

# SUPPORTING INFORMATION

## **ZnCl<sub>2</sub>-Based Deep Eutectic Solvent as Solvent-Catalyst in the Michael Addition Reaction of Pyrrole to Maleimide**

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## Experimental

### *Materials and equipment*

Thin layer chromatography (TLC) analyses were performed on commercial aluminum plates bearing a 0.25 mm Merck silica gel 60F254 layer, visualized with UV light at 254 nm or under iodine. Column chromatography was performed with SiO<sub>2</sub> (F60 (230–400 mesh)). Infra-red (IR) spectra were recorded on a Thermo Scientific modelo Nicolet iS10 spectrometer using ATR (Attenuated Total Reflection). Selected absorption maxima ( $\nu_{\text{max}}$ ) are reported in wavenumbers (cm<sup>-1</sup>). The melting point was recorded in degrees Celsius (°C), using a Fisher-Johns melting point apparatus, and is reported uncorrected. <sup>1</sup>H and <sup>13</sup>C-NMR spectra of solutions in CD<sub>3</sub>OD were recorded on a Mercury 400 spectrometer. Deuterated chloroform was used as received, and chemical shift values ( $\delta$ ) are reported in parts per million (ppm) relatives to the residual signals of this solvent [ $\delta$  7.2 for <sup>1</sup>H (CDCl<sub>3</sub>) and  $\delta$  77.2 ppm for <sup>13</sup>C (CDCl<sub>3</sub>)]. Abbreviations used in the NMR follow-up experiments: *s*, singlet; *d*, doublet; *t*, triplet and *m*, multiplet. The pyrrole **1**, maleimides **2**, ChCl, and ZnCl<sub>2</sub>·3H<sub>2</sub>O were obtained from commercial sources and used as received.

### Preparation of deep eutectic solvent (ChCl:ZnCl<sub>2</sub>)

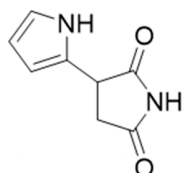
1.24 mmol of choline chloride and 2.5 mmol of ZnCl<sub>2</sub> were mixed in a 5 mL round-bottomed flask and heated for 15 minutes at 120°C until a clear liquid appeared. The mixture was allowed to stir for 15 min more, the colorless liquid was used directly for the reactions without purification.

### *Typical procedure for the pyrrole-maleimide Michael addition in ChCl:ZnCl<sub>2</sub>*

0.1 ml of water were added to the ChCl:ZnCl<sub>2</sub> (0.650 g) with stirring for 5 min, and then, the maleimide **2a** (0.072g, 0.74 mmol, 1 equiv) and pyrrole **1** (0.05 g, 0.74 mmol, 1 equiv)

were slowly added to the reaction mixture. The reaction mixture was stirred at room temperature for 2.5h. TLC monitored the reaction. After completion of the reaction, water was added, extraction was made with AcOEt, the organic phase was separated and dried on anhydrous Na<sub>2</sub>SO<sub>4</sub>, and the solvent was evaporated. The pure **3a** product was purified on a silica gel chromatographic column using the mixture of Hex/EtOAc (7:3, v/v) as the eluent.

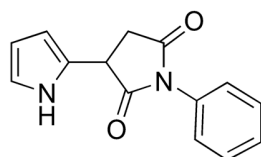
### 3-(1H-pyrrol-2-yl)pyrrolidine-2,5-dione **3a**



ACCORDING TO GENERAL PROCEDURE, **3a** WAS OBTAINED IN 82% YIELD (0.102G). BROWN CRYSTALS, RF 0.28 (Hex/EtOAc 6:4), MELTING POINT (MEASURED): 105-108°C;

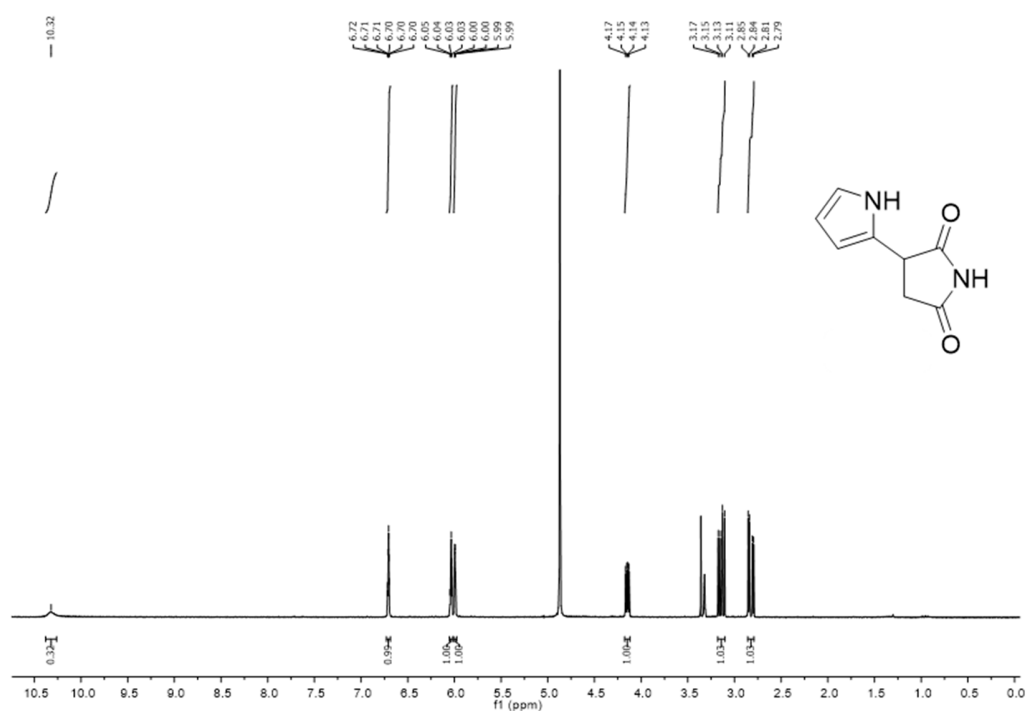
<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD; Me<sub>4</sub>Si) δ<sub>H</sub> = 10.32 (s, 1H), 6.71 (td, *J* = 2.7, 1.4 Hz, 3H), 6.04 (dd, *J* = 5.5, 2.8 Hz, 1H), 5.99 (dd, *J* = 2.4, 1.7 Hz, 1H), 4.15 (dd, *J* = 9.5, 5.3 Hz, 1H), 3.14 (dd, *J* = 18.2, 9.5 Hz, 1H), 2.82 (dd, *J* = 18.2, 5.3 Hz, 1H); <sup>13</sup>C {<sup>1</sup>H} NMR (100 MHz, CD<sub>3</sub>OD; Me<sub>4</sub>Si) δ<sub>C</sub> = 179.67, 178.62, 126.53, 118.22, 107.54, 105.49, 40.94, 36.72; IR (ν/cm<sup>-1</sup>) 3352, 1769, 1682, 1188.

### 1-phenyl-3-(1H-pyrrol-2-yl)pyrrolidine-2,5-dione **3b**



According to general procedure, **3b** was obtained in 87% yield (0.155g). Colorless crystals, rf 0.35 (Hex/EtOAc 7:3), melting point (measured): 178-180°C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, Me<sub>4</sub>Si) δ<sub>H</sub> = 9.13 (s, 1H), 7.43– 7.41 (m, 2H), 7.40-7.39 (ddd, *J* = 7.4, 3.7, 1.2

Hz, 1H), 7.29 – 7.26 (m, 2H), 6.83 (s, 1H), 6.22-6.20 (dd,  $J = 6.1, 2.8$  Hz, 1H), 6.10 – 6.08 (m, 1H), 4.27- 4.24 (dd,  $J = 9.3, 5.6$  Hz, 1H), 3.40 - 3.33 (dd,  $J = 18.3, 9.3$  Hz, 1H), 3.25 - 3.19 (dd,  $J = 18.3, 5.6$  Hz, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ,  $\text{Me}_4\text{Si}$ )  $\delta\text{C} = 176.94, 174.97, 131.78, 129.48, 129.08, 126.65, 125.41, 119.23, 108.71, 105.98, 38.71, 34.42$ ; IR ( $\text{v}/\text{cm}^{-1}$ ) 3318, 2940, 1685, 1396



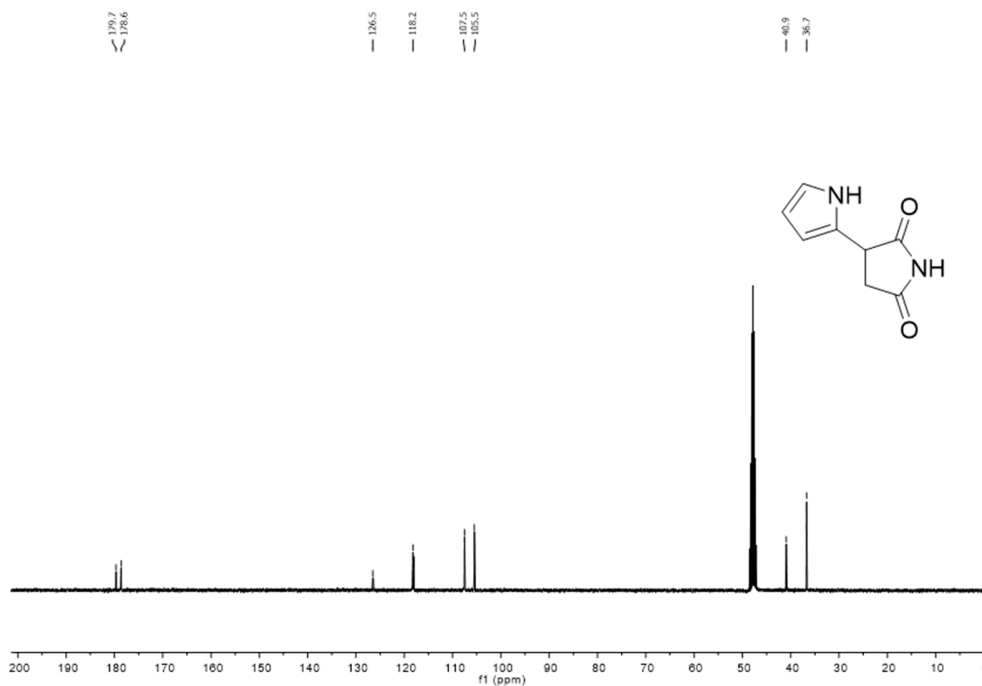


Figure S1. <sup>1</sup>H NMR (400MHz, CD<sub>3</sub>OD), <sup>13</sup>C{<sup>1</sup>H} NMR (100MHz, CD<sub>3</sub>OD) 3-(1H-pyrrol-2-yl)pyrrolidine-2,5-dione **3a**

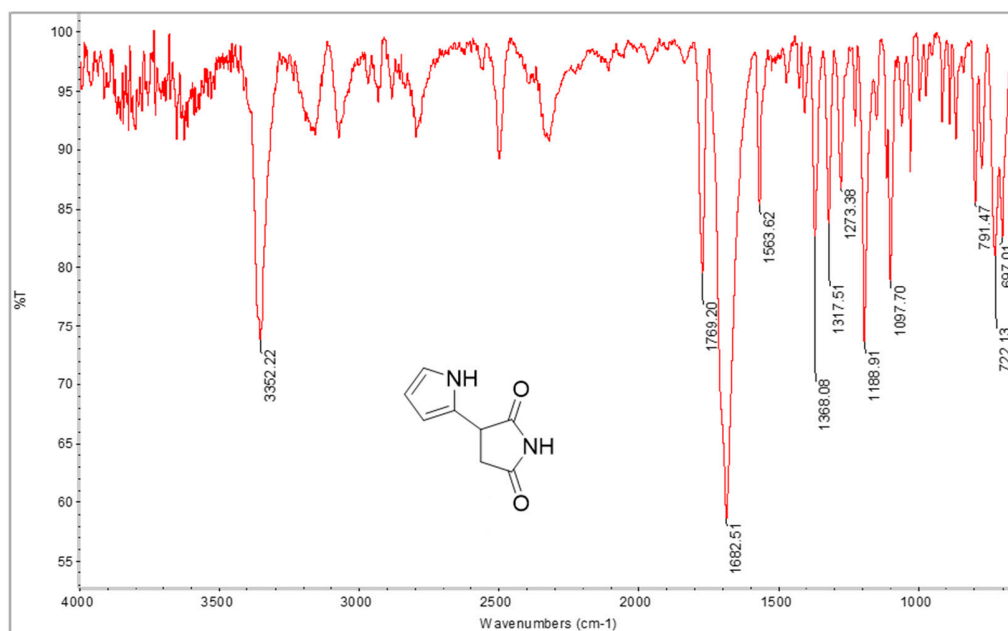


Figure S2. IR Spectrum 3-(1H-pyrrol-2-yl)pyrrolidine-2,5-dione **3a**

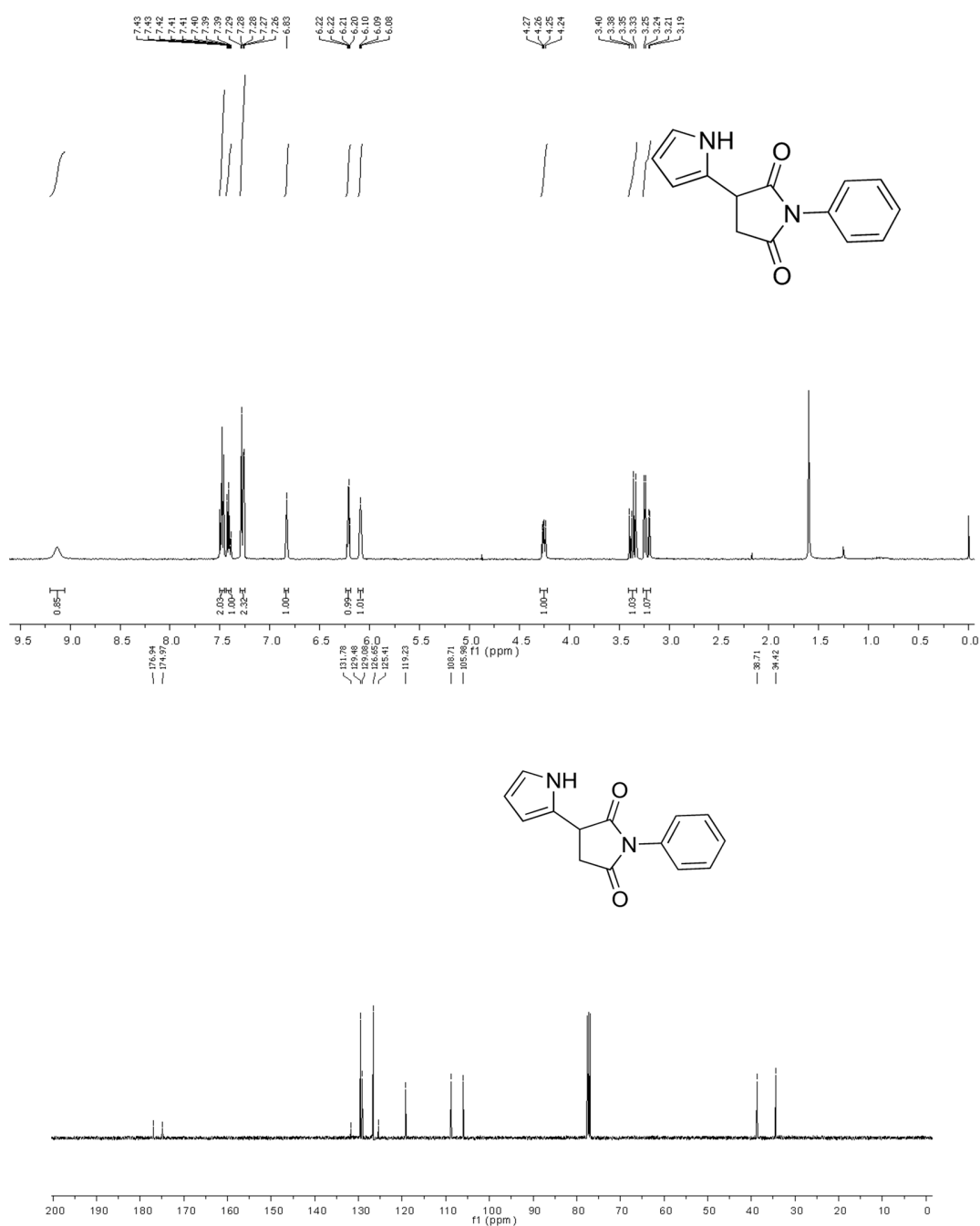


Figure S3 <sup>1</sup>H NMR (400MHz, CDCl<sub>3</sub>), <sup>13</sup>C{<sup>1</sup>H} NMR (100MHz, CDCl<sub>3</sub>) **1-PHENYL-3-(1H-PYRROL-2-YL)PYRROLIDINE-2,5-DIONE 3b**



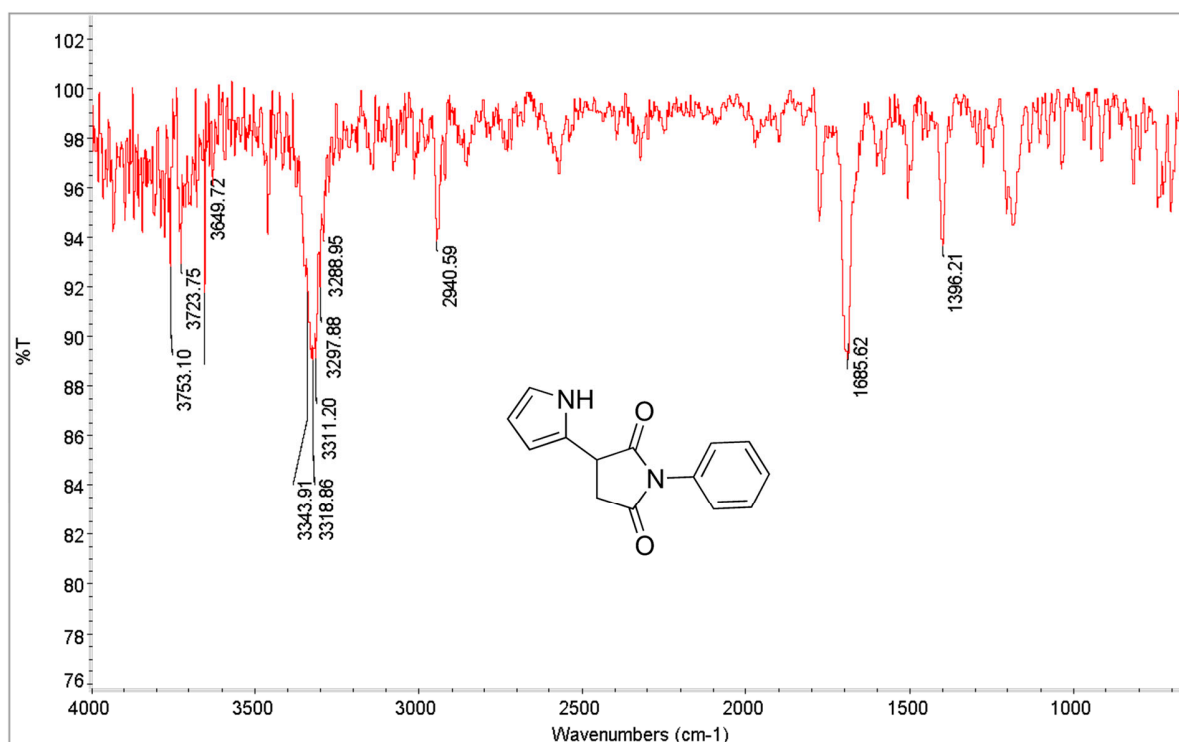


Figure S4. IR Spectrum 1-PHENYL-3-(1H-PYRROL-2-YL)PYRROLIDINE-2,5-DIONE **3B**

### Reference Gaussian 09

Gaussian 09, Revision B.01,

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

## Theoretical calculations

### *Energy and coordinates of Pirrol*

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.076524           |
| Thermal correction to Energy=                | 0.080526           |
| Thermal correction to Enthalpy=              | 0.081470           |
| Thermal correction to Gibbs Free Energy=     | 0.050727           |
| Sum of electronic and zero-point Energies=   | 0.117711           |
| Sum of electronic and thermal Energies=      | 0.121713           |
| Sum of electronic and thermal Enthalpies=    | 0.122657           |
| Sum of electronic and thermal Free Energies= | 0.091914           |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 50.531      | 14.763         | 64.705         |

|          |                 |             |             |
|----------|-----------------|-------------|-------------|
| Charge:0 | Multiplicity: 1 |             |             |
| C        | 0.00000000      | 1.13894600  | 0.33389500  |
| C        | 0.00000000      | 0.71289600  | -0.99413900 |
| C        | 0.00000000      | -0.71289600 | -0.99413900 |
| C        | 0.00000000      | -1.13894600 | 0.33389500  |
| N        | 0.00000000      | 0.00000000  | 1.14807800  |
| H        | 0.00000000      | 2.13405300  | 0.73293900  |
| H        | 0.00000000      | 1.33799600  | -1.86318700 |
| H        | 0.00000000      | -1.33799600 | -1.86318700 |
| H        | 0.00000000      | -2.13405300 | 0.73293900  |
| H        | 0.00000000      | 0.00000000  | 2.14687600  |

### *Energy and coordinates of Maleimide*

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                     | 0.063680           |
| Thermal correction to Energy=              | 0.069254           |
| Thermal correction to Enthalpy=            | 0.070198           |
| Thermal correction to Gibbs Free Energy=   | 0.034300           |
| Sum of electronic and zero-point Energies= | -0.018407          |

|  |           |
|--|-----------|
| Sum of electronic and thermal Energies=      | -0.012834 |
| Sum of electronic and thermal Enthalpies=    | -0.011890 |
| Sum of electronic and thermal Free Energies= | -0.047787 |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 43.457      | 20.306         | 75.553         |

Charge:0      Multiplicity: 1

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.00055600  | 1.28265100  | 0.66880100  |
| C | 0.00055600  | 1.28265100  | -0.66880100 |
| C | -0.00017900 | -0.14554100 | -1.18416400 |
| N | -0.00048800 | -0.95913900 | 0.00000000  |
| C | -0.00017900 | -0.14554100 | 1.18416400  |
| O | -0.00017900 | -0.57343900 | 2.30441300  |
| O | -0.00017900 | -0.57343900 | -2.30441300 |
| H | 0.00098500  | 2.10874300  | 1.36391100  |
| H | 0.00098500  | 2.10874300  | -1.36391100 |
| H | -0.00020500 | -1.97379100 | 0.00000000  |

### *Energy and coordinates of N-Phenyl Maleimide*

|  |                    |
|--|--------------------|
|  | (Hartree/Particle) |
| Zero-point correction=                       | 0.140030           |
| Thermal correction to Energy=                | 0.150379           |
| Thermal correction to Enthalpy=              | 0.151323           |
| Thermal correction to Gibbs Free Energy=     | 0.103037           |
| Sum of electronic and zero-point Energies=   | 0.105272           |
| Sum of electronic and thermal Energies=      | 0.115621           |
| Sum of electronic and thermal Enthalpies=    | 0.116565           |
| Sum of electronic and thermal Free Energies= | 0.068279           |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 94.364      | 39.805         | 101.627        |

Charge:0      Multiplicity: 1

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.02068500 | -0.66403500 | -0.06940200 |
|---|-------------|-------------|-------------|

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.02068600 | 0.66403200  | 0.06942000  |
| C | -1.59625700 | 1.17962300  | 0.11953500  |
| N | -0.75995200 | 0.00000100  | -0.00000800 |
| C | -1.59625600 | -1.17962100 | -0.11955700 |
| O | -1.21205000 | -2.31000100 | -0.22953700 |
| O | -1.21205300 | 2.31000100  | 0.22953600  |
| C | 0.68360600  | 0.00000100  | -0.00000300 |
| C | 1.38183600  | -1.19314500 | 0.25828500  |
| C | 2.77785200  | -1.18193100 | 0.25372000  |
| C | 3.48047700  | -0.00000100 | 0.00000500  |
| C | 2.77785500  | 1.18193000  | -0.25371500 |
| C | 1.38183900  | 1.19314600  | -0.25828700 |
| H | -3.84645700 | -1.35696500 | -0.14265400 |
| H | -3.84645800 | 1.35695900  | 0.14269400  |
| H | 0.84921200  | -2.12708800 | 0.45123900  |
| H | 3.32064600  | -2.10654000 | 0.45096800  |
| H | 4.56820200  | -0.00000200 | 0.00000800  |
| H | 3.32065200  | 2.10653800  | -0.45095900 |
| H | 0.84921800  | 2.12709000  | -0.45124500 |

### *Energy and coordinates of Choline chloride*

|  |                    |
|--|--------------------|
|  | (Hartree/Particle) |
| Zero-point correction=                       | 0.174838           |
| Thermal correction to Energy=                | 0.185135           |
| Thermal correction to Enthalpy=              | 0.186079           |
| Thermal correction to Gibbs Free Energy=     | 0.139259           |
| Sum of electronic and zero-point Energies=   | 0.058852           |
| Sum of electronic and thermal Energies=      | 0.069149           |
| Sum of electronic and thermal Enthalpies=    | 0.070093           |
| Sum of electronic and thermal Free Energies= | 0.023273           |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 116.174     | 38.440         | 98.540         |

Charge:0      Multiplicity: 1

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.01643700  | 0.78994400  | -0.80643600 |
| C  | 0.44319800  | 0.37871400  | 1.09187000  |
| H  | 2.59453400  | 1.47187500  | -0.16612500 |
| H  | 2.68736100  | 0.34525900  | -1.55552400 |
| C  | -0.38477200 | 1.60709500  | 0.57877100  |
| H  | -0.28828100 | -0.38079500 | 1.47039200  |
| H  | 1.07965900  | 0.68573600  | 1.94161500  |
| H  | -1.17932300 | 1.80527000  | 1.32867000  |
| H  | 0.25888100  | 2.49911800  | 0.48002000  |
| N  | 1.29292800  | -0.26498200 | 0.00136900  |
| C  | 0.43589000  | -1.08555800 | -0.93224200 |
| H  | -0.33380500 | -0.41247100 | -1.41589300 |
| H  | 1.01856000  | -1.57747100 | -1.71777300 |
| H  | -0.17010500 | -1.83920000 | -0.39141900 |
| C  | 2.31407600  | -1.17546200 | 0.65516800  |
| H  | 2.92725700  | -1.70120400 | -0.09618300 |
| H  | 2.99678800  | -0.61474000 | 1.31437000  |
| H  | 1.81472400  | -1.94930200 | 1.26777600  |
| H  | 1.26167300  | 1.40912900  | -1.35892100 |
| O  | -0.93161400 | 1.34684500  | -0.66348300 |
| Cl | -2.55180800 | -0.72247700 | 0.06889700  |
| H  | -1.83375600 | 0.53261700  | -0.49675400 |

### *Energy and coordinates of Zinc chloride*

|  |                    |
|--|--------------------|
|  | (Hartree/Particle) |
| Zero-point correction=                       | 0.002017           |
| Thermal correction to Energy=                | 0.006608           |
| Thermal correction to Enthalpy=              | 0.007552           |
| Thermal correction to Gibbs Free Energy=     | -0.024785          |
| Sum of electronic and zero-point Energies=   | -0.080082          |
| Sum of electronic and thermal Energies=      | -0.075491          |
| Sum of electronic and thermal Enthalpies=    | -0.074547          |
| Sum of electronic and thermal Free Energies= | -0.106884          |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 4.146       | 12.035         | 68.059         |

Charge:0      Multiplicity: 1

|    |            |            |             |
|----|------------|------------|-------------|
| Zn | 0.00000000 | 0.00000000 | 0.00000700  |
| Cl | 0.00000000 | 0.00000000 | -2.03593600 |
| Cl | 0.00000000 | 0.00000000 | 2.03592400  |

### *Energy and coordinates of Zinc zincate ( 2 ZnCl<sub>2</sub> . 3 H<sub>2</sub>O)*

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.118262           |
| Thermal correction to Energy=                | 0.144957           |
| Thermal correction to Enthalpy=              | 0.145902           |
| Thermal correction to Gibbs Free Energy=     | 0.058447           |
| Sum of electronic and zero-point Energies=   | -0.783931          |
| Sum of electronic and thermal Energies=      | -0.757236          |
| Sum of electronic and thermal Enthalpies=    | -0.756292          |
| Sum of electronic and thermal Free Energies= | -0.843747          |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 90.962      | 84.132         | 184.065        |

Charge:0      Multiplicity: 1

|    |             |             |             |
|----|-------------|-------------|-------------|
| Zn | -0.32830500 | -0.10237900 | -0.46168000 |
| Zn | 1.45309700  | -0.09869300 | -0.01696400 |
| Cl | 0.08996000  | 0.73640500  | 1.92090200  |
| Cl | 0.33653600  | -2.38088800 | -0.43790100 |
| Cl | 0.81327300  | 1.61928200  | -1.73851600 |
| Cl | 3.58183900  | -0.27087200 | 0.37265600  |
| O  | -0.80386100 | 3.06734100  | 0.27530500  |
| H  | -0.63393400 | 3.48553300  | -0.57084100 |
| O  | -1.62344800 | 0.04118000  | -2.02399300 |
| H  | -2.39951700 | -0.65790900 | -2.09953300 |
| O  | -1.31292000 | -1.77232900 | 2.61069500  |
| H  | -0.51504100 | -2.17825700 | 2.24118300  |
| O  | -2.15544400 | -0.44320200 | 0.50620700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.61100000 | 0.46927000  | 0.80154700  |
| O | -3.12079100 | -1.84813500 | -1.41404400 |
| H | -3.29622500 | -1.43303400 | -0.52811600 |
| O | -2.82298100 | 1.94792100  | 1.18407700  |
| H | -2.06198000 | 2.20005100  | 1.74615300  |
| H | -2.66440700 | 2.44005000  | 0.35198100  |
| H | 0.02951100  | 3.07903000  | 0.75836400  |
| H | -1.00641200 | -1.16354500 | 3.29641700  |
| H | -2.04127500 | -0.93651600 | 1.40911600  |
| H | -2.42273000 | -2.50346700 | -1.24176000 |
| H | -1.37249200 | 0.32199900  | -2.90254100 |

## Structures for the proposed reactions between Pirrol et Maleimide

### Transition state a) TS1

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.141535           |
| Thermal correction to Energy=                | 0.151409           |
| Thermal correction to Enthalpy=              | 0.152353           |
| Thermal correction to Gibbs Free Energy=     | 0.105257           |
| Sum of electronic and zero-point Energies=   | 0.137864           |
| Sum of electronic and thermal Energies=      | 0.147738           |
| Sum of electronic and thermal Enthalpies=    | 0.148682           |
| Sum of electronic and thermal Free Energies= | 0.101586           |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 95.011      | 37.667         | 99.123         |

|          |                 |             |             |
|----------|-----------------|-------------|-------------|
| Charge:0 | Multiplicity: 1 |             |             |
| C        | 2.30579600      | -0.75452800 | 0.00453000  |
| C        | 1.06778000      | -1.08094500 | 0.65096200  |
| C        | 0.20670200      | 0.03655200  | 0.71721000  |
| C        | 1.03411700      | 1.24687300  | 0.19948500  |
| N        | 2.24719700      | 0.71289000  | -0.24331700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 0.68229100  | 2.40558300  | 0.14581100  |
| O | 3.28955700  | -1.36329200 | -0.33906500 |
| N | -1.72892600 | -1.32707400 | -0.31281800 |
| C | -2.98485600 | -1.05563600 | 0.11335800  |
| C | -3.19198900 | 0.36456000  | 0.07503200  |
| H | -3.70463100 | -1.80640400 | 0.41938200  |
| C | -2.02474400 | 0.95682300  | -0.36716500 |
| H | -4.11259400 | 0.85284300  | 0.34515400  |
| H | -1.26726300 | -2.22788400 | -0.35076300 |
| H | -1.81413100 | 2.01114900  | -0.50096400 |
| C | -1.01435800 | -0.08473400 | -0.56824000 |
| H | -0.38374800 | -0.07350400 | -1.47394500 |
| H | -0.41884600 | 0.21716500  | 1.59749900  |
| H | 0.89938500  | -2.04214500 | 1.08042400  |
| H | 3.00846700  | 1.25595000  | -0.62885000 |

### Intermediate a) Int1

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.142427           |
| Thermal correction to Energy=                | 0.152525           |
| Thermal correction to Enthalpy=              | 0.153470           |
| Thermal correction to Gibbs Free Energy=     | 0.105524           |
| Sum of electronic and zero-point Energies=   | 0.135961           |
| Sum of electronic and thermal Energies=      | 0.146059           |
| Sum of electronic and thermal Enthalpies=    | 0.147004           |
| Sum of electronic and thermal Free Energies= | 0.099058           |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 95.711      | 38.517         | 100.911        |



|          |                 |             |             |
|----------|-----------------|-------------|-------------|
| Charge:0 | Multiplicity: 1 |             |             |
| C        | 2.01653200      | -0.98445500 | 0.15115900  |
| C        | 0.73519300      | -0.93374800 | 0.72458400  |
| C        | 0.16392000      | 0.43947200  | 0.66719100  |
| C        | 1.29358500      | 1.28606100  | 0.00797500  |
| N        | 2.32740100      | 0.41393300  | -0.29708500 |
| O        | 1.22947100      | 2.47376200  | -0.24849600 |
| O        | 2.84204300      | -1.84076200 | -0.08946200 |
| N        | -1.39740000     | -0.98643000 | -0.60342300 |
| C        | -2.66373900     | -1.23778000 | -0.31461000 |
| C        | -3.30953200     | -0.01086600 | 0.17553000  |
| H        | -3.15910100     | -2.20498700 | -0.41015400 |
| C        | -2.37653200     | 0.97366000  | 0.22755800  |
| H        | -4.35046000     | 0.03191000  | 0.45658400  |
| H        | -0.58133900     | -1.64096400 | -0.74537300 |
| H        | -2.48418600     | 2.00056400  | 0.55152200  |
| C        | -1.06103700     | 0.45042200  | -0.29801100 |
| H        | -0.79148900     | 0.98430500  | -1.25619700 |
| H        | -0.11166400     | 0.85548300  | 1.65611200  |
| H        | 0.39614300      | -1.67185700 | 1.41182600  |
| H        | 3.20963200      | 0.69243000  | -0.70534300 |

### Transition state a)TS2

|  |                    |
|--|--------------------|
|  | (Hartree/Particle) |
| Zero-point correction=                       | 0.140125           |
| Thermal correction to Energy=                | 0.149829           |
| Thermal correction to Enthalpy=              | 0.150773           |
| Thermal correction to Gibbs Free Energy=     | 0.104239           |
| Sum of electronic and zero-point Energies=   | 0.156379           |
| Sum of electronic and thermal Energies=      | 0.166082           |
| Sum of electronic and thermal Enthalpies=    | 0.167027           |
| Sum of electronic and thermal Free Energies= | 0.120492           |

|       |             |                |                |
|-------|-------------|----------------|----------------|
|       | E (Thermal) | CV             | S              |
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 94.019      | 37.556         | 97.940         |

|          |                 |             |             |
|----------|-----------------|-------------|-------------|
| Charge:0 | Multiplicity: 1 |             |             |
| C        | 2.30807600      | -0.72951900 | -0.23211500 |
| C        | 1.14684100      | -1.23661200 | 0.38894100  |
| C        | 0.25844400      | -0.11727500 | 0.87094900  |
| C        | 1.01276500      | 1.17092400  | 0.44368200  |
| N        | 2.18035700      | 0.76304800  | -0.18935700 |
| O        | 0.62666500      | 2.31374900  | 0.59320800  |
| O        | 3.28044200      | -1.18714000 | -0.79086200 |
| N        | -2.10371000     | -1.06567400 | 0.57541300  |
| C        | -3.25984900     | -0.62166100 | 0.04049700  |
| C        | -2.97410800     | 0.46277400  | -0.86099400 |
| H        | -4.24206200     | -1.02782200 | 0.26655600  |
| C        | -1.61182100     | 0.67560900  | -0.86016000 |
| H        | -3.72402200     | 1.01174800  | -1.40707500 |
| H        | -1.97704200     | -1.80717800 | 1.25215700  |
| H        | -1.05193700     | 1.43380100  | -1.39591400 |
| C        | -0.97499300     | -0.33923100 | -0.01214200 |
| H        | -0.26085000     | -1.17008000 | -0.70788700 |
| H        | 0.03965600      | -0.09814500 | 1.95295700  |
| H        | 1.10170500      | -2.22309600 | 0.78365100  |
| H        | 2.88903500      | 1.39623400  | -0.53756200 |

### *Succinimide a)P*

|  |                    |
|--|--------------------|
|  | (Hartree/Particle) |
| Zero-point correction=                       | 0.144407           |
| Thermal correction to Energy=                | 0.154517           |
| Thermal correction to Enthalpy=              | 0.155461           |
| Thermal correction to Gibbs Free Energy=     | 0.106484           |
| Sum of electronic and zero-point Energies=   | 0.045782           |
| Sum of electronic and thermal Energies=      | 0.055892           |
| Sum of electronic and thermal Enthalpies=    | 0.056836           |
| Sum of electronic and thermal Free Energies= | 0.007859           |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 96.961      | 38.204         | 103.081        |

|          |                 |             |             |
|----------|-----------------|-------------|-------------|
| Charge:0 | Multiplicity: 1 |             |             |
| C        | 2.30466600      | -0.73315000 | -0.11221000 |
| C        | 1.09546100      | -1.15028600 | 0.70118600  |
| C        | 0.22090000      | 0.11385200  | 0.88045700  |
| C        | 0.99186200      | 1.24357100  | 0.17159800  |
| N        | 2.17198000      | 0.66353800  | -0.38665900 |
| O        | 0.72662400      | 2.41066200  | 0.06809800  |
| O        | 3.23541900      | -1.39164400 | -0.49624300 |
| N        | -1.45495500     | -0.09568000 | -1.02333700 |
| C        | -2.83154400     | -0.29105100 | -1.17370600 |
| C        | -3.39429500     | -0.38948900 | 0.09923400  |
| H        | -3.30441100     | -0.34482100 | -2.13681000 |
| C        | -2.34805200     | -0.24268400 | 1.05339800  |
| H        | -4.43004900     | -0.54561700 | 0.32686300  |
| H        | -0.79903800     | 0.04097900  | -1.76757500 |
| H        | -2.46476400     | -0.26671800 | 2.11784100  |
| C        | -1.15471900     | -0.05848100 | 0.34871600  |
| H        | 0.54598200      | -1.97093100 | 0.19486600  |
| H        | 0.15107500      | 0.38281900  | 1.96908600  |
| H        | 1.40847100      | -1.57791400 | 1.67366700  |
| H        | 2.87154000      | 1.20136100  | -0.89485600 |

### *Transition state b)TS1*

|  |                    |
|--|--------------------|
|  | (Hartree/Particle) |
| Zero-point correction=                   | 0.144186           |
| Thermal correction to Energy=            | .160252            |
| Thermal correction to Enthalpy=          | 0.161196           |
| Thermal correction to Gibbs Free Energy= | 0.094857           |

|  |           |
|--|-----------|
| Sum of electronic and zero-point Energies=   | 0.022698  |
| Sum of electronic and thermal Energies=      | 0.038764  |
| Sum of electronic and thermal Enthalpies=    | 0.039708  |
| Sum of electronic and thermal Free Energies= | -0.026631 |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 100.559     | 54.409         | 139.622        |

|          |                 |             |             |
|----------|-----------------|-------------|-------------|
| Charge:0 | Multiplicity: 1 |             |             |
| C        | -0.01824300     | -0.17996400 | 0.58906800  |
| C        | -1.22862300     | -0.83386300 | 1.01108400  |
| C        | -2.30733700     | 0.05355000  | 0.95132800  |
| C        | -1.71566800     | 1.44503100  | 0.60819300  |
| N        | -0.33362200     | 1.21085400  | 0.36287900  |
| O        | -2.27500500     | 2.50629900  | 0.52666700  |
| O        | 1.10447100      | -0.66435600 | 0.43755600  |
| N        | -3.67445800     | -1.61455900 | -0.58234800 |
| C        | -5.01356700     | -1.64328300 | -0.34789300 |
| C        | -5.51152500     | -0.30291700 | -0.36685900 |
| H        | -5.58473900     | -2.55010200 | -0.18756300 |
| C        | -4.44209200     | 0.54760100  | -0.60610600 |
| H        | -6.54378900     | -0.02991000 | -0.22896400 |
| H        | -3.03734300     | -2.39937200 | -0.59722400 |
| Zn       | 2.92962700      | -0.10108100 | -0.11507000 |
| Cl       | 2.81390400      | 1.99605100  | -0.57705100 |
| Cl       | 4.03472800      | -1.91614400 | 0.00636900  |
| H        | -4.45664500     | 1.62729900  | -0.67666600 |
| C        | -3.22795100     | -0.24580100 | -0.67780000 |
| H        | -2.41850100     | -0.02377400 | -1.38069500 |
| H        | -3.16582400     | 0.00747000  | 1.62223300  |
| H        | -1.23619900     | -1.84851300 | 1.35507400  |
| H        | 0.33835700      | 1.93919300  | 0.10392300  |

### Intermediate b)/Int1

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.146002           |
| Thermal correction to Energy=                | 0.162094           |
| Thermal correction to Enthalpy=              | 0.163038           |
| Thermal correction to Gibbs Free Energy=     | 0.095537           |
| Sum of electronic and zero-point Energies=   | 0.012417           |
| Sum of electronic and thermal Energies=      | 0.028509           |
| Sum of electronic and thermal Enthalpies=    | 0.029453           |
| Sum of electronic and thermal Free Energies= | -0.038048          |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 101.715     | 54.735         | 142.067        |

|          |                 |             |             |
|----------|-----------------|-------------|-------------|
| Charge:0 | Multiplicity: 1 |             |             |
| C        | -0.05903200     | -0.13479900 | 0.54020000  |
| C        | -1.27151400     | -0.73474600 | 0.84997600  |
| C        | -2.37475100     | 0.25575900  | 0.77963200  |
| C        | -1.64925300     | 1.59876100  | 0.44735500  |
| N        | -0.29622400     | 1.29182800  | 0.28526800  |
| O        | -2.18536800     | 2.67391500  | 0.29965400  |
| O        | 1.08050600      | -0.63037900 | 0.44584200  |
| N        | -3.52083200     | -1.54984600 | -0.51327400 |
| C        | -4.81418800     | -1.84482500 | -0.44924900 |
| C        | -5.59094900     | -0.60974000 | -0.32373100 |
| H        | -5.23947100     | -2.85109200 | -0.48475600 |
| C        | -4.73109700     | 0.44238400  | -0.29254000 |
| H        | -6.67040600     | -0.59601300 | -0.25948000 |
| H        | -2.70263500     | -2.17368100 | -0.53194800 |
| Zn       | 2.87580900      | -0.15568100 | -0.06874500 |
| Cl       | 2.92911900      | 1.95008800  | -0.57624200 |
| Cl       | 4.03406400      | -1.95796300 | 0.02763700  |
| H        | -4.94045900     | 1.50409200  | -0.19558800 |
| C        | -3.31411700     | -0.06228100 | -0.41955100 |
| H        | -2.83197200     | 0.30002200  | -1.37614100 |
| H        | -2.95091700     | 0.34326800  | 1.72439400  |

|   |             |             |            |
|---|-------------|-------------|------------|
| H | -1.35783900 | -1.70651000 | 1.27567000 |
| H | 0.43300100  | 1.97899500  | 0.07602900 |

### Transition state b)TS2

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.142921           |
| Thermal correction to Energy=                | 0.158685           |
| Thermal correction to Enthalpy=              | 0.159629           |
| Thermal correction to Gibbs Free Energy=     | 0.094251           |
| Sum of electronic and zero-point Energies=   | 0.035552           |
| Sum of electronic and thermal Energies=      | 0.051315           |
| Sum of electronic and thermal Enthalpies=    | 0.052259           |
| Sum of electronic and thermal Free Energies= | -0.013119          |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 99.576      | 54.059         | 137.600        |

|          |                 |             |             |
|----------|-----------------|-------------|-------------|
| Charge:0 | Multiplicity: 1 |             |             |
| C        | 0.01677500      | -0.37886300 | -0.67144100 |
| C        | 1.18434300      | -1.12800100 | -0.90692600 |
| C        | 2.34787300      | -0.18896300 | -1.15853600 |
| C        | 1.71742300      | 1.22323300  | -1.04769500 |
| N        | 0.35296600      | 1.03306000  | -0.74066000 |
| O        | 2.27070700      | 2.28877100  | -1.16213900 |
| O        | -1.12806400     | -0.77322800 | -0.40041700 |
| N        | 4.37920800      | -1.36121600 | -0.11712100 |
| C        | 5.30961300      | -1.05497900 | 0.81438100  |
| C        | 4.84086400      | 0.05543000  | 1.59658000  |
| H        | 6.25554100      | -1.57716000 | 0.93563500  |
| C        | 3.60095800      | 0.42631100  | 1.11723900  |
| H        | 5.39780400      | 0.51371400  | 2.39917500  |
| H        | 4.42641900      | -2.08490000 | -0.82248200 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| Zn | -2.85178500 | -0.06615400 | 0.18973400  |
| Cl | -2.54887900 | 2.02051300  | 0.66674900  |
| Cl | -4.21690300 | -1.70905700 | 0.12782900  |
| H  | 2.97256900  | 1.24067300  | 1.45828700  |
| C  | 3.20837500  | -0.50952600 | 0.06157100  |
| H  | 2.17602400  | -1.24707300 | 0.48348300  |
| H  | 2.86480100  | -0.30873300 | -2.12850900 |
| H  | 1.16833400  | -2.14231700 | -1.24155300 |
| H  | -0.31335300 | 1.80053800  | -0.61000200 |

### Succinimide + ZnCl<sub>2</sub> b) P

|  |                    |
|--|--------------------|
|  | (Hartree/Particle) |
| Zero-point correction=                       | 0.147164           |
| Thermal correction to Energy=                | 0.163233           |
| Thermal correction to Enthalpy=              | 0.164177           |
| Thermal correction to Gibbs Free Energy=     | 0.097840           |
| Sum of electronic and zero-point Energies=   | -0.062618          |
| Sum of electronic and thermal Energies=      | -0.046550          |
| Sum of electronic and thermal Enthalpies=    | -0.045606          |
| Sum of electronic and thermal Free Energies= | -0.111942          |

|       |             |                |                |
|-------|-------------|----------------|----------------|
|       | E (Thermal) | CV             | S              |
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 102.430     | 54.678         | 139.617        |

|          |                 |             |             |
|----------|-----------------|-------------|-------------|
| Charge:0 | Multiplicity: 1 |             |             |
| C        | 0.04939100      | -0.24934000 | 0.43772500  |
| C        | -1.17164900     | -1.07082000 | 0.79198300  |
| C        | -2.32418700     | -0.05712700 | 0.97724200  |
| C        | -1.72558500     | 1.30035700  | 0.56589600  |
| N        | -0.32350100     | 1.09921500  | 0.31626100  |
| O        | -2.26042200     | 2.37069600  | 0.46371500  |
| O        | 1.17447500      | -0.70983700 | 0.28662200  |
| N        | -4.45228300     | 0.57947700  | -0.24731400 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -5.51102800 | -0.05919500 | -0.89569200 |
| C  | -5.28084400 | -1.43553300 | -0.84739900 |
| H  | -6.33024700 | 0.48267400  | -1.33305400 |
| C  | -4.05440600 | -1.65014400 | -0.15952700 |
| H  | -5.91267900 | -2.20099800 | -1.25329800 |
| H  | -4.33564300 | 1.57529000  | -0.13338300 |
| Zn | 3.04973100  | -0.05088900 | -0.17228500 |
| Cl | 2.80835600  | 2.04764300  | -0.47427200 |
| Cl | 4.06731100  | -1.89643300 | -0.04734200 |
| H  | -3.61590400 | -2.60524700 | 0.04561700  |
| C  | -3.54787900 | -0.39643500 | 0.20084900  |
| H  | -1.38405300 | -1.80724500 | -0.01852200 |
| H  | -2.60176600 | 0.00734700  | 2.06714000  |
| H  | -0.99798700 | -1.68788800 | 1.69741700  |
| H  | 0.31517800  | 1.86388800  | 0.05229000  |

### Transition state c)TS1

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.317936           |
| Thermal correction to Energy=                | 0.346915           |
| Thermal correction to Enthalpy=              | 0.347859           |
| Thermal correction to Gibbs Free Energy=     | 0.253110           |
| Sum of electronic and zero-point Energies=   | 0.037005           |
| Sum of electronic and thermal Energies=      | 0.065984           |
| Sum of electronic and thermal Enthalpies=    | 0.066928           |
| Sum of electronic and thermal Free Energies= | -0.027822          |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 217.693     | 100.118        | 199.417        |

|          |                                   |
|----------|-----------------------------------|
| Charge:0 | Multiplicity: 1                   |
| C        | -0.59614100 1.20968800 0.52763900 |



|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.55989200 | 0.26595100  | 1.05815800  |
| C  | -2.83588900 | 0.76868000  | 0.92324800  |
| C  | -2.71884000 | 2.20032200  | 0.38308400  |
| N  | -1.29602400 | 2.37806000  | 0.13777800  |
| O  | -3.52833000 | 3.05707900  | 0.18063700  |
| O  | 0.64014200  | 1.04588300  | 0.42239000  |
| N  | -3.73729000 | -1.41064600 | -0.49207300 |
| C  | -5.04733000 | -1.64660800 | -0.21385300 |
| C  | -5.80581000 | -0.46522700 | -0.48696200 |
| H  | -5.41639300 | -2.59526000 | 0.14642400  |
| C  | -4.91515900 | 0.50400400  | -0.93823500 |
| H  | -6.86681100 | -0.37103400 | -0.37094100 |
| C  | 3.41729200  | -2.17855000 | 1.17990900  |
| C  | 1.54359200  | -1.92754200 | -0.46693600 |
| H  | 3.61963200  | -1.08920900 | 1.13975000  |
| H  | 3.71507500  | -2.53756200 | 2.17809600  |
| C  | 2.46429100  | -2.30250900 | -1.62843000 |
| H  | 0.49371000  | -2.28163500 | -0.68440500 |
| H  | 1.45819900  | -0.81005000 | -0.40032300 |
| H  | 2.14678400  | -1.76629200 | -2.54566100 |
| H  | 3.53268100  | -2.07163300 | -1.44232700 |
| N  | 1.96272100  | -2.47800900 | 0.89213200  |
| C  | 1.74694600  | -3.97264100 | 0.93896000  |
| H  | 2.29380700  | -4.47398900 | 0.11069600  |
| H  | 2.06822000  | -4.40759900 | 1.89506700  |
| H  | 0.66912100  | -4.22609000 | 0.80032900  |
| C  | 1.11823500  | -1.81124700 | 1.95679500  |
| H  | 1.37700700  | -2.16145000 | 2.96642400  |
| H  | 1.22748400  | -0.70835500 | 1.92184800  |
| H  | 0.03284400  | -2.03069500 | 1.79858200  |
| H  | 4.08171500  | -2.66179600 | 0.43886200  |
| O  | 2.46547000  | -3.71301200 | -1.86264400 |
| H  | -2.88384900 | -2.11690200 | -0.33190100 |
| Cl | -1.54611800 | -3.11952700 | 0.14973500  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 1.59624100  | -4.00617500 | -2.22321500 |
| Zn | 2.13942800  | 2.22248600  | -0.14482000 |
| Cl | 1.56337500  | 4.27502800  | 0.04910500  |
| Cl | 3.63143000  | 0.77563600  | -0.71151800 |
| H  | -5.14553600 | 1.51175600  | -1.23432400 |
| C  | -3.59170000 | -0.05597400 | -0.89314600 |
| H  | -2.74620200 | 0.24843500  | -1.48809200 |
| H  | -3.73028800 | 0.45104500  | 1.45142200  |
| H  | -1.29528500 | -0.71880100 | 1.41697300  |
| H  | -0.88036200 | 3.24387200  | -0.21247700 |

### Intermediate c)Int1

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.319984           |
| Thermal correction to Energy=                | 0.348763           |
| Thermal correction to Enthalpy=              | 0.349707           |
| Thermal correction to Gibbs Free Energy=     | 0.256253           |
| Sum of electronic and zero-point Energies=   | -0.009101          |
| Sum of electronic and thermal Energies=      | 0.019678           |
| Sum of electronic and thermal Enthalpies=    | 0.020622           |
| Sum of electronic and thermal Free Energies= | -0.072831          |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 218.852     | 100.688        | 196.690        |

|          |                 |             |            |
|----------|-----------------|-------------|------------|
| Charge:0 | Multiplicity: 1 |             |            |
| C        | 0.32181100      | -1.18916600 | 0.42000900 |
| C        | 1.37677100      | -0.34544900 | 0.64544400 |
| C        | 2.67153500      | -1.09718500 | 0.56941300 |
| C        | 2.22009200      | -2.54704200 | 0.23958700 |
| N        | 0.80935700      | -2.53375300 | 0.18677200 |
| O        | 2.91340500      | -3.51995900 | 0.05071000 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| O  | -0.92953900 | -0.90348500 | 0.38792100  |
| N  | 4.05427700  | 0.83670400  | -0.25219700 |
| C  | 5.36704100  | 0.85888100  | -0.21464300 |
| C  | 5.94211900  | -0.48813200 | -0.44020100 |
| H  | 5.96360700  | 1.75187900  | -0.04238000 |
| C  | 4.91404200  | -1.34327800 | -0.62317800 |
| H  | 6.99918400  | -0.68675400 | -0.44166700 |
| C  | -2.95623100 | 2.44172700  | 1.25660100  |
| C  | -1.17674600 | 2.01961400  | -0.45730700 |
| H  | -3.22993500 | 1.36576800  | 1.32457500  |
| H  | -3.20693500 | 2.91211800  | 2.21954600  |
| C  | -2.06688900 | 2.52682500  | -1.59110900 |
| H  | -0.09978000 | 2.20940200  | -0.69101300 |
| H  | -1.26563700 | 0.88920600  | -0.39426900 |
| H  | -1.91044000 | 1.91259000  | -2.50030200 |
| H  | -3.14980000 | 2.51032700  | -1.34436600 |
| N  | -1.49323000 | 2.60920400  | 0.91393000  |
| C  | -1.13619900 | 4.07768500  | 0.93935000  |
| H  | -1.64022000 | 4.61780700  | 0.10503700  |
| H  | -1.41855200 | 4.55561500  | 1.88837300  |
| H  | -0.04727500 | 4.22799300  | 0.79521900  |
| C  | -0.67429600 | 1.87265700  | 1.95109300  |
| H  | -0.83443500 | 2.26789100  | 2.96368500  |
| H  | -0.92389600 | 0.78443400  | 1.95185500  |
| H  | 0.41537900  | 1.93053200  | 1.72355700  |
| H  | -3.60908200 | 2.88026800  | 0.47769400  |
| O  | -1.81421700 | 3.90726500  | -1.87375800 |
| H  | 3.13171100  | 1.93855200  | -0.09517700 |
| Cl | 2.30019900  | 3.08578500  | 0.04167100  |
| H  | -0.95394600 | 4.01873600  | -2.33417500 |
| Zn | -2.51126400 | -1.83005300 | -0.10219600 |
| Cl | -2.44167000 | -3.97332600 | 0.05504900  |
| Cl | -3.80019900 | -0.17274600 | -0.69069900 |
| H  | 4.91653600  | -2.41318500 | -0.78916500 |

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 3.60216700 | -0.56758400 | -0.53415400 |
| H | 3.06410300 | -0.56678600 | -1.52140300 |
| H | 3.19674200 | -1.09767600 | 1.55499600  |
| H | 1.34415300 | 0.69804100  | 0.85774200  |
| H | 0.22350900 | -3.35325800 | 0.03117700  |

### Transition state c)TS2

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.316591           |
| Thermal correction to Energy=                | 0.344927           |
| Thermal correction to Enthalpy=              | 0.345872           |
| Thermal correction to Gibbs Free Energy=     | 0.253404           |
| Sum of electronic and zero-point Energies=   | 0.042206           |
| Sum of electronic and thermal Energies=      | 0.070543           |
| Sum of electronic and thermal Enthalpies=    | 0.071487           |
| Sum of electronic and thermal Free Energies= | -0.020980          |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 216.445     | 99.341         | 194.615        |

|          |                 |             |             |
|----------|-----------------|-------------|-------------|
| Charge:0 | Multiplicity: 1 |             |             |
| C        | -0.10326100     | -1.27471200 | -0.53695700 |
| C        | -1.24829300     | -0.47081100 | -0.69853600 |
| C        | -2.46380700     | -1.36038500 | -0.95604200 |
| C        | -1.89075300     | -2.78549500 | -0.83982300 |
| N        | -0.47274700     | -2.64480000 | -0.59217200 |
| O        | -2.42246400     | -3.85798400 | -0.92430300 |
| O        | 1.06745000      | -0.85643000 | -0.32365200 |
| N        | -4.12794400     | 0.23397900  | 0.16153000  |
| C        | -5.10946100     | 0.12160000  | 1.07249400  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -5.04057500 | -1.17117100 | 1.71575100  |
| H  | -5.83180100 | 0.90150200  | 1.27834500  |
| C  | -3.95416000 | -1.83699300 | 1.18951300  |
| H  | -5.73290900 | -1.52036200 | 2.45738600  |
| C  | 2.51938900  | 3.07340100  | -1.03446500 |
| C  | 0.67898600  | 2.18641900  | 0.41348600  |
| H  | 3.04555200  | 2.09801500  | -0.95958400 |
| H  | 2.78474800  | 3.52247000  | -2.00497300 |
| C  | 1.30177500  | 2.79838400  | 1.66984700  |
| H  | -0.43892600 | 2.15547600  | 0.51108100  |
| H  | 1.01063200  | 1.10780700  | 0.33596900  |
| H  | 1.08911700  | 2.15297000  | 2.54593300  |
| H  | 2.40122400  | 2.93003100  | 1.59666500  |
| N  | 1.02425300  | 2.90102400  | -0.88984600 |
| C  | 0.35592000  | 4.25497900  | -0.93805300 |
| H  | 0.63517100  | 4.86404100  | -0.04960000 |
| H  | 0.61964300  | 4.81432300  | -1.84686000 |
| H  | -0.75347900 | 4.15717400  | -0.91617300 |
| C  | 0.52362200  | 2.05472700  | -2.04081100 |
| H  | 0.68620700  | 2.54253200  | -3.01343400 |
| H  | 1.02055100  | 1.06329600  | -2.05453600 |
| H  | -0.57551700 | 1.86246500  | -1.94571000 |
| H  | 2.92961000  | 3.72423200  | -0.23959800 |
| O  | 0.82176600  | 4.12360600  | 1.90677100  |
| H  | -3.71380300 | 1.24559300  | -0.34252300 |
| Cl | -2.79676200 | 2.55690700  | -0.61594000 |
| H  | -0.11523600 | 4.10790000  | 2.20772800  |
| Zn | 2.76943400  | -1.56722900 | 0.25248700  |
| Cl | 2.88131300  | -3.68938800 | 0.01202700  |
| Cl | 3.63575300  | 0.31091200  | 0.88072000  |
| H  | -3.61414700 | -2.83212100 | 1.42107800  |
| C  | -3.30053900 | -0.95135400 | 0.24179400  |
| H  | -2.04302000 | -0.34808200 | 0.62909900  |
| H  | -2.97109100 | -1.21410300 | -1.93046900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.24214400 | 0.54499700  | -1.05086300 |
| H | 0.16940600  | -3.43313100 | -0.48557600 |

### *Succinimide + ChCl + ZnCl<sub>2</sub> : c)P*

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.323057           |
| Thermal correction to Energy=                | 0.352081           |
| Thermal correction to Enthalpy=              | 0.353025           |
| Thermal correction to Gibbs Free Energy=     | 0.256845           |
| Sum of electronic and zero-point Energies=   | -0.033326          |
| Sum of electronic and thermal Energies=      | -0.004303          |
| Sum of electronic and thermal Enthalpies=    | -0.003359          |
| Sum of electronic and thermal Free Energies= | -0.099538          |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 220.934     | 100.048        | 202.427        |

|          |                 |             |             |
|----------|-----------------|-------------|-------------|
| Charge:0 | Multiplicity: 1 |             |             |
| C        | 0.82899000      | 1.22010500  | -0.43143200 |
| C        | 1.52321600      | -0.07072700 | -0.75403500 |
| C        | 3.01809500      | 0.27644100  | -0.93594900 |
| C        | 3.12877500      | 1.76357100  | -0.57402600 |
| N        | 1.76337900      | 2.24154800  | -0.32746600 |
| O        | 4.05336800      | 2.51570000  | -0.51202900 |
| O        | -0.39984800     | 1.31573100  | -0.27858800 |
| N        | 3.75189800      | -1.95761800 | 0.00011500  |
| C        | 4.77810600      | -2.46393600 | 0.79357400  |
| C        | 5.60838700      | -1.40171400 | 1.16904200  |
| H        | 4.85619100      | -3.50900500 | 1.03351100  |
| C        | 5.07847400      | -0.21500000 | 0.59844700  |
| H        | 6.48845200      | -1.46724500 | 1.77573700  |
| C        | -4.32783000     | -1.97536600 | -0.27327100 |
| C        | -2.03895400     | -1.91986600 | 0.69055200  |
| H        | -4.50250100     | -0.92527100 | 0.03063200  |
| H        | -4.95140100     | -2.16691700 | -1.16249400 |
| C        | -2.15606300     | -2.93579700 | 1.83124400  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -0.94787000 | -1.86667100 | 0.38360000  |
| H  | -2.29824400 | -0.89636400 | 1.05184300  |
| H  | -1.60687600 | -2.55269100 | 2.71708200  |
| H  | -3.20029100 | -3.15729900 | 2.12177200  |
| N  | -2.86336700 | -2.23478900 | -0.55280000 |
| C  | -2.69551300 | -3.66449100 | -1.00669800 |
| H  | -2.93762000 | -4.38675000 | -0.19913300 |
| H  | -3.30264300 | -3.88955000 | -1.89240100 |
| H  | -1.62482600 | -3.88019200 | -1.25906300 |
| C  | -2.39237400 | -1.31946200 | -1.66513800 |
| H  | -3.00185500 | -1.43032800 | -2.57379500 |
| H  | -2.41549300 | -0.25542200 | -1.35716700 |
| H  | -1.33682600 | -1.56088200 | -1.93408100 |
| H  | -4.69822100 | -2.62346200 | 0.54036500  |
| O  | -1.63418500 | -4.21089800 | 1.47764800  |
| H  | 2.98466200  | -2.49672300 | -0.39845000 |
| Cl | 0.61487800  | -3.03616800 | -0.75138000 |
| H  | -0.70317700 | -4.13048500 | 1.11109800  |
| Zn | -1.68596300 | 2.73833300  | 0.24665700  |
| Cl | -0.66331500 | 4.61291800  | 0.33665700  |
| Cl | -3.44760900 | 1.52037400  | 0.43205400  |
| H  | 5.49122700  | 0.77082800  | 0.69111800  |
| C  | 3.92699500  | -0.57116100 | -0.11638700 |
| H  | 1.36228100  | -0.81051600 | 0.07616900  |
| H  | 3.30955900  | 0.16706700  | -2.01862100 |
| H  | 1.09449200  | -0.59529000 | -1.63722800 |
| H  | 1.55277600  | 3.21822300  | -0.08557300 |

### *Transition state d)TS1*

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                     | 0.435827           |
| Thermal correction to Energy=              | 0.486188           |
| Thermal correction to Enthalpy=            | 0.487133           |
| Thermal correction to Gibbs Free Energy=   | 0.346987           |
| Sum of electronic and zero-point Energies= | -0.669342          |
| Sum of electronic and thermal Energies=    | -0.618981          |

Sum of electronic and thermal Enthalpies= -0.618037

Sum of electronic and thermal Free Energies= -0.758182

|          | E (Thermal)     | CV             | S              |
|----------|-----------------|----------------|----------------|
|          | KCal/Mol        | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total    | 305.088         | 172.410        | 294.961        |
| Charge:0 | Multiplicity: 1 |                |                |
| C        | 2.89007800      | -1.23485300    | 0.26211300     |
| C        | 3.49027500      | -0.46221500    | -0.79237200    |
| C        | 4.69823600      | 0.07224500     | -0.36516900    |
| C        | 4.99586400      | -0.53049900    | 1.02371400     |
| N        | 3.83482500      | -1.31771300    | 1.33649400     |
| O        | 5.95469000      | -0.42528200    | 1.73760300     |
| O        | 1.80470900      | -1.84757200    | 0.36826100     |
| N        | 3.93260200      | 2.61199100     | -0.90185400    |
| C        | 4.96334400      | 3.38016800     | -1.34593900    |
| C        | 6.04290500      | 3.28974600     | -0.41305900    |
| H        | 4.93129700      | 3.95961000     | -2.25766800    |
| C        | 5.64232900      | 2.43928900     | 0.61105500     |
| H        | 6.97916100      | 3.80605700     | -0.50231200    |
| C        | -3.66534500     | 1.48218900     | 0.70585900     |
| C        | -3.24214900     | 2.67902900     | 1.56057500     |
| H        | -4.04334600     | 0.65598700     | 1.35777200     |
| H        | -2.75233000     | 1.07623200     | 0.19038000     |
| H        | -2.27331500     | 2.46142900     | 2.05587100     |
| H        | -3.13697800     | 3.62496600     | 0.99187100     |
| N        | -4.70782600     | 1.80565100     | -0.36372200    |
| C        | -5.85708700     | 2.59140000     | 0.22696200     |
| H        | -5.51311300     | 3.55950300     | 0.64712500     |
| H        | -6.64034900     | 2.79445000     | -0.51788500    |
| H        | -6.30728700     | 2.05038900     | 1.08054800     |
| C        | -5.24988500     | 0.51093000     | -0.93044900    |
| H        | -5.98896200     | 0.68629100     | -1.72552700    |
| H        | -4.43818500     | -0.11906100    | -1.35948100    |
| H        | -5.72020000     | -0.11481400    | -0.14646600    |
| O        | -4.25702400     | 2.97604700     | 2.52856800     |
| H        | 3.00594300      | 2.46371700     | -1.38114000    |
| Cl       | -0.98960100     | 2.96603200     | -0.52274600    |
| H        | -4.18368200     | 2.38312000     | 3.30444000     |



|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 6.21034800  | 2.14461800  | 1.47875100  |
| C  | 4.32719700  | 1.93688700  | 0.29354800  |
| H  | 3.56200900  | 1.66982900  | 1.03049600  |
| H  | 5.52233600  | 0.37064800  | -1.00820600 |
| H  | 3.01398300  | -0.31660200 | -1.74884200 |
| Zn | -0.03441500 | -1.18980200 | -0.49551600 |
| Zn | -1.77067100 | -1.74083500 | 0.09850500  |
| Cl | -0.36059200 | -3.68530000 | 0.05757900  |
| Cl | -0.89730400 | -0.23965000 | 1.83788200  |
| Cl | -1.90401800 | -0.54557600 | -2.07581700 |
| Cl | -3.93775100 | -2.04495700 | 0.62077300  |
| O  | 0.81030200  | -1.69454700 | -2.38316600 |
| H  | 0.29391300  | -1.57432900 | -3.18521300 |
| O  | 0.58346300  | 0.74345200  | -0.50230300 |
| H  | 1.19414500  | 1.00049300  | 0.24373200  |
| O  | 1.47785300  | -1.43418900 | 3.03768200  |
| H  | 0.72059100  | -1.41204900 | 3.62772800  |
| O  | 1.91789400  | -3.95771300 | -1.82722500 |
| H  | 2.09595500  | -3.65393600 | -0.91482300 |
| O  | 1.74603100  | 1.11866800  | 1.91113600  |
| H  | 1.67681900  | 0.22331700  | 2.34268300  |
| O  | 1.64182600  | 2.19003900  | -2.32482500 |
| H  | 1.25310200  | 1.34221900  | -1.95080500 |
| H  | 0.96047400  | 2.85824200  | -2.18616900 |
| H  | 1.29406200  | -2.58991300 | -2.45756300 |
| H  | 1.20362500  | -1.98436200 | 2.27598800  |
| H  | 1.22011100  | -4.62096400 | -1.75069000 |
| H  | 1.02761700  | 1.63846800  | 2.27518600  |
| H  | -0.24311900 | 1.63425000  | -0.46053300 |
| C  | -4.06178800 | 2.59828100  | -1.47719900 |
| H  | -3.20535100 | 2.03691500  | -1.91944900 |
| H  | -4.77018600 | 2.83637200  | -2.28240800 |
| H  | -3.61954300 | 3.54321700  | -1.10222700 |
| H  | 3.64157100  | -1.74084100 | 2.24466500  |

### Intermediate d)Int1

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.438226           |
| Thermal correction to Energy=                | 0.487714           |
| Thermal correction to Enthalpy=              | 0.488659           |
| Thermal correction to Gibbs Free Energy=     | 0.352835           |
| Sum of electronic and zero-point Energies=   | -0.692394          |
| Sum of electronic and thermal Energies=      | -0.642906          |
| Sum of electronic and thermal Enthalpies=    | -0.641962          |
| Sum of electronic and thermal Free Energies= | -0.777785          |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 306.045     | 171.607        | 285.864        |

|          |                 |             |             |
|----------|-----------------|-------------|-------------|
| Charge:0 | Multiplicity: 1 |             |             |
| C        | 3.02277600      | -1.11158100 | 0.60110400  |
| C        | 3.79151600      | -0.40956700 | -0.28588300 |
| C        | 4.74720600      | 0.47935300  | 0.45303200  |
| C        | 4.55937300      | 0.04576600  | 1.93780400  |
| N        | 3.51303600      | -0.89646500 | 1.95191500  |
| O        | 5.16506000      | 0.44619500  | 2.90328400  |
| O        | 2.00012700      | -1.89374800 | 0.45992200  |
| N        | 3.01400100      | 2.13383000  | -0.33523100 |
| C        | 3.10565000      | 2.93022900  | -1.38291100 |
| C        | 4.50481900      | 3.37620600  | -1.55181200 |
| H        | 2.25728500      | 3.19345400  | -2.04643500 |
| C        | 5.25397400      | 2.80133000  | -0.58514800 |
| H        | 4.81209900      | 4.03631800  | -2.34735000 |
| C        | -4.52605100     | 0.78456500  | 1.01161600  |
| C        | -3.98161700     | 1.34965600  | 2.32704300  |
| H        | -5.58994900     | 0.48225100  | 1.13186000  |
| H        | -3.97288300     | -0.16956700 | 0.77675800  |
| H        | -3.84279900     | 0.53346100  | 3.06351000  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -3.01232900 | 1.87968500  | 2.21351600  |
| N  | -4.40881600 | 1.73627800  | -0.17782200 |
| C  | -5.37951500 | 2.88429500  | -0.00525100 |
| H  | -5.25527700 | 3.35060700  | 1.00108000  |
| H  | -5.21595700 | 3.67072300  | -0.76052300 |
| H  | -6.42606000 | 2.54898600  | -0.07835800 |
| C  | -4.75355100 | 0.97462600  | -1.44054800 |
| H  | -4.81308600 | 1.64113600  | -2.31574500 |
| H  | -3.97475900 | 0.20789800  | -1.67571000 |
| H  | -5.70517300 | 0.42541800  | -1.34981400 |
| O  | -4.86212000 | 2.35655700  | 2.83838500  |
| H  | 2.12907800  | 1.52249000  | -0.02784800 |
| Cl | -0.18194700 | 3.21522000  | -0.68088800 |
| H  | -5.58630000 | 1.95769300  | 3.36295100  |
| H  | 6.31333100  | 2.88696400  | -0.40247000 |
| C  | 4.36087900  | 1.96914600  | 0.32294800  |
| H  | 4.31783800  | 2.45097900  | 1.34529800  |
| H  | 5.80371000  | 0.31499400  | 0.14600300  |
| H  | 3.73716300  | -0.43907300 | -1.35148000 |
| Zn | 0.29124000  | -1.07016000 | -0.39423200 |
| Zn | -1.52983700 | -1.71140000 | -0.40559900 |
| Cl | -0.10247200 | -3.61742600 | -0.25093200 |
| Cl | -1.43185500 | -0.46943200 | 1.69149000  |
| Cl | -1.21519100 | -0.10991500 | -2.25019700 |
| Cl | -3.71011900 | -2.25602700 | -0.64506400 |
| O  | 1.38944300  | -1.25030500 | -2.27165800 |
| H  | 0.89909700  | -1.55959100 | -3.04945400 |
| O  | 0.77424200  | 0.83697400  | 0.22246700  |
| H  | 0.72138700  | 0.97639400  | 1.23151200  |
| O  | 0.90319000  | -2.02440800 | 2.97123500  |
| H  | -0.02049500 | -2.27751300 | 3.03006400  |
| O  | 2.59297300  | -3.41879200 | -1.68669200 |
| H  | 2.59143000  | -3.24532500 | -0.70609500 |
| O  | 0.95483800  | 0.73006000  | 2.84928200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.01753400  | -0.26996100 | 2.89824200  |
| O | 1.24968900  | 1.74884000  | -3.00117800 |
| H | 1.32831200  | 0.81472600  | -2.76591500 |
| H | 0.32490500  | 1.98410100  | -2.89107300 |
| H | 2.16372200  | -1.94505300 | -2.15749100 |
| H | 1.23127300  | -2.39959900 | 2.11758800  |
| H | 1.88305400  | -4.05226700 | -1.83335700 |
| H | 0.15211900  | 0.95298700  | 3.31775200  |
| H | 0.17375100  | 1.83818000  | -0.23745900 |
| C | -3.00642700 | 2.28354800  | -0.30816500 |
| H | -2.24741200 | 1.47514300  | -0.23844700 |
| H | -2.84030900 | 2.78192300  | -1.28122300 |
| H | -2.76259200 | 3.02134300  | 0.47854600  |
| H | 3.11187800  | -1.31613700 | 2.78618000  |

### Transition state d)TS2

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.440218           |
| Thermal correction to Energy=                | 0.490536           |
| Thermal correction to Enthalpy=              | 0.491480           |
| Thermal correction to Gibbs Free Energy=     | 0.352664           |
| Sum of electronic and zero-point Energies=   | -0.722043          |
| Sum of electronic and thermal Energies=      | -0.671725          |
| Sum of electronic and thermal Enthalpies=    | -0.670781          |
| Sum of electronic and thermal Free Energies= | -0.809597          |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 307.816     | 173.902        | 292.163        |

Charge:0 Multiplicity: 1

|   |            |             |            |
|---|------------|-------------|------------|
| C | 3.18766500 | -1.11089800 | 0.17045700 |
|---|------------|-------------|------------|

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 3.55134900  | -0.23683200 | -0.81680500 |
| C  | 4.62776800  | 0.69574500  | -0.32007300 |
| C  | 4.97553300  | 0.12320000  | 1.07712300  |
| N  | 4.02926200  | -0.91478100 | 1.33203600  |
| O  | 5.83017100  | 0.43691400  | 1.86671300  |
| O  | 2.25020900  | -1.99722300 | 0.26406600  |
| N  | 3.28014500  | 2.67822600  | -1.14225600 |
| C  | 2.94958800  | 3.97047300  | -0.71812000 |
| C  | 3.59653100  | 4.20403100  | 0.49472000  |
| H  | 2.28885700  | 4.60418400  | -1.28186400 |
| C  | 4.33474800  | 3.03272800  | 0.82969700  |
| H  | 3.55437700  | 5.10163000  | 1.07722900  |
| C  | -4.38079100 | 1.09443600  | 1.06357900  |
| C  | -3.71612600 | 1.95198800  | 2.14557100  |
| H  | -5.43392100 | 0.87006100  | 1.34546400  |
| H  | -3.86700400 | 0.09304900  | 1.02626700  |
| H  | -3.52020900 | 1.34344000  | 3.05028600  |
| H  | -2.75374500 | 2.40709900  | 1.82683900  |
| N  | -4.36255200 | 1.71892300  | -0.33097100 |
| C  | -5.32884800 | 2.88318700  | -0.37148200 |
| H  | -5.13286300 | 3.58016600  | 0.47847100  |
| H  | -5.23351500 | 3.45979000  | -1.30599300 |
| H  | -6.37435800 | 2.54846200  | -0.27907900 |
| C  | -4.79358800 | 0.67285100  | -1.33786000 |
| H  | -5.01620200 | 1.11684400  | -2.32061100 |
| H  | -3.98978300 | -0.08579000 | -1.50301800 |
| H  | -5.67623100 | 0.10378100  | -0.99882000 |
| O  | -4.54430800 | 3.07975400  | 2.45164800  |
| H  | 2.94467700  | 2.22986500  | -1.98337000 |
| Cl | -0.22757100 | 3.01276400  | -1.65138700 |
| H  | -5.19542600 | 2.86013500  | 3.14887000  |
| H  | 4.96133200  | 2.90470300  | 1.69176800  |
| C  | 4.12707800  | 2.09610800  | -0.18648100 |
| H  | 2.27516900  | 1.62535500  | 1.94316900  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 5.53956200  | 0.66426600  | -0.96659600 |
| H  | 3.20954200  | -0.22463800 | -1.82943500 |
| Zn | 0.27106600  | -1.37697800 | -0.05123100 |
| Zn | -1.60564400 | -1.81266900 | 0.02952300  |
| Cl | -0.24899100 | -3.74951900 | 0.59625300  |
| Cl | -1.30479300 | -0.03059900 | 1.68877200  |
| Cl | -1.25100300 | -0.60165600 | -2.07791400 |
| Cl | -3.81235100 | -2.27817600 | 0.02900000  |
| O  | 1.18862200  | -1.95415800 | -2.02906700 |
| H  | 0.64431700  | -2.41718600 | -2.68065000 |
| O  | 0.72510200  | 0.72796600  | -0.28727100 |
| H  | 1.69891600  | 0.86779900  | -0.48922200 |
| O  | 0.96089500  | -1.57188500 | 2.25412800  |
| H  | 0.29578300  | -1.93071900 | 2.86225700  |
| O  | 2.37997100  | -4.06507900 | -1.24432900 |
| H  | 2.63550200  | -3.67553200 | -0.36954900 |
| O  | 1.34357400  | 1.38507300  | 2.03628000  |
| H  | 1.31880200  | 0.47069700  | 2.38440300  |
| O  | 1.27733800  | 0.88102600  | -2.70381500 |
| H  | 1.39465200  | -0.08129600 | -2.49315300 |
| H  | 0.67616500  | 0.90779300  | -3.45494100 |
| H  | 1.98521800  | -2.59959200 | -1.84118400 |
| H  | 1.66578900  | -2.25497100 | 2.17741900  |
| H  | 1.57264100  | -4.56240600 | -1.07238000 |
| H  | 0.60756200  | 1.28543200  | 0.59541400  |
| H  | 0.26993300  | 1.74616200  | -1.59842700 |
| C  | -2.98122700 | 2.20590100  | -0.70324600 |
| H  | -2.20955900 | 1.42530800  | -0.51785900 |
| H  | -2.91380300 | 2.46833300  | -1.77435700 |
| H  | -2.67681800 | 3.09614400  | -0.12244600 |
| H  | 4.03340300  | -1.51002000 | 2.14505400  |

### Transition state d)TS3

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.439039           |
| Thermal correction to Energy=                | 0.487393           |
| Thermal correction to Enthalpy=              | 0.488337           |
| Thermal correction to Gibbs Free Energy=     | 0.356491           |
| Sum of electronic and zero-point Energies=   | -0.683625          |
| Sum of electronic and thermal Energies=      | -0.635271          |
| Sum of electronic and thermal Enthalpies=    | -0.634327          |
| Sum of electronic and thermal Free Energies= | -0.766174          |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 305.844     | 169.532        | 277.494        |

|          |                 |             |             |
|----------|-----------------|-------------|-------------|
| Charge:0 | Multiplicity: 1 |             |             |
| C        | -3.17732600     | -1.21139300 | -0.18760600 |
| C        | -3.58580700     | -0.30834200 | 0.75924400  |
| C        | -4.46045300     | 0.74247900  | 0.13901300  |
| C        | -4.74213800     | 0.17487900  | -1.28035500 |
| N        | -3.90350500     | -0.95459800 | -1.42851700 |
| O        | -5.47997100     | 0.60115200  | -2.13676400 |
| O        | -2.30608900     | -2.15491500 | -0.20304200 |
| N        | -3.02633200     | 2.58276000  | 1.16125400  |
| C        | -3.03881600     | 3.92362000  | 1.12121700  |
| C        | -3.83692000     | 4.35450500  | -0.00764800 |
| H        | -2.50954600     | 4.56198300  | 1.82645300  |
| C        | -4.27434300     | 3.23465400  | -0.67268400 |
| H        | -4.03182300     | 5.38480700  | -0.24698300 |
| C        | 4.32331500      | 1.26579900  | -0.98965400 |
| C        | 3.65296900      | 2.11734300  | -2.07229700 |
| H        | 5.38782300      | 1.07601500  | -1.25008700 |
| H        | 3.83464000      | 0.25033900  | -0.97984900 |
| H        | 3.46981700      | 1.50914100  | -2.97976500 |
| H        | 2.68303100      | 2.55705700  | -1.75278400 |
| N        | 4.25095600      | 1.86707200  | 0.41341100  |
| C        | 5.14470800      | 3.08596400  | 0.48680500  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 4.91899900  | 3.78413200  | -0.35396900 |
| H  | 4.99935700  | 3.63938800  | 1.42888100  |
| H  | 6.20946100  | 2.81687700  | 0.40502500  |
| C  | 4.72961300  | 0.83222900  | 1.40974300  |
| H  | 4.82261700  | 1.25421900  | 2.42281500  |
| H  | 4.00940100  | -0.01982600 | 1.48447300  |
| H  | 5.69642100  | 0.38921700  | 1.11953500  |
| O  | 4.46198200  | 3.26013700  | -2.37404200 |
| H  | -2.52402400 | 1.97813400  | 1.83638700  |
| Cl | -0.03715600 | 2.88711500  | 1.24492300  |
| H  | 5.14833000  | 3.04016700  | -3.03603900 |
| H  | -4.90051000 | 3.17107700  | -1.55276500 |
| C  | -3.69277500 | 2.04511300  | -0.02695100 |
| H  | -2.66528400 | 1.73347700  | -0.85236000 |
| H  | -5.41311400 | 0.89685700  | 0.69146400  |
| H  | -3.36548300 | -0.33232900 | 1.80441000  |
| Zn | -0.24888900 | -1.49141800 | 0.07463700  |
| Zn | 1.65914300  | -1.79060200 | -0.07712600 |
| Cl | 0.41868300  | -3.78345700 | -0.70378100 |
| Cl | 1.23174400  | 0.06715400  | -1.63765100 |
| Cl | 1.32730500  | -0.74726700 | 2.10848100  |
| Cl | 3.88960800  | -2.15198400 | -0.17651900 |
| O  | -1.11072800 | -2.12578300 | 2.03822500  |
| H  | -0.54633200 | -2.63047600 | 2.64204100  |
| O  | -0.80733000 | 0.49330600  | 0.30871300  |
| H  | -1.57518000 | 0.54413700  | 0.95469300  |
| O  | -0.98640700 | -1.61998100 | -2.16268400 |
| H  | -0.30979600 | -1.80093600 | -2.83541000 |
| O  | -2.41999600 | -4.18301500 | 1.26199000  |
| H  | -2.92475600 | -3.74145000 | 0.53666500  |
| O  | -1.61607500 | 1.51416700  | -1.72233300 |
| H  | -1.55827000 | 0.51688200  | -1.80459700 |
| O  | -1.39830800 | 0.70813000  | 2.79451400  |
| H  | -1.31414800 | -0.26921100 | 2.81040000  |
| H  | -0.51680000 | 1.05745000  | 2.98532900  |
| H  | -1.92923000 | -2.74232100 | 1.86277900  |
| H  | -1.58927600 | -2.39495200 | -2.15606200 |
| H  | -1.62824700 | -4.52972000 | 0.82537800  |
| H  | -0.82850200 | 1.71438700  | -1.12480800 |
| H  | -0.15831500 | 1.35447200  | 0.72682000  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.83561600  | 2.26122700  | 0.76405200  |
| H | 2.13316900  | 1.41203900  | 0.61517800  |
| H | 2.72971000  | 2.57180200  | 1.81804700  |
| H | 2.46393000  | 3.09729400  | 0.14045700  |
| H | -3.84910100 | -1.52674000 | -2.25669900 |

*Succinimide + ChCl + 2 ZnCl<sub>2</sub> • 3H<sub>2</sub>O d)P*

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.440893           |
| Thermal correction to Energy=                | 0.490659           |
| Thermal correction to Enthalpy=              | 0.491603           |
| Thermal correction to Gibbs Free Energy=     | 0.353616           |
| Sum of electronic and zero-point Energies=   | -0.743254          |
| Sum of electronic and thermal Energies=      | -0.693488          |
| Sum of electronic and thermal Enthalpies=    | -0.692544          |
| Sum of electronic and thermal Free Energies= | -0.830531          |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 307.893     | 171.366        | 290.418        |

|          |                 |             |             |
|----------|-----------------|-------------|-------------|
| Charge:0 | Multiplicity: 1 |             |             |
| C        | 4.00342500      | -1.53481800 | 0.69753400  |
| C        | 4.36485000      | -0.76757800 | -0.54760700 |
| C        | 5.20274000      | 0.44448100  | -0.08611900 |
| C        | 5.36764800      | 0.26861800  | 1.43531100  |
| N        | 4.60484800      | -0.90576300 | 1.80499700  |
| O        | 5.99793000      | 0.88861800  | 2.24171000  |
| O        | 3.30977900      | -2.53672700 | 0.79708600  |
| N        | 3.26011500      | 2.09985300  | -0.12991800 |
| C        | 3.05656100      | 3.42484200  | -0.51569000 |
| C        | 4.25739500      | 3.92248700  | -1.02993100 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 2.11009500  | 3.92749000  | -0.39103300 |
| C  | 5.22399300  | 2.88487600  | -0.95512900 |
| H  | 4.42414500  | 4.91049500  | -1.40863800 |
| C  | -4.80662500 | 0.71799400  | 0.88296000  |
| C  | -4.33652800 | 1.36253900  | 2.19119300  |
| H  | -5.87107600 | 0.40506500  | 0.96895100  |
| H  | -4.22992800 | -0.23716400 | 0.72632100  |
| H  | -4.22923200 | 0.59020500  | 2.97831500  |
| H  | -3.36720300 | 1.89681700  | 2.09854200  |
| N  | -4.64674500 | 1.60805600  | -0.34897500 |
| C  | -5.64573800 | 2.74309800  | -0.28879600 |
| H  | -5.57717400 | 3.26982200  | 0.69283700  |
| H  | -5.46019700 | 3.48761400  | -1.08112600 |
| H  | -6.68169900 | 2.38359300  | -0.39067200 |
| C  | -4.91797500 | 0.76944300  | -1.58065700 |
| H  | -4.88666200 | 1.37554100  | -2.50117500 |
| H  | -4.14982000 | -0.03223700 | -1.70323500 |
| H  | -5.89374100 | 0.25936600  | -1.53036700 |
| O  | -5.25173800 | 2.38483700  | 2.59840600  |
| H  | 2.54523700  | 1.47941000  | 0.25708100  |
| Cl | -0.39395000 | 3.05003000  | -0.72868600 |
| H  | -5.99818600 | 2.00739600  | 3.10776500  |
| H  | 6.24656100  | 2.95593000  | -1.26409700 |
| C  | 4.59676400  | 1.76347100  | -0.39624900 |
| H  | 6.22509000  | 0.40378000  | -0.54972200 |
| H  | 3.43088900  | -0.46358800 | -1.09429000 |
| Zn | 0.00093200  | -0.87359100 | -0.07266700 |
| Zn | -1.69070800 | -1.76115700 | -0.31615000 |
| Cl | 0.03683100  | -3.44150500 | -0.33520600 |
| Cl | -1.73738100 | -0.50017500 | 1.83927000  |
| Cl | -1.38397700 | -0.22028300 | -2.15833500 |
| Cl | -3.81323600 | -2.47866700 | -0.49286000 |
| O  | 1.49366200  | -0.79421500 | -1.53128000 |
| H  | 1.37120700  | -0.00168300 | -2.19308200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 0.69375100  | 0.88701700  | 0.55063600  |
| H | 0.63328300  | 1.10034100  | 1.52040800  |
| O | 0.84998100  | -1.82423800 | 1.85144100  |
| H | 0.26381400  | -2.50798100 | 2.23553200  |
| O | 2.47760200  | -3.07373200 | -1.94927900 |
| H | 2.64647800  | -3.11981900 | -0.98306000 |
| O | 0.67004700  | 0.67245100  | 3.21310900  |
| H | 0.77081500  | -0.27912600 | 3.01791900  |
| O | 1.15922500  | 1.45828100  | -2.82862100 |
| H | 1.61248400  | 2.11254700  | -2.27273500 |
| H | 0.21832400  | 1.69737700  | -2.78730500 |
| H | 1.64952500  | -1.61488300 | -2.10279500 |
| H | 1.70725900  | -2.30556100 | 1.67490400  |
| H | 1.89112200  | -3.80712500 | -2.15408800 |
| H | -0.21702000 | 0.78188300  | 3.55666300  |
| H | 0.19765600  | 1.87802400  | 0.00967000  |
| C | -3.25011000 | 2.17806400  | -0.43963800 |
| H | -2.47928600 | 1.41259200  | -0.21338300 |
| H | -3.01469200 | 2.55660500  | -1.45228000 |
| H | -3.08180200 | 3.01465300  | 0.26343400  |
| H | 4.90245800  | -1.40293300 | -1.27848800 |
| H | 4.51584400  | -1.23024700 | 2.76514300  |

## Structures for the proposed reactions between Pirrol et N-Phenyl Maleimide

### Transition state a) TS1

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.217556           |
| Thermal correction to Energy=                | 0.232344           |
| Thermal correction to Enthalpy=              | 0.233288           |
| Thermal correction to Gibbs Free Energy=     | 0.173763           |
| Sum of electronic and zero-point Energies=   | 0.257961           |
| Sum of electronic and thermal Energies=      | 0.272749           |
| Sum of electronic and thermal Enthalpies=    | 0.273693           |
| Sum of electronic and thermal Free Energies= | 0.214167           |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 145.798     | 57.304         | 125.283        |

|          |                 |             |             |
|----------|-----------------|-------------|-------------|
| Charge:0 | Multiplicity: 1 |             |             |
| C        | 0.29921700      | -1.13295900 | -1.01817900 |
| C        | 1.57427200      | -0.59156300 | -1.37426500 |
| C        | 1.68524500      | 0.77429400  | -1.04383100 |
| C        | 0.27588100      | 1.21538400  | -0.58339100 |
| N        | -0.51227900     | 0.03800000  | -0.51137900 |
| O        | -0.04649700     | 2.34193000  | -0.28083100 |
| O        | -0.16743100     | -2.24462300 | -1.02507300 |
| C        | -1.89831500     | 0.00189500  | -0.12862700 |
| C        | -2.51715800     | -1.23519300 | 0.13623900  |
| C        | -2.63360300     | 1.19585100  | 0.00015700  |
| C        | -3.85612300     | -1.26584100 | 0.52597100  |
| H        | -1.96505500     | -2.17232500 | 0.01765200  |
| C        | -3.97125800     | 1.14328000  | 0.39467100  |
| H        | -2.16929400     | 2.16390100  | -0.20536300 |
| C        | -4.58865300     | -0.08208700 | 0.66107800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.33303300 | -2.22533100 | 0.72394700  |
| H | -4.53628900 | 2.06974400  | 0.49217300  |
| H | -5.63106200 | -0.11543100 | 0.96610100  |
| N | 2.13525600  | 0.02716200  | 1.41545500  |
| C | 2.96110100  | -1.05086700 | 1.39873000  |
| C | 4.14016700  | -0.72202000 | 0.64620800  |
| H | 2.75877800  | -1.98326300 | 1.91502200  |
| C | 3.97214700  | 0.54470100  | 0.12403100  |
| H | 4.98754500  | -1.37537300 | 0.52929200  |
| H | 1.20357700  | 0.06395900  | 1.81155000  |
| H | 4.66373000  | 1.10307000  | -0.48403700 |
| C | 2.62496400  | 1.01644000  | 0.46274100  |
| H | 2.43273700  | 2.07135800  | 0.70728700  |
| H | 2.21595000  | 1.47988700  | -1.69370100 |
| H | 2.31570400  | -1.18268100 | -1.87042600 |

### Intermediate a) Int1

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.218996           |
| Thermal correction to Energy=                | 0.233905           |
| Thermal correction to Enthalpy=              | 0.234849           |
| Thermal correction to Gibbs Free Energy=     | 0.173900           |
| Sum of electronic and zero-point Energies=   | 0.258466           |
| Sum of electronic and thermal Energies=      | 0.273375           |
| Sum of electronic and thermal Enthalpies=    | 0.274320           |
| Sum of electronic and thermal Free Energies= | 0.213371           |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 146.777     | 57.825         | 128.278        |

| Charge:0 | Multiplicity: 1 |             |             |
|----------|-----------------|-------------|-------------|
| C        | -0.04458000     | 1.50070200  | 0.60820500  |
| C        | 1.28732100      | 1.19954400  | 0.91308600  |
| C        | 1.56621500      | -0.25034500 | 0.85165700  |
| C        | 0.18430500      | -0.88163100 | 0.52050300  |
| N        | -0.73659000     | 0.16172000  | 0.35072100  |
| O        | 0.01464700      | -2.07772400 | 0.37721900  |
| O        | -0.67491900     | 2.52668900  | 0.47315500  |
| C        | -2.12868900     | -0.02805700 | 0.04723600  |
| C        | -2.92191300     | 1.07681400  | -0.32161400 |
| C        | -2.70603800     | -1.31177900 | 0.10741300  |
| C        | -4.26997900     | 0.88930800  | -0.62292500 |
| H        | -2.48930000     | 2.08289300  | -0.35618200 |
| C        | -4.05697400     | -1.47868600 | -0.20047700 |
| H        | -2.10523500     | -2.18027700 | 0.38960100  |
| C        | -4.84537800     | -0.38483200 | -0.56725000 |
| H        | -4.87885100     | 1.74782400  | -0.90298600 |
| H        | -4.49652100     | -2.47375200 | -0.15161100 |
| H        | -5.89623000     | -0.52127200 | -0.80432000 |
| N        | 3.07706600      | 0.74424400  | -0.84533200 |
| C        | 4.40085400      | 0.72261400  | -0.83527900 |
| C        | 4.86635800      | -0.58967900 | -0.36767000 |
| H        | 5.05358200      | 1.54943000  | -1.12048500 |
| C        | 3.78129000      | -1.34075900 | -0.04711900 |
| H        | 5.91129900      | -0.84910400 | -0.29082000 |
| H        | 2.41662500      | 1.54986700  | -0.92729300 |
| H        | 3.73973200      | -2.35054900 | 0.34118200  |
| C        | 2.52276600      | -0.56304700 | -0.34570900 |
| H        | 1.94335000      | -1.06711000 | -1.17457100 |
| H        | 1.97404200      | -0.67526800 | 1.79131500  |
| H        | 1.91300800      | 1.89285200  | 1.42510500  |

### Transition state a)TS2

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.216333           |
| Thermal correction to Energy=                | 0.230890           |
| Thermal correction to Enthalpy=              | 0.231834           |
| Thermal correction to Gibbs Free Energy=     | 0.173064           |
| Sum of electronic and zero-point Energies=   | 0.279040           |
| Sum of electronic and thermal Energies=      | 0.293597           |
| Sum of electronic and thermal Enthalpies=    | 0.294541           |
| Sum of electronic and thermal Free Energies= | 0.235771           |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 144.886     | 57.046         | 123.693        |

|          |                 |             |             |
|----------|-----------------|-------------|-------------|
| Charge:0 | Multiplicity: 1 |             |             |
| C        | 0.19405800      | 1.85025600  | -0.15884900 |
| C        | -1.15933600     | 1.83505900  | -0.55024900 |
| C        | -1.59184100     | 0.46650700  | -0.99257100 |
| C        | -0.31702200     | -0.39933500 | -0.83959600 |
| N        | 0.70224200      | 0.42621400  | -0.33180400 |
| O        | -0.26418000     | -1.58758300 | -1.08402000 |
| O        | 0.93436100      | 2.69173900  | 0.29474500  |
| C        | 2.04616700      | -0.01956300 | -0.07622600 |
| C        | 2.89667000      | 0.75652200  | 0.73556500  |
| C        | 2.51426000      | -1.22915900 | -0.62517200 |
| C        | 4.19705300      | 0.32019900  | 0.98639600  |
| H        | 2.54955400      | 1.70757300  | 1.15267800  |
| C        | 3.81807400      | -1.65001100 | -0.35894500 |
| H        | 1.86440900      | -1.84467400 | -1.25181700 |
| C        | 4.66467700      | -0.88225200 | 0.44536700  |
| H        | 4.85284900      | 0.92629200  | 1.61009900  |
| H        | 4.17477900      | -2.58623600 | -0.78572700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 5.67886000  | -1.21462500 | 0.64703900  |
| N | -4.03066400 | 0.28492700  | -0.21891500 |
| C | -4.75789800 | -0.61225100 | 0.47951500  |
| C | -3.86722300 | -1.45441300 | 1.23202200  |
| H | -5.84263400 | -0.67529200 | 0.46307600  |
| C | -2.57343300 | -1.05397400 | 0.97159500  |
| H | -4.18790000 | -2.26877100 | 1.86153100  |
| H | -4.36814300 | 0.99959900  | -0.85042400 |
| H | -1.65134100 | -1.48619800 | 1.34390900  |
| C | -2.61118500 | 0.12748000  | 0.10208300  |
| H | -2.19454300 | 1.18841300  | 0.73488400  |
| H | -1.99222300 | 0.38566800  | -2.01938100 |
| H | -1.66428500 | 2.72663000  | -0.84223900 |

### *N-Phenyl succinimide a)P*

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.220618           |
| Thermal correction to Energy=                | 0.235546           |
| Thermal correction to Enthalpy=              | 0.236490           |
| Thermal correction to Gibbs Free Energy=     | 0.175941           |
| Sum of electronic and zero-point Energies=   | 0.170640           |
| Sum of electronic and thermal Energies=      | 0.185568           |
| Sum of electronic and thermal Enthalpies=    | 0.186512           |
| Sum of electronic and thermal Free Energies= | 0.125963           |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 147.807     | 57.723         | 127.436        |

|          |                 |            |             |
|----------|-----------------|------------|-------------|
| Charge:0 | Multiplicity: 1 |            |             |
| C        | -0.26273900     | 1.78418100 | -0.14107900 |
| C        | 1.17718400      | 1.96449500 | 0.29470800  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.61652600  | 0.64023400  | 0.94747600  |
| C | 0.35309300  | -0.24001300 | 0.97177200  |
| N | -0.69309200 | 0.47336400  | 0.27811800  |
| O | 0.22181000  | -1.32369400 | 1.47032200  |
| O | -0.94930300 | 2.57441900  | -0.73377700 |
| C | -2.02685200 | -0.05001500 | 0.06653300  |
| C | -3.10389000 | 0.83306700  | -0.12455100 |
| C | -2.23320300 | -1.44078400 | 0.04879200  |
| C | -4.38282600 | 0.31482600  | -0.33713400 |
| H | -2.95092700 | 1.91474400  | -0.12317900 |
| C | -3.52113300 | -1.93770500 | -0.16040500 |
| H | -1.40634400 | -2.13415000 | 0.21613600  |
| C | -4.59739700 | -1.06673300 | -0.35560200 |
| H | -5.21857000 | 0.99799800  | -0.48898800 |
| H | -3.68400400 | -3.01548000 | -0.16954600 |
| H | -5.59749300 | -1.46219100 | -0.51969800 |
| N | 2.60804700  | -0.53547500 | -1.07830500 |
| C | 3.83964900  | -1.07297900 | -1.46491600 |
| C | 4.73853000  | -0.89101100 | -0.41329500 |
| H | 3.99249000  | -1.53302300 | -2.42367400 |
| C | 4.04809100  | -0.23550500 | 0.64518700  |
| H | 5.76747600  | -1.19101500 | -0.39647300 |
| H | 1.76815700  | -0.54291300 | -1.62423700 |
| H | 4.46870600  | 0.03670600  | 1.59204300  |
| C | 2.73242500  | -0.02214100 | 0.22427700  |
| H | 1.81605700  | 2.24420400  | -0.56906100 |
| H | 1.93252800  | 0.81382400  | 2.01144500  |
| H | 1.26243800  | 2.82077900  | 0.99360300  |

### *Transition state b) TS1*

|                               |                    |
|-------------------------------|--------------------|
|                               | (Hartree/Particle) |
| Zero-point correction=        | 0.220538           |
| Thermal correction to Energy= | 0.241426           |

|  |          |
|--|----------|
| Thermal correction to Enthalpy=              | 0.242370 |
| Thermal correction to Gibbs Free Energy=     | 0.165408 |
| Sum of electronic and zero-point Energies=   | 0.143585 |
| Sum of electronic and thermal Energies=      | 0.164474 |
| Sum of electronic and thermal Enthalpies=    | 0.165418 |
| Sum of electronic and thermal Free Energies= | 0.088456 |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 151.497     | 73.834         | 161.981        |

|          |                 |             |             |
|----------|-----------------|-------------|-------------|
| Charge:0 | Multiplicity: 1 |             |             |
| C        | 0.09797900      | 0.11250100  | 0.65295900  |
| C        | -1.06323600     | -0.56299300 | 1.15478000  |
| C        | -2.18127000     | 0.26091500  | 1.07225300  |
| C        | -1.66434700     | 1.67117700  | 0.71906400  |
| N        | -0.25659600     | 1.50759500  | 0.43761200  |
| O        | -2.28684000     | 2.69666000  | 0.66714900  |
| O        | 1.24787500      | -0.28185500 | 0.39928600  |
| C        | 0.64274600      | 2.56672600  | 0.03925200  |
| C        | 0.27929800      | 3.90584700  | 0.26814700  |
| C        | 1.86813000      | 2.25518600  | -0.57448800 |
| C        | 1.14826000      | 4.92569900  | -0.12486800 |
| H        | -0.67154100     | 4.15971800  | 0.74145300  |
| C        | 2.72406800      | 3.29066100  | -0.95494500 |
| H        | 2.17100000      | 1.21759000  | -0.74408200 |
| C        | 2.36954100      | 4.62529300  | -0.73544000 |
| H        | 0.86778100      | 5.96443100  | 0.05036900  |
| H        | 3.67799500      | 3.04949400  | -1.42561900 |
| H        | 3.04240800      | 5.42580500  | -1.03595400 |
| N        | -3.15318500     | -1.55769700 | -0.62207300 |
| C        | -4.44280300     | -1.91171800 | -0.39071200 |
| C        | -5.23877700     | -0.72319900 | -0.31115600 |
| H        | -4.78618600     | -2.93544400 | -0.29820000 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -4.39774300 | 0.36479500  | -0.48866200 |
| H  | -6.30278700 | -0.70876100 | -0.15397100 |
| H  | -2.34368300 | -2.17290500 | -0.68879700 |
| Zn | 1.87229000  | -2.15677500 | 0.03052900  |
| Cl | 3.99620500  | -2.21938000 | 0.27360800  |
| Cl | 0.05083900  | -3.22473400 | -0.52584100 |
| H  | -4.66342500 | 1.41117800  | -0.49094100 |
| C  | -3.03810900 | -0.12256500 | -0.61870900 |
| H  | -2.30496700 | 0.32978700  | -1.29028400 |
| H  | -3.06343700 | 0.17106700  | 1.70493400  |
| H  | -1.03381200 | -1.57644000 | 1.51807200  |

### Intermediate b) Int1

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.222805           |
| Thermal correction to Energy=                | 0.243383           |
| Thermal correction to Enthalpy=              | 0.244327           |
| Thermal correction to Gibbs Free Energy=     | 0.169187           |
| Sum of electronic and zero-point Energies=   | 0.122986           |
| Sum of electronic and thermal Energies=      | 0.143564           |
| Sum of electronic and thermal Enthalpies=    | 0.144508           |
| Sum of electronic and thermal Free Energies= | 0.069368           |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 152.725     | 74.098         | 158.146        |

|          |                                   |
|----------|-----------------------------------|
| Charge:0 | Multiplicity: 1                   |
| C        | 0.22051900 0.18821000 -1.14153500 |
| C        | 1.54133400 0.17289000 -1.50487600 |
| C        | 2.22395700 1.42787400 -1.09114600 |
| C        | 1.07539200 2.29099800 -0.49075500 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| N  | -0.10007600 | 1.50907200  | -0.53875900 |
| O  | 1.21729000  | 3.39180900  | -0.00947500 |
| O  | -0.70503200 | -0.67494100 | -1.22411400 |
| C  | -1.41058800 | 1.95405700  | -0.13246400 |
| C  | -1.53273800 | 3.00327900  | 0.79621600  |
| C  | -2.55536200 | 1.33536900  | -0.66581400 |
| C  | -2.80557200 | 3.41528200  | 1.19646200  |
| H  | -0.64903800 | 3.50762800  | 1.19048500  |
| C  | -3.81729400 | 1.75732700  | -0.24535300 |
| H  | -2.46653300 | 0.52488800  | -1.39803100 |
| C  | -3.94851800 | 2.79433600  | 0.68446700  |
| H  | -2.90363300 | 4.22881600  | 1.91451300  |
| H  | -4.70589300 | 1.27102300  | -0.64902200 |
| H  | -4.93634200 | 3.11660200  | 1.00582500  |
| N  | 2.75753200  | 0.15609800  | 1.00392400  |
| C  | 3.50716100  | -0.93940700 | 0.98534600  |
| C  | 4.64556200  | -0.73699000 | 0.07720400  |
| H  | 3.31865200  | -1.85354100 | 1.56584600  |
| C  | 4.52661900  | 0.48195200  | -0.50135200 |
| H  | 5.41038200  | -1.48581600 | -0.07731200 |
| H  | 1.83543000  | 0.26740400  | 1.44956400  |
| Zn | -0.95139300 | -2.14400400 | -0.02035900 |
| Cl | -2.56756500 | -3.52225100 | -0.39015600 |
| Cl | 0.67484200  | -1.94966300 | 1.50798100  |
| H  | 5.17478400  | 0.95474900  | -1.22607900 |
| C  | 3.27968800  | 1.17517800  | 0.01428300  |
| H  | 3.51878300  | 2.13738900  | 0.54974400  |
| H  | 2.69597900  | 1.97086300  | -1.94260500 |
| H  | 2.02427100  | -0.61059100 | -2.04674500 |

### Transition state b)TS2

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.218570           |
| Thermal correction to Energy=                | 0.239301           |
| Thermal correction to Enthalpy=              | 0.240245           |
| Thermal correction to Gibbs Free Energy=     | 0.162391           |
| Sum of electronic and zero-point Energies=   | 0.154800           |
| Sum of electronic and thermal Energies=      | 0.175530           |
| Sum of electronic and thermal Enthalpies=    | 0.176474           |
| Sum of electronic and thermal Free Energies= | 0.098621           |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 150.163     | 73.879         | 163.856        |

|          |                 |             |             |
|----------|-----------------|-------------|-------------|
| Charge:0 | Multiplicity: 1 |             |             |
| C        | 1.01001900      | 0.15826200  | -0.38521200 |
| C        | -0.33737800     | 0.54222100  | -0.23477200 |
| C        | -1.23721300     | -0.55319500 | -0.78043500 |
| C        | -0.24846900     | -1.61523500 | -1.31899700 |
| N        | 1.05274500      | -1.14518800 | -1.01777700 |
| O        | -0.50001000     | -2.66117300 | -1.86307900 |
| O        | 2.03701400      | 0.75810200  | -0.02827600 |
| N        | -3.30639100     | -0.71820800 | 0.76610000  |
| C        | -3.82984700     | -1.66822800 | 1.57912100  |
| C        | -2.83014400     | -2.66659400 | 1.83952200  |
| H        | -4.84506800     | -1.65410600 | 1.96452800  |
| C        | -1.68306800     | -2.31111500 | 1.16370800  |
| H        | -2.99042900     | -3.54288400 | 2.44710600  |
| Zn       | 3.96161000      | 0.46898100  | 0.11304900  |
| Cl       | 4.33847800      | -1.60876800 | -0.34939900 |
| Cl       | 4.79463000      | 2.34684800  | 0.70594400  |
| H        | -0.74407500     | -2.84876900 | 1.12204100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.89567100 | -1.01295500 | 0.51875900  |
| H | -1.08489800 | -0.12388100 | 1.12162800  |
| H | -1.95172900 | -0.24084600 | -1.56543200 |
| H | -0.64258200 | 1.56387100  | -0.16555300 |
| H | 1.91012400  | -1.65330000 | -1.25413700 |
| C | -4.01225200 | 0.43567800  | 0.25685200  |
| C | -3.44925300 | 1.71374400  | 0.39018700  |
| C | -5.25799700 | 0.24555900  | -0.36562200 |
| C | -4.15138400 | 2.81481500  | -0.10749000 |
| H | -2.47565100 | 1.85407600  | 0.86668900  |
| C | -5.94337200 | 1.35967900  | -0.85398100 |
| H | -5.68004100 | -0.75257000 | -0.48416900 |
| C | -5.39390400 | 2.64083400  | -0.72556700 |
| H | -3.72203300 | 3.81516100  | -0.01313400 |
| H | -6.91048800 | 1.22766400  | -1.34330800 |
| H | -5.93518100 | 3.50631300  | -1.11283900 |

### *N\_ Phenyl succinimide ZnCl<sub>2</sub> b)P*

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.222901           |
| Thermal correction to Energy=                | 0.244124           |
| Thermal correction to Enthalpy=              | 0.245068           |
| Thermal correction to Gibbs Free Energy=     | 0.166084           |
| Sum of electronic and zero-point Energies=   | 0.063491           |
| Sum of electronic and thermal Energies=      | 0.084713           |
| Sum of electronic and thermal Enthalpies=    | 0.085658           |
| Sum of electronic and thermal Free Energies= | 0.006673           |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 153.190     | 74.522         | 166.237        |

| Charge:0 | Multiplicity: 1 |             |             |  |
|----------|-----------------|-------------|-------------|--|
| C        | 0.44101000      | -0.87794100 | -0.50496200 |  |
| C        | 1.79764200      | -1.44321000 | -0.86363800 |  |
| C        | 2.73592100      | -0.22857700 | -1.02946000 |  |
| C        | 1.90025800      | 0.98719800  | -0.58710200 |  |
| N        | 0.55564300      | 0.52291100  | -0.34049000 |  |
| O        | 2.25116600      | 2.12936900  | -0.47050000 |  |
| O        | -0.57186000     | -1.54923000 | -0.37966400 |  |
| C        | -0.53822700     | 1.39923500  | 0.04944500  |  |
| C        | -1.03801100     | 1.33073700  | 1.35895800  |  |
| C        | -1.06266800     | 2.29304700  | -0.89626800 |  |
| C        | -2.09593900     | 2.17344900  | 1.71557700  |  |
| H        | -0.61989500     | 0.63613400  | 2.09067100  |  |
| C        | -2.11451900     | 3.12963900  | -0.51464200 |  |
| H        | -0.66524000     | 2.33240200  | -1.90929200 |  |
| C        | -2.63116100     | 3.06952200  | 0.78472500  |  |
| H        | -2.50619300     | 2.12150200  | 2.72550400  |  |
| H        | -2.53857400     | 3.82672800  | -1.23826200 |  |
| H        | -3.45784200     | 3.72014500  | 1.07059700  |  |
| N        | 4.71694700      | 0.76577900  | 0.20445600  |  |
| C        | 5.88334300      | 0.32145100  | 0.83021000  |  |
| C        | 5.91682100      | -1.07172900 | 0.74349300  |  |
| H        | 6.58935100      | 0.99623100  | 1.27945300  |  |
| C        | 4.74649800      | -1.49542800 | 0.05474100  |  |
| H        | 6.68540800      | -1.71472500 | 1.12483400  |  |
| H        | 4.41222500      | 1.72438500  | 0.12002100  |  |
| Zn       | -2.56285200     | -1.22156400 | -0.01810300 |  |
| Cl       | -3.25547400     | -0.68890400 | -1.95769200 |  |
| Cl       | -2.65197600     | -1.62139300 | 2.07107500  |  |
| H        | 4.49393500      | -2.51002800 | -0.17573400 |  |
| C        | 4.00902900      | -0.35062900 | -0.26765300 |  |
| H        | 2.14386900      | -2.13648600 | -0.06121800 |  |
| H        | 2.98704400      | -0.08894600 | -2.11887600 |  |
| H        | 1.74557100      | -2.06787300 | -1.77909900 |  |

### Transition state c) TS1

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.393616           |
| Thermal correction to Energy=                | 0.427589           |
| Thermal correction to Enthalpy=              | 0.428533           |
| Thermal correction to Gibbs Free Energy=     | 0.322727           |
| Sum of electronic and zero-point Energies=   | 0.162408           |
| Sum of electronic and thermal Energies=      | 0.196380           |
| Sum of electronic and thermal Enthalpies=    | 0.197324           |
| Sum of electronic and thermal Free Energies= | 0.091519           |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 268.316     | 119.887        | 222.687        |

|          |                 |             |             |
|----------|-----------------|-------------|-------------|
| Charge:0 | Multiplicity: 1 |             |             |
| C        | -0.15988700     | 0.80015200  | -0.76147100 |
| C        | 1.04336700      | 1.39667000  | -1.29385900 |
| C        | 1.05755700      | 2.75176100  | -1.04644000 |
| C        | -0.28959000     | 3.13885300  | -0.42499700 |
| N        | -0.96811800     | 1.86026400  | -0.22052200 |
| O        | -0.76575800     | 4.20048800  | -0.15079100 |
| O        | -0.48510300     | -0.40054800 | -0.74667400 |
| C        | -2.28410700     | 1.67720500  | 0.34144700  |
| C        | -2.45552600     | 0.74736200  | 1.39085100  |
| C        | -3.36858500     | 2.40548300  | -0.17260300 |
| C        | -3.74964200     | 0.53642700  | 1.89585400  |
| H        | -1.59014200     | 0.30421600  | 1.90286600  |
| C        | -4.64265400     | 2.17977800  | 0.35266700  |
| H        | -3.21821100     | 3.13547400  | -0.96865300 |
| C        | -4.83696200     | 1.24123200  | 1.37376300  |
| H        | -3.89809200     | -0.17560300 | 2.71116400  |
| H        | -5.49423300     | 2.73608800  | -0.04353200 |
| H        | -5.83920500     | 1.06251400  | 1.76295100  |



|    |             |             |             |
|----|-------------|-------------|-------------|
| N  | 3.45007000  | 2.61082500  | 0.30229500  |
| C  | 4.18706200  | 3.72617000  | 0.05799100  |
| C  | 3.42193400  | 4.88344000  | 0.40981300  |
| H  | 5.19419500  | 3.69936700  | -0.33066800 |
| C  | 2.18779700  | 4.43868200  | 0.87188700  |
| H  | 3.76360700  | 5.89612700  | 0.33494700  |
| C  | 1.11909200  | -4.26172200 | -0.72398200 |
| C  | 1.76280000  | -2.23590500 | 0.59720300  |
| H  | 0.05740900  | -3.94355700 | -0.65895800 |
| H  | 1.24620900  | -4.81567800 | -1.66751000 |
| C  | 1.68497300  | -3.02614300 | 1.90372100  |
| H  | 2.55663100  | -1.43877100 | 0.68045400  |
| H  | 0.80596600  | -1.67098100 | 0.44262600  |
| H  | 1.32221900  | -2.36859400 | 2.71897700  |
| H  | 1.02072900  | -3.91269300 | 1.85385800  |
| N  | 2.05176700  | -3.07361500 | -0.64381100 |
| C  | 3.48309000  | -3.55837300 | -0.61460100 |
| H  | 3.68874900  | -4.11977700 | 0.32290500  |
| H  | 3.72001000  | -4.19906400 | -1.47488400 |
| H  | 4.19216400  | -2.69753000 | -0.62757500 |
| C  | 1.84160400  | -2.21303300 | -1.87094600 |
| H  | 1.98025200  | -2.78237300 | -2.80116700 |
| H  | 0.82641600  | -1.76301100 | -1.88075500 |
| H  | 2.56520800  | -1.36391800 | -1.89037000 |
| H  | 1.29444300  | -4.96905900 | 0.10803500  |
| O  | 2.95510900  | -3.58489800 | 2.25184200  |
| H  | 3.74616100  | 1.54393500  | 0.07593200  |
| Cl | 4.11702800  | -0.06152800 | -0.40529800 |
| H  | 3.59077500  | -2.87606400 | 2.50218400  |
| Zn | -2.25319200 | -1.31608200 | -0.30294300 |
| Cl | -3.70876000 | -1.00483800 | -1.87183500 |
| Cl | -1.50933000 | -2.74477600 | 1.19567700  |
| H  | 1.36785300  | 5.03994100  | 1.22130100  |
| C  | 2.16170200  | 3.00504400  | 0.75313600  |

|   |            |            |             |
|---|------------|------------|-------------|
| H | 1.55779400 | 2.32654300 | 1.33290000  |
| H | 1.66542100 | 3.50343100 | -1.54345500 |
| H | 1.83731700 | 0.81975900 | -1.74789700 |

### Intermediate c) Int1

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.395614           |
| Thermal correction to Energy=                | 0.428663           |
| Thermal correction to Enthalpy=              | 0.429608           |
| Thermal correction to Gibbs Free Energy=     | 0.326806           |
| Sum of electronic and zero-point Energies=   | 0.120982           |
| Sum of electronic and thermal Energies=      | 0.154031           |
| Sum of electronic and thermal Enthalpies=    | 0.154975           |
| Sum of electronic and thermal Free Energies= | 0.052174           |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 268.990     | 118.542        | 216.364        |

|          |                 |             |             |
|----------|-----------------|-------------|-------------|
| Charge:0 | Multiplicity: 1 |             |             |
| C        | -0.06990100     | 0.84767600  | -0.68339600 |
| C        | 1.20908200      | 1.21743500  | -0.99265500 |
| C        | 1.44854900      | 2.65512000  | -0.65372800 |
| C        | 0.08485300      | 3.13330600  | -0.08642000 |
| N        | -0.77520000     | 2.00312800  | -0.09760600 |
| O        | -0.20400900     | 4.23548100  | 0.31536100  |
| O        | -0.64789400     | -0.27657000 | -0.82147700 |
| C        | -2.15530900     | 1.96913900  | 0.30965600  |
| C        | -2.54672600     | 1.05384000  | 1.31534700  |
| C        | -3.09228800     | 2.81809300  | -0.30311900 |
| C        | -3.90607000     | 0.98829100  | 1.67389200  |
| H        | -1.79170900     | 0.53223000  | 1.92582400  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -4.43304100 | 2.73187300  | 0.07400400  |
| H  | -2.77255700 | 3.53156300  | -1.06237100 |
| C  | -4.84325100 | 1.81416600  | 1.05015800  |
| H  | -4.22184500 | 0.29379200  | 2.45587700  |
| H  | -5.16910600 | 3.38125700  | -0.40229600 |
| H  | -5.89597100 | 1.74428700  | 1.32031600  |
| N  | 3.85824800  | 2.28055900  | -0.02560300 |
| C  | 4.75406800  | 3.24022000  | -0.01900900 |
| C  | 4.16536700  | 4.53461600  | 0.40219000  |
| H  | 5.80063000  | 3.10825300  | -0.28345400 |
| C  | 2.85844800  | 4.32043900  | 0.66119700  |
| H  | 4.73085700  | 5.44701600  | 0.46748100  |
| C  | 0.50570200  | -4.29371200 | -0.72113500 |
| C  | 1.57397800  | -2.51418800 | 0.69114700  |
| H  | -0.48935600 | -3.81638100 | -0.56851600 |
| H  | 0.48372400  | -4.79066900 | -1.70391000 |
| C  | 1.42256000  | -3.39803000 | 1.92931100  |
| H  | 2.49318400  | -1.88261500 | 0.76846700  |
| H  | 0.71530400  | -1.78068300 | 0.65796000  |
| H  | 1.27003300  | -2.76885500 | 2.82815600  |
| H  | 0.57246200  | -4.10967900 | 1.86255500  |
| N  | 1.61622700  | -3.27178800 | -0.63742200 |
| C  | 2.94863400  | -3.96733800 | -0.79028200 |
| H  | 3.13000500  | -4.65343000 | 0.06689400  |
| H  | 3.00057400  | -4.54794400 | -1.72368000 |
| H  | 3.78199200  | -3.23661100 | -0.80148400 |
| C  | 1.42722800  | -2.25651500 | -1.74467600 |
| H  | 1.09049300  | -2.70440800 | -2.68760300 |
| H  | 0.64998900  | -1.51599100 | -1.39911700 |
| H  | 2.34783200  | -1.67546300 | -1.93784600 |
| H  | 0.61026500  | -5.07445600 | 0.05414200  |
| O  | 2.56273700  | -4.24732300 | 2.09903000  |
| H  | 4.03654100  | 0.85690600  | -0.31003200 |
| Cl | 4.34978000  | -0.51337200 | -0.48866400 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 3.31905900  | -3.74525500 | 2.47082900  |
| Zn | -2.39521700 | -0.97268100 | -0.27146100 |
| Cl | -4.01788900 | -0.91783300 | -1.73369000 |
| Cl | -1.72865300 | -2.44196600 | 1.29607300  |
| H  | 2.08561200  | 5.01042500  | 0.97221100  |
| C  | 2.54027500  | 2.84735300  | 0.41536300  |
| H  | 2.24282400  | 2.32962500  | 1.36685100  |
| H  | 1.69139000  | 3.24730700  | -1.56932100 |
| H  | 1.95469400  | 0.61739800  | -1.46329200 |

### Transition state c)TS2

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.392348           |
| Thermal correction to Energy=                | 0.425766           |
| Thermal correction to Enthalpy=              | 0.426710           |
| Thermal correction to Gibbs Free Energy=     | 0.321950           |
| Sum of electronic and zero-point Energies=   | 0.169739           |
| Sum of electronic and thermal Energies=      | 0.203157           |
| Sum of electronic and thermal Enthalpies=    | 0.204101           |
| Sum of electronic and thermal Free Energies= | 0.099341           |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 267.172     | 119.054        | 220.486        |

|          |                 |            |             |
|----------|-----------------|------------|-------------|
| Charge:0 | Multiplicity: 1 |            |             |
| C        | -0.28614900     | 0.64232100 | -0.65002800 |
| C        | 1.00494100      | 1.11328700 | -0.95459400 |
| C        | 0.99842500      | 2.63854100 | -1.01449000 |
| C        | -0.44839600     | 3.01419000 | -0.64194100 |
| N        | -1.14742600     | 1.76310500 | -0.39387500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -0.97255800 | 4.08836700  | -0.54970900 |
| O | -0.63484100 | -0.55752400 | -0.53564600 |
| C | -2.51783600 | 1.63420400  | 0.04608500  |
| C | -2.78289300 | 0.94642600  | 1.24810100  |
| C | -3.55378200 | 2.17291500  | -0.73127700 |
| C | -4.11640600 | 0.77700300  | 1.64461600  |
| H | -1.96896500 | 0.62913500  | 1.90831500  |
| C | -4.87392600 | 1.99711900  | -0.30945800 |
| H | -3.33124500 | 2.71975300  | -1.64724400 |
| C | -5.15702000 | 1.29375600  | 0.86713900  |
| H | -4.33904100 | 0.24353300  | 2.57006000  |
| H | -5.68905500 | 2.40545700  | -0.90835500 |
| H | -6.19121700 | 1.14725000  | 1.17642400  |
| N | 3.40274100  | 2.89020400  | -0.14757900 |
| C | 4.01125400  | 3.64488300  | 0.78299200  |
| C | 3.02547700  | 4.28439400  | 1.62558200  |
| H | 5.08622900  | 3.73973400  | 0.87098800  |
| C | 1.78470200  | 3.86012600  | 1.20194100  |
| H | 3.25415800  | 4.96742400  | 2.42071800  |
| C | 1.43921300  | -4.02136600 | -0.52270900 |
| C | 2.06232100  | -1.83395900 | 0.51540000  |
| H | 0.37851700  | -3.79006300 | -0.28244500 |
| H | 1.44709600  | -4.63108600 | -1.44040600 |
| C | 2.29665500  | -2.49062100 | 1.87754900  |
| H | 2.74040200  | -0.94957200 | 0.38814700  |
| H | 1.01070000  | -1.42472500 | 0.49022900  |
| H | 2.02467400  | -1.78341900 | 2.68666800  |
| H | 1.71153600  | -3.42201700 | 2.02451400  |
| N | 2.25144500  | -2.75632700 | -0.68536100 |
| C | 3.71147900  | -3.11005300 | -0.84734800 |
| H | 4.11402200  | -3.56262600 | 0.08588500  |
| H | 3.87599800  | -3.81050600 | -1.67859000 |
| H | 4.32328400  | -2.20148400 | -1.04742300 |
| C | 1.77679100  | -2.02852900 | -1.92439600 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 1.93003800  | -2.62293700 | -2.83694900 |
| H  | 0.69629300  | -1.77153800 | -1.85038500 |
| H  | 2.32468700  | -1.06378200 | -2.05637500 |
| H  | 1.82654000  | -4.64738400 | 0.30223100  |
| O  | 3.65166400  | -2.91823800 | 2.03311600  |
| H  | 3.89793900  | 1.96825800  | -0.77060500 |
| Cl | 4.33279100  | 0.45444300  | -1.09564700 |
| H  | 4.25271700  | -2.14602700 | 2.13559900  |
| Zn | -2.23779000 | -1.56546900 | 0.01833400  |
| Cl | -3.87602400 | -1.68048900 | -1.37823600 |
| Cl | -1.15470000 | -2.61058400 | 1.62294300  |
| H  | 0.82186500  | 4.14961500  | 1.58746100  |
| C  | 1.97811600  | 2.91796700  | 0.11220100  |
| H  | 1.75787900  | 1.50812500  | 0.34465400  |
| H  | 1.28838800  | 3.08384500  | -1.98697400 |
| H  | 1.73585900  | 0.55647300  | -1.51676800 |

*N-Phenyl succinimide + ChCl + ZnCl<sub>2</sub> c)P*

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.397703           |
| Thermal correction to Energy=                | 0.431908           |
| Thermal correction to Enthalpy=              | 0.432852           |
| Thermal correction to Gibbs Free Energy=     | 0.324831           |
| Sum of electronic and zero-point Energies=   | 0.093829           |
| Sum of electronic and thermal Energies=      | 0.128034           |
| Sum of electronic and thermal Enthalpies=    | 0.128978           |
| Sum of electronic and thermal Free Energies= | 0.020958           |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 271.026     | 120.108        | 227.348        |

| Charge:0 | Multiplicity: 1 |             |             |
|----------|-----------------|-------------|-------------|
| C        | -0.36043000     | 0.66798200  | -0.55662900 |
| C        | 0.92661300      | 1.34718000  | -0.91917100 |
| C        | 0.61864200      | 2.85818100  | -0.98531900 |
| C        | -0.82528700     | 3.00175500  | -0.48327700 |
| N        | -1.33342000     | 1.63415800  | -0.27096300 |
| O        | -1.51442500     | 3.95969000  | -0.31164600 |
| O        | -0.50063500     | -0.56134300 | -0.50106600 |
| C        | -2.67228900     | 1.32284700  | 0.19600100  |
| C        | -2.82845300     | 0.62880800  | 1.41027200  |
| C        | -3.77658400     | 1.71325500  | -0.57551400 |
| C        | -4.12305200     | 0.30161800  | 1.83244200  |
| H        | -1.96981600     | 0.40221800  | 2.04955200  |
| C        | -5.05840700     | 1.38310200  | -0.12744000 |
| H        | -3.64030400     | 2.26361100  | -1.50605900 |
| C        | -5.23218200     | 0.67295400  | 1.06593100  |
| H        | -4.26174000     | -0.24141700 | 2.76905200  |
| H        | -5.92743500     | 1.67639600  | -0.71851000 |
| H        | -6.23604100     | 0.40909800  | 1.39924100  |
| N        | 2.94881500      | 3.45497600  | -0.18764300 |
| C        | 3.55619700      | 4.42569100  | 0.60517500  |
| C        | 2.56280700      | 5.28766400  | 1.08277600  |
| H        | 4.61802100      | 4.44760000  | 0.77324000  |
| C        | 1.31605200      | 4.83280300  | 0.57936900  |
| H        | 2.71123700      | 6.14059200  | 1.71330000  |
| C        | 1.88634300      | -4.22469300 | 0.05954000  |
| C        | 2.37524500      | -1.84373600 | 0.59136300  |
| H        | 0.82127800      | -4.06869400 | 0.32875000  |
| H        | 1.92673700      | -5.02615100 | -0.69489400 |
| C        | 3.15847700      | -2.05236200 | 1.88298500  |
| H        | 2.78114000      | -0.86155600 | 0.09545500  |
| H        | 1.29703300      | -1.66474500 | 0.80388800  |
| H        | 2.84644200      | -1.29778800 | 2.63422500  |
| H        | 3.04984800      | -3.06180000 | 2.32160500  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| N  | 2.51714000  | -2.94563900 | -0.44311500 |
| C  | 3.96981400  | -3.19610800 | -0.77629700 |
| H  | 4.56157400  | -3.42871700 | 0.13548900  |
| H  | 4.09294900  | -4.00558300 | -1.50647500 |
| H  | 4.44168400  | -2.27270100 | -1.19231000 |
| C  | 1.80639900  | -2.50001600 | -1.70548700 |
| H  | 1.79370200  | -3.28899000 | -2.47102900 |
| H  | 0.76233000  | -2.19358100 | -1.49824800 |
| H  | 2.31846900  | -1.61021900 | -2.14112500 |
| H  | 2.39722700  | -4.59040400 | 0.96805700  |
| O  | 4.56655300  | -1.93632600 | 1.66845100  |
| H  | 3.42257700  | 2.67620500  | -0.64029200 |
| Cl | 3.87400500  | 0.27066300  | -0.99453100 |
| H  | 4.77874900  | -1.08218700 | 1.19826200  |
| Zn | -2.05322900 | -1.79818900 | -0.07364000 |
| Cl | -3.46272400 | -1.82537400 | -1.68172500 |
| Cl | -1.09469400 | -2.71408100 | 1.63371600  |
| H  | 0.35912200  | 5.28493500  | 0.75610400  |
| C  | 1.56674200  | 3.69386800  | -0.19770700 |
| H  | 1.70483300  | 1.11701500  | -0.14188900 |
| H  | 0.63972500  | 3.20871900  | -2.05596000 |
| H  | 1.38598000  | 0.95787800  | -1.85499600 |

### *Transition state d) TS1*

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                     | 0.511856           |
| Thermal correction to Energy=              | 0.567034           |
| Thermal correction to Enthalpy=            | 0.567978           |
| Thermal correction to Gibbs Free Energy=   | 0.418222           |
| Sum of electronic and zero-point Energies= | -0.544935          |
| Sum of electronic and thermal Energies=    | -0.489757          |



Sum of electronic and thermal Enthalpies= -0.488813  
 Sum of electronic and thermal Free Energies= -0.638569

|       | E (Thermal)<br>KCal/Mol | CV<br>Cal/Mol-Kelvin | S<br>Cal/Mol-Kelvin |
|-------|-------------------------|----------------------|---------------------|
| Total | 355.819                 | 192.064              | 315.187             |

Charge:0 Multiplicity: 1

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.58592000  | -0.04137700 | -0.72246000 |
| C | 2.60008400  | 1.24020000  | -1.36955800 |
| C | 3.75941000  | 1.93237600  | -1.06120000 |
| C | 4.67014600  | 0.97182500  | -0.27748200 |
| N | 3.89362600  | -0.24405500 | -0.12121900 |
| O | 5.78640200  | 1.13709300  | 0.12971300  |
| O | 1.72938500  | -0.94061800 | -0.63373300 |
| C | 4.34127400  | -1.44404200 | 0.53747200  |
| C | 3.76335800  | -2.68099300 | 0.19888500  |
| C | 5.35928800  | -1.37330200 | 1.50506700  |
| C | 4.20018100  | -3.84046400 | 0.84304800  |
| H | 2.97214200  | -2.74512200 | -0.55468300 |
| C | 5.78568800  | -2.54508500 | 2.13191000  |
| H | 5.82002200  | -0.41694700 | 1.76138800  |
| C | 5.20955300  | -3.77823300 | 1.80784100  |
| H | 3.74752900  | -4.79915000 | 0.58868800  |
| H | 6.57415600  | -2.49397800 | 2.88341300  |
| H | 5.54524300  | -4.68513400 | 2.30638000  |
| N | 2.45008200  | 4.11902900  | -0.20912400 |
| C | 3.14769100  | 5.26745000  | -0.42337600 |
| C | 4.44355700  | 5.13632500  | 0.16461700  |
| H | 2.74966300  | 6.12287900  | -0.95036000 |
| C | 4.52109000  | 3.86946600  | 0.73316200  |
| H | 5.20011100  | 5.89712800  | 0.16463100  |
| C | -4.38620800 | 0.59437000  | 1.09270800  |
| C | -4.20547400 | 1.73305900  | 2.09892000  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -4.42350600 | -0.38862800 | 1.62461600  |
| H  | -3.47558800 | 0.55684800  | 0.43467000  |
| H  | -3.15774400 | 1.74592400  | 2.46527200  |
| H  | -4.44358700 | 2.73639700  | 1.69249900  |
| N  | -5.61148200 | 0.73529200  | 0.19013700  |
| C  | -6.84078000 | 1.07990100  | 1.00058500  |
| H  | -6.72568900 | 2.05507900  | 1.51738000  |
| H  | -7.74514400 | 1.12160000  | 0.37637700  |
| H  | -6.99775800 | 0.34247600  | 1.81077200  |
| C  | -5.85384300 | -0.58004700 | -0.51859700 |
| H  | -6.71482900 | -0.52892600 | -1.20054800 |
| H  | -4.96852600 | -0.89101900 | -1.11779000 |
| H  | -6.02317800 | -1.40714900 | 0.19897300  |
| O  | -5.12699400 | 1.57779200  | 3.18644900  |
| H  | 1.49151400  | 3.89461700  | -0.56931300 |
| Cl | -2.40260600 | 2.93829200  | -0.08556800 |
| H  | -4.78395800 | 0.93944800  | 3.84520200  |
| H  | 5.35954700  | 3.43785000  | 1.25461400  |
| C  | 3.29050000  | 3.17193600  | 0.45370800  |
| H  | 2.83009900  | 2.41721400  | 1.10149300  |
| H  | 4.21591700  | 2.71605100  | -1.66305600 |
| H  | 1.77180800  | 1.59145300  | -1.97142000 |
| Zn | -0.38845700 | -0.69958600 | -0.85333600 |
| Zn | -1.78535900 | -1.83118000 | -0.18105900 |
| Cl | 0.13550200  | -3.23437800 | -0.51024700 |
| Cl | -1.20573500 | -0.37313200 | 1.68840700  |
| Cl | -2.53891800 | -0.52066500 | -2.15166600 |
| Cl | -3.69547700 | -2.84850400 | 0.43821700  |
| O  | 0.30139500  | -0.73423500 | -2.86804000 |
| H  | -0.31164800 | -0.71782200 | -3.60607100 |
| O  | -0.26121000 | 1.29577900  | -0.47487200 |
| H  | 0.31380000  | 1.52918600  | 0.31472800  |
| O  | 1.53336400  | -1.30268100 | 2.31809900  |
| H  | 0.73434200  | -1.69940300 | 2.67702600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.94719700  | -2.74212500 | -2.83055800 |
| H | 2.25852200  | -2.57193400 | -1.90812300 |
| O | 1.18378100  | 1.36373000  | 1.81607800  |
| H | 1.36250800  | 0.38800800  | 1.97629900  |
| O | 0.24586500  | 3.51757900  | -1.69241600 |
| H | 0.08247600  | 2.53104200  | -1.61672500 |
| H | -0.60326300 | 3.93391900  | -1.51002100 |
| H | 1.03452900  | -1.40835600 | -3.08817300 |
| H | 1.69013400  | -1.73591500 | 1.46318400  |
| H | 1.34804600  | -3.49751100 | -2.76712800 |
| H | 0.53000500  | 1.60536800  | 2.47273800  |
| H | -1.28193700 | 1.89559900  | -0.23753500 |
| C | -5.35641400 | 1.81166400  | -0.84059300 |
| H | -4.44410700 | 1.58059500  | -1.43928100 |
| H | -6.20153500 | 1.93365000  | -1.53159300 |
| H | -5.14185000 | 2.78968100  | -0.36434400 |

### Intermediate d) Int1

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.515650           |
| Thermal correction to Energy=                | 0.569886           |
| Thermal correction to Enthalpy=              | 0.570830           |
| Thermal correction to Gibbs Free Energy=     | 0.425004           |
| Sum of electronic and zero-point Energies=   | -0.564799          |
| Sum of electronic and thermal Energies=      | -0.510563          |
| Sum of electronic and thermal Enthalpies=    | -0.509619          |
| Sum of electronic and thermal Free Energies= | -0.655445          |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 357.609     | 191.003        | 306.916        |

| Charge:0 | Multiplicity: 1 |             |             |
|----------|-----------------|-------------|-------------|
| C        | 2.91247800      | 0.09577200  | -0.71460200 |
| C        | 3.03350400      | 1.37503100  | -1.17589600 |
| C        | 3.96968600      | 2.17376700  | -0.32802100 |
| C        | 4.54412600      | 1.12408900  | 0.65883400  |
| N        | 3.89738500      | -0.11269300 | 0.37501000  |
| O        | 5.35481400      | 1.31969300  | 1.53248800  |
| O        | 2.12516400      | -0.86989800 | -1.00854900 |
| C        | 4.25889600      | -1.37566800 | 0.95019600  |
| C        | 4.14659000      | -2.55131600 | 0.18443500  |
| C        | 4.71847200      | -1.43163600 | 2.27948600  |
| C        | 4.47795200      | -3.77831900 | 0.76197700  |
| H        | 3.81430300      | -2.50182100 | -0.85336800 |
| C        | 5.04942200      | -2.66770700 | 2.83506700  |
| H        | 4.83879700      | -0.51413300 | 2.86085200  |
| C        | 4.92479100      | -3.84268700 | 2.08514000  |
| H        | 4.39373100      | -4.69029100 | 0.17079000  |
| H        | 5.40954200      | -2.71451000 | 3.86308100  |
| H        | 5.18339800      | -4.80182700 | 2.52793300  |
| N        | 1.74721000      | 3.22647300  | 0.24251000  |
| C        | 1.31338500      | 4.38177000  | -0.22387700 |
| C        | 2.44147800      | 5.33148700  | -0.34876300 |
| H        | 0.26614600      | 4.59677300  | -0.49682600 |
| C        | 3.57228700      | 4.69796500  | 0.02961800  |
| H        | 2.31420300      | 6.34114800  | -0.70513900 |
| C        | -4.98010500     | -0.71863600 | 1.41552600  |
| C        | -4.42706300     | -0.54232100 | 2.83287700  |
| H        | -5.89788500     | -1.34655200 | 1.43354500  |
| H        | -4.23221300     | -1.30481300 | 0.80802100  |
| H        | -3.95173300     | -1.48123000 | 3.17834300  |
| H        | -3.67701100     | 0.27374000  | 2.91906900  |
| N        | -5.28654600     | 0.59417900  | 0.69604000  |
| C        | -6.48989300     | 1.25220400  | 1.33549500  |
| H        | -6.35091700     | 1.32526800  | 2.44032700  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -6.64716000 | 2.27249400  | 0.94943600  |
| H  | -7.41085100 | 0.67296400  | 1.16485000  |
| C  | -5.59331700 | 0.28855900  | -0.75490200 |
| H  | -5.92324500 | 1.18685900  | -1.30014500 |
| H  | -4.68627000 | -0.09236900 | -1.28724700 |
| H  | -6.36200700 | -0.49383000 | -0.86258100 |
| O  | -5.47320700 | -0.13828800 | 3.72448100  |
| H  | 1.16201100  | 2.25389800  | 0.31315700  |
| Cl | -1.60658900 | 3.18100000  | 0.80290700  |
| H  | -5.96718600 | -0.91296300 | 4.06098400  |
| H  | 4.58387100  | 5.06951600  | 0.06469200  |
| C  | 3.23709100  | 3.27813000  | 0.46665500  |
| H  | 3.43452100  | 3.16718700  | 1.57259800  |
| H  | 4.80606200  | 2.60799000  | -0.92448000 |
| H  | 2.51231600  | 1.79451100  | -2.01256000 |
| Zn | 0.00571000  | -0.49721700 | -0.78291200 |
| Zn | -1.66342600 | -1.50833700 | -0.98274700 |
| Cl | 0.17426100  | -2.89956300 | -1.68307700 |
| Cl | -1.63442300 | -1.02530000 | 1.40696800  |
| Cl | -2.05800700 | 0.65186300  | -2.02400300 |
| Cl | -3.63830700 | -2.57767900 | -1.30884600 |
| O  | 0.63566300  | 0.37304900  | -2.74928400 |
| H  | 0.05444000  | 0.24844900  | -3.51607000 |
| O  | 0.16950700  | 1.14245900  | 0.48017400  |
| H  | 0.33649900  | 0.87171900  | 1.44787400  |
| O  | 1.02959700  | -1.91018100 | 0.94754100  |
| H  | 0.54218300  | -2.72635100 | 1.14721900  |
| O  | 2.17714900  | -1.50451800 | -3.55110900 |
| H  | 2.46682000  | -1.71989200 | -2.63033600 |
| O  | 1.18810600  | -0.01575400 | 2.58361300  |
| H  | 1.88636100  | -0.41508800 | 2.03192500  |
| O  | -0.30028400 | 3.24750500  | -2.01073200 |
| H  | -0.00877500 | 2.35177900  | -2.23824400 |
| H  | -1.22572300 | 3.17068500  | -1.76282000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.52819800  | -0.05854100 | -3.03821100 |
| H | 1.84017000  | -2.20260100 | 0.44840800  |
| H | 1.48584800  | -2.13992000 | -3.75984800 |
| H | 0.54963900  | -0.73743600 | 2.71514000  |
| H | -0.79715600 | 1.95025300  | 0.58504100  |
| C | -4.10906300 | 1.53835000  | 0.75580800  |
| H | -3.17310400 | 1.03661400  | 0.42361000  |
| H | -4.23869800 | 2.41738300  | 0.10105100  |
| H | -3.91825800 | 1.91485800  | 1.77833600  |

### Transition state d)TS2

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.515213           |
| Thermal correction to Energy=                | 0.568312           |
| Thermal correction to Enthalpy=              | 0.569256           |
| Thermal correction to Gibbs Free Energy=     | 0.426421           |
| Sum of electronic and zero-point Energies=   | -0.563238          |
| Sum of electronic and thermal Energies=      | -0.510139          |
| Sum of electronic and thermal Enthalpies=    | -0.509195          |
| Sum of electronic and thermal Free Energies= | -0.652030          |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 356.621     | 188.657        | 300.622        |

|          |                 |             |             |
|----------|-----------------|-------------|-------------|
| Charge:0 | Multiplicity: 1 |             |             |
| C        | 2.77561700      | 0.07239000  | -0.88425300 |
| C        | 2.63410900      | 1.24505200  | -1.57630100 |
| C        | 3.38141500      | 2.35456600  | -0.90872900 |
| C        | 4.24689700      | 1.61762500  | 0.14820600  |
| N        | 3.83898800      | 0.24787400  | 0.13495900  |
| O        | 5.07553100      | 2.10278100  | 0.88010000  |
| O        | 2.14838100      | -1.03809300 | -0.90434100 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 4.45356600  | -0.81289900 | 0.87699300  |
| C  | 4.35385500  | -2.14059400 | 0.41554800  |
| C  | 5.14597900  | -0.52956900 | 2.07004500  |
| C  | 4.93147700  | -3.17183600 | 1.15774700  |
| H  | 3.84025800  | -2.36505000 | -0.52520600 |
| C  | 5.72023000  | -1.57447000 | 2.79358200  |
| H  | 5.25066000  | 0.50238700  | 2.41615400  |
| C  | 5.61101800  | -2.89640300 | 2.34777600  |
| H  | 4.85535700  | -4.19873600 | 0.79991500  |
| H  | 6.26006400  | -1.35487600 | 3.71502800  |
| H  | 6.06007200  | -3.70444200 | 2.92032600  |
| N  | 1.30364000  | 3.81614400  | -0.99247900 |
| C  | 1.02937200  | 5.06621400  | -0.60564200 |
| C  | 2.00937100  | 5.48368500  | 0.38299200  |
| H  | 0.18905500  | 5.65380100  | -0.97578200 |
| C  | 2.86115800  | 4.43505700  | 0.60923800  |
| H  | 2.02584200  | 6.46201200  | 0.83123300  |
| C  | -4.84067500 | -0.22692600 | 1.64962700  |
| C  | -4.24693000 | 0.53745900  | 2.83698400  |
| H  | -5.74034700 | -0.79794600 | 1.96866000  |
| H  | -4.09870800 | -1.00629900 | 1.31532900  |
| H  | -3.72640000 | -0.16046000 | 3.52167200  |
| H  | -3.52457700 | 1.32879100  | 2.53920400  |
| N  | -5.20632000 | 0.65711000  | 0.45781600  |
| C  | -6.40740500 | 1.50761200  | 0.81041800  |
| H  | -6.23478900 | 2.04147900  | 1.77501700  |
| H  | -6.60651900 | 2.26825400  | 0.03799500  |
| H  | -7.31604700 | 0.89868700  | 0.93786300  |
| C  | -5.54968800 | -0.23521400 | -0.71621200 |
| H  | -5.90217400 | 0.34793100  | -1.58177800 |
| H  | -4.65445000 | -0.80881800 | -1.06269600 |
| H  | -6.31471700 | -0.98568100 | -0.45931500 |
| O  | -5.27744800 | 1.25827100  | 3.52312100  |
| H  | 0.78028400  | 3.23537000  | -1.67869000 |
| Cl | -1.65591900 | 3.20936200  | -0.59661100 |
| H  | -5.72894700 | 0.68832400  | 4.17788600  |
| H  | 3.71751000  | 4.38459100  | 1.26926400  |
| C  | 2.40158200  | 3.26710900  | -0.17708200 |
| H  | 1.80089000  | 2.49853300  | 0.69568200  |
| H  | 4.03507500  | 2.92735700  | -1.60349500 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 2.09805200  | 1.37480100  | -2.49345400 |
| Zn | -0.00253300 | -1.00713300 | -0.62415400 |
| Zn | -1.62711500 | -1.99255500 | -0.30391200 |
| Cl | 0.30675100  | -3.47841900 | -0.34657300 |
| Cl | -1.49713100 | -0.45532000 | 1.60827300  |
| Cl | -2.09123600 | -0.46177200 | -2.17397200 |
| Cl | -3.57579700 | -3.10811700 | -0.05448900 |
| O  | 0.58756800  | -1.01349000 | -2.80493300 |
| H  | 0.05264900  | -1.52772300 | -3.42512700 |
| O  | -0.08283500 | 1.04544800  | -0.39870100 |
| H  | 0.49858000  | 1.47525700  | -1.08853400 |
| O  | 1.22427500  | -1.20737000 | 1.35195400  |
| H  | 0.81877000  | -1.68118400 | 2.09545100  |
| O  | 2.42215100  | -2.83728100 | -2.64201400 |
| H  | 2.77619200  | -2.54298300 | -1.76213300 |
| O  | 1.07862600  | 1.72286600  | 1.66167200  |
| H  | 1.37387300  | 0.77581200  | 1.55369200  |
| O  | -0.12378100 | 1.93278100  | -2.80706700 |
| H  | 0.07514400  | 1.00773500  | -3.06184500 |
| H  | -1.08795100 | 2.00292500  | -2.77817100 |
| H  | 1.53582800  | -1.41979700 | -2.87120300 |
| H  | 2.05054200  | -1.69510800 | 1.12673100  |
| H  | 1.80918300  | -3.55195800 | -2.44450600 |
| H  | 0.15458500  | 1.69666800  | 1.24866300  |
| H  | -1.01564900 | 1.74039400  | -0.47483700 |
| C  | -4.05582400 | 1.55502200  | 0.06843300  |
| H  | -3.12422700 | 0.97037400  | -0.09566500 |
| H  | -4.24694500 | 2.10703300  | -0.86821800 |
| H  | -3.82459500 | 2.30722800  | 0.84758500  |

### Intermediate b) Int2

|  |                    |
|--|--------------------|
|  | (Hartree/Particle) |
| Zero-point correction=                   | 0.516850           |
| Thermal correction to Energy=            | 0.571656           |
| Thermal correction to Enthalpy=          | 0.572600           |
| Thermal correction to Gibbs Free Energy= | 0.425039           |



|  |           |
|--|-----------|
| Sum of electronic and zero-point Energies=   | -0.602066 |
| Sum of electronic and thermal Energies=      | -0.547261 |
| Sum of electronic and thermal Enthalpies=    | -0.546317 |
| Sum of electronic and thermal Free Energies= | -0.693878 |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 358.719     | 192.939        | 310.569        |

|          |                 |             |             |
|----------|-----------------|-------------|-------------|
| Charge:0 | Multiplicity: 1 |             |             |
| C        | 2.77490100      | 0.13393900  | -0.86238600 |
| C        | 2.59114700      | 1.28442500  | -1.57645500 |
| C        | 3.49485000      | 2.37531300  | -1.07425900 |
| C        | 4.40726400      | 1.64653500  | -0.05981200 |
| N        | 3.91617800      | 0.29277700  | 0.04523100  |
| O        | 5.34528100      | 2.07431900  | 0.56132300  |
| O        | 2.10993200      | -0.96593800 | -0.81210700 |
| C        | 4.52314500      | -0.75903900 | 0.80386600  |
| C        | 4.33203600      | -2.10347500 | 0.42875000  |
| C        | 5.30339900      | -0.44751000 | 1.93510500  |
| C        | 4.90329400      | -3.12143100 | 1.19453200  |
| H        | 3.75568000      | -2.35310500 | -0.46822800 |
| C        | 5.86995000      | -1.47882400 | 2.68277100  |
| H        | 5.48471900      | 0.59531300  | 2.21024400  |
| C        | 5.66739100      | -2.81664100 | 2.32391200  |
| H        | 4.75586400      | -4.16090600 | 0.90143700  |
| H        | 6.47835000      | -1.23688200 | 3.55474200  |
| H        | 6.11153300      | -3.61349900 | 2.91550400  |
| N        | 1.53108900      | 3.96521000  | -0.96134500 |
| C        | 0.97520800      | 4.89146400  | -0.07053800 |
| C        | 1.80222900      | 4.96024400  | 1.04923400  |
| H        | 0.05587600      | 5.40701100  | -0.28462200 |
| C        | 2.88611900      | 4.05626600  | 0.85008100  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 1.66121300  | 5.58377400  | 1.90866800  |
| C  | -4.81678900 | -0.28800900 | 1.68402500  |
| C  | -4.21761600 | 0.52798300  | 2.83409900  |
| H  | -5.69505800 | -0.86956600 | 2.04351900  |
| H  | -4.06683000 | -1.06185900 | 1.35631100  |
| H  | -3.69072400 | -0.13949100 | 3.54415400  |
| H  | -3.49858000 | 1.30772700  | 2.50256600  |
| N  | -5.23555500 | 0.54708300  | 0.47474300  |
| C  | -6.46997200 | 1.35080200  | 0.82303300  |
| H  | -6.31055500 | 1.91477600  | 1.77330700  |
| H  | -6.71546000 | 2.08236900  | 0.03609200  |
| H  | -7.34802400 | 0.70349300  | 0.97670800  |
| C  | -5.55314800 | -0.38827600 | -0.67311300 |
| H  | -6.03167700 | 0.14060600  | -1.51217400 |
| H  | -4.62490100 | -0.86050700 | -1.07910100 |
| H  | -6.20501400 | -1.22280100 | -0.36387900 |
| O  | -5.24935600 | 1.27141600  | 3.49364200  |
| H  | 1.14071100  | 3.69866300  | -1.85283600 |
| Cl | -1.94755200 | 3.27061200  | -1.06330600 |
| H  | -5.66859900 | 0.74087100  | 4.20133100  |
| H  | 3.71252700  | 3.90433100  | 1.51756300  |
| C  | 2.70438900  | 3.44475700  | -0.39264200 |
| H  | 1.30385700  | 2.25961100  | 1.79050300  |
| H  | 4.13140200  | 2.80887000  | -1.88566600 |
| H  | 1.95472300  | 1.41491200  | -2.42744400 |
| Zn | 0.02505600  | -0.96719300 | -0.57963000 |
| Zn | -1.59192800 | -1.98341300 | -0.30720200 |
| Cl | 0.35614500  | -3.44092700 | -0.34187100 |
| Cl | -1.50009500 | -0.49058800 | 1.63316000  |
| Cl | -2.04292200 | -0.39293000 | -2.13199200 |
| Cl | -3.53111200 | -3.11867100 | -0.11206000 |
| O  | 0.61787500  | -0.94545000 | -2.77019100 |
| H  | 0.09087800  | -1.44457800 | -3.40762900 |
| O  | -0.18739800 | 1.17824600  | -0.42095600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.66865100  | 1.64006500  | -0.66561600 |
| O | 1.20280200  | -1.17212200 | 1.45123000  |
| H | 0.84642300  | -1.81098900 | 2.09066200  |
| O | 2.46018500  | -2.73031100 | -2.59837700 |
| H | 2.78065500  | -2.45063700 | -1.69686800 |
| O | 0.54954700  | 1.66608500  | 1.91155800  |
| H | 0.91054700  | 0.76638200  | 2.04927700  |
| O | -0.24662400 | 1.88648200  | -2.81122900 |
| H | 0.18664600  | 0.99224300  | -2.79138400 |
| H | -0.96241400 | 1.80635500  | -3.45179000 |
| H | 1.57238200  | -1.35167500 | -2.83547300 |
| H | 2.09476000  | -1.51561700 | 1.19410900  |
| H | 1.86415500  | -3.46882000 | -2.43981700 |
| H | -0.33649600 | 1.51512900  | 0.56366000  |
| H | -1.14957900 | 2.23085800  | -1.44891600 |
| C | -4.13606800 | 1.48880100  | 0.04116700  |
| H | -3.16094000 | 0.96110600  | -0.05854600 |
| H | -4.34986500 | 1.94427600  | -0.94227000 |
| H | -3.97685000 | 2.31166000  | 0.76226000  |

### *Transition state b) TS3*

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.513692           |
| Thermal correction to Energy=                | 0.567663           |
| Thermal correction to Enthalpy=              | 0.568608           |
| Thermal correction to Gibbs Free Energy=     | 0.423048           |
| Sum of electronic and zero-point Energies=   | -0.595689          |
| Sum of electronic and thermal Energies=      | -0.541717          |
| Sum of electronic and thermal Enthalpies=    | -0.540773          |
| Sum of electronic and thermal Free Energies= | -0.686333          |

|          | E (Thermal)     | CV             | S              |
|----------|-----------------|----------------|----------------|
|          | KCal/Mol        | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total    | 356.214         | 190.813        | 306.356        |
| Charge:0 | Multiplicity: 1 |                |                |
| C        | 2.75971700      | -0.08724300    | -0.74882300    |
| C        | 2.50058500      | 1.14619800     | -1.40252200    |
| C        | 3.59526600      | 2.13405300     | -1.07470800    |
| C        | 4.50550900      | 1.37043300     | -0.09106600    |
| N        | 3.96284800      | 0.01411600     | 0.02527800     |
| O        | 5.49871300      | 1.71883100     | 0.48254800     |
| O        | 2.05609700      | -1.13632900    | -0.70511100    |
| C        | 4.51885500      | -1.04949600    | 0.81602400     |
| C        | 4.26898900      | -2.38813600    | 0.45886200     |
| C        | 5.30494000      | -0.74997800    | 1.94419900     |
| C        | 4.79807100      | -3.41732400    | 1.24081700     |
| H        | 3.68533300      | -2.62649800    | -0.43517500    |
| C        | 5.82760500      | -1.79269400    | 2.70869000     |
| H        | 5.51910900      | 0.28992800     | 2.20912800     |
| C        | 5.57269900      | -3.12606300    | 2.36652800     |
| H        | 4.60970800      | -4.45435500    | 0.96340200     |
| H        | 6.44119900      | -1.56292600    | 3.58059000     |
| H        | 5.98410600      | -3.93173000    | 2.97065000     |
| N        | 1.86014000      | 3.96599900     | -0.82293700    |
| C        | 1.71965700      | 5.18331000     | -0.15339100    |
| C        | 2.88504600      | 5.41037000     | 0.58242900     |
| H        | 0.83061800      | 5.78067700     | -0.23512200    |
| C        | 3.75881700      | 4.30911300     | 0.36542700     |
| H        | 3.09070900      | 6.25775700     | 1.20267900     |
| C        | -5.02257800     | -0.13980000    | 1.54082300     |
| C        | -4.44897500     | 0.51498000     | 2.80160000     |
| H        | -5.95542200     | -0.69515900    | 1.78464200     |
| H        | -4.29685100     | -0.92333100    | 1.18208400     |
| H        | -4.00750300     | -0.25514800    | 3.46428300     |
| H        | -3.66721200     | 1.27532900     | 2.58846500     |
| N        | -5.30704100     | 0.83733400     | 0.40103000     |
| C        | -6.49011000     | 1.70800000     | 0.76482800     |
| H        | -6.33927300     | 2.16957900     | 1.76982300     |
| H        | -6.63086600     | 2.52604200     | 0.03923100     |
| H        | -7.42495300     | 1.12758300     | 0.81444600     |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -5.63460700 | 0.04222300  | -0.84542400 |
| H  | -5.96606500 | 0.69400200  | -1.66966000 |
| H  | -4.73938700 | -0.51306700 | -1.21821800 |
| H  | -6.41244400 | -0.71758900 | -0.66275100 |
| O  | -5.46705000 | 1.25605800  | 3.48244600  |
| H  | 1.16788700  | 3.53933200  | -1.42775900 |
| Cl | -1.63570200 | 3.29093700  | -0.47729600 |
| H  | -5.98488500 | 0.67783400  | 4.07943100  |
| H  | 4.73413800  | 4.17843900  | 0.79208500  |
| C  | 3.11117000  | 3.42060400  | -0.49956100 |
| H  | 0.29220100  | 1.41552800  | 0.73287800  |
| H  | 4.21100200  | 2.35929200  | -1.98958000 |
| H  | 2.04082800  | 1.18310700  | -2.38498600 |
| Zn | -0.13592700 | -0.87067700 | -0.57210100 |
| Zn | -1.79451400 | -1.85141300 | -0.43521000 |
| Cl | 0.07215400  | -3.40207200 | -0.60967300 |
| Cl | -1.65671500 | -0.54611400 | 1.64834400  |
| Cl | -2.09392200 | -0.14969900 | -2.17085900 |
| Cl | -3.78794000 | -2.90199400 | -0.34963900 |
| O  | 0.57270400  | -0.95744800 | -2.70151500 |
| H  | -0.00247200 | -1.34749400 | -3.37401400 |
| O  | 0.13213600  | 1.15954500  | -0.24905700 |
| H  | 1.20900500  | 1.47992800  | -0.78115200 |
| O  | 0.98290500  | -1.53067800 | 1.43679900  |
| H  | 0.57401300  | -2.26762800 | 1.92005900  |
| O  | 2.33779500  | -2.89143300 | -2.54688300 |
| H  | 2.57823700  | -2.73286200 | -1.60042300 |
| O  | 0.71794400  | 1.12612700  | 2.30892300  |
| H  | 0.90690800  | 0.16251500  | 2.29260800  |
| O  | -0.08098600 | 2.11909400  | -2.52381000 |
| H  | 0.13141600  | 1.20627100  | -2.78346500 |
| H  | -0.94889500 | 2.31175100  | -2.88516900 |
| H  | 1.44539200  | -1.51003400 | -2.74477600 |
| H  | 1.87600100  | -1.85259200 | 1.15737300  |
| H  | 1.74544000  | -3.64957700 | -2.54526600 |
| H  | -0.09113900 | 1.22884300  | 2.81348900  |
| H  | -0.77225100 | 2.19723100  | -0.66988600 |
| C  | -4.10976900 | 1.71443100  | 0.11853800  |
| H  | -3.18053900 | 1.11273400  | 0.00661100  |
| H  | -4.22302900 | 2.28772900  | -0.81878200 |

H            -3.91970900    2.44308200    0.92873100

*N-Phenyl succinimide + ChCl + 2 ZnCl<sub>2</sub> • 3H<sub>2</sub>O d)P*

|  | (Hartree/Particle) |
|--|--------------------|
| Zero-point correction=                       | 0.516965           |
| Thermal correction to Energy=                | 0.571622           |
| Thermal correction to Enthalpy=              | 0.572566           |
| Thermal correction to Gibbs Free Energy=     | 0.423305           |
| Sum of electronic and zero-point Energies=   | -0.620928          |
| Sum of electronic and thermal Energies=      | -0.566271          |
| Sum of electronic and thermal Enthalpies=    | -0.565327          |
| Sum of electronic and thermal Free Energies= | -0.714588          |

|       | E (Thermal) | CV             | S              |
|-------|-------------|----------------|----------------|
|       | KCal/Mol    | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 358.698     | 190.752        | 314.146        |

|          |                 |             |             |
|----------|-----------------|-------------|-------------|
| Charge:0 | Multiplicity: 1 |             |             |
| C        | 3.59611200      | -0.41475300 | -1.06561700 |
| C        | 3.77234000      | 0.98888000  | -1.57740600 |
| C        | 4.47719200      | 1.78136000  | -0.45924700 |
| C        | 4.73645700      | 0.76611900  | 0.66812600  |
| N        | 4.15929800      | -0.50432100 | 0.23858900  |
| O        | 5.31222400      | 0.90178200  | 1.70725200  |
| O        | 3.05382100      | -1.35211300 | -1.62996000 |
| C        | 4.14139400      | -1.70308100 | 1.04609200  |
| C        | 4.24837600      | -2.96084600 | 0.42799600  |
| C        | 4.00252500      | -1.59513800 | 2.44035200  |
| C        | 4.21504800      | -4.11168800 | 1.21855100  |
| H        | 4.36353600      | -3.04202000 | -0.65399700 |
| C        | 3.97632900      | -2.75808400 | 3.21199300  |
| H        | 3.92781100      | -0.61484100 | 2.92025200  |
| C        | 4.07853700      | -4.01542700 | 2.60672100  |
| H        | 4.30287500      | -5.09022900 | 0.74621900  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 3.87563900  | -2.67971300 | 4.29523500  |
| H  | 4.05880700  | -4.91665200 | 3.21668800  |
| N  | 2.38240900  | 2.84371400  | 0.53134300  |
| C  | 1.98128900  | 4.10902300  | 0.95830900  |
| C  | 3.03472800  | 5.00193900  | 0.73814800  |
| H  | 1.01391600  | 4.29343900  | 1.39934000  |
| C  | 4.11154400  | 4.27058900  | 0.17089700  |
| H  | 3.03524200  | 6.04952600  | 0.96121900  |
| C  | -4.97590200 | -0.65099500 | 1.43718800  |
| C  | -4.31362000 | -0.73388100 | 2.81646800  |
| H  | -5.94497200 | -1.19787700 | 1.44215300  |
| H  | -4.33040800 | -1.20091200 | 0.69532000  |
| H  | -3.93297800 | -1.75888700 | 2.99498500  |
| H  | -3.46762400 | -0.02551700 | 2.94562100  |
| N  | -5.21047700 | 0.77415800  | 0.93787400  |
| C  | -6.30940200 | 1.42273400  | 1.75129500  |
| H  | -6.09272500 | 1.32834500  | 2.84214500  |
| H  | -6.40271500 | 2.49728600  | 1.52111000  |
| H  | -7.28646400 | 0.94676900  | 1.57372100  |
| C  | -5.63704800 | 0.70651000  | -0.51380000 |
| H  | -5.89117800 | 1.70323600  | -0.91062500 |
| H  | -4.81698200 | 0.30849000  | -1.15966100 |
| H  | -6.50127800 | 0.03902200  | -0.66308000 |
| O  | -5.24119900 | -0.34737400 | 3.83595400  |
| H  | 1.80477600  | 1.99672300  | 0.55481200  |
| Cl | -1.37860900 | 3.14096500  | 1.00477400  |
| H  | -5.79756900 | -1.10443100 | 4.11166000  |
| H  | 5.06553300  | 4.67001200  | -0.10503400 |
| C  | 3.69717700  | 2.93747400  | 0.04962900  |
| H  | 5.47435300  | 2.15380100  | -0.81921600 |
| H  | 2.76633800  | 1.41974000  | -1.83621700 |
| Zn | -0.33178700 | -0.30671300 | -0.78436400 |
| Zn | -1.91416100 | -1.27608900 | -1.30620700 |
| Cl | -0.03869900 | -2.24077600 | -2.46685300 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| Cl | -1.65246400 | -1.43020500 | 1.17102300  |
| Cl | -2.21696700 | 1.03491300  | -1.95799500 |
| Cl | -3.91586900 | -2.24681700 | -1.63269400 |
| O  | 0.76704500  | 0.94915600  | -2.04702800 |
| H  | 0.40068600  | 1.92303700  | -2.05487900 |
| O  | 0.21305000  | 0.93793100  | 0.67611900  |
| H  | 0.33512900  | 0.56395900  | 1.59270900  |
| O  | 1.02838900  | -1.92385400 | 0.13730900  |
| H  | 0.58474000  | -2.78938200 | 0.24255500  |
| O  | 1.69705700  | -0.37305100 | -3.98561400 |
| H  | 2.14871200  | -0.92180100 | -3.30627300 |
| O  | 0.96953700  | -0.67038400 | 2.62758700  |
| H  | 1.34323900  | -1.20007400 | 1.89375200  |
| O  | -0.17038300 | 3.39266800  | -1.76797200 |
| H  | 0.28851600  | 3.75655900  | -0.99379300 |
| H  | -1.10188600 | 3.31777300  | -1.50122000 |
| H  | 0.83956000  | 0.68153100  | -3.02560900 |
| H  | 1.82454600  | -2.12380200 | -0.43796700 |
| H  | 1.08593200  | -0.96056900 | -4.44028700 |
| H  | 0.21639500  | -1.16597600 | 2.95246900  |
| H  | -0.51192900 | 1.91199700  | 0.86094000  |
| C  | -3.95507000 | 1.60867000  | 1.04235400  |
| H  | -3.06480600 | 1.05672800  | 0.67564300  |
| H  | -4.01254200 | 2.53268300  | 0.43696000  |
| H  | -3.73091200 | 1.91759400  | 2.08022600  |
| H  | 4.33047300  | 1.01177100  | -2.53321100 |