How does nucleophilic aromatic substitution really proceed in nitroarenes? Computational prediction and experimental verification

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Supporting Information

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Computational details

All calculations presented in this work were performed using Gaussian 09 package.[1] The starting structures were created using GaussView 5.0. The optimization of equilibrium and transition state structures has been performed using PBE1PBE hybrid functional[2] with 6-31+G(d) basis set and the electron energy in each single point has been recalculated using larger basis set 6-311+G(2d,p). This functional has been selected o the basis of the results and reasoning described below ("Method selection").Two sets of calculations have been performed: for the gas-phase reactions and for the solution phase reactions using PCM solvation model in DMF (dielectric constant ε = 37.219). No geometry restrictions have been applied. The thermal and ZPE corrections have been used in the calculations. Frequency analysis has been performed to find the proper ground state (no imaginary frequencies) and transition state (one imaginary frequency) structures. In the case when more than one transition state or stationary structure has been found the statistical contribution of energy has been calculated using standard Boltzmann equation.

The results of the calculations (geometries and energetic parameters) are given in the further part of this material.

Method selection

Four methods: PBE1PBE/6-311+G(2d,p)||PBE1PBE/6-31+G(d), M06-2X/6-311+G(d,p), CAM-B3LYP/6-311+G(d,p) and B3LYP/6-311+G(d,p) using PCM solvation model with a dielectric constant of *N*,*N*-dimethylformamide (ε = 37.2), a s well as without this model have been tested during their selection. The reaction of *p*-chloronitrobenzene with the anion of chloromethyl phenyl sulfone (**3** + **4** in the main text) has been selected as the model. The results are collected in tables S1 and S2.

All tested methods give similar trends of energy profiles for model reaction, i.e. an addition of the nucleophile into *ortho* and *para* positions in *p*-chloronitrobenzene. Especially, the most important parameter, i.e. the difference between activation Gibbs free energies of the addition of a nucleophile to the *ortho* and *para* positions in *p*-chloronitrobenzene has the same sign in all cases despite some differences in the absolute values.

Because none of the tested methods proved to be significantly better than others we have chosen the first of them: PBE0 (named PBE1PBE in Gaussian). This method proved to be very efficient in our previous works.[3,5] Especially, it reproduces with the reasonable accuracy proton affinities (PA)[5] values and other thermochemical parameters of compounds containing fluorine atoms and, especially, the fluoride anion. Other popular functionals, gave much higher errors. Our experience gathered during hundreds of calculations shows that the 6-31+G(d) basis set is sufficient to achieve good accuracy of the geometries and frequencies of the medium-sized organic anions and neutral molecules. Similarly, the 6-311+G(2d,p) basis set gives good accuracy for the energy of the molecule. Further extension of these basis sets does improve the results but makes the calculations significantly longer.

Comparison of the calculations performed for the gas-phase and solvent-phase reactions shows that the activation Gibbs free energies are much higher in solution but the differences between them are still comparable. Finally we decided to bas our work on the results of the PBE1PBE/6-311+G(2d,p)||PBE1PBE/6-31+G(d) using PCM(dimethylformamide) solvent model.

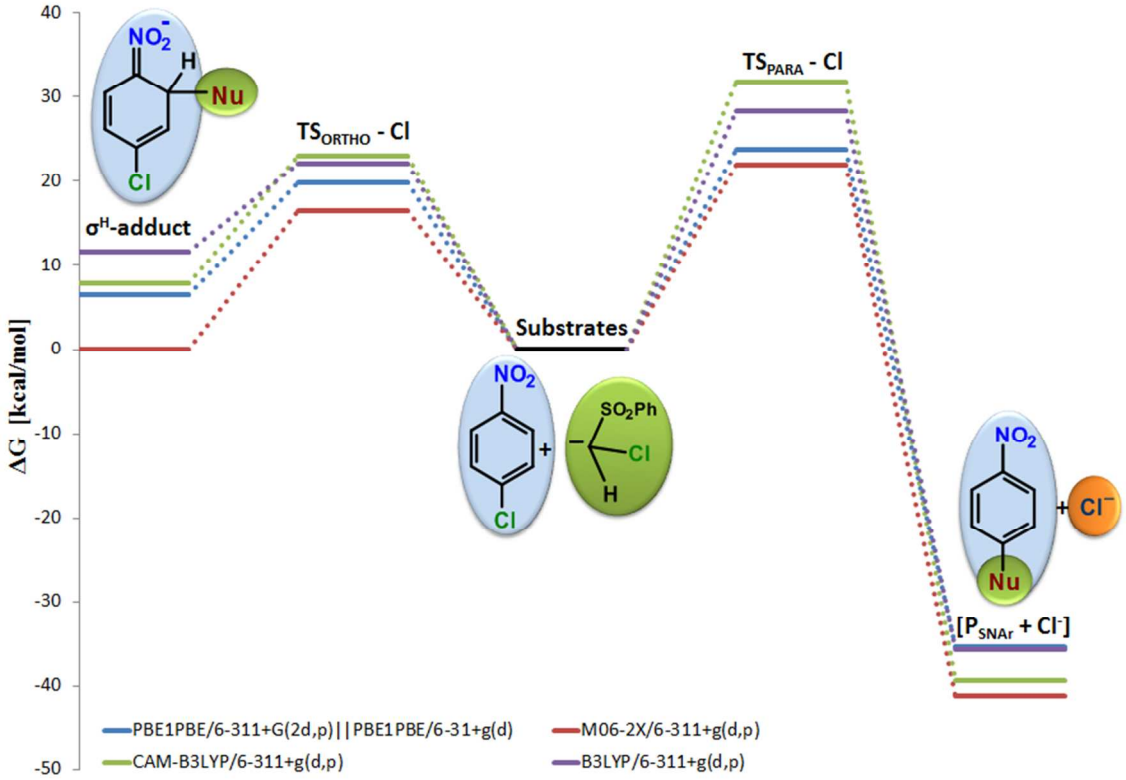

Figure S1. Energy profiles for model reaction, using PCM solvent model and DMF as the solvent.

Table S1. Calculated values of selected ΔG [kcal/mol] values for the reaction of *p*-chloro-nitrobenzene with the anion of chloromethyl phenyl sulfone, using PCM solvent model and DMF as the solvent.

	TS_{ortho}	σ^H-adduct	TS_{para}	TS_{para} - TS_{ortho}	$[P_{SNAr} + Cl^-]$
PBE1PBE/6-311+G(2d,p)|| PBE1PBE/6-31+G(d)	19.9	6.5	23.7	3.8	-35.5
M06-2X/6-311+G(d,p)	16.4	-0.02	22.0	5.6	-41.2
CAM-B3LYP/6-311+G(d,p)	23.0	7.9	31.8	8.8	-39.3
B3LYP/6-311+G(d,p)	22.2	11.7	28.3	6.1	-35.8

Table S2. Calculated values of selected ΔG [kcal/mol] values for the reaction of *p*-chloro-nitrobenzene with the anion of chloromethyl phenyl sulfone in the gas phase.

	TS_{ortho}	σ^H-adduct	TS_{para}	TS_{para} -TS_{ortho}	$[P_{SNAr} + Cl^-]$
PBE1PBE/6-311+G(2d,p)|| PBE1PBE/6-31+G(d)	6.2	-7.9	13.2	7.0	-39.9
M06-2X/6-311+G(d,p)	4.4	-9.1	9.5	5.1	-47.4
CAM-B3LYP/6-311+G(d,p)	9.1	-2.3	12.5	3.4	-44.3
B3LYP/6-311+G(d,p)	9.0	1.7	14.7	5.7	-40.5

Solution-phase kinetic data

Kinetic factors have been obtained using $\Delta G^{\ddagger}$ for each reaction, calculated at PBE1PBE/6-311+G(2d,p)||PBE1PBE/6-31+G(d) level of theory using PCM solvation model with a dielectric constant (ε = 37.219) of *N,N*-dimethylformamide. The reaction rates have been calculated using Eyring-Polanyi equation ($k = \frac{k_B T}{h} e^{-\frac{\Delta G^{\ddagger}}{RT}}$). The k_H of the reaction into *ortho* position has been taken for the relative rates calculations as a standard.

Table S3. Gibbs free energy values (ΔG in kcal mol^{-1}) for the reactions of nitroarenes **1** – **3** with anion **4** calculated at PBE1PBE/6-311+G(2d,p)||PBE1PBE/6-31+G(d) level of theory using PCM(dimethylformamide) solvation model.

X=	**TS_{ortho}** kcal mol^{-1}	**Stat. Factor** k_X	**Stat. Factor** $2k_X$	k_X/k_H	$\log(k_X/k_H)$	**Exp.** k_X/k_H	**Exp.** $\log(k_X/k_H)$
H	22.13	3.70×10^4	7.40×10^4	1.0	0.0	1	0
F	20.90	2.93×10^3	5.86×10^3	7.9	0.9	50	1.7
Cl	19.91	1.58×10^2	3.15×10^2	42.5	1.6	130	2.1

X=	**TS_{para}** kcal mol^{-1}	**Stat. Factor** k_X	**Stat. Factor** $2k_X$	k_X/k_H	$\log(k_X/k_H)$	**Exp.** k_X/k_H	**Exp.** $\log(k_X/k_H)$
H	21.85	5.96×10^4	-	0.8	-0.1	0.7	-0.15
F	21.39	1.29×10^3	-	1.7	0.2	-	-
Cl	23.71	2.58×10^5	-	0.03	-1.5	-	-

Gas phase results

Calculation for the gas-phase reactions have been performed at PBE1PBE/6-311+G(2d,p)||PBE1PBE/6-31+G(d) level of theory. The results are given in Tables S4 and S5 and in Figure S2.

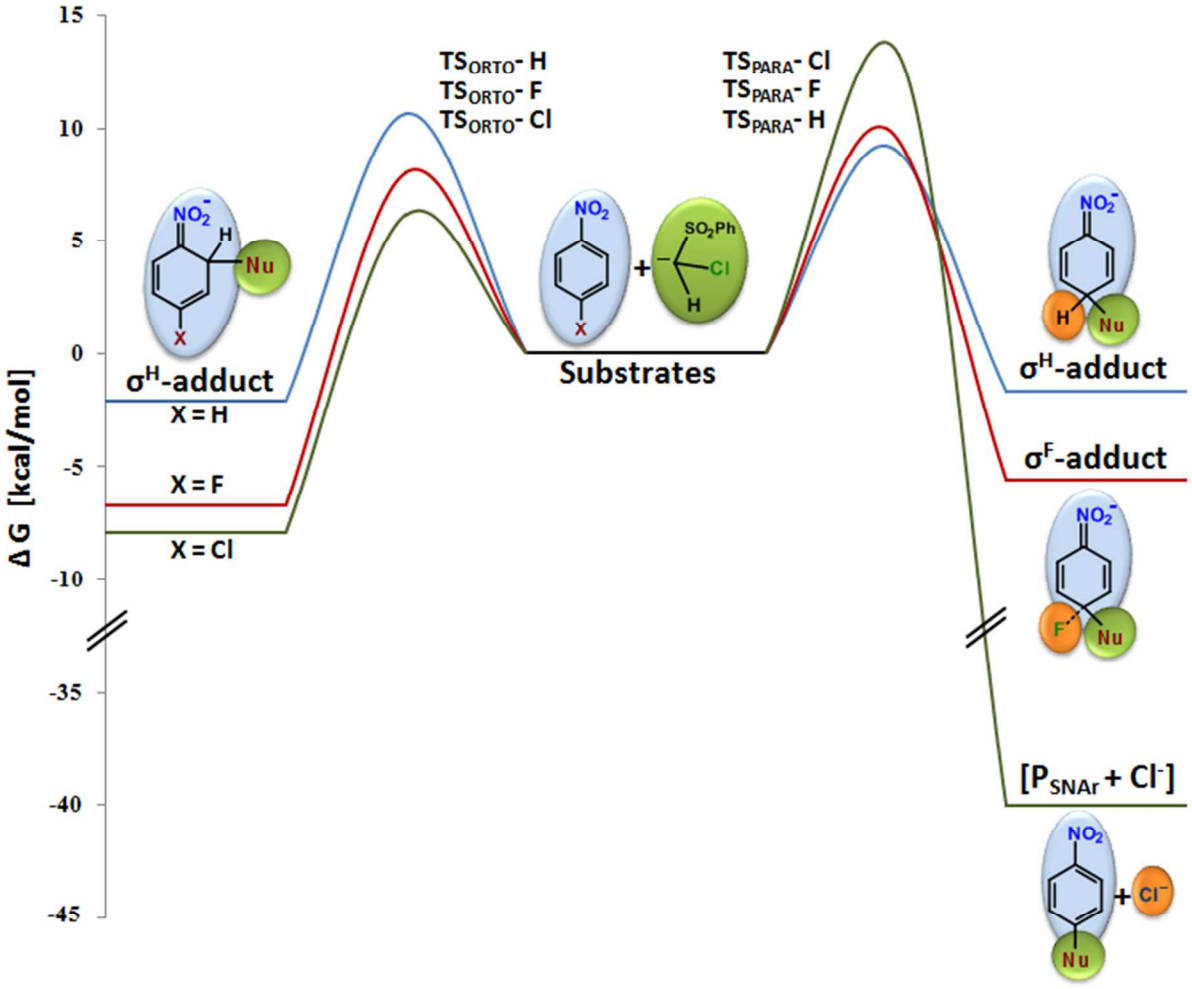

Figure S2. Calculated energy profiles for addition of the model nucleophile **4** at positions *ortho* and *para* of **1**, **2** and **3** to form σ^H,σ^F and σ^{Cl} adducts.

Table S4. Gibbs free energy values (ΔG in kcal mol^{-1}) for the reactions of nitroarenes **1 – 3** with anion **4** calculated at PBE1PBE/6-311+G(2d,p)||PBE1PBE/6-31+G(d) level of theory.

X=	TS_{ortho}-X	σ^{H}-adduct	TS_{para}-X	σ^{X}-adduct
H	10.7	-2.1	9.2	-1.7
F	8	-6.7	10	-5.6
				[P_{SNAr} + Cl^-]
Cl	6.2	-7.9	13.2	-39.9

Table S5. Kinetic factors for the gas-phase calculations.

	TS_{ortho}		**Stat. Factor**			**Exp.**	**Exp.**
X=	kcal mol^{-1}	k_X	$2k_X$	k_X/k_H	$\log(k_X/k_H)$	k_X/k_H	$\log(k_X/k_H)$
H	10.70	8.88×10^{4}	1.78×105	1.0	0.0	1	0
F	8.00	8.47×10^{6}	1.69×10^{7}	95.4	2.0	50	1.7
Cl	6.20	1.77×10^{8}	3.54×10^{8}	1992.1	3.3	130	2.11

	TS_{para}		**Stat. Factor**			**Exp.**	**Exp.**
X=	kcal mol^{-1}	k_X	$2k_X$	k_X/k_H	$\log(k_X/k_H)$	k_X/k_H	$\log(k_X/k_H)$
H	9.20	1.12×10^{6}	-	6.3	0.8	0.7	-0.15
F	10.00	2.89×10^{5}	-	1.6	0.2	-	-
Cl	13.20	1.30×10^{3}	-	0.0	-2.1	-	-

Geometries and energetic parameters calculated at PBE1PBE/6-311+G(2d,p)|| PBE1PBE/6-31+G(d) using SMD solvation model with a dielectric constant (ε = 37.219) of *N*,*N*-dimethylformamide as a solvent.

Substrates:

Nucleophile (chloromethyl phenyl sulfone)

C	-2.05906100	-0.00271100	-0.81478200
Cl	-2.02688400	1.78171100	-0.54684900
H	-1.71583300	-0.19486500	-1.83390300
S	-1.02548800	-0.83881800	0.26681800
O	-1.04192400	-2.25820200	-0.17250700
O	-1.40283500	-0.55220700	1.67180200
C	0.69799400	-0.32711900	0.15061000
C	1.49614900	-0.84459400	-0.87237100
C	1.19793200	0.64423100	1.01829400
C	2.80704400	-0.39703300	-1.01462800
H	1.09452900	-1.60154400	-1.54052000
C	2.51063800	1.09191000	0.86567500
H	0.56758700	1.03056400	1.81333900
C	3.31568800	0.57273300	-0.14734100
H	3.43448000	-0.80830900	-1.80132000
H	2.90461000	1.84464700	1.54386100
H	4.33923700	0.92026700	-0.26121600

Thermochemistry data [Hartree]

Electron Energy	-1278.643789
Thermal correction to Energy	0.116959
Zero-point correction	0.12702
Thermal correction to Enthalpy	0.127964
Thermal correction to Gibbs Free Energy	0.07945

Nitrobenzene

C	-0.24682900	0.00000000	0.00000700
C	0.42387800	-1.22064800	0.00001600
C	1.81444800	-1.21136900	0.00001400
C	2.50808700	0.00000000	0.00000200
C	1.81444800	1.21136900	-0.00000900
C	0.42387800	1.22064800	-0.00000500

N	-1.70509000	0.00000000	0.00001100
O	-2.28303800	1.07962800	0.00000700
O	-2.28303800	-1.07962800	-0.00003700
H	-0.13538400	-2.14916000	0.00002500
H	-0.13538400	2.14916000	-0.00001300
H	2.35655300	2.15219200	-0.00001900
H	2.35655300	-2.15219200	0.00002300
H	3.59443400	0.00000000	0.00000000

Thermochemistry data [Hartree]

Electron Energy	-436.3988393
Thermal correction to Energy	0.104134
Zero-point correction	0.110943
Thermal correction to Enthalpy	0.111888
Thermal correction to Gibbs Free Energy	0.072092

_p_-Fluoronitrobenzene

C	-0.67425200	0.00000000	0.00002800
C	-0.00088000	-1.22025800	0.00021400
C	1.38693600	-1.22138000	0.00021100
C	2.04919800	0.00000000	-0.00000600
C	1.38693600	1.22138000	-0.00020700
C	-0.00088000	1.22025800	-0.00017600
N	-2.12837200	0.00000000	0.00004900
O	-2.70580300	1.08010300	0.00019000
O	-2.70580200	-1.08010300	-0.00026300
H	-0.55757000	-2.15009000	0.00037500
H	-0.55757000	2.15009000	-0.00032200
H	1.95125000	2.14779600	-0.00038500
H	1.95124900	-2.14779600	0.00037700
F	3.39130400	0.00000000	-0.00002100

Thermochemistry data [Hartree]

Electron Energy	-535.5806944
Thermal correction to Energy	0.095774
Zero-point correction	0.103389
Thermal correction to Enthalpy	0.104334
Thermal correction to Gibbs Free Energy	0.062539

_p_-Chloronitrobenzene

C	-1.10119300	0.00000000	0.00007100
C	-0.42775700	1.21848000	-0.00005900
C	0.96042900	1.21785000	-0.00009800
C	1.64098600	0.00000000	0.00000500
C	0.96042900	-1.21785000	0.00014000
C	-0.42775700	-1.21848000	0.00016500
N	-2.55708800	0.00000000	0.00010800
O	-3.13318500	-1.08027600	-0.00020900
O	-3.13318500	1.08027600	0.00000200
H	-0.98240200	2.14962200	-0.00013400
H	-0.98240200	-2.14962200	0.00026600
H	1.50941700	-2.15345200	0.00022600
H	1.50941700	2.15345200	-0.00020900
Cl	3.37327800	0.00000000	-0.00003500

Thermochemistry data [Hartree]	
Electron Energy	-895.8633917
Thermal correction to Energy	0.094426
Zero-point correction	0.102404
Thermal correction to Enthalpy	0.103348
Thermal correction to Gibbs Free Energy	0.060288

Transition states for addition to the *ortho* position in nitrobenzene:

TS1

C	3.07512700	0.50753200	-0.08175900
C	2.20699000	-0.11559600	0.85171800
C	2.41037900	-1.50656100	1.06772400
C	3.27280500	-2.22773900	0.27540400
C	4.03305300	-1.59858000	-0.74226800
C	3.93794900	-0.23663500	-0.91283200
C	0.12114300	-0.04622100	-0.14722900
S	-1.16196300	-0.11793400	1.01646100
N	3.04487600	1.91083300	-0.20681500
O	3.81287400	2.47036800	-1.01067800

Cl	0.03460300	-1.32885300	-1.36089500
O	-0.96328900	1.05654900	1.89592300
O	-1.19086000	-1.45926300	1.63685100
O	2.24292100	2.55721000	0.48818300
H	1.74863500	0.49476100	1.61771300
H	4.52942300	0.28281300	-1.65898700
H	4.69963300	-2.18416800	-1.36876700
H	0.12877700	0.93145700	-0.62907600
H	1.83601500	-2.00083000	1.84593400
C	-2.76854200	0.09519300	0.24779100
C	-3.50204300	-1.02553300	-0.14299500
C	-3.23065700	1.38600500	-0.01818100
C	-4.71888000	-0.84794300	-0.80029500
H	-3.12911200	-2.02020000	0.08122800
C	-4.44844000	1.55216600	-0.67233700
H	-2.64731400	2.24708100	0.29590100
C	-5.19192500	0.43706900	-1.06510400
H	-5.29937900	-1.71621100	-1.10094800
H	-4.82000700	2.55375100	-0.87226000
H	-6.14209100	0.57132500	-1.57532500
H	3.38952100	-3.29603400	0.44408700

Thermochemistry data [Hartree]

Electron Energy	-1715.03131
Thermal correction to Energy	0.22157
Zero-point correction	0.23941
Thermal correction to Enthalpy	0.24036
Thermal correction to Gibbs Free Energy	0.17248

TS2

C	2.20640800	1.19918000	0.03714000
C	1.33092300	0.43060000	0.84364400
C	1.93819900	-0.51136200	1.71483800
C	3.28670200	-0.77719000	1.63957600
C	4.12176400	-0.07768300	0.73392300
C	3.58253200	0.90992000	-0.05877800
C	0.19569400	-0.95332400	-0.68430400
S	-1.33951800	-1.63708600	-0.20164100
N	1.67325200	2.26545200	-0.71680000

O	2.43187500	2.95974800	-1.41715500
Cl	1.33442800	-2.25295700	-1.10611800
O	-1.17163000	-2.36362900	1.07931000
O	-2.07488400	-2.39132500	-1.25414400
O	0.45114500	2.48018600	-0.66567300
H	0.34863800	0.82472100	1.06074800
H	4.19704400	1.48684500	-0.74141000
H	5.18206200	-0.30675000	0.67845800
H	0.03498000	-0.31592400	-1.55708700
H	1.31045000	-1.05182700	2.41739700
C	-2.28292700	-0.15333900	0.12048000
C	-2.93378900	0.48451300	-0.93505100
C	-2.35717200	0.33903300	1.42240100
C	-3.66276800	1.64391200	-0.67903300
H	-2.87875500	0.07399300	-1.93922900
C	-3.09480600	1.49541700	1.66882500
H	-1.85299500	-0.18568800	2.22882800
C	-3.74248000	2.14824000	0.61961500
H	-4.17355200	2.14994600	-1.49373300
H	-3.16391000	1.88514900	2.68080800
H	-4.31541500	3.05083700	0.81510700
H	3.72395900	-1.52317800	2.29960200

Thermochemistry data [Hartree]

Electron Energy	-1715.02472
Thermal correction to Energy	0.22131
Zero-point correction	0.23923
Thermal correction to Enthalpy	0.24018
Thermal correction to Gibbs Free Energy	0.17230

TS3

C	2.61957600	0.38148600	-0.45140000
C	1.22377800	0.56869500	-0.62936100
C	0.68927700	1.79544400	-0.14968100
C	1.45119800	2.64914700	0.61458300
C	2.81022300	2.36575000	0.89613700
C	3.39122900	1.24060100	0.35663100
C	0.24511800	-1.00839500	0.77529200
S	-1.29394300	-1.65899900	0.27572400

N	3.24371100	-0.71847300	-1.07272300
O	4.46929700	-0.88650100	-0.93457600
Cl	0.19277600	-0.28693700	2.39054200
O	-2.11431600	-2.27524200	1.34813900
O	-1.01070600	-2.48939500	-0.91847400
O	2.54923900	-1.50019500	-1.74354200
H	0.72984500	0.03591500	-1.43056300
H	4.43882900	1.01137800	0.51916900
H	3.39486200	3.04257800	1.51244200
H	0.97795600	-1.81600800	0.73913000
H	-0.34826100	2.03401600	-0.36679100
C	-2.22832100	-0.23906200	-0.28061000
C	-2.23345300	0.08169500	-1.63753400
C	-2.91922200	0.53969700	0.64831000
C	-2.93735000	1.20465300	-2.06825900
H	-1.70159300	-0.54877600	-2.34396100
C	-3.61348400	1.66494700	0.20807600
H	-2.91890400	0.26447400	1.69851300
C	-3.62143200	1.99844000	-1.14690000
H	-2.95221900	1.45815700	-3.12491300
H	-4.15345600	2.27826400	0.92446400
H	-4.16733000	2.87487700	-1.48607500
H	1.00925700	3.56844200	0.99276600

Thermochemistry data [Hartree]	
Electron Energy	-1715.02729
Thermal correction to Energy	0.22152
Zero-point correction	0.23927
Thermal correction to Enthalpy	0.24021
Thermal correction to Gibbs Free Energy	0.17329

σ^H adducts in *ortho* position in nitrobenzene:

ADDUCT 1

C	2.71327400	0.66902800	-0.04672600
C	1.69430000	-0.20378700	0.64419000
C	2.16243400	-1.63300900	0.73381600
C	3.24892900	-2.08684800	0.07712800
C	4.07196600	-1.22003400	-0.73881200
C	3.80945900	0.11624100	-0.76877200

C	0.30727100	-0.04916200	-0.03872100
S	-1.05791800	-0.72133800	0.98557300
N	2.57733200	2.00759900	0.06368400
O	3.41973900	2.80642900	-0.45876500
Cl	0.22994100	-0.75246100	-1.66948200
O	-0.89740900	-0.08523800	2.30294100
O	-1.09014400	-2.18715000	0.89519100
O	1.58006100	2.47950400	0.70848400
H	1.51461200	0.19768400	1.65442600
H	4.43966000	0.80154300	-1.32702300
H	4.90968700	-1.63408700	-1.29261100
H	0.08729500	1.01916100	-0.11765900
H	1.57639200	-2.30601000	1.35474500
C	-2.54128000	-0.08636100	0.23495400
C	-3.25795400	-0.89353900	-0.64711200
C	-2.95265200	1.20889000	0.54981800
C	-4.41782200	-0.38485400	-1.22690000
H	-2.91675300	-1.90087200	-0.86442100
C	-4.11214000	1.70492500	-0.04002800
H	-2.38374200	1.81117500	1.25217200
C	-4.84115300	0.90982400	-0.92555400
H	-4.99127000	-1.00196700	-1.91267500
H	-4.44906000	2.70989500	0.19747900
H	-5.74682400	1.30109100	-1.38097600
H	3.53059400	-3.13382000	0.17627200

Thermochemistry data [Hartree]

Electron Energy	-1715.06089
Thermal correction to Energy	0.22417
Zero-point correction	0.24181
Thermal correction to Enthalpy	0.24275
Thermal correction to Gibbs Free Energy	0.17614

ADDUCT 2

C	2.10994500	1.08975700	0.04879800
C	1.02009500	0.15903500	0.52711900
C	1.49254000	-0.69341100	1.67682900
C	2.78539000	-0.75526200	2.05445400
C	3.81760900	0.02143200	1.40251600
C	3.46753700	0.92631900	0.44667100
C	0.45789000	-0.65503600	-0.66639800
S	-1.14516000	-1.50737100	-0.36501500
N	1.75456600	2.11905200	-0.74905600
O	2.61067200	2.96452600	-1.16455300
Cl	1.59217300	-1.88627300	-1.27369900
O	-1.01460700	-2.42204500	0.77810500

O	-1.58612300	-2.04775600	-1.65959600
O	0.52966900	2.24534900	-1.08955900
H	0.16089700	0.77482500	0.84358400
H	4.20891900	1.56448000	-0.02406900
H	4.85483100	-0.09756800	1.70232400
H	0.23864300	0.03451000	-1.48586800
H	0.74039600	-1.28252400	2.19390600
C	-2.25312900	-0.19173800	0.09225300
C	-2.83985200	0.57675800	-0.91324300
C	-2.52318500	0.03099500	1.44209100
C	-3.71353700	1.59818100	-0.55071000
H	-2.62562800	0.37342200	-1.95822300
C	-3.40222600	1.05373900	1.78922100
H	-2.06294700	-0.59316500	2.20221700
C	-3.99199500	1.83591600	0.79586300
H	-4.18015900	2.20508500	-1.32125100
H	-3.62762500	1.23678100	2.83591200
H	-4.67649800	2.63321000	1.07228700
H	3.06343300	-1.39855500	2.88772500

Thermochemistry data [Hartree]

Electron Energy	-1715.05934
Thermal correction to Energy	0.22427
Zero-point correction	0.24186
Thermal correction to Enthalpy	0.24281
Thermal correction to Gibbs Free Energy	0.17668

ADDUCT 3

C	2.67433300	0.41660100	-0.27088900
C	1.20906500	0.24198800	-0.59443700
C	0.51943800	1.57729400	-0.71000300
C	1.09291100	2.73227800	-0.31427700
C	2.43837700	2.78288200	0.21279700
C	3.19976200	1.65294300	0.20017200
C	0.56202400	-0.72042400	0.43750800
S	-0.99435800	-1.55074900	-0.08304900
N	3.49264100	-0.64263300	-0.45438400
O	4.74268400	-0.56179300	-0.23113400
Cl	0.35303300	-0.00013600	2.05047700
O	-1.32640100	-2.51248200	0.97894600
O	-0.73659000	-2.04421900	-1.44476900
O	2.99672300	-1.74687200	-0.86011400
H	1.12194900	-0.31370700	-1.54161300
H	4.23443500	1.66689500	0.52859200
H	2.84413000	3.72350000	0.57394000
H	1.22058400	-1.58984700	0.54282800

H	-0.48075500	1.58859400	-1.13351300
C	-2.31617500	-0.36265100	-0.16722100
C	-2.68143700	0.14621400	-1.41329900
C	-2.98608800	0.00153500	1.00117100
C	-3.73480800	1.05378700	-1.48520500
H	-2.15439700	-0.17283300	-2.30736300
C	-4.03238600	0.91635700	0.91464800
H	-2.70218900	-0.43034300	1.95517800
C	-4.40330600	1.44171700	-0.32356800
H	-4.03455600	1.45459400	-2.44927800
H	-4.56302700	1.21195700	1.81515300
H	-5.22373600	2.15158600	-0.38448700
H	0.53566100	3.66214800	-0.41588300

Thermochemistry data [Hartree]

Electron Energy	-1715.05819
Thermal correction to Energy	0.22424
Zero-point correction	0.24180
Thermal correction to Enthalpy	0.24274
Thermal correction to Gibbs Free Energy	0.17669

Transition states for addition to the *para* position in nitrobenzene:

TS1

C	-2.27531600	1.46410400	1.11202200
C	-1.60945500	1.56435000	-0.14303600
C	-2.21784100	0.94661800	-1.26822800
C	-3.31615300	0.13122800	-1.11960100
C	-3.89318700	-0.03992900	0.15417000
C	-3.37216600	0.65082700	1.26851600
C	0.29735100	0.27109500	0.24211500
S	1.71629500	0.98302700	-0.44788400
Cl	-0.02673500	-1.37069200	-0.31284500
O	1.83035700	2.31278100	0.19502900
O	1.63140300	0.92219700	-1.92272100
H	-0.90762200	2.37445300	-0.29820400
H	-3.86295700	0.55316600	2.23098800
H	0.35555200	0.30237700	1.33022200
H	-1.78791900	1.09138800	-2.25534800
C	3.20423300	0.08248700	-0.01090700
C	3.64874700	-0.95315300	-0.83419800
C	3.85394100	0.37537200	1.19000800
C	4.76281900	-1.69812000	-0.45058900
H	3.13675000	-1.15960200	-1.76898200
C	4.96913800	-0.37159100	1.56113000
H	3.49471500	1.18717200	1.81611700

C	5.42268300	-1.40897800	0.74386200
H	5.11819500	-2.50208700	-1.08976800
H	5.48734800	-0.14079600	2.48817900
H	6.29280600	-1.99003800	1.03783100
H	-3.76295100	-0.36346200	-1.97549500
N	-5.02031700	-0.87019100	0.30792100
O	-5.47666300	-1.46507500	-0.68445500
O	-5.53349900	-0.99348200	1.43416400
H	-1.88945000	2.01485800	1.96580100

Thermochemistry data [Hartree]

Electron Energy	-1715.03150
Thermal correction to Energy	0.22148
Zero-point correction	0.23940
Thermal correction to Enthalpy	0.24035
Thermal correction to Gibbs Free Energy	0.17160

TS2

C	0.99146400	1.18703400	0.51880800
C	0.73244600	-0.02514600	1.21628700
C	1.82862700	-0.88312900	1.49647100
C	3.06649900	-0.64733900	0.94134200
C	3.26680600	0.49707800	0.14671100
C	2.22446600	1.42970600	-0.03830100
C	-0.48884300	-1.27453700	-0.38770600
S	-2.22353700	-1.26613500	-0.21169700
CL	0.13988000	-2.93425300	-0.44028800
O	-2.58460800	-1.87723500	1.08949400
O	-3.00996900	-1.75859700	-1.37618900
H	-0.16145400	-0.10496000	1.82205600
H	2.41669300	2.33793500	-0.59931100
H	-0.22012400	-0.75397100	-1.30999600
H	1.68134200	-1.75262000	2.12995800
C	-2.51712500	0.49335100	-0.09851100
C	-2.52660500	1.26305300	-1.26210600
C	-2.73179400	1.06814300	1.15277800
C	-2.73911800	2.63650000	-1.16390600
H	-2.38033900	0.79439200	-2.23127300
C	-2.95244200	2.44149300	1.23892500
H	-2.73394300	0.44309900	2.04098000
C	-2.95053600	3.22447300	0.08401500
H	-2.74634400	3.24598600	-2.06341200
H	-3.12585400	2.89952500	2.20893200
H	-3.12004400	4.29555000	0.15562800
H	3.89887500	-1.31787400	1.12664400

N	4.53636400	0.74290400	-0.42000300
O	4.70742800	1.77083100	-1.09655600
O	5.45231100	-0.07526600	-0.23285300
H	0.19090300	1.91112300	0.39186000

Thermochemistry data [Hartree]

Electron Energy	-1715.02503
Thermal correction to Energy	0.22134
Zero-point correction	0.23932
Thermal correction to Enthalpy	0.24026
Thermal correction to Gibbs Free Energy	0.17156

TS3

C	-1.84936700	-0.99065900	1.69870500
C	-0.74126700	-0.16379200	1.36570100
C	-0.98311300	0.98607300	0.57085800
C	-2.21839500	1.20713000	0.00513200
C	-3.27887900	0.31964300	0.27186500
C	-3.08648900	-0.77664200	1.13740900
C	0.50253700	-1.59156700	-0.05882400
S	2.22820900	-1.43916400	0.04893600
CL	-0.13477800	-1.37131200	-1.69050800
O	3.01391900	-1.99003800	-1.08432100
O	2.57454700	-1.92322700	1.40771700
H	0.14824600	-0.20533600	1.98224200
H	-3.92602600	-1.42196800	1.37283200
H	0.21581800	-2.56354300	0.34484400
H	-0.17295300	1.68466100	0.38046100
C	2.53468200	0.32286200	0.02319700
C	2.69065900	1.00370500	1.23009700
C	2.59540000	0.99597200	-1.19750300
C	2.90317400	2.38093500	1.21245600
H	2.65771000	0.45626500	2.16743300
C	2.79948600	2.37447800	-1.20362100
H	2.49417400	0.44797000	-2.12925100
C	2.95159900	3.06672000	-0.00161000
H	3.03293800	2.91729600	2.14867800
H	2.84672800	2.90677200	-2.14987400
H	3.11525500	4.14109100	-0.01159200
H	-2.39577800	2.07276800	-0.62415300
N	-4.54667300	0.55006200	-0.29882600
O	-4.70737900	1.53331300	-1.04283700
O	-5.47623700	-0.23689900	-0.04830500
H	-1.70850100	-1.82181800	2.38460400

Thermochemistry data [Hartree]	
Electron Energy	-1715.02747
Thermal correction to Energy	0.22143
Zero-point correction	0.23928
Thermal correction to Enthalpy	0.24023
Thermal correction to Gibbs Free Energy	0.17257

TS4

C	2.21793000	0.94578300	-1.26878700
C	1.60944700	1.56412000	-0.14399000
C	2.27524400	1.46468100	1.11115700
C	3.37216800	0.65160200	1.26818800
C	3.89328400	-0.03978200	0.15427900
C	3.31631100	0.13057500	-1.11962300
C	-0.29732500	0.27080300	0.24178200
S	-1.71626200	0.98274400	-0.44816600
O	-1.63156600	0.92155500	-1.92300200
O	-1.83006000	2.31266400	0.19445200
H	0.90747100	2.37400300	-0.29965600
H	3.76319500	-0.36458500	-1.97519900
H	1.88927600	2.01589800	1.96459000
C	-3.20429100	0.08253200	-0.01082500
C	-3.85430800	0.37630200	1.18970600
C	-3.64858900	-0.95373600	-0.83345400
C	-4.96958300	-0.37041200	1.56110900
H	-3.49524400	1.18857700	1.81528900
C	-4.76273100	-1.69844500	-0.44956100
H	-3.13637800	-1.16087800	-1.76796800
C	-5.42289900	-1.40842600	0.74451100
H	-5.48803300	-0.13892800	2.48785200
H	-5.11792800	-2.50289900	-1.08822600
H	-6.29308100	-1.98928400	1.03870100
H	3.86292000	0.55455800	2.23074200
N	5.02047500	-0.86988000	0.30857500
O	5.53364400	-0.99242600	1.43490000
O	5.47686700	-1.46535800	-0.68341600
H	1.78804800	1.08994000	-2.25601300
Cl	0.02664100	-1.37108800	-0.31293000
H	-0.35531700	0.30230300	1.32989000

Thermochemistry data [Hartree]	
Electron Energy	-1715.03150
Thermal correction to Energy	0.22148

Zero-point correction	0.23940
Thermal correction to Enthalpy	0.24035
Thermal correction to Gibbs Free Energy	0.17161

TS5

C	0.98311100	0.98607300	0.57083000
C	0.74126000	-0.16378700	1.36568200
C	1.84936400	-0.99064300	1.69870900
C	3.08648900	-0.77662800	1.13741900
C	3.27888100	0.31964700	0.27186100
C	2.21839500	1.20712700	0.00511100
C	-0.50252700	-1.59156500	-0.05882900
S	-2.22820100	-1.43916600	0.04894300
O	-2.57452500	-1.92322800	1.40772800
O	-3.01391300	-1.99004700	-1.08430800
H	-0.14825500	-0.20532400	1.98222100
H	2.39578000	2.07275800	-0.62418200
H	1.70849600	-1.82179200	2.38461800
C	-2.53468200	0.32285800	0.02320500
C	-2.59542700	0.99596200	-1.19749700
C	-2.69064000	1.00370400	1.23010400
C	-2.79952400	2.37446700	-1.20361700
H	-2.49421500	0.44795800	-2.12924500
C	-2.90316700	2.38093200	1.21246200
H	-2.65766800	0.45626900	2.16744300
C	-2.95162000	3.06671300	-0.00160600
H	-2.84678700	2.90675700	-2.14987100
H	-3.03291600	2.91729700	2.14868400
H	-3.11528500	4.14108200	-0.01159000
H	3.92602700	-1.42194500	1.37285900
N	4.54667700	0.55006300	-0.29882300
O	4.70738300	1.53330100	-1.04285200
O	5.47624600	-0.23688800	-0.04828000
H	0.17295200	1.68465800	0.38042000
Cl	0.13477400	-1.37130700	-1.69051800
H	-0.21581000	-2.56354700	0.34482800

Thermochemistry data [Hartree]

Electron Energy	-1715.02747
Thermal correction to Energy	0.22143
Zero-point correction	0.23928
Thermal correction to Enthalpy	0.24023
Thermal correction to Gibbs Free Energy	0.17257

TS6

C	-1.82862800	-0.88313100	1.49646900
C	-0.73244700	-0.02514800	1.21628700
C	-0.99146500	1.18703300	0.51880900
C	-2.22446700	1.42970600	-0.03829900
C	-3.26680700	0.49707800	0.14671100
C	-3.06650100	-0.64734100	0.94134000
C	0.48884400	-1.27453600	-0.38770700
S	2.22353700	-1.26613500	-0.21169400
O	3.00997200	-1.75860000	-1.37618300
O	2.58460400	-1.87723300	1.08949900
H	0.16145200	-0.10496300	1.82205600
H	-3.89887700	-1.31787600	1.12664100
H	-0.19090400	1.91112200	0.39186300
C	2.51712600	0.49335100	-0.09851000
C	2.73179400	1.06814400	1.15277800
C	2.52660800	1.26305100	-1.26210700
C	2.95244200	2.44149400	1.23892300
H	2.73394100	0.44310200	2.04098100
C	2.73912200	2.63649800	-1.16390800
H	2.38034200	0.79438900	-2.23127300
C	2.95053800	3.22447300	0.08401200
H	3.12585300	2.89952800	2.20892900
H	2.74634900	3.24598300	-2.06341500
H	3.12004700	4.29555000	0.15562300
H	-2.41669300	2.33793600	-0.59930800
N	-4.53636500	0.74290600	-0.42000200
O	-4.70742900	1.77083400	-1.09655400
O	-5.45231200	-0.07526400	-0.23285300
H	-1.68134400	-1.75262300	2.12995500
Cl	-0.13987900	-2.93425200	-0.44029300
H	0.22012700	-0.75396900	-1.30999600

Thermochemistry data [Hartree]

Electron Energy	-1715.02503
Thermal correction to Energy	0.22134
Zero-point correction	0.23932
Thermal correction to Enthalpy	0.24026
Thermal correction to Gibbs Free Energy	0.17156

σ^H adducts in *para* position in nitrobenzene:

ADDUCT 1

C	-1.94954000	0.06485200	1.69528100
C	-1.08330200	0.83718400	0.73438300
C	-1.81077500	1.17467300	-0.53921800
C	-3.05877200	0.73742800	-0.80934700
C	-3.79829300	-0.07279800	0.11984000
C	-3.19382400	-0.36030700	1.39123400
C	0.24232700	0.06016900	0.52022600
S	1.55609600	1.11813000	-0.21545400
Cl	0.05563100	-1.41858500	-0.44605000
O	1.65851000	2.27518000	0.68785300
O	1.28305100	1.33738700	-1.64092700
H	-0.74229000	1.76416400	1.22788400
H	-3.77435100	-0.91490800	2.12209400
H	0.65469400	-0.23632400	1.49012400
H	-1.29258100	1.79980900	-1.26173700
C	3.04696500	0.15906400	-0.07272400
C	3.49288800	-0.56723500	-1.17592500
C	3.73448100	0.15431200	1.14134800
C	4.65903100	-1.31875100	-1.05472800
H	2.94030900	-0.53453400	-2.10961500
C	4.89625000	-0.60534600	1.24849000
H	3.37585800	0.74287900	1.98091000
C	5.35521700	-1.33968600	0.15402200
H	5.02340000	-1.88699000	-1.90570400
H	5.44626700	-0.61775900	2.18503200
H	6.26380600	-1.92889800	0.24310800
H	-3.53992000	1.00941200	-1.74380200
N	-5.04028900	-0.51614400	-0.17762100
O	-5.57208700	-0.23596300	-1.30134100
O	-5.69216500	-1.22097100	0.66061400
H	-1.53082600	-0.14438700	2.67829900

Thermochemistry data [Hartree]

Electron Energy	-1715.06238
Thermal correction to Energy	0.22427
Zero-point correction	0.24193
Thermal correction to Enthalpy	0.24288
Thermal correction to Gibbs Free Energy	0.17580

ADDUCT 2

C	-1.40510800	-0.67269500	-1.38887300
C	-0.50496900	-0.30985100	-0.23505000
C	-1.26212000	-0.19769400	1.06133700
C	-2.60039800	-0.35299600	1.14518900
C	-3.40761700	-0.64589900	-0.00775100
C	-2.74166500	-0.81453000	-1.26952000
C	0.30708100	0.95139100	-0.61362100

S	1.81465900	1.25011400	0.40712100
Cl	-0.65652000	2.44638300	-0.58125500
O	1.44249300	1.32286700	1.82561600
O	2.52150000	2.38276800	-0.20674200
H	0.27195700	-1.09160500	-0.14428100
H	-3.34095800	-1.08002700	-2.13501600
H	0.70267200	0.84936700	-1.62940400
H	-0.68659000	0.01506100	1.95792200
C	2.78623100	-0.21802900	0.14869400
C	3.53150400	-0.33447100	-1.02529100
C	2.78834600	-1.21364800	1.12528900
C	4.28946400	-1.48507800	-1.22469300
H	3.53047800	0.46394600	-1.76165500
C	3.55748500	-2.35533300	0.91464800
H	2.20753800	-1.08893000	2.03427300
C	4.30091200	-2.49146200	-0.25801300
H	4.87690100	-1.59131900	-2.13206400
H	3.57573100	-3.13743000	1.66812100
H	4.89757200	-3.38534400	-0.41774400
H	-3.09689800	-0.26643600	2.10690800
N	-4.74784400	-0.78971300	0.09586900
O	-5.44841800	-1.06133900	-0.93335500
O	-5.32609600	-0.65364800	1.22317200
H	-0.92790800	-0.83303100	-2.35435200

Thermochemistry data [Hartree]

Electron Energy	-1715.06076
Thermal correction to Energy	0.22424
Zero-point correction	0.24191
Thermal correction to Enthalpy	0.24286
Thermal correction to Gibbs Free Energy	0.17556

ADDUCT 3

C	2.02602900	-1.64134400	-0.85907200
C	0.70949500	-0.90703500	-0.91041400
C	0.89336800	0.57850300	-0.75090100
C	2.07632400	1.14137400	-0.42356300
C	3.26618200	0.35713200	-0.24339400
C	3.19161100	-1.05010000	-0.52296700
C	-0.24629400	-1.55589300	0.12547800
S	-2.04701600	-1.38700100	-0.22724500
Cl	0.09855600	-1.08719200	1.80426100
O	-2.75274600	-2.13379100	0.82354900
O	-2.19460900	-1.80432900	-1.63026300
H	0.21676300	-1.12559300	-1.87324400
H	4.10809600	-1.63114400	-0.48632600
H	-0.14687200	-2.64690300	0.07455900
H	0.02999000	1.21786700	-0.91274400

C	-2.51962700	0.32072300	-0.09815900
C	-2.64162200	1.07535500	-1.26478400
C	-2.79167400	0.85864800	1.16027100
C	-3.03695000	2.40645300	-1.16255100
H	-2.43894100	0.62333900	-2.23090300
C	-3.17771900	2.19355800	1.24667700
H	-2.71330700	0.24306700	2.05044400
C	-3.29818500	2.96401300	0.08952300
H	-3.14303800	3.00638200	-2.06179700
H	-3.39172300	2.62901900	2.21843600
H	-3.60453000	4.00387100	0.16360000
H	2.15257900	2.21884300	-0.31270900
N	4.43420700	0.93486100	0.12027700
O	4.49191800	2.18799300	0.34018600
O	5.48741700	0.23085900	0.25111100
H	2.00685900	-2.70268300	-1.10130700

Thermochemistry data [Hartree]

Electron Energy	-1715.06028
Thermal correction to Energy	0.22429
Zero-point correction	0.24192
Thermal correction to Enthalpy	0.24286
Thermal correction to Gibbs Free Energy	0.17589

ADDUCT 4

C	-1.63525600	0.61232400	-1.50000200
C	-0.61846200	-0.07717200	-0.61916200
C	-1.26845200	-1.18000500	0.18130400
C	-2.60467400	-1.25711200	0.36573500
C	-3.50868700	-0.35305600	-0.28686700
C	-2.96646900	0.51364900	-1.29546600
C	0.05009600	0.97335100	0.31484300
S	1.44010900	0.35718500	1.36612300
O	0.89674200	-0.71747900	2.20784600
O	2.04934700	1.52434700	2.01726000
H	0.19049500	-0.48252000	-1.24700000
H	-3.65807400	1.05725100	-1.93239800
H	-0.62396000	-1.91487700	0.65194100
C	2.63280300	-0.34524300	0.25001700
C	3.62905200	0.47416200	-0.28166700
C	2.55647300	-1.70388700	-0.05767400
C	4.56486400	-0.08578000	-1.14746800
H	3.67535500	1.52403500	-0.01110000
C	3.50035900	-2.24998100	-0.92364400
H	1.78569900	-2.32590900	0.38707600
C	4.49874200	-1.44204600	-1.46820800
H	5.34948200	0.53749900	-1.56663500
H	3.45784900	-3.30764700	-1.16712400

H	5.23416500	-1.87354400	-2.14172100
H	-3.02383400	-2.04747100	0.98137100
N	-4.84130700	-0.40463200	-0.05141100
O	-5.63588500	0.36241000	-0.68272900
O	-5.30982300	-1.21593100	0.80883400
H	-1.25836400	1.22423000	-2.31431700
Cl	0.67070500	2.38074400	-0.59924900
H	-0.66875700	1.35174900	1.04893800

Thermochemistry data [Hartree]

Electron Energy	-1715.05851
Thermal correction to Energy	0.22439
Zero-point correction	0.24196
Thermal correction to Enthalpy	0.24290
Thermal correction to Gibbs Free Energy	0.17631

ADDUCT 5

C	-1.87420200	-2.05025800	0.43514200
C	-0.56589600	-1.45735700	0.90451700
C	-0.76226800	-0.03849800	1.37574300
C	-1.81787800	0.71169800	0.98867400
C	-2.88466200	0.14983100	0.20957900
C	-2.91613800	-1.27931900	0.05536700
C	0.44972800	-1.51641300	-0.26299000
S	2.11949300	-0.80152000	0.12383200
O	3.04668400	-1.27196100	-0.91552900
O	2.42286100	-1.08569300	1.53386500
H	-0.13321400	-2.06880100	1.70874900
H	-3.82492500	-1.73432600	-0.32738800
H	-0.01568700	0.38050700	2.04331900
C	1.95430100	0.96026100	-0.08584200
C	2.13607600	1.79042700	1.01754500
C	1.71781300	1.47232400	-1.36188500
C	2.06290300	3.16947900	0.83792300
H	2.33251800	1.36112000	1.99526900
C	1.63111500	2.85198500	-1.52364700
H	1.60941500	0.81163800	-2.21763400
C	1.80252400	3.69756900	-0.42650200
H	2.20637400	3.83024600	1.68804100
H	1.43836100	3.26630800	-2.50900700
H	1.73835400	4.77395600	-0.55986800
H	-1.90600900	1.74421200	1.31421700
N	-3.90307500	0.92322400	-0.24022100
O	-3.88789600	2.17940300	-0.04648300
O	-4.87716100	0.39953900	-0.86697800
H	-1.94543900	-3.13261800	0.37256000

Cl	0.74065600	-3.20269700	-0.78209400
H	0.08234200	-0.96531100	-1.13315500

Thermochemistry data [Hartree]

Electron Energy	-1715.05783
Thermal correction to Energy	0.22447
Zero-point correction	0.24199
Thermal correction to Enthalpy	0.24293
Thermal correction to Gibbs Free Energy	0.17671

Transition states for addition to the *ortho* position in *p*-fluoronitrobenzene:

TS1

C	2.88498600	0.88384400	-0.08817100
C	2.06504700	0.17932900	0.83036100
C	2.32858100	-1.20230600	0.99171100
C	3.21291800	-1.81438200	0.14377000
C	3.94683800	-1.13973700	-0.84866900
C	3.77651000	0.22240700	-0.95233400
C	-0.06380600	0.18097300	-0.18187500
S	-1.31654400	-0.00945600	0.99570800
N	2.77052400	2.28920700	-0.16636200
O	3.48717400	2.91583800	-0.96478000
Cl	-0.04968600	-1.09697100	-1.40466700
O	-1.22487100	1.18461700	1.86756500
O	-1.20343600	-1.34277600	1.62521100
O	1.94739200	2.85940600	0.56459600
H	1.56733600	0.73015300	1.61534000
H	4.33485600	0.79946000	-1.68085400
H	4.62777000	-1.68637100	-1.49213000
H	-0.14244900	1.15939500	-0.65569500
H	1.79738000	-1.78023600	1.74029900
C	-2.94890000	0.03299900	0.25126900
C	-3.58208800	-1.16126800	-0.09366700
C	-3.53230700	1.26715900	-0.04375300
C	-4.81993200	-1.11639400	-0.73439400
H	-3.11575000	-2.11018000	0.15282500
C	-4.76995100	1.30105700	-0.68068300
H	-3.02626800	2.18755300	0.23406700
C	-5.41336300	0.11101700	-1.02776200
H	-5.32194500	-2.04299000	-1.00023400
H	-5.23503300	2.25779600	-0.90331700
H	-6.37913400	0.14210700	-1.52527100
F	3.42796100	-3.14291300	0.27688600

Thermochemistry data [Hartree]

Electron Energy	-1814.21622

Thermal correction to Energy	0.21325
Zero-point correction	0.23192
Thermal correction to Enthalpy	0.23287
Thermal correction to Gibbs Free Energy	0.16323

TS2

C	1.91535000	1.46099100	-0.10753700
C	1.15548400	0.57358900	0.69331000
C	1.87229500	-0.38941700	1.43932600
C	3.21888300	-0.52896200	1.22502400
C	3.96380300	0.28163000	0.35074200
C	3.29537700	1.28522500	-0.31409700
C	-0.00301000	-0.77603000	-0.91159800
S	-1.42061100	-1.65107300	-0.39102600
N	1.25703100	2.53770700	-0.74446100
O	1.91373300	3.32109300	-1.44945800
Cl	1.22925100	-1.90708500	-1.52231800
O	-1.07354200	-2.50098200	0.77296700
O	-2.19482400	-2.34359900	-1.45870900
O	0.03483800	2.66457200	-0.58298300
H	0.15957500	0.86302200	0.99380200
H	3.82194500	1.95709100	-0.98252300
H	5.02820700	0.11566600	0.22411500
H	-0.29147300	-0.09042700	-1.71231900
H	1.35853600	-1.04323400	2.13604000
C	-2.44420700	-0.30494000	0.18960400
C	-3.22872500	0.39977300	-0.72303400
C	-2.44385200	0.01700500	1.54588300
C	-4.01782100	1.45331200	-0.26621600
H	-3.23013200	0.12076000	-1.77289600
C	-3.24326200	1.06703500	1.99371900
H	-1.83476700	-0.55761000	2.23779300
C	-4.02472600	1.78613600	1.08888600
H	-4.63229700	2.00998000	-0.96852900
H	-3.25578500	1.32221600	3.04991600
H	-4.64514700	2.60577600	1.44151600
F	3.89105000	-1.47892600	1.91350200

Thermochemistry data [Hartree]

Electron Energy	-1814.20975
Thermal correction to Energy	0.21293
Zero-point correction	0.23175
Thermal correction to Enthalpy	0.23269
Thermal correction to Gibbs Free Energy	0.16233

TS3

C	2.58001400	-0.02259200	-0.54661900
C	1.20185000	0.23555200	-0.76161200
C	0.74030600	1.53620500	-0.45118600
C	1.57711200	2.39887100	0.20757200
C	2.91150200	2.10306800	0.53569700
C	3.40843100	0.88001900	0.14306600
C	0.12967100	-1.10159000	0.88171500
S	-1.45278100	-1.71072500	0.49265900
N	3.12584500	-1.24292700	-1.00227600
O	4.33244400	-1.47599600	-0.82104600
Cl	0.14454300	-0.12154900	2.35775700
O	-2.30061100	-2.11269100	1.64345800
O	-1.24342000	-2.72112500	-0.57172000
O	2.37800200	-2.05289700	-1.56936600
H	0.66074500	-0.37540700	-1.46971500
H	4.43925800	0.60858300	0.34134100
H	3.51915000	2.82939900	1.06457600
H	0.80489100	-1.95332900	0.98041700
H	-0.27521500	1.83564700	-0.68956200
C	-2.29795500	-0.32345700	-0.25689100
C	-2.28776900	-0.19153700	-1.64514100
C	-2.93177600	0.61939300	0.55272300
C	-2.91626500	0.90661300	-2.22930800
H	-1.80316900	-0.94770700	-2.25577600
C	-3.55089700	1.71795500	-0.04093200
H	-2.94709300	0.49082700	1.63060300
C	-3.54141300	1.86336100	-1.42862800
H	-2.91837300	1.01340200	-3.31078000
H	-4.04565700	2.45824100	0.58208100
H	-4.02784600	2.72022500	-1.88726000
F	1.11460700	3.62545000	0.53913900

Thermochemistry data [Hartree]

Electron Energy	-1814.21239
Thermal correction to Energy	0.21324
Zero-point correction	0.23182
Thermal correction to Enthalpy	0.23276
Thermal correction to Gibbs Free Energy	0.16400

σ^H adducts in *ortho* position in *p*-fluoronitrobenzene:

ADDUCT 1

C	2.45670400	1.06620800	-0.05126300
C	1.52403800	0.10472900	0.64751300
C	2.11394800	-1.27757400	0.72272300
C	3.20679700	-1.59388600	0.01396600
C	3.95218600	-0.68683600	-0.81347700
C	3.57322900	0.62232200	-0.80869800

C	0.12311000	0.14232700	-0.02744500
S	-1.16609800	-0.66704900	0.99579200
N	2.21161900	2.39203900	0.07885100
O	2.96729200	3.25828300	-0.45797300
Cl	0.10609400	-0.54660900	-1.66497000
O	-1.07608500	-0.01364800	2.31106900
O	-1.03784300	-2.12771100	0.90867500
O	1.20105800	2.76825100	0.75579800
H	1.32334700	0.48521600	1.66082300
H	4.13031900	1.36502300	-1.37059700
H	4.80024200	-1.04927400	-1.38429700
H	-0.19573900	1.18614200	-0.09274700
H	1.62932600	-2.02390200	1.34412300
C	-2.70573100	-0.19747500	0.23860800
C	-3.32770200	-1.08186100	-0.64137800
C	-3.25323400	1.04948900	0.54176900
C	-4.53060800	-0.70226100	-1.23188800
H	-2.88030400	-2.04875900	-0.84938100
C	-4.45426500	1.41645100	-0.05918600
H	-2.75636400	1.71348000	1.24318300
C	-5.08925300	0.54311500	-0.94344100
H	-5.03129200	-1.38099000	-1.91641800
H	-4.89690300	2.38185400	0.16858300
H	-6.02754800	0.83411700	-1.40777100
F	3.70076200	-2.86132500	0.08410900

Thermochemistry data [Hartree]

Electron Energy	-1814.24639
Thermal correction to Energy	0.21584
Zero-point correction	0.23435
Thermal correction to Enthalpy	0.23530
Thermal correction to Gibbs Free Energy	0.16644

ADDUCT 2

C	1.81220000	1.36036400	-0.03468100
C	0.89248800	0.22451500	0.35352100
C	1.59602500	-0.77307300	1.23459700
C	2.92558600	-0.72341800	1.39680100
C	3.79812200	0.26688900	0.83106200
C	3.21904000	1.29442200	0.14811800
C	0.26217600	-0.40148700	-0.91906300
S	-1.21386500	-1.45881400	-0.62183900
N	1.24805100	2.48104600	-0.54525900
O	1.95111500	3.48668800	-0.86770500
Cl	1.41653200	-1.36376100	-1.87130100
O	-0.87454400	-2.52077500	0.33578700
O	-1.74217800	-1.83313000	-1.94176300
O	-0.01540500	2.51758800	-0.69805600

H	0.02943500	0.65412600	0.88815900
H	3.81953300	2.10249900	-0.25695100
H	4.86943400	0.19452900	0.98396100
H	-0.11303100	0.40316600	-1.55667300
H	1.01305500	-1.55081200	1.71636800
C	-2.37771300	-0.35553800	0.14975100
C	-3.10965000	0.52126600	-0.65138100
C	-2.54342800	-0.40218100	1.53348300
C	-4.02428500	1.37671500	-0.04384800
H	-2.97443900	0.52766600	-1.72889600
C	-3.46545900	0.45663000	2.12648300
H	-1.97013300	-1.10605900	2.12930700
C	-4.19975900	1.34475500	1.34028900
H	-4.60330000	2.06494100	-0.65285400
H	-3.61084500	0.42938500	3.20256800
H	-4.91698500	2.01353100	1.80823600
F	3.53308300	-1.65749400	2.18091700

Thermochemistry data [Hartree]

Electron Energy	-1814.24492
Thermal correction to Energy	0.21594
Zero-point correction	0.23441
Thermal correction to Enthalpy	0.23535
Thermal correction to Gibbs Free Energy	0.16727

ADDUCT 3

C	2.64014500	0.18584900	-0.27122400
C	1.16120700	0.05602900	-0.56252900
C	0.49964300	1.40781700	-0.60289200
C	1.13727700	2.49854800	-0.15310100
C	2.48670600	2.53169300	0.33319700
C	3.21215800	1.38138600	0.23757800
C	0.51915800	-0.93237600	0.45105100
S	-1.05616700	-1.72230400	-0.07548500
N	3.43149200	-0.88671300	-0.51934000
O	4.68395700	-0.84101000	-0.32511300
Cl	0.34542900	-0.25531100	2.08509100
O	-1.42380000	-2.67145000	0.98545300
O	-0.80094800	-2.22479900	-1.43417600
O	2.89856500	-1.95646000	-0.95504200
H	1.03822400	-0.45521900	-1.52970800
H	4.25614400	1.35660000	0.53270400
H	2.90068000	3.45632700	0.72035300
H	1.16622800	-1.81360800	0.51986300
H	-0.50818400	1.49735500	-0.99382900
C	-2.33813300	-0.49350200	-0.17401600
C	-2.67626700	0.02203800	-1.42512700
C	-3.00231700	-0.10038200	0.98827500

C	-3.69719100	0.96501300	-1.50858500
H	-2.15272200	-0.31807100	-2.31345800
C	-4.01584100	0.84944100	0.88991100
H	-2.73957700	-0.53662500	1.94642000
C	-4.36005900	1.38092000	-0.35345200
H	-3.97591200	1.37162800	-2.47649500
H	-4.54203600	1.16795500	1.78516900
H	-5.15515300	2.11822600	-0.42344500
F	0.49523700	3.69938800	-0.18160700

Thermochemistry data [Hartree]

Electron Energy	-1814.24382
Thermal correction to Energy	0.21600
Zero-point correction	0.23438
Thermal correction to Enthalpy	0.23533
Thermal correction to Gibbs Free Energy	0.16773

Transition states for addition to the *para* position in *p*-fluoronitrobenzene:

TS1

C	-2.13759400	-0.68516200	-1.46289300
C	-1.75943600	-1.48277800	-0.36045500
C	-2.46427100	-1.39534000	0.85821600
C	-3.37726500	-0.38031600	1.03647900
C	-3.65528200	0.50115100	-0.02161100
C	-3.05110500	0.32558500	-1.28108400
C	0.26117200	-0.43382000	0.28490400
S	1.65453200	-0.79061800	-0.68393000
Cl	0.54745000	-0.68879300	2.02114700
O	1.25930000	-0.46833600	-2.07467100
O	2.14091500	-2.15559000	-0.39191900
H	-3.32243600	0.98102700	-2.10114400
H	-0.03005200	0.60484100	0.11846800
H	-2.24076100	-2.09847500	1.65344400
C	3.02641200	0.29892400	-0.28979700
C	3.97969500	-0.10268900	0.64643500
C	3.07889400	1.56876700	-0.86814900
C	5.00198800	0.77731300	0.99991400
H	3.92641200	-1.09736500	1.07840300
C	4.10592700	2.43901800	-0.51139500
H	2.33003600	1.86385300	-1.59793400
C	5.06605000	2.04556700	0.42315700
H	5.75144300	0.46832500	1.72391300
H	4.15909900	3.42462100	-0.96643900
H	5.86562800	2.72797200	0.69924300
H	-3.89925800	-0.26575900	1.98005600
N	-4.59562100	1.54677000	0.16609300
O	-5.13361600	1.67773000	1.27354400

O	-4.84876800	2.30073800	-0.78281900
H	-1.65168600	-0.84363300	-2.41948900
F	-1.14355600	-2.65856500	-0.62924300

Thermochemistry data [Hartree]

Electron Energy	-1814.21380
Thermal correction to Energy	0.21295
Zero-point correction	0.23173
Thermal correction to Enthalpy	0.23267
Thermal correction to Gibbs Free Energy	0.16246

TS2

C	-1.92604300	-1.24399200	1.52527000
C	-0.81296000	-0.38013700	1.45745700
C	-0.93418300	0.89286700	0.86665300
C	-2.10211400	1.23014600	0.22024900
C	-3.18572200	0.33509300	0.21756700
C	-3.09224500	-0.90138900	0.87965600
C	0.50086500	-1.59947300	-0.15221500
S	2.22516000	-1.38941800	-0.27705600
Cl	-0.32934300	-1.30543200	-1.69473700
O	2.83960200	-1.78589800	-1.57081400
O	2.80023200	-2.00012600	0.94553300
H	-3.94891700	-1.56596200	0.89765900
H	0.32108900	-2.62556800	0.17814600
H	-0.09225300	1.57683000	0.89896200
C	2.48371500	0.37755000	-0.16144700
C	2.80079400	0.94060900	1.07350500
C	2.35242700	1.16941100	-1.30264400
C	2.98559100	2.31866200	1.16614200
H	2.90052100	0.30217800	1.94560200
C	2.52809400	2.54821200	-1.19735800
H	2.12445000	0.71280700	-2.26089800
C	2.84402300	3.12261200	0.03417000
H	3.24020600	2.76456900	2.12401800
H	2.42493100	3.17250500	-2.08091900
H	2.98565600	4.19749300	0.11076200
H	-2.20322100	2.19355700	-0.26718000
N	-4.38829500	0.68957100	-0.44186300
O	-4.45874200	1.78736700	-1.01192500
O	-5.33556400	-0.10899500	-0.43158600
H	-1.83687400	-2.18245700	2.06337100
F	0.15345100	-0.54997100	2.39058200

Thermochemistry data [Hartree]

Electron Energy	-1814.20992
Thermal correction to Energy	0.21274

Zero-point correction	0.23151
Thermal correction to Enthalpy	0.23246
Thermal correction to Gibbs Free Energy	0.16271

TS3

C	2.46427400	-1.39533700	0.85822800
C	1.75944300	-1.48279300	-0.36044500
C	2.13759800	-0.68518300	-1.46288800
C	3.05109700	0.32557600	-1.28108400
C	3.65526800	0.50115900	-0.02161000
C	3.37725700	-0.38030200	1.03648600
C	-0.26117200	-0.43384500	0.28490300
S	-1.65453500	-0.79062900	-0.68393200
O	-2.14093400	-2.15559500	-0.39192200
O	-1.25930100	-0.46835200	-2.07467400
H	3.89924600	-0.26573300	1.98006400
H	1.65169700	-0.84366700	-2.41948500
C	-3.02640200	0.29893000	-0.28980000
C	-3.07885900	1.56878000	-0.86813800
C	-3.97970100	-0.10267800	0.64641900
C	-4.10588000	2.43904400	-0.51138400
H	-2.32998900	1.86386200	-1.59791200
C	-5.00198200	0.77733600	0.99989800
H	-3.92643600	-1.09736000	1.07837700
C	-5.06601900	2.04559700	0.42315400
H	-4.15903300	3.42465300	-0.96641700
H	-5.75145000	0.46835200	1.72388600
H	-5.86558900	2.72801200	0.69924000
H	3.32242600	0.98101300	-2.10114900
N	4.59559600	1.54678900	0.16608800
O	4.84873800	2.30075200	-0.78283000
O	5.13358700	1.67776300	1.27353900
H	2.24076800	-2.09846800	1.65346100
Cl	-0.54745600	-0.68881700	2.02114500
H	0.03006100	0.60481400	0.11846800
F	1.14357700	-2.65858800	-0.62922500

Thermochemistry data [Hartree]

Electron Energy	-1814.21380
Thermal correction to Energy	0.21295
Zero-point correction	0.23173
Thermal correction to Enthalpy	0.23267
Thermal correction to Gibbs Free Energy	0.16246

TS4

C	0.93419300	0.89286400	0.86666200
C	0.81297200	-0.38014600	1.45745600
C	1.92605500	-1.24400100	1.52525800
C	3.09225500	-0.90139300	0.87964200
C	3.18572900	0.33509500	0.21756300
C	2.10212100	1.23014800	0.22025600
C	-0.50085900	-1.59946500	-0.15222400
S	-2.22515700	-1.38942100	-0.27705600
O	-2.80021700	-2.00013700	0.94553500
O	-2.83960400	-1.78590300	-1.57081000
H	2.20322600	2.19356200	-0.26716500
H	1.83688800	-2.18247100	2.06335100
C	-2.48372300	0.37754400	-0.16144000
C	-2.35248400	1.16940400	-1.30264300
C	-2.80076300	0.94060300	1.07352300
C	-2.52816000	2.54820400	-1.19735300
H	-2.12453800	0.71280000	-2.26090400
C	-2.98557100	2.31865400	1.16616400
H	-2.90045300	0.30217300	1.94562500
C	-2.84405100	3.12260300	0.03418500
H	-2.42503600	3.17249700	-2.08091900
H	-3.24015600	2.76456000	2.12404800
H	-2.98569200	4.19748300	0.11078000
H	3.94892700	-1.56596600	0.89763500
N	4.38829900	0.68957800	-0.44186900
O	4.45874500	1.78738000	-1.01192100
O	5.33556800	-0.10898900	-0.43160500
H	0.09226300	1.57682600	0.89898000
Cl	0.32933800	-1.30540000	-1.69474700
H	-0.32107500	-2.62556400	0.17812200
F	-0.15343600	-0.54998800	2.39058300

Thermochemistry data [Hartree]

Electron Energy	-1814.20992
Thermal correction to Energy	0.21274
Zero-point correction	0.23151
Thermal correction to Enthalpy	0.23246
Thermal correction to Gibbs Free Energy	0.16271

TS5

C	-1.91736200	-1.15701300	1.38662900
C	-0.80884700	-0.28567100	1.38574700
C	-0.93596600	1.02969800	0.88888800
C	-2.07682800	1.38536600	0.20835100
C	-3.13281200	0.46307600	0.08774800
C	-3.05763200	-0.79736300	0.70386200
C	0.45218800	-1.31916200	-0.36089000

S	2.18371700	-1.13768100	-0.55283800
O	2.71225300	-1.40608100	-1.91960900
O	2.88896300	-1.84706000	0.53956800
H	-3.90651000	-1.47012000	0.65238800
H	-0.11103500	1.72481400	1.00644900
C	2.36210300	0.62019500	-0.28036200
C	2.77889700	1.07758500	0.96821300
C	2.08094000	1.50580300	-1.32065900
C	2.91141200	2.44866800	1.17802200
H	2.99516800	0.36517700	1.75817100
C	2.20635600	2.87565500	-1.09736400
H	1.77806500	1.12970700	-2.29374400
C	2.62014900	3.34595200	0.14952600
H	3.24057500	2.81626400	2.14624800
H	1.98684700	3.57475700	-1.89971000
H	2.72059700	4.41480200	0.31880300
H	-2.17837500	2.37545100	-0.22191500
N	-4.30796400	0.82994800	-0.61834400
O	-4.36773800	1.95262500	-1.13680300
O	-5.23740400	0.01612400	-0.69870600
H	-1.83787300	-2.11838100	1.88269800
Cl	0.02058200	-3.05309500	-0.43952300
H	-0.02513100	-0.81118900	-1.20483400
F	0.14887600	-0.50966800	2.31547600

Thermochemistry data [Hartree]

Electron Energy	-1814.20805
Thermal correction to Energy	0.21294
Zero-point correction	0.23168
Thermal correction to Enthalpy	0.23263
Thermal correction to Gibbs Free Energy	0.16300

σ^F adducts in *para* position in *p*-chloronitrobenzene:

Adduct 1

C	2.02304900	0.53087200	-1.42913000
C	1.13999300	0.76292100	-0.26782100
C	1.70608300	0.28425200	1.00980000
C	2.99133700	-0.14284800	1.11535600
C	3.83696200	-0.23957900	-0.02452000
C	3.30336000	0.09398800	-1.29777400
C	-0.30517000	0.29993500	-0.58915500
S	-1.63609300	1.04222700	0.47494100
Cl	-0.40633400	-1.47185400	-0.53569800
O	-1.90520100	2.38439800	-0.05468700
O	-1.27112100	0.87203900	1.88730600
H	3.93217000	-0.01963100	-2.17513700

H	-0.57968300	0.61690300	-1.59880300
H	1.06549200	0.32135300	1.88479800
C	-3.08387100	0.05305000	0.15694900
C	-3.45853300	-0.92625100	1.07506800
C	-3.82854600	0.30664100	-0.99472600
C	-4.60928700	-1.67055700	0.82768000
H	-2.86214500	-1.09389900	1.96650800
C	-4.97241600	-0.45060000	-1.23309300
H	-3.52803400	1.08839300	-1.68605200
C	-5.36044200	-1.43596700	-0.32446700
H	-4.91848900	-2.43389700	1.53600400
H	-5.56430300	-0.26479000	-2.12473400
H	-6.25616500	-2.02146900	-0.51318600
H	3.38509100	-0.44068700	2.08203900
N	5.13482700	-0.68988300	0.09729800
O	5.58540900	-0.99582600	1.22888200
O	5.86079600	-0.78857800	-0.92291800
H	1.62495700	0.76608200	-2.41378600
F	0.93203400	2.23170100	-0.15384400

Thermochemistry data [Hartree]

Electron Energy	-1814.25003
Thermal correction to Energy	0.21536
Zero-point correction	0.23395
Thermal correction to Enthalpy	0.23490
Thermal correction to Gibbs Free Energy	0.16604

Adduct 2

C	-1.59725000	-0.34735600	-1.40838000
C	-0.73508300	-0.07996300	-0.24071100
C	-1.48152500	0.09424600	1.01941200
C	-2.80982300	-0.17828600	1.11390200
C	-3.57145200	-0.55673800	-0.02555000
C	-2.92570900	-0.60999600	-1.28932700
C	0.31782800	0.99844000	-0.57533200
S	1.79584600	1.14765400	0.54287600
Cl	-0.43765600	2.60429000	-0.65351500
O	1.36927200	1.04069100	1.94355100
O	2.49369500	2.36466100	0.10393900
H	-3.51473200	-0.84886300	-2.16917800
H	0.75394800	0.79372200	-1.55757500
H	-0.92255500	0.41208600	1.89333700
C	2.85862600	-0.22711300	0.15524200
C	3.62921700	-0.17396800	-1.00542600
C	2.94062700	-1.29353400	1.04696400
C	4.49456700	-1.22954100	-1.28252200
H	3.56557700	0.67958300	-1.67402800

C	3.82004300	-2.33492900	0.76415000
H	2.32795900	-1.30212100	1.94244600
C	4.58993400	-2.30530300	-0.39922400
H	5.10072000	-1.20516500	-2.18353800
H	3.90128100	-3.17146900	1.45232300
H	5.27134200	-3.12326100	-0.61678500
H	-3.31504100	-0.08572800	2.07019000
N	-4.92149800	-0.82026900	0.08493000
O	-5.58221900	-1.13158300	-0.93620500
O	-5.48082200	-0.75115300	1.20665600
H	-1.12144100	-0.37212600	-2.38638800
F	0.17007300	-1.26520700	-0.08047600

Thermochemistry data [Hartree]

Electron Energy	-1814.25057
Thermal correction to Energy	0.21548
Zero-point correction	0.23403
Thermal correction to Enthalpy	0.23497
Thermal correction to Gibbs Free Energy	0.16670

Adduct 3

C	1.90588300	-1.53403300	-0.71939000
C	0.66740300	-0.74272900	-0.55723200
C	0.89911600	0.58174500	0.05638000
C	2.14654400	1.08823300	0.23929900
C	3.30790400	0.32526400	-0.06201200
C	3.14338700	-1.00809000	-0.52341500
C	-0.44021400	-1.61528500	0.08959700
S	-2.23054400	-1.22401700	-0.24968700
Cl	-0.17895500	-1.73946700	1.83979200
O	-3.00108100	-1.88302900	0.81423100
O	-2.48112000	-1.61814900	-1.64049900
H	4.02607500	-1.61344200	-0.70374000
H	-0.38696400	-2.62885100	-0.32246800
H	0.03475900	1.17740000	0.33150900
C	-2.47660100	0.52659500	-0.08739500
C	-2.41273100	1.33108600	-1.22405100
C	-2.74081800	1.05136600	1.17818800
C	-2.61630100	2.70112900	-1.08331100
H	-2.20599600	0.88823300	-2.19249400
C	-2.93344600	2.42484400	1.30340200
H	-2.80158800	0.39706400	2.04219400
C	-2.87003500	3.24542700	0.17647000
H	-2.57525100	3.34357600	-1.95820500
H	-3.13939700	2.85216200	2.28054200
H	-3.02409800	4.31605500	0.28019800
H	2.27067200	2.08643200	0.64731400

N	4.56758900	0.85133900	0.13492200
O	4.69371800	2.02652400	0.55905000
O	5.58163800	0.15402400	-0.11478500
H	1.79839500	-2.56293900	-1.05588400
F	0.10393700	-0.52756800	-1.91533900

Thermochemistry data [Hartree]

Electron Energy	-1814.24820
Thermal correction to Energy	0.21547
Zero-point correction	0.23398
Thermal correction to Enthalpy	0.23492
Thermal correction to Gibbs Free Energy	0.16694

Adduct 4

C	-2.07323600	-1.24089500	-0.68295500
C	-1.14320800	-0.64833100	0.30417200
C	-1.66508600	0.60606800	0.90110900
C	-2.93043000	1.05091500	0.68339200
C	-3.81438300	0.37541200	-0.19989300
C	-3.33560500	-0.77601100	-0.87846500
C	0.30098800	-0.47226300	-0.23445500
S	1.61937800	-0.30303100	1.07186800
O	2.03514100	-1.62630700	1.54395200
O	1.15081900	0.69663000	2.04125200
H	-3.99489300	-1.28468800	-1.57480400
H	-1.00554200	1.15272700	1.56522200
C	2.97608900	0.41138300	0.16452700
C	2.98844700	1.78961200	-0.05174300
C	3.99542800	-0.41652700	-0.30267100
C	4.04916800	2.34675400	-0.76081400
H	2.19157100	2.41659200	0.33820100
C	5.05226400	0.15569200	-1.00690700
H	3.96282100	-1.48412300	-0.10963500
C	5.07656700	1.53125400	-1.23737200
H	4.07576600	3.41861000	-0.93466900
H	5.85709500	-0.47457500	-1.37422100
H	5.90312800	1.97169500	-1.78825300
H	-3.27449100	1.95432400	1.17713100
N	-5.09148900	0.84514200	-0.41912800
O	-5.49136800	1.87144600	0.18451500
O	-5.85002200	0.24292700	-1.21895900
H	-1.74004300	-2.12525700	-1.21539600
H	0.35482500	0.45922100	-0.80313100
Cl	0.85163700	-1.76669200	-1.32983000
F	-0.96625300	-1.64380000	1.39078300

Thermochemistry data [Hartree]

Electron Energy	-1814.24878

Thermal correction to Energy	0.21557
Zero-point correction	0.23408
Thermal correction to Enthalpy	0.23503
Thermal correction to Gibbs Free Energy	0.16676

Adduct 5

C	-1.78617300	0.65321700	-1.20565300
C	-0.89466700	0.09113900	-0.16568600
C	-1.64393700	-0.53343400	0.95200800
C	-2.99057600	-0.71387700	0.92249400
C	-3.78143400	-0.23998400	-0.15807400
C	-3.13125300	0.45634000	-1.21039000
C	0.17180200	1.09360500	0.33179300
S	1.60428800	0.43169200	1.32377200
O	1.09569200	-0.60496000	2.23149200
O	2.22423200	1.63351700	1.90170300
H	-3.72927500	0.84632900	-2.02806400
H	-1.06953300	-0.88919600	1.79939300
C	2.79644900	-0.31365000	0.23294200
C	3.82790900	0.47619200	-0.27421900
C	2.71846300	-1.68083600	-0.02877100
C	4.79771900	-0.12181600	-1.07499200
H	3.87387300	1.53367000	-0.03558500
C	3.69765700	-2.26534700	-0.82696600
H	1.91169000	-2.27308600	0.38889800
C	4.73098500	-1.48749800	-1.35110800
H	5.60805200	0.47941800	-1.47718400
H	3.65437300	-3.33034600	-1.03642900
H	5.49237000	-1.95022300	-1.97324500
H	-3.48368100	-1.21440400	1.74991900
N	-5.14807900	-0.41898500	-0.16681100
O	-5.82992400	0.02244700	-1.12500400
O	-5.70406300	-1.02529700	0.78238200
H	-1.32208400	1.18848000	-2.02708800
Cl	0.88069500	2.10596300	-0.95591900
H	-0.28739700	1.78122200	1.04814200
F	-0.06860300	-0.95970900	-0.81729600

Thermochemistry data [Hartree]

Electron Energy	-1814.24853
Thermal correction to Energy	0.21564
Zero-point correction	0.23410
Thermal correction to Enthalpy	0.23504
Thermal correction to Gibbs Free Energy	0.16719

Adduct 6

C	-1.82707200	-1.71485800	-0.48810100
C	-0.68176400	-1.28718700	0.35969800
C	-0.89767200	0.04216900	0.98278100
C	-2.04911900	0.74767300	0.83823000
C	-3.11483100	0.27519500	0.02544900
C	-2.96235000	-0.98411400	-0.62017600
C	0.64065700	-1.39028800	-0.43737800
S	2.18657900	-0.69446800	0.35153500
O	3.31428100	-1.26198900	-0.39912300
O	2.13986300	-0.86437000	1.80772800
H	-3.77505800	-1.35638500	-1.23591700
H	-0.12288700	0.41209700	1.64452000
C	2.13159900	1.04752300	-0.02556400
C	2.04744900	1.96410900	1.01982600
C	2.24714900	1.45591400	-1.35473400
C	2.06256900	3.32453400	0.72131100
H	1.97756000	1.61677700	2.04623800
C	2.24594100	2.81828900	-1.63946000
H	2.34746500	0.72851100	-2.15581200
C	2.15313600	3.74936400	-0.60387700
H	2.00185300	4.05128100	1.52629000
H	2.32722000	3.15169700	-2.66994800
H	2.15734600	4.81172400	-0.83160000
H	-2.16713000	1.69518800	1.35452500
N	-4.26483200	1.01348500	-0.12889300
O	-4.37701200	2.12592400	0.44686900
O	-5.20042100	0.57262800	-0.84447100
H	-1.73577100	-2.67242800	-0.99242600
Cl	1.00616300	-3.06481500	-0.92498900
H	0.53536200	-0.80890200	-1.35688200
F	-0.53000300	-2.26423300	1.43527100

Thermochemistry data [Hartree]

Electron Energy	-1814.24568
Thermal correction to Energy	0.21559
Zero-point correction	0.23406
Thermal correction to Enthalpy	0.23500
Thermal correction to Gibbs Free Energy	0.16693

Transition states for addition to the *ortho* position in *p*-chloronitrobenzene:

TS1

C	2.60651000	1.33862900	-0.10114200
C	1.86993300	0.53991000	0.80622500
C	2.27027600	-0.81239700	0.93806700
C	3.20313500	-1.33474000	0.07441500
C	3.84632600	-0.55816500	-0.91491500

C	3.54381300	0.78251500	-0.98941400
C	-0.26032500	0.31264200	-0.19753000
S	-1.48454400	0.00973200	0.98698900
N	2.36079700	2.73013400	-0.14351500
O	3.00266000	3.43639700	-0.93795700
Cl	-0.12594600	-0.96368400	-1.41421500
O	-1.49786500	1.20815700	1.85689500
O	-1.24646000	-1.30684900	1.61651600
O	1.50359100	3.20501900	0.61511800
H	1.31960400	1.02052300	1.60254300
H	4.03549200	1.42273600	-1.71340700
H	4.57026700	-1.00920500	-1.58476600
H	-0.43215000	1.27750400	-0.67491700
H	1.79855300	-1.43867100	1.68766400
C	-3.11757700	-0.09584500	0.25191500
C	-3.62031700	-1.33697500	-0.14041400
C	-3.83409100	1.07851500	0.01217600
C	-4.86180200	-1.40035200	-0.77212400
H	-3.05192100	-2.23934000	0.06283000
C	-5.07466400	1.00379300	-0.61576100
H	-3.42768400	2.03550000	0.32715600
C	-5.58827300	-0.23369900	-1.00947800
H	-5.26303100	-2.36429100	-1.07398600
H	-5.64350300	1.91247600	-0.79437200
H	-6.55702600	-0.28780800	-1.49914800
Cl	3.64862000	-3.01519000	0.21518500

Thermochemistry data [Hartree]

Electron Energy	-2174.49936
Thermal correction to Energy	0.21175
Zero-point correction	0.23090
Thermal correction to Enthalpy	0.23184
Thermal correction to Gibbs Free Energy	0.16002

TS2

C	1.53592400	1.75410500	-0.17071400
C	0.92726000	0.71316800	0.56720000
C	1.78657500	-0.24725800	1.15018200
C	3.12882500	-0.23301700	0.85059600
C	3.71574900	0.75232500	0.02685200
C	2.90790700	1.74665900	-0.47665900
C	-0.22145800	-0.59648400	-1.08931600
S	-1.49534100	-1.66459900	-0.55811200
N	0.73115500	2.81861100	-0.64150100
O	1.25930100	3.74232000	-1.28041400
Cl	1.05778400	-1.52080100	-1.91235800
O	-0.96127700	-2.59413600	0.46551300
O	-2.29864900	-2.31325300	-1.63145200

O	-0.48453600	2.79147200	-0.40469400
H	-0.06774000	0.85971400	0.96062200
H	3.31999200	2.53761700	-1.09344800
H	4.77802800	0.72737000	-0.19035100
H	-0.64485100	0.13296500	-1.78425300
H	1.37345300	-1.01421000	1.79669700
C	-2.58081800	-0.50302800	0.25970200
C	-3.52875400	0.19227000	-0.49047400
C	-2.46279600	-0.31183100	1.63570200
C	-4.36532500	1.10297000	0.15155800
H	-3.61656300	0.01485500	-1.55852500
C	-3.30961300	0.59536000	2.26929000
H	-1.72499800	-0.87606800	2.19905600
C	-4.25565500	1.30415700	1.52793300
H	-5.10713000	1.65075800	-0.42320200
H	-3.23049200	0.74766300	3.34228400
H	-4.91289500	2.01264900	2.02507100
Cl	4.16897600	-1.45082300	1.54080600

Thermochemistry data [Hartree]

Electron Energy	-2174.49288
Thermal correction to Energy	0.21164
Zero-point correction	0.23081
Thermal correction to Enthalpy	0.23175
Thermal correction to Gibbs Free Energy	0.16086

TS3

C	2.51603100	-0.47378400	-0.57353500
C	1.16438200	-0.11876700	-0.79642600
C	0.81117700	1.23187000	-0.56346500
C	1.71570400	2.08043500	0.03122000
C	3.02840100	1.68337100	0.36458800
C	3.42134200	0.40159700	0.04927100
C	-0.01941000	-1.25545600	0.93602700
S	-1.64910400	-1.74571600	0.57775500
N	2.95461600	-1.76413600	-0.95112500
O	4.14088400	-2.08049500	-0.76733000
Cl	0.09043700	-0.19682700	2.35205600
O	-2.52664900	-2.00845800	1.74631400
O	-1.53003000	-2.82782300	-0.42851900
O	2.13362100	-2.54552100	-1.45177100
H	0.56458200	-0.72795900	-1.45711500
H	4.43021400	0.06332200	0.25826700
H	3.71088500	2.37924400	0.84016200
H	0.58239800	-2.15424100	1.08000100
H	-0.18393300	1.58003800	-0.82088000
C	-2.37154500	-0.33431300	-0.25117700
C	-2.36406300	-0.29002800	-1.64496800

C	-2.90706200	0.71192700	0.50084100
C	-2.89451300	0.82353700	-2.29373000
H	-1.95690400	-1.12405800	-2.20907500
C	-3.42713300	1.82474500	-0.15758400
H	-2.92327800	0.65344800	1.58480700
C	-3.41930000	1.88234600	-1.55172200
H	-2.89845500	0.86267900	-3.37973800
H	-3.84390600	2.64524200	0.42036800
H	-3.82887000	2.75086700	-2.06067900
Cl	1.24979500	3.72890400	0.35806700

Thermochemistry data [Hartree]

Electron Energy	-2174.49553
Thermal correction to Energy	0.21171
Zero-point correction	0.23076
Thermal correction to Enthalpy	0.23170
Thermal correction to Gibbs Free Energy	0.16136

σ^H adducts in *ortho* position in *p*-chloronitrobenzene:

ADDUCT 1

C	2.11046100	1.49681700	-0.05463700
C	1.30254500	0.42477500	0.63311200
C	2.05680200	-0.87767100	0.69693800
C	3.18160500	-1.06991300	-0.01423500
C	3.80066600	-0.06080700	-0.83867100
C	3.26788300	1.19345900	-0.81739900
C	-0.09356600	0.29213200	-0.03853500
S	-1.27520800	-0.66173500	0.99108700
N	1.70946200	2.78272900	0.08904000
O	2.35922400	3.73803500	-0.43436400
Cl	-0.03206000	-0.39877500	-1.67374000
O	-1.25373100	-0.00329300	2.30669900
O	-0.97653400	-2.09713800	0.90091700
O	0.65876200	3.02771200	0.76494400
H	1.05924200	0.76323100	1.65220100
H	3.73170000	2.00080600	-1.37534800
H	4.68189800	-0.30025400	-1.42323300
H	-0.53324100	1.29085700	-0.10544100
H	1.65507400	-1.66793300	1.32321600
C	-2.86237600	-0.37219100	0.24162800
C	-3.37562200	-1.31476500	-0.64802100
C	-3.55421400	0.79713900	0.55865600
C	-4.61563700	-1.07480300	-1.23489800
H	-2.81696600	-2.21941800	-0.86645400
C	-4.79134400	1.02446600	-0.03820200
H	-3.13852800	1.50823000	1.26667000
C	-5.31851400	0.09172600	-0.93256900

H	-5.03231000	-1.80064300	-1.92730300
H	-5.34572600	1.92760500	0.20024800
H	-6.28516800	0.27412600	-1.39411300
Cl	4.00307200	-2.61844000	0.07281700

Thermochemistry data [Hartree]

Electron Energy	-2174.53024
Thermal correction to Energy	0.21456
Zero-point correction	0.23345
Thermal correction to Enthalpy	0.23439
Thermal correction to Gibbs Free Energy	0.16468

ADDUCT 2

C	-1.45335500	1.66057000	-0.07145700
C	-0.70287300	0.36337900	-0.25340900
C	-1.59566400	-0.71109600	-0.81936700
C	-2.92929100	-0.55075000	-0.88130300
C	-3.62229500	0.64939300	-0.48140900
C	-2.86998200	1.72458400	-0.11382400
C	-0.01021700	-0.04251600	1.07457600
S	1.29947600	-1.32590600	0.91570800
N	-0.72791400	2.78917900	0.11412700
O	-1.28785800	3.92011800	0.24103500
Cl	-1.15592600	-0.60736400	2.31262700
O	0.74871800	-2.50899100	0.23972500
O	1.90405000	-1.48287200	2.24621200
O	0.54132000	2.70252100	0.15809000
H	0.13790800	0.54666500	-0.94276800
H	-3.34103600	2.66898200	0.14001800
H	-4.70536900	0.68964700	-0.51208800
H	0.51823700	0.82708600	1.47421100
H	-1.12976000	-1.63143500	-1.15475600
C	2.50417500	-0.57486400	-0.15742100
C	3.41277300	0.33702300	0.38035600
C	2.52572000	-0.92880800	-1.50597700
C	4.36131100	0.91086000	-0.46131200
H	3.38540700	0.58478800	1.43733300
C	3.48325000	-0.34955200	-2.33481200
H	1.81504200	-1.65320000	-1.89240800
C	4.39497200	0.56887000	-1.81392900
H	5.07750000	1.62139100	-0.05881000
H	3.51773200	-0.61885800	-3.38652200
H	5.13984600	1.01817300	-2.46502500
Cl	-3.92364600	-1.84862200	-1.52052000

Thermochemistry data [Hartree]

Electron Energy	-2174.52875
Thermal correction to Energy	0.21464

Zero-point correction	0.23348
Thermal correction to Enthalpy	0.23443
Thermal correction to Gibbs Free Energy	0.16496

ADDUCT 3

C	2.63865100	-0.03974800	-0.26535500
C	1.15974500	-0.14945200	-0.55174000
C	0.51274800	1.21155400	-0.57425200
C	1.15044600	2.29992700	-0.10648700
C	2.50499800	2.29590200	0.38519800
C	3.21854200	1.14035400	0.26561100
C	0.50500100	-1.13945400	0.45154500
S	-1.07614200	-1.91241600	-0.08539400
N	3.41871700	-1.11550600	-0.53459900
O	4.67202600	-1.08432700	-0.34560400
Cl	0.33358500	-0.47326100	2.09018900
O	-1.45211200	-2.86731400	0.96715200
O	-0.82196600	-2.40478100	-1.44780800
O	2.87272000	-2.17248400	-0.98433200
H	1.02351800	-0.64360000	-1.52615300
H	4.26217300	1.10262400	0.56157900
H	2.93969800	3.20015700	0.79606100
H	1.14444200	-2.02667000	0.51493500
H	-0.49176200	1.29770100	-0.97430200
C	-2.34796600	-0.67257500	-0.17540300
C	-2.68136400	-0.14527000	-1.42297900
C	-3.01001100	-0.28307900	0.98939300
C	-3.69515400	0.80589700	-1.50006000
H	-2.16005700	-0.48296100	-2.31357400
C	-4.01629000	0.67502100	0.89733400
H	-2.75144500	-0.72835400	1.94451900
C	-4.35572400	1.21812000	-0.34231500
H	-3.97024200	1.22159800	-2.46514100
H	-4.54071200	0.99084000	1.79458100
H	-5.14532100	1.96175500	-0.40740500
Cl	0.33170300	3.85221200	-0.12753000

Thermochemistry data [Hartree]

Electron Energy	-2174.52766
Thermal correction to Energy	0.21465
Zero-point correction	0.23342
Thermal correction to Enthalpy	0.23437
Thermal correction to Gibbs Free Energy	0.16556

Transition states for addition to the *para* position in *p*-chloronitrobenzene:

TS1

C	-2.11289400	-0.64890900	-1.35788400
C	-1.79795200	-1.39728000	-0.19326000
C	-2.47719400	-1.10706200	1.01761200
C	-3.23035400	0.04028200	1.11981200
C	-3.40469400	0.86516200	-0.00397700
C	-2.86843500	0.49296300	-1.25223500
C	0.27908400	-0.47693100	0.36322900
S	1.65201900	-0.75070400	-0.66959000
Cl	0.62783400	-0.80613900	2.06915000
O	1.18490800	-0.43661400	-2.03818700
O	2.22437100	-2.08750200	-0.41093900
H	-3.07188700	1.10237600	-2.12582100
H	-0.05085200	0.55716300	0.25052000
H	-2.35524800	-1.76429900	1.87158600
C	2.96433600	0.41909900	-0.31009000
C	3.97271400	0.07149700	0.58944200
C	2.91704800	1.69254100	-0.88102500
C	4.95090900	1.01117000	0.91215400
H	3.99556600	-0.92674900	1.01577300
C	3.90013500	2.62275000	-0.55402200
H	2.12564700	1.94402000	-1.58161200
C	4.91571400	2.28397200	0.34261700
H	5.74387900	0.74564400	1.60635500
H	3.87603300	3.61227600	-1.00285700
H	5.68120200	3.01291300	0.59526500
H	-3.71299000	0.30088400	2.05541600
N	-4.18101300	2.04434500	0.10429400
O	-4.67295700	2.34132900	1.20267100
O	-4.34224400	2.74994900	-0.90196400
H	-1.69407000	-0.94786500	-2.31218000
Cl	-1.26934100	-3.05788000	-0.41950000

Thermochemistry data [Hartree]

Electron Energy	-2174.49230
Thermal correction to Energy	0.21149
Zero-point correction	0.23071
Thermal correction to Enthalpy	0.23165
Thermal correction to Gibbs Free Energy	0.15980

TS2

C	1.84292100	-0.43422200	1.75499800
C	0.73435200	-0.89085100	1.00120600
C	0.94927700	-1.36947900	-0.31762200
C	2.17362900	-1.21048900	-0.91795800
C	3.24113500	-0.64316000	-0.19442400

C	3.06919100	-0.27625300	1.15034300
C	-0.41828800	1.18871600	0.77494200
S	-1.45536300	1.52525200	-0.59828000
Cl	0.82010600	2.45545700	0.89984500
O	-0.67648900	1.39445900	-1.84998600
O	-2.25979000	2.77176800	-0.48217800
H	3.91265200	0.10860000	1.71301000
H	-1.03343200	1.20461700	1.67881300
H	0.12877100	-1.82958800	-0.85702500
C	-2.61165800	0.16592900	-0.52123500
C	-3.61088200	0.16890900	0.45259600
C	-2.51553700	-0.85993000	-1.45816000
C	-4.51395200	-0.89001400	0.49821500
H	-3.68895500	0.99035500	1.15941600
C	-3.43046000	-1.91037300	-1.40983800
H	-1.74232600	-0.82351300	-2.21964400
C	-4.42247100	-1.92889900	-0.42979400
H	-5.29416200	-0.90021200	1.25444800
H	-3.36793800	-2.71332600	-2.13935100
H	-5.13251100	-2.75087700	-0.39301600
H	2.33363000	-1.54081800	-1.93839600
N	4.50431100	-0.48863200	-0.80838600
O	5.43798600	-0.00230500	-0.15178400
O	4.64564400	-0.84029000	-1.98969800
H	1.71025100	-0.17661000	2.80075600
Cl	-0.59497100	-1.62019900	1.90378700

Thermochemistry data [Hartree]

Electron Energy	-2174.48542
Thermal correction to Energy	0.21155
Zero-point correction	0.23067
Thermal correction to Enthalpy	0.23162
Thermal correction to Gibbs Free Energy	0.16084

TS3

C	-1.93934100	-1.65243200	0.93048100
C	-0.80350300	-0.85345000	1.21736200
C	-0.90120800	0.55363500	1.08547800
C	-2.03169000	1.11833100	0.54244900
C	-3.12664300	0.30779400	0.19176700
C	-3.07024600	-1.08180000	0.39375900
C	0.54012200	-1.48504000	-0.65118800
S	2.23953900	-1.10550500	-0.79869600
Cl	-0.40021000	-0.88484200	-2.02541700
O	2.77392800	-1.11009400	-2.18393300
O	2.93892200	-1.95599900	0.19138500
H	-3.93226200	-1.69412900	0.15236400
H	0.44783100	-2.57058500	-0.57066100

H	-0.06771200	1.17846400	1.38950900
C	2.38532000	0.58796800	-0.24358600
C	2.79618500	0.84041700	1.06396900
C	2.08114200	1.63076900	-1.11959800
C	2.89943600	2.15956200	1.50173700
H	3.03166600	0.01015100	1.72179000
C	2.17714800	2.94581400	-0.66847000
H	1.78208500	1.41746400	-2.14121600
C	2.58487400	3.21051100	0.63950700
H	3.22617400	2.36570900	2.51755300
H	1.93972600	3.76437600	-1.34270000
H	2.66344100	4.23793100	0.98521600
H	-2.09899200	2.19312300	0.41344800
N	-4.29410300	0.89469600	-0.34320600
O	-4.32807800	2.12415900	-0.50873500
O	-5.25475900	0.16580400	-0.63659600
H	-1.90107500	-2.72074300	1.11900400
Cl	0.31465300	-1.48221600	2.42178700

Thermochemistry data [Hartree]

Electron Energy	-2174.48800
Thermal correction to Energy	0.21143
Zero-point correction	0.23053
Thermal correction to Enthalpy	0.23147
Thermal correction to Gibbs Free Energy	0.16136

TS4

C	2.47718200	-1.10705300	1.01762000
C	1.79794600	-1.39727200	-0.19325600
C	2.11290600	-0.64891000	-1.35788200
C	2.86845500	0.49295600	-1.25223300
C	3.40470500	0.86515900	-0.00397300
C	3.23034900	0.04028600	1.11982000
C	-0.27908300	-0.47692500	0.36322200
S	-1.65201800	-0.75068800	-0.66960200
O	-2.22436400	-2.08749200	-0.41097300
O	-1.18490300	-0.43656900	-2.03819100
H	3.71297900	0.30089100	2.05542700
H	1.69408800	-0.94787400	-2.31217900
C	-2.96434300	0.41910100	-0.31008700
C	-2.91708100	1.69254000	-0.88103200
C	-3.97270500	0.07149000	0.58946000
C	-3.90017700	2.62273600	-0.55402200
H	-2.12569200	1.94402400	-1.58163100
C	-4.95090900	1.01115100	0.91217800
H	-3.99553800	-0.92675500	1.01579500
C	-4.91574000	2.28395000	0.34263200
H	-3.87609500	3.61226000	-1.00286400

H	-5.74386700	0.74561700	1.60639000
H	-5.68123600	3.01288000	0.59528300
H	3.07192000	1.10236200	-2.12582100
N	4.18103200	2.04433600	0.10429900
O	4.34227900	2.74993400	-0.90196200
O	4.67296800	2.34132300	1.20268000
H	2.35522400	-1.76428400	1.87159800
Cl	-0.62783600	-0.80615200	2.06914000
H	0.05084500	0.55717400	0.25052800
Cl	1.26934000	-3.05787400	-0.41949900

Thermochemistry data [Hartree]

Electron Energy	-2174.49230
Thermal correction to Energy	0.21149
Zero-point correction	0.23071
Thermal correction to Enthalpy	0.23165
Thermal correction to Gibbs Free Energy	0.15980

TS5

C	0.90122200	0.55365600	1.08547300
C	0.80351100	-0.85342900	1.21736600
C	1.93934700	-1.65241600	0.93049000
C	3.07025300	-1.08179100	0.39376500
C	3.12665600	0.30780200	0.19176500
C	2.03170500	1.11834500	0.54244200
C	-0.54011700	-1.48504100	-0.65117100
S	-2.23953700	-1.10552000	-0.79868300
O	-2.93891300	-1.95600900	0.19140800
O	-2.77392700	-1.11012700	-2.18391900
H	2.09901300	2.19313500	0.41343600
H	1.90107700	-2.72072500	1.11901900
C	-2.38533300	0.58795900	-0.24359100
C	-2.08114600	1.63075200	-1.11960900
C	-2.79622100	0.84041900	1.06395500
C	-2.17716600	2.94580100	-0.66849500
H	-1.78207100	1.41743900	-2.14122000
C	-2.89948500	2.15956800	1.50170700
H	-3.03170900	0.01015800	1.72178000
C	-2.58491400	3.21050900	0.63947200
H	-1.93973700	3.76435800	-1.34273100
H	-3.22624100	2.36572300	2.51751600
H	-2.66349200	4.23793300	0.98516900
H	3.93226700	-1.69412400	0.15237400
N	4.29411900	0.89469600	-0.34320900
O	4.32809900	2.12415800	-0.50874400
O	5.25477300	0.16579900	-0.63659300
H	0.06772900	1.17849000	1.38950300

Cl	0.40020900	-0.88486300	-2.02541500
H	-0.44782000	-2.57058400	-0.57062700
Cl	-0.31464400	-1.48218000	2.42180000

Thermochemistry data [Hartree]

Electron Energy	-2174.48800
Thermal correction to Energy	0.21143
Zero-point correction	0.23053
Thermal correction to Enthalpy	0.23147
Thermal correction to Gibbs Free Energy	0.16136

TS6

C	-1.91819400	-1.48788800	1.00983300
C	-0.79967900	-0.66081800	1.28497500
C	-0.92102900	0.74244500	1.11351000
C	-2.01143800	1.25874700	0.45577200
C	-3.04756100	0.40225100	0.03759500
C	-3.00723800	-0.96730700	0.34880900
C	0.48372500	-1.25576800	-0.60853700
S	2.15785700	-0.82784500	-0.91290600
O	2.55474700	-0.82917300	-2.34765600
O	3.04587000	-1.59428500	-0.01082100
H	-3.84808800	-1.60087100	0.08846900
H	-0.12391400	1.39506700	1.45339700
C	2.17461800	0.87896000	-0.38743200
C	2.68588600	1.19808500	0.86902300
C	1.68432500	1.86477100	-1.24396900
C	2.69975800	2.53083400	1.27578300
H	3.06745100	0.41062800	1.51132500
C	1.69408800	3.19311900	-0.82356500
H	1.31111800	1.59971800	-2.22912000
C	2.20006500	3.52524200	0.43379900
H	3.10119300	2.79242200	2.25111500
H	1.31252200	3.96912100	-1.48156500
H	2.21025200	4.56318300	0.75589400
H	-2.09106100	2.32485700	0.27406400
N	-4.16960600	0.93523500	-0.64225200
O	-4.19897800	2.14929600	-0.89026300
O	-5.08798000	0.17251400	-0.97554100
H	-1.88691000	-2.53812500	1.27774100
Cl	0.24862200	-3.00050900	-0.87474400
H	-0.13677100	-0.70424000	-1.32085800
Cl	0.32387900	-1.23688700	2.50547700

Thermochemistry data [Hartree]

Electron Energy	-2174.48692
Thermal correction to Energy	0.21144
Zero-point correction	0.23063

Thermal correction to Enthalpy	0.23157
Thermal correction to Gibbs Free Energy	0.16064

Products of substitution of chlorine in *p*-chloronitrobenzene:

Product 1

C	-1.89947400	1.11250700	-0.02048000
C	-1.22453700	-0.03296000	0.41498600
C	-1.92641900	-1.22569500	0.62457200
C	-3.29447100	-1.27861100	0.39956600
C	-3.94333200	-0.12580000	-0.03544300
C	-3.26967500	1.07203300	-0.24858700
C	0.25959800	0.05414300	0.61151200
S	1.11382600	-0.72931800	-0.82714700
Cl	0.82165700	-0.70699900	2.11941100
O	0.72515900	0.08838700	-1.98387000
O	0.82043500	-2.16777600	-0.83284400
H	-3.80863100	1.95176300	-0.58083100
H	0.59719300	1.10130600	0.60868100
H	-1.40475600	-2.11297600	0.96829400
C	2.84620400	-0.50627000	-0.50400500
C	3.62600400	-1.62507900	-0.21766300
C	3.38265300	0.78079700	-0.55767100
C	4.98843100	-1.44709500	0.01013600
H	3.17234700	-2.61050000	-0.18131200
C	4.74461400	0.94131100	-0.31779500
H	2.74928300	1.64128700	-0.76194600
C	5.54405100	-0.16849000	-0.03903800
H	5.61404000	-2.30779000	0.22846700
H	5.18135700	1.93534500	-0.35112500
H	6.60698800	-0.03491400	0.14285800
H	-3.85311700	-2.19394100	0.55650500
N	-5.38310300	-0.17655300	-0.27203100
O	-5.96184900	-1.23647800	-0.07289800
O	-5.93920500	0.84266400	-0.65862000
H	-1.34540000	2.03684200	-0.16802600
Cl	0.95440100	3.52931700	0.37131500

Thermochemistry data [Hartree]

Electron Energy	-2174.59682
Thermal correction to Energy	0.21523
Zero-point correction	0.23507
Thermal correction to Enthalpy	0.23601
Thermal correction to Gibbs Free Energy	0.16168

Product 2

C	-0.94006400	-2.17742000	0.94507900
C	-0.04703800	-1.70203700	-0.02234800
C	-0.53157800	-0.99894500	-1.13043400
C	-1.89299600	-0.76770700	-1.27334700
C	-2.75691100	-1.24794400	-0.29474400
C	-2.30368400	-1.95155500	0.81601100
C	1.41771700	-1.94153500	0.18873200
S	2.22734400	-0.57016500	1.14853100
Cl	2.32796300	-2.24254000	-1.30470100
O	3.64619800	-0.92338900	1.26571100
O	1.40692000	-0.43011300	2.35751700
H	-3.00493400	-2.31776800	1.55664300
H	1.58504200	-2.79691900	0.85025800
H	0.15134200	-0.63763400	-1.89282400
C	2.07745500	0.89871900	0.17125900
C	0.95513000	1.71113100	0.33894900
C	3.08521300	1.20726700	-0.74408300
C	0.84122900	2.86338500	-0.43441700
H	0.19258100	1.45465200	1.06810500
C	2.95681700	2.36240100	-1.50994700
H	3.95384700	0.56390500	-0.84165400
C	1.83873100	3.18393200	-1.35612400
H	-0.03033800	3.50103300	-0.30460300
H	3.73337500	2.62256700	-2.22344900
H	1.74718600	4.08480600	-1.95697700
H	-2.28093900	-0.22428200	-2.12695600
N	-4.19098700	-1.01372100	-0.44362400
O	-4.57335800	-0.40221800	-1.43162400
O	-4.93592900	-1.44183800	0.42740400
H	-0.57071200	-2.72736800	1.80546200
Cl	-2.58254100	3.98595200	0.93265900

Thermochemistry data [Hartree]

Electron Energy	-2174.59155
Thermal correction to Energy	0.21530
Zero-point correction	0.23519
Thermal correction to Enthalpy	0.23614
Thermal correction to Gibbs Free Energy	0.16042

Product 3

C	-0.56169800	-0.66110400	1.01407100
C	0.18212500	-1.65878800	0.37505400
C	-0.46742100	-2.60948800	-0.42075600
C	-1.84520700	-2.56688100	-0.58508700
C	-2.55933600	-1.56421300	0.06227000
C	-1.94078200	-0.60868600	0.86191400
C	1.67541000	-1.73066700	0.48674700

S	2.53385500	-0.72102500	-0.81742300
O	1.94844300	-1.17658000	-2.08404200
O	3.97379100	-0.87130500	-0.58294700
H	-2.52788000	0.16073400	1.34987700
H	0.10393000	-3.38923700	-0.91534700
C	2.07779800	0.96821800	-0.54324100
C	2.85841500	1.74999200	0.30966800
C	0.94664300	1.47444100	-1.18517600
C	2.48807700	3.07460700	0.52348600
H	3.74119400	1.33182200	0.78265600
C	0.59088300	2.80124400	-0.96030500
H	0.36667900	0.84518500	-1.85317700
C	1.35744300	3.59558400	-0.10710600
H	3.08543100	3.70020200	1.18030000
H	-0.28679700	3.21305000	-1.44976500
H	1.07306900	4.63001600	0.06497100
H	-2.35942600	-3.29984200	-1.19562100
N	-4.01067200	-1.51850000	-0.09706500
O	-4.62906400	-0.66026300	0.51666000
O	-4.53273800	-2.34195900	-0.83657300
H	-0.06848000	0.07420200	1.64196500
Cl	2.30469200	-1.29677000	2.08849000
H	2.03920400	-2.73625000	0.25474700
Cl	-3.51242500	3.91155400	0.19407400

Thermochemistry data [Hartree]

Electron Energy	-2174.59104
Thermal correction to Energy	0.21530
Zero-point correction	0.23525
Thermal correction to Enthalpy	0.23620
Thermal correction to Gibbs Free Energy	0.15953

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