

Electronic Supplementary Material (ESI) for Dalton Transactions.

A Theoretical Study on the Oxidation of Alkenes to Aldehydes Catalyzed by Ruthenium Porphyrins Using O₂ as the Sole Oxidant

Lin-Lin Zhang,^{a†} Xiang-Yun Wang,^{a†} Kun-Yao Jiang,^a Bing-Yuan Zhao,^a Hui-Min Yan,^a Xiao-Yun Zhang,^a
Zhu-Xia Zhang,^a Zhen Guo^{*a} and Chi-Ming Che^{*b}

^a *College of Material Science & Engineering, Taiyuan University of Technology, Shanxi, 030024, P. R.China.*

^b *Department of Chemistry, The University of Hong Kong, Hong Kong, P. R.China.*

E-mail: guozhen@tyut.edu.cn; cmche@hku.hk

Table S1. The calculated free energies (ΔG_{solv} , kcal/mol) of the oxidative addition of styrene by dioxoruthenium porphyrin [Ru(Por)O₂] using different functionals(DFs)^{a,b}

	B3LYP	M06	PBE0	BP86
¹A+S	0.0	0.0	0.0	0.0
³A+S	30.6	22.7	29.6	29.4
¹I	-0.04	-3.0	0.8	-1.51
¹TS₁₋₁	10.4	9.1	9.9	5.92
¹B	2.03	-4.0	-1.7	2.9

a: $\Delta G_{\text{solv}} = \Delta E_{\text{solv(CPCM)}} + \Delta G_{\text{corr-gas}}$, where $\Delta E_{\text{solv(CPCM)}}$ refers to the solvation single point energy (DFs/6-311+G**:*Sdd*) and $\Delta G_{\text{corr-gas}}$ corresponds with the thermal correction to the free energy of the solute in the gas phase(M06L/6-31G*:*Sdd*). *b*: the D3 version of Grimme's dispersion was added in the single point calculations.

Table S2. The calculated free energies (ΔG_{solv} , kcal/mol) of the oxidative addition of styrene by dioxoruthenium porphyrin [Ru(Por)O₂] at the M06L/def2-TZVPP level of theory.^{a,b}

¹A+S	³A+S	¹I	¹TS₁₋₁	¹B
0.0	25.9	-1.9	11.0	6.0

a: $\Delta G_{\text{solv}} = \Delta E_{\text{solv(CPCM)}} + \Delta G_{\text{corr-gas}}$, where $\Delta E_{\text{solv(CPCM)}}$ refers to the solvation single point energy (M06L/def2-TZVPP) and $\Delta G_{\text{corr-gas}}$ corresponds with the thermal correction to the free energy of the solute in the gas phase(M06L/6-31G*:*Sdd*; *b*: the D3 version of Grimme's dispersion was added in the single point calculations;

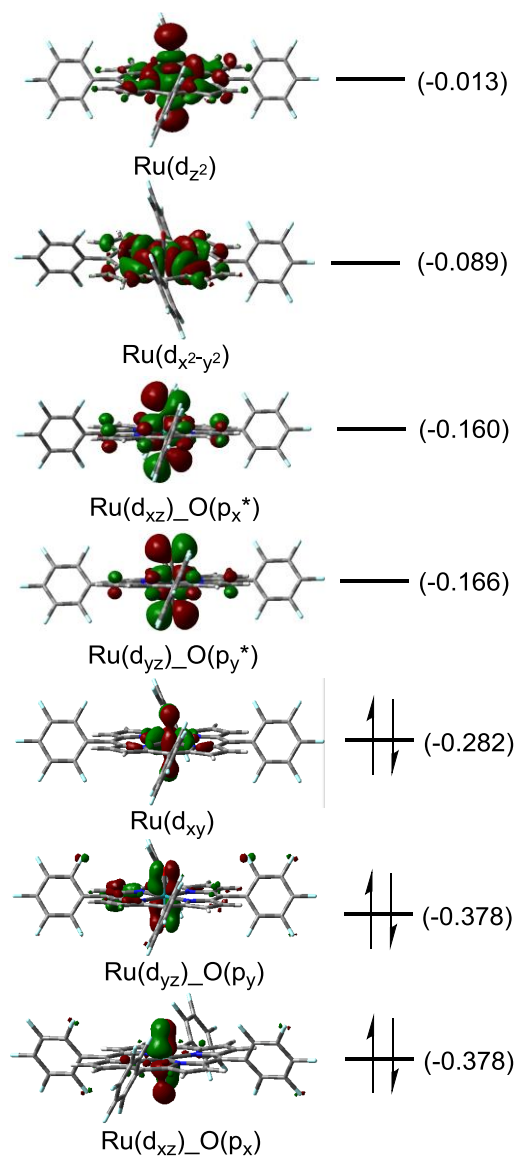


Figure S1. NBO analysis for the ^1A species with doubly occupied $\text{Ru}(\text{d}_{xy})$ orbital.

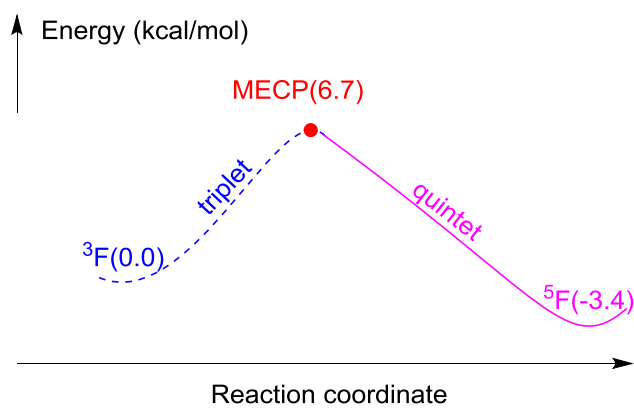
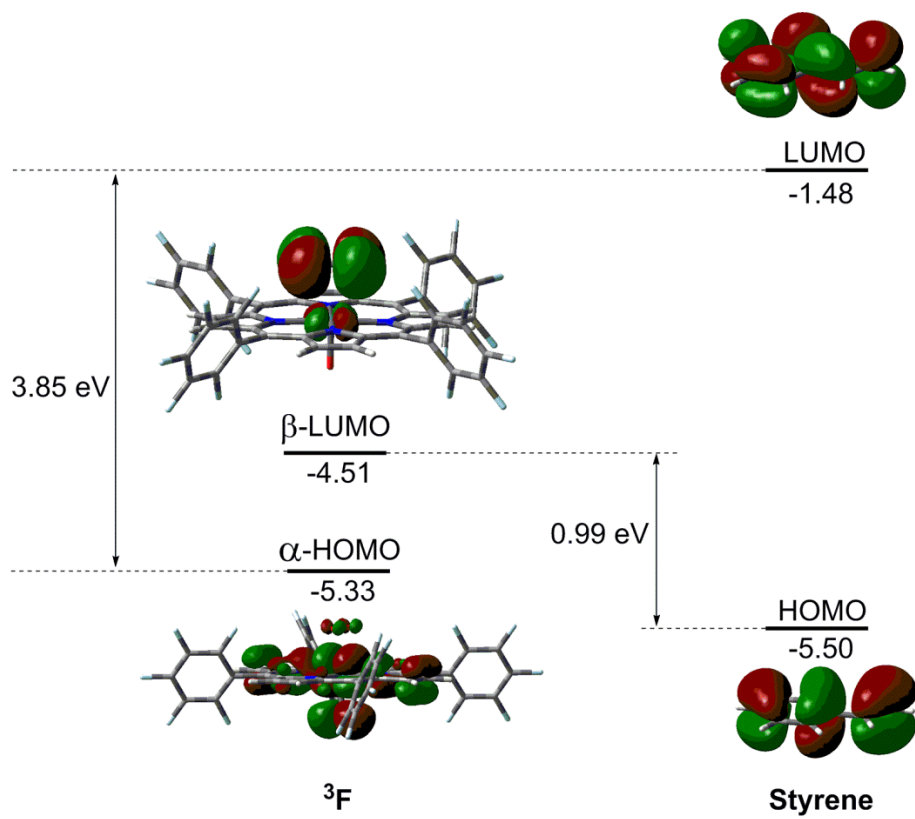
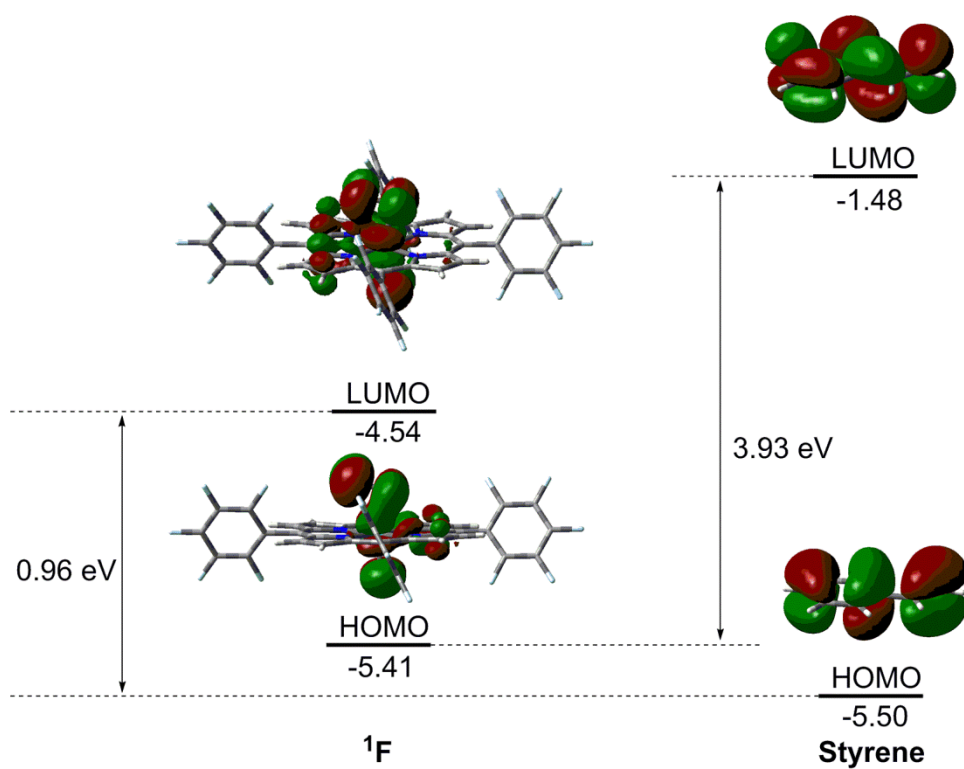


Figure S2. The relative energy of the triplet-quintet minimum energy crossing point (**MECP**) between ^3F and ^5F calculated at M06L/6-31G*:sdd level of theory.



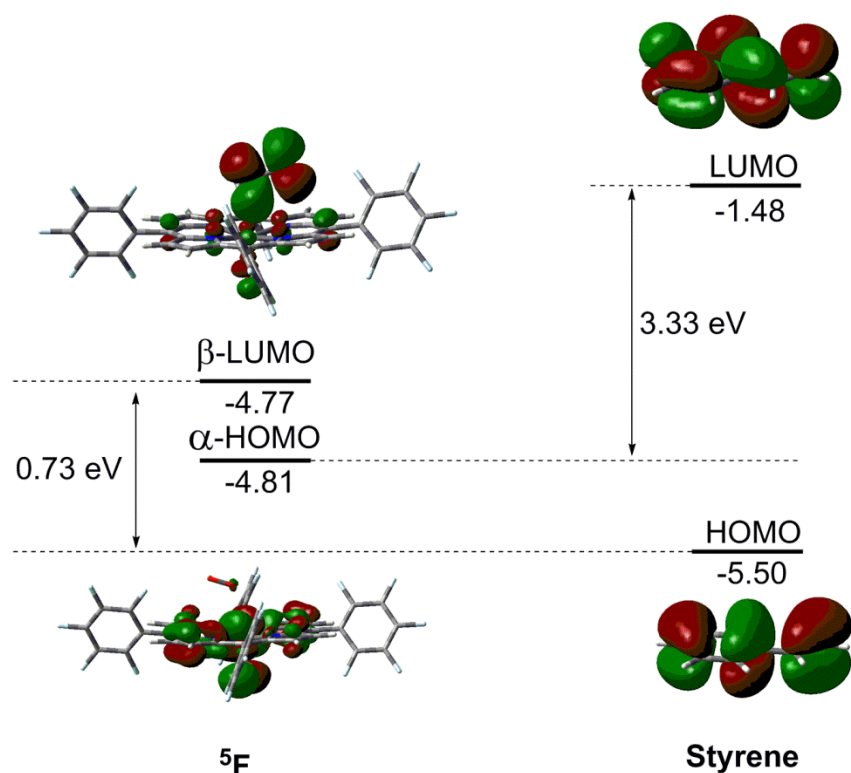
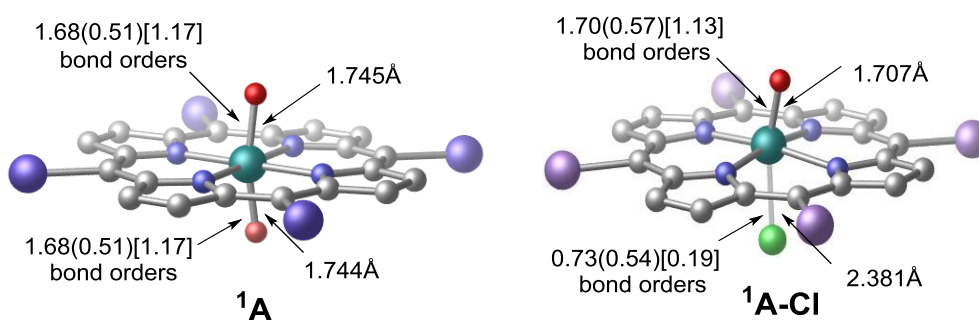


Figure S3. Energies of the HOMOs and LUMOs for $^{1,3,5}\text{F}$ and styrene. (In order to understand the reactivities between ruthenium porphyrin-superoxo $[\text{O}=\text{Ru}(\text{Por})\text{O}_2]$ ($^{1,3,5}\text{F}$) and styrene, frontier molecular orbital [FMO] analysis were calculated for $^{1,3,5}\text{F}$ and styrene. According to FMO theory, the smaller the HOMO-LUMO energy gap is, the easier the reaction will be. Thus, From Figure S3, we can see the LUMOs of species **F** generally lie lower in energy than HOMO of substrate, indicating that species **F** exhibits to be electrophilic in three spin states.



Species		^1A		$^1\text{A-Cl}$	
		O-Ru	O-Ru	Cl-Ru	O-Ru
Mayer Bond orders	Total bond order	1.68	1.68	0.73	1.70
	σ -contribution	0.51	0.51	0.54	0.57
	π -contribution	1.17	1.17	0.19	1.13

Figure S4. The analysis of atomic orbital symmetry based (AOSB) decomposition of $\text{Ru}=\text{O}$ and

Ru=Cl bond orders for $^1\mathbf{A}$ and $^1\mathbf{A-Cl}$ species.

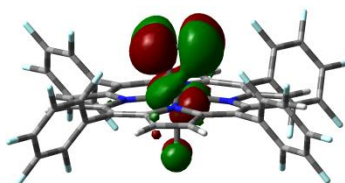


Figure S5. The $\pi^*(\text{O}_2)$ orbitals (β -Lumo+1) for $^3\mathbf{F-Cl}$ species.

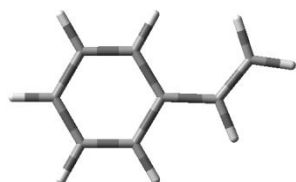
Calculations for All Stationary Points

$$\Delta G_{\text{solv}} = \Delta E_{\text{solv}}(\text{CPCM}) + \Delta G_{\text{corr-gas}}$$

ΔE_{solv} refers to the solvation single point energy by M06L/6-311+G(d,p):Sdd level of theory.

$\Delta G_{\text{corr-gas}}$ refers to the thermal correction to the free energy of the solute in the gas phase by M06L/6-31G(d):Sdd level of theory.

1. Coordinates of all stationary points in Fig. 2

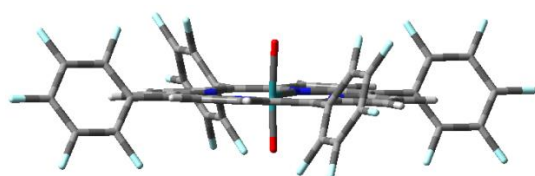


S

C	2.96248600	0.33519300	0.00022700
H	3.99343900	-0.00751600	0.00014200
H	2.81577100	1.41407200	0.00057600
C	1.94407200	-0.53255300	-0.00012700
H	2.17851800	-1.60017500	-0.00045700
C	0.51536900	-0.22477300	-0.00012500
C	0.01503200	1.08746800	-0.00015300
C	-0.40833700	-1.28031800	-0.00002700
C	-1.35141700	1.32884400	-0.00004400
H	0.70801200	1.92771500	-0.00031400
C	-1.77811700	-1.04094300	0.00010900
H	-0.03568300	-2.30512700	-0.00003100
C	-2.25602000	0.26627400	0.00010500
H	-1.71709300	2.35440600	-0.00008300
H	-2.47419300	-1.87800100	0.00015700
H	-3.32717900	0.45948300	0.00021700

$$\Delta E_{\text{solv}} = -309.621221314$$

$$\Delta G_{\text{solv}} = -309.518903314$$



	¹ A		
O	-0.12729300	-0.10680300	1.72816800
Ru	0.02448400	0.01945300	-0.00545300
N	-0.00886200	2.07740100	-0.01481400
C	-1.13317300	2.86308900	-0.04768800
C	-0.72022600	4.23459200	-0.14537400
C	0.64078100	4.25309900	-0.16305300
C	1.08895300	2.89281600	-0.07623600
C	-2.46524800	2.41854100	-0.00101100
C	-3.52045300	3.46165300	0.00347600
C	-3.65556000	4.36106800	1.06461700
C	-4.64317100	5.33902400	1.07949700
C	-5.53252700	5.43170700	0.01424100
C	-5.42703100	4.55016200	-1.05638400
C	-4.42829100	3.58325900	-1.05193800
F	-2.82402900	4.29347700	2.10763100
F	-4.74924000	6.17864200	2.10824700
F	-6.48254700	6.36171700	0.01942100
F	-6.27498700	4.64369900	-2.07955600
F	-4.34890800	2.75820500	-2.09878500
C	2.42876900	2.47082300	-0.07141700
C	2.87538300	1.13972900	-0.03510200
N	2.07820300	0.02549700	-0.01777800
C	2.88647000	-1.08381400	-0.00537000
C	4.25264000	-0.64410300	-0.01313400
C	4.24610500	0.71717600	-0.02326300
C	2.46550600	-2.42366800	-0.00114400
C	1.13513900	-2.88138200	-0.00121300
N	0.02757200	-2.09169400	0.00829500
C	-1.07638200	-2.89176300	0.02310000
C	-0.64177200	-4.26567900	0.01049400
C	0.71729700	-4.25985800	0.00400800
C	-2.41483300	-2.46088600	0.05785500
C	-3.45526700	-3.51886100	0.09905100
C	-3.58259700	-4.37790600	1.19344400
C	-4.55229800	-5.37300500	1.23920500
C	-5.43166300	-5.52294600	0.17221500
C	-5.33414800	-4.68140100	-0.93071500
C	-4.35296900	-3.69698400	-0.95690900
F	-2.75981300	-4.25506100	2.23827000
F	-4.65030500	-6.17524800	2.29837600
F	-6.36456600	-6.46976800	0.20613100
F	-6.17320100	-4.82902600	-1.95487500
F	-4.28147100	-2.90995400	-2.03306100

C	3.46693400	3.52974200	-0.11116700
C	3.62511700	4.43346900	0.94289600
C	4.59161600	5.43241300	0.91770700
C	5.43603000	5.54152000	-0.18217600
C	5.30619600	4.65630000	-1.24710600
C	4.32819500	3.66943600	-1.20244900
F	2.83523400	4.35052100	2.01650100
F	4.22360500	2.84143900	-2.24557200
F	6.11074000	4.76528100	-2.30321100
F	6.36638000	6.49070600	-0.21497600
F	4.72033500	6.27663500	1.94000500
O	-0.13223500	-0.12359400	-1.73694200
N	-2.09191900	-0.01337600	0.00045900
C	-2.87017800	-1.12993600	0.06434700
C	-4.24880700	-0.71895000	0.15697500
C	-4.26655500	0.63983500	0.14278600
C	-2.89859400	1.08051100	0.04087500
C	3.52859300	-3.45974100	0.00454000
C	3.71442200	-4.31875900	-1.08119900
C	4.70086400	-5.29820600	-1.08474700
C	5.53797500	-5.43193500	0.01764800
C	5.38102100	-4.59065100	1.11391800
C	4.38317500	-3.62292600	1.09762400
F	2.93142700	-4.21172700	-2.15777000
F	4.85392600	-6.10112500	-2.13656800
F	6.48684400	-6.36319400	0.02373300
F	6.17916300	-4.72311400	2.17225200
F	4.25447900	-2.83534500	2.16871000
H	-5.09742500	-1.38755700	0.23846400
H	-5.13168800	1.28834400	0.21118600
H	-1.38905900	5.08459900	-0.20681100
H	1.28561500	5.11998200	-0.24228600
H	5.10393400	1.37870400	-0.02250100
H	5.11763400	-1.29611200	-0.01506500
H	1.38027100	-5.11657400	0.00576800
H	-1.29554700	-5.12939900	0.00375800

$\Delta E_{\text{solv}} = -4142.32906061$

$\Delta G_{\text{solv}} = -4141.98358861$

³A

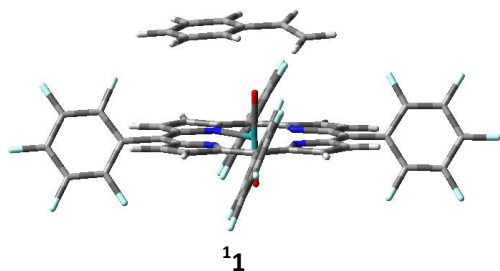
O	-0.22285300	-0.32215700	1.76207400
Ru	0.01743500	0.02196200	-0.03490000
N	-1.68672300	1.20744600	-0.01606000
C	-2.97391400	0.73175100	-0.04464200

C	-3.86832500	1.85732600	-0.12960400
C	-3.10965900	2.98424900	-0.14481200
C	-1.73632800	2.56777600	-0.06956500
C	-3.38376100	-0.61336400	-0.01379000
C	-4.84700400	-0.86368000	0.00236000
C	-5.64441900	-0.46861700	1.07964100
C	-7.01386500	-0.70561900	1.10703300
C	-7.61814400	-1.35912000	0.03820900
C	-6.85195700	-1.76778200	-1.04825200
C	-5.48472700	-1.51641200	-1.05579600
F	-5.09369400	0.15325500	2.12518900
F	-7.74752900	-0.31980100	2.15000700
F	-8.92707000	-1.59234300	0.05473200
F	-7.43285000	-2.38752400	-2.07455200
F	-4.77875200	-1.91416000	-2.11690000
C	-0.61494400	3.41170900	-0.06722500
C	0.72146100	2.99300900	-0.03227400
N	1.17129900	1.68482800	-0.02126900
C	2.55413500	1.72131800	-0.00417800
C	2.97349200	3.08755200	-0.00251500
C	1.85413400	3.86405900	-0.01145000
C	3.41406900	0.61546500	0.00128000
C	3.01606300	-0.73032100	0.00113200
N	1.72294200	-1.15939200	0.00351500
C	1.72822400	-2.53207800	0.02080100
C	3.09791600	-2.97703300	0.01692200
C	3.88851900	-1.87221200	0.01365500
C	0.61051600	-3.38538900	0.04183600
C	0.88513700	-4.84389600	0.09111900
C	1.49591200	-5.43723600	1.19873300
C	1.74900500	-6.80287800	1.25532300
C	1.38145200	-7.61324400	0.18633200
C	0.76766300	-7.05411900	-0.92953600
C	0.52876200	-5.68506600	-0.96593700
F	1.85340100	-4.68837300	2.24528200
F	2.33143400	-7.34034200	2.32629800
F	1.61678600	-8.92114900	0.23140900
F	0.42076300	-7.82999800	-1.95543700
F	-0.05671000	-5.17780800	-2.05325300
C	-0.87034600	4.87229100	-0.10732000
C	-1.51351600	5.52677000	0.94641300
C	-1.77008500	6.89274900	0.91761900
C	-1.37478300	7.64119100	-0.18608200
C	-0.73037900	7.02026700	-1.25093300

C	-0.48983900	5.65205000	-1.20248300
F	-1.89858400	4.83737200	2.02329900
F	0.12274600	5.08449900	-2.24527400
F	-0.35725000	7.73663600	-2.31024400
F	-1.61220500	8.94873300	-0.22315300
F	-2.38170800	7.48903300	1.93967700
O	-0.20539700	-0.29692900	-1.80567600
N	-1.20137900	-1.73325200	-0.03360000
C	-0.74530300	-3.00854500	0.02934700
C	-1.87899400	-3.89902700	0.11310200
C	-2.99532800	-3.12439000	0.09986400
C	-2.55656300	-1.75174400	0.00690100
C	4.87259100	0.88777700	0.01131000
C	5.68333400	0.54394100	-1.07308900
C	7.05271500	0.78352300	-1.07351200
C	7.64289600	1.38823600	0.03131400
C	6.86295900	1.74558100	1.12614500
C	5.49667600	1.49010400	1.10639000
F	5.14512300	-0.03222000	-2.15120900
F	7.79917000	0.44656000	-2.12407600
F	8.95110400	1.62487700	0.04075100
F	7.42956900	2.32055200	2.18582500
F	4.77598500	1.83954600	2.17558600
H	-1.82711900	-4.97867700	0.18847900
H	-4.02588600	-3.45306600	0.16233900
H	-4.94792900	1.79142600	-0.18752500
H	-3.45072200	4.01001100	-0.21509600
H	1.80635600	4.94612200	-0.00097700
H	4.00355300	3.42227700	0.00193500
H	4.97100300	-1.83455900	0.02112200
H	3.41634500	-4.01222200	0.01168600

$\Delta E_{\text{solv}} = -4142.28387188$

$\Delta G_{\text{solv}} = -4141.94143888$



C	-1.92548300	-5.46078700	0.70472800
C	-2.15837600	-4.54305600	-0.32227400
C	-2.93715300	-4.97829700	-1.39770700

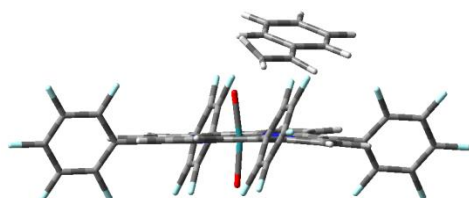
C	-3.46379900	-6.26366100	-1.45315400
C	-3.20981900	-7.15404600	-0.41525800
C	-2.43632100	-6.75302900	0.66883500
C	-1.60368300	-3.16692200	-0.27739500
C	-2.53300100	-2.11431700	-0.18687000
N	-2.22585200	-0.79065500	-0.17093600
C	-3.38252700	-0.07736200	-0.07629500
C	-4.48718900	-1.00357800	-0.04237100
C	-3.96458600	-2.25668900	-0.10147100
Ru	-0.26635600	0.01825900	-0.23146100
O	-0.53524800	0.10895500	-1.95123600
C	-3.48911200	1.32368100	-0.01634800
C	-4.85972900	1.88384800	0.09220400
C	-5.41626900	2.65362200	-0.93219200
C	-6.69671700	3.18700300	-0.83936900
C	-7.45786100	2.94925600	0.30027900
C	-6.93363000	2.18474200	1.33718600
C	-5.64860200	1.66683600	1.22454700
F	-4.71442800	2.89472300	-2.04228200
F	-7.20099500	3.91497800	-1.83467400
F	-8.68493100	3.45255700	0.39857200
F	-7.65939700	1.96209400	2.43219700
F	-5.17129600	0.94500400	2.24199300
F	-3.19115500	-4.15131400	-2.41502200
F	-4.19963400	-6.64985400	-2.49440800
F	-3.70544800	-8.38699900	-0.45940600
F	-2.19765900	-7.60431100	1.66548000
F	-1.19408800	-5.10513200	1.76508500
C	-2.43032800	2.24940600	-0.04173500
N	-1.10268600	1.95457700	-0.14453500
C	-0.39766600	3.11700600	-0.12010200
C	-1.32169200	4.21371700	0.00832000
C	-2.57101600	3.67959900	0.06017100
C	1.00425200	3.22594800	-0.18755900
C	1.92028300	2.16389900	-0.24847900
N	1.61587800	0.82320200	-0.27356800
C	2.78848300	0.11879500	-0.37179900
C	3.87741800	1.05160800	-0.37840300
C	3.34606900	2.30257900	-0.31694200
C	2.90707800	-1.27699200	-0.49590500
C	4.26922400	-1.81182400	-0.74593400
C	4.90204100	-2.71340100	0.11474800
C	6.18165900	-3.19866500	-0.12920900
C	6.86845600	-2.78950600	-1.26605100

C	6.26604700	-1.90337300	-2.15204600
C	4.98424000	-1.43479000	-1.88919100
F	4.28120300	-3.14934300	1.21476000
F	6.75208600	-4.05033400	0.72248000
F	8.09297800	-3.24705600	-1.50798400
F	6.91429000	-1.51951300	-3.25077600
F	4.43531600	-0.60243700	-2.77842800
C	1.55694700	4.60358300	-0.24449200
C	2.34401000	5.14152500	0.77568900
C	2.85851900	6.43123900	0.71123800
C	2.58139100	7.22586100	-0.39572400
C	1.79629400	6.72385200	-1.42811100
C	1.29898500	5.42853500	-1.34358600
F	2.62529600	4.41388500	1.86263700
F	3.60505500	6.91152300	1.70492500
F	3.06574500	8.46197700	-0.46677500
F	1.53355800	7.48118100	-2.49170300
F	0.55716300	4.97586000	-2.35662200
C	1.84487600	-2.19651400	-0.46366300
N	0.52050700	-1.88281000	-0.30885300
C	-0.20600000	-3.04624100	-0.35307400
C	0.70565500	-4.13936500	-0.53918000
C	1.96018000	-3.61822100	-0.61756600
O	-0.43213900	0.02463600	1.51000500
H	3.88386200	3.24286900	-0.30878400
H	4.92660600	0.78425900	-0.41017000
H	2.88513800	-4.15878800	-0.77385700
H	0.42112300	-5.18128400	-0.62346900
H	-4.50262300	-3.19691800	-0.08549100
H	-5.53345100	-0.72903900	0.01730300
H	-3.50907000	4.21009500	0.17093300
H	-1.04868600	5.26048200	0.06964700
C	1.02188100	-2.63481300	3.02754800
H	0.70537200	-3.67369400	3.07241300
H	0.26191800	-1.90295800	2.74982300
C	2.29046600	-2.28944400	3.28171100
H	3.00846600	-3.07857000	3.51692100
C	2.84489300	-0.93688900	3.24292600
C	2.02542500	0.20358800	3.24043800
C	4.23545600	-0.74950600	3.20670200
C	2.57429700	1.47596300	3.15901900
H	0.94637100	0.08910300	3.30430500
C	4.78671200	0.52598700	3.13226500
H	4.88677900	-1.62322500	3.23022800

C	3.95780700	1.64528900	3.10000800
H	1.91529900	2.34232100	3.14753400
H	5.86905100	0.64624600	3.10231300
H	4.38381800	2.64530200	3.03462600

$$\Delta E_{\text{solv}} = -4451.96982663$$

$$\Delta G_{\text{solv}} = -4451.49902663$$



¹TS1

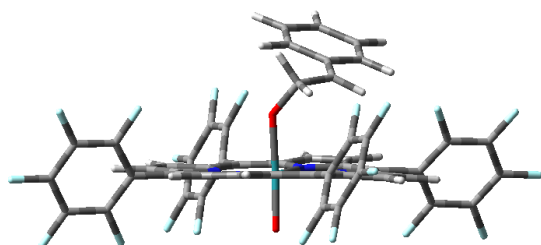
C	-2.83516800	-4.97532300	0.90928200
C	-2.98371700	-4.10688600	-0.17496700
C	-3.90679800	-4.47033800	-1.15801700
C	-4.65243900	-5.64075100	-1.06940000
C	-4.47819400	-6.48481700	0.02230900
C	-3.56443300	-6.15317200	1.01733400
C	-2.18772200	-2.85780300	-0.26231000
C	-2.89485700	-1.64420300	-0.18278200
N	-2.33766200	-0.40381000	-0.22497700
C	-3.33487400	0.51804500	-0.13432800
C	-4.59563100	-0.17434100	-0.04025500
C	-4.32367900	-1.50607300	-0.05453900
Ru	-0.27043300	0.01317500	-0.36284400
O	-0.53408100	0.08504500	-2.09532200
C	-3.16424300	1.91427600	-0.12038400
C	-4.39678400	2.73811400	-0.03677400
C	-4.79506800	3.55825000	-1.09526600
C	-5.94481300	4.33725900	-1.03029200
C	-6.73168000	4.30392100	0.11590000
C	-6.36287700	3.49756900	1.18734300
C	-5.20590300	2.73184200	1.10154000
F	-4.06374100	3.60922300	-2.21076200
F	-6.30133800	5.10747300	-2.05750600
F	-7.83513800	5.04316000	0.18792000
F	-7.11303400	3.47244800	2.28896500
F	-4.87375300	1.97585600	2.15266200
F	-4.08974900	-3.68764000	-2.22417400
F	-5.52295300	-5.96326000	-2.02519900
F	-5.18469300	-7.60781000	0.11479300
F	-3.40267500	-6.95897100	2.06633600
F	-1.97055400	-4.67918600	1.88688500

C	-1.94401800	2.60907000	-0.16228700
N	-0.70015900	2.05195200	-0.24390200
C	0.21854100	3.05666500	-0.21661000
C	-0.47264800	4.31689600	-0.11120000
C	-1.80227200	4.04120000	-0.07727100
C	1.61486200	2.89153300	-0.24697700
C	2.30742700	1.67043000	-0.29717200
N	1.74042300	0.42282300	-0.38388000
C	2.75227500	-0.49841200	-0.46995700
C	4.00718200	0.19310300	-0.40056100
C	3.73469500	1.52342400	-0.30355500
C	2.59162600	-1.88632400	-0.62179900
C	3.82342700	-2.68776900	-0.82321900
C	4.22351600	-3.68544200	0.06980100
C	5.37820500	-4.43500400	-0.11769000
C	6.17460200	-4.19800900	-1.23252000
C	5.80748400	-3.21585800	-2.14584700
C	4.64510300	-2.48215800	-1.93721900
F	3.49274900	-3.94566200	1.16547200
F	5.72822600	-5.37060100	0.76410200
F	7.28278200	-4.90733400	-1.42381200
F	6.56360400	-2.99286600	-3.21934700
F	4.32016000	-1.56131300	-2.84703000
C	2.42859200	4.13423000	-0.26758900
C	3.26397300	4.49789400	0.79002400
C	4.02425800	5.66125200	0.76577300
C	3.95387100	6.50366200	-0.33801400
C	3.12905500	6.17386700	-1.40800400
C	2.38348400	5.00124800	-1.36329800
F	3.35212400	3.71676000	1.87098200
F	4.80965900	5.97815900	1.79579600
F	4.67291600	7.62212000	-0.37019800
F	3.06480700	6.97752500	-2.46864100
F	1.60797200	4.71235500	-2.41056800
C	1.36737400	-2.57818900	-0.60415500
N	0.13794200	-2.00912400	-0.40812800
C	-0.79778000	-3.01182100	-0.40542600
C	-0.12518600	-4.26486000	-0.60673400
C	1.20225800	-3.99724700	-0.74559900
O	-0.37175400	0.01380300	1.47285400
H	4.44841600	2.33549500	-0.23640700
H	4.98280100	-0.27850800	-0.41300700
H	1.99850500	-4.70788000	-0.93047500
H	-0.60963200	-5.23231100	-0.66611600

H	-5.03247400	-2.32264200	0.01229500
H	-5.56833900	0.29748500	0.02965900
H	-2.61905800	4.74703200	0.01549900
H	0.00059300	5.28980300	-0.05149800
C	0.00837700	-1.24222200	2.72760600
H	-0.70693200	-2.01302900	2.44512900
H	-0.32927800	-0.60046600	3.53662500
C	1.36508300	-1.53175500	2.60514100
H	1.65620800	-2.42915700	2.05863700
C	2.41948400	-0.65932100	3.01909200
C	2.16897400	0.63766000	3.52583600
C	3.76608600	-1.07180100	2.89805600
C	3.21316000	1.45852300	3.91442800
H	1.14421700	1.00161000	3.57765000
C	4.80690500	-0.24324800	3.28864700
H	3.97239100	-2.06669000	2.50719100
C	4.53722700	1.02641100	3.79917200
H	3.00113200	2.45694500	4.29116400
H	5.83626000	-0.58518800	3.19250100
H	5.35282700	1.68103600	4.10056000

$\Delta E_{\text{solv}} = -4451.95372916$

$\Delta G_{\text{solv}} = -4451.48111116$



¹B

C	-3.11284600	-4.80463800	0.91109500
C	-3.20075000	-3.93536400	-0.17890600
C	-4.14134800	-4.24470600	-1.16375600
C	-4.96034900	-5.36478000	-1.07227300
C	-4.84470800	-6.21196100	0.02472600
C	-3.91595600	-5.93320800	1.02202100
C	-2.32801100	-2.73886800	-0.27217500
C	-2.95864000	-1.48419100	-0.19170400
N	-2.32922800	-0.27566400	-0.23876000
C	-3.27522800	0.69745700	-0.14174500
C	-4.57095400	0.08074800	-0.03418000
C	-4.37388800	-1.26515700	-0.04971700
Ru	-0.25523000	0.02779600	-0.45143100
O	-0.52566400	-0.02251000	-2.17571800

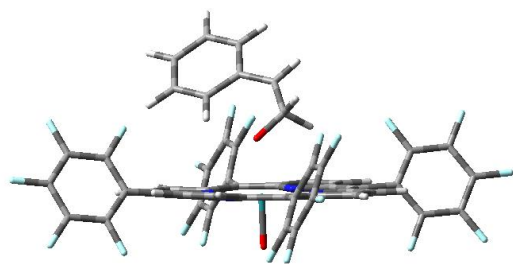
C	-3.02223900	2.08157300	-0.13363600
C	-4.20151500	2.97870400	-0.04206400
C	-4.56250200	3.81362400	-1.10234100
C	-5.66393500	4.65908000	-1.03131500
C	-6.43880400	4.68008900	0.12326500
C	-6.10649800	3.86065400	1.19665900
C	-4.99734800	3.02787500	1.10455000
F	-3.84203500	3.81444200	-2.22600600
F	-5.98645500	5.44133800	-2.06073700
F	-7.49588800	5.48386800	0.20174000
F	-6.84484300	3.88696500	2.30633000
F	-4.69810000	2.26156200	2.15825700
F	-4.27177400	-3.45671500	-2.23352100
F	-5.84696400	-5.63614100	-2.02919600
F	-5.62172000	-7.28718400	0.12091300
F	-3.80943100	-6.74188700	2.07609300
F	-2.23619400	-4.55809800	1.89171100
C	-1.76359500	2.69465700	-0.18645100
N	-0.55254000	2.05822500	-0.29127300
C	0.42418400	3.01499200	-0.25996000
C	-0.19229500	4.30934600	-0.13588500
C	-1.53546500	4.11268200	-0.09152500
C	1.80583900	2.77574100	-0.29481600
C	2.42274500	1.51556000	-0.34477400
N	1.77315200	0.30729000	-0.43520800
C	2.73114700	-0.67750400	-0.48854500
C	4.02455900	-0.06686500	-0.40580300
C	3.83435300	1.28038200	-0.32601200
C	2.49308000	-2.05521300	-0.61326100
C	3.67963600	-2.93076500	-0.77391400
C	4.01879500	-3.90873200	0.16422800
C	5.12772400	-4.73249500	0.01503200
C	5.93903600	-4.58997100	-1.10541700
C	5.63354800	-3.62697500	-2.06108100
C	4.51559000	-2.81820700	-1.88985900
F	3.27092500	-4.07140000	1.26783800
F	5.42068300	-5.64801500	0.93808600
F	7.00427500	-5.37065800	-1.26037000
F	6.40682000	-3.49344700	-3.13733200
F	4.24939900	-1.91602300	-2.83631200
C	2.69009300	3.96910100	-0.30149800
C	3.53448300	4.28179300	0.76554500
C	4.36101500	5.39928500	0.75133800
C	4.35037100	6.24717500	-0.35028600

C	3.51732100	5.96882700	-1.42835400
C	2.70503100	4.84110500	-1.39401800
F	3.56695400	3.49746300	1.84799200
F	5.15324800	5.66787600	1.79018400
F	5.13398700	7.32183900	-0.37248000
F	3.50848100	6.77788500	-2.48684200
F	1.92258700	4.60167300	-2.44862500
C	1.23134600	-2.67533700	-0.60102700
N	0.03928700	-2.02933200	-0.43032400
C	-0.95145000	-2.97798600	-0.41460100
C	-0.35293000	-4.27286800	-0.58354900
C	0.98933300	-4.08618000	-0.71190400
O	-0.31323100	-0.04301300	1.52158900
H	4.59620700	2.04753900	-0.25817300
H	4.96820600	-0.59984000	-0.40040700
H	1.74742300	-4.84407900	-0.86816400
H	-0.89376800	-5.21099000	-0.62641200
H	-5.12607900	-2.04150600	0.02360900
H	-5.51403500	0.60759300	0.04641300
H	-2.30859400	4.86350400	0.01935500
H	0.33939500	5.25135000	-0.07064400
C	-0.24532400	-1.06767400	2.50727400
H	-0.91139600	-1.90421700	2.24278200
H	-0.60220600	-0.63943100	3.45658400
C	1.16689300	-1.48378000	2.54284400
H	1.45002800	-2.40095900	2.02529600
C	2.20312700	-0.65016400	2.99506400
C	1.95234400	0.63132800	3.56371100
C	3.55678500	-1.07223100	2.88335700
C	2.99544500	1.42039600	4.00328900
H	0.92873700	0.99588900	3.61698500
C	4.59183100	-0.27367700	3.33433300
H	3.75916800	-2.04842400	2.44580800
C	4.31961600	0.97766100	3.89247200
H	2.78989800	2.40468300	4.41918900
H	5.62102300	-0.61668000	3.24323700
H	5.13482100	1.61297200	4.23323500

$$\Delta E_{\text{solv}} = -4451.96710749$$

$$\Delta G_{\text{solv}} = -4451.49316249$$

2. Coordinates of all stationary points in Fig. 3



³B

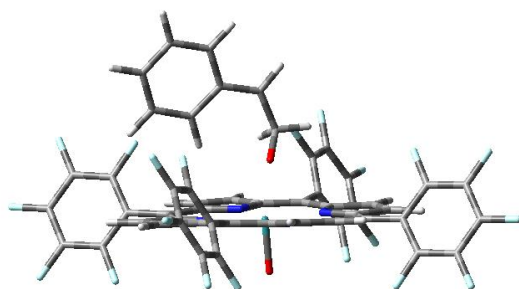
C	-1.65467000	-5.39696700	0.74389400
C	-1.96229100	-4.60404100	-0.36364600
C	-2.75079600	-5.18248800	-1.35987800
C	-3.21391900	-6.49027200	-1.26363700
C	-2.88367500	-7.25527100	-0.15004800
C	-2.09900400	-6.70824600	0.85994300
C	-1.47281100	-3.20654500	-0.45937600
C	-2.43059400	-2.18709800	-0.35115500
N	-2.16948400	-0.84173200	-0.34977200
C	-3.36069500	-0.18745500	-0.19001100
C	-4.41724500	-1.15831700	-0.09762400
C	-3.84442000	-2.38830900	-0.18742000
Ru	-0.32542800	0.04914500	-0.64517000
O	-0.47545300	0.04130200	-2.39838800
C	-3.52624200	1.20451000	-0.10607900
C	-4.90545000	1.70696300	0.11137500
C	-5.55848600	2.48121400	-0.85112300
C	-6.84678900	2.96638500	-0.65649000
C	-7.51790800	2.67501100	0.52604300
C	-6.89650500	1.90657300	1.50452400
C	-5.60588100	1.43746000	1.28962500
F	-4.94438000	2.77479700	-1.99951700
F	-7.44450900	3.69963900	-1.59499600
F	-8.75195500	3.13170600	0.72144100
F	-7.53681000	1.63576200	2.64221400
F	-5.03388100	0.71214000	2.25688200
F	-3.08189500	-4.47558000	-2.44254900
F	-3.96336700	-7.01699100	-2.23122200
F	-3.31911200	-8.50828100	-0.04974600
F	-1.78954000	-7.43837300	1.93160900
F	-0.91231100	-4.89280000	1.73832400
C	-2.50677100	2.16739500	-0.18213700
N	-1.18123200	1.91644100	-0.40551400
C	-0.51585600	3.11058300	-0.34082300
C	-1.46275600	4.15995600	-0.07368600
C	-2.68839300	3.58034600	0.01855700

C	0.86997300	3.28634900	-0.47249000
C	1.81943200	2.27190300	-0.67608200
N	1.55497800	0.93340300	-0.73442000
C	2.74875300	0.27658400	-0.84139200
C	3.81184300	1.24499100	-0.88921800
C	3.23914000	2.47425700	-0.79451100
C	2.92228200	-1.11727700	-0.83476600
C	4.31944000	-1.61534200	-0.88296000
C	4.88868200	-2.28244800	0.20477900
C	6.20197800	-2.73730600	0.18644800
C	6.98538300	-2.52478500	-0.94266000
C	6.44944600	-1.86398600	-2.04285600
C	5.13144600	-1.42289600	-2.00309700
F	4.16677500	-2.50214500	1.30799400
F	6.71582400	-3.36702200	1.24393200
F	8.24483300	-2.95342700	-0.97092400
F	7.19853500	-1.66515000	-3.12714000
F	4.64784400	-0.79461100	-3.07769300
C	1.39619400	4.66434200	-0.31512300
C	2.20433800	5.00076700	0.77413000
C	2.71487300	6.28118300	0.94759200
C	2.41248600	7.26948700	0.01662600
C	1.60657800	6.96935300	-1.07627100
C	1.11244400	5.67874700	-1.23160000
F	2.50376500	4.07577200	1.69535900
F	3.48118600	6.57013200	1.99980900
F	2.89309900	8.50030000	0.17156800
F	1.32270800	7.91582600	-1.97012400
F	0.34780900	5.42243100	-2.29550600
C	1.90528400	-2.08177000	-0.74780700
N	0.56513800	-1.82794700	-0.64565200
C	-0.08411100	-3.03104300	-0.59266000
C	0.88453200	-4.08991200	-0.67569900
C	2.10903200	-3.50527700	-0.76858800
O	-0.00920900	0.07442800	1.40346900
H	3.73748600	3.43657100	-0.80364500
H	4.86778800	1.01612300	-0.96996800
H	3.06901600	-3.99915200	-0.86208800
H	0.65789300	-5.14949100	-0.67613200
H	-4.34075600	-3.35040200	-0.14338100
H	-5.46976900	-0.92991600	0.02043200
H	-3.63365300	4.06739600	0.22671100
H	-1.22043400	5.20939900	0.04330400
C	-0.12825600	-0.99142700	2.23234800

H	-0.34745900	-1.95489800	1.71060200
H	-1.03911600	-0.87591800	2.86969600
C	0.96960200	-1.28726000	3.16937000
H	0.75926200	-2.12026200	3.84615100
C	2.21988500	-0.66304700	3.30697700
C	2.61779000	0.48557100	2.56122500
C	3.16400400	-1.23240700	4.21050000
C	3.90019500	0.99077900	2.69447300
H	1.89180500	0.96016800	1.90799200
C	4.43880200	-0.71907600	4.32760700
H	2.86687100	-2.10385400	4.79357700
C	4.81557100	0.39432000	3.56560400
H	4.18551000	1.87126700	2.12164900
H	5.14995200	-1.17664600	5.01224300
H	5.81905800	0.80454600	3.66542600

$\Delta E_{\text{solv}} = -4451.98848457$

$\Delta G_{\text{solv}} = -4451.51773757$



³TS2

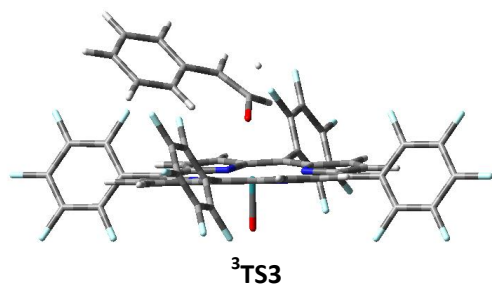
C	-2.26810000	-5.15557300	0.90583800
C	-2.46554100	-4.37318200	-0.23421400
C	-3.30953500	-4.88698800	-1.22038600
C	-3.93190600	-6.12295200	-1.08363000
C	-3.71002200	-6.88009100	0.06188800
C	-2.87337800	-6.39650200	1.06261300
C	-1.80550300	-3.05171700	-0.37293700
C	-2.63548900	-1.91807400	-0.33776000
N	-2.20833300	-0.62437500	-0.39262600
C	-3.30199300	0.18620000	-0.29464300
C	-4.47944400	-0.63572200	-0.19149000
C	-4.06826400	-1.93178100	-0.20558600
Ru	-0.23207800	0.01825100	-0.64053200
O	-0.49351100	0.01739300	-2.37535100
C	-3.28287600	1.59127700	-0.25974900
C	-4.59147100	2.27620700	-0.11183400
C	-5.10236700	3.09244300	-1.12415400
C	-6.32234600	3.74711200	-0.99733400

C	-7.06730100	3.59000500	0.16652700
C	-6.58669200	2.78463700	1.19348500
C	-5.36164900	2.14484900	1.04613300
F	-4.41432100	3.26191200	-2.25537700
F	-6.78441800	4.51578500	-1.98273600
F	-8.23727000	4.20923200	0.29818300
F	-7.29651400	2.63979800	2.31258600
F	-4.92387200	1.38945400	2.05885300
F	-3.53818000	-4.18717000	-2.33419600
F	-4.73025700	-6.58924000	-2.04306400
F	-4.29791600	-8.06512100	0.20166300
F	-2.66675300	-7.11853300	2.16362600
F	-1.47788000	-4.71001800	1.88920600
C	-2.14545900	2.41401700	-0.31647200
N	-0.85550800	1.99774500	-0.48423900
C	-0.04774600	3.09313100	-0.39798700
C	-0.86162000	4.26062300	-0.17981900
C	-2.15353100	3.84356100	-0.13772900
C	1.35490500	3.08143500	-0.47383000
C	2.16300100	1.94676400	-0.63989100
N	1.72670200	0.64802500	-0.69853300
C	2.82979300	-0.15658800	-0.82545400
C	4.00352700	0.66843500	-0.87482900
C	3.59333100	1.96083400	-0.75993000
C	2.82390900	-1.56002900	-0.82832300
C	4.14110200	-2.23680500	-0.91867000
C	4.65959700	-2.95726100	0.16025200
C	5.89275300	-3.59544800	0.09504000
C	6.64448100	-3.51419500	-1.07252700
C	6.15978600	-2.79869100	-2.16236900
C	4.92083300	-2.17346100	-2.07534100
F	3.96593000	-3.04006000	1.30041600
F	6.36322000	-4.27289700	1.14185500
F	7.82717300	-4.11857900	-1.14497500
F	6.88022600	-2.72387000	-3.28080400
F	4.48196600	-1.49530900	-3.13848800
C	2.05286900	4.38172300	-0.32834700
C	2.89110100	4.63203600	0.76215100
C	3.55343600	5.84404100	0.91758900
C	3.37959100	6.84766800	-0.02953800
C	2.54990700	6.63145000	-1.12447800
C	1.90310000	5.40862300	-1.26322200
F	3.07367300	3.69321600	1.69540800
F	4.34478900	6.05431000	1.96955700

F	4.00626600	8.01242900	0.11282800
F	2.38783000	7.59068100	-2.03525200
F	1.12171500	5.23019000	-2.33150700
C	1.69201300	-2.38094800	-0.70112300
N	0.39983500	-1.94468500	-0.57170400
C	-0.40752300	-3.05414500	-0.49007400
C	0.41337400	-4.23040000	-0.56330000
C	1.70244900	-3.81705800	-0.69638500
O	-0.26357600	0.14088400	1.37777200
H	4.21209000	2.85008300	-0.76273400
H	5.02029700	0.30658900	-0.97426800
H	2.58558600	-4.43673300	-0.79708800
H	0.04860200	-5.25024900	-0.53626500
H	-4.68499300	-2.81935700	-0.13055500
H	-5.49627500	-0.26950300	-0.11627000
H	-3.03657400	4.44978500	0.02576000
H	-0.49086300	5.27129700	-0.05915900
C	-0.49765900	-0.89398600	2.27607900
H	-0.11794600	-1.86828200	1.89766300
H	-1.58542300	-1.03368100	2.41811600
C	0.15162400	-0.56708900	3.57580300
H	-0.47658200	-0.49672500	4.46669600
C	1.51621500	-0.24014000	3.72603000
C	2.43879400	-0.31366600	2.64825700
C	2.01517400	0.14873600	4.99664000
C	3.77348200	-0.01419900	2.83856000
H	2.07568900	-0.60036800	1.66446600
C	3.35331400	0.45236900	5.17625700
H	1.32107400	0.20932200	5.83479100
C	4.24038700	0.37720500	4.09905600
H	4.46209900	-0.07398600	1.99616800
H	3.71424100	0.75350400	6.15783500
H	5.29100300	0.62401100	4.23952500

$\Delta E_{\text{solv}} = -4451.98002401$

$\Delta G_{\text{solv}} = -4451.50858301$



C	-0.83944900	-5.45605800	0.91820800
---	-------------	-------------	------------

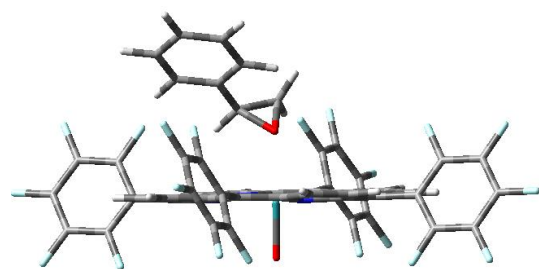
C	-1.26713300	-4.79731300	-0.23638600
C	-1.94544400	-5.56099300	-1.18735000
C	-2.18879400	-6.91798700	-1.00175700
C	-1.74263800	-7.54433300	0.15707800
C	-1.06310200	-6.81120400	1.12447900
C	-1.00198900	-3.34865300	-0.41657200
C	-2.10688900	-2.48449400	-0.35967900
N	-2.04896500	-1.11551500	-0.39132800
C	-3.32976500	-0.64650400	-0.27435500
C	-4.23236700	-1.76293200	-0.18765900
C	-3.47864600	-2.89387100	-0.22290400
Ru	-0.35014700	0.03393600	-0.66504500
O	-0.47571300	0.04082900	-2.42806100
C	-3.69879600	0.70585900	-0.20022400
C	-5.14367200	1.00564300	-0.04252000
C	-5.85603100	1.68636500	-1.03327700
C	-7.20786700	1.98206300	-0.89744400
C	-7.88358500	1.59116400	0.25329700
C	-7.20343400	0.91403700	1.25949900
C	-5.85054800	0.63587900	1.10409600
F	-5.23946800	2.07298900	-2.15210800
F	-7.86098100	2.62898400	-1.86243700
F	-9.17831000	1.86550300	0.39238500
F	-7.84869400	0.54799600	2.36791100
F	-5.22510600	-0.00154900	2.10002000
F	-2.38243400	-4.99142200	-2.31244400
F	-2.83729800	-7.62304200	-1.92782200
F	-1.96676200	-8.84274900	0.34196200
F	-0.64306800	-7.40880000	2.24052700
F	-0.19334700	-4.77172300	1.87534300
C	-2.82443000	1.80439600	-0.21743800
N	-1.46880400	1.74651900	-0.38932400
C	-0.98191900	3.01911900	-0.25576600
C	-2.07631800	3.91622400	0.00622700
C	-3.21168600	3.17020300	0.01832900
C	0.36949000	3.39013400	-0.33029400
C	1.45675400	2.53119100	-0.55831800
N	1.38497300	1.17196900	-0.68491900
C	2.66064400	0.70199700	-0.83222200
C	3.57417700	1.81373300	-0.82689300
C	2.83251000	2.94072900	-0.65721600
C	3.03539700	-0.65142400	-0.88931900
C	4.48550400	-0.93271800	-1.03281400
C	5.21948500	-1.56314600	-0.02536200

C	6.58173800	-1.81078700	-0.14519100
C	7.25117000	-1.41885900	-1.29882600
C	6.55220900	-0.78767100	-2.32198400
C	5.18822400	-0.55680600	-2.18121200
F	4.61527800	-1.95077600	1.10435000
F	7.25046400	-2.41136300	0.84125900
F	8.55641900	-1.64689600	-1.42311600
F	7.19182600	-0.41600400	-3.43049400
F	4.55025000	0.04759700	-3.18556900
C	0.69592000	4.81679700	-0.08877300
C	1.43377400	5.19993200	1.03449800
C	1.75718100	6.52679200	1.28951300
C	1.33308900	7.51538400	0.40768600
C	0.59411200	7.16891500	-0.71808500
C	0.28918600	5.83303100	-0.95571400
F	1.84912600	4.27443300	1.91052000
F	2.46042900	6.85852800	2.37347400
F	1.63384100	8.79053500	0.64061200
F	0.19314000	8.11691000	-1.56446800
F	-0.41256100	5.53521700	-2.05153100
C	2.17238800	-1.75380400	-0.78641200
N	0.81023100	-1.69052500	-0.64684500
C	0.34466000	-2.97404400	-0.56267500
C	1.45375900	-3.88481600	-0.65119200
C	2.57779300	-3.13353600	-0.79879600
O	-0.06684600	0.07050500	1.52918600
H	3.18787800	3.96364100	-0.61048200
H	4.65154100	1.74247900	-0.92099100
H	3.59490400	-3.48771200	-0.91691500
H	1.38112400	-4.96601900	-0.62937600
H	-3.82624400	-3.91851400	-0.16525300
H	-5.31032900	-1.69334900	-0.10324100
H	-4.22382900	3.51239600	0.19947900
H	-1.98889000	4.98340600	0.17127400
C	0.08672200	-1.05405500	2.16507500
H	-0.52670500	-1.93142600	1.86879200
H	-0.19426600	-0.95187600	3.31432900
C	1.29877500	-1.43568900	2.86249100
H	1.24555800	-2.41745300	3.34068600
C	2.44476400	-0.63655800	3.12403600
C	2.64223000	0.63558200	2.53050500
C	3.46912500	-1.18041100	3.93525100
C	3.83716500	1.30947300	2.73063600
H	1.84475200	1.06849400	1.93226500

C	4.65811100	-0.49992100	4.12144100
H	3.31807000	-2.15826200	4.39187100
C	4.84387600	0.74677200	3.51713100
H	3.98131900	2.28443800	2.26949000
H	5.44471200	-0.93259400	4.73541500
H	5.77804300	1.28507400	3.66813000

$$\Delta E_{\text{solv}} = -4451.98634274$$

$$\Delta G_{\text{solv}} = -4451.51616774$$



³E-C

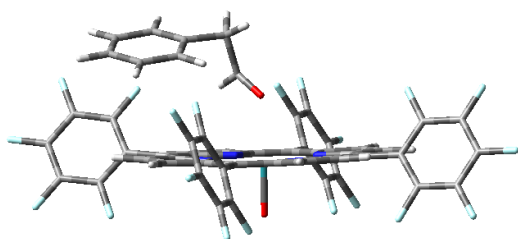
C	-4.03740700	-4.02740300	1.02355500
C	-3.94786900	-3.23131700	-0.12029100
C	-4.94133500	-3.39575100	-1.08750300
C	-5.97790700	-4.30900200	-0.92816900
C	-6.03419700	-5.09036500	0.22094000
C	-5.05910900	-4.95166900	1.20308100
C	-2.84249600	-2.25522500	-0.28470400
C	-3.18205900	-0.89407400	-0.25415700
N	-2.30023300	0.15210900	-0.34679900
C	-3.02835500	1.31017400	-0.25711700
C	-4.42022200	0.98080800	-0.11427400
C	-4.51347200	-0.37526900	-0.09969700
Ru	-0.26500900	0.01300100	-0.69113100
O	-0.40427800	0.01645300	-2.44607000
C	-2.49888000	2.60946800	-0.26520100
C	-3.45999500	3.73236400	-0.12888800
C	-3.66430200	4.64527600	-1.16652000
C	-4.55667700	5.70529100	-1.04954200
C	-5.27436800	5.87048000	0.13012300
C	-5.09258400	4.98005100	1.18286900
C	-4.19100600	3.93153500	1.04434600
F	-2.99302400	4.51304400	-2.31238400
F	-4.73318600	6.55746400	-2.05857600
F	-6.13212300	6.87986700	0.25305100
F	-5.77330600	5.14489800	2.31740700
F	-4.03026300	3.10216000	2.08171700
F	-4.91343900	-2.66494300	-2.20411100

F	-6.91061600	-4.44661000	-1.86957600
F	-7.02036900	-5.96832500	0.38179200
F	-5.11747600	-5.69475400	2.30815300
F	-3.11993400	-3.90756900	1.99217200
C	-1.13943700	2.94722300	-0.34881400
N	-0.10275100	2.06488800	-0.49876800
C	1.06013600	2.78853200	-0.45791100
C	0.74266000	4.18004500	-0.28178800
C	-0.61119300	4.27848500	-0.22013100
C	2.35854400	2.26085200	-0.53152400
C	2.69340600	0.90206300	-0.63431800
N	1.80212100	-0.13869000	-0.66717500
C	2.53104600	-1.29795200	-0.74467800
C	3.93112300	-0.97474100	-0.76729100
C	4.03058000	0.37949500	-0.70359000
C	2.00174500	-2.59719400	-0.75019300
C	2.97483600	-3.71700800	-0.79697400
C	3.19682200	-4.52148200	0.32178800
C	4.10411500	-5.57352300	0.30863800
C	4.82499800	-5.83696700	-0.85179800
C	4.63363900	-5.04941600	-1.98223900
C	3.71568400	-4.00492300	-1.94436600
F	2.52789300	-4.27889600	1.45871900
F	4.29527800	-6.32148800	1.39522200
F	5.69940200	-6.83910000	-0.87783800
F	5.32482400	-5.30394200	-3.09230400
F	3.55452400	-3.26711500	-3.04423100
C	3.48302200	3.22698600	-0.46760100
C	4.37443100	3.23726300	0.60850600
C	5.43280600	4.13549600	0.67941400
C	5.61598900	5.06210000	-0.34110700
C	4.74365400	5.08174200	-1.42381700
C	3.69602700	4.16920000	-1.47689300
F	4.22260500	2.36827800	1.61202400
F	6.26533000	4.12146600	1.72124500
F	6.62399800	5.92843200	-0.28118900
F	4.92239300	5.96689200	-2.40385000
F	2.88125900	4.21138800	-2.53369200
C	0.64474500	-2.93943800	-0.64329000
N	-0.39404200	-2.05024200	-0.52121500
C	-1.54899100	-2.78377200	-0.41953300
C	-1.22496200	-4.18199200	-0.47486600
C	0.12493700	-4.27766400	-0.61551900
O	-0.02762400	0.07923400	1.64618800

H	4.93667000	0.97324600	-0.70380600
H	4.74025100	-1.69417300	-0.81600200
H	0.71632100	-5.18162300	-0.70282600
H	-1.94166600	-4.99339900	-0.42769000
H	-5.41093900	-0.97270300	0.00800400
H	-5.22955400	1.69629500	-0.03228700
H	-1.20128300	5.17540600	-0.07341300
H	1.46618300	4.98199700	-0.19671700
C	-0.55687100	-0.82816800	2.61724800
H	-1.22872700	-1.59168300	2.21808500
H	-0.87646100	-0.33918200	3.53810400
C	0.86673100	-0.87401200	2.27534200
H	1.16608600	-1.68079700	1.60211300
C	1.95366800	-0.29337000	3.08999200
C	1.78266900	0.90872500	3.78339400
C	3.18258600	-0.95388200	3.15115800
C	2.82263000	1.42810800	4.54451800
H	0.83727800	1.44430000	3.70237600
C	4.22270000	-0.43263100	3.91534700
H	3.31835400	-1.88151100	2.59406900
C	4.04243400	0.75627200	4.61680100
H	2.68488000	2.36654100	5.07843100
H	5.17665400	-0.95389600	3.95750600
H	4.85653100	1.16789100	5.21025300

$\Delta E_{\text{solv}} = -4452.01960429$

$\Delta G_{\text{solv}} = -4451.54664829$



³E-D

C	-2.49188500	-5.24510100	0.65687200
C	-2.68716600	-4.32866900	-0.37869300
C	-3.57726400	-4.69607000	-1.39066200
C	-4.24538000	-5.91555500	-1.37655200
C	-4.02460600	-6.80698500	-0.33219100
C	-3.14282300	-6.47253300	0.68992600
C	-1.98422100	-3.02155500	-0.39715400
C	-2.77402600	-1.87255200	-0.23681600
N	-2.31596700	-0.58100700	-0.23057800
C	-3.39822300	0.23719200	-0.03866000

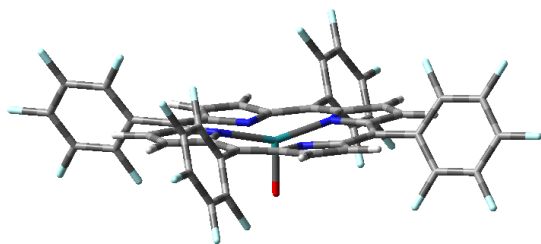
C	-4.58253100	-0.56929300	0.07849800
C	-4.19755400	-1.86776500	-0.03557500
Ru	-0.36772700	0.02435500	-0.57019200
O	-0.53721200	0.09231000	-2.32158200
C	-3.36029900	1.63766000	0.04173800
C	-4.65145100	2.33626700	0.26085000
C	-5.19940500	3.17562500	-0.71223500
C	-6.40588200	3.83898200	-0.51863100
C	-7.10052500	3.66556200	0.67360800
C	-6.58287400	2.83574500	1.66227200
C	-5.37131100	2.18894000	1.44861200
F	-4.56182400	3.35984800	-1.87044000
F	-6.90371800	4.63095600	-1.46777400
F	-8.25773600	4.29251300	0.86896700
F	-7.24479200	2.67373900	2.80828000
F	-4.89723500	1.40780300	2.42494500
F	-3.80719700	-3.86627200	-2.41063400
F	-5.08713200	-6.23877600	-2.35779200
F	-4.65656400	-7.97746700	-0.31018800
F	-2.93717300	-7.32363000	1.69549100
F	-1.65892900	-4.94977400	1.66205300
C	-2.21260400	2.43956300	-0.05251500
N	-0.93791600	1.98772200	-0.26746900
C	-0.11036000	3.07870100	-0.26617600
C	-0.89287600	4.26347300	-0.03802600
C	-2.18671900	3.86950900	0.09661000
C	1.28445600	3.05096700	-0.41923600
C	2.08152600	1.90298800	-0.54703500
N	1.62221800	0.61179400	-0.57083600
C	2.71459600	-0.21170600	-0.66149000
C	3.90616800	0.59237900	-0.68913000
C	3.51530800	1.89319500	-0.63893400
C	2.67685500	-1.61564200	-0.72044400
C	3.98362600	-2.31692400	-0.76355300
C	4.40072900	-3.12887300	0.29404000
C	5.65132700	-3.73246000	0.31692000
C	6.51794300	-3.55416000	-0.75555800
C	6.12587000	-2.77234000	-1.83693500
C	4.87313400	-2.16841300	-1.83083100
F	3.59263000	-3.33699200	1.34146500
F	6.02677200	-4.46773900	1.36569100
F	7.71762700	-4.12906100	-0.74747200
F	6.95129500	-2.61057200	-2.87049900
F	4.53467300	-1.42043300	-2.88360100

C	1. 97903000	4. 36343500	-0. 44328300
C	2. 84179300	4. 76694400	0. 57692300
C	3. 49878400	5. 99110600	0. 55256300
C	3. 29002100	6. 85795100	-0. 51450400
C	2. 43112800	6. 49197500	-1. 54514600
C	1. 79090600	5. 25825900	-1. 50016300
F	3. 05788600	3. 96557000	1. 63066900
F	4. 31551300	6. 34211200	1. 54664600
F	3. 91022200	8. 03421400	-0. 54828300
F	2. 23526100	7. 32049100	-2. 56972300
F	0. 97836100	4. 93706900	-2. 50822000
C	1. 52287300	-2. 41507100	-0. 69693200
N	0. 23686400	-1. 95833200	-0. 55307200
C	-0. 58918600	-3. 05303000	-0. 54829700
C	0. 20381700	-4. 24025400	-0. 70806000
C	1. 50330000	-3. 84779200	-0. 79638100
O	-0. 05374400	0. 02356600	1. 75379000
H	4. 15019300	2. 77147800	-0. 64894500
H	4. 92027800	0. 21353100	-0. 72896000
H	2. 37444200	-4. 47798800	-0. 93141500
H	-0. 18344400	-5. 25107100	-0. 75703000
H	-4. 82642800	-2. 74836100	0. 01967400
H	-5. 58646800	-0. 19109300	0. 22955800
H	-3. 04881400	4. 49455800	0. 29704500
H	-0. 49892300	5. 27065000	0. 03190100
C	0. 66392700	-0. 77246000	2. 34491500
H	0. 99736100	-1. 70592000	1. 84116200
H	0. 75381400	0. 35616300	4. 14860300
C	1. 24294300	-0. 51325200	3. 69720300
H	1. 09406300	-1. 39052000	4. 33981600
C	2. 71862200	-0. 28271100	3. 45282000
C	3. 16122800	0. 96250200	2. 99487200
C	3. 63363900	-1. 33033100	3. 57467100
C	4. 50567500	1. 16319300	2. 69994000
H	2. 44564500	1. 77422500	2. 86359800
C	4. 97548000	-1. 13502400	3. 26119300
H	3. 29027000	-2. 30972300	3. 90657400
C	5. 41455800	0. 11415700	2. 82918900
H	4. 83782600	2. 13918400	2. 35248300
H	5. 67475900	-1. 96592500	3. 34938700
H	6. 46468200	0. 27004300	2. 58815400

$$\Delta E_{\text{solv}} = - 4452.04851628$$

$$\Delta G_{\text{solv}} = - 4451.57619928$$

3. Coordinates of all stationary points in Fig. 5



¹E

Ru	0.00138600	-0.00319200	-0.37743100
N	0.51142400	1.92221200	0.06666000
C	-0.35303500	3.00991600	0.05080600
C	0.40412300	4.20850500	0.04530800
C	1.72709700	3.86135300	0.03405900
C	1.79817500	2.44534500	0.03140600
C	-1.75540700	2.96024700	-0.00872200
C	-2.48825400	4.24797100	0.03175400
C	-2.43035500	5.09289600	1.14342600
C	-3.12019400	6.29857600	1.18969900
C	-3.90166500	6.68330900	0.10530200
C	-3.98586800	5.86285300	-1.01448100
C	-3.28225200	4.66406600	-1.04064700
F	-1.69974700	4.74754100	2.20792500
F	-3.04756800	7.08035900	2.26639000
F	-4.56834300	7.83327200	0.14006300
F	-4.73238100	6.23320500	-2.05383900
F	-3.38068700	3.90274700	-2.13269500
C	2.99403600	1.71418200	-0.05959300
C	3.07683200	0.32932900	-0.14287000
N	2.00003100	-0.52477500	-0.19241500
C	2.51862600	-1.79754300	-0.12405100
C	3.95802100	-1.73805300	-0.09554000
C	4.30095100	-0.42926100	-0.09776400
C	1.76534200	-2.95835900	-0.00514300
C	0.36780500	-3.00519900	0.11521600
N	-0.49804800	-1.91869500	0.10767300
C	-1.78368000	-2.44281700	0.14945900
C	-1.70901000	-3.85647100	0.23255200
C	-0.38550600	-4.20212600	0.21891800
C	-2.98178500	-1.71395000	0.07647300
C	-4.25204600	-2.47321100	0.16263300
C	-4.60969900	-3.18040500	1.31337400
C	-5.80085100	-3.89096700	1.40211300
C	-6.67676300	-3.89792300	0.32174500
C	-6.35444500	-3.19823600	-0.83613300

C	-5.15398700	-2.50030200	-0.90449600
F	-3.79768000	-3.18292300	2.37522800
F	-6.11261900	-4.55407600	2.51518100
F	-7.82099500	-4.57140900	0.39620300
F	-7.19215500	-3.20734300	-1.87175500
F	-4.87378100	-1.84382500	-2.03235300
C	4.26418100	2.47806900	-0.04400300
C	4.65366300	3.23032200	1.06741100
C	5.84212600	3.95035200	1.09075800
C	6.68245100	3.92213800	-0.01718900
C	6.32756700	3.17846200	-1.13747100
C	5.13063500	2.47129200	-1.14049300
F	3.87602900	3.26895700	2.15349100
F	4.81800900	1.77280800	-2.23451100
F	7.13044200	3.15513600	-2.20026700
F	7.82397600	4.60406200	-0.00491600
F	6.18552700	4.65664100	2.16718900
O	-0.01155900	-0.01666100	-2.11352100
N	-1.99480800	0.52178400	-0.15875600
C	-3.06768200	-0.33172600	-0.04256200
C	-4.28796200	0.42731000	0.06076300
C	-3.94482400	1.73583800	0.03932400
C	-2.51010100	1.79495400	-0.07811300
C	2.49255300	-4.25253500	0.03306200
C	2.41633700	-5.16066800	-1.02490100
C	3.09186400	-6.37562800	-1.00064300
C	3.87295900	-6.70371600	0.10247300
C	3.97014000	-5.82004100	1.17198800
C	3.27943000	-4.61442800	1.12781500
F	1.67443400	-4.87303200	-2.09703600
F	3.00186000	-7.22214900	-2.02532700
F	4.52619800	-7.86162800	0.13425700
F	4.71553600	-6.13683500	2.23014300
F	3.38789400	-3.78816100	2.17294800
H	-5.27611700	0.00130000	0.18682300
H	-4.59622400	2.59517800	0.14426400
H	-0.01308100	5.20741500	0.01293700
H	2.58045200	4.52682200	-0.00965200
H	5.29501800	-0.00311900	-0.03502500
H	4.61624000	-2.59670600	-0.04409100
H	0.03389200	-5.19999600	0.25534100
H	-2.56165500	-4.52328700	0.26741500

$$\Delta E_{\text{solv}} = -4067.13727936$$

$$\Delta G_{\text{solv}} = -4066.79350336$$

³E

Ru	0.00239100	0.00005600	-0.23353600
N	-0.06932700	2.05304600	0.00805900
C	-1.20308300	2.83083700	-0.00226800
C	-0.82773500	4.21436400	-0.05209100
C	0.53088000	4.26311700	-0.06770000
C	1.00541400	2.90987600	-0.02806200
C	-2.51953100	2.35268000	0.03560700
C	-3.60989600	3.35916800	0.04172000
C	-3.78630200	4.24232400	1.10950500
C	-4.80557400	5.18737500	1.12379500
C	-5.68752800	5.25988400	0.05068200
C	-5.54264300	4.39154800	-1.02622500
C	-4.51182600	3.45859700	-1.02075400
F	-2.96293300	4.19014600	2.16125500
F	-4.94855500	6.01428700	2.15897400
F	-6.66805300	6.15826600	0.05473900
F	-6.38512400	4.46509200	-2.05560000
F	-4.39677000	2.64354500	-2.07171200
C	2.35328300	2.52665200	-0.02703800
C	2.82998000	1.20953900	0.01037600
N	2.05334700	0.07519000	0.00621500
C	2.91131400	-0.99902000	0.03409700
C	4.26442400	-0.52300300	0.06784900
C	4.21401800	0.83549200	0.06159100
C	2.52929300	-2.34718800	0.03282400
C	1.21207100	-2.82482800	0.04281900
N	0.07784300	-2.04779600	0.03522200
C	-0.99658800	-2.90549300	0.07192700
C	-0.52102500	-4.25857900	0.10106000
C	0.83758900	-4.20874800	0.09136900
C	-2.34396500	-2.52193600	0.10277400
C	-3.35885900	-3.60377900	0.15212900
C	-3.47294300	-4.45155900	1.25622900
C	-4.42057400	-5.46690700	1.31101400
C	-5.29271700	-5.64833000	0.24284000
C	-5.20977800	-4.81724300	-0.86930700
C	-4.24954700	-3.81226300	-0.90390700
F	-2.65706500	-4.29705600	2.30412300
F	-4.50592900	-6.25839000	2.37976900
F	-6.20552200	-6.61446100	0.28567700
F	-6.04346200	-4.99307400	-1.89335300
F	-4.19252000	-3.03405900	-1.98690900

C	3.36655800	3.61094200	-0.05388400
C	3.51567300	4.49866000	1.01413500
C	4.45949100	5.51910700	0.99801600
C	5.29132000	5.66540600	-0.10719000
C	5.17165000	4.79502700	-1.18557300
C	4.21586100	3.78593400	-1.14917800
F	2.73763800	4.37906000	2.09438300
F	4.12206900	2.97059500	-2.20237100
F	5.96639200	4.93791600	-2.24529700
F	6.20057800	6.63558900	-0.13225500
F	4.57860800	6.34884800	2.03393600
O	-0.00462300	-0.00467600	-1.98568300
N	-2.04383700	-0.07110500	0.03765300
C	-2.81926400	-1.20384400	0.11264400
C	-4.19814200	-0.82667000	0.23317300
C	-4.24713200	0.53196100	0.21588300
C	-2.89889700	1.00441800	0.08473900
C	3.61418100	-3.36052600	0.04110200
C	3.82366400	-4.20974900	-1.04798700
C	4.83255600	-5.16656200	-1.05189100
C	5.66760100	-5.28706300	0.05396500
C	5.48599200	-4.45547200	1.15405100
C	4.46602500	-3.51124500	1.13738400
F	3.04114100	-4.11617100	-2.12574400
F	5.00811400	-5.96156700	-2.10642800
F	6.63763000	-6.19682200	0.06017900
F	6.28220000	-4.57502300	2.21598300
F	4.31268900	-2.73247800	2.21332400
H	-5.02777400	-1.51527800	0.33974100
H	-5.12412000	1.16194100	0.30496500
H	-1.51753200	5.04930500	-0.07686900
H	1.15754000	5.14568600	-0.11019600
H	5.04782200	1.52624000	0.09854400
H	5.14780800	-1.14911900	0.09746700
H	1.52761600	-5.04313800	0.12722700
H	-1.14764700	-5.14160300	0.13260100

$\Delta E_{\text{solv}} = -4067.16383818$ $\Delta G_{\text{solv}} = -4066.82097118$

^5E

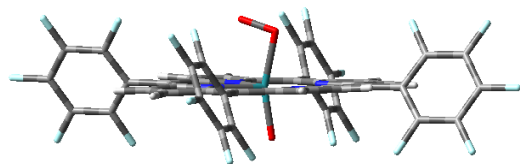
0 5

Ru	0.00270100	0.00218700	-0.19157000
N	-0.22744000	2.06812600	0.05766300
C	-1.41608300	2.75582100	0.02971600

C	-1.14752800	4.16046800	-0.10154400
C	0.20309300	4.30913500	-0.14952500
C	0.77806700	2.99853000	-0.04346100
C	-2.68837800	2.17633500	0.10207300
C	-3.85209900	3.08653100	0.10796500
C	-4.04930000	4.02087500	1.13056200
C	-5.14729000	4.87206300	1.15015300
C	-6.08838500	4.80115700	0.12851900
C	-5.92418300	3.88223000	-0.90326800
C	-4.81870100	3.04079900	-0.90373400
F	-3.17767300	4.10214700	2.14026100
F	-5.31050900	5.74362300	2.14454600
F	-7.14212300	5.61138600	0.13705000
F	-6.81940700	3.82487700	-1.88775700
F	-4.68217100	2.18782300	-1.91959800
C	2.14923400	2.71137100	-0.04073400
C	2.74273900	1.42052300	0.05437100
N	2.04996100	0.22908200	0.05520700
C	2.98893300	-0.77020900	0.13341600
C	4.28446700	-0.20568700	0.20297300
C	4.12954100	1.16413200	0.16079400
C	2.69697600	-2.17003200	0.09312100
C	1.42404100	-2.74955300	0.03285800
N	0.23520000	-2.06221700	0.03680300
C	-0.77133400	-2.99660300	0.02198600
C	-0.19670000	-4.31117700	-0.01265100
C	1.15435700	-4.15991700	0.00978100
C	-2.14167300	-2.70952700	0.07487100
C	-3.07675300	-3.85600000	0.08352500
C	-3.09574700	-4.78260100	1.13043200
C	-3.98017200	-5.85417000	1.14978300
C	-4.88240300	-6.01722400	0.10388100
C	-4.89378800	-5.10987700	-0.95075900
C	-4.00073900	-4.04524600	-0.94993200
F	-2.25874500	-4.64377600	2.16334600
F	-3.97781900	-6.71645900	2.16548300
F	-5.73243200	-7.03907800	0.11143400
F	-5.75221600	-5.27225800	-1.95583700
F	-4.02865000	-3.20222700	-1.98238700
C	3.08055100	3.85806800	-0.12142100
C	3.13778800	4.82869700	0.88354000
C	4.01729500	5.90277100	0.82114900
C	4.87375100	6.02496000	-0.26818000
C	4.84402900	5.07502700	-1.28450500

C	3.95665100	4.00886200	-1.20182700
F	2.34270900	4.73134500	1.95312300
F	3.94237600	3.12591400	-2.20111900
F	5.65723900	5.19890500	-2.33204200
F	5.71811800	7.04913000	-0.33918800
F	4.05254400	6.80710200	1.79882400
O	0.00439400	0.01893900	-1.94249600
N	-2.04135000	-0.22526200	0.06865800
C	-2.73051300	-1.41580700	0.15530900
C	-4.10565900	-1.15560400	0.35965700
C	-4.25735300	0.21581000	0.38024600
C	-2.97398100	0.77590400	0.18280200
C	3.85664900	-3.08843800	0.11417400
C	4.16010600	-3.90622700	-0.97861500
C	5.25264100	-4.76542200	-0.97381000
C	6.07651800	-4.82124300	0.14542900
C	5.80189500	-4.02095300	1.24988100
C	4.70350800	-3.17086200	1.22365500
F	3.39647600	-3.86868600	-2.07287800
F	5.52030900	-5.52636800	-2.03378100
F	7.12336900	-5.64042100	0.16170900
F	6.58376500	-4.08460500	2.32668000
F	4.45622700	-2.43048400	2.30757700
H	-4.87730200	-1.90369200	0.49581100
H	-5.17353600	0.77315500	0.53347500
H	-1.89799800	4.93932100	-0.16112200
H	0.76001600	5.23226700	-0.25447800
H	4.90929000	1.91441600	0.21124300
H	5.21414100	-0.75696300	0.26808700
H	1.90381200	-4.94191100	0.02184400
H	-0.75389800	-5.23958800	-0.03910500

$$\Delta E_{\text{solv}} = -4067.09778271 \quad \Delta G_{\text{solv}} = -4066.76270671$$



¹F

O	-0.04002500	-0.34314100	1.85194300
Ru	0.00094400	0.02744100	-0.10552300
N	-1.52810700	1.38491700	-0.09591800
C	-2.87389900	1.11513900	-0.12307200

C	-3.58414500	2.35756200	-0.20310600
C	-2.66025300	3.35920300	-0.20350700
C	-1.36686000	2.74869300	-0.12814900
C	-3.46495600	-0.15738100	-0.07304900
C	-4.94701100	-0.21599800	-0.07428100
C	-5.70040900	0.30906600	0.97906200
C	-7.08934700	0.25647200	0.98859500
C	-7.76036000	-0.34098900	-0.07315600
C	-7.03998700	-0.87692400	-1.13551800
C	-5.65164700	-0.80700600	-1.12643100
F	-5.08688300	0.87929900	2.01947300
F	-7.77912900	0.76444000	2.00877300
F	-9.08869200	-0.39927200	-0.07200400
F	-7.68279300	-1.44342500	-2.15560900
F	-4.99018100	-1.32305100	-2.16536200
C	-0.14161700	3.43514500	-0.10963200
C	1.13734900	2.85611100	-0.08828400
N	1.41222100	1.51085300	-0.09612100
C	2.77576300	1.35574600	-0.07708000
C	3.38105700	2.65590600	-0.07105800
C	2.37623800	3.57545400	-0.06586200
C	3.46973800	0.13569600	-0.05915800
C	2.88681200	-1.14176700	-0.02706600
N	1.54892400	-1.39923900	0.00464600
C	1.37593400	-2.75272400	0.03137200
C	2.67255000	-3.38156300	0.02320900
C	3.60168500	-2.39094300	-0.00526400
C	0.14622400	-3.43369900	0.06815600
C	0.20850000	-4.91603400	0.12634100
C	0.73625300	-5.58190800	1.23527600
C	0.80235100	-6.96904500	1.29857300
C	0.32644100	-7.72708000	0.23391300
C	-0.20807800	-7.09481900	-0.88367300
C	-0.25876800	-5.70629600	-0.92680000
F	1.19514000	-4.88291400	2.27708000
F	1.30867700	-7.57503300	2.37177700
F	0.38219500	-9.05469900	0.28390500
F	-0.65853600	-7.82124500	-1.90548300
F	-0.77056700	-5.12993000	-2.01704100
C	-0.20709400	4.91788900	-0.11829200
C	-0.75183000	5.62906800	0.95405500
C	-0.82285900	7.01751500	0.95623100
C	-0.33477000	7.73102400	-0.13345300
C	0.21599500	7.05299500	-1.21590200

C	0.26999300	5.66416900	-1.19868800
F	-1.22353800	4.97462200	2.01763500
F	0.79613800	5.04326900	-2.25836700
F	0.67842700	7.73547500	-2.26243600
F	-0.39478800	9.05926400	-0.14097900
F	-1.34596600	7.66667900	1.99511800
O	0.02840000	-0.28775800	-1.79928000
N	-1.42336000	-1.52760000	-0.02623600
C	-1.13716100	-2.85861100	0.05077000
C	-2.37585100	-3.59066300	0.13522900
C	-3.38502000	-2.68196400	0.09677400
C	-2.77793400	-1.38107900	-0.01107200
C	4.95250100	0.19967500	-0.06587400
C	5.69567500	-0.26966800	-1.15162800
C	7.08497200	-0.22470900	-1.16751100
C	7.76637000	0.30735000	-0.07787900
C	7.05572300	0.78556700	1.01800300
C	5.66699200	0.72328500	1.01424600
F	5.07133200	-0.78051000	-2.21603800
F	7.76479300	-0.67902400	-2.21922400
F	9.09508300	0.35868600	-0.08397000
F	7.70769000	1.29030300	2.06446400
F	5.01473600	1.18346700	2.08546100
H	-2.46205400	-4.66665200	0.22681400
H	-4.44968100	-2.87495600	0.15060700
H	-4.66120400	2.45850200	-0.26079800
H	-2.84737900	4.42459900	-0.26182500
H	2.47371800	4.65400200	-0.04364500
H	4.44684300	2.84928000	-0.06763600
H	4.67968300	-2.49724600	-0.00769600
H	2.85047900	-4.45004600	0.03150800
O	-0.04706200	0.90437600	2.20163500

$\Delta E_{\text{solv}} = -4218.32516742$ $\Delta G_{\text{solv}} = -4217.97761842$

³F

O	0.16955800	-0.61164500	2.06308200
Ru	0.00199400	0.00163400	-0.05433700
N	-1.97915400	-0.58791400	0.02582200
C	-2.43128400	-1.88043200	-0.02153100
C	-3.86670000	-1.86253700	-0.09237600
C	-4.25596400	-0.55992900	-0.10601200
C	-3.06609000	0.24377800	-0.04358700
C	-1.63521600	-3.03878600	-0.04215300

C	-2.34717300	-4.34022700	-0.03851000
C	-3.13845100	-4.73509000	1.04364600
C	-3.81396600	-5.94973700	1.05847600
C	-3.70093800	-6.80985800	-0.02870100
C	-2.91856900	-6.44886000	-1.12046700
C	-2.25682300	-5.22632300	-1.11548000
F	-3.25946100	-3.93690400	2.10810800
F	-4.55902000	-6.29859100	2.10649300
F	-4.34032900	-7.97565900	-0.02462900
F	-2.81716400	-7.27025600	-2.16441300
F	-1.52172900	-4.90637200	-2.18355500
C	-3.03523700	1.64787600	-0.09672300
C	-1.88473100	2.45581500	-0.12502000
N	-0.59673200	2.00667300	-0.11254700
C	0.23582800	3.08767600	-0.09961500
C	-0.56442400	4.28262200	-0.13382500
C	-1.86807900	3.89427100	-0.14102200
C	1.63930300	3.04129200	-0.03761900
C	2.43452600	1.88448100	0.02154900
N	1.98082400	0.59164600	0.04398700
C	3.06960500	-0.23997300	0.04629400
C	4.26095400	0.56415700	0.05604100
C	3.87150400	1.86681300	0.04896100
C	3.03923900	-1.64486800	0.02006300
C	4.34618100	-2.34567900	0.06606100
C	5.18217300	-2.25903000	1.18237700
C	6.40710600	-2.91365800	1.23839600
C	6.82097400	-3.68659300	0.15868900
C	6.01087800	-3.79690600	-0.96648500
C	4.79271200	-3.12800000	-1.00221300
F	4.80986800	-1.53287700	2.24056700
F	7.18040000	-2.81459100	2.31899400
F	7.98936700	-4.31978800	0.20230200
F	6.40981900	-4.53405400	-2.00202000
F	4.04221100	-3.24804600	-2.10026400
C	-4.34420600	2.34530900	-0.13471700
C	-5.23705800	2.28005600	0.93829700
C	-6.46631700	2.92846400	0.91411100
C	-6.82731700	3.67229700	-0.20427100
C	-5.96077500	3.75929100	-1.28863200
C	-4.73951700	3.09680900	-1.24450000
F	-4.91740800	1.58074400	2.03082700
F	-3.93576200	3.19184600	-2.30704600
F	-6.30961000	4.46711700	-2.36209300

F	-7.99940400	4.29936500	-0.23630300
F	-7.29456000	2.85033300	1.95468700
O	0.00470900	0.00037800	-1.78178500
N	0.60261100	-2.00497700	-0.10242500
C	1.89006500	-2.45288500	-0.04091400
C	1.87346800	-3.89039000	0.01184400
C	0.57010600	-4.27920200	-0.00397100
C	-0.23002100	-3.08535200	-0.06660100
C	2.35083000	4.34487700	-0.03691300
C	3.14643200	4.74265400	-1.11379300
C	3.81920000	5.95921300	-1.12213900
C	3.69710200	6.81709200	-0.03418400
C	2.90936400	6.45229400	1.05245800
C	2.25163400	5.22762900	1.04089700
F	3.27856300	3.94344700	-2.17577100
F	4.57133000	6.31117100	-2.16401100
F	4.33342100	7.98468500	-0.03243600
F	2.79811300	7.27229200	2.09670400
F	1.50724600	4.90313200	2.10203000
H	2.74871100	-4.52562000	0.07652500
H	0.18447000	-5.29045500	0.04493900
H	-4.50083800	-2.73896600	-0.15018400
H	-5.26643500	-0.17590900	-0.17713600
H	-2.74409100	4.53155400	-0.14613800
H	-0.17956300	5.29520500	-0.14592600
H	4.50818000	2.74312200	0.05569100
H	5.27415400	0.18091800	0.05509500
O	-0.17929200	0.61684600	2.06163200

$$\Delta E_{\text{solv}} = -4218.33633524 \quad \Delta G_{\text{solv}} = -4217.99072424$$

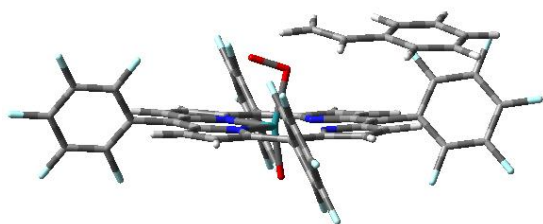
⁵F

O	0.10822200	0.31018700	2.29788600
Ru	-0.01029800	-0.02864900	-0.36527900
N	0.76573300	-1.93014400	-0.09274700
C	2.09519900	-2.27412900	-0.12411200
C	2.21346700	-3.70447200	-0.13496200
C	0.95302800	-4.21277500	-0.10346400
C	0.04659200	-3.10024900	-0.07720100
C	3.16979100	-1.37350200	-0.13202800
C	4.53842400	-1.94597500	-0.13031300
C	5.02133300	-2.69050800	0.94858400
C	6.30352300	-3.22709700	0.95832500
C	7.14274700	-3.01653300	-0.13069700

C	6.69482800	-2.27483700	-1.21869700
C	5.40644300	-1.75246800	-1.20816900
F	4.24527900	-2.89927200	2.01668200
F	6.73629200	-3.92982200	2.00460900
F	8.37231800	-3.52286000	-0.13082600
F	7.49814000	-2.07705900	-2.26293100
F	5.00488300	-1.05002900	-2.26978900
C	-1.35180500	-3.19943900	-0.05030000
C	-2.25321400	-2.12541300	-0.04631600
N	-1.91471000	-0.79523900	-0.10054900
C	-3.08718400	-0.07969600	-0.09509700
C	-4.19552400	-0.98940500	-0.02799200
C	-3.68215800	-2.24734200	0.01296600
C	-3.19009300	1.31822200	-0.13552600
C	-2.11624500	2.21948800	-0.14927600
N	-0.78618100	1.87807500	-0.16906500
C	-0.06813200	3.04561700	-0.09987700
C	-0.97547100	4.15689600	-0.05377200
C	-2.23613900	3.64838500	-0.08394700
C	1.33015100	3.14189600	-0.04332700
C	1.90397300	4.50259200	0.10041000
C	1.70586800	5.24662400	1.26563000
C	2.23561800	6.52158900	1.42403800
C	2.99396800	7.07917300	0.39964100
C	3.21499300	6.36102800	-0.77099900
C	2.67036100	5.08907800	-0.90847500
F	0.99148800	4.73051200	2.27099800
F	2.03106900	7.20606700	2.54881600
F	3.50839200	8.29746500	0.54019100
F	3.93917800	6.89750100	-1.75190000
F	2.89786600	4.42544400	-2.04415200
C	-1.93034400	-4.56567100	-0.01195300
C	-1.74386900	-5.40481900	1.08910700
C	-2.27766300	-6.68729900	1.13736700
C	-3.02800600	-7.15744000	0.06473300
C	-3.23528600	-6.34576700	-1.04557800
C	-2.68620500	-5.06874900	-1.07357900
F	-1.03578100	-4.97921900	2.13955100
F	-2.89788300	-4.31744500	-2.15690400
F	-3.94946200	-6.79878000	-2.07500300
F	-3.54663700	-8.38143000	0.10096400
F	-2.08412300	-7.46259400	2.20379200
O	-0.03353800	-0.10206000	-2.11797800
N	1.89802500	0.74316000	-0.16339500

C	2.23459700	2.07031200	-0.06627400
C	3.65994200	2.18952600	0.05529600
C	4.17287100	0.93072200	0.02058300
C	3.06733800	0.02486100	-0.11155300
C	-4.55527100	1.90017100	-0.12928000
C	-5.04392000	2.61410900	-1.22618500
C	-6.31850200	3.16935700	-1.23408200
C	-7.14123500	3.01347900	-0.12350800
C	-6.68421000	2.30906100	0.98532300
C	-5.40379400	1.76825700	0.97231400
F	-4.27927100	2.77883800	-2.30807400
F	-6.75864300	3.84117800	-2.29695000
F	-8.36306000	3.53824300	-0.12131600
F	-7.47007400	2.16659300	2.05215500
F	-4.98955200	1.10786400	2.05843100
H	4.20276200	3.11994500	0.17103800
H	5.21304700	0.63950600	0.10531800
H	3.14541500	-4.25570600	-0.16860900
H	0.66304300	-5.25656800	-0.10721900
H	-4.22850800	-3.18007800	0.08425700
H	-5.24018200	-0.70373100	-0.01013100
H	-3.16967700	4.19682100	-0.04492700
H	-0.68563600	5.19950800	-0.00186100
O	0.51710000	1.39537000	2.68670500

$$\Delta E_{\text{solv}} = -4218.34159207 \quad \Delta G_{\text{solv}} = -4217.99971307$$



¹₂

C	6.29477600	1.60423700	2.41649300
C	4.98120500	1.88439100	2.79688300
C	4.03594400	0.86937200	2.87311400
C	4.38825600	-0.46193800	2.59619900
C	5.71592900	-0.72715900	2.22833500
C	6.65903900	0.29043200	2.13180000
C	3.43004600	-1.56522700	2.63639000
C	2.13821400	-1.50155200	2.97963200
O	-0.07043000	0.31405500	1.49420000
Ru	-0.52526500	-0.01608300	-0.41692300

N	-0.67557800	-2.05575900	-0.34445100
C	0.34073900	-2.96662400	-0.48907700
C	-0.22160300	-4.28493300	-0.45413700
C	-1.56525800	-4.15265500	-0.27037000
C	-1.85188200	-2.75050300	-0.19927800
C	1.70291200	-2.66639800	-0.63919400
C	2.64435200	-3.80492700	-0.77230000
C	2.86220700	-4.70827300	0.27079300
C	3.75938400	-5.76396400	0.15782300
C	4.47072800	-5.93431500	-1.02513800
C	4.28009600	-5.05085600	-2.08229200
C	3.37487300	-4.00460700	-1.94674300
F	2.20692700	-4.56580100	1.42872900
F	3.94793700	-6.60455900	1.17425200
F	5.33259300	-6.93965100	-1.14501400
F	4.95855500	-5.21778400	-3.21626800
F	3.21391500	-3.17580700	-2.98062000
C	-3.12734500	-2.18667100	-0.03694200
C	-3.43984600	-0.81689300	-0.03430500
N	-2.54465200	0.21334000	-0.18557200
C	-3.24373900	1.39460800	-0.14518900
C	-4.63488800	1.09207400	0.02228600
C	-4.75310800	-0.26301100	0.10552200
C	-2.69596200	2.68433100	-0.23545200
C	-1.32974500	2.99275900	-0.34351200
N	-0.31711200	2.08235600	-0.38814700
C	0.86486000	2.75872200	-0.43862100
C	0.58515100	4.17218400	-0.43494700
C	-0.76507100	4.31644200	-0.37597100
C	2.14966200	2.18633300	-0.47825300
C	3.29811800	3.12369100	-0.42159200
C	3.53424300	3.89282300	0.71931200
C	4.63880600	4.72702600	0.83165600
C	5.53985300	4.81823000	-0.22299700
C	5.32367600	4.08006100	-1.38211700
C	4.21197000	3.24966300	-1.47023000
F	2.70228600	3.81254100	1.76401700
F	4.85761800	5.40654900	1.95891400
F	6.60541500	5.60814400	-0.12396200
F	6.17792900	4.17793700	-2.39992200
F	4.03557200	2.55524300	-2.59722400
C	-4.25630500	-3.13427500	0.13703200
C	-4.34961000	-3.95194900	1.26628500
C	-5.39652200	-4.84993200	1.44031400

C	-6.38935200	-4.94152500	0.47063300
C	-6.32670700	-4.14041600	-0.66459500
C	-5.26657900	-3.25492500	-0.82026900
F	-3.41497600	-3.88498200	2.21738000
F	-5.22995700	-2.50721700	-1.92715300
F	-7.27428100	-4.23356400	-1.59650300
F	-7.39747300	-5.79400800	0.62800300
F	-5.45944500	-5.61522300	2.52886400
O	-0.47891100	0.15352000	-2.13055600
N	1.56622300	-0.21324900	-0.54896900
C	2.46232200	0.81721600	-0.54232300
C	3.79396700	0.26938900	-0.61370300
C	3.66958400	-1.07945000	-0.69616500
C	2.26307100	-1.37938400	-0.64735600
C	-3.63965200	3.82853800	-0.18910800
C	-3.81348000	4.66914100	-1.29131700
C	-4.68248700	5.75373500	-1.26037300
C	-5.40975900	6.01682300	-0.10429400
C	-5.26052700	5.19814000	1.01028200
C	-4.38034500	4.12335600	0.95804800
F	-3.13333500	4.44055800	-2.41761400
F	-4.82816300	6.53586000	-2.32892000
F	-6.24611700	7.04991300	-0.06463600
F	-5.95143900	5.45394600	2.12045300
F	-4.25150400	3.36313000	2.04924300
H	4.71407500	0.83925400	-0.56111300
H	4.46713700	-1.81235900	-0.73569400
H	0.33937500	-5.20552900	-0.56227700
H	-2.30017900	-4.94586000	-0.20516300
H	-5.66189500	-0.83445000	0.24991200
H	-5.43221200	1.82342000	0.07447400
H	-1.33015300	5.24035000	-0.34700500
H	1.33117200	4.95662300	-0.47999200
H	1.50131100	-2.38210200	2.95139800
H	1.65751300	-0.57684000	3.29045300
H	3.83938400	-2.53574800	2.34033500
H	3.00736600	1.11327500	3.14009400
H	6.00257400	-1.75658200	2.00722000
H	4.69212000	2.90575400	3.03760500
H	7.68122700	0.05662000	1.83868800
H	7.02864100	2.40655100	2.35241900
O	-0.94838200	-0.51591400	1.96773100

$$\Delta E_{\text{solv}} = -4527.10575234 \quad \Delta G_{\text{solv}} = -4526.63612434$$

C	-5.31634800	-1.43955900	2.64523300
C	-3.99856100	-1.76115100	2.97250500
C	-3.03518500	-0.76518800	3.07915700
C	-3.36780100	0.58328700	2.86326200
C	-4.69332200	0.88533100	2.50911900
C	-5.65904500	-0.11066300	2.40968900
C	-2.40687800	1.67662400	3.00547000
C	-1.20255600	1.62179800	3.58587100
O	-0.05881800	-0.61068100	1.72080800
Ru	0.39013500	-0.00122800	-0.38106200
N	-0.11239700	2.01005800	-0.28005100
C	-1.34389500	2.56548500	-0.50425200
C	-1.20768400	3.99587900	-0.51076100
C	0.10230900	4.27842700	-0.27508000
C	0.79716500	3.02456700	-0.15932900
C	-2.53846800	1.84895200	-0.69089500
C	-3.76672400	2.60242400	-1.04589600
C	-4.35948800	3.56054200	-0.21992600
C	-5.51923600	4.23814400	-0.57760800
C	-6.12426000	3.96822100	-1.79923000
C	-5.56232400	3.02384100	-2.65098100
C	-4.40179100	2.36045300	-2.27094200
F	-3.82575400	3.85681300	0.97332100
F	-6.05597400	5.13652200	0.24761900
F	-7.23393800	4.61011300	-2.15120900
F	-6.13276900	2.76846900	-3.82705700
F	-3.89054100	1.47052500	-3.12400500
C	2.19252800	2.88692600	-0.03683900
C	2.93782000	1.69573100	-0.11468300
N	2.42310600	0.43875800	-0.26646600
C	3.46094500	-0.44907600	-0.30431400
C	4.69401700	0.28317800	-0.19849300
C	4.37225500	1.59777100	-0.05987600
C	3.33677500	-1.84714100	-0.37451000
C	2.12798100	-2.56459000	-0.37045300
N	0.87711400	-2.01406100	-0.35672300
C	-0.03670700	-3.02830300	-0.27164300
C	0.66964200	-4.27908600	-0.23456500
C	1.99970600	-3.99509700	-0.30588700
C	-1.43476600	-2.88251800	-0.24319900
C	-2.22845800	-4.12180700	-0.04034100
C	-2.30112700	-4.71119500	1.22236000

C	-3.06301400	-5.84847000	1.46116800
C	-3.77028700	-6.42862000	0.41302500
C	-3.71592000	-5.86591800	-0.85813400
C	-2.94940100	-4.72488900	-1.07088500
F	-1.64020200	-4.16593200	2.25013800
F	-3.12708600	-6.37836300	2.68240800
F	-4.50202900	-7.51857800	0.62745500
F	-4.39453000	-6.42384300	-1.85983900
F	-2.92234700	-4.20034900	-2.29833000
C	2.95358200	4.14325300	0.17691900
C	2.79477600	4.88208400	1.35244100
C	3.48525300	6.06719700	1.57690500
C	4.36646700	6.53988400	0.60994800
C	4.54651400	5.82861100	-0.57167600
C	3.83941300	4.64920900	-0.77669400
F	1.95829000	4.45171200	2.30211300
F	4.02445900	3.99900200	-1.92908000
F	5.38436500	6.28644900	-1.50112900
F	5.03481000	7.67126400	0.81511500
F	3.31448600	6.74760700	2.70960700
O	0.46215700	0.06918500	-2.10373400
N	-1.63683500	-0.43369300	-0.45988000
C	-2.16604400	-1.69124400	-0.36921900
C	-3.59920800	-1.59279000	-0.44193700
C	-3.90437500	-0.27877400	-0.60973100
C	-2.66503800	0.45093400	-0.60804400
C	4.58774400	-2.64347100	-0.41175300
C	4.92294800	-3.40971500	-1.53115600
C	6.08602000	-4.16935500	-1.58276000
C	6.95138600	-4.17270500	-0.49408500
C	6.64610800	-3.42223600	0.63635600
C	5.47400500	-2.67568900	0.66759500
F	4.11497600	-3.42575200	-2.59412300
F	6.37958800	-4.88589100	-2.66684300
F	8.06841400	-4.89336200	-0.53295400
F	7.47023700	-3.43283200	1.68343500
F	5.20343100	-1.98021400	1.77645500
H	-4.28984200	-2.42364200	-0.35969900
H	-4.89061200	0.16456400	-0.67830300
H	-2.01118200	4.70293800	-0.67511900
H	0.56413400	5.25726400	-0.22312300
H	5.05459100	2.42946700	0.06637500
H	5.68568100	-0.15252800	-0.21462100
H	2.82441500	-4.69793300	-0.29711800

H	0.20578800	-5.25690600	-0.17537300
H	-0.56101200	2.49897700	3.63488400
H	-0.80343900	0.70891600	4.02442800
H	-2.74270500	2.63647800	2.61292800
H	-2.00932400	-1.03367500	3.32782200
H	-4.96369900	1.92764700	2.33645100
H	-3.71818400	-2.79716300	3.15637200
H	-6.68371900	0.15257600	2.15053600
H	-6.06950200	-2.22256900	2.57183800
O	0.75792300	0.37085900	1.78229700

$\Delta E_{\text{solv}} = -4527.11447018$ $\Delta G_{\text{solv}} = -4526.64520818$

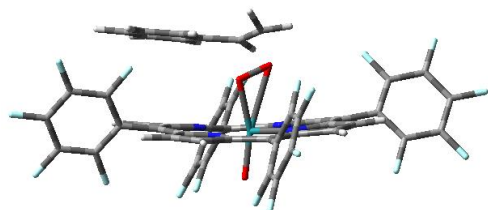
⁵2

C	5.74354100	0.73929300	1.99420200
C	4.59274200	1.39473100	2.43369300
C	3.52964600	0.67372900	2.96074500
C	3.60044500	-0.72508000	3.08433600
C	4.75420400	-1.37093900	2.60969600
C	5.81458600	-0.64928800	2.07218600
C	2.55643300	-1.52209300	3.72448000
C	1.52985700	-1.06388400	4.45226500
O	-0.11157000	0.09481000	1.82684700
Ru	-0.46391500	0.03877300	-0.73478900
N	-0.18956900	-2.00568700	-0.55903900
C	1.00051700	-2.68108900	-0.67097100
C	0.74677700	-4.09340600	-0.65363100
C	-0.59660400	-4.25915500	-0.52630200
C	-1.18172100	-2.94958100	-0.45885900
C	2.26626500	-2.09083500	-0.78206500
C	3.44767100	-2.98704200	-0.81063400
C	3.79395800	-3.75820400	0.30017900
C	4.95703700	-4.51596100	0.34330200
C	5.80063900	-4.53905800	-0.76161800
C	5.47315600	-3.80192600	-1.89516600
C	4.31039300	-3.03953500	-1.90802800
F	3.01043500	-3.76057000	1.38526400
F	5.27384300	-5.19815100	1.44505200
F	6.91639700	-5.26246800	-0.73588000
F	6.27562700	-3.82987800	-2.95819000
F	4.03851200	-2.32970200	-3.00513600
C	-2.54989700	-2.68215400	-0.30781100
C	-3.13648100	-1.41094900	-0.21832700
N	-2.46857300	-0.21423000	-0.28998300

C	-3.40377200	0.78094500	-0.14314300
C	-4.70099000	0.18883000	0.02202400
C	-4.53533800	-1.16000900	-0.01494400
C	-3.13541500	2.15683500	-0.12969500
C	-1.86770400	2.74663100	-0.23870800
N	-0.68708200	2.07327900	-0.43018100
C	0.31675400	3.00940000	-0.42439900
C	-0.25049700	4.31281300	-0.22970000
C	-1.59647300	4.15124200	-0.11633400
C	1.68347000	2.73829300	-0.56325000
C	2.61617600	3.89085100	-0.47484800
C	2.90203100	4.48150200	0.75609600
C	3.79772000	5.53686200	0.87670800
C	4.43069700	6.02749500	-0.26090100
C	4.16817100	5.45867100	-1.50292100
C	3.26888400	4.40142300	-1.59686600
F	2.32177300	4.01484100	1.86911000
F	4.06169500	6.07057700	2.06945800
F	5.29074800	7.03697700	-0.15949800
F	4.77785500	5.92945600	-2.58983400
F	3.04502700	3.86592300	-2.79813400
C	-3.46131800	-3.85010400	-0.21717300
C	-3.41628000	-4.73204200	0.86484900
C	-4.26392100	-5.82981800	0.95676300
C	-5.19534000	-6.06237100	-0.04954600
C	-5.26997100	-5.20001800	-1.13809200
C	-4.40708200	-4.11242900	-1.21129700
F	-2.53941000	-4.53103700	1.85371200
F	-4.50175400	-3.30651200	-2.27149900
F	-6.16037000	-5.42553200	-2.10317900
F	-6.01356900	-7.10782100	0.03000400
F	-4.19635700	-6.65245600	2.00316700
O	-0.66972100	0.05671300	-2.47751100
N	1.58821200	0.28047300	-0.73338400
C	2.26502600	1.47442000	-0.71157200
C	3.67524100	1.22253100	-0.78928800
C	3.83986600	-0.12484800	-0.83940600
C	2.53128600	-0.71405100	-0.80150400
C	-4.28830600	3.07390100	0.05036900
C	-4.68252500	3.95097400	-0.96303300
C	-5.75349000	4.82349800	-0.80573500
C	-6.46334800	4.82955600	0.39025600
C	-6.09629900	3.96859400	1.41907000
C	-5.01802200	3.10971300	1.24069700

F	-4.02376800	3.96716600	-2.12401300
F	-6.10810200	5.64626900	-1.79173800
F	-7.49131400	5.65820500	0.54983900
F	-6.77153900	3.98003600	2.56815800
F	-4.68263200	2.30440300	2.25399200
H	4.44917400	1.98093700	-0.76560600
H	4.77500900	-0.67072300	-0.85592200
H	1.50329500	-4.86478700	-0.73611300
H	-1.14445800	-5.19284200	-0.48603400
H	-5.29821100	-1.92107700	0.09706200
H	-5.62651900	0.73547600	0.15629700
H	-2.34156700	4.91921400	0.05443400
H	0.31154000	5.23834600	-0.18402500
H	0.81700600	-1.74336500	4.91102500
H	1.36236300	-0.00164100	4.62626500
H	2.67219100	-2.60184200	3.61879100
H	2.63477600	1.20277100	3.28869500
H	4.82196600	-2.45584900	2.69626300
H	4.52331100	2.47980500	2.36811200
H	6.70349900	-1.17381600	1.72269300
H	6.57557200	1.30946100	1.58380300
O	-0.66743800	-0.75297700	2.51194900

$\Delta E_{\text{solv}} = -4527.11517431$ $\Delta G_{\text{solv}} = -4526.65113131$



¹TS4

C	-4.74791200	-1.34728400	3.05423400
C	-3.41856800	-1.75209200	3.18660300
C	-2.38620200	-0.83224200	3.07274400
C	-2.66038800	0.53252600	2.79949000
C	-4.01775600	0.91266200	2.64009900
C	-5.04003300	-0.00696400	2.78265700
C	-1.63604300	1.51706400	2.70331000
C	-0.31807600	1.33813100	3.15350600
O	0.36790900	-0.55914100	1.52192000
Ru	0.32715500	0.02141700	-0.45313500
N	-0.11513600	2.03204600	-0.41580900
C	-1.35090700	2.60030200	-0.59233400

C	-1. 19724900	4. 02925600	-0. 61661400
C	0. 12203500	4. 29890100	-0. 41848200
C	0. 80329800	3. 03898000	-0. 30770800
C	-2. 56611900	1. 90356300	-0. 68477300
C	-3. 79722500	2. 69598900	-0. 92890100
C	-4. 27847100	3. 64620200	-0. 02540300
C	-5. 43776100	4. 37610400	-0. 25792200
C	-6. 15725500	4. 16414700	-1. 42851700
C	-5. 70957500	3. 22617600	-2. 35229800
C	-4. 54413700	2. 51204800	-2. 09769600
F	-3. 62659000	3. 88032100	1. 12517100
F	-5. 86583200	5. 26800400	0. 63525800
F	-7. 26970900	4. 85412600	-1. 66260400
F	-6. 39334100	3. 02509600	-3. 47731100
F	-4. 14257800	1. 62881900	-3. 01318100
C	2. 18925200	2. 87197300	-0. 15235100
C	2. 88873000	1. 65446100	-0. 18212600
N	2. 32835100	0. 41137700	-0. 33879600
C	3. 34474900	-0. 51458800	-0. 33545800
C	4. 59301300	0. 18006600	-0. 20058300
C	4. 31211500	1. 50710300	-0. 08392300
C	3. 19627700	-1. 90731100	-0. 41730300
C	1. 97815300	-2. 61044600	-0. 44963800
N	0. 74254800	-2. 04159900	-0. 44549200
C	-0. 18505300	-3. 03343000	-0. 34876800
C	0. 49734900	-4. 30189700	-0. 33196100
C	1. 83100200	-4. 04174000	-0. 39979800
C	-1. 57760000	-2. 85341700	-0. 25958400
C	-2. 39225700	-4. 08242300	-0. 08212600
C	-2. 34231800	-4. 80480700	1. 11176500
C	-3. 10140500	-5. 95129300	1. 31313400
C	-3. 93752100	-6. 40460300	0. 29820700
C	-4. 00881200	-5. 70925600	-0. 90413000
C	-3. 23759200	-4. 56567900	-1. 08238800
F	-1. 55222200	-4. 39109000	2. 11008600
F	-3. 03920800	-6. 61277400	2. 46905300
F	-4. 67002500	-7. 50045800	0. 47865100
F	-4. 80788000	-6. 14649700	-1. 87675000
F	-3. 32554900	-3. 92342200	-2. 24953400
C	2. 98277300	4. 10686500	0. 06056000
C	2. 81676100	4. 87187600	1. 21794700
C	3. 53842000	6. 03812000	1. 44187900
C	4. 46181400	6. 46401700	0. 49273600
C	4. 65241900	5. 72496700	-0. 67000600

C	3.91318800	4.56525100	-0.87456700
F	1.94189400	4.48519800	2.15392500
F	4.11200400	3.88593100	-2.00756700
F	5.53143700	6.13824100	-1.58213000
F	5.16081900	7.57700100	0.69711800
F	3.35873800	6.74371500	2.55806100
O	0.17860400	-0.13269500	-2.17445700
N	-1.71807500	-0.39211200	-0.40039800
C	-2.27545900	-1.63696000	-0.31536400
C	-3.71037700	-1.50285300	-0.35247200
C	-3.98576400	-0.18556100	-0.52555800
C	-2.72551500	0.51189800	-0.55654100
C	4.43479200	-2.72508700	-0.42151900
C	4.79549100	-3.48256900	-1.53861500
C	5.94216700	-4.26831200	-1.55723100
C	6.76455100	-4.30733300	-0.43644700
C	6.43317200	-3.56570600	0.69236300
C	5.27809500	-2.79246400	0.68998800
F	4.02867200	-3.46523200	-2.63146300
F	6.26115400	-4.97605200	-2.64024900
F	7.86607800	-5.05307500	-0.44325600
F	7.21651900	-3.60972700	1.76985600
F	4.98283900	-2.10394000	1.79664600
H	-4.41983000	-2.31591000	-0.25588600
H	-4.96180200	0.28194200	-0.58250700
H	-1.99662900	4.74461100	-0.76527400
H	0.59624000	5.27273900	-0.38255100
H	5.01877700	2.31701300	0.05080200
H	5.57050300	-0.28645100	-0.18591700
H	2.64414700	-4.75789200	-0.39469100
H	0.01664600	-5.27202300	-0.28219400
H	0.28854900	2.23433200	3.27493300
H	-0.14270100	0.58357000	3.92008700
H	-1.90712100	2.48194200	2.27495600
H	-1.35318200	-1.16284200	3.16812200
H	-4.24184900	1.95727000	2.43018500
H	-3.18404900	-2.79459100	3.39181100
H	-6.07548600	0.31388700	2.67864700
H	-5.55331400	-2.07129000	3.16448600
O	0.77597100	0.63080000	1.97949600

$\Delta E_{\text{solv}} = -4527.08630102$ $\Delta G_{\text{solv}} = -4526.61103402$

³TS4

C	-4.88241700	-1.47320400	3.12234400
C	-3.54637500	-1.84653500	3.28819200
C	-2.52900800	-0.91877000	3.11979100
C	-2.82646300	0.41747300	2.76105900
C	-4.18486500	0.76571100	2.56927300
C	-5.19605000	-0.16066000	2.76313000
C	-1.82161100	1.42180500	2.59209500
C	-0.48770600	1.31964300	3.01525400
O	0.24815000	-0.76375900	1.58093700
Ru	0.33433400	0.02295100	-0.39110600
N	-0.07272100	2.05413900	-0.35124300
C	-1.28394400	2.65221200	-0.56885800
C	-1.09536300	4.07652300	-0.57897800
C	0.22600100	4.31118100	-0.34473000
C	0.87229600	3.03275600	-0.22267200
C	-2.50959700	1.97768500	-0.70762700
C	-3.71791900	2.79267000	-0.98702100
C	-4.22588300	3.72785500	-0.08317300
C	-5.36097000	4.48330500	-0.35081300
C	-6.02861000	4.31037500	-1.55808700
C	-5.55501400	3.38519800	-2.48198900
C	-4.41456700	2.64503100	-2.19117100
F	-3.62663300	3.91643800	1.10396500
F	-5.81659000	5.36047800	0.54328900
F	-7.11774700	5.02452500	-1.82642700
F	-6.19066800	3.22063700	-3.64056100
F	-3.98718800	1.77312000	-3.10560900
C	2.25552100	2.82945800	-0.05881400
C	2.93915900	1.60150100	-0.10929900
N	2.36386300	0.37156400	-0.27198000
C	3.36116900	-0.56484600	-0.31859500
C	4.62618500	0.10775400	-0.18410700
C	4.36637900	1.43399000	-0.03455400
C	3.18350500	-1.95269700	-0.44883200
C	1.95078100	-2.62908000	-0.51229200
N	0.72647500	-2.03803400	-0.50461700
C	-0.22181100	-3.01081700	-0.41212500
C	0.43463000	-4.29364200	-0.41517700
C	1.77276300	-4.05899300	-0.48520500
C	-1.60923100	-2.80238000	-0.30867600
C	-2.44566100	-4.01113600	-0.09701900
C	-2.40560800	-4.68990200	1.12258400
C	-3.19943100	-5.80214500	1.37425800
C	-4.05641400	-6.26888100	0.38314500

C	-4.11464400	-5.61951700	-0.84549200
C	-3.31126900	-4.50709600	-1.07266500
F	-1.59426500	-4.26345900	2.09741000
F	-3.15049000	-6.41675100	2.55665900
F	-4.82130700	-7.33340300	0.61145200
F	-4.93422500	-6.06938200	-1.79526800
F	-3.39207700	-3.90440500	-2.26170600
C	3.06997600	4.04867300	0.16999100
C	2.91736200	4.79894500	1.33861300
C	3.65559700	5.95152600	1.57842700
C	4.58183700	6.37918500	0.63292900
C	4.75845800	5.65546200	-0.54155300
C	4.00274300	4.50922400	-0.76166500
F	2.03873200	4.41066800	2.27093600
F	4.18756600	3.84641200	-1.90657000
F	5.63985000	6.07109000	-1.45041000
F	5.29667000	7.47942800	0.85174300
F	3.48838700	6.64263400	2.70568000
O	0.32999300	0.01243500	-2.12703500
N	-1.70747700	-0.33709000	-0.43166700
C	-2.28770900	-1.57278900	-0.36469600
C	-3.71726000	-1.41291900	-0.42779700
C	-3.96675200	-0.08796900	-0.59895400
C	-2.69631100	0.58830400	-0.60049300
C	4.40497400	-2.79445800	-0.47401300
C	4.74590700	-3.54164700	-1.60446000
C	5.87928700	-4.34577200	-1.64264500
C	6.70866200	-4.41491300	-0.52847100
C	6.39685300	-3.68489200	0.61339900
C	5.25484100	-2.89277700	0.63052100
F	3.97304900	-3.49496500	-2.69235900
F	6.17915800	-5.04201600	-2.73863600
F	7.79757300	-5.17872000	-0.55382200
F	7.18614800	-3.75849400	1.68499900
F	4.97792300	-2.21850600	1.75056900
H	-4.44387100	-2.21311700	-0.35500400
H	-4.93374700	0.39486700	-0.68139600
H	-1.87325000	4.81233100	-0.74418900
H	0.72374100	5.27260700	-0.29405000
H	5.08644200	2.23163300	0.10231000
H	5.59679100	-0.37303800	-0.19892000
H	2.57087200	-4.79196000	-0.49522500
H	-0.06600000	-5.25419800	-0.37591800
H	0.10462000	2.23306500	3.03474900

H	-0.25064900	0.61695100	3.81259700
H	-2.13099200	2.34921700	2.11100300
H	-1.49014800	-1.22562100	3.22826900
H	-4.42250300	1.79125400	2.28629600
H	-3.29653500	-2.87112900	3.55688900
H	-6.23526400	0.13475400	2.62820700
H	-5.67564200	-2.20393000	3.27068600
O	0.62824600	0.49562300	1.85574600

$\Delta E_{\text{solv}} = -4527.09637547$ $\Delta G_{\text{solv}} = -4526.62230847$

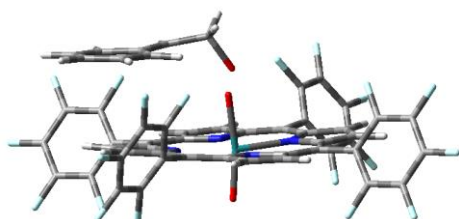
⁵TS4

C	-5.26251600	-0.92750900	2.57269900
C	-4.01184700	-1.51968800	2.76784300
C	-2.89782100	-0.74079800	3.03236700
C	-3.00586200	0.67051600	3.11525400
C	-4.27917900	1.25005600	2.88370800
C	-5.38768200	0.46302600	2.62423600
C	-1.91352300	1.52338900	3.45053500
C	-0.61338200	1.09785800	3.79966700
O	-0.05940900	-0.10240000	1.66494400
Ru	0.38553700	-0.03663500	-0.66162700
N	0.16229600	2.01838400	-0.51557400
C	-1.01283900	2.71731600	-0.60639700
C	-0.72600800	4.12545200	-0.60100600
C	0.62250100	4.25984900	-0.49421500
C	1.17724000	2.93564000	-0.43089000
C	-2.29483600	2.15247800	-0.68526000
C	-3.44948800	3.08278900	-0.74127700
C	-3.76908000	3.92757700	0.32339600
C	-4.87185700	4.77189800	0.29881800
C	-5.69129900	4.79471500	-0.82404400
C	-5.40017000	3.97216000	-1.90685700
C	-4.29147700	3.13425900	-1.85604500
F	-3.01056100	3.93500000	1.42955300
F	-5.15298800	5.54750300	1.34731700
F	-6.75050300	5.59869000	-0.86150100
F	-6.18098300	3.99671200	-2.98599600
F	-4.04571300	2.35973300	-2.91413100
C	2.54008900	2.63540800	-0.29164300
C	3.10011400	1.35124600	-0.21077300
N	2.40774700	0.17068000	-0.28093600
C	3.32061100	-0.84576700	-0.16538100
C	4.63443300	-0.28408400	-0.01298000

C	4.49764000	1.06814600	-0.03170900
C	3.02366700	-2.21666600	-0.18207800
C	1.74402400	-2.78206000	-0.28818900
N	0.57222500	-2.08492900	-0.42624600
C	-0.44872900	-2.99859300	-0.42887200
C	0.10048500	-4.32039900	-0.30462900
C	1.45076400	-4.18705800	-0.21610300
C	-1.81592300	-2.69562600	-0.51446100
C	-2.76389100	-3.83500800	-0.44179100
C	-2.91173700	-4.57749000	0.73109300
C	-3.80512200	-5.63682900	0.82999500
C	-4.58238700	-5.97948900	-0.27137800
C	-4.46226800	-5.25925500	-1.45496400
C	-3.55949000	-4.20367500	-1.52859500
F	-2.19281200	-4.26096200	1.81767900
F	-3.92984300	-6.31571400	1.97114800
F	-5.44268400	-6.99111100	-0.19037800
F	-5.20731900	-5.58890700	-2.50921600
F	-3.47062400	-3.53295900	-2.67848800
C	3.47734600	3.78298900	-0.20212100
C	3.46231200	4.65558900	0.88812800
C	4.33253700	5.73525500	0.98173800
C	5.25813500	5.95878500	-0.03170200
C	5.30389900	5.10533400	-1.12858900
C	4.41801100	4.03628800	-1.20334000
F	2.59272700	4.46333100	1.88640900
F	4.48593100	3.24001600	-2.27258500
F	6.18904000	5.32227900	-2.10093900
F	6.09841000	6.98720900	0.04911400
F	4.29249300	6.54914600	2.03733100
O	0.57691900	-0.04637300	-2.41318200
N	-1.67633500	-0.23706700	-0.66037700
C	-2.37661500	-1.41496200	-0.61472700
C	-3.78386900	-1.12730000	-0.62582000
C	-3.91748200	0.22431300	-0.66949600
C	-2.59355100	0.78170100	-0.68748400
C	4.16289200	-3.15881200	-0.04837900
C	4.53011700	-4.00796200	-1.09508700
C	5.58934500	-4.90138800	-0.98150900
C	6.31561200	-4.95742500	0.20303100
C	5.97644700	-4.12472400	1.26390400
C	4.90909900	-3.24457300	1.12899000
F	3.85668600	-3.97707600	-2.24725100
F	5.91810200	-5.69675200	-1.99905700

F	7.33315600	-5.80645300	0.32127100
F	6.66811100	-4.18301100	2.40240500
F	4.60175400	-2.46694700	2.17269300
H	-4.57508200	-1.86630400	-0.57324400
H	-4.83852800	0.79509800	-0.65590500
H	-1.46342600	4.91570700	-0.67778000
H	1.19258600	5.18086200	-0.46816000
H	5.27939900	1.81085000	0.07405600
H	5.55046300	-0.85194500	0.09692700
H	2.18457400	-4.97528900	-0.09624500
H	-0.47404700	-5.23904100	-0.28696000
H	0.04153500	1.82593100	4.27365700
H	-0.47472600	0.08029300	4.16230800
H	-2.09015400	2.59670500	3.38780800
H	-1.92849000	-1.21930800	3.16157100
H	-4.37401700	2.33407600	2.93425700
H	-3.90637000	-2.60116500	2.71749500
H	-6.35789600	0.93001500	2.46372100
H	-6.13474000	-1.54796500	2.37404400
O	0.35599200	0.91815500	2.32597400

$$\Delta E_{\text{solv}} = -4527.097017 \quad \Delta G_{\text{solv}} = -4526.628626$$



¹G

C	-5.35719100	-0.96338400	2.80641700
C	-4.11836100	-1.60928400	2.86531900
C	-2.94169200	-0.88108800	2.88249300
C	-2.97158100	0.54582800	2.86495400
C	-4.24836400	1.17536300	2.74796700
C	-5.41163700	0.43428600	2.73136600
C	-1.82948300	1.34274900	3.00914000
C	-0.47530100	0.87012500	3.33587600
O	0.05473900	-0.22140100	1.39088800
Ru	0.39598700	-0.02652500	-0.56612800
N	0.28778700	2.03984200	-0.45151100
C	-0.84818500	2.79656700	-0.56011200
C	-0.48444700	4.18905200	-0.53989800
C	0.86529400	4.25104000	-0.39988800

C	1. 34686600	2. 89653200	-0. 34098300
C	-2. 15960700	2. 30874700	-0. 64571300
C	-3. 25685100	3. 30283900	-0. 75658800
C	-3. 57645800	4. 18536100	0. 27666500
C	-4. 61815900	5. 09967500	0. 17802100
C	-5. 37832400	5. 14828800	-0. 98509400
C	-5. 09060100	4. 28274700	-2. 03470300
C	-4. 04174100	3. 37823700	-1. 91140800
F	-2. 88048100	4. 16434400	1. 42345300
F	-4. 89879600	5. 91859900	1. 19227800
F	-6. 37938100	6. 01745200	-1. 09147500
F	-5. 81654200	4. 32982600	-3. 15045600
F	-3. 79443000	2. 56467400	-2. 93902800
C	2. 68947700	2. 51950500	-0. 19803800
C	3. 17480400	1. 20313400	-0. 16000900
N	2. 41991900	0. 06156100	-0. 28117400
C	3. 27147900	-1. 01437900	-0. 20797100
C	4. 60866300	-0. 52965800	-0. 04188600
C	4. 54829200	0. 83123700	-0. 00117500
C	2. 90076100	-2. 36721500	-0. 27729900
C	1. 59249000	-2. 85896000	-0. 39684100
N	0. 46310100	-2. 09538300	-0. 49522900
C	-0. 61356800	-2. 94073600	-0. 48957300
C	-0. 13882900	-4. 29838000	-0. 42196000
C	1. 21751100	-4. 24816800	-0. 36372400
C	-1. 96243700	-2. 55966200	-0. 50328000
C	-2. 97189400	-3. 64137900	-0. 39204100
C	-3. 11194000	-4. 37243500	0. 78885900
C	-4. 08372100	-5. 35311100	0. 94170700
C	-4. 94200800	-5. 63528700	-0. 11554000
C	-4. 82528500	-4. 93055900	-1. 30893200
C	-3. 84883900	-3. 94802200	-1. 43428400
F	-2. 31292400	-4. 11649900	1. 83385200
F	-4. 20784800	-6. 00834500	2. 09680300
F	-5. 87666100	-6. 57259800	0. 01706300
F	-5. 64688400	-5. 20272200	-2. 32188100
F	-3. 77111600	-3. 28343500	-2. 58877300
C	3. 68516800	3. 61057700	-0. 05991400
C	3. 68888300	4. 45486500	1. 05310500
C	4. 61057200	5. 48571600	1. 19373000
C	5. 56814000	5. 68832200	0. 20582700
C	5. 59462700	4. 86317000	-0. 91318900
C	4. 65778000	3. 84329600	-1. 03529100
F	2. 78782000	4. 28231300	2. 02506700

F	4.70624500	3.07546200	-2.12699200
F	6.50885200	5.06178300	-1.86230000
F	6.45695300	6.67011000	0.33153500
F	4.58871800	6.27252900	2.26966300
O	0.36577300	0.01860000	-2.31468300
N	-1.70286300	-0.11413000	-0.60464200
C	-2.45801700	-1.24584900	-0.54906300
C	-3.84878400	-0.87539500	-0.52261100
C	-3.90268300	0.48191400	-0.58295300
C	-2.54629300	0.95690200	-0.62665000
C	3.98885700	-3.37149000	-0.17832200
C	4.30225500	-4.21197000	-1.24943100
C	5.31233700	-5.16386500	-1.16814900
C	6.04341900	-5.28910300	0.00810200
C	5.75727600	-4.46728400	1.09277900
C	4.73803200	-3.52777300	0.99043500
F	3.62308700	-4.11452000	-2.39494400
F	5.58992900	-5.94871800	-2.20882700
F	7.01489500	-6.19366000	0.09608200
F	6.45302600	-4.59289800	2.22292400
F	4.48169900	-2.76295200	2.05614300
H	-4.68199800	-1.56439600	-0.44891300
H	-4.78729100	1.10773200	-0.56436100
H	-1.17578600	5.01848100	-0.62999000
H	1.48446500	5.13887100	-0.35270300
H	5.37325500	1.52131300	0.12810700
H	5.49381600	-1.14960300	0.03442000
H	1.90558400	-5.08159100	-0.28660000
H	-0.76736800	-5.18109100	-0.41883400
H	0.02007800	1.56141700	4.02920200
H	-0.44804100	-0.14208900	3.75796900
H	-1.94517900	2.41736300	2.86903300
H	-1.98142200	-1.39442400	2.89081100
H	-4.28458400	2.26403400	2.71199700
H	-4.07373800	-2.69592000	2.90259400
H	-6.37472700	0.93777800	2.66810000
H	-6.27627100	-1.54610900	2.80357700
O	0.40205200	0.90475100	2.18878800

$$\Delta E_{\text{solv}} = -4527.10018352 \quad \Delta G_{\text{solv}} = -4526.62585252$$

³G

C	-4.89696300	-0.76836900	2.79898600
C	-3.64552400	-1.38830900	2.83978900

C	-2.48923800	-0.63896400	2.97863100
C	-2.55290900	0.77871000	3.09217400
C	-3.83936300	1.38564400	3.02611500
C	-4.98473400	0.62546600	2.88843800
C	-1.41729300	1.58701500	3.31126100
C	-0.02961900	1.08911400	3.42655500
O	0.14003400	-0.09405300	1.46479300
Ru	0.32199800	-0.05333900	-0.56720100
N	0.09480400	2.00584000	-0.51069700
C	-1.08682100	2.68699100	-0.60220500
C	-0.80756700	4.09730100	-0.65284700
C	0.54105000	4.24448900	-0.57076700
C	1.10570100	2.92670200	-0.47103100
C	-2.36873200	2.11318100	-0.63624700
C	-3.52440900	3.04225000	-0.68598000
C	-3.78966700	3.94554600	0.34655400
C	-4.88549000	4.79917800	0.32497000
C	-5.75466600	4.77121400	-0.75973000
C	-5.51699200	3.89253900	-1.81079400
C	-4.41241500	3.04917200	-1.76621900
F	-2.97817700	4.01068400	1.41109700
F	-5.10986300	5.63704200	1.33788000
F	-6.80795100	5.58276800	-0.79240200
F	-6.34251600	3.87064600	-2.85621300
F	-4.21476600	2.22828500	-2.80004100
C	2.47311200	2.64010900	-0.34779900
C	3.04413600	1.36052600	-0.26396400
N	2.36145500	0.17497700	-0.31468900
C	3.27372200	-0.83847700	-0.19532900
C	4.58675000	-0.26820300	-0.07453500
C	4.44441700	1.08445200	-0.10749400
C	2.98205100	-2.21205200	-0.18617400
C	1.70529900	-2.78957400	-0.26607500
N	0.52426300	-2.10832600	-0.38200700
C	-0.48939000	-3.02666600	-0.38335700
C	0.07586700	-4.34461800	-0.28120900
C	1.42538500	-4.19851400	-0.20365200
C	-1.86087400	-2.73498000	-0.45381400
C	-2.79738200	-3.88444000	-0.39715800
C	-2.91437800	-4.67060000	0.75113000
C	-3.79061500	-5.74631000	0.82612300
C	-4.58406300	-6.05911500	-0.27254500
C	-4.49549200	-5.29499700	-1.43114500
C	-3.60808400	-4.22551000	-1.48235800

F	-2.17731700	-4.38635500	1.83363100
F	-3.88195000	-6.47122500	1.94117100
F	-5.42848600	-7.08519800	-0.21309700
F	-5.25356100	-5.59761400	-2.48411200
F	-3.54604100	-3.51563500	-2.61072500
C	3.39957200	3.79662000	-0.27555400
C	3.37362800	4.68248400	0.80434900
C	4.23254100	5.77223500	0.88494400
C	5.15672100	5.99286200	-0.13058700
C	5.21284600	5.12647300	-1.21691400
C	4.33849500	4.04733900	-1.27897300
F	2.50577800	4.49278700	1.80370900
F	4.41494000	3.23860500	-2.33888100
F	6.09612800	5.34091900	-2.19136200
F	5.98593400	7.03075700	-0.06183800
F	4.18333200	6.59849200	1.93000100
O	0.40434800	-0.07946700	-2.32037000
N	-1.74637200	-0.27514900	-0.58711400
C	-2.43274200	-1.45657800	-0.53979300
C	-3.84309200	-1.17733300	-0.53998800
C	-3.98448100	0.17298900	-0.57812000
C	-2.66261200	0.73940800	-0.61025500
C	4.13108700	-3.14408500	-0.06300200
C	4.49167900	-3.99547800	-1.11006700
C	5.56091600	-4.87803500	-1.00670900
C	6.30453900	-4.91963500	0.16770200
C	5.97301100	-4.08341700	1.22828500
C	4.89530700	-3.21420000	1.10389700
F	3.80163800	-3.97678700	-2.25311200
F	5.88298400	-5.67588100	-2.02432400
F	7.33168700	-5.75794900	0.27635000
F	6.68226100	-4.12748700	2.35615900
F	4.59687500	-2.43102900	2.14520500
H	-4.62903900	-1.92137500	-0.48165200
H	-4.90865800	0.73804400	-0.55648800
H	-1.55010100	4.87993000	-0.75147800
H	1.10573700	5.16891100	-0.58946700
H	5.22525800	1.83124100	-0.02789500
H	5.50761500	-0.83035700	0.02386600
H	2.16798600	-4.98100400	-0.10276800
H	-0.48825600	-5.26957200	-0.27117800
H	0.60742600	1.78345900	3.98401000
H	0.05191600	0.08821600	3.86881300
H	-1.55869000	2.66851200	3.31377600

H	-1.52137400	-1.13508300	2.98449100
H	-3.90659300	2.46879100	3.11054100
H	-3.57146200	-2.47114700	2.76134900
H	-5.95770100	1.11333600	2.85466200
H	-5.80012600	-1.36724700	2.69309400
O	0.60278900	1.04841100	2.12280000

$$\Delta E_{\text{solv}} = -4527.12176686 \quad \Delta G_{\text{solv}} = -4526.64731586$$

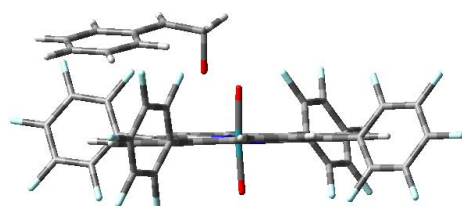
⁵G

C	5.35659600	0.98350800	2.62910000
C	4.11319400	1.59406900	2.81925800
C	2.96973700	0.83120900	2.98677100
C	3.03616600	-0.58826100	2.97886300
C	4.30829900	-1.18407500	2.75648900
C	5.44337300	-0.41155200	2.59163800
C	1.91973800	-1.42729000	3.20875800
C	0.57113100	-0.96912400	3.56425600
O	0.07549500	0.19323400	1.63456300
Ru	-0.39259800	0.02821800	-0.64032100
N	-0.19663100	-2.02778200	-0.46332000
C	0.96570600	-2.74637200	-0.56295200
C	0.65695500	-4.14963400	-0.53934500
C	-0.69179500	-4.26137500	-0.41102200
C	-1.22504600	-2.92786100	-0.35846900
C	2.25606200	-2.20175800	-0.66245000
C	3.39471800	-3.14827600	-0.76165900
C	3.73247500	-4.02203800	0.27359700
C	4.81390500	-4.89038800	0.19209100
C	5.59543100	-4.90425800	-0.95760900
C	5.28845500	-4.04952400	-2.01059900
C	4.20031000	-3.19031700	-1.90399600
F	3.01433400	-4.03688700	1.40681500
F	5.11111600	-5.69866300	1.21049300
F	6.63395000	-5.73027200	-1.04856500
F	6.03331100	-4.06467000	-3.11482800
F	3.93596500	-2.38767000	-2.93615100
C	-2.58339600	-2.60551600	-0.22235200
C	-3.12759500	-1.31247200	-0.17341300
N	-2.41931300	-0.14348900	-0.26841400
C	-3.31859300	0.88776900	-0.18589600
C	-4.64101900	0.34762100	-0.02931400
C	-4.52231900	-1.00638300	-0.01093000
C	-3.00230700	2.25446400	-0.23225300

C	-1. 71393100	2. 80068700	-0. 33979900
N	-0. 55202900	2. 08457500	-0. 45580500
C	0. 48311800	2. 98023100	-0. 44606900
C	-0. 04545200	4. 31225100	-0. 34329700
C	-1. 39943800	4. 20192400	-0. 27818700
C	1. 84721200	2. 65319400	-0. 49858100
C	2. 81378000	3. 77487500	-0. 39802600
C	2. 96243000	4. 49005500	0. 79137300
C	3. 88677200	5. 51827500	0. 92631400
C	4. 68962100	5. 86135500	-0. 15635300
C	4. 56528000	5. 17082200	-1. 35717400
C	3. 63465300	4. 14285200	-1. 46569600
F	2. 21742500	4. 17427800	1. 85980000
F	4. 01733200	6. 16444400	2. 08579200
F	5. 57849200	6. 84452600	-0. 04156900
F	5. 33466100	5. 50108700	-2. 39360100
F	3. 54574400	3. 49603800	-2. 62928300
C	-3. 53488400	-3. 73888600	-0. 10612100
C	-3. 52625700	-4. 58795000	1. 00265200
C	-4. 40875300	-5. 65495500	1. 12241100
C	-5. 33971900	-5. 88987600	0. 11640600
C	-5. 37860200	-5. 06031000	-0. 99896800
C	-4. 48071100	-4. 00346400	-1. 09951700
F	-2. 65082900	-4. 38437100	1. 99353200
F	-4. 54140100	-3. 23101500	-2. 18651600
F	-6. 26843600	-5. 28859400	-1. 96432000
F	-6. 19140200	-6. 90646600	0. 22175200
F	-4. 37496900	-6. 44588300	2. 19536600
O	-0. 58254200	0. 00243100	-2. 39435900
N	1. 67240100	0. 19595300	-0. 63292200
C	2. 39030300	1. 36453200	-0. 58111200
C	3. 79305100	1. 05530600	-0. 58138400
C	3. 90677000	-0. 29776200	-0. 63489400
C	2. 57518400	-0. 83612400	-0. 66041200
C	-4. 12909400	3. 21454400	-0. 12593100
C	-4. 47242100	4. 05225700	-1. 18999700
C	-5. 52042100	4. 96172300	-1. 10269800
C	-6. 25883900	5. 04679700	0. 07255900
C	-5. 94292300	4. 22686500	1. 15041000
C	-4. 88676100	3. 32993200	1. 04174400
F	-3. 78711800	3. 99349900	-2. 33393800
F	-5. 82687400	5. 74477500	-2. 13654100
F	-7. 26568500	5. 91132600	0. 16611400
F	-6. 64583600	4. 31356600	2. 28003300

F	-4.60136700	2.56627500	2.10176200
H	4.59536000	1.78108600	-0.51834500
H	4.81910000	-0.88233900	-0.62182900
H	1.38009900	-4.95275900	-0.61677800
H	-1.27559700	-5.17303500	-0.36660800
H	-5.31515900	-1.73509300	0.10829000
H	-5.55031500	0.92993800	0.05828000
H	-2.12178100	5.00334300	-0.17775400
H	0.54470900	5.22097900	-0.32268700
H	0.01395700	-1.69688800	4.16020700
H	0.53857300	0.01533400	4.04065600
H	2.06392700	-2.50230300	3.11382700
H	2.00731400	1.32630800	3.10595900
H	4.37505500	-2.27150300	2.74164100
H	4.03701100	2.67944800	2.84259900
H	6.40733500	-0.89350600	2.43672900
H	6.25120600	1.59157000	2.50707500
O	-0.31346400	-0.84726200	2.35622800

$\Delta E_{\text{solv}} = -4527.10041602$ $\Delta G_{\text{solv}} = -4526.62974102$



¹TS5

C	5.95696600	0.63722600	2.28587700
C	4.77337900	1.37976500	2.35450000
C	3.58190600	0.77239200	2.69996000
C	3.54137800	-0.61353400	3.02131000
C	4.75885200	-1.34596000	2.95085500
C	5.93968200	-0.73056700	2.58130700
C	2.35376300	-1.26496500	3.40103800
C	1.02265700	-0.65517300	3.27137000
O	-0.29442200	0.04385200	1.38375900
Ru	-0.45842700	0.01760800	-0.53541200
N	-0.22909500	-2.02774000	-0.53653000
C	0.95396700	-2.71087600	-0.63918400
C	0.67746300	-4.11913400	-0.62374600
C	-0.67046600	-4.26464200	-0.50627900
C	-1.23953700	-2.94685400	-0.43682700
C	2.22781500	-2.13847600	-0.75599500

C	3.39548500	-3.05363600	-0.76404900
C	3.74883800	-3.77021500	0.38066300
C	4.89500800	-4.55243300	0.44105700
C	5.71378100	-4.65421400	-0.67827100
C	5.38088900	-3.96830200	-1.84184800
C	4.23506300	-3.18058100	-1.87234600
F	2.98716700	-3.69620200	1.47845200
F	5.21789500	-5.18732400	1.56996900
F	6.81346300	-5.40207500	-0.63645400
F	6.16270300	-4.06828100	-2.91622400
F	3.95778300	-2.51927000	-2.99822100
C	-2.60653500	-2.65942100	-0.29176800
C	-3.18300100	-1.38130600	-0.19568800
N	-2.50579000	-0.19665500	-0.22872500
C	-3.41423800	0.81486600	-0.08700800
C	-4.72864700	0.24141000	0.03337200
C	-4.58554300	-1.10905900	-0.02438400
C	-3.12072400	2.18751100	-0.04911600
C	-1.84313300	2.76519400	-0.14596000
N	-0.67429300	2.08759800	-0.33499400
C	0.34322900	2.99669800	-0.35391700
C	-0.20492300	4.31312500	-0.16533400
C	-1.55165400	4.17087700	-0.03655600
C	1.70364100	2.70057900	-0.53038100
C	2.65099600	3.84539800	-0.50942600
C	3.02349400	4.45159600	0.69000100
C	3.92985100	5.50427300	0.73479500
C	4.48490200	5.97743900	-0.44979300
C	4.13493800	5.39355300	-1.66281800
C	3.22770400	4.33918100	-1.68010200
F	2.52016900	4.00411600	1.84832300
F	4.27872300	6.05131300	1.89980500
F	5.35535600	6.98305600	-0.42139800
F	4.67008200	5.84689400	-2.79539300
F	2.91971300	3.79000500	-2.85606000
C	-3.53261900	-3.81735400	-0.21858500
C	-3.50873600	-4.70786300	0.85727600
C	-4.37012100	-5.79624000	0.93279800
C	-5.29515300	-6.01019100	-0.08324200
C	-5.34935600	-5.13887600	-1.16565800
C	-4.47232900	-4.06172200	-1.22302300
F	-2.63898400	-4.52617200	1.85587700
F	-4.54758700	-3.24763100	-2.27888500
F	-6.23337800	-5.34660300	-2.14092100

F	-6.12661400	-7.04664400	-0.01913900
F	-4.32189600	-6.62775500	1.97362700
O	-0.71222600	0.16145400	-2.26169500
N	1.59349900	0.23979100	-0.69589800
C	2.27030400	1.42865600	-0.69399200
C	3.67687500	1.16142800	-0.82961700
C	3.82798500	-0.18860100	-0.88070800
C	2.51456100	-0.76522000	-0.78916100
C	-4.26324500	3.11845500	0.12592500
C	-4.63125300	4.01506400	-0.88046400
C	-5.69325100	4.89906500	-0.72703400
C	-6.42230300	4.89644000	0.45724000
C	-6.08313200	4.01501600	1.47805400
C	-5.01288500	3.14504500	1.30438000
F	-3.95657500	4.03885900	-2.03239800
F	-6.02211000	5.74057300	-1.70665000
F	-7.44233300	5.73608400	0.61306100
F	-6.77726600	4.01756600	2.61616300
F	-4.70613700	2.31985000	2.30980100
H	4.45764800	1.91345300	-0.84912400
H	4.75659200	-0.74340600	-0.94299600
H	1.42143400	-4.90254400	-0.70900500
H	-1.23165900	-5.19096000	-0.47817300
H	-5.36539000	-1.85784700	0.04658700
H	-5.64857200	0.80172400	0.14887100
H	-2.28448500	4.95154300	0.12942400
H	0.36885400	5.23248600	-0.14044600
H	0.23488600	-1.18618800	3.82145000
H	0.97766900	0.41377700	3.52467700
H	2.40585200	-2.32931200	3.62312900
H	2.66363900	1.35711400	2.71295100
H	4.73940800	-2.41293400	3.17387500
H	4.78623600	2.44461600	2.12710400
H	6.85879000	-1.31096200	2.52379100
H	6.88985500	1.12236500	2.00539300
O	0.86698100	-0.82167000	1.86376700

$\Delta E_{\text{solv}} = -4527.10179762$ $\Delta G_{\text{solv}} = -4526.62781562$

³TS5

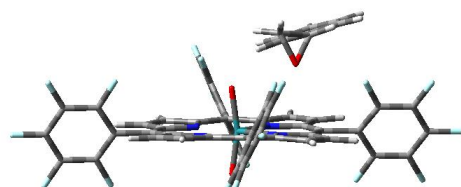
C	4.78318800	0.81609500	2.90157300
C	3.57329300	1.50822300	2.91335300
C	2.36548100	0.82071500	2.94185100
C	2.36434400	-0.58209700	2.94209400

C	3.58589500	-1.27017600	2.90009800
C	4.78907400	-0.57548000	2.89091800
C	1.15767200	-1.39803800	3.10031400
C	-0.11221600	-0.94689400	3.66213800
O	-0.17102500	0.25048800	1.49068600
Ru	-0.30480000	0.03841000	-0.59600000
N	-0.15675300	-2.02317100	-0.52822800
C	0.99684500	-2.75600800	-0.61137300
C	0.66198600	-4.15347400	-0.63956100
C	-0.69268200	-4.24442600	-0.55496600
C	-1.20435200	-2.90413500	-0.47705900
C	2.29950700	-2.22948000	-0.64493000
C	3.41857600	-3.20281300	-0.67298600
C	3.64689100	-4.09821600	0.37455900
C	4.70087000	-5.00281600	0.36847600
C	5.56996100	-5.03218600	-0.71633100
C	5.37333400	-4.15857800	-1.78006200
C	4.30761900	-3.26543300	-1.75057500
F	2.83822600	-4.10266300	1.44967400
F	4.88708400	-5.83275400	1.39630100
F	6.58510000	-5.89199300	-0.73508600
F	6.20041800	-4.19080300	-2.82384200
F	4.14909400	-2.45214000	-2.79579000
C	-2.55957400	-2.56035000	-0.35274200
C	-3.08514500	-1.26041100	-0.28626300
N	-2.35814500	-0.10474000	-0.34788700
C	-3.23328100	0.93997500	-0.23386800
C	-4.57047400	0.42135200	-0.10574400
C	-4.47840300	-0.93382700	-0.12751700
C	-2.89059500	2.30131800	-0.23179800
C	-1.59337900	2.83253500	-0.30594900
N	-0.43848900	2.10514400	-0.39906100
C	0.60876500	2.98377100	-0.40638700
C	0.09372500	4.32451200	-0.32794200
C	-1.26123300	4.23110800	-0.26047200
C	1.96798200	2.63298500	-0.46527600
C	2.94806900	3.74479600	-0.39797000
C	3.06128700	4.54978100	0.73790900
C	3.98017600	5.58805400	0.82477000
C	4.82178200	5.84780800	-0.25123600
C	4.73705900	5.06701600	-1.39872300
C	3.80673400	4.03508100	-1.46161800
F	2.27827300	4.32182700	1.80375100
F	4.06655500	6.32728300	1.93190800

F	5.70776300	6.83818500	-0.18069200
F	5.54039600	5.31866700	-2.43170800
F	3.75154800	3.31172600	-2.58131900
C	-3.52631600	-3.68190800	-0.25175500
C	-3.53729100	-4.53193300	0.85616900
C	-4.43183000	-5.58929600	0.96843700
C	-5.35688700	-5.81320900	-0.04545700
C	-5.37768200	-4.98185900	-1.15986000
C	-4.46728300	-3.93471300	-1.25243300
F	-2.66972100	-4.33656000	1.85778800
F	-4.51136600	-3.16059200	-2.33870500
F	-6.26243900	-5.19971700	-2.13248400
F	-6.22081300	-6.82070300	0.05210300
F	-4.41656000	-6.38077300	2.04221300
O	-0.43337400	0.11601100	-2.36684900
N	1.76298100	0.17729700	-0.61680800
C	2.49144600	1.33286700	-0.54709000
C	3.89268700	1.00249800	-0.51921500
C	3.98700100	-0.35080400	-0.56864800
C	2.64439100	-0.86770800	-0.62933500
C	-4.00509200	3.27589000	-0.11688500
C	-4.33692400	4.13123300	-1.17009300
C	-5.37386300	5.05243600	-1.07228000
C	-6.11415800	5.13016000	0.10216000
C	-5.81078100	4.29128000	1.16875500
C	-4.76481000	3.38371800	1.04979700
F	-3.65026700	4.08027300	-2.31368200
F	-5.66863000	5.85361200	-2.09607500
F	-7.11122900	6.00565500	0.20553400
F	-6.51653200	4.36954600	2.29793600
F	-4.49340300	2.59957000	2.09895800
H	4.70469200	1.71617200	-0.43985400
H	4.89055200	-0.94849900	-0.53560500
H	1.37133600	-4.96794800	-0.72760300
H	-1.29332600	-5.14641500	-0.56213200
H	-5.28637500	-1.65056400	-0.03972300
H	-5.46914700	1.01897500	-0.00959200
H	-1.97333100	5.04392400	-0.18032400
H	0.69065000	5.22883800	-0.33024900
H	-0.77952800	-1.63883800	4.17272000
H	-0.22950000	0.10641100	3.90738300
H	1.31757800	-2.47570100	3.07088100
H	1.42649500	1.36864900	2.93433400
H	3.58476400	-2.35831300	2.89548500

H	3.56471600	2.59503100	2.91228700
H	5.72938400	-1.12294800	2.87284800
H	5.72298900	1.36562700	2.89470500
O	-0.10656800	-1.15882500	2.22834200

$$\Delta E_{\text{solv}} = -4527.10344139 \quad \Delta G_{\text{solv}} = -4526.63007839$$



¹A-C

C	4.34655000	1.69600500	3.05013600
C	2.97143200	1.68070600	2.81710100
C	2.26629400	0.48326800	2.84657100
C	2.92575600	-0.71866500	3.13150300
C	4.30591900	-0.69588700	3.35001000
C	5.01482500	0.50249800	3.30717300
C	2.19767200	-2.00803200	3.22542700
C	0.76138900	-2.11052100	3.49036800
O	-0.43915600	0.03729600	1.26816000
Ru	-0.33036400	0.03232900	-0.47714200
N	0.38716200	-1.88053400	-0.61404800
C	1.69946600	-2.24201700	-0.75753500
C	1.76997000	-3.67090300	-0.86044900
C	0.50339400	-4.14962600	-0.73291400
C	-0.37022400	-3.02155200	-0.57013500
C	2.79520200	-1.36641600	-0.76668800
C	4.14803500	-1.95844300	-0.91020000
C	4.69215400	-2.81221100	0.05308500
C	5.97046600	-3.34434200	-0.06918400
C	6.74393000	-3.02757700	-1.18018500
C	6.23190000	-2.18438400	-2.16035300
C	4.95006700	-1.66625300	-2.01767400
F	3.98367600	-3.14544500	1.13528200
F	6.45928100	-4.14947600	0.87430000
F	7.96836100	-3.53101700	-1.30628600
F	6.96738700	-1.88546700	-3.23024800
F	4.49002300	-0.86519900	-2.98232600
C	-1.76250200	-3.09825200	-0.40663200
C	-2.66009200	-2.01655300	-0.33453000
N	-2.31179300	-0.70359600	-0.38130100
C	-3.44198300	0.05110300	-0.27570500

C	-4.57321100	-0.83750000	-0.18299700
C	-4.09160400	-2.10863400	-0.20155300
C	-3.50131200	1.45563800	-0.23317600
C	-2.41165800	2.34530800	-0.25473500
N	-1.09526600	2.00136800	-0.33154700
C	-0.34702400	3.13495400	-0.28030100
C	-1.23139200	4.26682500	-0.17594300
C	-2.50124100	3.78070000	-0.15750100
C	1.05891000	3.18742300	-0.32245200
C	1.67954800	4.53143300	-0.21156700
C	1.59155500	5.27395200	0.96813300
C	2.16521700	6.53362100	1.09303100
C	2.85395900	7.08086600	0.01550000
C	2.96358600	6.36615600	-1.17272100
C	2.37698700	5.10960900	-1.27467100
F	0.94815600	4.76892300	2.02697800
F	2.06709100	7.21306300	2.23488200
F	3.40953500	8.28440800	0.12257200
F	3.62123700	6.89188000	-2.20498300
F	2.49729400	4.45217300	-2.43042900
C	-2.33448400	-4.45928500	-0.26167800
C	-2.01617500	-5.25055700	0.84590400
C	-2.53724100	-6.52843800	1.01037600
C	-3.40586400	-7.04277500	0.05334300
C	-3.74361100	-6.27966100	-1.05934200
C	-3.20532000	-5.00618200	-1.20601500
F	-1.19034600	-4.78157200	1.78522100
F	-3.54123200	-4.30243500	-2.29082000
F	-4.57062800	-6.77580900	-1.97882100
F	-3.91290300	-8.26323000	0.20221000
F	-2.21832800	-7.25861900	2.07848600
O	-0.63194200	0.20461700	-2.18514000
N	1.58188700	0.77406700	-0.54896700
C	1.93460600	2.09747200	-0.44717900
C	3.36689500	2.18417700	-0.46795500
C	3.85310900	0.91902000	-0.58603100
C	2.72896100	0.03105100	-0.64126700
C	-4.85153800	2.06484400	-0.12663500
C	-5.38667800	2.83229500	-1.16380800
C	-6.64546400	3.41562700	-1.07403400
C	-7.40573700	3.23264400	0.07620000
C	-6.90195100	2.47294300	1.12659600
C	-5.63792500	1.90501700	1.01666500
F	-4.68342000	3.02444100	-2.28258300

F	-7.12972900	4.14029600	-2.08184100
F	-8.61262100	3.78357000	0.17174100
F	-7.62688200	2.30253900	2.23182200
F	-5.17927200	1.19068500	2.04825400
H	3.93751900	3.10049800	-0.37347100
H	4.89222000	0.61298700	-0.60045100
H	2.67796700	-4.24238500	-1.00930900
H	0.18500100	-5.18467700	-0.76450200
H	-4.65986400	-3.02849200	-0.13638600
H	-5.60873300	-0.52810000	-0.10857700
H	-3.42121600	4.34708500	-0.07575300
H	-0.92092900	5.30389300	-0.12827500
H	0.37047600	-2.99746000	3.99594400
H	0.16435200	-1.20349500	3.60656400
H	2.82204700	-2.85715800	3.52063500
H	1.19608600	0.47683700	2.63947500
H	4.82670500	-1.63196200	3.55709400
H	2.43984000	2.60936000	2.61111900
H	6.08949700	0.50276700	3.48244700
H	4.89510000	2.63672100	3.02687600
O	1.26795000	-2.32995700	2.18834200

$$\Delta E_{\text{solv}} = -4527.17142417 \quad \Delta G_{\text{solv}} = -4526.69483017$$

³A-C

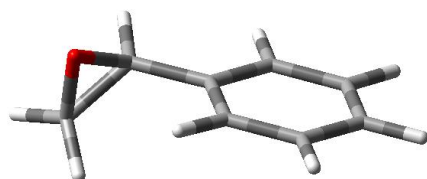
C	5.04772800	1.30692500	2.87124600
C	3.69841600	1.61967300	2.70867100
C	2.72837400	0.62794300	2.79545100
C	3.09918400	-0.69433600	3.06706400
C	4.45450400	-1.00456000	3.21120900
C	5.42543900	-0.01080100	3.11298500
C	2.09097600	-1.76966900	3.22467100
C	0.69695800	-1.52575000	3.59506700
O	-0.14432700	0.34145400	1.36231800
Ru	-0.40742500	0.01740200	-0.54407300
N	0.05390100	-1.96753300	-0.51966100
C	1.31130000	-2.51900700	-0.63948300
C	1.18440800	-3.94711000	-0.66464700
C	-0.13626900	-4.24219900	-0.53262900
C	-0.84510600	-2.99836900	-0.43900100
C	2.52205000	-1.82147900	-0.71835500
C	3.77023700	-2.61445300	-0.84136000
C	4.21610100	-3.45657200	0.17956300
C	5.40923000	-4.16311500	0.08746400

C	6. 19290900	-4. 03979500	-1. 05435400
C	5. 77668000	-3. 21331400	-2. 09265300
C	4. 57937900	-2. 51624700	-1. 97680000
F	3. 49208600	-3. 60144600	1. 29434900
F	5. 80788900	-4. 94876900	1. 08841700
F	7. 33682600	-4. 71091300	-1. 15363700
F	6. 52395300	-3. 09970700	-3. 18981200
F	4. 21067500	-1. 73183400	-2. 99226700
C	-2. 23604500	-2. 86757100	-0. 31543700
C	-2. 94684400	-1. 65963700	-0. 26651300
N	-2. 39673500	-0. 40399000	-0. 33006000
C	-3. 42371900	0. 50720300	-0. 20985500
C	-4. 66190000	-0. 20855400	-0. 10162200
C	-4. 36845800	-1. 53670700	-0. 12245100
C	-3. 29338700	1. 90079800	-0. 16810500
C	-2. 08415200	2. 61704900	-0. 20420000
N	-0. 84629000	2. 06104500	-0. 31363300
C	0. 08053600	3. 06754500	-0. 28667600
C	-0. 61374200	4. 32060800	-0. 16825800
C	-1. 94573800	4. 04407000	-0. 11263900
C	1. 47553000	2. 92042200	-0. 38136200
C	2. 28048600	4. 16749700	-0. 32538200
C	2. 35799400	4. 93239300	0. 84018800
C	3. 11431200	6. 09619200	0. 91143600
C	3. 81966300	6. 52213200	-0. 20915900
C	3. 76506900	5. 78267200	-1. 38583200
C	2. 99968000	4. 62279100	-1. 43270100
F	1. 70327100	4. 53969600	1. 93948700
F	3. 17355200	6. 79923700	2. 04200800
F	4. 54803200	7. 63355000	-0. 15482000
F	4. 43833600	6. 19428700	-2. 45909300
F	2. 96621800	3. 93791500	-2. 57766700
C	-3. 02193000	-4. 12134000	-0. 20849800
C	-2. 88558700	-4. 96979600	0. 89327200
C	-3. 60879300	-6. 15149600	1. 00664600
C	-4. 50345800	-6. 50672000	0. 00269900
C	-4. 66578700	-5. 68194900	-1. 10542000
C	-3. 92641200	-4. 50834500	-1. 20005500
F	-2. 04090500	-4. 65351800	1. 87896300
F	-4. 09944000	-3. 74172100	-2. 28049500
F	-5. 51841300	-6. 02548400	-2. 07014600
F	-5. 20309700	-7. 63340800	0. 10224200
F	-3. 45862100	-6. 93925700	2. 07106800
O	-0. 34009300	0. 28385900	-2. 28321500

N	1.65466700	0.46779200	-0.57935100
C	2.19154100	1.72000300	-0.51844700
C	3.62781500	1.60978200	-0.58010300
C	3.92557400	0.28846700	-0.67203400
C	2.67367400	-0.42397900	-0.67007500
C	-4.53951200	2.69828700	-0.04917000
C	-4.96508800	3.53449300	-1.08409800
C	-6.12524500	4.29437200	-0.98693900
C	-6.89485200	4.22483000	0.16940100
C	-6.49865000	3.40185800	1.21831800
C	-5.33123200	2.65623700	1.10066700
F	-4.24985900	3.61872600	-2.20870400
F	-6.50758600	5.08002000	-1.99281700
F	-8.00815300	4.94489600	0.27221600
F	-7.23330300	3.34149300	2.32854900
F	-4.97353100	1.88248800	2.12974700
H	4.32353500	2.43847400	-0.51976900
H	4.90883300	-0.16585200	-0.69763900
H	2.00562900	-4.64403600	-0.77854200
H	-0.59396200	-5.22405300	-0.52047200
H	-5.06251400	-2.36424800	-0.03947300
H	-5.64062100	0.24649300	-0.01112000
H	-2.76229600	4.74950400	-0.01520000
H	-0.14383700	5.29645000	-0.14091100
H	0.13834200	-2.29642000	4.13108300
H	0.34574600	-0.50255000	3.73916200
H	2.50855100	-2.74849400	3.47577600
H	1.67881300	0.87065700	2.62634900
H	4.74704400	-2.03704300	3.40806000
H	3.39362200	2.64680200	2.51323100
H	6.47699400	-0.26683400	3.23195000
H	5.80280100	2.08886000	2.80506400
O	1.03527100	-1.85020400	2.25740600

$$\Delta E_{\text{solv}} = -4527.12667317 \quad \Delta G_{\text{solv}} = -4526.65344617$$

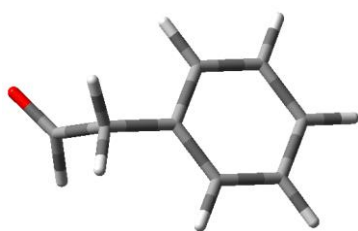
4. Coordinates of all stationary points in Fig. 8



C			
0	2.47428600	-0.40362200	-0.64793100

C	2.57569300	-0.05691700	0.72210100
H	3.48991300	0.46326800	1.00905700
H	2.22444600	-0.81738500	1.42174500
C	1.59528000	0.60151400	-0.14705800
H	1.83216500	1.61051800	-0.49246300
C	0.14990600	0.27551300	-0.08753800
C	-0.28673200	-1.05298600	-0.06721500
C	-0.79371200	1.30473000	-0.03539800
C	-1.64472700	-1.34335900	0.01590500
H	0.44870500	-1.85057100	-0.13837700
C	-2.15307800	1.01344100	0.05171100
H	-0.45889500	2.33993700	-0.06548700
C	-2.58194500	-0.31188000	0.07924100
H	-1.97519100	-2.37848300	0.02539000
H	-2.87753300	1.82222400	0.09131300
H	-3.64201300	-0.54087100	0.14178000

$\Delta E_{\text{solv}} = -384.82332618$ $\Delta G_{\text{solv}} = -384.71625818$

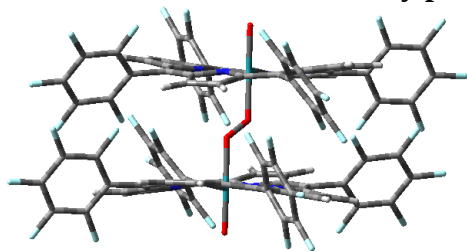


D

O	-3.22376500	0.62187000	-0.45531800
C	-2.36299600	-0.22544300	-0.47121600
H	-2.12213500	-0.79043900	-1.40787100
H	-1.84710300	-0.04047900	1.58474000
C	-1.49015800	-0.59212600	0.70742400
H	-1.60236600	-1.66797700	0.90419300
C	-0.05238400	-0.27519100	0.38704200
C	0.37795200	1.05630600	0.37350400
C	0.85479300	-1.27946000	0.04128200
C	1.69060600	1.37295500	0.04100800
H	-0.32872600	1.84683100	0.62784900
C	2.16911900	-0.96418000	-0.29367800
H	0.52867900	-2.31996300	0.04492800
C	2.59052500	0.36268400	-0.29316000
H	2.01252400	2.41282300	0.04114100
H	2.86630500	-1.75896900	-0.55314800
H	3.61820000	0.60993700	-0.55252800

$$\Delta E_{\text{solv}} = -384.853798285 \quad \Delta G_{\text{solv}} = -384.750721285$$

5. Coordinates of all stationary points in Fig. 10



¹H

O	0.22864100	-0.59010900	0.22362100
O	-0.22864100	0.59010900	-0.22362100
Ru	-0.37590700	1.14474000	-2.15709500
Ru	0.37590700	-1.14474000	2.15709500
N	1.02666900	2.60922600	-1.68027700
C	2.38163500	2.43710100	-1.70848900
C	0.77395000	3.93012100	-1.44672400
C	3.01261900	3.71899800	-1.53814000
C	2.02594500	4.63591700	-1.36693800
H	4.08172900	3.89468200	-1.53136200
H	2.14277800	5.69030600	-1.14975500
N	-1.88088200	2.46351000	-1.69731400
C	-1.72242600	3.78867000	-1.35741700
C	-3.22873300	2.22772400	-1.84139700
C	-3.01794300	4.39149400	-1.25259300
C	-3.93990600	3.43550000	-1.54881100
H	-3.21023400	5.43173000	-1.02287200
H	-5.01428300	3.56020400	-1.60041100
C	-0.50431600	4.48060300	-1.24392700
N	-1.77631100	-0.32038600	-2.54370900
C	-3.12498100	-0.12304600	-2.68422100
C	-1.49793100	-1.59959100	-2.95057600
C	-3.71333100	-1.31393400	-3.23220400
C	-2.71217000	-2.21435400	-3.40766600
H	-4.77048100	-1.46925400	-3.40935800
H	-2.79546200	-3.22177200	-3.79670900
C	-3.81649100	1.04099400	-2.31260500
N	1.14340400	-0.26650900	-2.34941600
C	2.45728100	-0.05109800	-2.03493900
C	0.96477200	-1.61032900	-2.52124000
C	3.13441600	-1.31848900	-1.99972500
C	2.21641800	-2.27755600	-2.30025900
H	4.18239400	-1.46655300	-1.77664300
H	2.37991300	-3.34612100	-2.35786200

C	3. 05037900	1. 20301400	-1. 79620900
C	-0. 24767800	-2. 23242800	-2. 86980800
N	1. 77631100	0. 32038600	2. 54370900
C	3. 12498100	0. 12304600	2. 68422100
C	1. 49793100	1. 59959100	2. 95057600
C	3. 71333100	1. 31393400	3. 23220400
C	2. 71217000	2. 21435400	3. 40766600
H	4. 77048100	1. 46925400	3. 40935800
H	2. 79546200	3. 22177200	3. 79670900
N	1. 88088200	-2. 46351000	1. 69731400
C	1. 72242600	-3. 78867000	1. 35741700
C	3. 22873300	-2. 22772400	1. 84139700
C	3. 01794300	-4. 39149400	1. 25259300
C	3. 93990600	-3. 43550000	1. 54881100
H	3. 21023400	-5. 43173000	1. 02287200
H	5. 01428300	-3. 56020400	1. 60041100
N	-1. 02666900	-2. 60922600	1. 68027700
C	-0. 77395000	-3. 93012100	1. 44672400
C	-2. 38163500	-2. 43710100	1. 70848900
C	-2. 02594500	-4. 63591700	1. 36693800
C	-3. 01261900	-3. 71899800	1. 53814000
H	-2. 14277800	-5. 69030600	1. 14975500
H	-4. 08172900	-3. 89468200	1. 53136200
N	-1. 14340400	0. 26650900	2. 34941600
C	-2. 45728100	0. 05109800	2. 03493900
C	-0. 96477200	1. 61032900	2. 52124000
C	-3. 13441600	1. 31848900	1. 99972500
C	-2. 21641800	2. 27755600	2. 30025900
H	-4. 18239400	1. 46655300	1. 77664300
H	-2. 37991300	3. 34612100	2. 35786200
C	3. 81649100	-1. 04099400	2. 31260500
C	0. 50431600	-4. 48060300	1. 24392700
C	-3. 05037900	-1. 20301400	1. 79620900
C	0. 24767800	2. 23242800	2. 86980800
C	-4. 50767100	-1. 22266600	1. 52722500
C	-5. 46163100	-0. 75491400	2. 43516800
C	-4. 98797300	-1. 69375700	0. 30175100
C	-6. 82057800	-0. 74229900	2. 13589700
C	-6. 33548500	-1. 67254200	-0. 02831000
C	-7. 25928000	-1. 20594800	0. 90000100
C	0. 58152100	-5. 91784200	0. 88336900
C	0. 06606800	-6. 92172100	1. 71009600
C	1. 19066800	-6. 34585100	-0. 30040200
C	0. 11415300	-8. 26722800	1. 36227400

C	1. 27614600	-7. 68517600	-0. 65774800
C	0. 72227700	-8. 65271400	0. 17246300
C	5. 29432400	-1. 03066700	2. 45621300
C	5. 91653000	-0. 83944400	3. 69440600
C	6. 14275100	-1. 22490900	1. 36297100
C	7. 29993400	-0. 80476100	3. 83223200
C	7. 52702000	-1. 22189700	1. 47758700
C	8. 11089600	-0. 99676500	2. 71863300
C	0. 23338300	3. 69319600	3. 11002600
C	-0. 55469200	4. 30269600	4. 09036600
C	1. 03082500	4. 53875600	2. 33304600
C	-0. 55790700	5. 68107100	4. 28146100
C	1. 03680800	5. 91646800	2. 49628200
C	0. 24393400	6. 49061800	3. 48357700
C	-0. 58152100	5. 91784200	-0. 88336900
C	-0. 06606800	6. 92172100	-1. 71009600
C	-1. 19066800	6. 34585100	0. 30040200
C	-0. 11415300	8. 26722800	-1. 36227400
C	-1. 27614600	7. 68517600	0. 65774800
C	-0. 72227700	8. 65271400	-0. 17246300
C	-5. 29432400	1. 03066700	-2. 45621300
C	-5. 91653000	0. 83944400	-3. 69440600
C	-6. 14275100	1. 22490900	-1. 36297100
C	-7. 29993400	0. 80476100	-3. 83223200
C	-7. 52702000	1. 22189700	-1. 47758700
C	-8. 11089600	0. 99676500	-2. 71863300
C	-0. 23338300	-3. 69319600	-3. 11002600
C	0. 55469200	-4. 30269600	-4. 09036600
C	-1. 03082500	-4. 53875600	-2. 33304600
C	0. 55790700	-5. 68107100	-4. 28146100
C	-1. 03680800	-5. 91646800	-2. 49628200
C	-0. 24393400	-6. 49061800	-3. 48357700
C	4. 50767100	1. 22266600	-1. 52722500
C	4. 98797300	1. 69375700	-0. 30175100
C	5. 46163100	0. 75491400	-2. 43516800
C	6. 33548500	1. 67254200	0. 02831000
C	6. 82057800	0. 74229900	-2. 13589700
C	7. 25928000	1. 20594800	-0. 90000100
O	0. 22439500	-1. 57260600	3. 83633800
O	-0. 22439500	1. 57260600	-3. 83633800
F	5. 18041300	-0. 68868600	4. 79844100
F	7. 85254400	-0. 61228900	5. 02837000
F	9. 43338900	-0. 98212200	2. 84356900
F	8. 28934800	-1. 42630500	0. 40280600

F	5.62904900	-1.43132600	0.14099000
F	4.13356700	2.16773900	0.60853800
F	6.74296100	2.07139300	1.23841600
F	8.55443100	1.19731200	-0.60012000
F	7.70420700	0.29833800	-3.02761600
F	5.08326900	0.30635800	-3.63423200
F	-0.48808700	-6.60582200	2.88341100
F	-0.39620600	-9.19062300	2.17467300
F	0.78842100	-9.93737800	-0.15956700
F	1.87917800	-8.03977200	-1.79285100
F	1.72609000	-5.45120500	-1.14537400
F	-1.81077800	-4.02283100	-1.37983600
F	-1.77468400	-6.69101100	-1.69303800
F	-0.24847500	-7.80906000	-3.65507400
F	1.31266000	-6.22879900	-5.23212300
F	1.32587300	-3.56115100	-4.88861300
F	-5.08326900	-0.30635800	3.63423200
F	-7.70420700	-0.29833800	3.02761600
F	-8.55443100	-1.19731200	0.60012000
F	-6.74296100	-2.07139300	-1.23841600
F	-4.13356700	-2.16773900	-0.60853800
F	-5.62904900	1.43132600	-0.14099000
F	-8.28934800	1.42630500	-0.40280600
F	-9.43338900	0.98212200	-2.84356900
F	-7.85254400	0.61228900	-5.02837000
F	-5.18041300	0.68868600	-4.79844100
F	-1.32587300	3.56115100	4.88861300
F	-1.31266000	6.22879900	5.23212300
F	0.24847500	7.80906000	3.65507400
F	1.77468400	6.69101100	1.69303800
F	1.81077800	4.02283100	1.37983600
F	-1.72609000	5.45120500	1.14537400
F	-1.87917800	8.03977200	1.79285100
F	-0.78842100	9.93737800	0.15956700
F	0.39620600	9.19062300	-2.17467300
F	0.48808700	6.60582200	-2.88341100

$$\Delta E_{\text{solv}} = -8286.39346455 \quad \Delta G_{\text{solv}} = -8285.65214855$$

³H

O	0.37611900	-0.46464500	0.24750000
O	-0.37611900	0.46464500	-0.24750000
Ru	-0.41218100	1.16967600	-2.26713800
Ru	0.41218100	-1.16967600	2.26713800

N	0.98184000	2.60529800	-1.72389100
C	2.33860500	2.43142400	-1.73098200
C	0.73222100	3.92992900	-1.48982500
C	2.97117900	3.70903700	-1.54737800
C	1.98504000	4.62882500	-1.38844500
H	4.04065600	3.88079500	-1.52533500
H	2.10304300	5.68491500	-1.18224700
N	-1.92276300	2.49155900	-1.82212600
C	-1.76523400	3.81090000	-1.46488100
C	-3.27019000	2.26301500	-1.98234900
C	-3.05858100	4.42072000	-1.37083300
C	-3.98080000	3.47237700	-1.68879400
H	-3.24643800	5.45934800	-1.12853600
H	-5.05426600	3.60067100	-1.75161200
C	-0.54420100	4.48904500	-1.31022900
N	-1.82940100	-0.28858600	-2.67785900
C	-3.17529300	-0.09072600	-2.82305400
C	-1.55361400	-1.57397400	-3.05541100
C	-3.76765300	-1.28970400	-3.35248200
C	-2.76851800	-2.19631800	-3.50553800
H	-4.82233900	-1.44110100	-3.54408200
H	-2.85203900	-3.21091900	-3.87614800
C	-3.86197300	1.07663100	-2.44868800
N	1.09745200	-0.24812500	-2.41723900
C	2.41114200	-0.04771300	-2.09158900
C	0.91146000	-1.59061200	-2.60407400
C	3.08303200	-1.31773100	-2.07212300
C	2.16076000	-2.26647400	-2.38805300
H	4.12965400	-1.47341900	-1.84616400
H	2.32114700	-3.33359600	-2.46763300
C	3.00569500	1.19753500	-1.81849200
C	-0.30442200	-2.20893100	-2.94737700
N	1.82940100	0.28858600	2.67785900
C	3.17529300	0.09072600	2.82305400
C	1.55361400	1.57397400	3.05541100
C	3.76765300	1.28970400	3.35248200
C	2.76851800	2.19631800	3.50553800
H	4.82233900	1.44110100	3.54408200
H	2.85203900	3.21091900	3.87614800
N	1.92276300	-2.49155900	1.82212600
C	1.76523400	-3.81090000	1.46488100
C	3.27019000	-2.26301500	1.98234900
C	3.05858100	-4.42072000	1.37083300
C	3.98080000	-3.47237700	1.68879400

H	3.24643800	-5.45934800	1.12853600
H	5.05426600	-3.60067100	1.75161200
N	-0.98184000	-2.60529800	1.72389100
C	-0.73222100	-3.92992900	1.48982500
C	-2.33860500	-2.43142400	1.73098200
C	-1.98504000	-4.62882500	1.38844500
C	-2.97117900	-3.70903700	1.54737800
H	-2.10304300	-5.68491500	1.18224700
H	-4.04065600	-3.88079500	1.52533500
N	-1.09745200	0.24812500	2.41723900
C	-2.41114200	0.04771300	2.09158900
C	-0.91146000	1.59061200	2.60407400
C	-3.08303200	1.31773100	2.07212300
C	-2.16076000	2.26647400	2.38805300
H	-4.12965400	1.47341900	1.84616400
H	-2.32114700	3.33359600	2.46763300
C	3.86197300	-1.07663100	2.44868800
C	0.54420100	-4.48904500	1.31022900
C	-3.00569500	-1.19753500	1.81849200
C	0.30442200	2.20893100	2.94737700
C	-4.45254300	-1.21352000	1.50064900
C	-5.44049900	-0.76456200	2.38047200
C	-4.88411800	-1.67892000	0.25428000
C	-6.78911600	-0.76687200	2.03735100
C	-6.22169000	-1.67998600	-0.11537100
C	-7.18074700	-1.23526900	0.78784800
C	0.61652700	-5.91713300	0.91207900
C	0.10346400	-6.94400000	1.71016200
C	1.21302700	-6.30701300	-0.29082300
C	0.14759200	-8.27827600	1.32032800
C	1.29764700	-7.63507800	-0.68851200
C	0.74824000	-8.62718000	0.11530500
C	5.34350500	-1.05787600	2.53784300
C	6.02018900	-0.85511100	3.74435600
C	6.14060600	-1.24592900	1.40477500
C	7.40836400	-0.80714700	3.81635000
C	7.52839600	-1.23307700	1.45492500
C	8.16766300	-0.99707000	2.66652000
C	0.29919900	3.67801900	3.13730100
C	-0.48168400	4.32661600	4.09732100
C	1.09587700	4.48874300	2.32252300
C	-0.48025900	5.71117900	4.23602100
C	1.10757300	5.87181700	2.43561700
C	0.32445400	6.48522600	3.40702800

C	-0.61652700	5.91713300	-0.91207900
C	-0.10346400	6.94400000	-1.71016200
C	-1.21302700	6.30701300	0.29082300
C	-0.14759200	8.27827600	-1.32032800
C	-1.29764700	7.63507800	0.68851200
C	-0.74824000	8.62718000	-0.11530500
C	-5.34350500	1.05787600	-2.53784300
C	-6.02018900	0.85511100	-3.74435600
C	-6.14060600	1.24592900	-1.40477500
C	-7.40836400	0.80714700	-3.81635000
C	-7.52839600	1.23307700	-1.45492500
C	-8.16766300	0.99707000	-2.66652000
C	-0.29919900	-3.67801900	-3.13730100
C	0.48168400	-4.32661600	-4.09732100
C	-1.09587700	-4.48874300	-2.32252300
C	0.48025900	-5.71117900	-4.23602100
C	-1.10757300	-5.87181700	-2.43561700
C	-0.32445400	-6.48522600	-3.40702800
C	4.45254300	1.21352000	-1.50064900
C	4.88411800	1.67892000	-0.25428000
C	5.44049900	0.76456200	-2.38047200
C	6.22169000	1.67998600	0.11537100
C	6.78911600	0.76687200	-2.03735100
C	7.18074700	1.23526900	-0.78784800
O	0.26516500	-1.57783200	3.95527600
O	-0.26516500	1.57783200	-3.95527600
F	5.33451500	-0.70387100	4.88050200
F	8.01496300	-0.60353300	4.98417800
F	9.49441300	-0.97107500	2.72911500
F	8.24179100	-1.43786400	0.34701600
F	5.57099200	-1.45210500	0.20793200
F	3.98997900	2.12560600	0.63170200
F	6.59157100	2.08195800	1.33626500
F	8.46620500	1.24757700	-0.44737600
F	7.70724300	0.33942600	-2.90170900
F	5.10617800	0.32239100	-3.59519000
F	-0.44779900	-6.66130300	2.89344700
F	-0.36103700	-9.22599500	2.10542100
F	0.81156900	-9.90115200	-0.25614000
F	1.89487600	-7.95486100	-1.83715100
F	1.73517000	-5.38498900	-1.11355800
F	-1.86846300	-3.93168100	-1.38612300
F	-1.84551000	-6.61744800	-1.60609000
F	-0.34104700	-7.80908000	-3.53141200

F	1.22941100	-6.29755300	-5.16757300
F	1.25307900	-3.61764300	-4.92496600
F	-5.10617800	-0.32239100	3.59519000
F	-7.70724300	-0.33942600	2.90170900
F	-8.46620500	-1.24757700	0.44737600
F	-6.59157100	-2.08195800	-1.33626500
F	-3.98997900	-2.12560600	-0.63170200
F	-5.57099200	1.45210500	-0.20793200
F	-8.24179100	1.43786400	-0.34701600
F	-9.49441300	0.97107500	-2.72911500
F	-8.01496300	0.60353300	-4.98417800
F	-5.33451500	0.70387100	-4.88050200
F	-1.25307900	3.61764300	4.92496600
F	-1.22941100	6.29755300	5.16757300
F	0.34104700	7.80908000	3.53141200
F	1.84551000	6.61744800	1.60609000
F	1.86846300	3.93168100	1.38612300
F	-1.73517000	5.38498900	1.11355800
F	-1.89487600	7.95486100	1.83715100
F	-0.81156900	9.90115200	0.25614000
F	0.36103700	9.22599500	-2.10542100
F	0.44779900	6.66130300	-2.89344700

$$\Delta E_{\text{solv}} = - 8286.41851374 \quad \Delta G_{\text{solv}} = - 8285.68398074$$

⁵H

O	0.15502500	-0.61368700	0.13877000
O	-0.15502500	0.61368700	-0.13877000
Ru	-0.38699900	1.18694700	-2.31476700
Ru	0.38699900	-1.18694700	2.31476700
N	1.00093200	2.62553900	-1.75274500
C	2.35707500	2.45399500	-1.76231600
C	0.75093600	3.94935000	-1.51177500
C	2.98910000	3.73095000	-1.57553200
C	2.00217700	4.64947800	-1.41127300
H	4.05857900	3.90340700	-1.55667500
H	2.11927600	5.70498900	-1.20188200
N	-1.89952400	2.50267400	-1.82524100
C	-1.74350000	3.82263100	-1.46755200
C	-3.24737100	2.27199000	-1.96411900
C	-3.03740000	4.42958000	-1.35814100
C	-3.96004000	3.47851400	-1.66322500
H	-3.22537300	5.46751300	-1.11372000
H	-5.03495400	3.60124900	-1.71017400

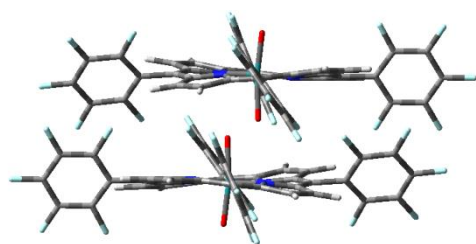
C	-0.52490400	4.50526400	-1.32162100
N	-1.79618400	-0.27917900	-2.64077900
C	-3.14853500	-0.08572700	-2.77744100
C	-1.52518400	-1.56919500	-3.02507900
C	-3.74059300	-1.28449700	-3.30005700
C	-2.74117800	-2.18990000	-3.46379500
H	-4.79690600	-1.43702600	-3.48159400
H	-2.82695800	-3.20402400	-3.83486900
C	-3.83911400	1.08073500	-2.41526600
N	1.11943800	-0.23082600	-2.44846800
C	2.43270000	-0.02527300	-2.11799000
C	0.93761100	-1.57840100	-2.60738900
C	3.10491100	-1.29514100	-2.07280000
C	2.18495300	-2.25021900	-2.37502600
H	4.15032000	-1.44586300	-1.83917800
H	2.34335000	-3.31962000	-2.42652700
C	3.02555100	1.22037100	-1.84866200
C	-0.27695400	-2.20382300	-2.93625600
N	1.79618400	0.27917900	2.64077900
C	3.14853500	0.08572700	2.77744100
C	1.52518400	1.56919500	3.02507900
C	3.74059300	1.28449700	3.30005700
C	2.74117800	2.18990000	3.46379500
H	4.79690600	1.43702600	3.48159400
H	2.82695800	3.20402400	3.83486900
N	1.89952400	-2.50267400	1.82524100
C	1.74350000	-3.82263100	1.46755200
C	3.24737100	-2.27199000	1.96411900
C	3.03740000	-4.42958000	1.35814100
C	3.96004000	-3.47851400	1.66322500
H	3.22537300	-5.46751300	1.11372000
H	5.03495400	-3.60124900	1.71017400
N	-1.00093200	-2.62553900	1.75274500
C	-0.75093600	-3.94935000	1.51177500
C	-2.35707500	-2.45399500	1.76231600
C	-2.00217700	-4.64947800	1.41127300
C	-2.98910000	-3.73095000	1.57553200
H	-2.11927600	-5.70498900	1.20188200
H	-4.05857900	-3.90340700	1.55667500
N	-1.11943800	0.23082600	2.44846800
C	-2.43270000	0.02527300	2.11799000
C	-0.93761100	1.57840100	2.60738900
C	-3.10491100	1.29514100	2.07280000
C	-2.18495300	2.25021900	2.37502600

H	-4.15032000	1.44586300	1.83917800
H	-2.34335000	3.31962000	2.42652700
C	3.83911400	-1.08073500	2.41526600
C	0.52490400	-4.50526400	1.32162100
C	-3.02555100	-1.22037100	1.84866200
C	0.27695400	2.20382300	2.93625600
C	-4.46935200	-1.23635600	1.51656500
C	-5.46613300	-0.78141300	2.38316300
C	-4.88756100	-1.70214900	0.26567700
C	-6.81044900	-0.77851900	2.02331100
C	-6.22023200	-1.69694200	-0.12106000
C	-7.18854900	-1.24725300	0.76970500
C	0.59964800	-5.93185200	0.91899300
C	0.08990900	-6.96218600	1.71489900
C	1.19817600	-6.31778800	-0.28434500
C	0.13793900	-8.29548000	1.32220900
C	1.28678200	-7.64475100	-0.68467500
C	0.73989700	-8.64017800	0.11668600
C	5.32067700	-1.05776000	2.50707700
C	5.99332800	-0.85035500	3.71511300
C	6.12187400	-1.24819700	1.37769800
C	7.38124300	-0.80051000	3.79152900
C	7.50952400	-1.23436200	1.43217200
C	8.14468200	-0.99341500	2.64487600
C	0.27395600	3.67259700	3.12206500
C	-0.49962500	4.32224200	4.08745800
C	1.06969900	4.48211400	2.30469900
C	-0.48851900	5.70604900	4.23242700
C	1.09306900	5.86427100	2.42626400
C	0.31850600	6.47840900	3.40406700
C	-0.59964800	5.93185200	-0.91899300
C	-0.08990900	6.96218600	-1.71489900
C	-1.19817600	6.31778800	0.28434500
C	-0.13793900	8.29548000	-1.32220900
C	-1.28678200	7.64475100	0.68467500
C	-0.73989700	8.64017800	-0.11668600
C	-5.32067700	1.05776000	-2.50707700
C	-5.99332800	0.85035500	-3.71511300
C	-6.12187400	1.24819700	-1.37769800
C	-7.38124300	0.80051000	-3.79152900
C	-7.50952400	1.23436200	-1.43217200
C	-8.14468200	0.99341500	-2.64487600
C	-0.27395600	-3.67259700	-3.12206500
C	0.49962500	-4.32224200	-4.08745800

C	-1.06969900	-4.48211400	-2.30469900
C	0.48851900	-5.70604900	-4.23242700
C	-1.09306900	-5.86427100	-2.42626400
C	-0.31850600	-6.47840900	-3.40406700
C	4.46935200	1.23635600	-1.51656500
C	4.88756100	1.70214900	-0.26567700
C	5.46613300	0.78141300	-2.38316300
C	6.22023200	1.69694200	0.12106000
C	6.81044900	0.77851900	-2.02331100
C	7.18854900	1.24725300	-0.76970500
O	0.25200700	-1.65662300	3.99092500
O	-0.25200700	1.65662300	-3.99092500
F	5.30369400	-0.69483900	4.84828500
F	7.98369400	-0.59181700	4.96058200
F	9.47114300	-0.96539600	2.71168300
F	8.22621200	-1.44117500	0.32671400
F	5.55635100	-1.45852500	0.17965300
F	3.98468500	2.15289500	0.60954600
F	6.57607800	2.09703900	1.34690800
F	8.46963900	1.25355000	-0.41280000
F	7.73735700	0.34465700	-2.87487800
F	5.14421500	0.33566100	-3.59984700
F	-0.46119200	-6.68425200	2.89932400
F	-0.36780600	-9.24630400	2.10538600
F	0.80694100	-9.91313900	-0.25752700
F	1.88540500	-7.96044400	-1.83377400
F	1.71807800	-5.39310100	-1.10579200
F	-1.83149900	-3.92594300	-1.35873900
F	-1.83331600	-6.60879300	-1.59759600
F	-0.34510200	-7.80143300	-3.53509200
F	1.22975800	-6.29309000	-5.16988400
F	1.27054400	-3.61427200	-4.91630100
F	-5.14421500	-0.33566100	3.59984700
F	-7.73735700	-0.34465700	2.87487800
F	-8.46963900	-1.25355000	0.41280000
F	-6.57607800	-2.09703900	-1.34690800
F	-3.98468500	-2.15289500	-0.60954600
F	-5.55635100	1.45852500	-0.17965300
F	-8.22621200	1.44117500	-0.32671400
F	-9.47114300	0.96539600	-2.71168300
F	-7.98369400	0.59181700	-4.96058200
F	-5.30369400	0.69483900	-4.84828500
F	-1.27054400	3.61427200	4.91630100
F	-1.22975800	6.29309000	5.16988400

F	0.34510200	7.80143300	3.53509200
F	1.83331600	6.60879300	1.59759600
F	1.83149900	3.92594300	1.35873900
F	-1.71807800	5.39310100	1.10579200
F	-1.88540500	7.96044400	1.83377400
F	-0.80694100	9.91313900	0.25752700
F	0.36780600	9.24630400	-2.10538600
F	0.46119200	6.68425200	-2.89932400

$\Delta E_{\text{solv}} = -8286.40648084$ $\Delta G_{\text{solv}} = -8285.67299984$



¹TS6

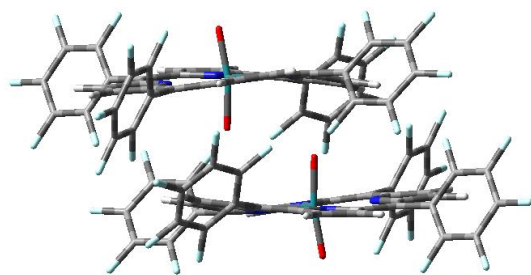
O	0.26131000	-0.72100200	0.24716500
O	-0.26131000	0.72100200	-0.24716500
Ru	-0.37920100	1.10383800	-2.08729200
Ru	0.37920100	-1.10383800	2.08729200
N	1.03430500	2.59600900	-1.61074200
C	2.38383800	2.42910800	-1.65360500
C	0.77089000	3.91541300	-1.39721000
C	3.01238400	3.71596400	-1.49748100
C	2.02188500	4.62878200	-1.32794200
H	4.08058000	3.89722200	-1.50065900
H	2.13485100	5.68636900	-1.12405200
N	-1.90062600	2.46442600	-1.68401700
C	-1.73526300	3.78347600	-1.34938100
C	-3.23879200	2.23362100	-1.84524900
C	-3.03166600	4.39825500	-1.26407200
C	-3.95431700	3.44707500	-1.56736200
H	-3.21994400	5.44045100	-1.03917600
H	-5.02776200	3.57444500	-1.63226100
C	-0.51179200	4.46655300	-1.21783000
N	-1.76812900	-0.33078100	-2.52455200
C	-3.11820400	-0.12134600	-2.68385900
C	-1.48651700	-1.60488200	-2.95042400
C	-3.69618900	-1.30039000	-3.26026900
C	-2.69496700	-2.20362600	-3.43351100
H	-4.74732800	-1.44459700	-3.47543900
H	-2.77607900	-3.20193100	-3.84601000

C	-3.81617100	1.04080000	-2.31886300
N	1.14760200	-0.27674400	-2.33959900
C	2.45964100	-0.05768700	-2.01215100
C	0.97423200	-1.62019800	-2.51988500
C	3.13948900	-1.32477300	-1.98278300
C	2.22689600	-2.28446700	-2.29419400
H	4.18566900	-1.47164300	-1.75071500
H	2.39442500	-3.35215500	-2.35581000
C	3.05204900	1.19345100	-1.75842500
C	-0.23660000	-2.24011000	-2.87354000
O	-0.21987400	1.70150600	-3.72065500
N	1.76812900	0.33078100	2.52455200
C	3.11820400	0.12134600	2.68385900
C	1.48651700	1.60488200	2.95042400
C	3.69618900	1.30039000	3.26026900
C	2.69496700	2.20362600	3.43351100
H	4.74732800	1.44459700	3.47543900
H	2.77607900	3.20193100	3.84601000
N	1.90062600	-2.46442600	1.68401700
C	1.73526300	-3.78347600	1.34938100
C	3.23879200	-2.23362100	1.84524900
C	3.03166600	-4.39825500	1.26407200
C	3.95431700	-3.44707500	1.56736200
H	3.21994400	-5.44045100	1.03917600
H	5.02776200	-3.57444500	1.63226100
N	-1.03430500	-2.59600900	1.61074200
C	-0.77089000	-3.91541300	1.39721000
C	-2.38383800	-2.42910800	1.65360500
C	-2.02188500	-4.62878200	1.32794200
C	-3.01238400	-3.71596400	1.49748100
H	-2.13485100	-5.68636900	1.12405200
H	-4.08058000	-3.89722200	1.50065900
N	-1.14760200	0.27674400	2.33959900
C	-2.45964100	0.05768700	2.01215100
C	-0.97423200	1.62019800	2.51988500
C	-3.13948900	1.32477300	1.98278300
C	-2.22689600	2.28446700	2.29419400
H	-4.18566900	1.47164300	1.75071500
H	-2.39442500	3.35215500	2.35581000
C	3.81617100	-1.04080000	2.31886300
C	0.51179200	-4.46655300	1.21783000
C	-3.05204900	-1.19345100	1.75842500
O	0.21987400	-1.70150600	3.72065500
C	0.23660000	2.24011000	2.87354000

C	-4.51161300	-1.21487800	1.50486400
C	-5.45484400	-0.74880600	2.42539200
C	-5.00773400	-1.69339500	0.28812700
C	-6.81774300	-0.74118300	2.14566600
C	-6.36055300	-1.67976000	-0.02109400
C	-7.27226500	-1.21055700	0.91786100
C	0.58841900	-5.90858500	0.87344400
C	0.07266700	-6.90288000	1.71114300
C	1.19892700	-6.34858300	-0.30476300
C	0.12217800	-8.25217800	1.37833200
C	1.28409800	-7.69156500	-0.64819800
C	0.73061800	-8.65009400	0.19279100
C	5.29291000	-1.02580700	2.47592100
C	5.90691900	-0.84491600	3.71949800
C	6.14815300	-1.21171300	1.38646600
C	7.28937300	-0.80954500	3.86630100
C	7.53172000	-1.20575200	1.50942000
C	8.10740500	-0.99027400	2.75601100
C	0.22489300	3.69920200	3.12059600
C	-0.57650800	4.30813600	4.09073300
C	1.03394000	4.54566600	2.35584100
C	-0.58470700	5.68645200	4.28128900
C	1.03139500	5.92384600	2.51570500
C	0.22402100	6.49721000	3.49166800
C	-0.58841900	5.90858500	-0.87344400
C	-0.07266700	6.90288000	-1.71114300
C	-1.19892700	6.34858300	0.30476300
C	-0.12217800	8.25217800	-1.37833200
C	-1.28409800	7.69156500	0.64819800
C	-0.73061800	8.65009400	-0.19279100
C	-5.29291000	1.02580700	-2.47592100
C	-5.90691900	0.84491600	-3.71949800
C	-6.14815300	1.21171300	-1.38646600
C	-7.28937300	0.80954500	-3.86630100
C	-7.53172000	1.20575200	-1.50942000
C	-8.10740500	0.99027400	-2.75601100
C	-0.22489300	-3.69920200	-3.12059600
C	0.57650800	-4.30813600	-4.09073300
C	-1.03394000	-4.54566600	-2.35584100
C	0.58470700	-5.68645200	-4.28128900
C	-1.03139500	-5.92384600	-2.51570500
C	-0.22402100	-6.49721000	-3.49166800
C	4.51161300	1.21487800	-1.50486400
C	5.00773400	1.69339500	-0.28812700

C	5.45484400	0.74880600	-2.42539200
C	6.36055300	1.67976000	0.02109400
C	6.81774300	0.74118300	-2.14566600
C	7.27226500	1.21055700	-0.91786100
F	-5.06219000	-0.29848300	3.61925000
F	-7.68982200	-0.29739600	3.04879600
F	-8.57135700	-1.20610100	0.63596400
F	-6.78646900	-2.08813000	-1.22129100
F	-4.16465600	-2.16730500	-0.63355400
F	-0.48308900	-6.57392200	2.87988300
F	-0.38768100	-9.16708200	2.20065700
F	0.79746500	-9.93833400	-0.12520900
F	1.73642400	-5.46209900	-1.15677400
F	1.88818600	-8.05864100	-1.77874400
F	5.64181400	-1.41280100	0.16075500
F	8.30140900	-1.39929500	0.43792200
F	9.42907600	-0.97361400	2.88909000
F	7.83428500	-0.62626100	5.06743600
F	5.16337700	-0.70384700	4.82008100
F	1.83526100	4.03105700	1.41983600
F	1.77694900	6.69941100	1.72098000
F	0.22268300	7.81587100	3.66113200
F	-1.35212200	6.23310900	5.22234800
F	-1.35698300	3.56579000	4.87952100
F	0.48308900	6.57392200	-2.87988300
F	0.38768100	9.16708200	-2.20065700
F	-0.79746500	9.93833400	0.12520900
F	-1.88818600	8.05864100	1.77874400
F	-1.73642400	5.46209900	1.15677400
F	-5.64181400	1.41280100	-0.16075500
F	-8.30140900	1.39929500	-0.43792200
F	-9.42907600	0.97361400	-2.88909000
F	-7.83428500	0.62626100	-5.06743600
F	-5.16337700	0.70384700	-4.82008100
F	-1.83526100	-4.03105700	-1.41983600
F	-1.77694900	-6.69941100	-1.72098000
F	-0.22268300	-7.81587100	-3.66113200
F	1.35212200	-6.23310900	-5.22234800
F	1.35698300	-3.56579000	-4.87952100
F	5.06219000	0.29848300	-3.61925000
F	7.68982200	0.29739600	-3.04879600
F	8.57135700	1.20610100	-0.63596400
F	4.16465600	2.16730500	0.63355400
F	6.78646900	2.08813000	1.22129100

$$\Delta E_{\text{solv}} = -8286.38448269 \quad \Delta G_{\text{solv}} = -8285.64537169$$



¹A-¹A

O	0.36446500	-1.62370200	0.34412900
O	-0.36446500	1.62370200	-0.34412900
Ru	-0.31079100	1.70971400	-2.08846200
Ru	0.31079100	-1.70971400	2.08846200
N	1.11632300	3.24172100	-1.76725500
C	2.45983700	3.06537200	-1.65002100
C	0.83689700	4.56960600	-1.64104000
C	3.07963800	4.35513600	-1.49010900
C	2.08351400	5.27952700	-1.47945500
H	4.14445000	4.52831300	-1.38726200
H	2.18358200	6.34956300	-1.34508800
N	-1.85993800	3.13208000	-1.88505800
C	-1.68429900	4.46982600	-1.68754900
C	-3.19455000	2.86947700	-1.93966800
C	-2.98477100	5.08905400	-1.61891800
C	-3.91236800	4.10429300	-1.76408400
H	-3.16829300	6.14886000	-1.48991100
H	-4.99089600	4.21009300	-1.77767900
C	-0.44966900	5.14368200	-1.59012600
N	-1.70617800	0.24926800	-2.42913100
C	-3.06938500	0.41941000	-2.46453800
C	-1.42621800	-1.05395100	-2.75208000
C	-3.66502800	-0.83394200	-2.83007600
C	-2.65803000	-1.72473900	-3.03549300
H	-4.72618100	-1.03352700	-2.91071300
H	-2.75573300	-2.76412500	-3.32276100
C	-3.76878900	1.61071000	-2.19825400
N	1.21051400	0.33816400	-2.21615100
C	2.51311300	0.56535200	-1.84475000
C	1.04230400	-1.00807900	-2.38672600
C	3.17619400	-0.70381600	-1.74788600
C	2.28200900	-1.66620100	-2.09617000
H	4.19774900	-0.85461600	-1.43584000

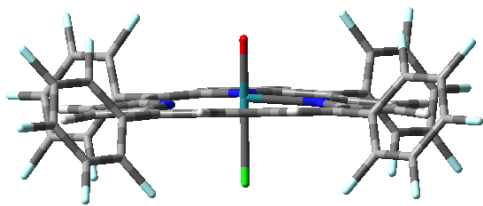
H	2.43985700	-2.73864400	-2.10037600
C	3.11534700	1.81869000	-1.62251600
C	-0.15801800	-1.65209300	-2.72361800
N	1.70617800	-0.24926800	2.42913100
C	3.06938500	-0.41941000	2.46453800
C	1.42621800	1.05395100	2.75208000
C	3.66502800	0.83394200	2.83007600
C	2.65803000	1.72473900	3.03549300
H	4.72618100	1.03352700	2.91071300
H	2.75573300	2.76412500	3.32276100
N	1.85993800	-3.13208000	1.88505800
C	1.68429900	-4.46982600	1.68754900
C	3.19455000	-2.86947700	1.93966800
C	2.98477100	-5.08905400	1.61891800
C	3.91236800	-4.10429300	1.76408400
H	3.16829300	-6.14886000	1.48991100
H	4.99089600	-4.21009300	1.77767900
N	-1.11632300	-3.24172100	1.76725500
C	-0.83689700	-4.56960600	1.64104000
C	-2.45983700	-3.06537200	1.65002100
C	-2.08351400	-5.27952700	1.47945500
C	-3.07963800	-4.35513600	1.49010900
H	-2.18358200	-6.34956300	1.34508800
H	-4.14445000	-4.52831300	1.38726200
N	-1.21051400	-0.33816400	2.21615100
C	-2.51311300	-0.56535200	1.84475000
C	-1.04230400	1.00807900	2.38672600
C	-3.17619400	0.70381600	1.74788600
C	-2.28200900	1.66620100	2.09617000
H	-4.19774900	0.85461600	1.43584000
H	-2.43985700	2.73864400	2.10037600
C	3.76878900	-1.61071000	2.19825400
C	0.44966900	-5.14368200	1.59012600
C	-3.11534700	-1.81869000	1.62251600
C	0.15801800	1.65209300	2.72361800
C	-4.56152200	-1.78093900	1.28254300
C	-5.49881800	-1.15969900	2.11799300
C	-5.03946000	-2.24109600	0.05000900
C	-6.81370600	-0.93329900	1.72444600
C	-6.34448300	-2.01339800	-0.37054000
C	-7.23788400	-1.36433300	0.47246800
C	0.50923500	-6.61141000	1.36865800
C	-0.01037100	-7.51867400	2.29557900
C	1.06260400	-7.15185600	0.20584200

C	0.00200700	-8.89100700	2.07059200
C	1.08323100	-8.51679400	-0.04668900
C	0.55097400	-9.39138900	0.89461900
C	5.25176500	-1.50991700	2.19932800
C	5.96457000	-1.13494800	3.34291400
C	6.00453000	-1.70722600	1.03864300
C	7.33710800	-0.91170200	3.32269300
C	7.37700500	-1.49698800	0.99274800
C	8.04690800	-1.08411200	2.13871900
C	0.07394600	3.11055100	2.96015100
C	-0.73398300	3.64589100	3.96777900
C	0.74186400	4.02223500	2.13704700
C	-0.88989200	5.01729500	4.14181300
C	0.60709200	5.39278200	2.30034600
C	-0.22305900	5.89389300	3.29431200
C	-0.50923500	6.61141000	-1.36865800
C	0.01037100	7.51867400	-2.29557900
C	-1.06260400	7.15185600	-0.20584200
C	-0.00200700	8.89100700	-2.07059200
C	-1.08323100	8.51679400	0.04668900
C	-0.55097400	9.39138900	-0.89461900
C	-5.25176500	1.50991700	-2.19932800
C	-5.96457000	1.13494800	-3.34291400
C	-6.00453000	1.70722600	-1.03864300
C	-7.33710800	0.91170200	-3.32269300
C	-7.37700500	1.49698800	-0.99274800
C	-8.04690800	1.08411200	-2.13871900
C	-0.07394600	-3.11055100	-2.96015100
C	0.73398300	-3.64589100	-3.96777900
C	-0.74186400	-4.02223500	-2.13704700
C	0.88989200	-5.01729500	-4.14181300
C	-0.60709200	-5.39278200	-2.30034600
C	0.22305900	-5.89389300	-3.29431200
C	4.56152200	1.78093900	-1.28254300
C	5.03946000	2.24109600	-0.05000900
C	5.49881800	1.15969900	-2.11799300
C	6.34448300	2.01339800	0.37054000
C	6.81370600	0.93329900	-1.72444600
C	7.23788400	1.36433300	-0.47246800
F	-5.32356100	0.95661400	-4.50061100
F	-7.97526800	0.53890500	-4.42988700
F	-9.35606900	0.86640500	-2.10536300
F	-8.04153900	1.65946600	0.15174000
F	-5.40792900	2.09610100	0.09743400

F	-5.13417100	-0.72785500	3.32714600
F	-7.66730700	-0.31145800	2.53350000
F	-8.48855900	-1.14357900	0.07454500
F	-6.73837000	-2.39258400	-1.59030300
F	-4.22917200	-2.88906500	-0.78952600
F	-1.39540600	2.83308200	4.79597700
F	-1.67897800	5.49143800	5.10496500
F	-0.39195500	7.20777700	3.40975900
F	1.52401100	3.58578100	1.14960800
F	1.22238800	6.24005500	1.46932600
F	-1.58157200	6.34081300	0.72711100
F	-1.60506700	8.98744700	1.17813300
F	-0.56703000	10.70193800	-0.67116700
F	0.50025200	9.72898200	-2.97637500
F	0.54632700	7.07586700	-3.43564600
F	5.32356100	-0.95661400	4.50061100
F	7.97526800	-0.53890500	4.42988700
F	9.35606900	-0.86640500	2.10536300
F	8.04153900	-1.65946600	-0.15174000
F	5.40792900	-2.09610100	-0.09743400
F	4.22917200	2.88906500	0.78952600
F	6.73837000	2.39258400	1.59030300
F	8.48855900	1.14357900	-0.07454500
F	7.66730700	0.31145800	-2.53350000
F	5.13417100	0.72785500	-3.32714600
F	1.39540600	-2.83308200	-4.79597700
F	1.67897800	-5.49143800	-5.10496500
F	-1.22238800	-6.24005500	-1.46932600
F	-1.52401100	-3.58578100	-1.14960800
F	0.39195500	-7.20777700	-3.40975900
F	-0.54632700	-7.07586700	3.43564600
F	-0.50025200	-9.72898200	2.97637500
F	0.56703000	-10.70193800	0.67116700
F	1.60506700	-8.98744700	-1.17813300
F	1.58157200	-6.34081300	-0.72711100
O	-0.23015700	2.22897700	-3.75036000
O	0.23015700	-2.22897700	3.75036000

$$\Delta E_{\text{solv}} = -8286.40636079 \quad \Delta G_{\text{solv}} = -8285.67029879$$

6. Coordinates of all stationary points in Fig. 11



¹A-Cl

C	-4.42303600	-3.67015700	-0.96986400
C	-3.50139100	-3.48722300	0.06708100
C	-3.61609600	-4.32088700	1.18488500
C	-4.59949000	-5.29831200	1.27060100
C	-5.49901300	-5.45936000	0.21880800
C	-5.41243200	-4.64317700	-0.90708600
C	-2.45346800	-2.44632000	-0.01660300
C	-1.11179200	-2.87169600	-0.00760200
N	-0.02018300	-2.05047300	-0.09543200
C	1.10938300	-2.85124000	-0.03855700
C	0.69253300	-4.21033900	0.07546100
C	-0.67288800	-4.22562500	0.08236200
Ru	-0.04023700	-0.00006500	-0.25085800
C	2.44791500	-2.43496200	-0.10750200
C	3.48619200	-3.48817700	-0.13047900
C	4.45057600	-3.57873800	0.88018100
C	5.43567200	-4.55814200	0.86545400
C	5.47548200	-5.47448500	-0.18355600
C	4.53178300	-5.40844500	-1.20665900
C	3.55189000	-4.42482900	-1.16872300
F	4.42403000	-2.71879800	1.89970000
F	6.32981600	-4.62901600	1.84253600
F	6.41069800	-6.40884500	-0.20777700
F	4.57779600	-6.27628300	-2.20908300
F	2.66552500	-4.37298100	-2.16627100
F	-2.77346800	-4.17508800	2.21027400
F	-4.69158200	-6.06964800	2.34589800
F	-6.43774000	-6.38798000	0.28991900
F	-6.26641200	-4.80144200	-1.90972400
F	-4.35428900	-2.90045400	-2.05853100
C	2.89127600	-1.09950900	-0.16049700
N	2.09365600	0.00006300	-0.07926800
C	2.89111600	1.09975400	-0.16065900
C	4.25857100	0.67959300	-0.30914400
C	4.25868300	-0.67917200	-0.30901000
C	2.44758700	2.43515200	-0.10783100
C	1.10900700	2.85126000	-0.03855800

N	-0.02045800	2.05034400	-0.09516300
C	-1.11214600	2.87139200	-0.00701100
C	-0.67343100	4.22538000	0.08300200
C	0.69198900	4.21029800	0.07567000
C	-2.45376900	2.44585500	-0.01584300
C	-3.50179400	3.48662100	0.06829900
C	-4.42357300	3.66988300	-0.96846500
C	-5.41298100	4.64286200	-0.90523500
C	-5.49944500	5.45866500	0.22094400
C	-4.59976700	5.29730300	1.27255800
C	-3.61636300	4.31993100	1.18638600
F	-4.35493400	2.90057300	-2.05742000
F	-6.26708500	4.80144000	-1.90772100
F	-6.43819100	6.38723400	0.29249000
F	-4.69171200	6.06829800	2.34811300
F	-2.77356900	4.17383500	2.21159500
C	3.48561100	3.48858900	-0.13145800
C	3.55051000	4.42507700	-1.16990700
C	4.53004700	5.40901900	-1.20850000
C	5.47423100	5.47555800	-0.18588200
C	5.43522800	4.55939700	0.86331700
C	4.45046800	3.57966700	0.87870500
F	2.66371500	4.37280000	-2.16704900
F	4.57529700	6.27671700	-2.21107800
F	6.40914200	6.41020400	-0.21070200
F	6.32980100	4.63071700	1.83996900
F	4.42471200	2.71989900	1.89839100
C	-2.87011500	1.11524300	-0.07227100
N	-2.04640700	-0.00018700	-0.16554700
C	-2.86996500	-1.11574100	-0.07267800
C	-4.22620400	-0.67996300	0.03028400
C	-4.22629100	0.67923700	0.03057000
O	0.27316000	0.00013800	-1.92903000
H	1.35615900	5.06235300	0.14316400
H	-1.31943200	5.09207800	0.13699700
H	-5.08212600	1.33507000	0.12584600
H	-5.08198000	-1.33591700	0.12525100
H	-1.31878300	-5.09241900	0.13608700
H	1.35678100	-5.06232100	0.14308000
H	5.10995900	-1.33968500	-0.41465000
H	5.10972400	1.34027200	-0.41473800
Cl	0.13369700	-0.00011600	2.12383100

$\Delta E_{\text{solv}} = -4527.12496889$

$\Delta G_{\text{solv}} = -4526.78173489$

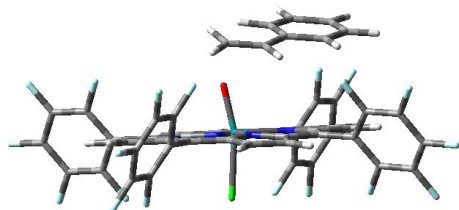
³A-Cl

C	-4.58399400	-3.46220100	-0.90006400
C	-3.60367400	-3.35999400	0.09546900
C	-3.69609400	-4.23687500	1.18410800
C	-4.71630600	-5.17384100	1.28248700
C	-5.67184600	-5.25585000	0.27107400
C	-5.60598800	-4.39907100	-0.82655100
C	-2.51932200	-2.36123000	0.00123800
C	-1.19814500	-2.84819300	-0.04672800
N	-0.07584000	-2.07417500	-0.11610600
C	1.00140000	-2.91139500	-0.12016400
C	0.53962900	-4.27070800	-0.05713600
C	-0.81855900	-4.23169400	-0.02731300
Ru	-0.01270500	0.01516700	-0.23150600
C	2.35729000	-2.51658800	-0.14098000
C	3.36399500	-3.59703400	-0.17197400
C	4.29973700	-3.75502600	0.85890200
C	5.24278100	-4.77415100	0.83922300
C	5.27240700	-5.66033900	-0.23628100
C	4.35813900	-5.52678100	-1.28006600
C	3.41608200	-4.50803600	-1.23521100
F	4.27879900	-2.92977000	1.90561300
F	6.10591500	-4.91267700	1.83599400
F	6.16982600	-6.62957800	-0.26632500
F	4.39826700	-6.36465600	-2.30705100
F	2.56070500	-4.38957200	-2.25211200
F	-2.80488600	-4.16400700	2.17322800
F	-4.79146700	-5.98115200	2.33166900
F	-6.64403300	-6.14693900	0.35309800
F	-6.51137500	-4.48618700	-1.79135100
F	-4.53241700	-2.65967300	-1.96446100
C	2.84165600	-1.19089300	-0.12433700
N	2.07787300	-0.05993600	-0.08174400
C	2.92420200	1.01018500	-0.10988800
C	4.27776100	0.54037900	-0.18408000
C	4.22713900	-0.81808400	-0.19414700
C	2.52998600	2.36410200	-0.11276800
C	1.20255100	2.84039000	-0.10597500
N	0.06592600	2.06987100	-0.12789100
C	-1.00459200	2.92300300	-0.07277600
C	-0.52960800	4.27338000	-0.04653000
C	0.83058200	4.22108700	-0.05047400
C	-2.35817400	2.53470600	-0.03623800

C	-3.37089600	3.60737200	0.03766000
C	-4.33378700	3.76188600	-0.96811200
C	-5.29202600	4.76528200	-0.91553700
C	-5.31095600	5.63748500	0.17146400
C	-4.37265900	5.50407700	1.19342300
C	-3.41614800	4.50029900	1.11608900
F	-4.32645000	2.94423800	-2.02214300
F	-6.18040700	4.90089400	-1.89034100
F	-6.22187000	6.59254100	0.23347600
F	-4.40443200	6.32658300	2.23291800
F	-2.54257900	4.37924600	2.11667900
C	3.60803100	3.37383900	-0.11600800
C	3.74579600	4.29033800	-1.16651800
C	4.76230700	5.23589800	-1.18342200
C	5.66754800	5.28734800	-0.12458200
C	5.55495700	4.39215700	0.93798700
C	4.53751600	3.44704900	0.92981100
F	2.90089300	4.24745800	-2.19839200
F	4.88058900	6.08046800	-2.19888400
F	6.63512700	6.18713900	-0.12868400
F	6.41159800	4.45227200	1.94809100
F	4.44001500	2.61037300	1.96303400
C	-2.83241200	1.20711900	-0.03686600
N	-2.05969000	0.07791900	-0.13302700
C	-2.90187800	-1.00352200	-0.01428100
C	-4.24135900	-0.53538300	0.14965900
C	-4.19931600	0.82716500	0.13614100
O	0.14876500	-0.10424500	-1.95067000
H	1.51777800	5.05600900	-0.00908400
H	-1.15096900	5.15911700	-0.02622200
H	-5.02997800	1.50973300	0.26211100
H	-5.11278700	-1.16202300	0.28863900
H	-1.49932900	-5.07211600	0.00854900
H	1.17160200	-5.14887700	-0.02871100
H	5.06103800	-1.50432800	-0.26464800
H	5.15923000	1.16582400	-0.24095700
Cl	0.05268100	-0.07831900	2.16167300

$\Delta E_{\text{solv}} = -4527.12768864$

$\Delta G_{\text{solv}} = -4526.78660964$



¹1-Cl

C	-2.67671500	-5.13311000	0.72487700
C	-2.80349600	-4.16651600	-0.27688600
C	-3.68633000	-4.44535300	-1.32537800
C	-4.41423800	-5.62834500	-1.37573400
C	-4.26697800	-6.56855500	-0.35922800
C	-3.39413000	-6.32177600	0.69772400
C	-2.03529900	-2.90064800	-0.23054300
C	-2.77366000	-1.70580600	-0.13659900
N	-2.24054200	-0.45523400	-0.12667400
C	-3.26943200	0.43989600	-0.05005900
C	-4.51107400	-0.28451700	-0.01592500
C	-4.20534300	-1.60852800	-0.05610500
Ru	-0.16765900	0.00489900	-0.07529500
C	-3.14945000	1.84091800	-0.02447400
C	-4.40795200	2.62136300	0.04684800
C	-4.80900300	3.45306600	-1.00281200
C	-5.98971200	4.18431800	-0.94644700
C	-6.79944500	4.09259500	0.18277500
C	-6.42550300	3.27392500	1.24562300
C	-5.24166300	2.55134500	1.16629900
F	-4.05097700	3.55235800	-2.09657500
F	-6.35024800	4.96187200	-1.96029200
F	-7.92595200	4.78538400	0.24693300
F	-7.19459400	3.19401100	2.32565400
F	-4.89836400	1.77723400	2.20129000
F	-3.83595300	-3.56755700	-2.31865300
F	-5.23934200	-5.86861100	-2.38675900
F	-4.95557200	-7.69809300	-0.39716100
F	-3.25651100	-7.21519500	1.67037600
F	-1.84584800	-4.92030900	1.75492600
C	-1.94856700	2.56687700	-0.06140100
N	-0.68226300	2.04582500	-0.12611300
C	0.19375700	3.08484100	-0.14433300
C	-0.53385600	4.32059400	-0.07369300
C	-1.85405300	4.00030400	-0.01670200
C	1.59698500	2.96568000	-0.19369700
C	2.31271300	1.76596700	-0.20907200

N	1. 78021900	0. 47912100	-0. 19458600
C	2. 84202200	-0. 40409300	-0. 30851400
C	4. 05783100	0. 33965700	-0. 32420900
C	3. 73518500	1. 66330500	-0. 27241300
C	2. 73817700	-1. 79611800	-0. 42423300
C	3. 98753400	-2. 56499900	-0. 63213500
C	4. 40041600	-3. 56600800	0. 25254300
C	5. 56396000	-4. 29814200	0. 05706900
C	6. 35177200	-4. 04322900	-1. 06246300
C	5. 96791500	-3. 06062800	-1. 97093000
C	4. 79852200	-2. 34159000	-1. 75140800
F	3. 66633700	-3. 84497700	1. 34368400
F	5. 92625200	-5. 23192400	0. 92855000
F	7. 46269300	-4. 73383600	-1. 26177100
F	6. 71069200	-2. 82238500	-3. 04399500
F	4. 44930800	-1. 42067700	-2. 65163800
C	2. 36976300	4. 22873900	-0. 27644500
C	3. 23498300	4. 64048500	0. 73928100
C	3. 95279600	5. 82699000	0. 66131800
C	3. 81041300	6. 63992600	-0. 46016500
C	2. 95478100	6. 25983100	-1. 49102400
C	2. 24761400	5. 06730800	-1. 38940000
F	3. 38416200	3. 88097500	1. 83289200
F	4. 76275800	6. 19005900	1. 65047500
F	4. 48836100	7. 77367100	-0. 54551900
F	2. 82371600	7. 03196800	-2. 56218900
F	1. 43828500	4. 72248000	-2. 39190300
C	1. 53372100	-2. 51263100	-0. 40291700
N	0. 27947300	-1. 96406900	-0. 21352000
C	-0. 63947200	-2. 99997700	-0. 30606700
C	0. 07165200	-4. 21734600	-0. 53290000
C	1. 40028100	-3. 91848600	-0. 60140000
O	-0. 38761200	0. 05134100	1. 63284500
H	4. 41753400	2. 50392500	-0. 28788800
H	5. 05003400	-0. 09153100	-0. 37401900
H	2. 21575200	-4. 60406500	-0. 79327600
H	-0. 38658100	-5. 19020300	-0. 65995500
H	-4. 89223800	-2. 44518100	-0. 03474200
H	-5. 49626200	0. 16220300	0. 02637700
H	-2. 69343200	4. 67969300	0. 06120400
H	-0. 09236300	5. 30910000	-0. 05265300
C	-0. 26312400	-1. 91563300	3. 15262100
H	-0. 86389200	-2. 77524700	2. 86488000
H	-0. 77764300	-1. 12314800	3. 68731400

C	1.07958300	-1.90521700	2.93749300
H	1.53485300	-2.79223800	2.48953900
C	1.97703800	-0.80732200	3.20083400
C	1.52001300	0.46337800	3.62992400
C	3.35710800	-0.98198000	2.97419000
C	2.41103300	1.51285800	3.78976700
H	0.46506600	0.61536800	3.84195900
C	4.24512200	0.06710300	3.15235300
H	3.71600600	-1.95894900	2.65804600
C	3.77327900	1.32083700	3.55028000
H	2.04902400	2.48797600	4.10757000
H	5.30893600	-0.08513000	2.98159400
H	4.46753800	2.14792600	3.68050700
Cl	-0.46237100	0.13543300	-2.41774100

$\Delta E_{\text{solv}} = -4836.78148959$

$\Delta G_{\text{solv}} = -4836.31013859$

³1-Cl

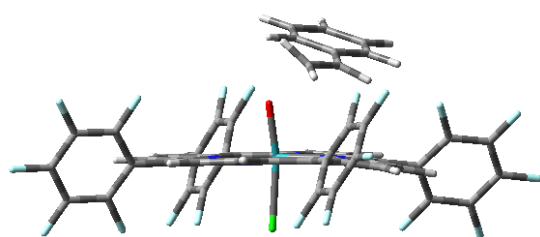
C	-2.82237800	-5.03299300	0.86800400
C	-2.98353500	-4.07067200	-0.13544500
C	-3.91727700	-4.34452600	-1.14216000
C	-4.66181600	-5.51763200	-1.14918000
C	-4.48403600	-6.45012700	-0.12968700
C	-3.56102800	-6.20798600	0.88591300
C	-2.18247100	-2.82792600	-0.13293000
C	-2.87778400	-1.60953000	-0.05349300
N	-2.29924500	-0.36863700	-0.05708900
C	-3.30675800	0.54938100	-0.02379200
C	-4.57094200	-0.13306600	0.00765600
C	-4.30563400	-1.46528300	0.01058400
Ru	-0.26114400	0.03256500	-0.05548700
C	-3.14183400	1.95346700	-0.04107600
C	-4.37217300	2.77297300	-0.01561200
C	-4.69721700	3.62650100	-1.07712400
C	-5.85436000	4.39487200	-1.06846800
C	-6.71371100	4.32829900	0.02614800
C	-6.41415000	3.49403000	1.10134700
C	-5.25697400	2.72768300	1.06810500
F	-3.89626300	3.69919800	-2.13998000
F	-6.14764200	5.18359200	-2.09377400
F	-7.81576500	5.05885500	0.04578100
F	-7.22755200	3.44230500	2.14862500
F	-4.98160000	1.94792600	2.11677900
F	-4.09123800	-3.48031800	-2.14217100

F	-5.53121100	-5.75707200	-2.12168900
F	-5.19016100	-7.56793300	-0.12583800
F	-3.39702900	-7.09341500	1.86038900
F	-1.94634900	-4.82136600	1.85712000
C	-1.91725900	2.64580200	-0.08501400
N	-0.67599300	2.07068400	-0.12514900
C	0.24380600	3.07839600	-0.11178700
C	-0.43923000	4.33986100	-0.04764900
C	-1.77210700	4.07283900	-0.03196100
C	1.64782900	2.91555200	-0.11993600
C	2.34394100	1.69134100	-0.14378200
N	1.76965100	0.45092200	-0.18560500
C	2.77621500	-0.45912000	-0.32922400
C	4.03919900	0.22480400	-0.32673500
C	3.77321200	1.55207500	-0.22049800
C	2.60368000	-1.85118900	-0.49554100
C	3.81605300	-2.64193500	-0.80122400
C	4.24139200	-3.71439000	-0.00867400
C	5.37980700	-4.45034500	-0.30679600
C	6.12242600	-4.13381700	-1.44221500
C	5.72207600	-3.08266000	-2.26320600
C	4.58502200	-2.35350600	-1.93806400
F	3.55751700	-4.05092900	1.09551900
F	5.76162100	-5.44709000	0.48151200
F	7.20505000	-4.83169600	-1.73893000
F	6.41955300	-2.78924500	-3.35189500
F	4.21670000	-1.36978000	-2.75735600
C	2.45881600	4.15300400	-0.15666200
C	3.35668000	4.47886500	0.86527100
C	4.12107000	5.63722700	0.83157700
C	4.00397500	6.50400500	-0.25261800
C	3.12368800	6.20690600	-1.29058300
C	2.36320800	5.04566400	-1.23202700
F	3.48217100	3.67067400	1.92289200
F	4.95311700	5.92418800	1.82600700
F	4.72894800	7.60912500	-0.29611200
F	3.02129900	7.02699300	-2.32788200
F	1.54024700	4.77781800	-2.24552500
C	1.37701700	-2.54270400	-0.44264100
N	0.14653200	-1.97634300	-0.19859700
C	-0.78053100	-2.98117400	-0.24829400
C	-0.11903300	-4.22006600	-0.51808100
C	1.20973200	-3.94669600	-0.65471700
O	-0.20904800	0.08058000	1.69473900

H	4.48712500	2.36560400	-0.21113900
H	5.01061900	-0.24877700	-0.39364900
H	1.99715100	-4.64836800	-0.89622300
H	-0.60517000	-5.18094100	-0.63071300
H	-5.02129400	-2.27649300	0.04288700
H	-5.54337900	0.34177700	0.01879800
H	-2.58386200	4.78611300	0.03135500
H	0.03592600	5.31133400	-0.00038200
C	0.01344800	-1.92258000	3.21636000
H	-0.66735800	-2.72807200	2.95066300
H	-0.40972600	-1.09780400	3.78087300
C	1.33546700	-2.01087900	2.92851300
H	1.69302700	-2.92094800	2.44012200
C	2.33918900	-1.00235900	3.18147200
C	2.01551700	0.28749500	3.65645200
C	3.69258400	-1.29856400	2.92031500
C	3.00691900	1.23444200	3.84927300
H	0.97847200	0.54100500	3.86048800
C	4.68358300	-0.34883700	3.12211500
H	3.95220500	-2.29647100	2.57234000
C	4.34287400	0.92427300	3.57839500
H	2.74417800	2.22610900	4.21027000
H	5.72452300	-0.59804000	2.92527400
H	5.11526600	1.67578600	3.73077300
Cl	-0.34126100	0.11368600	-2.45812100

$\Delta E_{\text{solv}} = -4836.77645924$

$\Delta G_{\text{solv}} = -4836.30847324$



¹TS1-Cl

C	-2.60098000	-5.08447800	0.89369300
C	-2.79549300	-4.18748700	-0.16066800
C	-3.71639900	-4.54964500	-1.14806200
C	-4.41656700	-5.74935200	-1.08972100
C	-4.20156100	-6.61922100	-0.02354700
C	-3.28967600	-6.28712900	0.97573600
C	-2.04769900	-2.91009900	-0.21089900
C	-2.79604000	-1.72165800	-0.13726300
N	-2.27483100	-0.46437400	-0.16775100

C	-3.30622500	0.42012600	-0.09160300
C	-4.54426200	-0.31072100	-0.02848500
C	-4.22872500	-1.63298100	-0.03806800
Ru	-0.19828300	0.01754800	-0.13955600
C	-3.18602900	1.82485100	-0.07590200
C	-4.44715200	2.60372700	-0.02955000
C	-4.83375600	3.42177400	-1.09518000
C	-6.01580800	4.15241800	-1.06516500
C	-6.84154500	4.07435900	0.05330800
C	-6.48171300	3.27024700	1.13192700
C	-5.29600400	2.54836000	1.07895200
F	-4.05932200	3.50990800	-2.17814500
F	-6.36212900	4.91738700	-2.09357500
F	-7.96978800	4.76662700	0.09259000
F	-7.26552900	3.20389100	2.20251300
F	-4.96585800	1.78958000	2.12974800
F	-3.93051300	-3.73945900	-2.18586700
F	-5.27948600	-6.07223200	-2.04495900
F	-4.86429800	-7.76333300	0.04038600
F	-3.09003700	-7.11304800	1.99649200
F	-1.73400200	-4.78129200	1.87112700
C	-1.98899200	2.55355300	-0.09631200
N	-0.71505800	2.03761300	-0.13476300
C	0.15254500	3.08574500	-0.12841800
C	-0.58575300	4.31697400	-0.06298300
C	-1.90328500	3.98844000	-0.04217500
C	1.55624500	2.97476100	-0.15871600
C	2.27544900	1.77778000	-0.21309800
N	1.73935100	0.49356000	-0.24527000
C	2.80601000	-0.38980900	-0.38734100
C	4.02071400	0.35731800	-0.38265400
C	3.69819200	1.67726100	-0.28237700
C	2.70715000	-1.77570600	-0.53835600
C	3.95785200	-2.53378200	-0.77529800
C	4.38453300	-3.54478600	0.09064200
C	5.54710800	-4.27141600	-0.12748300
C	6.32058100	-3.99887800	-1.25296600
C	5.92407000	-3.00404300	-2.14246400
C	4.75578000	-2.29028900	-1.89930800
F	3.66508700	-3.83570500	1.19027700
F	5.92315900	-5.21499800	0.72796100
F	7.43124000	-4.68338200	-1.47468300
F	6.65483700	-2.74809800	-3.21967700
F	4.39622600	-1.35508800	-2.77964700

C	2.33128900	4.23907900	-0.18239600
C	3.19373100	4.59926600	0.85542800
C	3.92030500	5.78263200	0.83518000
C	3.79163500	6.64602400	-0.24938700
C	2.94159300	6.31745800	-1.30206100
C	2.22590900	5.12636700	-1.25864200
F	3.33569100	3.79000500	1.91443300
F	4.72730700	6.09470300	1.84457100
F	4.47784900	7.77782200	-0.27935000
F	2.82480800	7.13582000	-2.34014100
F	1.42485900	4.83170700	-2.28365500
C	1.50619200	-2.50661900	-0.50617600
N	0.26282200	-1.97030400	-0.26342900
C	-0.64993900	-3.00516700	-0.33014900
C	0.05550900	-4.22097300	-0.59079300
C	1.37890100	-3.91229500	-0.71517900
O	-0.45472100	-0.02232900	1.60973800
H	4.38075000	2.51771800	-0.27045500
H	5.01323900	-0.07083000	-0.45188700
H	2.19063700	-4.59000500	-0.94720500
H	-0.40341400	-5.19512400	-0.70686200
H	-4.90994900	-2.47302700	0.01244700
H	-5.53249800	0.12894500	0.01593100
H	-2.74826000	4.66265200	0.01813600
H	-0.15191800	5.30834600	-0.02693900
C	-0.18112800	-1.55213700	2.83919000
H	-0.85063600	-2.31882600	2.45517000
H	-0.59797100	-0.91263400	3.61011300
C	1.19148100	-1.71271500	2.70606900
H	1.56108900	-2.59674700	2.18244500
C	2.16255300	-0.74831200	3.10499600
C	1.79159400	0.52881300	3.59819000
C	3.53834900	-1.03879700	2.94277000
C	2.75872700	1.46770500	3.90057100
H	0.73936400	0.77788400	3.71558900
C	4.50103300	-0.09666200	3.26219100
H	3.82544900	-2.01910000	2.56880900
C	4.11398200	1.16025000	3.73335600
H	2.46801800	2.45091100	4.26148100
H	5.55595100	-0.33209900	3.14118700
H	4.86844400	1.90756100	3.97115300
Cl	-0.53639100	0.07807700	-2.46363500

$$\Delta E_{\text{solv}} = -4836.78102773$$

$$\Delta G_{\text{solv}} = -4836.30846173$$

³TS1-CI

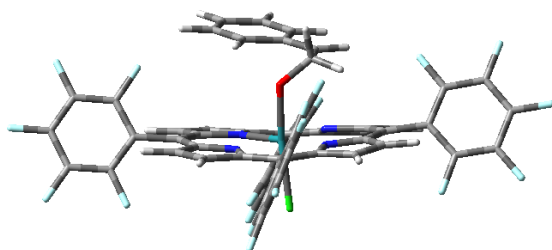
C	-2.55977500	-5.08342600	1.03181000
C	-2.81692600	-4.19821200	-0.02115900
C	-3.76914700	-4.58645700	-0.96964700
C	-4.44206700	-5.79865600	-0.87289300
C	-4.17018900	-6.65290700	0.19348400
C	-3.22521200	-6.29524100	1.15333000
C	-2.08388700	-2.91742600	-0.10966400
C	-2.83224400	-1.73114900	-0.04602100
N	-2.30671500	-0.46628700	-0.08504100
C	-3.35048000	0.40843800	-0.06312000
C	-4.58548500	-0.32618600	-0.00999700
C	-4.26469500	-1.64572000	0.02822900
Ru	-0.28933300	0.01959300	-0.12061000
C	-3.24204000	1.81908800	-0.09280800
C	-4.50416600	2.58981300	-0.09334900
C	-4.84125300	3.42118700	-1.16855400
C	-6.02462100	4.14848800	-1.18702300
C	-6.89911000	4.06254000	-0.10598600
C	-6.58782500	3.25061000	0.98278000
C	-5.40365700	2.52574500	0.97682900
F	-4.02433800	3.51319900	-2.21748000
F	-6.32762100	4.91725800	-2.22479200
F	-8.02646100	4.75429100	-0.11159900
F	-7.41565700	3.18190200	2.01808300
F	-5.11742000	1.76925500	2.04005500
F	-4.03227100	-3.79706400	-2.01136700
F	-5.33203100	-6.14939300	-1.79190800
F	-4.80924500	-7.80657500	0.29454500
F	-2.97222800	-7.10651200	2.17284400
F	-1.66202800	-4.75304600	1.96862800
C	-2.04758600	2.56250600	-0.11779500
N	-0.78454900	2.03874400	-0.13814300
C	0.09289800	3.08345600	-0.09795900
C	-0.64315900	4.31741900	-0.03278600
C	-1.96241500	3.99647200	-0.05116900
C	1.49948400	2.97327800	-0.09457800
C	2.24506600	1.77703200	-0.16121700
N	1.71972500	0.51920600	-0.25488300
C	2.76183100	-0.34635200	-0.42960000
C	3.99681100	0.38651700	-0.39970200
C	3.67830100	1.69761100	-0.23765000
C	2.64201500	-1.73817500	-0.62563400

C	3.88081500	-2.47822800	-0.95031000
C	4.35071000	-3.53741100	-0.16574900
C	5.51304000	-4.23007200	-0.47416500
C	6.23623000	-3.87955400	-1.61224100
C	5.79341000	-2.83834000	-2.42372500
C	4.63218300	-2.15266000	-2.08803500
F	3.68595100	-3.89956100	0.94397800
F	5.93691400	-5.21595900	0.30699300
F	7.34249700	-4.53546400	-1.91898500
F	6.47495200	-2.51229800	-3.51330700
F	4.22590900	-1.17566800	-2.89681400
C	2.26806200	4.23825400	-0.07057400
C	3.13385300	4.54839800	0.98277600
C	3.86473500	5.72811900	1.01250700
C	3.74523500	6.63387200	-0.03884200
C	2.89643900	6.35337200	-1.10700300
C	2.16951300	5.16905000	-1.11195500
F	3.26129200	3.69999500	2.00868100
F	4.66759500	5.99800100	2.03596400
F	4.43870000	7.76026000	-0.02262800
F	2.79244400	7.21079800	-2.11372100
F	1.37711100	4.91852900	-2.15383400
C	1.44515900	-2.48120200	-0.55752900
N	0.20453500	-1.96966100	-0.25311100
C	-0.68022400	-3.01296900	-0.27387000
C	0.01992100	-4.22152200	-0.57853200
C	1.32854700	-3.88895200	-0.77688200
O	-0.23760000	0.08719100	1.67255600
H	4.35934000	2.53794200	-0.19554800
H	4.98627500	-0.04505000	-0.48764400
H	2.13384300	-4.55362700	-1.06142200
H	-0.43014900	-5.20151900	-0.67753400
H	-4.94603100	-2.48458800	0.08528400
H	-5.57731600	0.10676700	-0.00493500
H	-2.80479700	4.67464300	-0.00145900
H	-0.20933900	5.30704600	0.03169900
C	0.09563300	-1.46429500	2.95052000
H	-0.64237400	-2.18865500	2.61480900
H	-0.23385500	-0.77994100	3.72433400
C	1.43504900	-1.69154600	2.71206200
H	1.71143500	-2.57878600	2.13786000
C	2.50312000	-0.81706700	3.09125500
C	2.26411500	0.46355300	3.64285900
C	3.84105600	-1.22146300	2.88061700

C	3.32128100	1.28831600	3.98031600
H	1.24091400	0.80736300	3.77783400
C	4.89561700	-0.39086800	3.22494300
H	4.03090000	-2.20868300	2.46475600
C	4.63914400	0.86654100	3.77320000
H	3.12788500	2.27254300	4.39947200
H	5.92099700	-0.72000800	3.07113700
H	5.46536000	1.52088200	4.04365900
Cl	-0.42399100	0.12181100	-2.50567300

$\Delta E_{\text{solv}} = -4836.77596049$

$\Delta G_{\text{solv}} = -4836.30654549$



¹B-Cl

C	-1.22841000	-5.42506900	1.21717000
C	-1.58846300	-4.70088300	0.07759300
C	-2.30149400	-5.37936100	-0.91388000
C	-2.64782000	-6.71911700	-0.77630600
C	-2.27663600	-7.41067100	0.37409600
C	-1.56382700	-6.76192500	1.37990700
C	-1.19973000	-3.27728800	-0.04769100
C	-2.23947600	-2.31971600	-0.09925600
N	-2.05926200	-0.97299400	-0.16226400
C	-3.29398700	-0.39090700	-0.22425800
C	-4.29525800	-1.42021400	-0.22067900
C	-3.64494400	-2.61286800	-0.11599300
Ru	-0.20665800	0.03691500	-0.13956200
C	-3.55048600	0.99317200	-0.24815100
C	-4.96979700	1.41578500	-0.31668900
C	-5.45836000	2.12261400	-1.41972800
C	-6.78533900	2.52804000	-1.50016000
C	-7.65722800	2.23135500	-0.45588100
C	-7.19884100	1.53424600	0.65907000
C	-5.86868200	1.13740500	0.71656000
F	-4.64160200	2.41764600	-2.43245400
F	-7.22515100	3.19009600	-2.56375000
F	-8.92351800	2.61412000	-0.52218600
F	-8.02848300	1.26098400	1.66053200
F	-5.44929300	0.48244900	1.80491500

F	-2.65462800	-4.74297500	-2.03152600
F	-3.31954800	-7.34279300	-1.73574800
F	-2.60140200	-8.68650900	0.51293700
F	-1.21620800	-7.41898800	2.48089100
F	-0.54880500	-4.81470100	2.20275700
C	-2.58755400	2.01359700	-0.18436400
N	-1.23019500	1.84409500	-0.14504600
C	-0.67298900	3.07712200	-0.00892200
C	-1.71086800	4.07585600	0.04575700
C	-2.89142000	3.42001600	-0.07338000
C	0.70835200	3.32729800	0.07896600
C	1.72113900	2.36468400	-0.00679300
N	1.53522200	0.98658000	-0.11447800
C	2.79620700	0.41833700	-0.27540200
C	3.77138800	1.45168300	-0.23240300
C	3.11625200	2.64006300	-0.05324900
C	3.06505800	-0.94466600	-0.49365900
C	4.42686500	-1.28270600	-0.97411500
C	5.29250100	-2.17563500	-0.33582600
C	6.55656700	-2.47129500	-0.83075900
C	6.99160600	-1.87278000	-2.00902100
C	6.15467100	-0.98701100	-2.68140500
C	4.89524600	-0.70707300	-2.16505300
F	4.92370800	-2.78689300	0.80182100
F	7.34890500	-3.31690800	-0.17958100
F	8.19439700	-2.14716300	-2.48833700
F	6.55747500	-0.42246500	-3.81254100
F	4.11593700	0.13180400	-2.84913700
C	1.13710300	4.73497800	0.25287600
C	1.78579000	5.14849300	1.41821200
C	2.20038000	6.45972800	1.60798500
C	1.96452900	7.39988600	0.60778300
C	1.31805000	7.02128100	-0.56598900
C	0.91391300	5.70109000	-0.73169700
F	2.00988300	4.26212300	2.40132600
F	2.81029400	6.81981100	2.73276400
F	2.35443800	8.65439400	0.77444900
F	1.09846500	7.91721700	-1.51992000
F	0.30469800	5.36092100	-1.86809900
C	2.11689800	-1.97073800	-0.37945600
N	0.78218600	-1.76735700	-0.08330300
C	0.17423200	-3.01729500	-0.12064000
C	1.17265500	-4.01448700	-0.36310700
C	2.35732000	-3.37007600	-0.55520600

O	-0.55825400	0.05868600	1.77398400
H	3.55848500	3.62704100	0.01205200
H	4.84063600	1.30109700	-0.32584900
H	3.30885400	-3.81862500	-0.80900000
H	0.98520800	-5.07842500	-0.44273100
H	-4.08703400	-3.59980800	-0.06558900
H	-5.36395900	-1.25907600	-0.28468300
H	-3.88679400	3.84610400	-0.06175300
H	-1.55527600	5.14064900	0.16555900
C	-0.42348800	-1.12586000	2.52420100
H	-1.10268000	-1.91326000	2.15346200
H	-0.76175900	-0.89510900	3.55028000
C	0.96131800	-1.64434800	2.57923500
H	1.09495700	-2.72734500	2.52280800
C	2.10102200	-0.86636300	2.81303900
C	2.05897500	0.54928500	2.99354000
C	3.36043200	-1.52584800	2.87811800
C	3.22464700	1.24780300	3.22904700
H	1.10379200	1.06779300	2.94034400
C	4.52096100	-0.81256900	3.10396800
H	3.39156300	-2.60462000	2.74026900
C	4.45260700	0.57275800	3.28132600
H	3.19494000	2.32422900	3.37023400
H	5.47812500	-1.32595000	3.14384100
H	5.36519100	1.13571700	3.46915700
Cl	-0.39744100	-0.06557400	-2.45128800

$\Delta E_{\text{solv}} = -4836.80729717$

$\Delta G_{\text{solv}} = -4836.33322517$

³B-Cl

C	-1.24659700	-5.40671200	1.29639200
C	-1.60993400	-4.69566900	0.14958100
C	-2.31877100	-5.38826500	-0.83492800
C	-2.65955600	-6.72798500	-0.68306300
C	-2.28467200	-7.40610800	0.47403300
C	-1.57457700	-6.74377500	1.47271300
C	-1.22173000	-3.27309100	0.01096400
C	-2.25147000	-2.31527100	-0.05909800
N	-2.07611200	-0.96093100	-0.15318600
C	-3.31824500	-0.38804400	-0.23617600
C	-4.31216200	-1.42376600	-0.21467700
C	-3.65736900	-2.60834600	-0.07723900
Ru	-0.26848800	0.04047700	-0.16883700
C	-3.57909000	0.98997500	-0.27953400

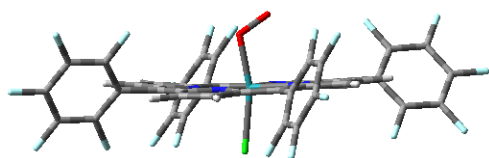
C	-4.99565000	1.41837900	-0.35951800
C	-5.47232000	2.12275800	-1.46918800
C	-6.79580100	2.53683500	-1.56151600
C	-7.67740300	2.24996000	-0.52266600
C	-7.23143400	1.55535800	0.59869600
C	-5.90372800	1.15179900	0.66878000
F	-4.64517100	2.40960300	-2.47662900
F	-7.22284700	3.19755300	-2.63123000
F	-8.94090000	2.64004400	-0.60014400
F	-8.07023500	1.29137000	1.59497300
F	-5.49679300	0.50003100	1.76372600
F	-2.67585400	-4.76538900	-1.95942300
F	-3.32903400	-7.36465600	-1.63582200
F	-2.60338700	-8.68223100	0.62589000
F	-1.22247300	-7.38805800	2.58006200
F	-0.56839600	-4.78307300	2.27452500
C	-2.61050400	2.00554600	-0.21262800
N	-1.24804200	1.82480100	-0.17468100
C	-0.67106700	3.06394300	-0.01794900
C	-1.70582300	4.05220200	0.04315300
C	-2.89626600	3.40366700	-0.09296900
C	0.70459000	3.32355700	0.07614200
C	1.72705600	2.36660800	-0.02769400
N	1.54247900	1.01282200	-0.14323000
C	2.77780400	0.44129900	-0.31620600
C	3.77487300	1.46979500	-0.28399500
C	3.12984300	2.65471100	-0.09174100
C	3.03833200	-0.93180000	-0.51104300
C	4.38265900	-1.27722700	-1.03334200
C	5.27194100	-2.16303300	-0.41813600
C	6.52128700	-2.45511000	-0.95103500
C	6.91595300	-1.86152600	-2.14580400
C	6.05292800	-0.98532000	-2.79753000
C	4.80877900	-0.70879500	-2.24372000
F	4.94180000	-2.77193500	0.73270400
F	7.33751300	-3.29398300	-0.32041800
F	8.10448000	-2.13341000	-2.66140300
F	6.41643300	-0.42741000	-3.94526100
F	4.00112000	0.11626900	-2.91096800
C	1.12734200	4.72698900	0.29274800
C	1.78705700	5.09354400	1.46803600
C	2.21184600	6.39407300	1.70296700
C	1.97489100	7.37206700	0.74013200
C	1.31791600	7.04093400	-0.44200800

C	0.90529100	5.72986400	-0.65413300
F	2.01449700	4.16960700	2.41564300
F	2.83353800	6.70852800	2.83517500
F	2.37377400	8.61738500	0.95031200
F	1.09725200	7.97301200	-1.36078800
F	0.28724300	5.43646900	-1.79960400
C	2.09402500	-1.95772500	-0.35915800
N	0.76233600	-1.77194800	-0.01594900
C	0.15680100	-3.01649200	-0.06366400
C	1.15132000	-4.00597500	-0.32683000
C	2.33187400	-3.35256400	-0.54309000
O	-0.42643700	0.12743900	1.81392200
H	3.56959700	3.64292700	-0.02926400
H	4.84177000	1.30767100	-0.38469700
H	3.27699200	-3.79792500	-0.82528800
H	0.96755300	-5.07030400	-0.41191700
H	-4.09519300	-3.59593500	-0.00662500
H	-5.38124500	-1.26846100	-0.28633600
H	-3.88712800	3.84061400	-0.08455900
H	-1.55004600	5.11531100	0.17703500
C	-0.32456900	-1.04303500	2.55290400
H	-1.01685000	-1.82803000	2.19851900
H	-0.64126800	-0.82689000	3.59276800
C	1.04951100	-1.59038900	2.60933100
H	1.14795700	-2.67968600	2.62484100
C	2.22372700	-0.84702300	2.78781400
C	2.24080100	0.57208600	2.93921600
C	3.45229000	-1.55853200	2.87171800
C	3.43060500	1.22036000	3.19241100
H	1.31226300	1.12977100	2.84550500
C	4.64115700	-0.89328000	3.10581500
H	3.43840000	-2.64019300	2.75287800
C	4.62828200	0.49311700	3.27190700
H	3.44454600	2.29947300	3.31792800
H	5.57480000	-1.44661900	3.16170800
H	5.56165500	1.01929400	3.46441600
Cl	-0.17463400	-0.13703900	-2.47018100

$$\Delta E_{\text{solv}} = -4836.82118461$$

$$\Delta G_{\text{solv}} = -4836.34675461$$

7. Coordinates of all stationary points in Fig. 13



¹F-Cl

O	-0.09518500	0.19614500	1.92693300
Ru	0.02810400	-0.03553300	-0.01303800
N	2.03356400	-0.20207500	-0.03005200
C	2.95239700	0.83693400	-0.10822500
C	4.26343400	0.28237900	-0.24839900
C	4.14379700	-1.07313600	-0.22643200
C	2.75527800	-1.37612800	-0.08335000
C	2.65823500	2.20490200	-0.05601000
C	3.79859700	3.14343800	-0.08323100
C	4.78395200	3.12439200	0.91262000
C	5.85219600	4.01130500	0.90245300
C	5.95916000	4.94314900	-0.12840500
C	4.99777100	4.98533500	-1.13677900
C	3.93187100	4.09600600	-1.10195500
F	4.69410000	2.25375400	1.91989600
F	6.76213700	3.98243000	1.86684000
F	6.97451600	5.78872600	-0.15037000
F	5.10936800	5.86462700	-2.12302400
F	3.03357400	4.14372900	-2.08634700
C	2.20279700	-2.66732600	-0.03610500
C	0.83026300	-2.96822500	0.00301800
N	-0.18498500	-2.03521600	0.00346300
C	-1.38154600	-2.74567800	0.00789600
C	-1.08504800	-4.14535900	0.02673600
C	0.26793900	-4.28171400	0.04161200
C	-2.66704300	-2.19695300	-0.03772400
C	-2.98337900	-0.81480200	-0.04281500
N	-2.07237500	0.18817200	0.03871500
C	-2.76268400	1.36850000	0.05439900
C	-4.16879000	1.09059900	-0.02727700
C	-4.30674300	-0.26352500	-0.07518300
C	-2.19922400	2.65833500	0.13334500
C	-3.14115600	3.79404900	0.21783000
C	-4.02956700	3.92186800	1.29346200
C	-4.91748500	4.98531400	1.38669000
C	-4.93987300	5.94932000	0.38019900
C	-4.07310200	5.84726200	-0.70667400
C	-3.18504200	4.78178700	-0.77468700
F	-4.01522400	3.02015300	2.27689500

F	-5.73544300	5.09156200	2.42538900
F	-5.78484600	6.96271000	0.45653800
F	-4.10591000	6.75983900	-1.66831100
F	-2.37855100	4.69601700	-1.83330600
C	3.14699400	-3.80289000	-0.04286100
C	4.09473600	-3.96432100	0.97618700
C	4.98623800	-5.02886000	0.98447700
C	4.95070000	-5.96062700	-0.05147500
C	4.02464800	-5.82449500	-1.08418100
C	3.13709700	-4.75687700	-1.06852600
F	4.13898800	-3.09163000	1.98376700
F	2.27221800	-4.63683500	-2.07768000
F	4.00257500	-6.70542600	-2.07510800
F	5.79779600	-6.97477900	-0.05485300
F	5.86180200	-5.16658200	1.97062800
N	0.20153800	2.07143500	0.00907800
C	-0.82209200	2.96897800	0.12314300
C	-0.27644400	4.29077400	0.25028500
C	1.07904200	4.17045900	0.18821500
C	1.36349300	2.77374300	0.03126100
C	-3.80559500	-3.13982400	-0.07001800
C	-4.67855600	-3.18340100	-1.16365900
C	-5.75547200	-4.05908600	-1.20500800
C	-5.98483600	-4.91432300	-0.12861300
C	-5.13625000	-4.89198500	0.97661300
C	-4.06028300	-4.01428100	0.99309500
F	-4.47018100	-2.38137800	-2.20903200
F	-6.55836000	-4.09099900	-2.25984400
F	-7.00912600	-5.74913300	-0.15657700
F	-5.36270200	-5.70003100	2.00357100
F	-3.26732400	-4.00141500	2.06666600
H	-0.84837500	5.19986300	0.38478600
H	1.81385800	4.96182800	0.26342500
H	5.17472200	0.85475300	-0.36503900
H	4.93819400	-1.80229200	-0.32088000
H	0.83109200	-5.20516500	0.07359900
H	-1.81976700	-4.93994000	0.02670400
H	-5.22875700	-0.82819700	-0.12328000
H	-4.95686300	1.83223300	-0.05834000
O	0.59292100	-0.65479300	2.56456300
Cl	-0.20729200	0.20501400	-2.29676700

$\Delta E_{\text{solv}} = -4602.25998991$

$\Delta G_{\text{solv}} = -4601.91551891$

³F-Cl

O	0.07564100	0.63145700	-2.23746000
Ru	0.00421700	0.00037900	-0.20317600
N	-2.06504600	0.18151000	-0.16652600
C	-2.77454400	1.34669800	-0.07395000
C	-4.17189900	1.04539700	0.06946000
C	-4.28775700	-0.30708300	0.08287300
C	-2.96193600	-0.84527400	-0.04968900
C	-2.22284400	2.64360000	-0.02935100
C	-3.17216000	3.77335900	0.00710000
C	-4.09988500	3.97381000	-1.02399500
C	-4.99824200	5.03200300	-1.00513700
C	-4.99219200	5.91639200	0.07206500
C	-4.08716200	5.74078400	1.11735700
C	-3.18962100	4.68220500	1.07372500
F	-4.11392300	3.14964400	-2.07299900
F	-5.85285600	5.20881300	-2.00357000
F	-5.84686000	6.92367800	0.10229300
F	-4.09410600	6.57669600	2.14664900
F	-2.34760200	4.52467300	2.09548600
C	-2.64232300	-2.21657000	0.02564400
C	-1.34334500	-2.76936400	0.05024100
N	-0.17356000	-2.06324600	-0.00936400
C	0.85877600	-2.95977000	0.01363400
C	0.32006300	-4.28327700	0.10814400
C	-1.03659400	-4.16687800	0.11474600
C	2.23273800	-2.63945500	-0.03426300
C	2.78275400	-1.34449000	-0.10128400
N	2.06918400	-0.17737900	-0.16318200
C	2.97316100	0.84837300	-0.14668600
C	4.30480900	0.30969900	-0.11039500
C	4.18766800	-1.04257300	-0.09881100
C	2.65361700	2.22054400	-0.09916900
C	3.78247400	3.17249100	-0.11370700
C	4.67553300	3.22146800	-1.19183400
C	5.74080600	4.11120900	-1.22001000
C	5.94009000	4.97525400	-0.14455800
C	5.07262800	4.94777300	0.94591700
C	4.00713100	4.05720800	0.94915600
F	4.49549000	2.41461100	-2.23949900
F	6.56067400	4.14919900	-2.26174200
F	6.95352000	5.82323700	-0.15940800
F	5.27179700	5.76337400	1.97221700
F	3.20063000	4.03752200	2.01066400

C	-3.77500700	-3.16153200	0.10396000
C	-4.72122700	-3.24008000	-0.92604300
C	-5.79117400	-4.12317600	-0.87162000
C	-5.94189200	-4.94817100	0.24184600
C	-5.02244100	-4.88792300	1.28768900
C	-3.95379000	-4.00466000	1.20818900
F	-4.59009200	-2.46739600	-2.00589200
F	-3.09857100	-3.95075600	2.23019200
F	-5.17635500	-5.66489300	2.35131800
F	-6.95966700	-5.78870400	0.30681500
F	-6.66222800	-4.18981700	-1.86938400
N	0.18391800	2.05880600	0.01158100
C	1.35466100	2.76822100	-0.02732300
C	1.04942100	4.16622000	-0.06150300
C	-0.30704300	4.28383000	-0.04560800
C	-0.84747600	2.95937700	-0.00108700
C	3.18077900	-3.77424000	0.00491600
C	4.07316100	-3.94514900	1.06975100
C	4.95922800	-5.01383600	1.11563300
C	4.97091500	-5.94009000	0.07444100
C	4.09631700	-5.79556400	-1.00111700
C	3.21298400	-4.72438600	-1.02239000
F	4.06883600	-3.07873900	2.08378600
F	5.78502400	-5.15988500	2.14306800
F	5.81340600	-6.95825000	0.10730000
F	4.11618500	-6.67357800	-1.99511500
F	2.39134900	-4.59812800	-2.06710900
H	1.77603100	4.96618600	-0.12051800
H	-0.88644200	5.19701700	-0.08793100
H	-4.96307000	1.77494800	0.18500500
H	-5.19199500	-0.88818000	0.21011700
H	-1.76249100	-4.96858100	0.15375400
H	0.89983400	-5.19553400	0.16319500
H	4.98743300	-1.77132400	-0.07971800
H	5.21754100	0.89036100	-0.07742100
O	-0.05417700	-0.64037300	-2.11323600
Cl	-0.01779000	-0.04082500	2.10552300

$\Delta E_{\text{solv}} = -4602.27209039$

$\Delta G_{\text{solv}} = -4601.92863439$

⁵F-Cl

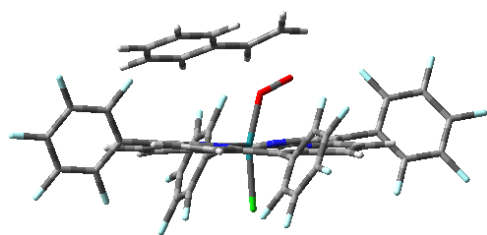
O	0.05866600	-0.25921200	2.22299400
Ru	-0.00471900	0.02235100	-0.29660500
N	-1.64396800	1.22316300	-0.00203800

C	-2.96655800	0.82801500	-0.09111400
C	-3.80227700	1.98127100	-0.16360700
C	-2.99185700	3.07619600	-0.10267900
C	-1.64908700	2.60676700	-0.00036400
C	-3.42601100	-0.49459900	-0.10061500
C	-4.88853500	-0.71925700	-0.12780800
C	-5.71480300	-0.27593500	0.90998800
C	-7.08736200	-0.48993300	0.89633200
C	-7.66469900	-1.16378800	-0.17740900
C	-6.86884000	-1.61859500	-1.22626800
C	-5.49789000	-1.39542800	-1.19011300
F	-5.18192700	0.36084000	1.95675700
F	-7.84520200	-0.06557300	1.89965100
F	-8.97077000	-1.37322300	-0.20011500
F	-7.42089600	-2.25528700	-2.25119700
F	-4.75493600	-1.83632100	-2.20814100
C	-0.51959700	3.43046400	0.06693300
C	0.80296600	2.97320300	0.08036400
N	1.20494800	1.65078700	0.00065900
C	2.58817600	1.66265500	-0.01685400
C	3.05086900	3.00939400	0.06490300
C	1.95305100	3.81399400	0.14318800
C	3.41697200	0.53714400	-0.10308500
C	2.96223600	-0.78460900	-0.14092800
N	1.63683200	-1.18250400	-0.11759800
C	1.64226600	-2.56311600	-0.06657100
C	2.98946400	-3.03249700	-0.09166700
C	3.80153600	-1.93846200	-0.13769200
C	0.51188100	-3.38343600	0.03056300
C	0.74022800	-4.83601200	0.20110000
C	1.36807900	-5.32502000	1.35079000
C	1.58831000	-6.68292300	1.54304800
C	1.17443100	-7.58674500	0.56691800
C	0.54479000	-7.12982000	-0.58880900
C	0.33394200	-5.76665400	-0.75877900
F	1.75938500	-4.47156300	2.30236100
F	2.17990000	-7.12138600	2.64710900
F	1.37813100	-8.88265800	0.73928100
F	0.15561100	-7.99306100	-1.51826200
F	-0.26909300	-5.34718400	-1.87381000
C	-0.74356100	4.89399700	0.10743400
C	-1.40946200	5.49596200	1.17958100
C	-1.63240800	6.86659800	1.22690400
C	-1.18623100	7.66931200	0.17962000

C	-0.52210300	7.09902000	-0.90386100
C	-0.30888200	5.72628200	-0.92867600
F	-1.84291900	4.74465200	2.19539000
F	0.32104100	5.19982100	-1.98250100
F	-0.10535100	7.86361100	-1.90521400
F	-1.39497000	8.97536900	0.21329000
F	-2.26083200	7.41179300	2.26075900
N	-1.21620100	-1.61528800	-0.10389300
C	-0.81342000	-2.93255300	0.00919400
C	-1.96182900	-3.77023400	0.13245900
C	-3.06078600	-2.96519700	0.07811000
C	-2.59962700	-1.62267700	-0.06169800
C	4.88176900	0.75623100	-0.12821900
C	5.64668400	0.39852300	-1.24240300
C	7.02223300	0.59206500	-1.27879000
C	7.66389300	1.15473300	-0.17796600
C	6.92944500	1.51831800	0.94831100
C	5.55504900	1.31549300	0.96163600
F	5.05039000	-0.14208000	-2.30815600
F	7.72272000	0.24927700	-2.35228200
F	8.97341800	1.34279100	-0.20132900
F	7.54287800	2.04632000	2.00011500
F	4.87056900	1.66278500	2.05586400
H	-1.94036000	-4.84528100	0.25781400
H	-4.09891700	-3.26321500	0.15441300
H	-4.88002200	1.96519100	-0.26597800
H	-3.28769700	4.11682400	-0.14649900
H	1.93403000	4.89273200	0.23175600
H	4.08938500	3.31467000	0.06049900
H	4.88397800	-1.92314200	-0.15150100
H	3.28694400	-4.07361700	-0.08008100
O	0.27050100	-1.38629700	2.65917600
Cl	-0.03313700	0.15142200	-2.52715200

$\Delta E_{\text{solv}} = -4602.27826145$

$\Delta G_{\text{solv}} = -4601.93768445$



12-Cl

C	3.43516100	0.84424800	3.32951800
---	------------	------------	------------

C	2.10985900	0.94365300	3.75553700
C	1.28516300	-0.17106500	3.72606700
C	1.76355100	-1.41333400	3.24569600
C	3.10108300	-1.48574100	2.80632700
C	3.93146700	-0.37810100	2.86652900
C	0.94342600	-2.60292400	3.19753900
C	-0.28567600	-2.75115800	3.73734200
O	-0.54280900	-0.21202900	1.60698600
Ru	-0.17492600	0.11344400	-0.27196800
N	-0.25244200	-1.97685400	-0.30743100
C	0.79831300	-2.82687500	-0.46920700
C	0.31074700	-4.17665100	-0.49559700
C	-1.04068700	-4.11569200	-0.32064900
C	-1.38909100	-2.72819700	-0.22565400
C	2.14608600	-2.42946800	-0.59406100
C	3.14522200	-3.47831100	-0.91346900
C	3.45461900	-4.51977600	-0.03661500
C	4.38802100	-5.49935100	-0.35038200
C	5.04136600	-5.45147100	-1.57922500
C	4.75749500	-4.42672100	-2.47830800
C	3.82027300	-3.45774800	-2.13928900
F	2.85371400	-4.58733200	1.16258700
F	4.66293300	-6.46913000	0.51407100
F	5.93391900	-6.37799100	-1.88990700
F	5.37733100	-4.38290100	-3.65045700
F	3.56333100	-2.48998400	-3.02013400
C	-2.71039800	-2.23184700	-0.16078500
C	-3.10197600	-0.88478800	-0.26520400
N	-2.25625900	0.19333700	-0.33171200
C	-3.02170300	1.31277500	-0.40838300
C	-4.40882100	0.93853800	-0.43674800
C	-4.45827500	-0.41555500	-0.31475700
C	-2.52510900	2.63380500	-0.38419200
C	-1.18154200	2.99540200	-0.24782000
N	-0.10095000	2.12227300	-0.16820500
C	1.03397200	2.89920300	-0.03960800
C	0.65457100	4.27822300	-0.00030200
C	-0.69850500	4.33645500	-0.13415200
C	2.34952500	2.42063300	-0.02627700
C	3.43060700	3.42499200	0.11106000
C	3.58293200	4.16032400	1.28961200
C	4.58546800	5.10969300	1.44034100
C	5.46517200	5.34784100	0.38714400
C	5.33699700	4.63588900	-0.80265900

C	4.32657800	3.68936700	-0.92851600
F	2.75085400	3.94720700	2.31766800
F	4.71212300	5.78235300	2.57864100
F	6.42446500	6.25023800	0.51912200
F	6.17165700	4.86739600	-1.80802600
F	4.21781600	3.02655200	-2.08196200
C	-3.78242400	-3.23997400	0.00186800
C	-3.86969900	-3.99586500	1.17447900
C	-4.85935600	-4.95195500	1.36017000
C	-5.79038000	-5.17587900	0.34861600
C	-5.72671900	-4.44285900	-0.83417900
C	-4.73066300	-3.48702300	-0.99490600
F	-2.99035000	-3.78752200	2.16040700
F	-4.68193500	-2.80675600	-2.14203500
F	-6.60869500	-4.66540100	-1.80021500
F	-6.73633600	-6.08663700	0.51186900
F	-4.92392900	-5.64555300	2.49066300
N	1.85536100	0.01750800	-0.24795500
C	2.72517100	1.07701200	-0.17789000
C	4.06887400	0.59716700	-0.30716200
C	4.00241400	-0.74650300	-0.50993400
C	2.62268700	-1.12048800	-0.47162400
C	-3.51238300	3.73357000	-0.48228600
C	-3.50835500	4.61264900	-1.57005000
C	-4.43026000	5.64654900	-1.67918700
C	-5.38345100	5.82273900	-0.67923100
C	-5.40844800	4.96816600	0.42021000
C	-4.47833200	3.94008200	0.50703200
F	-2.60418900	4.46166300	-2.53994200
F	-4.40936500	6.46042900	-2.72732300
F	-6.26457800	6.80591500	-0.77196600
F	-6.30954900	5.14549400	1.37909400
F	-4.51077000	3.14376000	1.58035000
H	4.96020800	1.20995500	-0.25345300
H	4.83032300	-1.43232600	-0.64311800
H	0.91553700	-5.06381000	-0.63659600
H	-1.74038800	-4.94219700	-0.30419900
H	-5.34287400	-1.03752300	-0.27239800
H	-5.24390400	1.62239500	-0.52081900
H	-1.31812300	5.22431000	-0.14680100
H	1.34025000	5.11069100	0.09814700
H	-0.83745700	-3.67930100	3.62059300
H	-0.75372800	-1.98712800	4.35201900
H	1.37610200	-3.44989800	2.66284800

H	0.25887200	-0.09141800	4.07759000
H	3.48141800	-2.43967000	2.44168900
H	1.72593500	1.89457900	4.11842100
H	4.96936900	-0.45963300	2.55064700
H	4.08484800	1.71652700	3.37068800
O	-1.38354400	-0.99074900	2.11493400
Cl	-0.22718900	0.00194800	-2.55647700

$\Delta E_{\text{solv}} = -4911.923432$

$\Delta G_{\text{solv}} = -4911.450558$

³2-Cl

C	-3.51114700	-1.06663100	3.41088800
C	-2.18317700	-1.12027800	3.84061900
C	-1.39132800	0.01527100	3.79487800
C	-1.90779600	1.23616900	3.30139800
C	-3.24670900	1.26324000	2.85656500
C	-4.04294000	0.13221300	2.92682700
C	-1.12396600	2.44801000	3.23643300
C	0.10893100	2.63540600	3.75772100
O	0.43185700	0.03929900	1.64676700
Ru	0.21952300	-0.06327500	-0.36080500
N	0.26505400	1.99167600	-0.32677500
C	-0.80601000	2.83849600	-0.45050800
C	-0.33605700	4.19173200	-0.44766800
C	1.01819400	4.14737400	-0.29431700
C	1.39221200	2.76626400	-0.23678800
C	-2.15150300	2.43945100	-0.57571500
C	-3.15764300	3.48619500	-0.87803500
C	-3.48618400	4.50468700	0.01859400
C	-4.43052700	5.47798900	-0.28148300
C	-5.07629300	5.44595200	-1.51507600
C	-4.77409400	4.44322900	-2.43306500
C	-3.82680900	3.47948400	-2.10752500
F	-2.89364900	4.55451400	1.22192000
F	-4.72396000	6.42613700	0.60052600
F	-5.97903800	6.36682500	-1.81221500
F	-5.38719900	4.41457400	-3.60908600
F	-3.55213400	2.53230400	-3.00473800
C	2.71361700	2.29005800	-0.18528500
C	3.10944800	0.94095900	-0.28302700
N	2.26345800	-0.13319500	-0.36578900
C	3.04575800	-1.26834200	-0.41458800
C	4.42562500	-0.88124100	-0.41592900
C	4.46569900	0.47389700	-0.30398800
C	2.57138100	-2.58459800	-0.39709900

C	1. 21632700	-2. 96846000	-0. 27769200
N	0. 14831600	-2. 11460700	-0. 21408800
C	-0. 98508800	-2. 88818000	-0. 08139500
C	-0. 60330700	-4. 26926600	-0. 04422000
C	0. 75247700	-4. 31839200	-0. 16647000
C	-2. 30355400	-2. 41729600	-0. 06224200
C	-3. 37841800	-3. 42962100	0. 06291100
C	-3. 51814800	-4. 19906200	1. 22193700
C	-4. 51989200	-5. 15176100	1. 35595400
C	-5. 40798600	-5. 36425300	0. 30435000
C	-5. 28934100	-4. 62226700	-0. 86824300
C	-4. 28235300	-3. 67046800	-0. 97688000
F	-2. 67936700	-4. 01624600	2. 24905100
F	-4. 63626000	-5. 85374400	2. 47739400
F	-6. 36430400	-6. 27135500	0. 42031200
F	-6. 12899400	-4. 83148000	-1. 87395400
F	-4. 18114700	-2. 98277900	-2. 11601300
C	3. 77788800	3. 30125900	-0. 00656200
C	3. 83704100	4. 06816600	1. 16191000
C	4. 82430800	5. 02347400	1. 36338300
C	5. 78210000	5. 23545100	0. 37411600
C	5. 74748200	4. 49145700	-0. 80324800
C	4. 75300000	3. 53736600	-0. 98031000
F	2. 93344600	3. 87236100	2. 12788900
F	4. 73177300	2. 84533300	-2. 12143000
F	6. 65474600	4. 70319900	-1. 74793300
F	6. 72576900	6. 14526900	0. 55332900
F	4. 86269600	5. 72716800	2. 48863800
N	-1. 85122600	0. 00256800	-0. 26907000
C	-2. 69850700	-1. 06581600	-0. 20135700
C	-4. 05078000	-0. 60894300	-0. 32230200
C	-4. 00305000	0. 74047400	-0. 50725700
C	-2. 62449100	1. 12338700	-0. 46999900
C	3. 56930900	-3. 67627700	-0. 46430500
C	3. 58561700	-4. 56690200	-1. 54300000
C	4. 50960000	-5. 60094400	-1. 62552200
C	5. 44449400	-5. 76624800	-0. 60611300
C	5. 44887700	-4. 90075000	0. 48507700
C	4. 51734700	-3. 87185200	0. 54503000
F	2. 69891200	-4. 42462600	-2. 53010600
F	4. 50981600	-6. 42476800	-2. 66577800
F	6. 32802400	-6. 74898600	-0. 67290100
F	6. 33204600	-5. 06810800	1. 46203200
F	4. 52980900	-3. 06685800	1. 61153200

H	-4.93382400	-1.23335300	-0.26904100
H	-4.83987300	1.41778000	-0.62862700
H	-0.95445500	5.07377000	-0.55659400
H	1.70412700	4.98497700	-0.26388100
H	5.34741200	1.09886900	-0.24723800
H	5.26755300	-1.55880900	-0.47673900
H	1.37992100	-5.20071400	-0.17532700
H	-1.28419500	-5.10669200	0.04322700
H	0.63064700	3.57936800	3.62679000
H	0.61350200	1.88503100	4.35953900
H	-1.58998000	3.28117700	2.70856800
H	-0.35865400	-0.03172900	4.13220000
H	-3.65285900	2.20075100	2.47524100
H	-1.77151000	-2.05481700	4.21489200
H	-5.08025400	0.17659500	2.60117200
H	-4.13396400	-1.95761800	3.46509400
O	1.25833100	0.86948700	2.14024500
Cl	0.09823500	-0.10294300	-2.67496500

$\Delta E_{\text{solv}} = -4911.92063532$

$\Delta G_{\text{solv}} = -4911.44991632$

⁵2-Cl

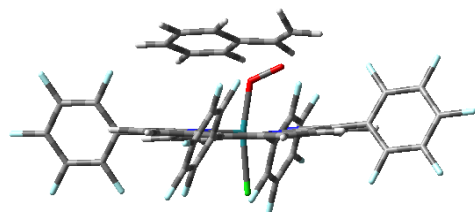
C	3.32287800	1.60189900	3.36365800
C	2.02982900	1.48887900	3.87641800
C	1.40377100	0.25240600	3.91674600
C	2.05037800	-0.90493400	3.42718100
C	3.34891600	-0.76522100	2.89911600
C	3.98305900	0.46805900	2.88457900
C	1.43408500	-2.21630400	3.44866200
C	0.26600800	-2.54370100	4.03685300
O	-0.33249600	-0.18385300	1.74608600
Ru	-0.22680100	0.04034400	-0.56462400
N	0.14872100	-1.96591200	-0.46759400
C	1.38002500	-2.58418900	-0.58205700
C	1.19295600	-3.99999200	-0.59267200
C	-0.14165400	-4.23571500	-0.44241000
C	-0.79561200	-2.96692200	-0.37586300
C	2.61412600	-1.92998800	-0.65923900
C	3.82893500	-2.75354400	-0.87452300
C	4.28708000	-3.67711900	0.06729400
C	5.42609000	-4.44438800	-0.14236800
C	6.14248200	-4.29490800	-1.32692300
C	5.71574900	-3.38083400	-2.28669900
C	4.57202000	-2.62617600	-2.05266100
F	3.62593700	-3.83898200	1.22445800

F	5.83514700	-5.30844100	0.77952200
F	7.23029100	-5.01904400	-1.53840600
F	6.39659400	-3.23818000	-3.41665700
F	4.18238300	-1.75830600	-2.98874300
C	-2.18071500	-2.78564000	-0.28545800
C	-2.84252100	-1.55079600	-0.34755700
N	-2.23442700	-0.31784300	-0.41945600
C	-3.24159300	0.62854300	-0.42131400
C	-4.50585200	-0.03585100	-0.40543700
C	-4.26051200	-1.37529100	-0.32975200
C	-3.05896200	2.01429800	-0.36711200
C	-1.81640200	2.65516300	-0.25905100
N	-0.58451900	2.03605400	-0.24951100
C	0.36316600	3.03089300	-0.11834600
C	-0.29371100	4.29630800	-0.03203500
C	-1.63510500	4.06524100	-0.11908200
C	1.75196900	2.84889500	-0.11472300
C	2.59670900	4.06001800	0.02430000
C	2.60786800	4.80508000	1.20592800
C	3.39087100	5.94383200	1.35026100
C	4.18766900	6.36493800	0.28859100
C	4.19592800	5.64643200	-0.90417100
C	3.40384900	4.51017800	-1.02403500
F	1.85034000	4.42046100	2.24089100
F	3.38686700	6.62509600	2.49089000
F	4.93873200	7.44795900	0.41376300
F	4.95173300	6.05115300	-1.91731500
F	3.42315900	3.84098900	-2.17932700
C	-3.00361500	-4.00132300	-0.08900200
C	-2.89122900	-4.74205200	1.09080500
C	-3.64254700	-5.88912300	1.31127500
C	-4.53569400	-6.31869500	0.33240000
C	-4.67078900	-5.60132500	-0.85372000
C	-3.90682500	-4.45683800	-1.05179100
F	-2.04334700	-4.33838500	2.04482900
F	-4.04723800	-3.78642500	-2.19846200
F	-5.51856600	-6.01596800	-1.78717500
F	-5.25759600	-7.41075500	0.53069100
F	-3.51871000	-6.57058700	2.44467400
N	1.78767400	0.38773400	-0.38320000
C	2.40297300	1.61902200	-0.26764400
C	3.81868100	1.44542400	-0.34083700
C	4.05676200	0.11622200	-0.52526200
C	2.79111000	-0.54535300	-0.54413000

C	-4.26715300	2.87317900	-0.38839100
C	-4.51341900	3.74051400	-1.45641600
C	-5.63849100	4.55543000	-1.49447300
C	-6.54973000	4.51419500	-0.44225700
C	-6.32966000	3.66359800	0.63808800
C	-5.19676100	2.85913600	0.65462700
F	-3.65183700	3.79686600	-2.47517100
F	-5.84942000	5.36524200	-2.52491600
F	-7.62556600	5.28552400	-0.46864700
F	-7.19419700	3.63015600	1.64565800
F	-5.00172700	2.05882300	1.70801000
H	4.55112300	2.23807600	-0.25026100
H	5.01868300	-0.37431200	-0.61394100
H	1.98029600	-4.73466400	-0.70457100
H	-0.64148200	-5.19623500	-0.41461000
H	-4.99079300	-2.17233200	-0.27336800
H	-5.47092200	0.45401200	-0.43176300
H	-2.43208000	4.79762300	-0.08630300
H	0.20387200	5.25300000	0.06710300
H	-0.12552200	-3.55543700	3.98124100
H	-0.31680200	-1.83529500	4.62100900
H	1.98682100	-3.00139300	2.92891900
H	0.40031500	0.17274000	4.32976800
H	3.86002300	-1.65099500	2.52283000
H	1.51514100	2.36932600	4.25426300
H	4.99655200	0.55176100	2.49697900
H	3.82087100	2.56999900	3.35186200
O	-1.11999400	-1.04948200	2.17204600
Cl	-0.20472100	0.20243200	-2.80563500

$\Delta E_{\text{solv}} = -4911.92093208$

$\Delta G_{\text{solv}} = -4911.45086308$



¹TS4-Cl

C	3.76815300	0.56112300	3.19245000
C	2.48049200	0.90428400	3.61606300
C	1.48374200	-0.05172600	3.63169300
C	1.74371700	-1.38199300	3.18613300
C	3.06564900	-1.70279800	2.76808000

C	4.06172500	-0.75003600	2.79140600
C	0.72805300	-2.35564700	3.11042800
C	-0.60767800	-2.09700500	3.45813700
O	-0.44890000	-0.14692900	1.69124700
Ru	-0.19808400	0.13372300	-0.26207700
N	-0.43157000	-1.94613100	-0.25265100
C	0.56443300	-2.87577500	-0.35257500
C	-0.02103700	-4.18466000	-0.39280100
C	-1.37343700	-4.02156300	-0.30149800
C	-1.61983300	-2.61284800	-0.22875200
C	1.94330500	-2.59564300	-0.45919700
C	2.84911700	-3.74313300	-0.72022900
C	3.05306000	-4.76692800	0.20571600
C	3.88963000	-5.84581600	-0.04809000
C	4.55152900	-5.92161000	-1.27059900
C	4.37108500	-4.91969300	-2.22013400
C	3.52741000	-3.85042900	-1.93923300
F	2.43542300	-4.72426600	1.40208300
F	4.06327700	-6.79407800	0.86599600
F	5.35299200	-6.94355400	-1.52746400
F	4.99769800	-4.99246600	-3.38727000
F	3.36759800	-2.91077000	-2.87109400
C	-2.90203800	-2.01772500	-0.21083400
C	-3.17766500	-0.64805000	-0.28779800
N	-2.24252900	0.36533000	-0.31949000
C	-2.92544900	1.54228100	-0.35350300
C	-4.34011500	1.27524200	-0.38896000
C	-4.49420900	-0.07141600	-0.32362500
C	-2.33553100	2.81803600	-0.29704900
C	-0.96405900	3.07164700	-0.18317400
N	0.04129200	2.11405800	-0.15229600
C	1.25004600	2.80287500	-0.05302700
C	0.97803200	4.20244500	0.01306700
C	-0.37250300	4.36671600	-0.06741600
C	2.52196400	2.23022100	-0.08448400
C	3.68361200	3.15301500	-0.04471500
C	4.00295700	3.87922200	1.10388800
C	5.08660600	4.74737500	1.15099400
C	5.88421100	4.90607500	0.02056200
C	5.59269400	4.19664900	-1.14163500
C	4.50168300	3.33485900	-1.16287400
F	3.25460500	3.73968600	2.20847300
F	5.36666300	5.41577400	2.26526200
F	6.92145900	5.72896300	0.05222200

F	6.35155400	4.34929500	-2.21968300
F	4.24045500	2.66838900	-2.28867700
C	-4.05521900	-2.94309500	-0.11409900
C	-4.25105200	-3.71752000	1.03185700
C	-5.31460300	-4.60170700	1.15204900
C	-6.21722300	-4.72910600	0.09885500
C	-6.04939800	-3.97345700	-1.05879200
C	-4.97722400	-3.09319700	-1.15350900
F	-3.39933600	-3.60483700	2.06180100
F	-4.83196000	-2.38756800	-2.27639800
F	-6.90551800	-4.10240400	-2.06481400
F	-7.23555000	-5.56926100	0.19980500
F	-5.47762800	-5.31711200	2.25971700
N	1.85778400	-0.13022200	-0.19891200
C	2.79731400	0.85455300	-0.20374800
C	4.10533000	0.27858500	-0.36521000
C	3.93514000	-1.06248700	-0.49818300
C	2.52816800	-1.32672600	-0.39375700
C	-3.23971800	3.99125600	-0.33531900
C	-3.20268200	4.90200300	-1.39551600
C	-4.04734600	6.00445700	-1.44480200
C	-4.95756300	6.21683100	-0.41266700
C	-5.01586300	5.33000400	0.65930300
C	-4.16118500	4.23518200	0.68689000
F	-2.33906400	4.71825400	-2.39674300
F	-3.99399100	6.84931200	-2.46763100
F	-5.76657300	7.26458000	-0.44914300
F	-5.87726700	5.53886200	1.64873700
F	-4.22671600	3.40591900	1.73401200
H	5.03698200	0.83129700	-0.37944400
H	4.70357800	-1.81456400	-0.63162900
H	0.52183000	-5.11584400	-0.49868100
H	-2.13285700	-4.79354900	-0.32413200
H	-5.42355600	-0.62581100	-0.30350400
H	-5.11874400	2.02546500	-0.44591200
H	-0.91950300	5.30113500	-0.04676900
H	1.72804500	4.97955100	0.09377100
H	-1.33922900	-2.89110500	3.34034800
H	-0.82358000	-1.41142600	4.27348000
H	0.97126300	-3.30795500	2.64003900
H	0.49242800	0.21460300	3.98726400
H	3.27406900	-2.71965000	2.44091000
H	2.26779200	1.91881400	3.94174200
H	5.07136500	-1.00815100	2.48147900

H	4.55410500	1.31487300	3.19569500
O	-1.31286300	-0.98733800	2.17408200
Cl	-0.07467700	-0.06952700	-2.54434000

$\Delta E_{\text{solv}} = -4911.9170215$

$\Delta G_{\text{solv}} = -4911.4420695$

³TS4-Cl

C	-3.72650200	-0.81159900	3.28312000
C	-2.42404000	-1.09224200	3.70407000
C	-1.46567200	-0.09555600	3.69165900
C	-1.78686500	1.20897300	3.22649700
C	-3.11394200	1.46486500	2.79475500
C	-4.07267100	0.47299800	2.84450400
C	-0.81548900	2.24320300	3.14682600
C	0.48790100	2.12095300	3.58115500
O	0.46944000	-0.03825300	1.69246400
Ru	0.21039500	-0.07787700	-0.35896600
N	0.37987500	1.97108900	-0.31117600
C	-0.64416000	2.88234300	-0.39310200
C	-0.09386300	4.20422500	-0.39913700
C	1.26158700	4.07800700	-0.30861700
C	1.55590700	2.67813600	-0.26771700
C	-2.01236200	2.57336300	-0.48754500
C	-2.95550200	3.69794800	-0.71133200
C	-3.19198300	4.67945900	0.25165000
C	-4.06601300	5.73714200	0.03740500
C	-4.73619200	5.83071200	-1.17943800
C	-4.52653300	4.86843100	-2.16342700
C	-3.64409100	3.82086100	-1.92235500
F	-2.56838200	4.61347900	1.44327400
F	-4.26911300	6.64732600	0.98356600
F	-5.57486200	6.83169300	-1.39759200
F	-5.16324900	4.95764000	-3.32403600
F	-3.45848000	2.91570700	-2.88364900
C	2.84722400	2.12873600	-0.24473800
C	3.15470700	0.76060100	-0.31378200
N	2.24546000	-0.26655800	-0.36706800
C	2.95861200	-1.44708900	-0.37471500
C	4.35849400	-1.14313000	-0.38485600
C	4.47990600	0.21086700	-0.32239400
C	2.41116600	-2.73329700	-0.31312100
C	1.04080800	-3.02900800	-0.20398300
N	0.01773200	-2.11188000	-0.18696700
C	-1.16413400	-2.82087000	-0.09016800

C	-0.86094200	-4.22001400	-0.02255400
C	0.49295900	-4.34731300	-0.08924200
C	-2.45190300	-2.27878600	-0.11415600
C	-3.59086700	-3.22960700	-0.06956700
C	-3.86776100	-3.98859800	1.06941000
C	-4.92772100	-4.88541100	1.11984200
C	-5.74351900	-5.04332800	0.00252300
C	-5.49249600	-4.30495800	-1.15101900
C	-4.42452200	-3.41488500	-1.17609700
F	-3.09923500	-3.85750300	2.16077300
F	-5.16767700	-5.58291300	2.22564200
F	-6.75807200	-5.89380500	0.03806300
F	-6.26670800	-4.45801600	-2.21812600
F	-4.20121800	-2.72439100	-2.29610200
C	3.97733400	3.07894800	-0.12458800
C	4.13872500	3.85282100	1.02745900
C	5.18368300	4.75629700	1.16823900
C	6.10394300	4.90168900	0.13304900
C	5.97223600	4.14512500	-1.02862700
C	4.91683500	3.24768700	-1.14514300
F	3.27056200	3.72408800	2.04091800
F	4.80680800	2.53789900	-2.27032900
F	6.84622000	4.28961500	-2.01721700
F	7.10514600	5.75964000	0.25477500
F	5.31279600	5.47309000	2.27956900
N	-1.85073700	0.11635700	-0.24135900
C	-2.75954600	-0.90796200	-0.23078500
C	-4.07975500	-0.37171200	-0.37682100
C	-3.95403900	0.97865600	-0.50727800
C	-2.55785400	1.28557300	-0.42363500
C	3.35010900	-3.88080400	-0.33063200
C	3.36002300	-4.78885600	-1.39308100
C	4.22903100	-5.87303700	-1.42311500
C	5.11810900	-6.06735300	-0.36918800
C	5.13066300	-5.18142900	0.70481800
C	4.25080200	-4.10599400	0.71363300
F	2.51577200	-4.62202700	-2.41392700
F	4.21926400	-6.71730700	-2.44788800
F	5.95135500	-7.09672900	-0.38717400
F	5.97323100	-5.37146200	1.71427600
F	4.27420100	-3.27561000	1.76172400
H	-4.99559100	-0.95009900	-0.37770900
H	-4.74829600	1.70494700	-0.63339000
H	-0.66402300	5.12157800	-0.47982600

H	1.99765400	4.87271200	-0.30844200
H	5.39720300	0.78476100	-0.28550000
H	5.15726600	-1.87316700	-0.41840700
H	1.06876000	-5.26397900	-0.06271500
H	-1.59197200	-5.01571400	0.05017300
H	1.19590100	2.92767400	3.41929400
H	0.77442800	1.38189000	4.32159700
H	-1.10447000	3.15300800	2.61912500
H	-0.45805900	-0.31489800	4.03285000
H	-3.36350600	2.46430500	2.44149900
H	-2.16710600	-2.09150800	4.04486800
H	-5.09198600	0.68314800	2.52929200
H	-4.48167500	-1.59538200	3.31059700
O	1.26899500	0.87655200	2.12814900
Cl	0.05000400	-0.09768000	-2.65379500

$\Delta E_{\text{solv}} = -4911.92115405$

$\Delta G_{\text{solv}} = -4911.45015005$

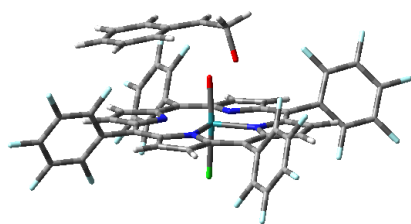
⁵TS4-Cl

C	5.09614000	0.93733200	2.71820200
C	3.85062000	1.54418800	2.91234600
C	2.72552800	0.77410900	3.14943500
C	2.81682000	-0.64141700	3.20112700
C	4.08580000	-1.23454100	2.97229200
C	5.20625400	-0.45625900	2.74260000
C	1.71248000	-1.48749300	3.50633800
C	0.41774700	-1.05575800	3.85024200
O	0.04290600	0.07385700	1.60518100
Ru	-0.33315700	0.03043900	-0.52835600
N	-0.11709600	-1.99930500	-0.45132700
C	1.06148100	-2.70619900	-0.56379600
C	0.76786900	-4.10430600	-0.61880100
C	-0.58354700	-4.24085200	-0.51929600
C	-1.13948300	-2.92873900	-0.39792200
C	2.34663200	-2.15204100	-0.61884500
C	3.49564600	-3.08598700	-0.67251500
C	3.77101100	-3.96721800	0.37615500
C	4.85756000	-4.83145400	0.35109700
C	5.70235500	-4.83500900	-0.75564400
C	5.45481600	-3.97356400	-1.82110200
C	4.36232100	-3.11510800	-1.76950500
F	2.98019400	-3.98507300	1.46069800
F	5.09625400	-5.64316600	1.37631000
F	6.74153400	-5.65473200	-0.79286800

F	6.25719700	-3.97896700	-2.87818300
F	4.14920800	-2.30009000	-2.80398700
C	-2.49918700	-2.64579100	-0.24652300
C	-3.05307000	-1.35756700	-0.14218000
N	-2.35399900	-0.17716700	-0.18537400
C	-3.27493200	0.84276400	-0.08144800
C	-4.58338300	0.28094800	0.03716700
C	-4.44543600	-1.07628900	0.01401500
C	-2.99171200	2.21616000	-0.10061500
C	-1.71080300	2.77603900	-0.21711600
N	-0.53090900	2.07539800	-0.32826600
C	0.48387100	2.99671400	-0.37051800
C	-0.06930800	4.31227800	-0.30442400
C	-1.42397500	4.17579400	-0.20174800
C	1.85764200	2.70460500	-0.44576700
C	2.79778300	3.84883000	-0.39890400
C	2.90544100	4.64584200	0.74346600
C	3.78360400	5.71935700	0.81336200
C	4.58204100	6.02051300	-0.28742600
C	4.50042300	5.24476500	-1.44096700
C	3.61561600	4.17295600	-1.48469100
F	2.16078700	4.36345700	1.82259100
F	3.87159100	6.44910000	1.92042200
F	5.42358600	7.04150300	-0.23349800
F	5.26128900	5.53382100	-2.48938400
F	3.55694200	3.44277200	-2.59955600
C	-3.43176600	-3.79579300	-0.18148400
C	-3.38518000	-4.70945000	0.87503700
C	-4.25087400	-5.79351900	0.94745100
C	-5.19679700	-5.98191900	-0.05693300
C	-5.26969100	-5.08867800	-1.12266200
C	-4.39202900	-4.01222300	-1.17389800
F	-2.48977000	-4.54538300	1.85567800
F	-4.47706400	-3.17286700	-2.20872400
F	-6.16818200	-5.27295400	-2.08242900
F	-6.02737500	-7.01150600	0.00229500
F	-4.18539500	-6.64206200	1.96759800
N	1.70355400	0.23595900	-0.57484200
C	2.40942100	1.42517800	-0.53038100
C	3.80926400	1.13580000	-0.53920400
C	3.94734900	-0.21818300	-0.58210800
C	2.63420100	-0.78206200	-0.60182600
C	-4.13514100	3.15213200	0.01333400
C	-4.47909400	4.00804100	-1.03707300

C	-5.54917400	4.88984500	-0.94334500
C	-6.30408900	4.92910300	0.22613100
C	-5.98577100	4.08965800	1.29065000
C	-4.91142100	3.21650800	1.17372900
F	-3.77214900	3.98551300	-2.16948600
F	-5.85797200	5.68661200	-1.95941000
F	-7.32550600	5.76569500	0.32646000
F	-6.70191600	4.13245500	2.40854700
F	-4.61905000	2.42583000	2.21183400
H	4.59855500	1.87651100	-0.49702700
H	4.87027800	-0.78471400	-0.57890400
H	1.50210200	-4.89160200	-0.73672300
H	-1.15416600	-5.16085700	-0.54219700
H	-5.23059100	-1.81776500	0.09169700
H	-5.50295600	0.84631500	0.12089600
H	-2.15967800	4.96585100	-0.11766500
H	0.49855500	5.23389000	-0.33868800
H	-0.26875300	-1.78048600	4.28077400
H	0.26654000	-0.03516300	4.19665000
H	1.88159700	-2.56254500	3.44109700
H	1.76409600	1.26299400	3.29723900
H	4.16743000	-2.31968500	3.00843000
H	3.76331000	2.62798200	2.89388800
H	6.17463300	-0.92922500	2.59261500
H	5.97993500	1.55055900	2.55220500
O	-0.53667700	-0.85680400	2.29997400
Cl	-0.60421900	0.09565600	-2.77684800

$\Delta E_{\text{solv}} = -4911.91100275$ $\Delta G_{\text{solv}} = -4911.44409175$



¹G-Cl

C	4.36461200	1.07759200	2.82822500
C	3.04564800	1.50033100	3.03416300
C	2.04612000	0.56892900	3.21583200
C	2.34303900	-0.83339200	3.16673500
C	3.70931000	-1.23019900	2.97700100
C	4.69714200	-0.28937200	2.82257300
C	1.36490700	-1.80643900	3.28996700
C	-0.08855100	-1.52034500	3.42522000

O	-0.12259700	-0.12673100	1.57869300
Ru	-0.30453500	0.06785200	-0.33406200
N	0.12023900	-1.96503900	-0.44036900
C	1.36069800	-2.52888600	-0.56426500
C	1.21299100	-3.95121300	-0.70246800
C	-0.11949500	-4.22720100	-0.62545400
C	-0.79414300	-2.97464800	-0.45903100
C	2.59053900	-1.84159700	-0.56719900
C	3.81719300	-2.66259100	-0.72252100
C	4.18925400	-3.62893800	0.21560000
C	5.33428600	-4.40193000	0.07688000
C	6.14644200	-4.22496300	-1.03995000
C	5.80336400	-3.27859900	-2.00124600
C	4.65103600	-2.51692700	-1.83707200
F	3.42813200	-3.83652900	1.30824500
F	5.65676500	-5.29989500	1.00331400
F	7.24163000	-4.95522400	-1.18523500
F	6.57135400	-3.11330500	-3.07069300
F	4.34670800	-1.62972400	-2.78415700
C	-2.18940800	-2.81753900	-0.34139900
C	-2.87109100	-1.60045400	-0.29446400
N	-2.28685900	-0.34061500	-0.30593200
C	-3.30669500	0.57566500	-0.25433600
C	-4.56283200	-0.12033600	-0.22803600
C	-4.29322700	-1.45279900	-0.22990400
C	-3.15187800	1.96816700	-0.21087300
C	-1.92414900	2.64666000	-0.18681900
N	-0.68667400	2.05574300	-0.20748700
C	0.25411400	3.08231400	-0.16267600
C	-0.43297300	4.33681000	-0.10038700
C	-1.76608200	4.07226700	-0.11305100
C	1.63895600	2.93115700	-0.19735000
C	2.46108100	4.16438500	-0.13155600
C	2.49676900	4.95717400	1.01729700
C	3.26343200	6.11284900	1.09546600
C	4.02207900	6.50315000	-0.00510200
C	4.01025200	5.73508800	-1.16641400
C	3.23439400	4.58219100	-1.21805100
F	1.78164400	4.59800600	2.09639400
F	3.28231000	6.83750000	2.20976600
F	4.75926800	7.60199200	0.05558400
F	4.73360500	6.10861000	-2.21477400
F	3.23888300	3.86361300	-2.34148900
C	-2.98450100	-4.06063200	-0.21184900

C	-2.82502200	-4.87555300	0.91222600
C	-3.54248300	-6.05288600	1.07554500
C	-4.45113600	-6.43922400	0.09320000
C	-4.63461400	-5.64801900	-1.03786400
C	-3.90357000	-4.47334100	-1.17872800
F	-1.96383000	-4.51491800	1.87587400
F	-4.09252400	-3.73350800	-2.27304400
F	-5.49758300	-6.02152000	-1.97536400
F	-5.14270300	-7.56012400	0.23696400
F	-3.37357400	-6.80415000	2.15945400
N	1.75557300	0.48057700	-0.33560700
C	2.33515300	1.70664100	-0.30064600
C	3.76503900	1.56336500	-0.36337900
C	4.02465700	0.23003000	-0.46382300
C	2.76379600	-0.45311000	-0.45593700
C	-4.38312700	2.79253000	-0.17378600
C	-4.70937200	3.65488300	-1.22438200
C	-5.86030500	4.43364300	-1.20427700
C	-6.71904100	4.35878900	-0.11088500
C	-6.42088100	3.51111900	0.95259000
C	-5.26319200	2.74418600	0.91047500
F	-3.90206300	3.74310700	-2.28410200
F	-6.14749200	5.24024500	-2.21953500
F	-7.81988000	5.09530000	-0.08132500
F	-7.23592200	3.44579200	2.00034200
F	-4.99375900	1.94485400	1.94899400
H	4.48120800	2.37641500	-0.34835400
H	4.99603500	-0.24529500	-0.53010500
H	2.01954800	-4.65689100	-0.85772800
H	-0.59899900	-5.19503700	-0.70673200
H	-5.00687900	-2.26615600	-0.20205600
H	-5.53739900	0.35146100	-0.20994400
H	-2.57734900	4.78875900	-0.07554200
H	0.04341700	5.30860800	-0.06567500
H	-0.64452900	-2.38117400	3.80663600
H	-0.30938900	-0.64460200	4.04742300
H	1.66454200	-2.85106700	3.19215300
H	1.02764000	0.89842900	3.39052500
H	3.94293100	-2.29128400	2.95694000
H	2.80919000	2.56112400	3.05430100
H	5.73133200	-0.59533300	2.68433800
H	5.15053300	1.81952300	2.69618900
O	-0.65545400	-1.33329200	2.11442700
C1	-0.13022300	0.09522200	-2.64603900

$\Delta E_{\text{solv}} = - 4911.93975502$

$\Delta G_{\text{solv}} = - 4911.46323002$

³G-Cl

C	-4.05076000	-0.86195600	2.88798200
C	-2.78580800	-1.41461600	3.11502500
C	-1.70063600	-0.58701000	3.32361800
C	-1.86629700	0.83288800	3.29351100
C	-3.16893500	1.36625400	3.05646200
C	-4.24335000	0.52835500	2.86342600
C	-0.80535900	1.71370600	3.48281100
C	0.61024700	1.30444900	3.50239000
O	0.45966800	-0.05171500	1.63305100
Ru	0.21419800	-0.03742600	-0.38795300
N	-0.60610700	1.84477600	-0.32327900
C	-1.93395900	2.16692500	-0.48306400
C	-2.06358400	3.59140900	-0.52763600
C	-0.81485000	4.11894400	-0.36775300
C	0.10108300	3.02423000	-0.27572500
C	-2.98823300	1.24464700	-0.59115300
C	-4.33336300	1.75365600	-0.95761200
C	-5.07851500	2.62805400	-0.16420300
C	-6.33146600	3.09414100	-0.54241500
C	-6.87823800	2.68396600	-1.75464700
C	-6.16457800	1.81461900	-2.57450100
C	-4.91209700	1.36449800	-2.17257500
F	-4.59353300	3.04906200	1.01746100
F	-7.00817900	3.91890200	0.25168400
F	-8.07289500	3.11927800	-2.12543100
F	-6.67791300	1.42541200	-3.73477100
F	-4.25276900	0.54000200	-2.98714400
C	1.49636900	3.15433600	-0.23641700
C	2.42080400	2.10665100	-0.36217000
N	2.10867100	0.77407200	-0.42978000
C	3.28631400	0.07488000	-0.50309900
C	4.37644900	1.00520200	-0.53829000
C	3.84517800	2.25517200	-0.42230300
C	3.41312100	-1.32365800	-0.46789200
C	2.35505100	-2.23264200	-0.32217200
N	1.01512100	-1.91586200	-0.26692800
C	0.32216400	-3.08519300	-0.07140900
C	1.25231600	-4.17147600	-0.00179700
C	2.50138100	-3.64751300	-0.16478600
C	-1.07185800	-3.20841700	0.01119000

C	-1.61706900	-4.56816700	0.25324800
C	-1.52983300	-5.15194500	1.51753100
C	-2.02121000	-6.42502300	1.77753900
C	-2.62258500	-7.14496700	0.74823200
C	-2.72953000	-6.58849600	-0.52359000
C	-2.22664700	-5.31259100	-0.75791400
F	-0.96495900	-4.46629800	2.52488100
F	-1.92871800	-6.95230200	2.99453100
F	-3.09937200	-8.35897300	0.98225500
F	-3.30568000	-7.27741400	-1.50160200
F	-2.34102600	-4.79596900	-1.98245700
C	2.02266500	4.51729700	0.00836200
C	1.79535000	5.13143700	1.24256500
C	2.26044700	6.40760700	1.52849800
C	2.97743600	7.10316800	0.55783400
C	3.22357400	6.51831900	-0.68148400
C	2.74552500	5.23838800	-0.94290100
F	1.11444300	4.47108000	2.19700200
F	2.98996900	4.69840600	-2.13857900
F	3.90405500	7.18623800	-1.60513900
F	3.42772200	8.32194600	0.81631200
F	2.03360200	6.96263400	2.71554000
N	-1.67441100	-0.82915500	-0.26070200
C	-1.99039700	-2.16193000	-0.13012300
C	-3.41297800	-2.31296200	-0.18792200
C	-3.94297600	-1.07357200	-0.39815600
C	-2.85576700	-0.14267300	-0.43651400
C	4.78125200	-1.89018400	-0.54759400
C	5.17184800	-2.67742000	-1.63453000
C	6.44855100	-3.21946100	-1.72708200
C	7.36999200	-2.97818300	-0.71171700
C	7.00936400	-2.20232100	0.38663600
C	5.72663800	-1.67310100	0.45790100
F	4.30473800	-2.92375200	-2.61901200
F	6.79302500	-3.95928000	-2.77499500
F	8.59028000	-3.48867100	-0.78853300
F	7.88639700	-1.98087900	1.36052600
F	5.40111900	-0.94286900	1.53124600
H	-3.94619700	-3.25221200	-0.09709700
H	-4.99012000	-0.81340800	-0.50301300
H	-2.98852100	4.13451000	-0.67407300
H	-0.53834600	5.16657100	-0.36783500
H	4.38124300	3.19556600	-0.39327400
H	5.42300400	0.74207500	-0.62763500

H	3.44346300	-4.18197000	-0.16614700
H	0.98714400	-5.21283000	0.13720000
H	1.28986200	2.08114600	3.85792700
H	0.84684700	0.34604500	3.97351100
H	-1.00579000	2.78533200	3.42254800
H	-0.72417100	-1.01708600	3.52038500
H	-3.29380000	2.44635100	3.03107100
H	-2.65500100	-2.49372800	3.13362600
H	-5.23377600	0.94024500	2.68728800
H	-4.90327900	-1.52226100	2.73852100
O	0.84946500	1.22376900	2.07914900
Cl	0.12179700	-0.07271500	-2.67891200

$\Delta E_{\text{solv}} = -4911.94964815$ $\Delta G_{\text{solv}} = -4911.47441315$

⁵G-Cl

C	5.02857100	0.99761200	2.83656300
C	3.75495700	1.55335400	2.99651900
C	2.63236600	0.74422300	3.06178300
C	2.74792400	-0.67060900	2.97572600
C	4.05145000	-1.20758300	2.78265000
C	5.16615200	-0.38943500	2.72549000
C	1.64582900	-1.55074000	3.10342900
C	0.26587700	-1.14552800	3.45429600
O	-0.09670900	0.11807500	1.59010000
Ru	-0.32479100	0.03639100	-0.36226800
N	-0.07593200	-2.00783100	-0.32271700
C	1.10166800	-2.68932500	-0.50131800
C	0.82991100	-4.09266300	-0.57385900
C	-0.51396900	-4.24909600	-0.41457300
C	-1.07538500	-2.94085100	-0.25866200
C	2.37920900	-2.10366900	-0.60857600
C	3.53382700	-3.01125800	-0.77445900
C	3.86082000	-3.98722600	0.17427000
C	4.95690100	-4.82532500	0.02171600
C	5.75385300	-4.71157200	-1.11553200
C	5.45316200	-3.75659900	-2.08413100
C	4.35893100	-2.91992900	-1.90381900
F	3.12626400	-4.11584800	1.28670600
F	5.24982900	-5.72550000	0.95212400
F	6.79627900	-5.50930600	-1.27331700
F	6.20676300	-3.65473000	-3.17042800
F	4.08830900	-2.02390100	-2.85226300
C	-2.45275700	-2.66636000	-0.12715700

C	-3.04400200	-1.38765500	-0.09230500
N	-2.36780100	-0.20110800	-0.17030100
C	-3.30208600	0.79977300	-0.13185400
C	-4.61035800	0.22360900	-0.02844600
C	-4.44951100	-1.12676800	0.01941300
C	-3.02475200	2.18154100	-0.19685800
C	-1.74478300	2.76815800	-0.26731600
N	-0.55618200	2.08419200	-0.30703400
C	0.44597200	3.01426100	-0.29045200
C	-0.12550200	4.32683900	-0.25439400
C	-1.48003400	4.17414500	-0.23741300
C	1.82911900	2.73245100	-0.32131800
C	2.74847000	3.88507000	-0.21520100
C	2.77448500	4.67870200	0.93677900
C	3.64240100	5.75438800	1.06698400
C	4.50386900	6.06784600	0.01750100
C	4.49859200	5.30026500	-1.14530500
C	3.63050300	4.22025500	-1.24824500
F	1.97181600	4.38171900	1.96510000
F	3.66104100	6.47578500	2.18107300
F	5.33138300	7.09359900	0.12757700
F	5.31501000	5.60697500	-2.14456900
F	3.63780200	3.50379000	-2.37241900
C	-3.35599400	-3.83215500	-0.02719600
C	-3.25364000	-4.73244000	1.04006700
C	-4.09277500	-5.83272700	1.15326900
C	-5.05891700	-6.06021400	0.17507700
C	-5.18133800	-5.18703600	-0.90382800
C	-4.33737700	-4.08720700	-0.99241200
F	-2.34218100	-4.52799200	1.99479800
F	-4.46173800	-3.27627900	-2.04392600
F	-6.09356400	-5.41392400	-1.83964900
F	-5.86028500	-7.10753500	0.27131300
F	-3.98416000	-6.66058300	2.18464500
N	1.72934000	0.27653100	-0.50697900
C	2.41367400	1.45766600	-0.42816500
C	3.82505200	1.19300500	-0.42765000
C	3.97699400	-0.15405500	-0.52109900
C	2.66095700	-0.72242100	-0.56615400
C	-4.17968500	3.10407800	-0.17221700
C	-4.44770700	3.95370800	-1.25253800
C	-5.53206400	4.82159900	-1.24861400
C	-6.37266700	4.86277200	-0.13817500
C	-6.12709100	4.03602100	0.95639100

C	-5.04288200	3.16906200	0.92765800
F	-3.66174200	3.92469700	-2.32927500
F	-5.77293400	5.60385800	-2.29232900
F	-7.40451300	5.68946800	-0.12174000
F	-6.92076400	4.08795600	2.01844000
F	-4.81701000	2.40016700	1.99557200
H	4.60516600	1.93799300	-0.33675200
H	4.90395600	-0.71297400	-0.51708300
H	1.56432700	-4.86921500	-0.74434700
H	-1.07301300	-5.17600600	-0.43531700
H	-5.22432700	-1.87574600	0.12008700
H	-5.54155200	0.77390500	0.00572800
H	-2.22766600	4.95580800	-0.19404400
H	0.43049000	5.25600900	-0.25356600
H	-0.26083400	-1.92229800	4.01927600
H	0.22116200	-0.20599400	4.01892800
H	1.82871900	-2.61652600	2.96298000
H	1.64893600	1.19731000	3.17650100
H	4.16179500	-2.28981100	2.72144300
H	3.63988000	2.63201500	3.08723500
H	6.15455800	-0.83012900	2.60645300
H	5.90700600	1.63945200	2.80687600
O	-0.59701800	-0.99967300	2.29100800
Cl	-0.50539300	-0.00918700	-2.68112900

$\Delta E_{\text{solv}} = - 4911.92383375$ $\Delta G_{\text{solv}} = - 4911.45285675$