

Supporting Information (SI)

The reaction of acetamiprid with OH radicals in the environment: A theoretical study

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Table S1. The method to calculate rate constant following the conventional transition state theory

The rate constant (k) was calculated by using the conventional transition state theory (TST) (at 298.15 K, 1M standard state) according to the equation (1):¹⁻⁵

$$k = \sigma \kappa \frac{k_B T}{h} e^{-(\Delta G^\ddagger)/RT} \quad (1)$$

Where: σ is the reaction symmetry number,^{6,7}

κ contains the tunneling corrections calculated using the Eckart barrier,⁸

k_B is the Boltzmann constant,

h is the Planck constant,

$\Delta G^\ddagger$ is the Gibbs free energy of activation.

The Marcus Theory was used to estimate the reaction barriers of SET reactions.⁹⁻¹² The free energy of reaction $\Delta G^\ddagger$ for the SET pathway was computed following the equations (2,3).

$$\Delta G_{\text{SET}}^\ddagger = \frac{\lambda}{4} \left(1 + \frac{\Delta G_{\text{SET}}^0}{\lambda} \right)^2 \quad (2)$$

$$\lambda \approx \Delta E_{\text{SET}} - \Delta G_{\text{SET}}^0 \quad (3)$$

where ΔG_{SET} is the Gibbs energy of reaction, ΔE_{SET} is the non-adiabatic energy difference between reactants and vertical products for SET.^{13,14}

For rate constants that were close to the diffusion limit a correction was applied to yield realistic results¹⁵. The apparent rate constants (k_{app}) were calculated following the Collins–Kimball theory in the solvents at 298.15K;¹⁶ the steady-state Smoluchowski rate constant (k_D) for an irreversible bimolecular diffusion–controlled reaction was calculated following the literature as corroding to equations (4,5).^{15,17}

$$k_{\text{app}} = \frac{k_{\text{TST}} k_D}{k_{\text{TST}} + k_D} \quad (4)$$

$$k_D = 4\pi R_{AB} D_{AB} N_A \quad (5)$$

where R_{AB} is the reaction distance, N_A is the Avogadro constant, and $D_{AB} = D_A + D_B$ (D_{AB} is the mutual diffusion coefficient of the reactants A and B),^{16,18} where D_A or D_B is estimated using the

Stokes–Einstein formulation (6).^{19,20}

$$D_{A \text{ or } B} = \frac{k_B T}{6\pi\eta a_{A \text{ or } B}} \quad (6)$$

η is the viscosity of the solvents (i.e. $\eta(\text{H}_2\text{O}) = 8.91 \times 10^{-4} \text{ Pa s}$, $\eta(\text{pentyl ethanoate}) = 8.62 \times 10^{-4} \text{ Pa s}$) and a is the radius of the solute.

The kinetic study requires different considerations. Water (dielectric constants, $\epsilon = 78.35$) and pentyl ethanoate ($\epsilon = 4.73$) are the *de facto* standard solvents in the literature to mimic the polar and nonpolar environments.^{15,21-23} All transition states were characterized by the existence of only one single imaginary frequency. Intrinsic coordinate calculations (IRCs) were performed to ensure that each transition state is connected correctly with the pre-complex and post-complex.

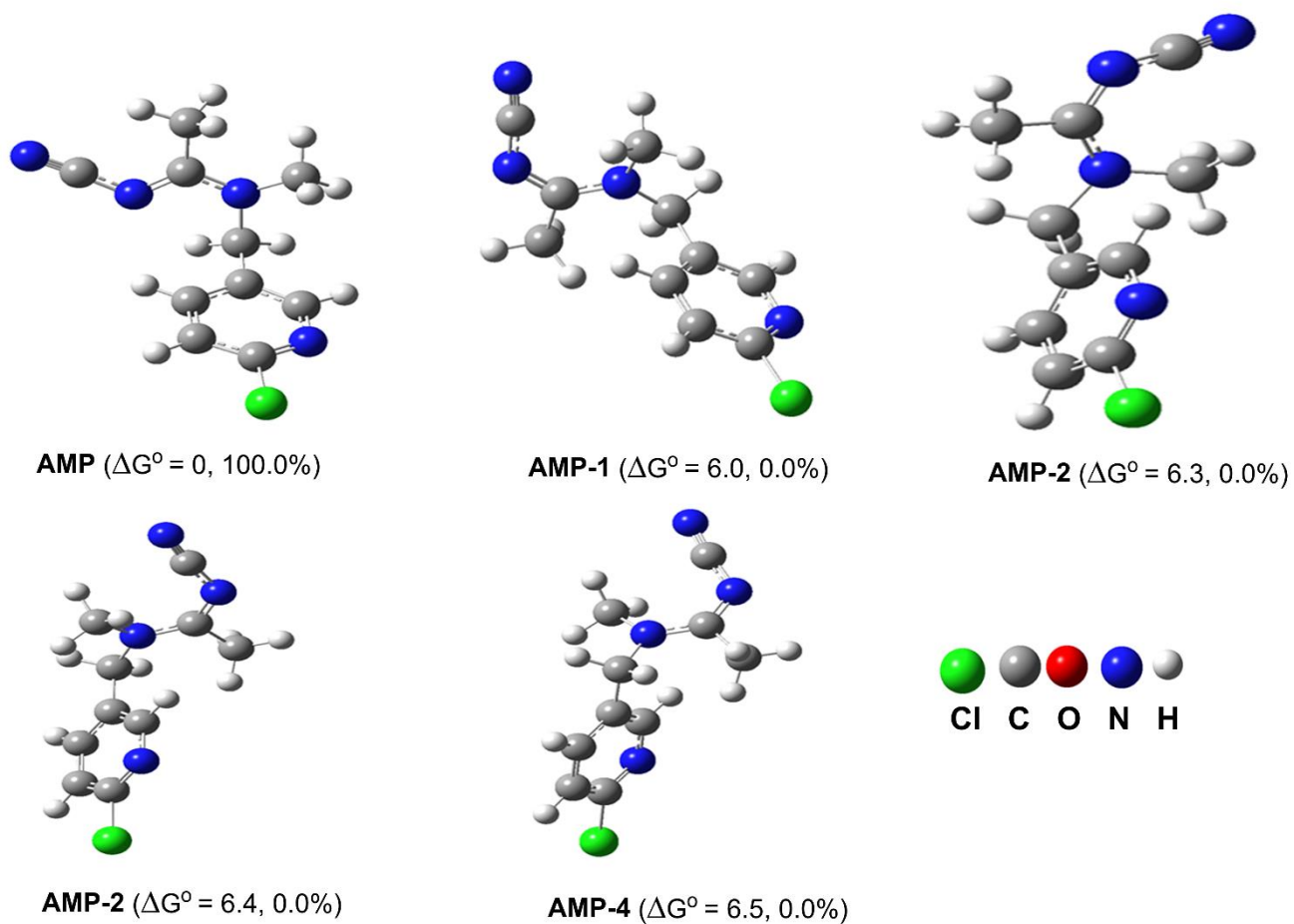


Figure S1. The typical conformers of AMP and the relative free energies ΔG° (in kcal/mol) compared to the AMP conformer

Table S2: The Cartesian coordinates, energies and imaginary frequency of AMP, RC and TS of the reaction between AMP with HO^{*} in the studied media (G: the gas phase; P: pentyl ethanoate; W: water)

Name				AMP-G
Cartesian Coordinates				Frequency and Energy
Cl	-5.12883800	1.54695900	0.62260600	Zero-point correction= 0.203661 (Hartree/Particle)
N	0.96685100	-0.91907100	-0.22803400	Thermal correction to Energy= 0.218079
N	-3.53048200	-0.34294200	-0.21218200	Thermal correction to Enthalpy= 0.219024
N	1.92881300	1.12528000	-0.52565700	Thermal correction to Gibbs Free Energy= 0.160012
N	3.59931300	2.87919700	0.02686700	Sum of electronic and zero-point Energies= -1066.578294
C	0.05790500	-0.64003000	-1.34504300	Sum of electronic and thermal Energies= -1066.563876
C	-1.23929000	-0.02464600	-0.87858200	Sum of electronic and thermal Enthalpies= -1066.562932
C	1.85493400	0.02062500	0.16439300	Sum of electronic and thermal Free Energies= -1066.621943
C	0.60982900	-2.05410300	0.61159900	
C	-1.35197900	1.34405200	-0.61551100	
C	-2.36402000	-0.81174600	-0.66262800	
C	2.70744300	-0.27466900	1.36939900	
C	-2.55424000	1.84827200	-0.15198000	
C	-3.60133800	0.94514800	0.03149100	
C	2.83892500	2.03816600	-0.20246900	
H	-0.13881300	-1.58950100	-1.84768900	
H	0.57245600	0.02187400	-2.03810100	
H	-0.17070000	-1.79101400	1.33345500	
H	1.47719700	-2.43451600	1.14494300	
H	0.23271600	-2.85203800	-0.02854800	
H	-0.50086600	1.99588500	-0.77694800	
H	-2.33459200	-1.87922900	-0.86810500	
H	3.37804900	0.55950100	1.56337200	
H	3.30297300	-1.17457000	1.20475500	
H	2.08022200	-0.43632600	2.24820600	
H	-2.69246800	2.89943800	0.06039700	
Name				AMP-P
Cartesian Coordinates				Frequency and Energy
Cl	-5.27367900	1.42714500	0.46153400	Zero-point correction= 0.203954 (Hartree/Particle)
N	0.94117300	-0.83438100	-0.16133100	Thermal correction to Energy= 0.218213
N	-3.62112600	-0.37155500	-0.46814200	Thermal correction to Enthalpy= 0.219157
N	2.07146100	1.09278700	-0.61317300	Thermal correction to Gibbs Free Energy= 0.160687
N	3.86117100	2.75800700	-0.23577800	Sum of electronic and zero-point Energies= -1066.607481
C	0.05229300	-0.60064800	-1.30420500	Sum of electronic and thermal Energies= -1066.593222
C	-1.27518000	-0.03112200	-0.86724700	Sum of electronic and thermal Enthalpies= -1066.592278
C	1.90912300	0.03404400	0.15263500	Sum of electronic and thermal Free Energies= -1066.650748
C	0.57983300	-1.94591400	0.71466200	
C	-1.39296300	1.29000600	-0.42702500	
C	-2.42245800	-0.81377900	-0.86632400	
C	2.74852500	-0.25697200	1.36330500	
C	-2.62515500	1.76455300	-0.01192200	
C	-3.69399300	0.87281700	-0.05916500	
C	3.04030200	1.94967300	-0.37438800	
H	-0.10129200	-1.55877100	-1.80378600	
H	0.55251800	0.07668000	-1.99233300	
H	-0.08018300	-1.61479800	1.52165100	
H	1.46637100	-2.41030900	1.14055600	
H	0.05699200	-2.69410900	0.12005800	
H	-0.52441400	1.94034000	-0.41778200	

H	-2.38474400	-1.84487700	-1.20621700	
H	3.44074500	0.56040700	1.55206800	
H	3.32174300	-1.17415200	1.21010900	
H	2.11540000	-0.39641000	2.24130100	
H	-2.76246400	2.78133400	0.33094000	
Name				AMP-W
Cartesian Coordinates				Frequency and Energy
Cl	-5.13181000	1.93356300	-0.12885900	Zero-point correction= 0.203603 (Hartree/Particle)
N	0.96652900	-0.95214500	-0.07245500	Thermal correction to Energy= 0.217914
N	-3.55893000	0.26470200	-1.39232400	Thermal correction to Enthalpy= 0.218858
N	1.93402700	0.94354500	-0.89404700	Thermal correction to Gibbs Free Energy= 0.160139
N	3.58358100	2.78640200	-0.83020800	Sum of electronic and zero-point Energies= -1066.602724
C	0.00120900	-0.93237500	-1.16518800	Sum of electronic and thermal Energies= -1066.588413
C	-1.26446000	-0.17962600	-0.81607200	Sum of electronic and thermal Enthalpies= -1066.587469
C	1.86098600	0.03043400	0.06021600	Sum of electronic and thermal Free Energies= -1066.646188
C	0.68093300	-1.87284300	1.03073400	
C	-1.35572400	0.71857200	0.24370400	
C	-2.39996000	-0.37028000	-1.59630500	
C	2.72273100	0.03231500	1.28373600	
C	-2.55037900	1.38581600	0.47467000	
C	-3.60388300	1.11038000	-0.38421700	
C	2.83122100	1.89833400	-0.80788700	
H	-0.24574900	-1.96511200	-1.41316200	
H	0.46859200	-0.48206200	-2.03932500	
H	0.13811500	-1.36768900	1.83381400	
H	1.60097100	-2.29719000	1.42759100	
H	0.06643300	-2.68201800	0.64248600	
H	-0.50866400	0.90250800	0.89629700	
H	-2.37847900	-1.06881300	-2.42674500	
H	3.38814600	0.89250400	1.28635500	
H	3.32008300	-0.88090000	1.32175000	
H	2.09609100	0.06153800	2.17794200	
H	-2.66160900	2.09043800	1.28749900	
Name				RC-G
Cartesian Coordinates				Frequency and Energy
Cl	-5.65479400	1.06897200	-0.00155400	Zero-point correction= 0.214643 (Hartree/Particle)
N	0.66396700	-0.99162200	-0.11465500	Thermal correction to Energy= 0.232039
N	-3.81097800	-0.40574600	-1.11688800	Thermal correction to Enthalpy= 0.232983
N	1.67860000	1.01862200	0.20857400	Thermal correction to Gibbs Free Energy= 0.163942
N	3.31061100	2.49994100	1.33779700	Sum of electronic and zero-point Energies= -1142.306685
C	-0.03978300	-0.45866300	-1.28659300	Sum of electronic and thermal Energies= -1142.289290
C	-1.44252300	-0.01981000	-0.95028200	Sum of electronic and thermal Enthalpies= -1142.288345
C	1.54156600	-0.23500000	0.56350000	Sum of electronic and thermal Free Energies= -1142.357386
C	0.33206300	-2.36345300	0.24385300	
C	-1.68038300	1.10842300	-0.15834400	
C	-2.54635000	-0.73160200	-1.39993900	
C	2.30741700	-0.87116500	1.69251300	
C	-2.98236400	1.46164800	0.14256800	
C	-4.00127400	0.65541800	-0.36944900	
C	2.56184700	1.77769100	0.83284900	
H	-0.06630100	-1.25111200	-2.03924700	
H	0.54337000	0.37269200	-1.67784600	
H	-0.73357400	-2.51737600	0.06533700	
H	0.52241600	-2.55585300	1.29599200	

H	0.89910600	-3.07549200	-0.36336800	
H	-0.84555500	1.69797300	0.20549900	
H	-2.41607100	-1.60996200	-2.02750300	
H	3.12301500	-0.22044000	2.00110300	
H	2.71255500	-1.83841600	1.39515800	
H	1.64854800	-1.02265600	2.55112200	
H	-3.21877400	2.32748900	0.74559000	
O	5.40672800	3.73733300	2.96436200	
H	4.69586900	3.38349700	2.38908400	
Name				RC-P
Cartesian Coordinates				Frequency and Energy
Cl	-5.66190600	1.13777400	-0.09902300	Zero-point correction= 0.214483 (Hartree/Particle)
N	0.65035300	-1.00231100	-0.07109700	Thermal correction to Energy= 0.230817
N	-3.79732500	-0.29200600	-1.24307000	Thermal correction to Enthalpy= 0.231762
N	1.73810300	0.96617000	0.26973300	Thermal correction to Gibbs Free Energy= 0.166668
N	3.38702200	2.43048900	1.37425400	Sum of electronic and zero-point Energies= -1142.339770
C	-0.02687500	-0.44710800	-1.24851300	Sum of electronic and thermal Energies= -1142.323436
C	-1.43204300	0.00070500	-0.93142300	Sum of electronic and thermal Enthalpies= -1142.322492
C	1.55311100	-0.29680700	0.60910700	Sum of electronic and thermal Free Energies= -1142.387586
C	0.31505600	-2.38632600	0.25231500	
C	-1.67940800	1.06305000	-0.05755700	
C	-2.52907500	-0.63818800	-1.49392800	
C	2.29267300	-0.97369600	1.72645800	
C	-2.98457100	1.43460100	0.21291300	
C	-3.99241100	0.70793900	-0.41713200	
C	2.62709800	1.70316900	0.88489700	
H	-0.04829900	-1.22950800	-2.01065000	
H	0.56522000	0.38551300	-1.62294100	
H	-0.72600900	-2.55818000	-0.02234300	
H	0.41592400	-2.57817000	1.31741900	
H	0.94983500	-3.07801600	-0.30843500	
H	-0.85244300	1.59632800	0.39955300	
H	-2.38954700	-1.46700600	-2.18217600	
H	3.12538600	-0.35728600	2.05857700	
H	2.67191400	-1.94485100	1.40708100	
H	1.61943200	-1.13114000	2.57308200	
H	-3.22124300	2.25322000	0.87912900	
O	5.30400800	4.10542400	2.66057100	
H	4.63497300	3.53754700	2.21243200	
Name				RC-W
Cartesian Coordinates				Frequency and Energy
Cl	-4.78231100	2.44822100	0.21663700	Zero-point correction= 0.213035 (Hartree/Particle)
N	0.87806400	-1.22792900	-0.12452400	Thermal correction to Energy= 0.230076
N	-3.31799900	0.95198000	-1.35518200	Thermal correction to Enthalpy= 0.231020
N	1.90015700	0.77208100	-0.49843400	Thermal correction to Gibbs Free Energy= 0.165306
N	3.50821000	2.56472700	0.06504800	Sum of electronic and zero-point Energies= -1142.335640
C	-0.06135600	-0.92164700	-1.19770000	Sum of electronic and thermal Energies= -1142.318599
C	-1.22480800	-0.06648100	-0.74153000	Sum of electronic and thermal Enthalpies= -1142.317655
C	1.78371500	-0.32055600	0.24274800	Sum of electronic and thermal Free Energies= -1142.383369
C	0.54880300	-2.36845100	0.73388000	
C	-1.32776000	0.48719300	0.53093600	
C	-2.25173300	0.19865200	-1.64200800	
C	2.60532500	-0.59088400	1.46372700	
C	-2.42699400	1.27304000	0.84947300	

C	-3.37761100	1.46095900	-0.14186600	
C	2.78067100	1.68428800	-0.16410000	
H	-0.43494000	-1.86665000	-1.59185200	
H	0.47000500	-0.41401700	-2.00161000	
H	0.01123000	-3.09961700	0.13446300	
H	-0.08249400	-2.05797400	1.57078400	
H	1.45345100	-2.83491900	1.11668000	
H	-0.56476200	0.31766500	1.28346100	
H	-2.21529900	-0.21405400	-2.64522000	
H	3.27194800	0.24264600	1.67340100	
H	3.19997300	-1.49519100	1.31788900	
H	1.95082800	-0.75196200	2.32314200	
H	-2.54065400	1.72187900	1.82703500	
O	0.96897300	2.29978900	2.08880800	
H	1.78632300	2.74853900	1.79514900	
Name				C2-RAF-G
Cartesian Coordinates				Frequency and Energy
Cl	-5.15574700	1.65785300	0.69673000	Zero-point correction= 0.214752 (Hartree/Particle)
N	0.85818400	-0.96926700	-0.25382700	Thermal correction to Energy= 0.231070
N	-3.65832600	-0.29313000	-0.18352900	Thermal correction to Enthalpy= 0.232014
N	1.91341300	0.97666900	-0.77875500	Thermal correction to Gibbs Free Energy= 0.167605
N	3.48559700	2.86338400	-0.56596100	Sum of electronic and zero-point Energies= -1142.291761
C	-0.09343600	-0.74080500	-1.34545000	Sum of electronic and thermal Energies= -1142.275443
C	-1.35802300	-0.07714500	-0.85737900	Sum of electronic and thermal Enthalpies= -1142.274499
C	1.82568900	-0.06551600	0.00240200	Sum of electronic and thermal Free Energies= -1142.338908
C	0.51611400	-2.03178200	0.68233900	
C	-1.39970600	1.28985400	-0.56441400	v = -650.47
C	-2.51844700	-0.81149300	-0.64925100	
C	2.71815500	-0.31353600	1.18823000	
C	-2.57236100	1.84441900	-0.08436300	
C	-3.66343600	0.99125100	0.08543400	
C	2.93088100	1.82107700	-0.65367600	
H	-0.32742900	-1.71239400	-1.78608300	
H	0.40190400	-0.12809700	-2.09548400	
H	-0.14057000	-1.67152200	1.48094100	
H	1.41105900	-2.46836100	1.11964000	
H	-0.00748000	-2.81512400	0.13475300	
H	-0.51723400	1.90104200	-0.71876100	
H	-2.54287200	-1.87523000	-0.87303200	
H	3.37669700	0.53594900	1.34412300	
H	3.34092100	-1.19259400	1.01111700	
H	2.11742800	-0.48155400	2.08365600	
H	-2.65672200	2.89648300	0.15062400	
O	4.50027200	0.72684300	-0.88313800	
H	5.21955500	1.35975000	-1.03012700	
Name				C4-RAF-G
Cartesian Coordinates				Frequency and Energy
Cl	-5.19131800	1.46661500	0.52109000	Zero-point correction= 0.215593 (Hartree/Particle)
N	0.92487400	-0.89902300	-0.21521900	Thermal correction to Energy= 0.231311
N	-3.61507400	-0.34418500	-0.50219200	Thermal correction to Enthalpy= 0.232255
N	2.00502500	1.08681300	-0.64964100	Thermal correction to Gibbs Free Energy= 0.170412
N	3.63176000	2.88369500	-0.10770000	Sum of electronic and zero-point Energies= -1142.280912
C	0.04711200	-0.65210800	-1.36036700	Sum of electronic and thermal Energies= -1142.265194
C	-1.26049300	-0.06495400	-0.88565700	Sum of electronic and thermal Enthalpies= -1142.264250

C	2.02645000	-0.03882600	0.05013700	Sum of electronic and thermal Free Energies= v =-463.47	-1142.326093	
C	0.61744800	-2.01850600	0.65841200			
C	-1.32465700	1.23814800	-0.38149700			
C	-2.43463500	-0.80499400	-0.92226300			
C	2.64946600	-0.13095900	1.41736200			
C	-2.54059000	1.72969600	0.05547600			
C	-3.64615500	0.88086700	-0.03077400			
C	2.89007800	2.02392000	-0.33706000			
H	-0.11907500	-1.60711300	-1.86332400			
H	0.56014300	0.03648900	-2.02763600			
H	0.39706500	-1.66266100	1.66692700			
H	1.46737300	-2.70173700	0.68423800			
H	-0.25588600	-2.53588900	0.26664200			
H	-0.42587800	1.84544900	-0.34577200			
H	-2.43709400	-1.81819400	-1.31676400			
H	3.61792600	0.36595100	1.37675300			
H	2.79488100	-1.15849000	1.73934000			
H	2.01817800	0.40314000	2.13249800			
H	-2.64721500	2.73170200	0.44774600			
O	2.93980900	-1.33096100	-0.80368000			
H	2.97697600	-0.94178600	-1.69068400			
Name				C5-FHT-G		
Cartesian Coordinates				Frequency and Energy		
Cl	-5.33704800	1.37482700	0.43136000	Zero-point correction=	0.210207 (Hartree/Particle)	
N	0.86998300	-0.95779300	-0.20257700	Thermal correction to Energy=	0.226357	
N	-3.72660400	-0.16487700	-0.93175100	Thermal correction to Enthalpy=	0.227301	
N	2.05194600	0.97755100	-0.50666500	Thermal correction to Gibbs Free Energy=	0.163200	
N	3.71312800	2.59264300	0.38225000	Sum of electronic and zero-point Energies=	-1142.295849	
C	0.00316900	-0.60639700	-1.32916700	Sum of electronic and thermal Energies=	-1142.279699	
C	-1.32507300	-0.06761200	-0.85401600	Sum of electronic and thermal Enthalpies=	-1142.278754	
C	1.84931700	-0.12130900	0.18251200	Sum of electronic and thermal Free Energies=	-1142.342856	
C	0.47319600	-2.11785000	0.59291800	v =-1482.54		
C	-1.39566900	0.97831400	0.07123900			
C	-2.52177500	-0.59901300	-1.31384600			
C	2.64372600	-0.43738500	1.40177200			
C	-2.63338900	1.43923900	0.47864400			
C	-3.76006200	0.82044700	-0.06660100			
C	2.95803200	1.82053100	-0.03866700			
H	-0.15006300	-1.50288200	-1.93447600			
H	0.52654100	0.13185900	-1.93379600			
H	-0.40406000	-2.56007900	0.12433800			
H	0.19952500	-1.83187200	1.61046000			
H	1.26406800	-2.86936200	0.62078800			
H	-0.48807600	1.42583800	0.46438500			
H	-2.52155700	-1.41813300	-2.02840600			
H	3.70033500	-0.21681500	1.26086000			
H	2.48267800	-1.41171200	1.84980500			
H	2.28110500	0.36225400	2.23113700			
H	-2.73984000	2.24588000	1.19069400			
O	1.98507300	1.48986500	2.86454700			
H	2.58904100	2.11074100	2.41279200			
Name				C7-FHT-G		
Cartesian Coordinates				Frequency and Energy		
Cl	-5.37235400	1.54941600	0.03532300	Zero-point correction=	0.210734 (Hartree/Particle)	

N	0.85522300	-0.77023700	0.10375300	Thermal correction to Energy=	0.227493
N	-3.69725000	-0.33145800	-0.65599600	Thermal correction to Enthalpy=	0.228437
N	1.99046500	1.11273200	-0.48348500	Thermal correction to Gibbs Free Energy=	0.162217
N	3.83503600	2.75570800	-0.21465900	Sum of electronic and zero-point Energies=	-1142.296720
C	0.03566400	-0.67517800	-1.10937800	Sum of electronic and thermal Energies=	-1142.279961
C	-1.31312400	-0.06549800	-0.82627100	Sum of electronic and thermal Enthalpies=	-1142.279017
C	1.88234100	0.09045500	0.31515300	Sum of electronic and thermal Free Energies=	-1142.345237
C	0.60275600	-1.88525900	0.96366000	ν =-744.10	
C	-1.43354900	1.27535600	-0.44726400		
C	-2.47787900	-0.81477900	-0.91422000		
C	2.81109100	-0.20612200	1.45840300		
C	-2.68654100	1.79256100	-0.17833700		
C	-3.77696200	0.92862200	-0.30144500		
C	2.99355500	1.96839100	-0.31116300		
H	-0.07882700	-1.68655700	-1.50781200		
H	0.58516200	-0.07817200	-1.83449100		
H	0.78178800	-1.65837400	2.01224200		
H	1.31444100	-2.73808000	0.67395000		
H	-0.42019300	-2.23393000	0.82540900		
H	-0.54657600	1.89645200	-0.37513100		
H	-2.43905000	-1.85922500	-1.21364900		
H	3.68352400	0.44157500	1.40173200		
H	3.12493500	-1.25093100	1.42505800		
H	2.30714400	-0.02012600	2.41034200		
H	-2.83363400	2.82360800	0.11238400		
O	2.57426300	-3.43859500	0.16322000		
H	2.45009800	-4.33558600	0.51453800		
Name				C8-FHT-G	
Cartesian Coordinates				Frequency and Energy	
Cl	-4.83444200	2.20105600	0.58640100	Zero-point correction=	0.209566 (Hartree/Particle)
N	0.96964600	-1.04760200	-0.19326700	Thermal correction to Energy=	0.226493
N	-3.30054100	0.10189100	0.33738200	Thermal correction to Enthalpy=	0.227437
N	1.51132600	1.15168700	-0.13050100	Thermal correction to Gibbs Free Energy=	0.161898
N	2.71164500	3.11971000	0.79550900	Sum of electronic and zero-point Energies=	-1142.291387
C	0.01057800	-0.74483000	-1.23279200	Sum of electronic and thermal Energies=	-1142.274460
C	-1.18417000	0.06949500	-0.80374000	Sum of electronic and thermal Enthalpies=	-1142.273516
C	1.67225200	-0.03351200	0.37358300	Sum of electronic and thermal Free Energies=	-1142.339055
C	1.09624800	-2.42729500	0.26199900	ν =-741.06	
C	-1.32140800	1.42258100	-1.11354600		
C	-2.20738900	-0.53659200	-0.08389700		
C	2.58347900	-0.35649800	1.52491600		
C	-2.45261600	2.09897100	-0.69092400		
C	-3.39885400	1.37696600	0.03465600		
C	2.17267800	2.18055100	0.38949300		
H	-0.30787500	-1.68881500	-1.67563900		
H	0.56450300	-0.15065500	-2.07128100		
H	0.43141000	-2.63468200	1.10645000		
H	2.12082600	-2.64826600	0.55367700		
H	0.83318000	-3.09141800	-0.55984200		
H	-0.53921700	1.92403100	-1.67172200		
H	-2.15308700	-1.59313000	0.16890600		
H	2.93057800	0.56517100	1.98767900		
H	3.45479900	-0.91238400	1.16996700		
H	2.07002200	-0.96372400	2.27140800		

H	-2.60570200	3.14840600	-0.90112300	
O	1.00606500	0.43893500	-3.30273500	
H	0.38166800	0.02957700	-3.92406200	
Name				C9-RAF-G
Cartesian Coordinates				Frequency and Energy
Cl	-4.74493200	1.71419300	1.07381600	Zero-point correction= 0.214638 (Hartree/Particle)
N	0.93727200	-0.92844500	-0.27912300	Thermal correction to Energy= 0.231008
N	-3.30803200	-0.24126300	0.11830900	Thermal correction to Enthalpy= 0.231953
N	1.80537000	1.17250800	-0.40203000	Thermal correction to Gibbs Free Energy= 0.168730
N	3.31215700	2.98951800	0.37263600	Sum of electronic and zero-point Energies= -1142.296320
C	0.10249300	-0.63246200	-1.44493500	Sum of electronic and thermal Energies= -1142.279949
C	-1.20154300	0.02991600	-1.05356700	Sum of electronic and thermal Enthalpies= -1142.279005
C	1.74718700	0.02951600	0.22324100	Sum of electronic and thermal Free Energies= -1142.342228
C	0.63263000	-2.14640400	0.46024000	v =-442.98
C	-1.27989400	1.43036700	-0.84588000	
C	-2.25051800	-0.74621100	-0.50146200	
C	2.53227600	-0.29041600	1.46669200	
C	-2.38014300	1.96146700	-0.21019700	
C	-3.35769600	1.07162200	0.25110200	
C	2.62809100	2.11792100	0.04016000	
H	-0.11254000	-1.56988700	-1.95732800	
H	0.65221700	0.01677900	-2.12163500	
H	-0.14816600	-1.98274900	1.21120100	
H	1.52062800	-2.53695700	0.95236200	
H	0.28258900	-2.89923900	-0.24523400	
H	-0.47851800	2.06246800	-1.20716900	
H	-2.23313700	-1.82594000	-0.62138700	
H	3.11091900	0.57763100	1.77471200	
H	3.21682500	-1.12048200	1.28040800	
H	1.86207900	-0.57769600	2.27894700	
H	-2.49316000	3.02516300	-0.05160200	
O	-1.85117300	-0.13774100	-2.95195300	
H	-2.64984600	0.41157800	-2.93571400	
Name				C10-RAF-G
Cartesian Coordinates				Frequency and Energy
Cl	-5.00813600	2.16348300	0.26380100	Zero-point correction= 0.214618 (Hartree/Particle)
N	0.92758800	-0.82166100	-0.38760200	Thermal correction to Energy= 0.231034
N	-2.98986200	0.52536900	0.46476700	Thermal correction to Enthalpy= 0.231979
N	1.67366400	1.20499000	0.29828900	Thermal correction to Gibbs Free Energy= 0.168418
N	3.03396100	2.67823600	1.76528300	Sum of electronic and zero-point Energies= -1142.295626
C	0.21496000	-0.12776400	-1.45195600	Sum of electronic and thermal Energies= -1142.279210
C	-1.03742500	0.56071600	-0.98482700	Sum of electronic and thermal Enthalpies= -1142.278265
C	1.68632200	-0.09007000	0.45428400	Sum of electronic and thermal Free Energies= -1142.341826
C	0.79973700	-2.27395000	-0.30837000	v =-486.73
C	-1.55304100	1.66746400	-1.64893400	
C	-1.80486500	0.00089300	0.06204600	
C	2.47939800	-0.81272600	1.50826200	
C	-2.78073900	2.17534000	-1.26974900	
C	-3.45182900	1.53753100	-0.21009600	
C	2.41328400	1.96238400	1.10159000	
H	-0.07833700	-0.87610800	-2.19369600	
H	0.88072100	0.59822700	-1.92108800	
H	0.89220400	-2.61240100	0.72185600	
H	1.55903400	-2.77477000	-0.91711000	

H	-0.19310800	-2.54817100	-0.66530100	
H	-0.99382000	2.12969400	-2.45467500	
H	-1.35044400	-0.69572500	0.75468100	
H	3.18375900	-0.12719300	1.97514000	
H	3.02294700	-1.65463600	1.07840900	
H	1.81002800	-1.19760000	2.28183200	
H	-3.22231100	3.03693900	-1.75102300	
O	-2.32956400	-1.56954600	-1.09913300	
H	-3.24373100	-1.60716200	-0.77833200	
Name				C12-RAF-G
Cartesian Coordinates				Frequency and Energy
Cl	-4.98128500	1.49321000	0.84307200	Zero-point correction= 0.214425 (Hartree/Particle)
N	0.96946900	-0.92088300	-0.19764200	Thermal correction to Energy= 0.230844
N	-3.50357200	-0.36093300	-0.26652100	Thermal correction to Enthalpy= 0.231788
N	1.95416600	1.10979900	-0.51136400	Thermal correction to Gibbs Free Energy= 0.167783
N	3.62551100	2.86199100	0.04551400	Sum of electronic and zero-point Energies= -1142.283064
C	0.09701900	-0.65802900	-1.34673700	Sum of electronic and thermal Energies= -1142.266645
C	-1.20581600	-0.02051100	-0.93019700	Sum of electronic and thermal Enthalpies= -1142.265700
C	1.85509800	0.02101000	0.19909700	Sum of electronic and thermal Free Energies= -1142.329706
C	0.58257000	-2.03729500	0.65420900	
C	-1.31144900	1.34727200	-0.68482300	v =-612.25
C	-2.34538500	-0.81502000	-0.70138200	
C	2.67372400	-0.25639800	1.43117300	
C	-2.52167700	1.86048600	-0.24958200	
C	-3.62108400	0.96962700	-0.11054700	
C	2.86389700	2.02271700	-0.18502800	
H	-0.09392100	-1.61591600	-1.83563000	
H	0.63738900	-0.01361600	-2.03690500	
H	-0.21368100	-1.75606800	1.35174400	
H	1.43356800	-2.41254600	1.21675200	
H	0.21746500	-2.84554400	0.02001300	
H	-0.45189200	1.99275100	-0.82179000	
H	-2.28898700	-1.89023700	-0.86162500	
H	3.34453300	0.57730000	1.62650500	
H	3.26742400	-1.16288900	1.29922600	
H	2.02287000	-0.39714900	2.29628800	
H	-2.66877600	2.91214000	-0.04811000	
O	-4.28011400	1.61517800	-1.82841800	
H	-3.74895700	1.10158600	-2.45746200	
Name				C13-RAF-G
Cartesian Coordinates				Frequency and Energy
Cl	-4.99271200	1.61493500	0.78672600	Zero-point correction= 0.214637 (Hartree/Particle)
N	0.99510000	-0.95523700	-0.23487800	Thermal correction to Energy= 0.231173
N	-3.43432900	-0.30958400	-0.02102600	Thermal correction to Enthalpy= 0.232117
N	1.88453000	1.13067400	-0.43855200	Thermal correction to Gibbs Free Energy= 0.167787
N	3.48495900	2.92031400	0.20191000	Sum of electronic and zero-point Energies= -1142.291655
C	0.09064700	-0.65006300	-1.34796200	Sum of electronic and thermal Energies= -1142.275119
C	-1.19309400	-0.00538700	-0.87909800	Sum of electronic and thermal Enthalpies= -1142.274174
C	1.84586900	-0.00142700	0.20688600	Sum of electronic and thermal Free Energies= -1142.338504
C	0.66860700	-2.13342900	0.55616500	
C	-1.31809700	1.37229600	-0.74382400	v =-533.69
C	-2.28933000	-0.79210300	-0.52036200	
C	2.69686400	-0.31508900	1.40787200	
C	-2.54268600	1.91615400	-0.31358000	

C	-3.53021800	0.98921400	0.10864600	
C	2.75755200	2.06302200	-0.06918300	
H	-0.12695200	-1.59278900	-1.85427500	
H	0.61663800	0.00427100	-2.03978600	
H	-0.12341600	-1.92543100	1.28384300	
H	1.54462500	-2.50592900	1.08105700	
H	0.32328500	-2.91800200	-0.11747000	
H	-0.49558400	2.02763600	-1.00303500	
H	-2.24727300	-1.87288600	-0.63147400	
H	3.33593200	0.53350000	1.64176400	
H	3.32522200	-1.18636900	1.21372100	
H	2.06784900	-0.53336300	2.27308900	
H	-2.62524100	2.95365100	-0.02614200	
O	-3.33344800	2.43667200	-2.06917500	
H	-3.26683400	1.60075500	-2.55687800	
Name				C14-RAF-G
Cartesian Coordinates				Frequency and Energy
Cl	-5.02512800	1.73219000	0.77613900	Zero-point correction= 0.214511 (Hartree/Particle)
N	0.97674700	-0.93303200	-0.25500400	Thermal correction to Energy= 0.230969
N	-3.43712900	-0.21535400	0.05791200	Thermal correction to Enthalpy= 0.231914
N	1.80522100	1.18539100	-0.33719900	Thermal correction to Gibbs Free Energy= 0.167829
N	3.36833300	2.97408800	0.39200300	Sum of electronic and zero-point Energies= -1142.289200
C	0.05314400	-0.58865000	-1.34213900	Sum of electronic and thermal Energies= -1142.272741
C	-1.21664600	0.04367300	-0.83345500	Sum of electronic and thermal Enthalpies= -1142.271797
C	1.81061700	0.01293500	0.23247100	Sum of electronic and thermal Free Energies= -1142.335882
C	0.70090600	-2.16915800	0.46396900	
C	-1.36468800	1.45834800	-0.82255400	v = -579.76
C	-2.29291600	-0.72186600	-0.41712800	
C	2.69477400	-0.35465600	1.39382000	
C	-2.54649200	1.99022000	-0.26173000	
C	-3.53388900	1.09977900	0.12934300	
C	2.65987400	2.11594000	0.07681100	
H	-0.17578600	-1.51285500	-1.87583400	
H	0.55433800	0.09438200	-2.02528800	
H	-0.07531800	-2.03064900	1.22448200	
H	1.59991100	-2.55206700	0.94054400	
H	0.35707800	-2.91633800	-0.25128800	
H	-0.48758200	2.08177900	-0.93330800	
H	-2.24702800	-1.80676500	-0.46803200	
H	3.31371800	0.49538400	1.67230000	
H	3.34387500	-1.19160600	1.12949100	
H	2.09068000	-0.64930100	2.25410800	
H	-2.69167700	3.05803200	-0.17370900	
O	-1.66929900	1.64877900	-2.73544300	
H	-2.59771200	1.37639800	-2.81410300	
Name				C2-RAF-P
Cartesian Coordinates				Frequency and Energy
Cl	-5.29359000	1.53524900	0.58638000	Zero-point correction= 0.214579 (Hartree/Particle)
N	0.84365500	-0.88452400	-0.20692200	Thermal correction to Energy= 0.230850
N	-3.73237300	-0.32876300	-0.37186000	Thermal correction to Enthalpy= 0.231794
N	1.99936800	0.97808500	-0.82345300	Thermal correction to Gibbs Free Energy= 0.167896
N	3.63901900	2.80593800	-0.72584400	Sum of electronic and zero-point Energies= -1142.317855
C	-0.09548700	-0.69161300	-1.31618400	Sum of electronic and thermal Energies= -1142.301585
C	-1.38931700	-0.07510400	-0.84400400	Sum of electronic and thermal Enthalpies= -1142.300641

C	1.85834800	-0.03878700	-0.00018100	Sum of electronic and thermal Free Energies= v =-671.51	-1142.364538	
C	0.51031600	-1.93998000	0.74699900			
C	-1.44730600	1.25300300	-0.41251500			
C	-2.56223600	-0.81700300	-0.80057300			
C	2.74611800	-0.29206300	1.18443800			
C	-2.64902200	1.77471400	0.03367300			
C	-3.74974600	0.92093100	0.02593000			
C	3.04417300	1.77626100	-0.75287900			
H	-0.28859100	-1.66925900	-1.76153900			
H	0.38272600	-0.05810500	-2.05971400			
H	-0.00114100	-1.53528100	1.62475000			
H	1.40430900	-2.47548500	1.06193600			
H	-0.15452200	-2.64688300	0.25313900			
H	-0.55609100	1.87176900	-0.43456400			
H	-2.57094800	-1.85231400	-1.12914800			
H	3.45431900	0.52179800	1.31075400			
H	3.30593300	-1.21911700	1.04295000			
H	2.14267400	-0.39171500	2.08870600			
H	-2.74002800	2.79845800	0.37118800			
O	4.56744500	0.65204000	-1.00526900			
H	5.33607600	1.24477400	-1.02943600			
Name				C4-RAF-P		
Cartesian Coordinates				Frequency and Energy		
Cl	-5.21401200	1.44054300	0.51504300	Zero-point correction=	0.215502 (Hartree/Particle)	
N	0.94074300	-0.88779700	-0.21116500	Thermal correction to Energy=	0.231150	
N	-3.59668600	-0.36606200	-0.45546800	Thermal correction to Enthalpy=	0.232094	
N	2.01169300	1.11273400	-0.59436200	Thermal correction to Gibbs Free Energy=	0.170682	
N	3.64359500	2.90610100	-0.10876400	Sum of electronic and zero-point Energies=	-1142.314090	
C	0.05728100	-0.62818000	-1.35263400	Sum of electronic and thermal Energies=	-1142.298442	
C	-1.25443800	-0.04838500	-0.87653500	Sum of electronic and thermal Enthalpies=	-1142.297498	
C	2.01201700	-0.03058800	0.08373600	Sum of electronic and thermal Free Energies=	-1142.358910	
C	0.61572600	-2.01278700	0.65488900	v =-478.34		
C	-1.34690300	1.26910100	-0.42072100			
C	-2.41022800	-0.81920500	-0.87260400			
C	2.66941600	-0.17255700	1.42594600			
C	-2.56878100	1.75290300	0.01358200			
C	-3.64901500	0.87491000	-0.03040700			
C	2.89889800	2.03559900	-0.30205300			
H	-0.11029400	-1.58132500	-1.85666400			
H	0.56049000	0.06092400	-2.02612100			
H	0.31392700	-1.65216700	1.64109800			
H	1.48060600	-2.66879700	0.74987900			
H	-0.20608300	-2.56783200	0.20725300			
H	-0.46846600	1.90535800	-0.41577600			
H	-2.38979100	-1.84550800	-1.22793100			
H	3.65310700	0.29324200	1.38014700			
H	2.78816500	-1.20962800	1.72568300			
H	2.06626000	0.35715300	2.16875900			
H	-2.68885000	2.76745100	0.36917200			
O	2.96357800	-1.33210700	-0.85436500			
H	2.89454100	-0.97099400	-1.75322500			
Name				C5-FHT-P		
Cartesian Coordinates				Frequency and Energy		
Cl	-5.35142600	1.50049700	0.32913900	Zero-point correction=	0.209396 (Hartree/Particle)	

N	0.88211900	-0.82657100	-0.10584700	Thermal correction to Energy=	0.226121
N	-3.72484600	-0.22764900	-0.76658600	Thermal correction to Enthalpy=	0.227065
N	2.05077500	1.07029100	-0.60569600	Thermal correction to Gibbs Free Energy=	0.160885
N	3.88294700	2.69415200	-0.25214400	Sum of electronic and zero-point Energies=	-1142.325342
C	-0.00252300	-0.61463500	-1.25374800	Sum of electronic and thermal Energies=	-1142.308617
C	-1.33062200	-0.03439700	-0.83373900	Sum of electronic and thermal Enthalpies=	-1142.307673
C	1.90505100	-0.00540700	0.14169000	Sum of electronic and thermal Free Energies=	-1142.373853
C	0.58595000	-1.99063900	0.72648800	v =-1130.33	
C	-1.40941300	1.17724300	-0.14241900		
C	-2.51930200	-0.69376400	-1.11456500		
C	2.80753200	-0.33808900	1.28109400		
C	-2.64721500	1.67351900	0.22593100		
C	-3.76179000	0.91380200	-0.12204500		
C	3.04283100	1.90501000	-0.38553900		
H	-0.15424000	-1.58126200	-1.73928900		
H	0.50015900	0.04936500	-1.95443800		
H	-0.47306200	-2.22332500	0.61710600		
H	0.77109400	-1.77956000	1.77790200		
H	1.17408600	-2.85663600	0.41108500		
H	-0.50620800	1.72761800	0.10053000		
H	-2.51089500	-1.64174200	-1.64474300		
H	3.69124400	0.29373900	1.31603800		
H	3.06301900	-1.39476200	1.34853600		
H	2.19723200	-0.12744200	2.27156300		
H	-2.75498300	2.60842900	0.75892400		
O	1.42224800	0.34735200	3.30879300		
H	1.75788500	1.26176100	3.33651100		
Name				C7-FHT-P	
Cartesian Coordinates				Frequency and Energy	
Cl	-5.36616900	1.50926600	0.06009300	Zero-point correction=	0.210598 (Hartree/Particle)
N	0.89585900	-0.75679000	0.09236700	Thermal correction to Energy=	0.227234
N	-3.66170800	-0.35647500	-0.60650200	Thermal correction to Enthalpy=	0.228178
N	1.99690600	1.15136300	-0.47214300	Thermal correction to Gibbs Free Energy=	0.162810
N	3.76614600	2.86330100	-0.22144500	Sum of electronic and zero-point Energies=	-1142.328449
C	0.06418900	-0.65971800	-1.11514900	Sum of electronic and thermal Energies=	-1142.311813
C	-1.28636500	-0.05820500	-0.81874600	Sum of electronic and thermal Enthalpies=	-1142.310869
C	1.89389500	0.11532200	0.32496000	Sum of electronic and thermal Free Energies=	-1142.376237
C	0.65914100	-1.89433400	0.93519500	v =-770.80	
C	-1.42490400	1.28890000	-0.47297000		
C	-2.43867100	-0.83135700	-0.87100300		
C	2.80730600	-0.15660600	1.48299000		
C	-2.68219900	1.79671700	-0.19714500		
C	-3.75424500	0.91129800	-0.28316700		
C	2.95859200	2.03523500	-0.30100300		
H	-0.05219500	-1.67157000	-1.50911500		
H	0.59912300	-0.06131700	-1.84939200		
H	0.87905000	-1.69840400	1.98146400		
H	1.33744800	-2.75267700	0.58960500		
H	-0.37069800	-2.23118000	0.82271300		
H	-0.55174100	1.93147100	-0.42929900		
H	-2.38451500	-1.88173500	-1.14302900		
H	3.66597500	0.51047600	1.45167300		
H	3.15496100	-1.19065200	1.45892700		
H	2.27509300	0.00581000	2.42389900		

H	-2.83608800	2.83400800	0.06841800	
O	2.39626500	-3.69808400	0.03613900	
H	2.21109400	-4.46729400	0.60353300	
Name				C8-FHT-P
Cartesian Coordinates				Frequency and Energy
Cl	-4.83730400	2.22695400	0.62522900	Zero-point correction= 0.209444 (Hartree/Particle)
N	0.94344500	-1.03554700	-0.18695200	Thermal correction to Energy= 0.226395
N	-3.22400800	0.17639200	0.47024300	Thermal correction to Enthalpy= 0.227339
N	1.46334100	1.16381600	-0.04343300	Thermal correction to Gibbs Free Energy= 0.161760
N	2.61964800	3.13712200	0.90120800	Sum of electronic and zero-point Energies= -1142.325568
C	0.00780900	-0.70264300	-1.23694900	Sum of electronic and thermal Energies= -1142.308616
C	-1.18633500	0.10949300	-0.79889300	Sum of electronic and thermal Enthalpies= -1142.307672
C	1.64138700	-0.05037400	0.41121600	Sum of electronic and thermal Free Energies= -1142.373251
C	1.12006800	-2.43657000	0.19949000	
C	-1.39765000	1.42082800	-1.21807100	v =-785.78
C	-2.13205900	-0.46440200	0.04339600	
C	2.56717200	-0.41912600	1.53001400	
C	-2.52878300	2.09767700	-0.79074700	
C	-3.39412700	1.41118700	0.05429700	
C	2.10301400	2.18348500	0.49145700	
H	-0.31029700	-1.62887800	-1.71343700	
H	0.57396700	-0.08848800	-2.04644100	
H	0.63653900	-2.64136100	1.15800800	
H	2.17759500	-2.69013200	0.26719200	
H	0.66470600	-3.06461000	-0.56269200	
H	-0.67474200	1.90370900	-1.86602600	
H	-2.01065200	-1.48542900	0.39551800	
H	2.93707100	0.47544400	2.02641500	
H	3.42071100	-0.97719200	1.13669400	
H	2.05830500	-1.05034500	2.26010100	
H	-2.73190700	3.11753000	-1.08817100	
O	1.07863700	0.45842600	-3.29804400	
H	0.63005000	-0.14734000	-3.91366700	
Name				C9-RAF-P
Cartesian Coordinates				Frequency and Energy
Cl	-4.73693000	1.76647500	1.06202500	Zero-point correction= 0.214573 (Hartree/Particle)
N	0.92692300	-0.91961300	-0.26230600	Thermal correction to Energy= 0.230908
N	-3.28082100	-0.20456000	0.16749400	Thermal correction to Enthalpy= 0.231852
N	1.79725000	1.17809800	-0.36196000	Thermal correction to Gibbs Free Energy= 0.168499
N	3.27097000	3.01695100	0.39117200	Sum of electronic and zero-point Energies= -1142.327495
C	0.10353300	-0.62024100	-1.43762200	Sum of electronic and thermal Energies= -1142.311160
C	-1.20115900	0.04356600	-1.05053200	Sum of electronic and thermal Enthalpies= -1142.310216
C	1.73578000	0.01591900	0.25136900	Sum of electronic and thermal Free Energies= -1142.373569
C	0.67962900	-2.18558400	0.42529100	
C	-1.29698600	1.45011400	-0.90325200	v =-430.87
C	-2.22670600	-0.72633500	-0.44643100	
C	2.51337200	-0.32048700	1.49060300	
C	-2.39332600	1.99682800	-0.27203800	
C	-3.34508900	1.11254200	0.24164100	
C	2.60019900	2.12470200	0.07505300	
H	-0.10570100	-1.56002800	-1.94594300	
H	0.65898100	0.02961300	-2.10969200	
H	-0.05659000	-2.06645600	1.22607800	
H	1.60080500	-2.58531800	0.84397200	

H	0.29946900	-2.90256800	-0.30013200	
H	-0.51763400	2.08121600	-1.31197900	
H	-2.18863700	-1.80999100	-0.50815700	
H	3.06508300	0.54870900	1.84154500	
H	3.22223400	-1.12532300	1.28292100	
H	1.84094300	-0.65751300	2.28169600	
H	-2.51692400	3.06577600	-0.16247400	
O	-1.90577300	-0.17194300	-2.93410500	
H	-2.68945900	0.40020600	-2.89962900	
Name				C10-RAF-P
Cartesian Coordinates				Frequency and Energy
Cl	-5.20890300	1.52748100	0.60559800	Zero-point correction= 0.214889 (Hartree/Particle)
N	0.92958900	-0.83032700	-0.17624100	Thermal correction to Energy= 0.231263
N	-3.62596800	-0.29977300	-0.36680500	Thermal correction to Enthalpy= 0.232207
N	2.01977900	1.13434900	-0.55128500	Thermal correction to Gibbs Free Energy= 0.168504
N	3.78474600	2.81341400	-0.12017900	Sum of electronic and zero-point Energies= -1142.324050
C	0.03942200	-0.56654900	-1.31084500	Sum of electronic and thermal Energies= -1142.307676
C	-1.26688000	0.02931500	-0.85380100	Sum of electronic and thermal Enthalpies= -1142.306732
C	1.88432800	0.04193700	0.16986900	Sum of electronic and thermal Free Energies= -1142.370435
C	0.58597100	-1.98056900	0.65637000	
C	-1.36780400	1.35946300	-0.43431300	v =-514.91
C	-2.44434000	-0.75360700	-0.86678800	
C	2.73811100	-0.28507000	1.36081100	
C	-2.58691900	1.84260400	-0.00407100	
C	-3.67064800	0.94207600	0.00878900	
C	2.97717000	1.99714000	-0.28579500	
H	-0.14519600	-1.51288100	-1.82003900	
H	0.54355900	0.10918400	-1.99835900	
H	-0.09372700	-1.69459800	1.46440000	
H	1.47851000	-2.43438100	1.08063100	
H	0.09384400	-2.72186200	0.02829000	
H	-0.49295900	1.99995500	-0.44977600	
H	-2.38005300	-1.82543600	-1.00832400	
H	3.42134800	0.53344800	1.57550100	
H	3.32141600	-1.18791800	1.16600700	
H	2.11508500	-0.46746400	2.23813200	
H	-2.71630500	2.86414200	0.32753200	
O	-2.56485400	-0.55794900	-2.84651000	
H	-2.82792700	0.37565900	-2.90044900	
Name				C12-RAF-P
Cartesian Coordinates				Frequency and Energy
Cl	-5.28785900	1.19862000	0.51179600	Zero-point correction= 0.214419 (Hartree/Particle)
N	0.93134300	-0.83575300	-0.09117700	Thermal correction to Energy= 0.230795
N	-3.66872300	-0.43432700	-0.73936200	Thermal correction to Enthalpy= 0.231740
N	2.07247400	1.03940200	-0.70290500	Thermal correction to Gibbs Free Energy= 0.168061
N	3.86804200	2.72421900	-0.46285600	Sum of electronic and zero-point Energies= -1142.317623
C	0.05576100	-0.70538100	-1.25678200	Sum of electronic and thermal Energies= -1142.301246
C	-1.28273400	-0.11876100	-0.88433800	Sum of electronic and thermal Enthalpies= -1142.300302
C	1.90738200	0.04896800	0.14746100	Sum of electronic and thermal Free Energies= -1142.363980
C	0.57218600	-1.87448900	0.87213900	
C	-1.39075400	1.14242200	-0.30302100	v =-604.61
C	-2.46420700	-0.86173500	-1.06749500	
C	2.74317200	-0.14894600	1.37870000	
C	-2.64254100	1.62541300	0.03661500	

C	-3.76943900	0.82028500	-0.27348900	
C	3.04451700	1.91043900	-0.53610300	
H	-0.07999800	-1.69930700	-1.68705500	
H	0.55441100	-0.07318900	-1.98959100	
H	-0.02522900	-1.46543200	1.69168300	
H	1.46077900	-2.35545200	1.27663900	
H	-0.01748200	-2.62965600	0.35438100	
H	-0.50567100	1.73965400	-0.11240100	
H	-2.40558700	-1.86750600	-1.47570000	
H	3.44328300	0.67421700	1.50151000	
H	3.30690200	-1.08152900	1.30249500	
H	2.10736000	-0.21009900	2.26376000	
H	-2.78612100	2.59699500	0.48936800	
O	-4.09251800	1.90495200	-1.88523500	
H	-3.34064300	1.65800800	-2.44920700	
Name				C13-RAF-P
Cartesian Coordinates				Frequency and Energy
Cl	-4.91172200	1.79585000	0.84537000	Zero-point correction= 0.214785 (Hartree/Particle)
N	0.98138500	-0.96111000	-0.22800000	Thermal correction to Energy= 0.231154
N	-3.35742800	-0.18365400	0.16809700	Thermal correction to Enthalpy= 0.232098
N	1.82095200	1.14756000	-0.33474600	Thermal correction to Gibbs Free Energy= 0.168768
N	3.32558400	2.98359300	0.36268100	Sum of electronic and zero-point Energies= -1142.324947
C	0.08156400	-0.62999400	-1.33929000	Sum of electronic and thermal Energies= -1142.308578
C	-1.18157400	0.04757600	-0.85981400	Sum of electronic and thermal Enthalpies= -1142.307634
C	1.80766500	-0.02687500	0.25838700	Sum of electronic and thermal Free Energies= -1142.370964
C	0.76892900	-2.23522800	0.45454200	
C	-1.32943800	1.42683100	-0.88072300	$\nu = -501.87$
C	-2.23500600	-0.71058700	-0.34185200	
C	2.65613300	-0.37786800	1.44567400	
C	-2.53534600	2.00541000	-0.43745300	
C	-3.47069300	1.11945900	0.14878500	
C	2.64213300	2.09273900	0.07105100	
H	-0.16157800	-1.56336000	-1.84797400	
H	0.61322600	0.01724900	-2.03407000	
H	0.06588700	-2.12893000	1.28620200	
H	1.70926200	-2.63327600	0.82981900	
H	0.36297400	-2.94680100	-0.26228800	
H	-0.54102400	2.06137700	-1.26708400	
H	-2.17428200	-1.79514100	-0.32629100	
H	3.23065600	0.48620900	1.77178500	
H	3.34789800	-1.18367400	1.19068800	
H	2.02861800	-0.71896100	2.27141000	
H	-2.61357500	3.06854700	-0.26308200	
O	-3.47718900	2.29021200	-2.19098900	
H	-3.33554700	1.41885200	-2.59585400	
Name				C14-RAF-P
Cartesian Coordinates				Frequency and Energy
Cl	-5.26648900	1.43849600	0.51507600	Zero-point correction= 0.214387 (Hartree/Particle)
N	0.92628300	-0.84350400	-0.15981100	Thermal correction to Energy= 0.230859
N	-3.62686600	-0.37306500	-0.41506600	Thermal correction to Enthalpy= 0.231804
N	2.01590600	1.10969000	-0.59538700	Thermal correction to Gibbs Free Energy= 0.167519
N	3.78268900	2.79850500	-0.21215900	Sum of electronic and zero-point Energies= -1142.321381
C	0.03539600	-0.62168800	-1.30385600	Sum of electronic and thermal Energies= -1142.304909
C	-1.28819600	-0.05632400	-0.86709400	Sum of electronic and thermal Enthalpies= -1142.303965

C	1.88166000	0.03953100	0.15753000	Sum of electronic and thermal Free Energies= -1142.368249 v =-580.44
C	0.59578000	-1.97487400	0.70328600	
C	-1.39967900	1.31956500	-0.52362300	
C	-2.43208500	-0.83192800	-0.81889600	
C	2.73774500	-0.25303400	1.35602400	
C	-2.63881500	1.78043500	-0.02968700	
C	-3.69766500	0.88672400	-0.03510600	
C	2.97299300	1.98013900	-0.35550500	
H	-0.11197400	-1.58247000	-1.79943700	
H	0.51961100	0.06601800	-1.99488100	
H	-0.06723100	-1.67127000	1.51845500	
H	1.49565600	-2.42303800	1.11842400	
H	0.08857600	-2.72788400	0.10145700	
H	-0.50243300	1.89978000	-0.34619900	
H	-2.40011200	-1.87616800	-1.11478500	
H	3.41471800	0.57552600	1.55119100	
H	3.32806600	-1.15556400	1.18178000	
H	2.11677300	-0.42016100	2.23778400	
H	-2.76336200	2.80212600	0.30304200	
O	-1.43088100	2.05288600	-2.33979100	
H	-2.31813700	1.78657300	-2.63558500	
Name				C2-RAF-W
Cartesian Coordinates				Frequency and Energy
Cl	-5.23685600	1.86251200	0.12019900	Zero-point correction= 0.213914 (Hartree/Particle) Thermal correction to Energy= 0.230436 Thermal correction to Enthalpy= 0.231380 Thermal correction to Gibbs Free Energy= 0.165869 Sum of electronic and zero-point Energies= -1142.320344 Sum of electronic and thermal Energies= -1142.303822 Sum of electronic and thermal Enthalpies= -1142.302878 Sum of electronic and thermal Free Energies= -1142.368389 v =-611.49
N	0.88052200	-0.94743400	-0.14878900	
N	-3.72652200	0.17355900	-1.19059500	
N	1.91230200	0.87355200	-1.05835100	
N	3.48439100	2.76352600	-1.16505500	
C	-0.12577600	-0.91849600	-1.20471300	
C	-1.38098600	-0.18447800	-0.78866800	
C	1.83553500	-0.02052700	-0.08463200	
C	0.60740700	-1.83936400	0.98134100	
C	-1.40933500	0.76360200	0.23102500	
C	-2.57076400	-0.44306000	-1.45999800	
C	2.75045200	-0.03804800	1.10064600	
C	-2.59924100	1.41172800	0.52922400	
C	-3.71203500	1.06731300	-0.22430800	
C	2.91112400	1.72259700	-1.08165200	
H	-0.37411700	-1.94898700	-1.46103900	
H	0.30539400	-0.44820900	-2.08653200	
H	0.14086300	-1.29549400	1.80644400	
H	1.52409100	-2.31114700	1.32988200	
H	-0.07337900	-2.61544000	0.63852000	
H	-0.51613600	0.99965900	0.80046100	
H	-2.59782100	-1.18307700	-2.25349600	
H	3.41375900	0.82350900	1.08947000	
H	3.35021100	-0.95102300	1.09604200	
H	2.16320300	-0.02443900	2.02088900	
H	-2.66373500	2.15221600	1.31488500	
O	4.52828800	0.68167900	-1.39160900	
H	5.18324300	1.09079600	-0.80283700	
Name				C4-RAF-W
Cartesian Coordinates				Frequency and Energy
Cl	-5.27199100	1.35801300	0.45144300	Zero-point correction= 0.214699 (Hartree/Particle)

N	0.94355400	-0.83949100	-0.19122900	Thermal correction to Energy=	0.230717
N	-3.61620300	-0.39960700	-0.55052600	Thermal correction to Enthalpy=	0.231661
N	2.06099100	1.13779500	-0.59706300	Thermal correction to Gibbs Free Energy=	0.168472
N	3.78763200	2.84040000	-0.10847300	Sum of electronic and zero-point Energies=	-1142.315302
C	0.06424300	-0.59711200	-1.34007100	Sum of electronic and thermal Energies=	-1142.299284
C	-1.26233600	-0.04519100	-0.87619400	Sum of electronic and thermal Enthalpies=	-1142.298340
C	2.02399000	-0.00412600	0.08383900	Sum of electronic and thermal Free Energies=	-1142.361529
C	0.58439700	-1.93255400	0.70589200	ν =-468.34	
C	-1.37850600	1.24609700	-0.35921800		
C	-2.40911700	-0.82389500	-0.94664700		
C	2.71785800	-0.17227200	1.40105900		
C	-2.61784000	1.70142100	0.05680800		
C	-3.68714400	0.82155800	-0.06870700		
C	2.99687000	2.00558900	-0.29776200		
H	-0.08307200	-1.55507000	-1.84112300		
H	0.56028400	0.09428800	-2.01568300		
H	0.31349200	-1.53481300	1.68630200		
H	1.42121400	-2.62225400	0.80962600		
H	-0.26559500	-2.46036600	0.27974700		
H	-0.50749100	1.88775900	-0.28633200		
H	-2.36153000	-1.83273400	-1.34313500		
H	3.71651300	0.25714800	1.32779900		
H	2.80118200	-1.21260000	1.70053000		
H	2.15099900	0.37983400	2.15614000		
H	-2.75656700	2.69554800	0.45952700		
O	2.95362400	-1.35735700	-0.90636500		
H	2.78705000	-1.05390700	-1.81379100		
Name				C5-FHT-W	
Cartesian Coordinates				Frequency and Energy	
Cl	-5.05200000	2.05863700	0.31041200	Zero-point correction=	0.209904 (Hartree/Particle)
N	0.91555200	-1.04685700	-0.17577600	Thermal correction to Energy=	0.226368
N	-3.53245500	0.62166500	-1.26430400	Thermal correction to Enthalpy=	0.227313
N	1.90700400	0.94600500	-0.70048800	Thermal correction to Gibbs Free Energy=	0.162269
N	3.55271900	2.74375500	-0.26873400	Sum of electronic and zero-point Energies=	-1142.325299
C	-0.06393200	-0.83336500	-1.23438800	Sum of electronic and thermal Energies=	-1142.308835
C	-1.28813200	-0.08286900	-0.75550400	Sum of electronic and thermal Enthalpies=	-1142.307891
C	1.85151200	-0.13092000	0.06843400	Sum of electronic and thermal Free Energies=	-1142.372935
C	0.64128900	-2.13369600	0.77273700	ν =-1244.26	
C	-1.36167300	0.56443600	0.47443500		
C	-2.40541500	-0.02318000	-1.58212200		
C	2.76630300	-0.33755200	1.22211600		
C	-2.52398300	1.23805800	0.82425000		
C	-3.56331100	1.22368600	-0.09333000		
C	2.80402400	1.86737100	-0.43111000		
H	-0.36086400	-1.81152800	-1.61452400		
H	0.40948400	-0.28906000	-2.04988700		
H	-0.30776800	-2.58695600	0.49580000		
H	0.55982900	-1.75060000	1.79062500		
H	1.41962500	-2.89665700	0.72866800		
H	-0.52688900	0.55106200	1.16777600		
H	-2.39539700	-0.51850800	-2.54772400		
H	3.71106400	0.18745000	1.10096500		
H	2.90852200	-1.37403700	1.51494800		
H	2.23896500	0.17134400	2.14865800		

H	-2.62064100	1.75210100	1.77093600	
O	1.51016500	1.01788000	2.99054100	
H	1.39404800	1.75923700	2.36712300	
Name				C7-FHT-W
Cartesian Coordinates				Frequency and Energy
Cl	-5.08779200	2.17829900	-0.36630700	Zero-point correction= 0.210671 (Hartree/Particle)
N	0.87159900	-0.96237800	0.01219700	Thermal correction to Energy= 0.226930
N	-3.45259600	0.58151800	-1.64533700	Thermal correction to Enthalpy= 0.227875
N	1.77621300	0.92797800	-0.87134500	Thermal correction to Gibbs Free Energy= 0.163598
N	3.40916900	2.78781800	-0.91890700	Sum of electronic and zero-point Energies= -1142.328095
C	-0.09038100	-1.00385100	-1.08396200	Sum of electronic and thermal Energies= -1142.311835
C	-1.32029000	-0.16436000	-0.81605100	Sum of electronic and thermal Enthalpies= -1142.310891
C	1.79022100	0.01248900	0.07628600	Sum of electronic and thermal Free Energies= -1142.375168
C	0.70289500	-1.92198900	1.07350000	
C	-1.51361400	0.56977600	0.34982400	v =-1011.13
C	-2.32348000	-0.12103300	-1.77899400	
C	2.75826700	-0.00348300	1.21558900	
C	-2.67991600	1.30608000	0.50798500	
C	-3.59999700	1.26337700	-0.52793000	
C	2.67001600	1.89270000	-0.84743000	
H	-0.38044200	-2.04632200	-1.22475800	
H	0.39597400	-0.66793400	-1.99845600	
H	0.90826400	-1.50250000	2.05543800	
H	1.41556500	-2.80796600	0.92541700	
H	-0.30343600	-2.33603600	1.03891800	
H	-0.76798900	0.57627500	1.13835200	
H	-2.21382500	-0.67830100	-2.70395100	
H	3.58368200	0.67865800	1.02321200	
H	3.14867700	-1.00936500	1.37398200	
H	2.24624200	0.31268100	2.12892300	
H	-2.86792700	1.88987900	1.39861100	
O	2.56822000	-3.81317900	0.92021100	
H	3.10822900	-3.35205700	1.58685000	
Name				C8-FHT-W
Cartesian Coordinates				Frequency and Energy
Cl	-4.80086700	2.16102100	0.68226400	Zero-point correction= 0.209059 (Hartree/Particle)
N	1.03415400	-0.98367500	-0.29570800	Thermal correction to Energy= 0.225961
N	-2.55614300	0.84971800	0.96606900	Thermal correction to Enthalpy= 0.226905
N	1.75330500	1.12498600	0.15820800	Thermal correction to Gibbs Free Energy= 0.161453
N	3.06373900	2.79672700	1.42860600	Sum of electronic and zero-point Energies= -1142.328577
C	0.16535300	-0.44798500	-1.31697300	Sum of electronic and thermal Energies= -1142.311675
C	-1.07805200	0.23388800	-0.82390600	Sum of electronic and thermal Enthalpies= -1142.310731
C	1.75553900	-0.15475300	0.47328200	Sum of electronic and thermal Free Energies= -1142.376183
C	0.86052900	-2.39704600	0.05552800	
C	-1.93802200	0.83808600	-1.74284800	v =-1012.60
C	-1.43443100	0.26995000	0.51772100	
C	2.51046200	-0.73821700	1.62410100	
C	-3.10006900	1.44157900	-1.29741400	
C	-3.34065800	1.40783400	0.07187300	
C	2.46977500	1.96787100	0.86885700	
H	-0.08331900	-1.24263000	-2.01952200	
H	0.75757700	0.32548700	-1.93852600	
H	0.13696200	-2.50377000	0.86794300	
H	1.80929400	-2.84005800	0.34857800	

H	0.48942900	-2.92281900	-0.82105000	
H	-1.69462000	0.83414900	-2.80058400	
H	-0.80851400	-0.18783200	1.27621600	
H	2.99023400	0.04613300	2.20500000	
H	3.27455300	-1.42669100	1.25599100	
H	1.83131800	-1.30018300	2.26851400	
H	-3.79312300	1.92071300	-1.97541200	
O	1.27909600	1.12811500	-3.07584600	
H	0.66210200	0.79902900	-3.75400600	
Name				C9-RAF-W
Cartesian Coordinates				Frequency and Energy
Cl	-4.84867000	1.53035800	1.02516900	Zero-point correction= 0.214319 (Hartree/Particle)
N	0.95071600	-0.87956400	-0.28094600	Thermal correction to Energy= 0.230734
N	-3.34400900	-0.35198100	0.02713900	Thermal correction to Enthalpy= 0.231678
N	1.99016300	1.14006100	-0.51219100	Thermal correction to Gibbs Free Energy= 0.168029
N	3.59372100	2.89100400	0.18253500	Sum of electronic and zero-point Energies= -1142.327860
C	0.11564200	-0.59826900	-1.45288600	Sum of electronic and thermal Energies= -1142.311445
C	-1.20117800	0.01894000	-1.04055100	Sum of electronic and thermal Enthalpies= -1142.310501
C	1.80938100	0.03095400	0.18498900	Sum of electronic and thermal Free Energies= -1142.374150
C	0.57252500	-2.04800700	0.51684900	
C	-1.30180700	1.40114400	-0.74805700	v =-369.74
C	-2.25224600	-0.80860500	-0.57861400	
C	2.52344400	-0.26710500	1.46695700	
C	-2.43082700	1.88214000	-0.12485600	
C	-3.41063300	0.95231900	0.23009100	
C	2.85674000	2.03374500	-0.09571900	
H	-0.06735000	-1.54189600	-1.96529200	
H	0.64760300	0.07268200	-2.12086600	
H	-0.13647200	-1.77543300	1.30340900	
H	1.45016300	-2.50761100	0.96534800	
H	0.10588800	-2.77436900	-0.14563100	
H	-0.50182800	2.07010400	-1.04116200	
H	-2.20018900	-1.87897800	-0.74879700	
H	3.14496500	0.57438300	1.76431800	
H	3.15496700	-1.14961400	1.34475700	
H	1.80070700	-0.47601600	2.25769000	
H	-2.56137200	2.93328000	0.09322600	
O	-1.89230200	-0.00003700	-2.98085900	
H	-2.71430700	0.50112400	-2.85144200	
Name				C10-RAF-W
Cartesian Coordinates				Frequency and Energy
Cl	-5.16443400	2.03940900	-0.32849100	Zero-point correction= 0.215151 (Hartree/Particle)
N	0.81851700	-1.06360400	0.06106000	Thermal correction to Energy= 0.231143
N	-3.50791500	0.49275500	-1.62126200	Thermal correction to Enthalpy= 0.232087
N	1.36909400	0.82041100	-1.08889100	Thermal correction to Gibbs Free Energy= 0.169907
N	2.73637000	2.84698000	-1.48362400	Sum of electronic and zero-point Energies= -1142.329399
C	-0.25424100	-1.28900200	-0.90092600	Sum of electronic and thermal Energies= -1142.313407
C	-1.43589900	-0.37663300	-0.69378900	Sum of electronic and thermal Enthalpies= -1142.312463
C	1.59806200	0.00702200	-0.06602100	Sum of electronic and thermal Free Energies= -1142.374643
C	0.88384700	-1.92186800	1.24951900	
C	-1.67581300	0.31115400	0.49493100	v =-545.71
C	-2.33805400	-0.18469500	-1.76208500	
C	2.66566800	0.23922700	0.95324300	
C	-2.81029400	1.09054900	0.60437200	

C	-3.68605100	1.11577300	-0.49330600	
C	2.12951900	1.88260600	-1.25152500	
H	-0.57825400	-2.32620000	-0.80123900	
H	0.12973300	-1.16481000	-1.91492100	
H	0.93151100	-1.32057300	2.15705500	
H	1.74993100	-2.58445100	1.20541500	
H	-0.02097000	-2.52390900	1.28165200	
H	-0.98809100	0.23534100	1.33034000	
H	-2.25629200	-0.80220800	-2.64738900	
H	3.38849800	0.96735100	0.59084900	
H	3.17784900	-0.69082200	1.19859400	
H	2.20401000	0.62574100	1.86685900	
H	-3.03824800	1.64514200	1.50435000	
O	-1.16726400	1.25423400	-2.61552600	
H	-0.32039400	1.12686400	-2.14089200	
Name				C12-RAF-W
Cartesian Coordinates				Frequency and Energy
Cl	-5.34729000	1.41746400	-0.13093000	Zero-point correction= 0.214688 (Hartree/Particle)
N	0.93216200	-0.99646200	-0.04139300	Thermal correction to Energy= 0.230840
N	-3.63239400	-0.04243600	-1.47211200	Thermal correction to Enthalpy= 0.231785
N	1.75128900	0.90824200	-0.98933300	Thermal correction to Gibbs Free Energy= 0.168760
N	3.28055000	2.85174200	-1.07481900	Sum of electronic and zero-point Energies= -1142.321348
C	-0.04952600	-1.09452500	-1.11250100	Sum of electronic and thermal Energies= -1142.305195
C	-1.32999200	-0.35579600	-0.81384400	Sum of electronic and thermal Enthalpies= -1142.304251
C	1.76501400	0.04706000	0.01360900	Sum of electronic and thermal Free Energies= -1142.367275
C	0.72953100	-1.87099200	1.11719100	
C	-1.47157900	0.55719200	0.21965900	v =-535.06
C	-2.45719300	-0.62155800	-1.62077300	
C	2.65710400	0.17006500	1.20845300	
C	-2.69197800	1.19737600	0.39050600	
C	-3.71966100	0.91437700	-0.53364400	
C	2.58761500	1.92124500	-0.98206900	
H	-0.27065200	-2.15050800	-1.27511200	
H	0.38471000	-0.70472800	-2.03330700	
H	0.16843000	-1.35794500	1.90246600	
H	1.68371700	-2.20893000	1.51605500	
H	0.16506800	-2.74132700	0.78984200	
H	-0.65657700	0.77157200	0.90200400	
H	-2.38359700	-1.37156100	-2.40274300	
H	3.26312100	1.07088200	1.14580200	
H	3.31497100	-0.69910600	1.27292700	
H	2.05525100	0.20564100	2.11918800	
H	-2.85875500	1.91337000	1.18372300	
O	-3.23076000	2.60049600	-1.54431800	
H	-2.33047400	2.39117900	-1.84470000	
Name				C13-RAF-W
Cartesian Coordinates				Frequency and Energy
Cl	-4.87378300	2.28940700	-0.87455700	Zero-point correction= 0.214714 (Hartree/Particle)
N	0.86797100	-1.13031900	0.03318800	Thermal correction to Energy= 0.230996
N	-3.28270100	0.51132900	-1.93115000	Thermal correction to Enthalpy= 0.231940
N	1.33299500	0.75879300	-1.14061400	Thermal correction to Gibbs Free Energy= 0.168689
N	2.44287500	2.94332800	-1.48281300	Sum of electronic and zero-point Energies= -1142.327603
C	-0.19345600	-1.41107600	-0.93134900	Sum of electronic and thermal Energies= -1142.311322
C	-1.35789000	-0.45188500	-0.82357800	Sum of electronic and thermal Enthalpies= -1142.310378

C	1.55352200	0.01055100	-0.07238700	Sum of electronic and thermal Free Energies= v =-441.99	-1142.373628
C	0.92817900	-1.94851500	1.24701300		
C	-1.61260800	0.30744200	0.30322500		
C	-2.21604300	-0.30437400	-1.91428900		
C	2.51604000	0.36692000	1.01572800		
C	-2.66018900	1.24870800	0.28212400		
C	-3.49226700	1.23274500	-0.86014800		
C	1.95517400	1.90768800	-1.27107800		
H	-0.53284700	-2.43195600	-0.75826600		
H	0.21183500	-1.36335800	-1.94258000		
H	0.34848400	-1.49616900	2.05610300		
H	1.95840200	-2.07892300	1.57098900		
H	0.51421700	-2.92737400	1.01829600		
H	-0.98670600	0.24478300	1.18662900		
H	-2.04265200	-0.87542900	-2.82037300		
H	2.96351900	1.34076700	0.83003500		
H	3.30785000	-0.38325200	1.07225200		
H	1.99983000	0.38560600	1.97798700		
H	-2.98868000	1.73968800	1.18654500		
O	-1.57381200	2.90173100	-0.21441700		
H	-0.96879400	2.47914700	-0.84753400		
Name				C14-RAF-W	
Cartesian Coordinates				Frequency and Energy	
Cl	-5.38604900	1.25293800	0.26951800	Zero-point correction=	0.214014 (Hartree/Particle)
N	0.92831900	-0.80926000	-0.17229300	Thermal correction to Energy=	0.230510
N	-3.70513800	-0.38473200	-0.88822000	Thermal correction to Enthalpy=	0.231454
N	2.19870400	0.94583600	-0.90377400	Thermal correction to Gibbs Free Energy=	0.167410
N	4.06674800	2.55269700	-0.68602100	Sum of electronic and zero-point Energies=	-1142.323093
C	0.02941200	-0.69106900	-1.32158800	Sum of electronic and thermal Energies=	-1142.306597
C	-1.31212100	-0.15531100	-0.90468700	Sum of electronic and thermal Enthalpies=	-1142.305652
C	1.92833000	0.04988600	0.03201700	Sum of electronic and thermal Free Energies=	-1142.369697
C	0.49617800	-1.74761700	0.86631100	v =-553.24	
C	-1.41837400	1.07584400	-0.20424100		
C	-2.47977900	-0.81960500	-1.22749700		
C	2.69740700	-0.06752500	1.31174200		
C	-2.69706100	1.48975100	0.22330300		
C	-3.77805200	0.72989600	-0.18689900		
C	3.20258400	1.77378700	-0.73454300		
H	-0.09084900	-1.67874300	-1.76892700		
H	0.48382100	-0.02808900	-2.05560800		
H	-0.07425300	-1.23520200	1.64517600		
H	1.35007300	-2.25268800	1.31237200		
H	-0.14023600	-2.49599900	0.39687400		
H	-0.54099700	1.51763800	0.25371500		
H	-2.44075000	-1.75232700	-1.77929600		
H	3.41663900	0.74301300	1.40353100		
H	3.23214800	-1.01990000	1.33444100		
H	2.01676800	-0.04209800	2.16438600		
H	-2.82536000	2.38530000	0.81566900		
O	-1.20070900	2.31298700	-1.74026500		
H	-1.98947700	2.07561100	-2.25801700		

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