

Supporting Information

On the Mechanism of Intermolecular Nitrogen-Atom Transfer from a Lattice-Isolated Diruthenium Nitride Intermediate

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A. General Considerations

Materials Unless otherwise noted, all reactions were carried out under ambient atmosphere at 23 °C using as-received reagents. MeCN was obtained as ACS reagent grade, chlorobenzene was obtained from BTC, and NMR solvents were purchased from Cambridge Isotope Laboratories. H₂esp was prepared according to literature procedures.¹

Characterization Details NMR spectra were recorded on Varian Inova 500 (¹H NMR, 499.43 MHz) at 25 °C and spectra were referenced against residual solvent signals: CD₃CN (1.94 ppm, ¹H).² ¹H NMR data are reported as follows: chemical shift (δ , ppm), multiplicity (s (singlet), d (doublet), t (triplet), m (multiplet), br (broad), integration. *In situ* IR spectra were measured in a KBr pellet with a Bruker VERTEX 70, were blanked against air, and were determined as the average of 64 scans. IR data are reported as follows: wavenumber (cm⁻¹), peak intensity (s, strong; m, medium; w, weak).

Powder X-ray Diffraction (PXRD) PXRD measurements were carried out on a Bruker D8 Advance Eco X-ray diffractometer (Cu K α , 1.5418 Å; 40 kV, 25 mA) fitted with a LynxEye detector. The angular range was measured from 5.00 to 30.00° or 3.00 to 25.00° (2 θ) with steps of 0.010° and a measurement time of 0.3 second per step.

Single-Crystal X-Ray Diffraction Details A Bruker APEX 2 Duo X-ray (three-circle) diffractometer was used for crystal screening, unit cell determination, and data collection for the X-ray crystal structure of **3**. Crystal suitable for X-ray diffraction were mounted on a MiTeGen dual-thickness micro-mount and placed under a 110 K N₂ stream (Oxford). The X-ray radiation employed was generated from a Mo sealed X-ray tube (K α = 0.70173 Å with a potential of 40 kV and a current of 40 mA). Bruker AXS APEX II software was used for data collection and reduction. Absorption corrections were applied using SADABS.³ A solution was obtained using XT/XS in APEX2 and refined in Olex2.⁴⁻⁶ Hydrogen atoms were placed in idealized positions and were set riding on the respective parent atoms. All non-hydrogen atoms were refined with anisotropic thermal parameters. The structure was refined (weighted least squares refinement on F²) to convergence.⁴

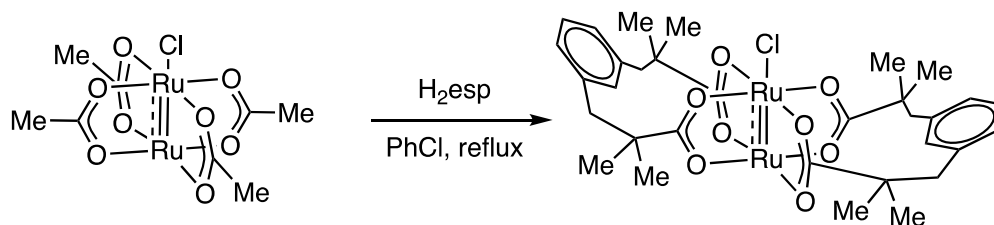
Computational Methods Free energies of stationary points for modeled reaction routes were calculated using density functional theory (DFT) within the Gaussian 16 software package,⁷ and visualization of optimized structures was made using ChemCraft.⁸

Reaction species were geometry optimized with the B3LYP⁹ functional including the GD3¹⁰ dispersion correction term with two basis sets: def2-TZVP¹¹ for Ru, N and O and def2-SVP¹¹ for C and H. Two spin states, low (doublet) and intermediate (quartet) were evaluated for reactants, transition states, intermediates and products of all pertinent species; test calculations suggested that sextet spin states were much higher in energy. The lowest free energy spin multiplicities were selected to calculate the thermodynamics, ΔG_{rxn} , and free energy barriers, ΔG^\ddagger , to study the mechanisms of reaction. Solvation effects were obtained from single-point gas-phase optimized geometries using the SMD solvation model^{9, 12} with toluene ($\epsilon \sim 2.37$) as the continuum solvent. Free energies are calculated in Kcal mol⁻¹ and corrections to the electronic energy assumed 1 atm and 298.15 K.

The analytic Hessian was used to identify the correct number of imaginary frequencies for all optimized species. Ground states are characterized by possession of no imaginary frequencies, and transition states have one imaginary frequency via harmonic frequency calculations. Changing magnetic properties of optimized stationary points were examined via spin density maps for these species in their various spin states.

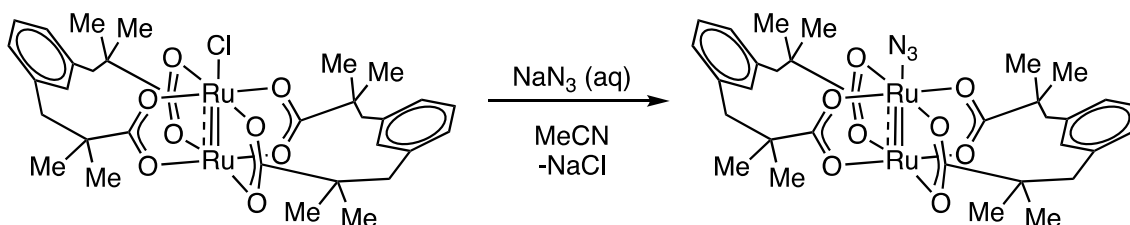
B. Synthesis and Characterization

Synthesis of Ru(esp)₂Cl



Ru₂(esp)₂Cl was prepared by a method similar to that reported by Musaev and Dubois.¹³ In a 50-mL round bottom flask equipped with a condenser, Ru₂(OAc)₄Cl (200 mg, 0.422 mmol) and H₂esp (300 mg, 1.08 mmol) were refluxed in chlorobenzene (20 mL) for 18 h. The reaction was cooled to 23 °C and placed in a freezer (-22 °C) to promote the precipitation of the product. The mixture was then filtered through a frit and the solids washed with chlorobenzene then diethyl ether before drying under reduced pressure to afford a red solid (277 mg, 0.351 mmol, 83% yield). Characterization is consistent with previously reported data.¹³

Synthesis of Ru₂(esp)₂N₃ (3)



To a mixture of Ru₂(esp)₂Cl (15 mg, 0.019 mmol) in MeCN (5 mL), an aqueous solution of NaN₃ (1.5 mg NaN₃ in 0.37 mL H₂O, 0.023 mmol) was added. The mixture immediately darkened and became homogenous. Volatiles were removed under reduced pressure at 23 °C. Acetone was added to the residue and the mixture was filtered into a pre-weighed 20 mL vial and dried under reduced pressure at 23 °C. Yield: 11 mg (0.014 mmol, 73% yield). IR $\nu(\text{N}_3)$: 2000 (s), 2020(s) cm⁻¹ (KBr). ¹H NMR (499.43 MHz, d₆-DMSO): δ 32.58, 13.18, 12.15, 11.08, 8.48 (all peaks are broad and featureless. NMR shifts are in good agreement with previously reported Ru₂(esp)₂SbF₆).¹³ Single-crystals suitable for single-crystal X-ray diffraction were grown by blowing a stream of N₂ over a DMF solution of 3.

C. Supporting Data

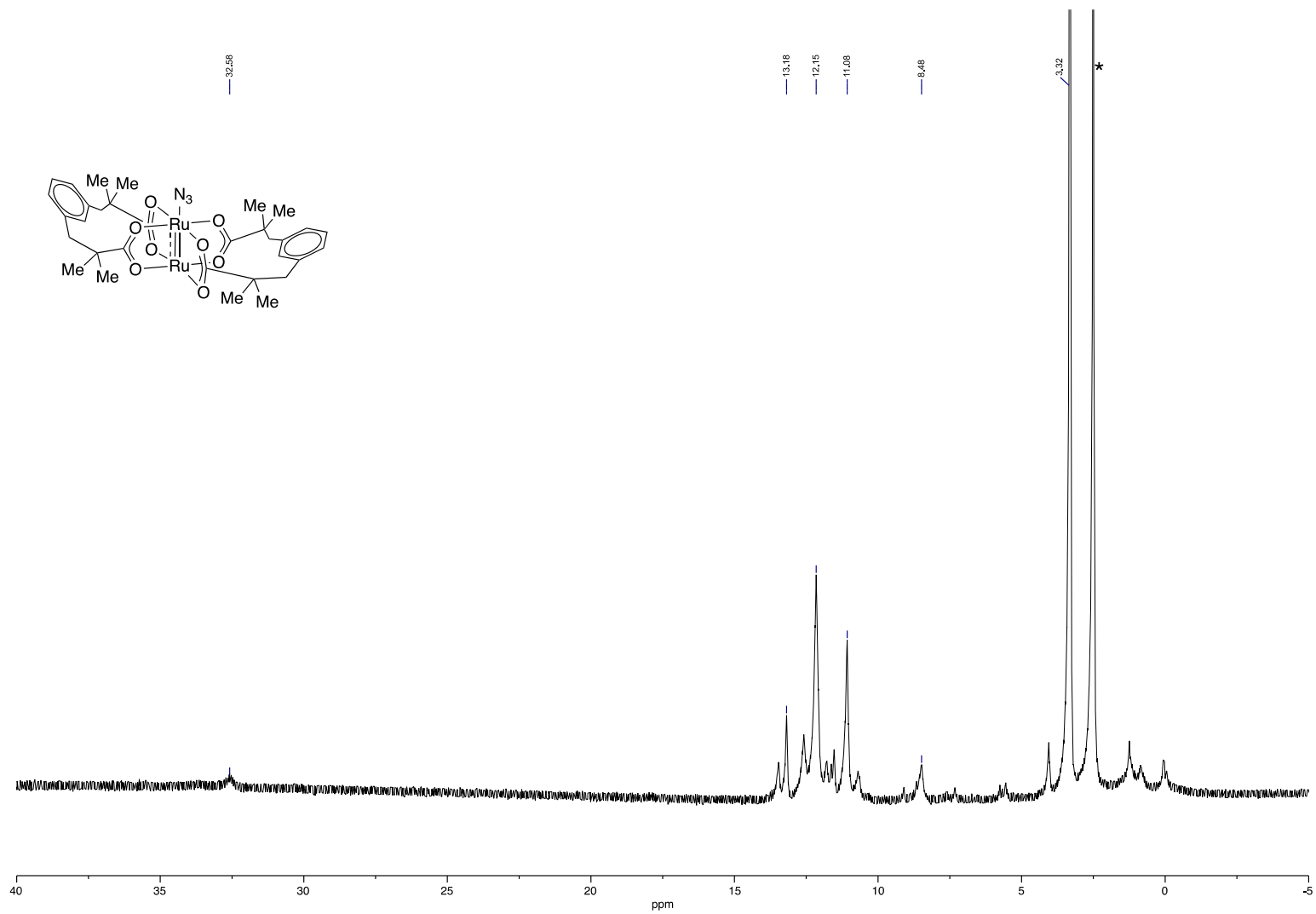


Figure S1. ¹H NMR spectrum of **3** in d₆-DMSO (499.43 MHz) at 25 °C. Residual solvent peak (d₅-DMSO) is marked with *.

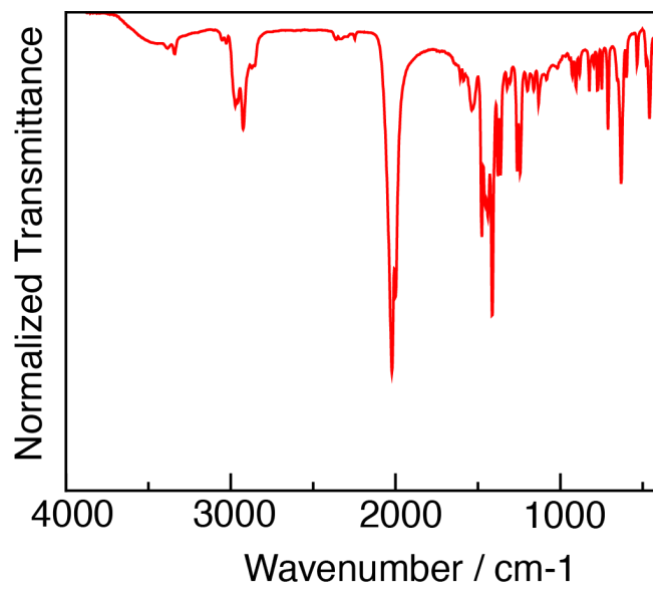


Figure S2. Solid state IR spectrum of a KBr pellet of **3**.

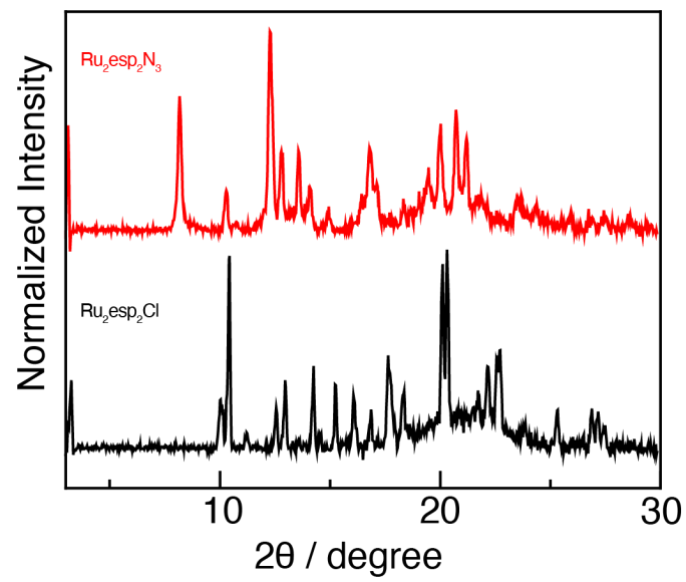


Figure S3. Powder XRD patterns of **3** (top) and Ru₂esp₂Cl (bottom).

D. X-ray experimental details of 3 (CCDC 2221722)

Crystal data	
Chemical formula	C ₆₄ H ₈₀ N ₆ O ₁₆ Ru ₄
<i>M</i> _r	1593.62
Crystal system, space group	triclinic, <i>P</i> 1
Temperature (K)	110
<i>a</i> , <i>b</i> , <i>c</i> (Å)	11.2116(9), 17.297(1), 19.843(1)
α , β , γ (°)	64.903(2), 89.935(2), 74.563(2)
<i>V</i> (Å ³)	3331.4(5)
<i>Z</i>	2
Radiation type	Mo K α
μ (mm ⁻¹)	0.96
Crystal size (mm)	0.04 × 0.04 × 0.02
Data collection	
Diffractometer	Bruker APEX-II CCD
Absorption correction	Multi-scan <i>SADABS-2016/2</i> (Bruker,2016/2) was used for absorption correction. <i>wR</i> ² (int) was 0.1207 before and 0.0825 after correction. The Ratio of minimum to maximum transmission is 0.8884. The $\lambda/2$ correction factor is not present.
<i>T</i> _{min} , <i>T</i> _{max}	0.6622, 0.7454
No. of measured, independent, and observed [<i>I</i> > 2 <i>s</i> (<i>I</i>)] reflections	157822, 13694, 11184
<i>R</i> _{int}	0.116
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.627
Refinement	
<i>R</i> [<i>F</i> ² > 2 <i>s</i> (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.084, 0.185, 1.25
No. of reflections	13694
No. of parameters	821
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	1.81, -2.09

E. Computational Data

Cartesian Coordinates (Å) of Optimized Stationary Points. The first column denotes the atomic number of the atom of interest. Lowest energy spin state for that stationary point is indicated.

Quartet Azide Complex

44	-0.033332000	-0.000130000	0.975247000
44	-0.132917000	-0.000398000	-1.344804000
8	-0.035530000	2.048131000	0.893603000
8	-0.139135000	2.021109000	-1.348349000
7	0.218800000	0.000576000	3.010528000
8	-2.077062000	-0.004450000	1.022192000
8	2.003241000	0.004203000	0.802437000
8	-0.026749000	-2.048382000	0.893742000
8	-2.146913000	-0.004608000	-1.220851000
8	1.886494000	0.003859000	-1.437349000
8	-0.130567000	-2.021902000	-1.348209000
6	-0.085315000	2.641770000	-0.224527000
6	-2.720340000	-0.005685000	-0.069701000
6	2.553965000	0.005242000	-0.338454000
6	-0.074225000	-2.642281000	-0.224352000
6	4.035379000	0.008002000	-0.405262000
6	4.785359000	0.009740000	0.784061000
6	4.687471000	0.008862000	-1.649501000
6	6.178922000	0.012332000	0.722385000
6	6.081447000	0.011445000	-1.702818000
6	6.827381000	0.013183000	-0.518286000
1	4.266670000	0.009034000	1.744761000
1	4.091807000	0.007489000	-2.563562000
1	6.762005000	0.013689000	1.646276000
1	6.589337000	0.012107000	-2.670276000
1	7.919645000	0.015203000	-0.562431000
6	-0.080733000	4.126465000	-0.242509000
6	-0.017432000	4.840678000	0.965912000
6	-0.138311000	4.818150000	-1.463792000
6	-0.011901000	6.235417000	0.949247000
6	-0.132811000	6.213240000	-1.473921000
6	-0.069612000	6.922550000	-0.268991000
1	0.027482000	4.290501000	1.907115000
1	-0.186590000	4.251666000	-2.394846000
1	0.038017000	6.789932000	1.889330000
1	-0.177549000	6.750650000	-2.424230000
1	-0.064961000	8.015596000	-0.279288000
6	-4.203819000	-0.008309000	-0.024930000
6	-4.947271000	-0.009650000	-1.216859000
6	-4.865467000	-0.009439000	1.214734000
6	-6.341494000	-0.012104000	-1.166824000
6	-6.259598000	-0.011897000	1.258119000
6	-6.998400000	-0.013230000	0.069074000
1	-4.421526000	-0.008747000	-2.172723000
1	-4.275199000	-0.008371000	2.132458000
1	-6.919201000	-0.013145000	-2.094251000
1	-6.773335000	-0.012773000	2.222389000

1	-8.090875000	-0.015147000	0.105882000
6	-0.064078000	-4.126949000	-0.242227000
6	-0.119143000	-4.818943000	-1.463452000
6	0.001948000	-4.840822000	0.966247000
6	-0.108437000	-6.214004000	-1.473467000
6	0.012684000	-6.235532000	0.949696000
6	-0.042527000	-6.922975000	-0.268483000
1	-0.169592000	-4.252719000	-2.394548000
1	0.044851000	-4.290404000	1.907404000
1	-0.151225000	-6.751656000	-2.423729000
1	0.064713000	-6.789779000	1.889822000
1	-0.033811000	-8.015997000	-0.278691000
7	1.300623000	0.003466000	3.537982000
7	2.309466000	0.006091000	4.075659000

Doublet Benzylic C-H Activation TS

44	0.390771000	0.016119000	0.902973000
44	0.830367000	-0.047331000	-1.469034000
8	-0.650830000	1.763672000	0.532276000
8	-0.252892000	1.669424000	-1.683748000
7	-0.167971000	-0.150230000	2.570128000
8	-1.306842000	-1.096987000	0.379618000
8	2.102978000	1.121196000	1.100547000
8	1.517945000	-1.727515000	1.007569000
8	-0.825433000	-1.152354000	-1.821026000
8	2.504163000	1.059873000	-1.111562000
8	1.910144000	-1.743327000	-1.2111725000
1	-1.203397000	0.238894000	2.841795000
6	-0.761181000	2.217439000	-0.648591000
6	-1.548587000	-1.459493000	-0.806901000
6	2.801655000	1.412429000	0.080947000
6	2.033255000	-2.231648000	-0.032325000
6	-3.584441000	0.578458000	2.470688000
6	-4.406521000	-0.392326000	3.099977000
6	-3.919427000	0.968380000	1.147465000
1	-4.162269000	-0.716187000	4.115559000
1	-3.289764000	1.699082000	0.639230000
6	-5.521691000	-0.917136000	2.451526000
6	-5.031687000	0.436906000	0.503929000
1	-6.147275000	-1.655436000	2.960509000
1	-5.268680000	0.752136000	-0.515327000
6	-5.844300000	-0.503901000	1.151932000
6	2.837168000	-3.476636000	0.119423000
6	3.005520000	-4.053698000	1.389047000
6	3.427073000	-4.076305000	-1.005149000
1	2.540514000	-3.577138000	2.253458000
1	3.287461000	-3.618050000	-1.985219000
6	3.758101000	-5.220003000	1.529618000
6	4.178821000	-5.242880000	-0.858975000
1	3.887892000	-5.667639000	2.517979000
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6	4.345214000	-5.815559000	0.407083000
1	4.934351000	-6.729540000	0.519517000
6	4.038493000	2.212939000	0.288577000
6	4.837207000	2.568692000	-0.810589000

6	4.410223000	2.613523000	1.582745000
1	4.537104000	2.249998000	-1.809808000
1	3.781540000	2.329041000	2.427902000
6	5.996819000	3.319633000	-0.614812000
6	5.570917000	3.363719000	1.772819000
1	6.617118000	3.595733000	-1.470972000
1	5.859186000	3.673916000	2.780118000
6	6.364735000	3.717629000	0.675497000
1	7.273889000	4.305452000	0.826780000
6	-1.546264000	3.469391000	-0.841906000
6	-1.838063000	3.918668000	-2.140316000
6	-2.005107000	4.199533000	0.267111000
1	-1.473910000	3.344520000	-2.993408000
1	-1.766569000	3.848989000	1.271547000
6	-2.588133000	5.080846000	-2.324461000
6	-2.751647000	5.362785000	0.078463000
1	-2.817342000	5.425283000	-3.335791000
1	-3.105270000	5.928146000	0.943925000
6	-3.045896000	5.803532000	-1.216861000
1	-3.633044000	6.713798000	-1.363379000
6	-2.746949000	-2.309555000	-1.045372000
6	-3.559415000	-2.692644000	0.032753000
6	-3.061663000	-2.736235000	-2.346560000
1	-3.317713000	-2.338483000	1.035193000
1	-2.421595000	-2.429647000	-3.175055000
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6	-4.179131000	-3.542579000	-2.563587000
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1	-4.423216000	-3.873927000	-3.575914000
6	-4.984512000	-3.928648000	-1.485101000
1	-5.858537000	-4.562616000	-1.656683000
1	-6.713742000	-0.923281000	0.640737000
6	-2.446662000	1.142000000	3.147129000
1	-2.001185000	2.055200000	2.748730000
1	-2.357058000	0.994834000	4.228147000

Singlet Dinitrogen

7	0.000000000	0.000000000	0.545451000
7	0.000000000	0.000000000	-0.545451000

Singlet Toluene

1	-0.011998000	0.737828000	2.154672000
6	0.030406000	2.426491000	0.000000000
1	-0.463211000	2.844002000	0.891258000
1	-0.463211000	2.844002000	-0.891258000
1	1.070949000	2.796393000	0.000000000
6	-0.005411000	0.917155000	0.000000000
6	-0.008011000	0.195285000	-1.204492000
6	-0.008011000	-1.202532000	-1.207281000
6	-0.007284000	-1.907884000	0.000000000
6	-0.008011000	-1.202532000	1.207281000
6	-0.008011000	0.195285000	1.204492000
1	-0.011998000	0.737828000	-2.154672000
1	-0.012177000	-1.743384000	-2.157501000
1	-0.010175000	-3.000901000	0.000000000

1 -0.012177000 -1.743384000 2.157501000

Doublet Ru₂N Intermediate

44 0.031944000 0.000046000 1.246095000
44 -0.046520000 -0.000164000 -1.197119000
8 0.066898000 -2.063458000 1.059616000
8 -0.036008000 -2.035200000 -1.191206000
7 -0.239329000 -0.000639000 2.874538000
8 2.068961000 0.002716000 1.088320000
8 -2.079266000 -0.002591000 1.043777000
8 0.061572000 2.063543000 1.059637000
8 2.004071000 0.002719000 -1.162451000
8 -2.070158000 -0.003009000 -1.212840000
8 -0.041737000 2.034938000 -1.191159000
6 0.021180000 -2.642745000 -0.069962000
6 2.632992000 0.003503000 -0.055057000
6 -2.664033000 -0.003567000 -0.078663000
6 0.014076000 2.642691000 -0.069961000
6 -4.154764000 -0.005320000 -0.082025000
6 -4.862644000 -0.005980000 1.131300000
6 -4.854177000 -0.006360000 -1.299982000
6 -6.257772000 -0.007678000 1.123524000
6 -6.249612000 -0.008059000 -1.302015000
6 -6.952368000 -0.008715000 -0.091753000
1 -4.306339000 -0.005189000 2.069847000
1 -4.291789000 -0.005858000 -2.234718000
1 -6.806852000 -0.008210000 2.068268000
1 -6.792235000 -0.008887000 -2.250523000
1 -8.045549000 -0.010048000 -0.095489000
6 0.038777000 -4.131438000 -0.081350000
6 0.099140000 -4.847491000 1.125779000
6 -0.005948000 -4.822176000 -1.303573000
6 0.114965000 -6.242331000 1.107545000
6 0.010239000 -6.217288000 -1.315887000
6 0.070721000 -6.928219000 -0.111871000
1 0.132526000 -4.299008000 2.068278000
1 -0.053659000 -4.253253000 -2.233142000
1 0.161616000 -6.797978000 2.047225000
1 -0.024779000 -6.753323000 -2.267423000
1 0.083066000 -8.021236000 -0.123693000
6 4.120399000 0.005445000 -0.086177000
6 4.792845000 0.006359000 -1.319467000
6 4.854333000 0.006403000 1.111756000
6 6.187627000 0.008220000 -1.351802000
6 6.248810000 0.008264000 1.073383000
6 6.916411000 0.009171000 -0.156933000
1 4.209991000 0.005620000 -2.241608000
1 4.320528000 0.005706000 2.063220000
1 6.709470000 0.008943000 -2.311797000
1 6.818472000 0.009023000 2.005773000
1 8.009191000 0.010632000 -0.184456000
6 0.027982000 4.131420000 -0.081380000
6 -0.018731000 4.822031000 -1.303603000
6 0.086767000 4.847639000 1.125729000
6 -0.006101000 6.217180000 -1.315933000

6	0.099037000	6.242514000	1.107479000
6	0.052816000	6.928274000	-0.111935000
1	-0.065236000	4.252981000	-2.233154000
1	0.121672000	4.299256000	2.068231000
1	-0.042698000	6.753116000	-2.267464000
1	0.144432000	6.798288000	2.047145000
1	0.062373000	8.021319000	-0.123769000

Quartet Imido + Benzyl Radical Pair

44	-0.022477000	0.000739000	1.201525000
44	0.016187000	-0.000803000	-1.205167000
8	2.058699000	-0.072842000	1.063249000
8	2.048534000	-0.073046000	-1.192171000
7	0.209932000	-0.008192000	2.994161000
8	0.043354000	2.059315000	1.023777000
8	-0.101671000	-2.057574000	1.023638000
8	-2.071753000	0.072978000	1.120457000
8	0.077633000	2.024708000	-1.223761000
8	-0.066656000	-2.025391000	-1.223970000
8	-2.013690000	0.071635000	-1.131690000
6	2.646443000	-0.093848000	-0.058595000
6	0.079085000	2.640551000	-0.100287000
6	-0.108501000	-2.639807000	-0.100437000
6	-2.640686000	0.093611000	-0.012492000
6	-0.168607000	-4.126390000	-0.119842000
6	-0.236538000	-4.843711000	1.086115000
6	-0.158159000	-4.814771000	-1.344059000
6	-0.292826000	-6.237420000	1.064775000
6	-0.214021000	-6.208937000	-1.359528000
6	-0.281338000	-6.921139000	-0.156677000
1	-0.245819000	-4.296079000	2.029783000
1	-0.105758000	-4.245267000	-2.273020000
1	-0.346389000	-6.793989000	2.003561000
1	-0.205285000	-6.743200000	-2.312682000
1	-0.325416000	-8.013307000	-0.170983000
6	4.135974000	-0.145860000	-0.069148000
6	4.850433000	-0.170265000	1.139901000
6	4.830219000	-0.170734000	-1.289865000
6	6.244571000	-0.218929000	1.126304000
6	6.224801000	-0.219446000	-1.298629000
6	6.933254000	-0.243546000	-0.092063000
1	4.300486000	-0.150744000	2.081777000
1	4.264200000	-0.151529000	-2.222152000
1	6.797638000	-0.237804000	2.068541000
1	6.762299000	-0.238726000	-2.249833000
1	8.025694000	-0.281647000	-0.100903000
6	0.123828000	4.127658000	-0.119671000
6	0.183638000	4.813466000	-1.343889000
6	0.105790000	4.848099000	1.086234000
6	0.226026000	6.208094000	-1.359439000
6	0.147656000	6.242314000	1.064813000
6	0.208030000	6.923401000	-0.156668000
1	0.196702000	4.241583000	-2.272782000
1	0.057548000	4.302550000	2.029922000
1	0.273096000	6.740328000	-2.312605000

1	0.132776000	6.801355000	2.003541000
1	0.240844000	8.015963000	-0.171061000
6	-4.127164000	0.146141000	-0.049700000
6	-4.801618000	0.170856000	-1.281462000
6	-4.858552000	0.171136000	1.149535000
6	-6.195798000	0.220039000	-1.311263000
6	-6.252241000	0.220195000	1.113799000
6	-6.922019000	0.244673000	-0.115159000
1	-4.221513000	0.151178000	-2.205089000
1	-4.321429000	0.151646000	2.099115000
1	-6.719132000	0.239254000	-2.270323000
1	-6.819694000	0.239510000	2.047394000
1	-8.014208000	0.283132000	-0.140643000
1	1.194916000	-0.044881000	3.307668000

Doublet Benzyl Radical

1	-0.000008000	0.795989000	2.169216000
6	0.000203000	2.406832000	0.000000000
1	0.000243000	2.969050000	0.936579000
1	0.000243000	2.969050000	-0.936579000
6	-0.000122000	0.997768000	0.000000000
6	-0.000034000	0.252560000	-1.220234000
6	-0.000034000	-1.135804000	-1.213847000
6	-0.000027000	-1.843112000	0.000000000
6	-0.000034000	-1.135804000	1.213847000
6	-0.000034000	0.252560000	1.220234000
1	-0.000008000	0.795989000	-2.169216000
1	-0.000016000	-1.682160000	-2.160899000
1	0.000061000	-2.935759000	0.000000000
1	-0.000016000	-1.682160000	2.160899000

Doublet Ru₂-N(H)benzyl Intermediate

44	-0.324466000	-0.025592000	0.706318000
44	-0.873948000	0.045417000	-1.548837000
8	0.451929000	1.904662000	0.466527000
8	-0.063394000	1.925138000	-1.716554000
8	-2.145849000	0.828738000	1.161507000
8	1.471768000	-0.904664000	0.122180000
8	-1.122175000	-1.918163000	0.830798000
8	-2.677493000	0.867784000	-1.016215000
8	0.943320000	-0.763963000	-2.051645000
8	-1.658278000	-1.840238000	-1.344755000
6	0.448164000	2.454109000	-0.679207000
6	-2.939796000	1.104347000	0.206894000
6	1.745662000	-1.060053000	-1.107062000
6	-1.611131000	-2.438490000	-0.222584000
6	3.085993000	-1.608976000	-1.456046000
6	4.041824000	-1.819040000	-0.448066000
6	3.403385000	-1.901228000	-2.792259000
6	5.303188000	-2.316156000	-0.777966000
6	4.664261000	-2.404150000	-3.115657000
6	5.615638000	-2.611331000	-2.109633000
1	3.794060000	-1.577513000	0.585101000
1	2.652896000	-1.728983000	-3.565365000
1	6.044647000	-2.468230000	0.010030000

1	4.908291000	-2.633811000	-4.155873000
1	6.604141000	-3.001937000	-2.365753000
6	1.093240000	3.791773000	-0.814079000
6	1.718830000	4.387981000	0.293075000
6	1.091136000	4.453304000	-2.052336000
6	2.336170000	5.632522000	0.160982000
6	1.707600000	5.698832000	-2.179799000
6	2.330889000	6.289630000	-1.074713000
1	1.715735000	3.864751000	1.250340000
1	0.604277000	3.978262000	-2.905314000
1	2.823159000	6.092720000	1.024264000
1	1.703717000	6.211445000	-3.144887000
1	2.814431000	7.264676000	-1.176905000
6	-4.249045000	1.733033000	0.538786000
6	-5.147506000	2.071409000	-0.485869000
6	-4.588236000	1.989982000	1.876974000
6	-6.372550000	2.661947000	-0.173227000
6	-5.814689000	2.580073000	2.185103000
6	-6.707738000	2.916924000	1.161481000
1	-4.871999000	1.866301000	-1.521373000
1	-3.881505000	1.720660000	2.663297000
1	-7.069632000	2.924800000	-0.972727000
1	-6.076553000	2.778409000	3.227365000
1	-7.667968000	3.379399000	1.404616000
6	-2.162034000	-3.819471000	-0.133380000
6	-2.692429000	-4.441069000	-1.275224000
6	-2.151340000	-4.504354000	1.092491000
6	-3.205959000	-5.735774000	-1.190044000
6	-2.666655000	-5.798619000	1.173244000
6	-3.193953000	-6.415836000	0.033136000
1	-2.694682000	-3.898004000	-2.221446000
1	-1.737775000	-4.008960000	1.972179000
1	-3.617497000	-6.217520000	-2.080398000
1	-2.657986000	-6.329202000	2.128555000
1	-3.596940000	-7.429937000	0.098109000
7	0.443994000	0.059559000	2.490373000
1	0.463920000	0.975373000	2.936018000
1	1.309519000	-1.818768000	2.536787000
6	1.431458000	-0.842008000	3.030470000
1	1.227595000	-1.003296000	4.108006000
6	2.880221000	-0.393909000	2.870328000
6	3.235457000	0.726551000	2.106967000
1	2.461325000	1.314509000	1.613392000
6	4.580545000	1.070391000	1.936066000
1	4.838653000	1.941077000	1.327512000
6	5.588720000	0.298735000	2.519605000
1	6.639293000	0.564448000	2.377465000
6	5.241966000	-0.820497000	3.285205000
6	3.897939000	-1.159470000	3.460768000
1	3.633632000	-2.038935000	4.056334000
1	6.021518000	-1.431965000	3.747612000

Doublet Arene CH Activation TS

44	0.244940000	0.064531000	0.745980000
44	0.920016000	-0.014511000	-1.572742000

8	2.201094000	-0.554454000	1.190228000
8	2.796126000	-0.531745000	-0.979818000
8	0.852212000	2.021283000	0.757621000
8	-0.330518000	-1.924691000	0.405569000
8	-1.611786000	0.684387000	0.121893000
8	1.465995000	1.948516000	-1.401952000
8	0.377039000	-1.972322000	-1.729143000
8	-0.987035000	0.592610000	-2.035397000
6	3.036428000	-0.739985000	0.258836000
6	1.326561000	2.559716000	-0.292300000
6	-0.152624000	-2.513167000	-0.702260000
6	-1.850699000	0.795637000	-1.119644000
6	-0.597722000	-3.932485000	-0.813599000
6	-1.083791000	-4.611445000	0.315912000
6	-0.535647000	-4.594284000	-2.050353000
6	-1.506956000	-5.936729000	0.206831000
6	-0.962326000	-5.918863000	-2.155730000
6	-1.448548000	-6.591377000	-1.028785000
1	-1.115023000	-4.092692000	1.275184000
1	-0.152861000	-4.057245000	-2.919405000
1	-1.881039000	-6.462746000	1.088588000
1	-0.915145000	-6.430232000	-3.120325000
1	-1.780817000	-7.629362000	-1.113194000
6	4.401881000	-1.216560000	0.626178000
6	4.722932000	-1.455853000	1.972205000
6	5.368225000	-1.429634000	-0.369934000
6	5.998949000	-1.904039000	2.316034000
6	6.643060000	-1.878178000	-0.021429000
6	6.960100000	-2.115723000	1.320810000
1	3.961511000	-1.285752000	2.734955000
1	5.106347000	-1.238858000	-1.411660000
1	6.246256000	-2.089401000	3.364270000
1	7.393277000	-2.043055000	-0.798819000
1	7.959270000	-2.466755000	1.592119000
6	1.740665000	3.988025000	-0.216409000
6	2.262400000	4.629884000	-1.351100000
6	1.610575000	4.696455000	0.989234000
6	2.648970000	5.968748000	-1.278848000
6	1.999277000	6.034835000	1.056676000
6	2.518181000	6.672424000	-0.076141000
1	2.359062000	4.067257000	-2.280782000
1	1.204779000	4.184855000	1.863294000
1	3.054602000	6.466371000	-2.163154000
1	1.898062000	6.584039000	1.995986000
1	2.822145000	7.721069000	-0.021298000
6	-3.227310000	1.203051000	-1.519127000
6	-3.582285000	1.268499000	-2.875576000
6	-4.174960000	1.520027000	-0.531714000
6	-4.876779000	1.642365000	-3.240414000
6	-5.466192000	1.898077000	-0.902101000
6	-5.819727000	1.957660000	-2.255289000
1	-2.834727000	1.022945000	-3.631508000
1	-3.886782000	1.464521000	0.518038000
1	-5.152017000	1.690247000	-4.296898000
1	-6.199268000	2.150546000	-0.131846000

1	-6.832099000	2.253034000	-2.543339000
1	-0.870828000	-0.839859000	3.148403000
6	-2.068642000	-0.382410000	2.843887000
6	-2.567809000	0.688350000	3.575845000
1	-1.890765000	1.331310000	4.143236000
6	-3.946638000	0.927874000	3.551620000
1	-4.356283000	1.769298000	4.117838000
6	-4.809922000	0.112382000	2.801242000
6	-4.259623000	-0.954835000	2.067147000
6	-2.886873000	-1.202624000	2.068198000
1	-2.454170000	-2.000348000	1.464709000
1	-4.917527000	-1.588091000	1.464762000
7	-0.108549000	-0.201849000	2.512785000
6	-6.295734000	0.369846000	2.759992000
1	-6.661108000	0.404149000	1.720499000
1	-6.852049000	-0.435501000	3.269304000
1	-6.560445000	1.319665000	3.247721000

Triplet Ru₂ Imido Intermediate

44	-0.022477000	0.000739000	1.201525000
44	0.016187000	-0.000803000	-1.205167000
8	2.058699000	-0.072842000	1.063249000
8	2.048534000	-0.073046000	-1.192171000
7	0.209932000	-0.008192000	2.994161000
8	0.043354000	2.059315000	1.023777000
8	-0.101671000	-2.057574000	1.023638000
8	-2.071753000	0.072978000	1.120457000
8	0.077633000	2.024708000	-1.223761000
8	-0.066656000	-2.025391000	-1.223970000
8	-2.013690000	0.071635000	-1.131690000
6	2.646443000	-0.093848000	-0.058595000
6	0.079085000	2.640551000	-0.100287000
6	-0.108501000	-2.639807000	-0.100437000
6	-2.640686000	0.093611000	-0.012492000
6	-0.168607000	-4.126390000	-0.119842000
6	-0.236538000	-4.843711000	1.086115000
6	-0.158159000	-4.814771000	-1.344059000
6	-0.292826000	-6.237420000	1.064775000
6	-0.214021000	-6.208937000	-1.359528000
6	-0.281338000	-6.921139000	-0.156677000
1	-0.245819000	-4.296079000	2.029783000
1	-0.105758000	-4.245267000	-2.273020000
1	-0.346389000	-6.793989000	2.003561000
1	-0.205285000	-6.743200000	-2.312682000
1	-0.325416000	-8.013307000	-0.170983000
6	4.135974000	-0.145860000	-0.069148000
6	4.850433000	-0.170265000	1.139901000
6	4.830219000	-0.170734000	-1.289865000
6	6.244571000	-0.218929000	1.126304000
6	6.224801000	-0.219446000	-1.298629000
6	6.933254000	-0.243546000	-0.092063000
1	4.300486000	-0.150744000	2.081777000
1	4.264200000	-0.151529000	-2.222152000
1	6.797638000	-0.237804000	2.068541000
1	6.762299000	-0.238726000	-2.249833000

1	8.025694000	-0.281647000	-0.100903000
6	0.123828000	4.127658000	-0.119671000
6	0.183638000	4.813466000	-1.343889000
6	0.105790000	4.848099000	1.086234000
6	0.226026000	6.208094000	-1.359439000
6	0.147656000	6.242314000	1.064813000
6	0.208030000	6.923401000	-0.156668000
1	0.196702000	4.241583000	-2.272782000
1	0.057548000	4.302550000	2.029922000
1	0.273096000	6.740328000	-2.312605000
1	0.132776000	6.801355000	2.003541000
1	0.240844000	8.015963000	-0.171061000
6	-4.127164000	0.146141000	-0.049700000
6	-4.801618000	0.170856000	-1.281462000
6	-4.858552000	0.171136000	1.149535000
6	-6.195798000	0.220039000	-1.311263000
6	-6.252241000	0.220195000	1.113799000
6	-6.922019000	0.244673000	-0.115159000
1	-4.221513000	0.151178000	-2.205089000
1	-4.321429000	0.151646000	2.099115000
1	-6.719132000	0.239254000	-2.270323000
1	-6.819694000	0.239510000	2.047394000
1	-8.014208000	0.283132000	-0.140643000
1	1.194916000	-0.044881000	3.307668000

Doublet Ru₂NH + Aryl Radical Pair

1	-0.012414000	0.675754000	2.158645000
6	0.030006000	2.356573000	0.000000000
1	-0.464513000	2.773768000	0.890728000
1	-0.464513000	2.773768000	-0.890728000
1	1.069989000	2.727656000	0.000000000
6	-0.005604000	0.846276000	0.000000000
6	-0.008169000	0.130259000	-1.209415000
6	-0.008169000	-1.275249000	-1.225007000
6	-0.006791000	-1.909537000	0.000000000
6	-0.008169000	-1.275249000	1.225007000
6	-0.008169000	0.130259000	1.209415000
1	-0.012414000	0.675754000	-2.158645000
1	-0.012879000	-1.823346000	-2.171584000
1	-0.012879000	-1.823346000	2.171584000

Doublet Ru₂-N(H)aryl Intermediate

44	-0.324466000	-0.025592000	0.706318000
44	-0.873948000	0.045417000	-1.548837000
8	0.451929000	1.904662000	0.466527000
8	-0.063394000	1.925138000	-1.716554000
8	-2.145849000	0.828738000	1.161507000
8	1.471768000	-0.904664000	0.122180000
8	-1.122175000	-1.918163000	0.830798000
8	-2.677493000	0.867784000	-1.016215000
8	0.943320000	-0.763963000	-2.051645000
8	-1.658278000	-1.840238000	-1.344755000
6	0.448164000	2.454109000	-0.679207000
6	-2.939796000	1.104347000	0.206894000
6	1.745662000	-1.060053000	-1.107062000

6	-1.611131000	-2.438490000	-0.222584000
6	3.085993000	-1.608976000	-1.456046000
6	4.041824000	-1.819040000	-0.448066000
6	3.403385000	-1.901228000	-2.792259000
6	5.303188000	-2.316156000	-0.777966000
6	4.664261000	-2.404150000	-3.115657000
6	5.615638000	-2.611331000	-2.109633000
1	3.794060000	-1.577513000	0.585101000
1	2.652896000	-1.728983000	-3.565365000
1	6.044647000	-2.468230000	0.010030000
1	4.908291000	-2.633811000	-4.155873000
1	6.604141000	-3.001937000	-2.365753000
6	1.093240000	3.791773000	-0.814079000
6	1.718830000	4.387981000	0.293075000
6	1.091136000	4.453304000	-2.052336000
6	2.336170000	5.632522000	0.160982000
6	1.707600000	5.698832000	-2.179799000
6	2.330889000	6.289630000	-1.074713000
1	1.715735000	3.864751000	1.250340000
1	0.604277000	3.978262000	-2.905314000
1	2.823159000	6.092720000	1.024264000
1	1.703717000	6.211445000	-3.144887000
1	2.814431000	7.264676000	-1.176905000
6	-4.249045000	1.733033000	0.538786000
6	-5.147506000	2.071409000	-0.485869000
6	-4.588236000	1.989982000	1.876974000
6	-6.372550000	2.661947000	-0.173227000
6	-5.814689000	2.580073000	2.185103000
6	-6.707738000	2.916924000	1.161481000
1	-4.871999000	1.866301000	-1.521373000
1	-3.881505000	1.720660000	2.663297000
1	-7.069632000	2.924800000	-0.972727000
1	-6.076553000	2.778409000	3.227365000
1	-7.667968000	3.379399000	1.404616000
6	-2.162034000	-3.819471000	-0.133380000
6	-2.692429000	-4.441069000	-1.275224000
6	-2.151340000	-4.504354000	1.092491000
6	-3.205959000	-5.735774000	-1.190044000
6	-2.666655000	-5.798619000	1.173244000
6	-3.193953000	-6.415836000	0.033136000
1	-2.694682000	-3.898004000	-2.221446000
1	-1.737775000	-4.008960000	1.972179000
1	-3.617497000	-6.217520000	-2.080398000
1	-2.657986000	-6.329202000	2.128555000
1	-3.596940000	-7.429937000	0.098109000
7	0.443994000	0.059559000	2.490373000
1	0.463920000	0.975373000	2.936018000
1	1.309519000	-1.818768000	2.536787000
6	1.431458000	-0.842008000	3.030470000
1	1.227595000	-1.003296000	4.108006000
6	2.880221000	-0.393909000	2.870328000
6	3.235457000	0.726551000	2.106967000
1	2.461325000	1.314509000	1.613392000
6	4.580545000	1.070391000	1.936066000
1	4.838653000	1.941077000	1.327512000

6	5.588720000	0.298735000	2.519605000
1	6.639293000	0.564448000	2.377465000
6	5.241966000	-0.820497000	3.285205000
6	3.897939000	-1.159470000	3.460768000
1	3.633632000	-2.038935000	4.056334000
1	6.021518000	-1.431965000	3.747612000

Doublet TS for Electrophilic Attack

44	-0.202835000	-0.029306000	0.788393000
44	-0.642450000	-0.050620000	-1.598549000
8	-1.977439000	1.081169000	0.945714000
8	-2.387625000	0.947257000	-1.261110000
7	-0.002313000	0.071151000	2.547442000
8	-1.285304000	-1.804870000	0.872613000
8	0.839668000	1.721461000	0.411869000
8	1.498387000	-1.134741000	0.373115000
8	-1.655691000	-1.807674000	-1.345377000
8	0.359501000	1.727120000	-1.785403000
8	1.104733000	-1.095270000	-1.842278000
6	-2.676060000	1.333914000	-0.080892000
6	-1.758418000	-2.323356000	-0.185323000
6	0.890661000	2.236061000	-0.747960000
6	1.795067000	-1.426305000	-0.828000000
6	1.222537000	0.399765000	3.695748000
6	1.895973000	1.576061000	3.176273000
6	2.005543000	-0.828166000	3.679579000
1	1.397924000	2.542404000	3.275994000
1	1.593032000	-1.710944000	4.172946000
6	3.074544000	1.464829000	2.466509000
6	3.191649000	-0.902377000	2.986902000
1	3.508362000	2.351717000	1.998211000
1	3.734062000	-1.850197000	2.946280000
6	3.735655000	0.226794000	2.325810000
6	4.956047000	0.096609000	1.462513000
1	5.515885000	1.042337000	1.398346000
1	5.632148000	-0.693797000	1.823809000
1	4.662518000	-0.185320000	0.435191000
1	0.590134000	0.555119000	4.575282000
6	3.038507000	-2.217072000	-1.061142000
6	3.637504000	-2.917129000	-0.002637000
6	3.613951000	-2.262978000	-2.340728000
1	3.169027000	-2.881583000	0.980490000
1	3.132356000	-1.723299000	-3.157762000
6	4.805493000	-3.649196000	-0.219465000
6	4.789527000	-2.985779000	-2.551272000
1	5.264679000	-4.199593000	0.605581000
1	5.241157000	-3.011615000	-3.546034000
6	5.386741000	-3.679270000	-1.492293000
1	6.304756000	-4.248297000	-1.660677000
6	-2.487160000	-3.618807000	-0.058008000
6	-2.637401000	-4.222223000	1.201017000
6	-3.024042000	-4.239475000	-1.197218000
1	-2.216525000	-3.727585000	2.077704000
1	-2.901366000	-3.759129000	-2.169053000
6	-3.318163000	-5.434899000	1.317122000

6	-3.703217000	-5.452674000	-1.076631000
1	-3.434657000	-5.901768000	2.298365000
1	-4.119834000	-5.933576000	-1.965159000
6	-3.851332000	-6.051725000	0.179518000
1	-4.384328000	-7.001707000	0.272243000
6	-3.926287000	2.127595000	0.104527000
6	-4.301750000	2.560387000	1.386485000
6	-4.730170000	2.445415000	-1.001807000
1	-3.667955000	2.304284000	2.236860000
1	-4.427785000	2.101618000	-1.992063000
6	-5.470048000	3.304196000	1.557862000
6	-5.897327000	3.190162000	-0.826015000
1	-5.760373000	3.638996000	2.556870000
1	-6.520956000	3.436124000	-1.689118000
6	-6.268819000	3.620315000	0.452892000
1	-7.183741000	4.203058000	0.588906000
6	1.624114000	3.526591000	-0.900373000
6	2.029474000	4.248980000	0.233343000
6	1.909618000	4.025589000	-2.181012000
1	1.785043000	3.859297000	1.221365000
1	1.582132000	3.459355000	-3.054262000
6	2.718938000	5.453502000	0.087236000
6	2.605578000	5.227119000	-2.323645000
1	3.026741000	6.015626000	0.972444000
1	2.830848000	5.609688000	-3.322208000
6	3.011687000	5.942121000	-1.191216000
1	3.553914000	6.884420000	-1.305161000

Quartet Aziridine-like Intermediate

44	-0.248377000	0.004631000	0.786436000
44	-0.743328000	0.040704000	-1.571429000
8	0.669466000	1.839258000	0.454716000
8	0.220274000	1.822671000	-1.753543000
7	0.288773000	-0.115711000	2.510008000
8	-2.039133000	0.979886000	1.052690000
8	1.499251000	-0.958050000	0.190852000
8	-1.239862000	-1.817877000	0.841709000
8	-2.480796000	1.010001000	-1.151709000
8	0.978195000	-0.933430000	-2.000720000
8	-1.701013000	-1.737999000	-1.362005000
6	0.737806000	2.342605000	-0.705318000
6	-2.774978000	1.277454000	0.064350000
6	1.747790000	-1.227039000	-1.019761000
6	-1.753428000	-2.298253000	-0.210264000
6	1.450160000	0.182965000	3.339616000
6	2.358056000	1.267938000	2.823882000
6	2.170210000	-1.126959000	3.547724000
1	1.918350000	2.259454000	2.718087000
1	1.585471000	-1.947049000	3.968492000
6	3.651021000	1.029615000	2.466764000
6	3.478924000	-1.301072000	3.175547000
1	4.252482000	1.848979000	2.059166000
1	3.943571000	-2.281167000	3.326347000
6	4.260931000	-0.256637000	2.614815000
6	5.674607000	-0.481624000	2.162874000

1	6.339666000	0.334911000	2.491877000
1	6.081172000	-1.430095000	2.546758000
1	5.738066000	-0.520067000	1.059661000
1	1.000312000	0.508204000	4.306482000
6	3.020576000	-1.935724000	-1.332483000
6	3.393811000	-2.162125000	-2.667152000
6	3.849400000	-2.378572000	-0.290055000
6	4.590940000	-2.820177000	-2.953293000
6	5.044188000	-3.037730000	-0.581082000
6	5.417421000	-3.258095000	-1.911985000
1	2.738800000	-1.815476000	-3.467707000
1	3.542875000	-2.194266000	0.739015000
1	4.881726000	-2.992822000	-3.992420000
1	5.687637000	-3.379922000	0.233178000
1	6.354419000	-3.773578000	-2.138678000
6	1.473992000	3.629440000	-0.870025000
6	2.093234000	4.239377000	0.232784000
6	1.557678000	4.233088000	-2.135302000
6	2.788280000	5.438236000	0.071675000
6	2.252832000	5.433031000	-2.292631000
6	2.868888000	6.036978000	-1.190879000
1	2.023755000	3.762102000	1.209645000
1	1.074038000	3.749809000	-2.985248000
1	3.268653000	5.908555000	0.933168000
1	2.315196000	5.899795000	-3.278723000
1	3.413239000	6.976629000	-1.316171000
6	-4.059196000	1.980221000	0.334898000
6	-4.432940000	2.282215000	1.654830000
6	-4.900293000	2.342054000	-0.729950000
6	-5.637280000	2.940582000	1.904672000
6	-6.103527000	3.001116000	-0.474732000
6	-6.473292000	3.300874000	0.841300000
1	-3.770716000	1.993980000	2.472642000
1	-4.598183000	2.100522000	-1.749972000
1	-5.926740000	3.174013000	2.932192000
1	-6.756497000	3.282143000	-1.304640000
1	-7.416551000	3.816739000	1.039210000
6	-2.467040000	-3.602634000	-0.107925000
6	-2.565119000	-4.254336000	1.132477000
6	-3.042563000	-4.183458000	-1.249558000
6	-3.233124000	-5.475513000	1.227441000
6	-3.709421000	-5.405326000	-1.149473000
6	-3.805604000	-6.052328000	0.087683000
1	-2.113476000	-3.790547000	2.010800000
1	-2.958858000	-3.666704000	-2.206630000
1	-3.308705000	-5.980688000	2.193506000
1	-4.156281000	-5.855696000	-2.039236000
1	-4.328535000	-7.009301000	0.164111000

Quartet 1,2 H transfer TS

44	0.194529000	0.010886000	0.632259000
44	0.971454000	0.001485000	-1.631169000
8	-1.069122000	-1.523341000	0.048924000
8	-0.323114000	-1.512842000	-2.074328000
7	-0.601427000	-0.038397000	2.347780000

8	1.665714000	-1.375023000	1.044818000
8	-1.202421000	1.392556000	-0.010391000
8	1.526676000	1.538809000	0.992403000
8	2.382340000	-1.355530000	-1.089917000
8	-0.459310000	1.362481000	-2.135377000
8	2.244079000	1.501848000	-1.141458000
6	-1.089596000	-1.945194000	-1.147379000
6	2.444536000	-1.762258000	0.124394000
6	-1.262568000	1.759308000	-1.221252000
6	2.265515000	1.962626000	0.055415000
1	-1.494654000	-1.295250000	2.568611000
6	-3.121494000	-0.068437000	1.856037000
6	-1.959243000	-0.219538000	2.745967000
6	-4.395425000	0.052915000	2.366285000
1	-5.233335000	0.140550000	1.667013000
6	-2.263359000	-0.143004000	4.181748000
6	-4.660834000	0.080901000	3.757630000
1	-1.418968000	-0.204999000	4.871355000
6	-3.555750000	-0.018497000	4.638793000
1	-3.734261000	0.017480000	5.717965000
1	-2.948970000	-0.087585000	0.783176000
6	-6.062988000	0.256683000	4.273093000
1	-6.368250000	1.319350000	4.244584000
1	-6.792382000	-0.299997000	3.662550000
1	-6.160197000	-0.081818000	5.315975000
6	3.501326000	-2.754156000	0.469208000
6	4.375531000	-3.227747000	-0.522539000
6	3.626403000	-3.217439000	1.789369000
6	5.363967000	-4.157000000	-0.195257000
6	4.616628000	-4.145931000	2.111726000
6	5.485895000	-4.616972000	1.120797000
1	4.268221000	-2.859092000	-1.543631000
1	2.941693000	-2.839143000	2.550033000
1	6.042830000	-4.524312000	-0.968845000
1	4.712578000	-4.504187000	3.139660000
1	6.261167000	-5.344462000	1.375347000
6	3.220808000	3.064529000	0.357094000
6	3.286730000	3.601463000	1.653465000
6	4.057450000	3.569517000	-0.651453000
6	4.181887000	4.633708000	1.935620000
6	4.950980000	4.602273000	-0.364124000
6	5.014483000	5.135257000	0.928299000
1	2.630906000	3.199164000	2.427148000
1	3.996300000	3.143465000	-1.653840000
1	4.231625000	5.049784000	2.944863000
1	5.601016000	4.993721000	-1.150520000
1	5.715186000	5.944140000	1.151493000
6	-2.348771000	2.704712000	-1.603319000
6	-3.294533000	3.109306000	-0.645951000
6	-2.437720000	3.184283000	-2.919900000
6	-4.318578000	3.985808000	-1.006122000
6	-3.462437000	4.063147000	-3.274000000
6	-4.403325000	4.464525000	-2.318863000
1	-3.216923000	2.725496000	0.372697000
1	-1.697680000	2.859677000	-3.652869000

1	-5.053803000	4.298579000	-0.260542000
1	-3.528868000	4.436850000	-4.298750000
1	-5.205578000	5.152489000	-2.598469000
6	-2.078838000	-3.004222000	-1.492527000
6	-2.080179000	-3.575530000	-2.775252000
6	-3.020878000	-3.426149000	-0.539345000
6	-3.011610000	-4.563390000	-3.097884000
6	-3.952904000	-4.410889000	-0.868092000
6	-3.948289000	-4.982008000	-2.146044000
1	-1.345569000	-3.235841000	-3.506789000
1	-3.017846000	-2.968407000	0.451021000
1	-3.008593000	-5.008695000	-4.095783000
1	-4.686517000	-4.734881000	-0.125807000
1	-4.678044000	-5.754862000	-2.401277000

Quartet-Ru₂NCl Product

44	0.000134000	-0.000059000	1.029833000
44	0.000129000	-0.000069000	-1.283375000
8	-1.446638000	1.447148000	0.951494000
8	-1.426887000	1.427418000	-1.291142000
17	0.000141000	0.000047000	3.383184000
8	-1.447197000	-1.446712000	0.951478000
8	1.447389000	1.446663000	0.951436000
8	1.446863000	-1.447295000	0.951460000
8	-1.427470000	-1.426970000	-1.291163000
8	1.427622000	1.426952000	-1.291206000
8	1.427120000	-1.427574000	-1.291175000
6	-1.867387000	1.868018000	-0.165271000
6	-1.868160000	-1.867362000	-0.165290000
6	1.868262000	1.867395000	-0.165333000
6	1.867572000	-1.868214000	-0.165310000
6	2.917628000	2.916475000	-0.182141000
6	3.420102000	3.419130000	1.030109000
6	3.408493000	3.406869000	-1.403471000
6	4.406513000	4.405219000	1.016476000
6	4.395154000	4.393190000	-1.410085000
6	4.894511000	4.892727000	-0.201690000
1	3.028652000	3.028034000	1.970714000
1	3.009495000	3.007744000	-2.337113000
1	4.797117000	4.795954000	1.959068000
1	4.777010000	4.774638000	-2.360128000
1	5.667578000	5.665525000	-0.209275000
6	-2.916407000	2.917435000	-0.182089000
6	-3.418879000	3.420096000	1.030162000
6	-3.406940000	3.408163000	-1.403419000
6	-4.404940000	4.406535000	1.016530000
6	-4.393242000	4.394843000	-1.410032000
6	-4.892597000	4.894382000	-0.201637000
1	-3.027679000	3.028749000	1.970766000
1	-3.007948000	3.009031000	-2.337060000
1	-4.795534000	4.797281000	1.959121000
1	-4.774816000	4.776574000	-2.360074000
1	-5.665379000	5.667465000	-0.209224000
6	-2.917828000	-2.916138000	-0.182099000
6	-3.408828000	-3.406398000	-1.403428000

6	-3.420458000	-3.418636000	1.030153000
6	-4.395771000	-4.392438000	-1.410040000
6	-4.407153000	-4.404440000	1.016521000
6	-4.895282000	-4.891819000	-0.201644000
1	-3.009711000	-3.007394000	-2.337070000
1	-3.028901000	-3.027646000	1.970756000
1	-4.777726000	-4.773788000	-2.360083000
1	-4.797879000	-4.795053000	1.959113000
1	-5.668570000	-5.664396000	-0.209229000
6	2.916481000	-2.917742000	-0.182109000
6	3.406915000	-3.408578000	-1.403434000
6	3.418941000	-3.420405000	1.030147000
6	4.393105000	-4.395371000	-1.410041000
6	4.404893000	-4.406952000	1.016521000
6	4.892451000	-4.894910000	-0.201642000
1	3.007935000	-3.009443000	-2.337079000
1	3.027818000	-3.028976000	1.970748000
1	4.774599000	-4.777189000	-2.360080000
1	4.795481000	-4.797697000	1.959115000
1	5.665146000	-5.668079000	-0.209224000

Singlet Benzylamine

1	0.078528000	-2.311598000	0.027873000
6	-1.918679000	-0.480018000	-0.377024000
1	-2.120917000	-1.553772000	-0.189063000
1	-2.179184000	-0.298049000	-1.435355000
6	-0.437154000	-0.223332000	-0.184608000
6	0.068471000	1.087162000	-0.205099000
6	1.435961000	1.324580000	-0.051577000
6	2.322599000	0.255758000	0.125527000
6	1.829706000	-1.051278000	0.151065000
6	0.458524000	-1.285806000	0.000362000
1	-0.627366000	1.919293000	-0.334489000
1	1.814351000	2.350280000	-0.070360000
1	3.392826000	0.442830000	0.246472000
1	2.512675000	-1.892826000	0.294740000
7	-2.734066000	0.430957000	0.432115000
1	-2.566898000	0.280268000	1.420934000
1	-3.722123000	0.284481000	0.262567000

Singlet p-Toluidine

1	1.206161000	2.153430000	-0.020187000
6	2.914160000	-0.000466000	0.007340000
1	3.327246000	0.906154000	-0.462198000
1	3.326486000	-0.873104000	-0.523740000
1	3.302637000	-0.036987000	1.041003000
6	1.404407000	0.000903000	-0.014684000
6	0.672769000	-1.197195000	-0.010364000
6	-0.721849000	-1.205680000	0.002740000
6	-1.445691000	0.000195000	0.010617000
6	-0.722769000	1.205895000	0.002709000
6	0.672514000	1.198055000	-0.010369000
1	1.207244000	-2.152133000	-0.020592000
1	-1.261368000	-2.157531000	0.006824000
1	-1.262139000	2.157813000	0.006588000

7	-2.841832000	-0.000813000	0.078159000
1	-3.296795000	-0.837550000	-0.251368000
1	-3.297894000	0.835356000	-0.251372000

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