.984256 -0.279559
I 0.261353 1.928870 -1.931401
I -3.226500 1.911118 -2.397728
I -2.665367 -0.903046 -1.152958
I -1.886918 -3.515188 0.012420

ENERGY AND THERMAL PARAMETERS
HF=-1457.1148126
Zero-point vibrational energy 25792.2 (Joules/Mol)
Zero-point correction= 0.009824 (Hartree/Particle)
Thermal correction to Energy= 0.032239
Thermal correction to Enthalpy= 0.033184
Thermal correction to Gibbs Free Energy= -0.057700
Sum of electronic and zero-point Energies= -1457.104989
Sum of electronic and thermal Energies= -1457.082573
Sum of electronic and thermal Enthalpies= -1457.081629
Sum of electronic and thermal Free Energies= -1457.173488

$8{\cdot}I_2$
CARTESIAN COORDINATES
P -0.151609 0.903282 1.211685
P -0.228472 -2.086307 -0.881389
P 2.316607 -0.213691 -1.257315
P 1.158984 -0.926452 0.608624
I 1.673728 2.375704 2.171955
I 4.471641 0.557332 -0.237170
I -1.241145 -0.081297 3.273740
I 1.400683 -3.987353 -1.279838
I 1.118082 1.874822 -2.076561
I -3.042141 2.843771 -1.624141
I -3.228123 0.226741 -0.765443
I -1.998635 -3.113351 0.606253

ENERGY AND THERMAL PARAMETERS

HF=-1457.1290546
Zero-point vibrational energy 25250.9 (Joules/Mol)
Zero-point correction= 0.009618 (Hartree/Particle)
Thermal correction to Energy= 0.032957
Thermal correction to Enthalpy= 0.033901
Thermal correction to Gibbs Free Energy= -0.060877
Sum of electronic and zero-point Energies= -1457.119437
Sum of electronic and thermal Energies= -1457.096098
Sum of electronic and thermal Enthalpies= -1457.095154
Sum of electronic and thermal Free Energies= -1457.190872

8

CARTESIAN COORDINATES

P 0.013041 0.394340 1.323864
P 0.444292 -2.479047 -0.877934
P 2.279497 0.178539 -1.522777
P 1.612986 -0.944593 0.362475
I 1.528534 2.094885 2.415473
I 4.345195 1.303501 -0.630622
I -0.706975 -1.137251 3.198690
I 0.408680 -4.394854 0.751933
I 0.633681 2.076562 -1.921839
I -1.973630 -1.698480 -1.007464

ENERGY AND THERMAL PARAMETERS
HF=-1434.2072092
Zero-point vibrational energy 23872.6 (Joules/Mol)
Zero-point correction= 0.009093 (Hartree/Particle)
Thermal correction to Energy= 0.027311
Thermal correction to Enthalpy= 0.028255
Thermal correction to Gibbs Free Energy= -0.048569
Sum of electronic and zero-point Energies= -1434.198117
Sum of electronic and thermal Energies= -1434.179898
Sum of electronic and thermal Enthalpies= -1434.178954
Sum of electronic and thermal Free Energies= -1434.2567166

4th P-P cleavage
Pathway IVa

5'2I_2

CARTESIAN COORDINATES

P 1.006166 -0.989465 -1.533300
P -1.055931 0.066256 -1.318291
P -1.090534 1.593656 0.448888
P 2.282533 0.414157 -0.146548
I 0.889985 -2.936053 0.024877
I -3.328890 2.614153 0.071722
I 2.252912 2.512862 -1.528950
I -2.812196 -1.621712 -1.105667
I -1.331723 0.096151 2.419888
I 4.491455 -0.673295 -0.663664
I -1.328606 1.389523 -3.489994
I -1.506571 3.230334 -6.121824
I 0.720146 4.910931 -4.581591
I 2.775057 6.244828 -2.980485

ENERGY AND THERMAL PARAMETERS
HF=-1480.0756436
Zero-point vibrational energy 28799.9 (Joules/Mol)
Zero-point correction= 0.010969 (Hartree/Particle)
Thermal correction to Energy= 0.038869
Thermal correction to Enthalpy= 0.039813

Thermal correction to Gibbs Free Energy= -0.067853
Sum of electronic and zero-point Energies= -1480.064674
Sum of electronic and thermal Energies= -1480.036775
Sum of electronic and thermal Enthalpies= -1480.035830
Sum of electronic and thermal Free Energies= -1480.143497

$(5{\cdot}2I_2)^{\ddagger}$

CARTESIAN COORDINATES

P 1.543234 -0.316637 -1.749508	I -1.645195 -1.783871 -2.976148
P -0.591473 -0.761825 -1.018079	I -4.110527 -0.852568 1.074969
P -2.407874 0.891250 1.565551	I 4.517665 0.498194 0.260593
P 2.094086 1.140286 0.024749	I -1.807766 1.827878 -0.928642
I 1.797399 -2.561520 -0.531482	I -1.134534 3.648244 -4.134858
I -3.634716 2.827247 2.506694	I 0.511227 1.171358 -4.957641
I 2.097051 3.200201 -1.403675	I 2.055722 -1.318136 -5.554923

ENERGY AND THERMAL PARAMETERS
HF=-1480.0487628
Zero-point vibrational energy 26496.8 (Joules/Mol)
Zero-point correction= 0.010092 (Hartree/Particle)
Thermal correction to Energy= 0.038609
Thermal correction to Enthalpy= 0.039554
Thermal correction to Gibbs Free Energy= -0.071481
Sum of electronic and zero-point Energies= -1480.038671
Sum of electronic and thermal Energies= -1480.010153
Sum of electronic and thermal Enthalpies= -1480.009209
Sum of electronic and thermal Free Energies= -1480.120244

$(5\text{-}9)_{TS}$

Imaginary Frequency at -15.1 cm^{-1}
CARTESIAN COORDINATES

P 0.085772 1.267129 -0.855333	I 2.811464 -1.023670 -2.525357
P 1.393846 -0.667035 -0.562097	I 4.539925 0.881672 0.763115
P 2.636384 -0.576352 1.415328	I -0.861816 4.287549 1.024474
P 0.401982 2.143385 1.313626	I -0.392227 -2.461803 -0.352740
I 1.577437 2.828880 -2.095822	I -3.238481 -4.031451 -0.133740
I 3.508997 -2.907863 1.442529	I -4.051949 -0.865302 -0.380145
I -1.157504 0.586738 2.509262	I -4.083430 2.019622 -0.561504

ENERGY AND THERMAL PARAMETERS
HF=-1480.0726774
Zero-point vibrational energy 28571.7 (Joules/Mol)
Zero-point correction= 0.010882 (Hartree/Particle)
Thermal correction to Energy= 0.037903
Thermal correction to Enthalpy= 0.038847
Thermal correction to Gibbs Free Energy= -0.064652
Sum of electronic and zero-point Energies= -1480.061795
Sum of electronic and thermal Energies= -1480.034775
Sum of electronic and thermal Enthalpies= -1480.033830
Sum of electronic and thermal Free Energies= -1480.137329

$9{\cdot}I_2{\cdot}9$

CARTESIAN COORDINATES

P 0.897274 1.539246 1.135600
P -1.481064 -0.833632 0.251568
P -2.491920 -1.471939 -1.732499
P -0.358781 2.296529 -0.668171
I -0.221771 2.955703 2.870369
I -3.920955 -3.451074 -1.178132
I 0.797985 0.865400 -2.402541
I -3.159618 -0.988995 2.086949
I -4.071454 0.484982 -1.887774
I 0.362935 4.648265 -1.128487
I 0.055910 -2.787711 0.489689
I 4.054724 -3.758485 0.012810
I 3.941763 -0.994388 0.353859
I 3.232170 2.517998 0.84776

ENERGY AND THERMAL PARAMETERS

HF=-1480.0837291
Zero-point vibrational energy 27890.2 (Joules/Mol)
Zero-point correction= 0.010623 (Hartree/Particle)
Thermal correction to Energy= 0.038761
Thermal correction to Enthalpy= 0.039705
Thermal correction to Gibbs Free Energy= -0.070188
Sum of electronic and zero-point Energies= -1480.073106
Sum of electronic and thermal Energies= -1480.044968
Sum of electronic and thermal Enthalpies= -1480.044024
Sum of electronic and thermal Free Energies= -1480.153917

9

CARTESIAN COORDINATES

P -0.775759 -0.536464 0.390384
P -1.658171 1.031323 -1.068620
I -2.470837 -0.903391 2.194860
I -1.637188 2.974140 0.535581
I -4.070898 0.454666 -1.402357
I -0.978047 -2.521274 -1.148147

ENERGY AND THERMAL PARAMETERS

HF=-728.5716266
Zero-point vibrational energy 12338.4 (Joules/Mol)
Zero-point correction= 0.004699 (Hartree/Particle)
Thermal correction to Energy= 0.015070
Thermal correction to Enthalpy= 0.016014
Thermal correction to Gibbs Free Energy= -0.039245
Sum of electronic and zero-point Energies= -728.566927
Sum of electronic and thermal Energies= -728.556557
Sum of electronic and thermal Enthalpies= -728.555613
Sum of electronic and thermal Free Energies= -728.610872

Pathway IVabis

$(5\text{-}10)_{TS}$

Imaginary Frequency at -9.36 cm^{-1}

CARTESIAN COORDINATES

P 2.489038 0.942704 -1.149918
P 1.204348 -0.973351 -0.868716
P 0.471611 -1.193160 1.354384
P 1.961026 2.100618 0.838018
I 4.787689 0.256375 -0.468225
I -1.188985 -3.017996 1.105787
I -0.484949 2.515088 0.487572
I 2.460724 -2.922150 -1.658227
I 2.477056 -2.196116 2.428661
I 3.119234 4.228994 0.159805
I -0.881341 -0.530090 -2.237978
I -3.910397 0.308317 -3.128180
I -4.009284 0.449637 0.110288
I -3.660369 0.448130 2.995728

ENERGY AND THERMAL PARAMETERS

HF=-1480.0746496
Zero-point vibrational energy 28748.2 (Joules/Mol)

Zero-point correction= 0.010950 (Hartree/Particle)
Thermal correction to Energy= 0.037928
Thermal correction to Enthalpy= 0.038872
Thermal correction to Gibbs Free Energy= -0.064790
Sum of electronic and zero-point Energies= -1480.063700
Sum of electronic and thermal Energies= -1480.036721
Sum of electronic and thermal Enthalpies= -1480.035777
Sum of electronic and thermal Free Energies= -1480.139439

7·I_2·10

CARTESIAN COORDINATES

P 2.691635 0.586764 -1.228593
P 0.972248 -1.004058 -0.972202
P -0.821915 -1.117501 1.345033
P 2.410336 1.694201 0.815982
I 4.755824 -0.600770 -0.440946
I -1.565518 -3.439388 0.776106
I 0.005955 2.451302 0.629127
I 1.909974 -3.082813 -1.973883
I 1.182033 -1.405343 2.851884
I 3.792186 3.722406 0.205446
I -0.587333 -0.052043 -2.674820
I -4.298475 1.778684 -2.570259
I -3.789626 0.909604 0.068408
I -2.702125 -0.296045 3.077918

ENERGY AND THERMAL PARAMETERS
HF=-1480.0823409
Zero-point vibrational energy 27316.8 (Joules/Mol)
Zero-point correction= 0.010404 (Hartree/Particle)
Thermal correction to Energy= 0.038663
Thermal correction to Enthalpy= 0.039607
Thermal correction to Gibbs Free Energy= -0.069387
Sum of electronic and zero-point Energies= -1480.071937
Sum of electronic and thermal Energies= -1480.043678
Sum of electronic and thermal Enthalpies= -1480.042734
Sum of electronic and thermal Free Energies= -1480.151728

Pathway IVb

6·2I_2

CARTESIAN COORDINATES

P 0.942218 0.307364 1.825790
P -0.462068 -1.426261 1.546840
P -1.246031 0.784058 1.632316
I -0.236536 -2.177598 -0.790518
I 2.393885 0.892318 -0.037786
I -1.597109 1.668555 -0.642944
I 1.890544 0.535820 4.230257
I 2.812753 0.677757 7.200365
I 0.444910 -1.450658 7.903082
I -1.678166 -3.335656 8.431996

ENERGY AND THERMAL PARAMETERS
HF=-1104.2904143
Zero-point vibrational energy 20526.1 (Joules/Mol)
Zero-point correction= 0.007818 (Hartree/Particle)
Thermal correction to Energy= 0.027089
Thermal correction to Enthalpy= 0.028033
Thermal correction to Gibbs Free Energy= -0.056744
Sum of electronic and zero-point Energies= -1104.282596
Sum of electronic and thermal Energies= -1104.263325
Sum of electronic and thermal Enthalpies= -1104.262381
Sum of electronic and thermal Free Energies= -1104.347159

$(6\text{-}10)_{TS}$

Imaginary Frequency at -7.9 cm^{-1}

CARTESIAN COORDINATES

P -1.279477 -1.187516 -0.041987
P -1.321837 0.493908 1.458788
P -1.042416 0.908387 -0.837113
I -3.679977 0.797429 2.109951
I -3.369072 -2.374792 -0.493294
I -3.196506 1.520214 -1.868614
I 1.058353 -2.242795 -0.019081
I 4.223910 -2.313419 0.062417
I 3.543794 0.938128 0.028800
I 2.478129 3.610856 0.00103

ENERGY AND THERMAL PARAMETERS

HF=-1104.2891603
Zero-point vibrational energy 20338.8 (Joules/Mol)
Zero-point correction= 0.007747 (Hartree/Particle)
Thermal correction to Energy= 0.026123
Thermal correction to Enthalpy= 0.027067
Thermal correction to Gibbs Free Energy= -0.053006
Sum of electronic and zero-point Energies= -1104.281414
Sum of electronic and thermal Energies= -1104.263037
Sum of electronic and thermal Enthalpies= -1104.262093
Sum of electronic and thermal Free Energies= -1104.342166

10·I_2

CARTESIAN COORDINATES

P 1.283157 -2.002748 0.640369
P 0.772910 -0.238171 -0.764496
P 0.569190 1.360471 0.900663
I 3.049701 0.033492 -1.780705
I 1.081906 -3.864746 -1.054755
I 2.733298 1.295593 2.181796
I -0.936229 -1.980922 1.864210
I -4.583946 -0.328750 -0.117744
I -2.802144 1.683263 -0.722806
I 0.714058 3.412818 -0.587

ENERGY AND THERMAL PARAMETERS

HF=-1104.3153882
Zero-point vibrational energy 19826.0 (Joules/Mol)
Zero-point correction= 0.007551 (Hartree/Particle)
Thermal correction to Energy= 0.026921
Thermal correction to Enthalpy= 0.027865
Thermal correction to Gibbs Free Energy= -0.056880
Sum of electronic and zero-point Energies= -1104.307837
Sum of electronic and thermal Energies= -1104.288468
Sum of electronic and thermal Enthalpies= -1104.287523
Sum of electronic and thermal Free Energies= -1104.372268

10

CARTESIAN COORDINATES

P -1.334046 1.976527 0.600929
P -0.749692 0.232969 -0.804029
P -0.498938 -1.382545 0.820309
I -3.020491 -0.055084 -1.828942
I -1.053328 3.867404 -1.052839
I -2.559185 -1.225732 2.278467
I 0.790646 1.987191 1.981758
I -0.846065 -3.427429 -0.598453

ENERGY AND THERMAL PARAMETERS

HF=-1081.3914951
Zero-point vibrational energy 17999.4 (Joules/Mol)
Zero-point correction= 0.006856 (Hartree/Particle)
Thermal correction to Energy= 0.021189
Thermal correction to Enthalpy= 0.022133
Thermal correction to Gibbs Free Energy= -0.044557

Sum of electronic and zero-point Energies= -1081.384639
Sum of electronic and thermal Energies= -1081.370306
Sum of electronic and thermal Enthalpies= -1081.369362
Sum of electronic and thermal Free Energies= -1081.436052

Pathway IVc

$(8^{\cdot}2I_2)_{centr}$

CARTESIAN COORDINATES

P -0.076667 1.305781 -0.479328
P -1.616450 -1.883983 1.070678
P 1.800293 -1.943992 0.485511
P 0.179439 -0.384154 1.104882
I 1.982844 2.633972 0.016383
I 3.901856 -0.942551 1.356392
I -1.949803 2.538964 0.624070
I -3.219583 -0.906846 2.706019
I 1.855878 -1.598470 -2.006196
I -2.576154 -1.408825 -1.211214
I 0.591501 0.483933 3.432901
I 0.736810 1.741671 6.468436
I -2.369357 1.213029 6.262110
I -5.192107 0.556871 5.714957

ENERGY AND THERMAL PARAMETERS
HF=-1480.0786181
Zero-point vibrational energy 28486.7 (Joules/Mol)
Zero-point correction= 0.010850 (Hartree/Particle)
Thermal correction to Energy= 0.038799
Thermal correction to Enthalpy= 0.039744
Thermal correction to Gibbs Free Energy= -0.067643
Sum of electronic and zero-point Energies= -1480.067768
Sum of electronic and thermal Energies= -1480.039819
Sum of electronic and thermal Enthalpies= -1480.038874
Sum of electronic and thermal Free Energies= -1480.147218

$(8^{\cdot}2I_2)_{lat}$

CARTESIAN COORDINATES

P -0.076667 1.305781 -0.479328
P -1.616450 -1.883983 1.070678
P 1.800293 -1.943992 0.485511
P 0.179439 -0.384154 1.104882
I 1.982844 2.633972 0.016383
I 3.901856 -0.942551 1.356392
I -1.949803 2.538964 0.624070
I -3.219583 -0.906846 2.706019
I 1.855878 -1.598470 -2.006196
I -2.576154 -1.408825 -1.211214
I 0.591501 0.483933 3.432901
I 0.736810 1.741671 6.468436
I -2.369357 1.213029 6.262110
I -5.192107 0.556871 5.714957

ENERGY AND THERMAL PARAMETERS
HF=-1480.0786181
Zero-point vibrational energy 28486.7 (Joules/Mol)
Zero-point correction= 0.010850 (Hartree/Particle)
Thermal correction to Energy= 0.038799
Thermal correction to Enthalpy= 0.039744
Thermal correction to Gibbs Free Energy= -0.067643
Sum of electronic and zero-point Energies= -1480.067768
Sum of electronic and thermal Energies= -1480.039819
Sum of electronic and thermal Enthalpies= -1480.038874
Sum of electronic and thermal Free Energies= -1480.146261

(8-10)$_{TS}$

Imaginary Frequency at -10.8 cm^{-1}

CARTESIAN COORDINATES

P 2.905864 0.428840 1.260284	I -1.576626 2.249395 1.696509
P -0.294647 2.011118 -0.407888	I 3.961648 0.636774 -2.338534
P 1.591022 -0.183200 -2.333912	I 1.556113 3.714835 -0.304212
P 1.011571 0.087711 -0.061189	I -0.593952 -1.670624 0.656326
I 3.798409 -1.908934 1.140729	I -3.601715 -3.223586 1.062958
I 1.728265 -2.645765 -2.580784	I -4.239358 -0.504058 -0.496595
I 1.809012 0.612472 3.489577	I -4.307805 2.086122 -1.877771

ENERGY AND THERMAL PARAMETERS

HF=-1480.0730403

Zero-point vibrational energy 28137.9 (Joules/Mol)

Zero-point correction= 0.010717 (Hartree/Particle)

Thermal correction to Energy= 0.037854

Thermal correction to Enthalpy= 0.038798

Thermal correction to Gibbs Free Energy= -0.066399

Sum of electronic and zero-point Energies= -1480.062323

Sum of electronic and thermal Energies= -1480.035187

Sum of electronic and thermal Enthalpies= -1480.034242

Sum of electronic and thermal Free Energies= -1480.140396

7·I$_2$·10

CARTESIAN COORDINATES

P 2.913439 -0.090655 0.842045	I -1.749581 2.579568 2.125694
P -0.656123 2.712457 -0.132428	I 1.608146 0.854315 -2.786808
P 0.252221 -0.949082 -1.629572	I 1.286160 4.279640 0.178760
P 0.652711 -0.145847 0.461180	I -0.446836 -1.831236 1.892547
I 3.637861 -2.393034 1.504574	I -3.542957 -2.174250 -1.424755
I 1.488026 -3.111485 -1.977521	I -3.337071 0.594594 -1.658482
I 2.785083 1.166121 3.027482	I -2.358980 4.110294 -1.553316

ENERGY AND THERMAL PARAMETERS

HF=-1480.0836558

Zero-point vibrational energy 27286.4 (Joules/Mol)

Zero-point correction= 0.010393 (Hartree/Particle)

Thermal correction to Energy= 0.038707

Thermal correction to Enthalpy= 0.039651

Thermal correction to Gibbs Free Energy= -0.072806

Sum of electronic and zero-point Energies= -1480.073263

Sum of electronic and thermal Energies= -1480.044949

Sum of electronic and thermal Enthalpies= -1480.044005

Sum of electronic and thermal Free Energies= -1480.157419

Pathway V

10·2I$_2$

CARTESIAN COORDINATES

P -0.773313 2.288950 -0.387336	I 1.706468 2.317749 -0.047440
P -1.053573 0.081041 -1.115423	I -1.863985 -3.124111 0.760962
P -0.555975 -1.039877 0.854527	I 1.973839 -1.691616 0.984387
I -3.545469 0.119130 -1.099747	I 5.000715 -2.371889 1.075479
I -1.124941 3.315537 -2.671293	I 5.465031 0.821185 0.711451
I -1.300441 0.269562 2.818695	I 5.617744 3.686739 0.362038

ENERGY AND THERMAL PARAMETERS
HF=-1127.2517581
Zero-point vibrational energy 22997.2 (Joules/Mol)
Zero-point correction= 0.008759 (Hartree/Particle)
Thermal correction to Energy= 0.032741
Thermal correction to Enthalpy= 0.033686
Thermal correction to Gibbs Free Energy= -0.063727
Sum of electronic and zero-point Energies= -1127.242999
Sum of electronic and thermal Energies= -1127.219017
Sum of electronic and thermal Enthalpies= -1127.218072
Sum of electronic and thermal Free Energies= -1127.315485

$(10\text{-}9)_{TS}$
Imaginary Frequency at -13.7 cm^{-1}
CARTESIAN COORDINATES

P -2.092515 0.679147 1.950468	I 0.132883 -0.113591 2.785352
P -1.603491 0.459512 -0.323722	I -0.903429 -2.003354 -2.981650
P -0.702952 -1.696244 -0.523088	I 0.306163 1.847310 -1.142842
I -3.776280 0.746580 -1.421340	I 3.577176 2.484919 -1.670608
I -2.100403 3.163123 2.114405	I 3.529045 -0.268087 -0.035454
I -2.573567 -2.991684 0.515382	I 3.055269 -2.711031 1.516298

ENERGY AND THERMAL PARAMETERS
HF=-1127.2580603
Zero-point vibrational energy 22906.2 (Joules/Mol)
Zero-point correction= 0.008725 (Hartree/Particle)
Thermal correction to Energy= 0.031817
Thermal correction to Enthalpy= 0.032762
Thermal correction to Gibbs Free Energy= -0.060761
Sum of electronic and zero-point Energies= -1127.249336
Sum of electronic and thermal Energies= -1127.226243
Sum of electronic and thermal Enthalpies= -1127.225299
Sum of electronic and thermal Free Energies= -1127.318821

$7{\cdot}I_2{\cdot}9$
CARTESIAN COORDINATES

P -2.152445 0.820173 0.947521	I -0.159045 1.133246 2.449646
P -0.968545 0.839265 -1.044412	I -1.198208 -3.617017 -1.592550
P -0.534724 -2.255028 0.419098	I 1.970317 -2.401051 0.508228
I -2.926288 0.617443 -2.580070	I 5.265632 0.004538 -0.053251
I -3.442954 2.960755 1.049650	I 3.058812 1.578324 -0.687996
I -1.356429 -3.572849 2.406094	I -0.112922 3.206800 -1.369458

ENERGY AND THERMAL PARAMETERS
HF=-1127.261763
Zero-point vibrational energy 21601.2 (Joules/Mol)
Zero-point correction= 0.008227 (Hartree/Particle)
Thermal correction to Energy= 0.032604
Thermal correction to Enthalpy= 0.033548
Thermal correction to Gibbs Free Energy= -0.067622
Sum of electronic and zero-point Energies= -1127.253536
Sum of electronic and thermal Energies= -1127.229159
Sum of electronic and thermal Enthalpies= -1127.228215
Sum of electronic and thermal Free Energies= -1127.329385

9·I_2

CARTESIAN COORDINATES
P 1.901042 -0.955527 -1.397820
P 1.891283 0.739323 0.196423
I 3.984924 -2.222311 -0.885404
I 3.826138 2.093847 -0.539621
I 2.362460 -0.167081 2.447208
I 0.023724 -2.311060 -0.468067
I -0.469735 2.095195 -0.041865
I -3.060635 3.478213 -0.46655

ENERGY AND THERMAL PARAMETERS
HF=-751.5021299
Zero-point vibrational energy 15012.6 (Joules/Mol)
Zero-point correction= 0.005718 (Hartree/Particle)
Thermal correction to Energy= 0.020885
Thermal correction to Enthalpy= 0.021829
Thermal correction to Gibbs Free Energy= -0.049265
Sum of electronic and zero-point Energies= -751.496412
Sum of electronic and thermal Energies= -751.481245
Sum of electronic and thermal Enthalpies= -751.480301
Sum of electronic and thermal Free Energies= -751.551395

9·2I_2

CARTESIAN COORDINATES
P 0.605770 1.958137 -0.766292
P -0.735918 0.041100 -0.801828
I 1.005892 2.224224 1.673968
I -2.828652 0.795402 0.250764
I 0.234956 -1.798806 0.513990
I 2.677330 0.987755 -1.747817
I -0.984132 -0.603122 -3.272534
I -0.672686 -1.273120 -6.370170
I 2.436292 -0.901185 -5.588742
I 5.104847 -0.470484 -4.512040

ENERGY AND THERMAL PARAMETERS
HF=-774.4347148
Zero-point vibrational energy 17390.1 (Joules/Mol)
Zero-point correction= 0.006624 (Hartree/Particle)
Thermal correction to Energy= 0.026636
Thermal correction to Enthalpy= 0.027580
Thermal correction to Gibbs Free Energy= -0.058278
Sum of electronic and zero-point Energies= -774.428091
Sum of electronic and thermal Energies= -774.408079
Sum of electronic and thermal Enthalpies= -774.407134
Sum of electronic and thermal Free Energies= -774.492993

(9-7)$_{TS}$

Imaginary Frequency at -8.5 cm^{-1}
CARTESIAN COORDINATES
P 1.073222 -1.297061 -0.394355
P 1.836132 0.919136 -0.156360
I 3.223166 -2.542119 -0.473061
I 2.975840 1.345076 -2.296499
I 3.434094 1.166791 1.704059
I 0.159709 -1.622167 1.888127
I -0.363847 2.232000 0.065628
I -3.434638 2.968006 0.195293
I -3.550938 -0.304899 -0.262984
I -3.259140 -3.137062 -0.668850

ENERGY AND THERMAL PARAMETERS
HF=-774.4319634
Zero-point vibrational energy 17177.6 (Joules/Mol)
Zero-point correction= 0.006543 (Hartree/Particle)
Thermal correction to Energy= 0.025691
Thermal correction to Enthalpy= 0.026636
Thermal correction to Gibbs Free Energy= -0.056226
Sum of electronic and zero-point Energies= -774.425421
Sum of electronic and thermal Energies= -774.406272
Sum of electronic and thermal Enthalpies= -774.405328
Sum of electronic and thermal Free Energies= -774.488189

7·I_2·7
CARTESIAN COORDINATES
P 0.356536 -1.589168 -0.053725
P 1.740055 1.064745 -0.061532
I 2.540465 -2.790717 -0.336897
I 2.470709 1.335331 -2.450803
I 3.598552 2.049761 1.325507
I 0.027924 -1.408549 2.426651
I -0.214685 2.607829 0.211410
I -4.328311 2.180517 0.004155
I -3.294592 -0.378737 -0.431890
I -1.402052 -3.386513 -0.774175

ENERGY AND THERMAL PARAMETERS
HF=-774.4407882
Zero-point vibrational energy 15821.0 (Joules/Mol)
Zero-point correction= 0.006026 (Hartree/Particle)
Thermal correction to Energy= 0.026450
Thermal correction to Enthalpy= 0.027394
Thermal correction to Gibbs Free Energy= -0.062589
Sum of electronic and zero-point Energies= -774.434762
Sum of electronic and thermal Energies= -774.414339
Sum of electronic and thermal Enthalpies= -774.413394
Sum of electronic and thermal Free Energies= -774.503377

11
CARTESIAN COORDINATES
P -2.537279 -1.947159 0.528242
P -3.222812 -1.146659 -1.480809
C -3.625188 -0.868635 1.705336
C -4.512320 0.166624 -0.893315
H -4.831550 0.722549 -1.786627
H -3.288835 -1.077332 2.731167
C -1.726318 -0.004127 -1.901843
C -0.844792 -1.033278 0.680442
H -1.778107 0.845283 -1.203285
H -1.878019 0.370768 -2.923462
H -4.638055 -1.290423 1.595324
H -5.370821 -0.435203 -0.551718
C -0.418293 -0.732839 -1.756847
H 0.180069 -0.913808 -2.652742
C -0.008954 -1.210766 -0.557588
H 0.921042 -1.778928 -0.481873
H -0.341978 -1.422968 1.576306
H -1.079831 0.030051 0.842441
C -3.596606 0.598179 1.387855
C -4.006110 1.076053 0.188270
H -3.161834 1.278613 2.123891
H -3.899508 2.139704 -0.037767

ENERGY AND THERMAL PARAMETERS
HF=-994.5085365
Zero-point vibrational energy 462763.3 (Joules/Mol)
Zero-point correction= 0.176257 (Hartree/Particle)
Thermal correction to Energy= 0.186508
Thermal correction to Enthalpy= 0.187452
Thermal correction to Gibbs Free Energy= 0.141396
Sum of electronic and zero-point Energies= -994.332279

Sum of electronic and thermal Energies= -994.322029
Sum of electronic and thermal Enthalpies= -994.321085
Sum of electronic and thermal Free Energies= -994.36714

11'I_2

CARTESIAN COORDINATES

P -2.594240 0.850822 -0.947320
P -2.460375 -0.879634 0.462368
C -3.065734 2.155639 0.383487
C -2.666560 -0.175206 2.186687
H -2.695542 -1.011971 2.896758
H -3.390856 3.042479 -0.178375
C -3.941888 -1.966737 0.094821
C -4.320527 0.380155 -1.654563
H -4.788206 -1.449189 0.576307
H -3.787010 -2.931680 0.593744
H -2.112350 2.410013 0.874641
H -1.757047 0.415141 2.380265
C -4.138388 -2.104952 -1.396853
H -4.097919 -3.108849 -1.819762
C -4.318321 -1.028520 -2.194604
H -4.420391 -1.165741 -3.272272
H -4.535786 1.116664 -2.440041
H -5.061860 0.497461 -0.849719
C -4.102398 1.718667 1.386825
C -3.925016 0.660591 2.210160
H -5.048664 2.262170 1.412393
H -4.723457 0.345574 2.883353
I -0.330187 -2.210513 0.162891
I 2.401125 -4.030682 -0.275591

ENERGY AND THERMAL PARAMETERS
HF=-1017.4697245
Zero-point vibrational energy 468219.6 (Joules/Mol)
Zero-point correction= 0.178335 (Hartree/Particle)
Thermal correction to Energy= 0.193243
Thermal correction to Enthalpy= 0.194187
Thermal correction to Gibbs Free Energy= 0.132023
Sum of electronic and zero-point Energies= -1017.291389
Sum of electronic and thermal Energies= -1017.276481
Sum of electronic and thermal Enthalpies= -1017.275537
Sum of electronic and thermal Free Energies= -1017.337701

11'2I_2

CARTESIAN COORDINATES

P 2.597297 0.803860 0.937316
P 2.604418 -0.903160 -0.513484
C 2.877210 2.151111 -0.395000
C 2.615460 -0.188640 -2.233742
H 2.697073 -1.013077 -2.953650
H 3.152737 3.052336 0.170693
C 4.166421 -1.882199 -0.222042
C 4.396019 0.480372 1.537827
H 4.941541 -1.291096 -0.738494
H 4.067273 -2.850809 -0.727568
H 1.877595 2.337823 -0.820114
H 1.639112 0.303092 -2.365267
C 4.436899 -2.010377 1.259862
H 4.511084 -3.017230 1.670117
C 4.550787 -0.927296 2.059691
H 4.714794 -1.062698 3.129640
H 4.580244 1.226289 2.322315
H 5.084402 0.675366 0.702046
C 3.893273 1.829245 -1.460715
C 3.780687 0.774042 -2.298790
H 4.773081 2.471003 -1.533043
H 4.566647 0.555700 -3.022073
I 0.658166 -2.313127 -0.187506
I -3.279334 -2.112333 0.255103
I -2.111825 0.728245 0.251573
I -0.853086 3.495505 0.241310

ENERGY AND THERMAL PARAMETERS
HF=-1040.4114371
Zero-point vibrational energy 471225.3 (Joules/Mol)
Zero-point correction= 0.179480 (Hartree/Particle)
Thermal correction to Energy= 0.199216
Thermal correction to Enthalpy= 0.200160

Thermal correction to Gibbs Free Energy= 0.120840
Sum of electronic and zero-point Energies= -1040.231957
Sum of electronic and thermal Energies= -1040.212221
Sum of electronic and thermal Enthalpies= -1040.211277
Sum of electronic and thermal Free Energies= -1040.290597

$(11\text{-}12)_{TS}$

Imaginary Frequency at -22.2 cm^{-1}

CARTESIAN COORDINATES

P -0.786566 1.510003 -0.242929	H -5.096939 1.357893 -1.797251
P -3.466681 -0.696773 0.424657	C -3.355874 2.330371 -1.119403
C -0.611386 0.631509 1.473226	H -3.199761 2.794179 -2.096097
C -3.241460 -0.851556 2.305060	H -1.987943 3.683170 -0.167400
H -4.189835 -1.124662 2.786572	H -2.734928 2.526334 0.955097
H 0.434425 0.784624 1.775291	C -1.559760 1.071469 2.544434
C -4.711564 0.743553 0.308577	C -2.708165 0.443554 2.888497
C -2.329772 2.645423 -0.057815	H -1.317119 2.009646 3.049643
H -4.527118 1.350283 1.207917	H -3.334563 0.911234 3.651687
H -5.744714 0.376360 0.348508	I -4.898558 -2.725095 -0.062405
H -0.725562 -0.436087 1.235559	I 4.991346 -1.477639 0.230940
H -2.534932 -1.685376 2.447642	I 3.281471 0.788406 0.152454
C -4.425622 1.519527 -0.950935	I 1.059681 3.338551 0.10017

ENERGY AND THERMAL PARAMETERS
HF=-1040.3809557
Zero-point vibrational energy 470126.2 (Joules/Mol)
Zero-point correction= 0.179062 (Hartree/Particle)
Thermal correction to Energy= 0.198021
Thermal correction to Enthalpy= 0.198965
Thermal correction to Gibbs Free Energy= 0.123087
Sum of electronic and zero-point Energies= -1040.201894
Sum of electronic and thermal Energies= -1040.182935
Sum of electronic and thermal Enthalpies= -1040.181991
Sum of electronic and thermal Free Energies= -1040.257869

$12{\cdot}I_2$

CARTESIAN COORDINATES

P -0.199965 1.655604 -1.045692	H -4.533101 1.719679 -2.301619
P -3.889474 -0.632126 -0.213254	C -2.709494 2.535424 -1.667647
C -0.593324 0.173195 0.077903	H -2.516159 2.900033 -2.679533
C -3.301383 -0.876128 1.583008	H -1.254423 3.857879 -0.787637
H -4.167584 -0.776632 2.251693	H -1.964095 2.709455 0.386334
H 0.345330 -0.406005 0.105117	C -1.076355 0.475970 1.465816
C -4.303001 1.237468 -0.155979	C -2.209276 0.060125 2.071784
C -1.633555 2.834229 -0.653172	H -0.414608 1.116647 2.054680
H -3.769807 1.653609 0.709279	H -2.366318 0.417960 3.093132
H -5.382030 1.367245 0.002954	I -6.196885 -1.699627 -0.034615
H -1.310459 -0.430642 -0.504724	I 4.934910 -2.483825 -0.169559
H -2.967052 -1.925765 1.641227	I 3.510782 -0.049951 0.105161
C -3.861929 1.859695 -1.449937	I 1.643354 2.781585 0.390478

ENERGY AND THERMAL PARAMETERS

HF=-1040.384748
Zero-point vibrational energy 469478.3 (Joules/Mol)
Zero-point correction= 0.178815 (Hartree/Particle)
Thermal correction to Energy= 0.198825
Thermal correction to Enthalpy= 0.199769
Thermal correction to Gibbs Free Energy= 0.120203
Sum of electronic and zero-point Energies= -1040.205933
Sum of electronic and thermal Energies= -1040.185923
Sum of electronic and thermal Enthalpies= -1040.184979
Sum of electronic and thermal Free Energies= -1040.264545

12

CARTESIAN COORDINATES

P 0.138203 0.692916 0.658846	C 3.487620 0.621365 2.295255
P 4.269277 -0.711840 -0.014977	H 3.923874 0.022629 3.099475
C 1.080861 0.132284 -0.902746	C 2.211706 1.044874 2.450284
C 4.233877 0.116107 -1.732262	H 1.692709 0.765019 3.370799
H 5.221166 0.555471 -1.930141	H 0.818454 2.623631 2.006256
H 0.298492 -0.292379 -1.553841	H 2.014769 2.353980 0.706386
C 4.363014 0.845922 1.094192	C 1.864877 1.187634 -1.624978
C 1.403061 1.859563 1.473119	C 3.178925 1.190270 -1.937046
H 4.020626 1.692076 0.483014	H 1.287308 2.067735 -1.919971
H 5.406906 1.024788 1.385225	H 3.553100 2.083301 -2.445388
H 1.707627 -0.712918 -0.571224	I 6.685516 -1.531071 -0.004834
H 4.096015 -0.709873 -2.450203	I -1.428685 2.421213 -0.389937

ENERGY AND THERMAL PARAMETERS
HF=-1017.4589108
Zero-point vibrational energy 467964.9 (Joules/Mol)
Zero-point correction= 0.178238 (Hartree/Particle)
Thermal correction to Energy= 0.193164
Thermal correction to Enthalpy= 0.194108
Thermal correction to Gibbs Free Energy= 0.132863
Sum of electronic and zero-point Energies= -1017.280672
Sum of electronic and thermal Energies= -1017.265747
Sum of electronic and thermal Enthalpies= -1017.264803
Sum of electronic and thermal Free Energies= -1017.326048

I_2

CARTESIAN COORDINATES

I 0.000000 0.000000 -0.006327	I 0.000000 0.000000 2.736327

ENERGY AND THERMAL PARAMETERS
HF=-22.9138694
Zero-point vibrational energy 1168.4 (Joules/Mol)
Zero-point correction= 0.000445 (Hartree/Particle)
Thermal correction to Energy= 0.003374
Thermal correction to Enthalpy= 0.004318
Thermal correction to Gibbs Free Energy= -0.025389
Sum of electronic and zero-point Energies= -22.913424
Sum of electronic and thermal Energies= -22.910496
Sum of electronic and thermal Enthalpies= -22.909552
Sum of electronic and thermal Free Energies= -22.939259

$P(CH_3)_3$

CARTESIAN COORDINATES

P -1.085096 -0.108215 -0.253067
C -2.940931 -0.256020 0.002602
H -3.389079 0.748417 0.045985
H -3.388827 -0.797780 -0.844431
H -3.173571 -0.794086 0.936866
C -0.605624 -1.907076 0.003313
H 0.490777 -1.994633 0.046467
H -1.034776 -2.305140 0.938136
H -0.967461 -2.510726 -0.843013
C -0.605744 0.568762 1.433273
H -1.037322 -0.040508 2.245135
H 0.490562 0.572423 1.531636
H -0.965008 1.604484 1.532097

ENERGY AND THERMAL PARAMETERS

HF=-461.010921
Zero-point vibrational energy 286876.2 (Joules/Mol)
Zero-point correction= 0.109265 (Hartree/Particle)
Thermal correction to Energy= 0.116179
Thermal correction to Enthalpy= 0.117124
Thermal correction to Gibbs Free Energy= 0.079712
Sum of electronic and zero-point Energies= -460.901656
Sum of electronic and thermal Energies= -460.894741
Sum of electronic and thermal Enthalpies= -460.893797
Sum of electronic and thermal Free Energies= -460.931209

$P(CH_3)_3 \cdot I_2$

CARTESIAN COORDINATES

P -1.193645 -0.000739 -0.000279
C -1.823495 0.940927 -1.438257
H -1.453665 1.973134 -1.384440
H -1.466332 0.468429 -2.362590
H -2.923415 0.935387 -1.414699
C -1.827979 -1.715424 -0.097416
H -1.471099 -2.283007 0.771996
H -2.927842 -1.689411 -0.102198
H -1.461014 -2.183843 -1.020024
C -1.823574 0.774417 1.533922
H -2.923452 0.768246 1.511829
H -1.463585 0.203964 2.400146
H -1.456350 1.807343 1.593460
I 1.318350 -0.002665 -0.000186
I 4.693497 0.004140 0.006333

ENERGY AND THERMAL PARAMETERS

HF=-483.9790958
Zero-point vibrational energy 294598.9 (Joules/Mol)
Zero-point correction= 0.112207 (Hartree/Particle)
Thermal correction to Energy= 0.123462
Thermal correction to Enthalpy= 0.124406
Thermal correction to Gibbs Free Energy= 0.071108
Sum of electronic and zero-point Energies= -483.866889
Sum of electronic and thermal Energies= -483.855634
Sum of electronic and thermal Enthalpies= -483.854690
Sum of electronic and thermal Free Energies= -483.907988

$P(CH_3)_3 \cdot 2I_2$

CARTESIAN COORDINATES

P 2.072502 0.802772 0.282009
C 1.631024 -0.726881 -0.610649
H 1.498545 -0.477604 -1.673840
H 2.438211 -1.461453 -0.494562
H 0.695478 -1.128290 -0.200196
C 0.734135 2.030844 0.101743
H 1.005062 2.944834 0.645480
H 0.612188 2.250307 -0.969315
H -0.196192 1.615755 0.509936
C 3.628736 1.483166 -0.386386
H 3.885645 2.401166 0.157778
H 4.429204 0.741181 -0.270923
H 3.474866 1.708543 -1.452030
I 2.357261 0.304554 2.653802
I 2.362931 -0.079022 6.377920
I 0.118931 2.002172 5.858094

I -2.038626 4.014156 5.250644

ENERGY AND THERMAL PARAMETERS
HF=-506.9200525
Zero-point vibrational energy 298097.2 (Joules/Mol)
Zero-point correction= 0.113539 (Hartree/Particle)
Thermal correction to Energy= 0.129541
Thermal correction to Enthalpy= 0.130486
Thermal correction to Gibbs Free Energy= 0.060250
Sum of electronic and zero-point Energies= -506.806513
Sum of electronic and thermal Energies= -506.790511
Sum of electronic and thermal Enthalpies= -506.789567

$[P(CH_3)_3I]^+$

CARTESIAN COORDINATES

P -1.194254 -0.264383 0.015591	H -0.948141 -2.480091 0.895173
C -3.016059 -0.249162 -0.007871	H -0.946880 -2.487747 -0.905467
H -3.371787 0.788874 -0.003275	C -0.574851 0.613606 1.487076
H -3.374690 -0.769860 -0.904785	H -0.953616 0.084365 2.374167
H -3.365063 -0.770954 0.895742	H 0.522408 0.604891 1.483845
C -0.573630 -1.977118 -0.008849	H -0.946569 1.645968 1.478583
H 0.523634 -1.967394 -0.006234	I -0.386104 0.878205 -1.965295

ENERGY AND THERMAL PARAMETERS
HF=-472.3255965
Zero-point vibrational energy 295582.2 (Joules/Mol)
Zero-point correction= 0.112581 (Hartree/Particle)
Thermal correction to Energy= 0.121045
Thermal correction to Enthalpy= 0.121989
Thermal correction to Gibbs Free Energy= 0.078680
Sum of electronic and zero-point Energies= -472.213015
Sum of electronic and thermal Energies= -472.204552
Sum of electronic and thermal Enthalpies= -472.203607

I_3^-
CARTESIAN COORDINATES
I 0.000000 0.000000 -0.356780
I 0.000000 0.000000 2.709962
I 0.000000 0.000000 5.776818

ENERGY AND THERMAL PARAMETERS
HF=-34.5770037
Zero-point vibrational energy 1715.1 (Joules/Mol)
Zero-point correction= 0.000653 (Hartree/Particle)
Thermal correction to Energy= 0.006179
Thermal correction to Enthalpy= 0.007123
Thermal correction to Gibbs Free Energy= -0.032343
Sum of electronic and zero-point Energies= -34.576350
Sum of electronic and thermal Energies= -34.570824
Sum of electronic and thermal Enthalpies= -34.569880
Sum of electronic and thermal Free Energies= -34.609347