Supporting Information

Experimental procedure for the preparation of **3-Tol-*p*** and **4-Tol-*p***.

Table S1. Crystal and refinement data for **4-Tol-*p***.

Table S2. Selected natural charges and Wiberg bond indices for species **A1-D** and associated transition structures for the conversion of cluster **B** to **A1**.

Figure S1: Graph of $\ln[I_3/(I_3+I_4)]$ vs reaction time at 25˚C.

Figure S2: Graph of $\ln[I_3/(I_3+I_4)]$ vs reaction time at 35˚C.

Figure S3: Graph of $\ln[I_3/(I_3+I_4)]$ vs reaction time at 55˚C.

Figure S4: Graph of $\ln[I_3/(I_3+I_4)]$ vs reaction time at 65˚C.

Figure S5: Graph of $\ln[I_3/(I_3+I_4)]$ vs reaction time at 75˚C.

Figure S6: Eyring plot for conversion of **3-Tol-*p*** to **4-Tol-*p***.

Figure S7. M06-optimized structures for the conversion of **B** to **A1** and transition state structures **TSBC**, **TSCD**, **TSDA2**, **TSA2A1**, and **TSBA3**.

M06 geometries and energies for all optimized minima and transition structures.

IR and ^{1}H NMR spectra of **3-Tol-*p***

IR and ^{1}H NMR spectra of **4-Tol-*p***

Variable-temperature ^{1}H NMR spectrum of **4-Tol-*p*** from 25˚C to 90˚C in toluene-d_8

Experimental procedure for the preparation of **3-Tol-p** and **4-Tol-p**.

Cluster **1** (150 mg, 0.159 mmol) and the ditelluride **2** (70 mg, 0.160 mmol) were stirred in DCM (15 mL) at room temperature for 1 h. Column chromatographic separation on silica gel using DCM and hexane (20:80, v/v) as eluent afforded **4-Tol-p** (9.5 mg, 7%) followed by **3-Tol-p** (80.6 mg, 60%).

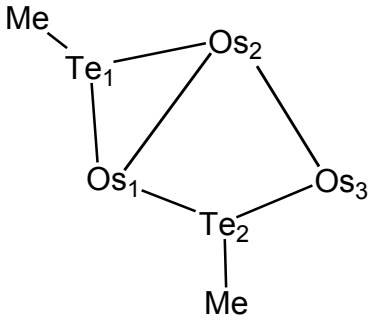
3-Tol-p: ν_{CO}/cm^{-1} (cyclohexane): 2105w, 2058s, 2041m, 2026s, 2010w, 1988w, 1971w, 1964w and 195w. ^{1}H NMR ($CDCl_3$): 6.9-7.5 (m, 8H, aromatic), 2.379 (s, 3H, Me), 2.362 (s, 3H, Me).

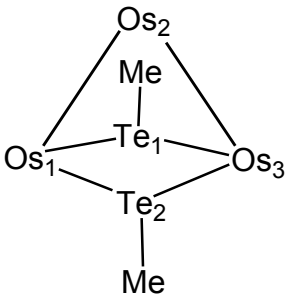
4-Tol-p: ν_{CO}/cm^{-1} (DCM): 2098m, 2056vs, 2009s, 1980m. ^{1}H NMR ($CDCl_3$): 6.6-7.2 (m, 8H, aromatic), 2.289 (s, 6H, Me).

Table S1. Crystal and refinement data for **4-Tol-*p***.

Empirical formula	C24 H14 O10 Os3 Te2	
Formula weight	1288.15	
Temperature	103(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	$I\bar{4}2d$	
Unit cell dimensions	a = 14.1313(6) Å	α= 90°.
	b = 14.1313(6) Å	β= 90°.
	c = 28.8408(13) Å	γ = 90°.
Volume	5759.3(6) $Å^3$	
Z	8	
Density (calculated)	2.971 Mg/m^3	
Absorption coefficient	15.242 mm^{-1}	
F(000)	4560	
Crystal size	0.240 x 0.200 x 0.180 mm^3	
Theta range for data collection	3.815 to 26.372°.	
Index ranges	-17<=h<=17, -17<=k<=17, -35<=l<=36	
Reflections collected	35019	
Independent reflections	2952 [R(int) = 0.0646]	
Completeness to theta = 25.242°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.170 and 0.121	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2952 / 0 / 178	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2sigma(I)]	R1 = 0.0168, wR2 = 0.0355	
R indices (all data)	R1 = 0.0180, wR2 = 0.0358	
Absolute structure parameter	0.000(4)	
Largest diff. peak and hole	0.982 and -0.667 $e.Å^{-3}$	

Table S2. Selected natural charges and Wiberg bond indices for species **A1**-**D** and associated transition structures for the conversion of cluster **B** to **A1**.[a]





Natural Charge

species	Os_1	Os_2	Os_3	Te_1	Te_2
B	-1.60	-1.33	-1.60	0.78	0.84
TSBC	-1.21	-1.54	-1.36	0.78	0.41
C	-1.31	-1.28	-1.53	0.81	0.37
TSCD	-1.20	-1.37	-1.51	0.79	0.37
D	-1.61	-1.32	-1.60	0.80	0.84
TSDA2	-1.57	-1.26	-1.45	0.84	0.82
A2	-1.55	-1.40	-1.55	0.75	0.82
TSA2A1	-1.49	-1.40	-1.49	0.49	0.81
A1	-1.56	-1.40	-1.56	0.80	0.80
TSBA3	-1.55	-1.22	-1.48	0.83	0.78
A3	-1.51	-1.40	-1.51	0.75	0.75

Table S2. Con't.

Wiberg bond indices

species	Os_1-Os_2	Os_2-Os_3	Os_1-Os_3	Os_1-Te_1	Os_2-Te_1	Os_3-Te_1	Os_1-Te_2	Os_2-Te_2	Os_3-Te_2
B	0.47	0.40	0.04	0.80	0.79	0.02	0.77	0.06	0.77
TSBC	0.60	0.33	0.21	0.78	0.78	0.03	0.20	0.03	0.75
C	0.65	0.28	0.30	0.79	0.78	0.04	0.06	0.01	0.77
TSCD	0.61	0.33	0.21	0.78	0.78	0.03	0.18	0.03	0.73
D	0.47	0.40	0.03	0.81	0.79	0.02	0.77	0.06	0.77
TSDA2	0.47	0.20	0.03	0.79	0.44	0.50	0.76	0.03	0.77
A2	0.41	0.41	0.11	0.76	0.05	0.76	0.77	0.07	0.77
TSA2A1	0.43	0.43	0.09	0.71	0.06	0.71	0.76	0.08	0.76
A1	0.42	0.42	0.10	0.76	0.07	0.76	0.76	0.07	0.76
TSBA3	0.47	0.20	0.03	0.79	0.38	0.55	0.76	0.03	0.78
A3	0.39	0.39	0.13	0.76	0.05	0.75	0.76	0.05	0.76

[a] Atom numbers based on the numbering scheme for the different Os_3 clusters examined in this study.

The kinetics for the isomerization of **3-Tol-*p*** to **4-Tol-*p*** was obtained by monitoring the sum of the intensities for the two distinct methyl resonances at 2.379 and 2.362 ppm for the former (**I_3**), against the single methyl resonance at 2.289 ppm for the latter (**I_4**).

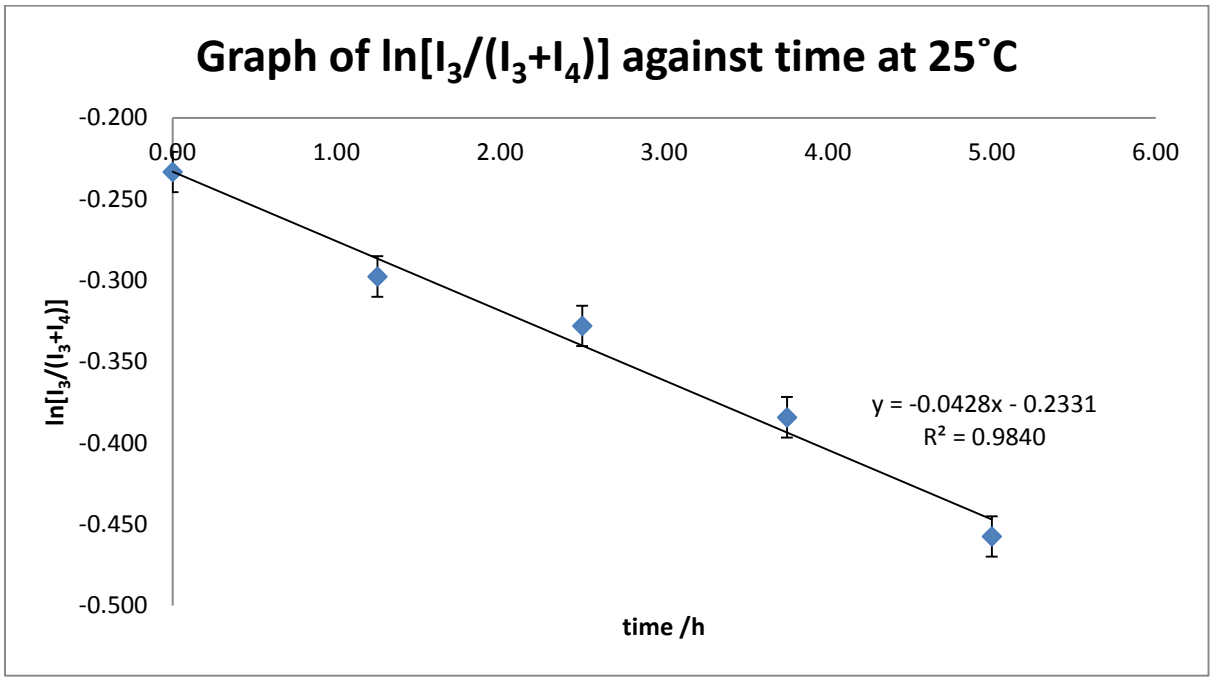


Figure S1: Graph of ln[I_3/(I_3+I_4)] vs reaction time at 25˚C.

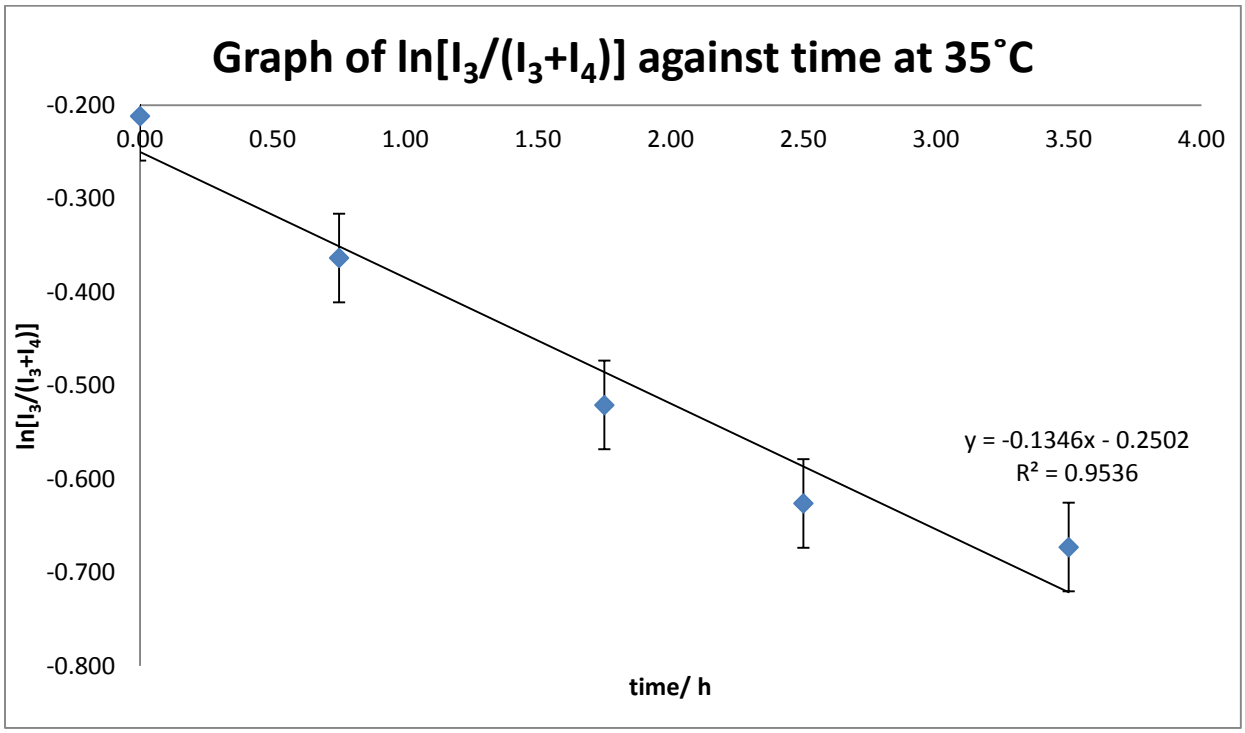


Figure S2: Graph of ln[I_3/(I_3+I_4)] vs reaction time at 35˚C.

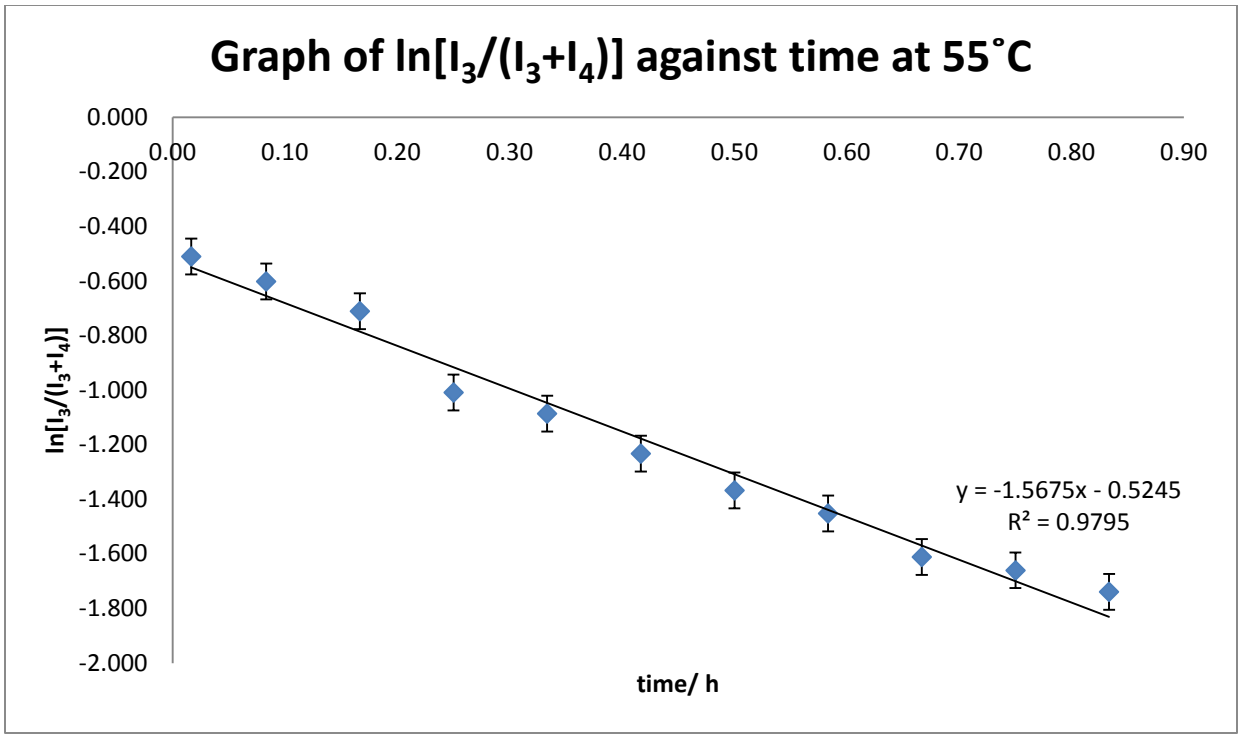


Figure S3: Graph of ln[I_3/(I_3+I_4)] vs reaction time at 55˚C.

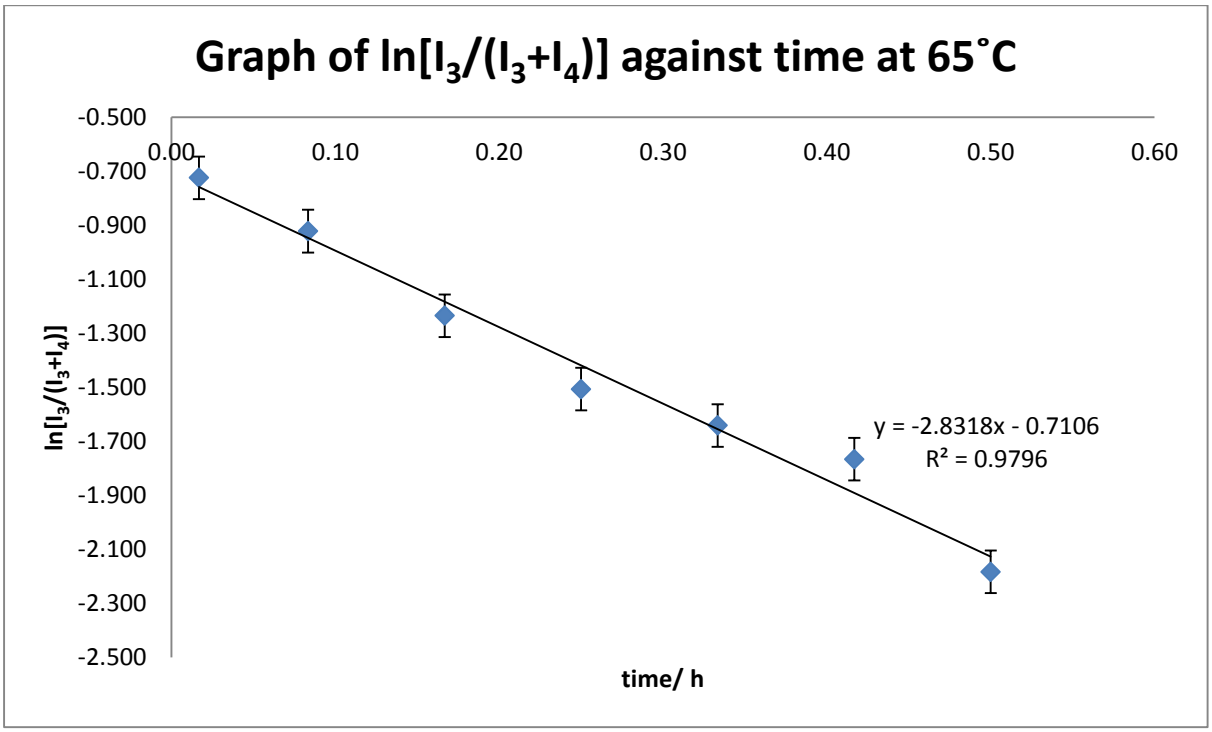


Figure S4: Graph of ln[I_3/(I_3+I_4)] vs reaction time at 65˚C.

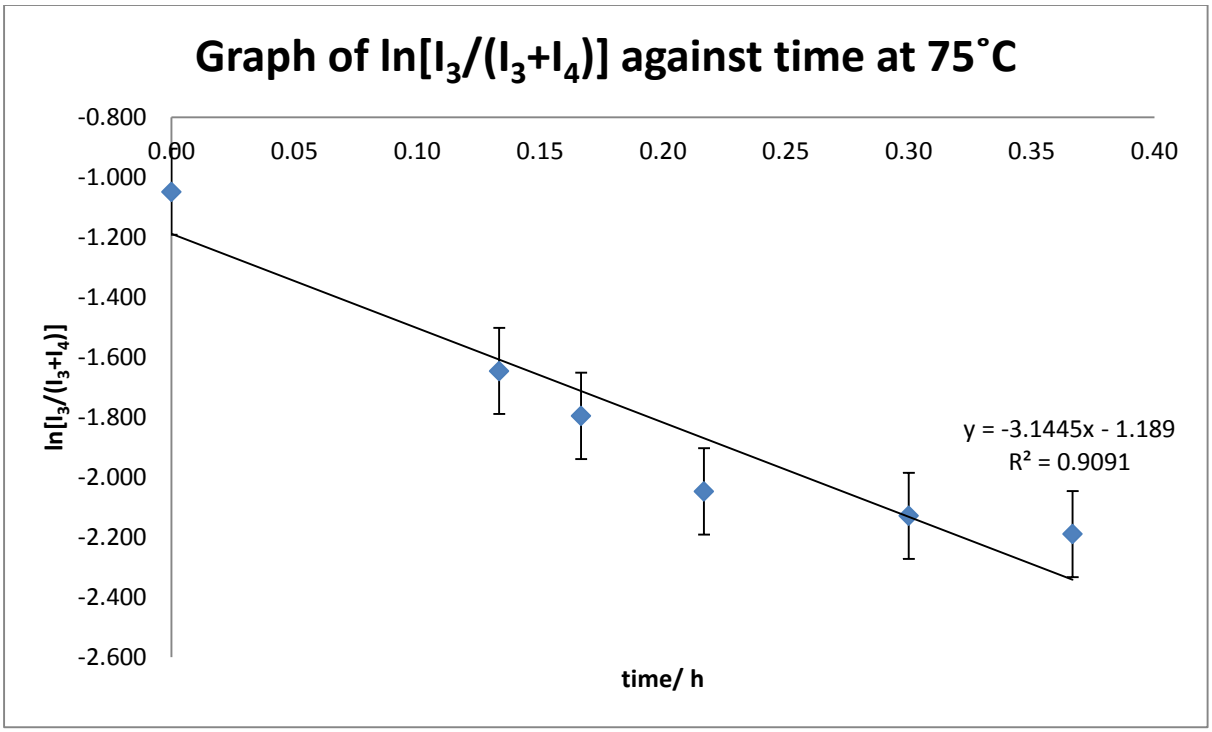


Figure S5: Graph of $\ln[I_3/(I_3+I_4)]$ vs reaction time at 75˚C.

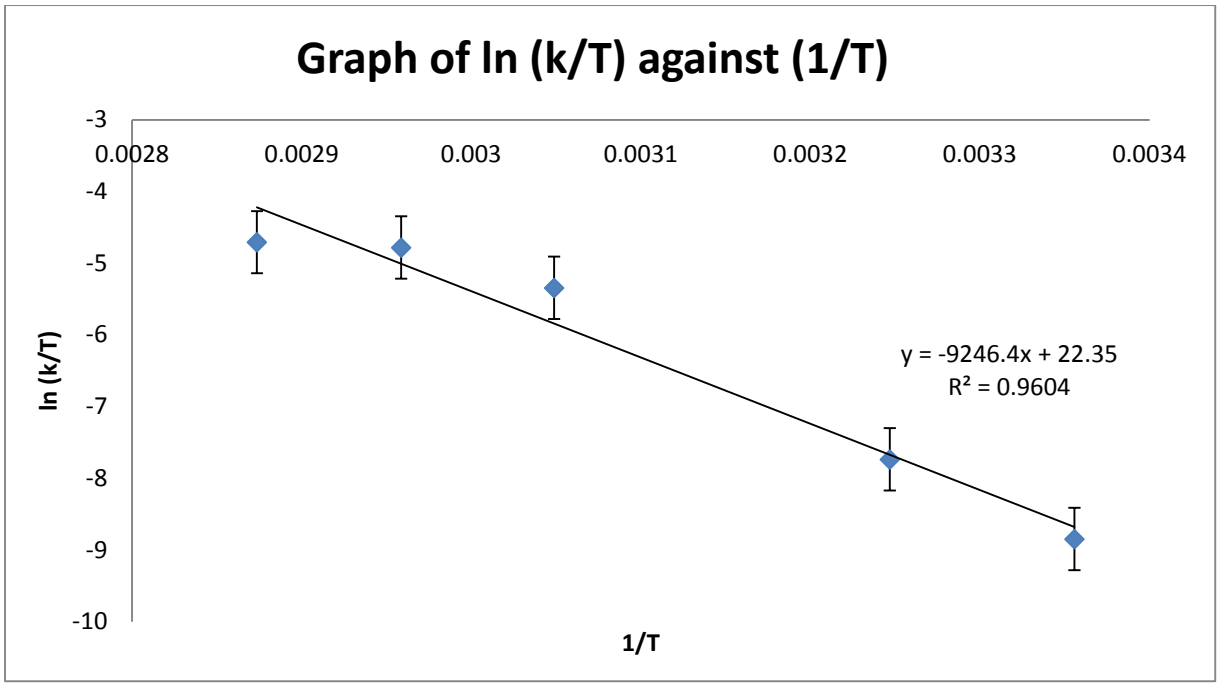


Figure S6: Eyring plot for conversion of **3-Tol-*p*** to **4-Tol-*p***.

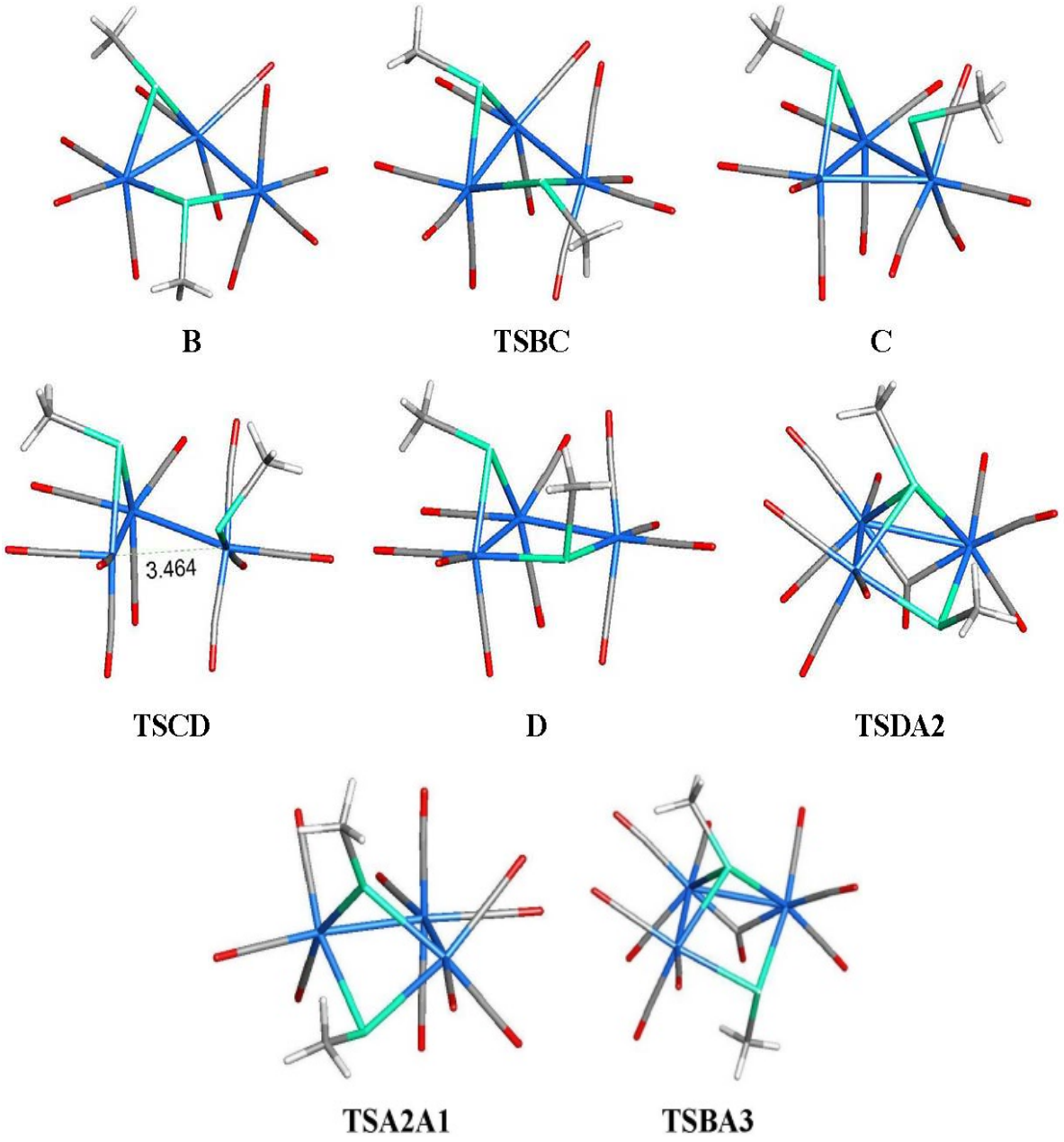


Figure S7. M06-optimized structures for the conversion of **B** to **A1** and transition state structures **TSBC**, **TSCD**, **TSDA2**, **TSA2A1**, and **TSBA3**.

M06 geometries and energies for all optimized minima and transition structures

Species A1
SCF Done: E(RM06) = -1501.13537888
No imaginary frequency
Zero-point correction = 0.162096 (Hartree/Particle)
Thermal correction to Energy = 0.198045
Thermal correction to Enthalpy = 0.198990
Thermal correction to Gibbs Free Energy = 0.089806
Sum of electronic and zero-point Energies = -1500.973283
Sum of electronic and thermal Energies = -1500.937333
Sum of electronic and thermal Enthalpies = -1500.936389
Sum of electronic and thermal Free Energies = -1501.045573

Coordinates: **A1**

Os	1.62950000	4.69090000	8.50300000
Os	-0.58340000	2.29040000	6.94380000
Os	1.38200000	1.75890000	9.16950000
O	1.65410000	7.62180000	7.57980000
O	4.65450000	4.16050000	8.48880000
O	1.46180000	5.11490000	11.54050000
O	-2.49390000	3.15800000	4.69850000
O	-2.56910000	0.73930000	8.69960000
O	0.62350000	-0.21780000	5.64530000
O	3.52050000	1.16030000	6.97950000
O	3.56100000	2.02220000	11.34400000
O	-0.84880000	2.52620000	11.20970000
O	0.55610000	-1.21670000	9.26750000
C	1.64380000	6.52490000	7.93040000
C	3.52290000	4.36250000	8.49800000
C	1.53180000	4.96060000	10.40350000
C	-1.77610000	2.82950000	5.53690000
C	-1.82710000	1.31620000	8.03770000
C	0.16330000	0.71710000	6.13060000
C	2.72140000	1.41010000	7.76410000
C	2.75120000	1.93120000	10.53420000
C	-0.04190000	2.26950000	10.43530000
C	0.85830000	-0.10910000	9.22500000
Te	-1.17180000	4.58830000	8.44020000
Te	1.53140000	3.77460000	5.85480000
C	-1.79910000	6.10490000	7.03320000
H	-0.93880000	6.62490000	6.60180000
H	-2.40210000	5.64720000	6.24060000
H	-2.41570000	6.81990000	7.58890000
C	0.61860000	5.34930000	4.68920000
H	0.96500000	6.32450000	5.05030000

H	0.94580000	5.21070000	3.65290000
H	-0.47290000	5.29390000	4.73670000

Species A2
SCF Done: E(RM06) = -1501.13223991
No imaginary frequency
Zero-point correction = 0.161996 (Hartree/Particle)
Thermal correction to Energy = 0.197985
Thermal correction to Enthalpy = 0.198930
Thermal correction to Gibbs Free Energy = 0.089351
Sum of electronic and zero-point Energies = -1500.970244
Sum of electronic and thermal Energies = -1500.934255
Sum of electronic and thermal Enthalpies = -1500.933310
Sum of electronic and thermal Free Energies = -1501.042889

Coordinates: **A2**

Os	1.73330000	4.78540000	8.19760000
Os	-0.48380000	2.42990000	6.61990000
Os	1.20620000	1.93800000	9.08370000
O	2.31910000	7.59120000	7.08040000
O	4.64370000	3.98870000	8.75120000
O	1.02940000	5.54840000	11.08510000
O	-1.99500000	2.99900000	4.00140000
O	-2.83420000	1.45070000	8.33210000
O	0.56820000	-0.34870000	5.85530000
O	3.53460000	0.99040000	7.23360000
O	3.10350000	2.24930000	11.50160000
O	-1.16510000	3.01300000	10.78420000
O	0.12580000	-0.94170000	9.37070000
C	2.08200000	6.54360000	7.49090000
C	3.55100000	4.28320000	8.54780000
C	1.31710000	5.25950000	10.00850000
C	-1.43230000	2.80500000	4.98530000
C	-1.94800000	1.79470000	7.68290000
C	0.17390000	0.69130000	6.14710000
C	2.67070000	1.36220000	7.89190000
C	2.40680000	2.14450000	10.59360000
C	-0.30300000	2.65750000	10.11420000
C	0.52430000	0.12920000	9.24710000
Te	-0.95250000	5.10070000	7.39620000
Te	1.87040000	3.60560000	5.66190000
C	-2.26300000	5.19180000	9.11020000
H	-2.96820000	6.00350000	8.90270000
H	-2.80700000	4.25010000	9.23160000
H	-1.69650000	5.41620000	10.01930000
C	1.17560000	5.15440000	4.32360000

H	1.99840000	5.85980000	4.16060000
H	0.89830000	4.68550000	3.37250000
H	0.31140000	5.68730000	4.73600000

Species A3
SCF Done: E(RM06) = -1501.12131002
No imaginary frequency
Zero-point correction = 0.162783 (Hartree/Particle)
Thermal correction to Energy = 0.198370
Thermal correction to Enthalpy = 0.199314
Thermal correction to Gibbs Free Energy = 0.091308
Sum of electronic and zero-point Energies = -1500.958527
Sum of electronic and thermal Energies = -1500.922940
Sum of electronic and thermal Enthalpies = -1500.921996
Sum of electronic and thermal Free Energies = -1501.030002

Coordinates: **A3**

Os	1.75130000	4.76470000	8.15110000
Os	-0.36540000	2.49420000	6.49180000
Os	1.10440000	1.94670000	9.10090000
O	2.48010000	7.62980000	7.30290000
O	4.62080000	3.81850000	8.66320000
O	1.05710000	5.43840000	11.05960000
O	-1.90520000	2.92100000	3.86400000
O	-2.73930000	1.43630000	8.11550000
O	0.82600000	-0.22990000	5.74600000
O	3.51920000	0.85960000	7.46780000
O	2.90110000	2.23170000	11.59680000
O	-1.31890000	3.06130000	10.70350000
O	-0.05170000	-0.90900000	9.31780000
C	2.18340000	6.55630000	7.58550000
C	3.53750000	4.16820000	8.48940000
C	1.32530000	5.17230000	9.97210000
C	-1.31390000	2.80040000	4.84170000
C	-1.83610000	1.81530000	7.51000000
C	0.37580000	0.78800000	6.04040000
C	2.61870000	1.30410000	8.02490000
C	2.23680000	2.14550000	10.66220000
C	-0.43690000	2.69410000	10.06640000
C	0.36750000	0.15710000	9.21810000
Te	-0.90390000	5.16510000	7.25660000
Te	1.83830000	3.93030000	5.44730000
C	-2.29180000	5.21020000	8.91110000
H	-2.80810000	4.25140000	9.01220000
H	-1.77560000	5.45960000	9.84280000
H	-3.01260000	5.99680000	8.66440000

C	3.53100000	2.63290000	5.10380000
H	4.26700000	2.73220000	5.90670000
H	3.21020000	1.59080000	5.01730000
H	3.96580000	2.96780000	4.15630000

Species B
SCF Done: E(RM06) = -1501.12167931
No imaginary frequency
Zero-point correction = 0.161374 (Hartree/Particle)
Thermal correction to Energy = 0.197661
Thermal correction to Enthalpy = 0.198605
Thermal correction to Gibbs Free Energy = 0.087911
Sum of electronic and zero-point Energies = -1500.960305
Sum of electronic and thermal Energies = -1500.924018
Sum of electronic and thermal Enthalpies = -1500.923074
Sum of electronic and thermal Free Energies = -1501.033768

Coordinates: **B**

Os	4.42950000	8.29590000	15.23300000
Os	2.41390000	6.12190000	14.38030000
Os	2.03700000	7.53100000	11.80920000
Te	4.36180000	8.91820000	12.51020000
Te	3.75100000	5.37280000	12.06230000
O	3.96010000	7.23900000	18.09420000
O	2.04230000	10.29520000	15.46970000
O	6.60380000	10.42310000	15.81880000
O	6.40680000	5.98060000	14.55110000
O	0.20410000	4.12160000	13.71680000
O	0.51820000	7.69400000	16.20730000
O	3.77890000	4.29270000	16.45110000
O	2.36270000	8.63600000	8.94460000
O	0.24320000	9.65620000	13.10610000
O	-0.32320000	5.71560000	11.09260000
C	4.15180000	7.62000000	17.03050000
C	2.89410000	9.53530000	15.39050000
C	5.79160000	9.64730000	15.58640000
C	5.65950000	6.81500000	14.79400000
C	1.03880000	4.88850000	13.92740000
C	1.24870000	7.12830000	15.51640000
C	3.28150000	4.98970000	15.68070000
C	2.26930000	8.20330000	10.00740000
C	0.92100000	8.85810000	12.62440000
C	0.55870000	6.39860000	11.37760000
C	2.66580000	3.64670000	11.34940000
H	3.08460000	3.36980000	10.37630000

H	2.81720000	2.83000000	12.06340000
H	1.59750000	3.85790000	11.24770000
C	3.74650000	10.98370000	12.54230000
H	4.50720000	11.56640000	13.07530000
H	3.68320000	11.32260000	11.50210000
H	2.77170000	11.09970000	13.02710000

Species TSBC
SCF Done: E(RM06) = -1501.08269217
One imaginary frequency (41*i*)
Zero-point correction= 0.161017 (Hartree/Particle)
Thermal correction to Energy= 0.196638
Thermal correction to Enthalpy= 0.197583
Thermal correction to Gibbs Free Energy= 0.088536
Sum of electronic and zero-point Energies= -1500.921675
Sum of electronic and thermal Energies= -1500.886054
Sum of electronic and thermal Enthalpies= -1500.885110
Sum of electronic and thermal Free Energies= -1500.994156

Coordinates: **TSBC**

Os	1.48230000	4.61430000	8.55810000
Os	0.43730000	2.18210000	6.34670000
Os	-0.35110000	2.68150000	9.34480000
O	2.85320000	7.00380000	7.11890000
O	4.00710000	3.02780000	9.29260000
O	1.62490000	6.00770000	11.22850000
O	-2.65180000	2.60940000	6.18670000
O	0.24160000	-0.62280000	7.61480000
O	0.43660000	0.98460000	3.50710000
O	3.55780000	2.34290000	6.26310000
O	1.83720000	0.69560000	10.16450000
O	-0.79720000	3.55000000	12.22830000
O	-2.82200000	0.81550000	9.18830000
C	2.31480000	6.10150000	7.57950000
C	3.05860000	3.59750000	8.98030000
C	1.58340000	5.48110000	10.20300000
C	-1.52410000	2.45750000	6.30410000
C	0.31400000	0.45070000	7.21640000
C	0.46040000	1.46090000	4.54840000
C	2.42170000	2.29800000	6.40000000
C	1.01540000	1.43530000	9.84060000
C	-0.62820000	3.21190000	11.13890000
C	-1.92090000	1.52880000	9.23700000
Te	-1.23630000	5.14330000	8.42190000
Te	0.58620000	4.75100000	5.10460000
C	-1.59410000	6.35490000	10.17720000

H	-1.22930000	5.86520000	11.08510000
H	-1.08630000	7.31660000	10.04440000
H	-2.67440000	6.51810000	10.25400000
C	1.64180000	4.14890000	3.30970000
H	1.90730000	5.07080000	2.77950000
H	2.56300000	3.61300000	3.56570000
H	1.00740000	3.53160000	2.66510000

Species C
SCF Done: E(RM06) = -1501.08546118
No imaginary frequency
Zero-point correction = 0.161236 (Hartree/Particle)
Thermal correction to Energy = 0.197637
Thermal correction to Enthalpy = 0.198581
Thermal correction to Gibbs Free Energy = 0.086523
Sum of electronic and zero-point Energies = -1500.924225
Sum of electronic and thermal Energies = -1500.887824
Sum of electronic and thermal Enthalpies = -1500.886880
Sum of electronic and thermal Free Energies = -1500.998938

Coordinates: **C**

Os	1.68030000	4.38250000	8.75570000
Os	0.94950000	2.35920000	6.39750000
Os	-0.46310000	2.75070000	9.28070000
O	3.49150000	6.45380000	7.31260000
O	3.83210000	2.41600000	9.71390000
O	1.69970000	5.86800000	11.40230000
O	-2.12230000	2.57700000	5.87240000
O	1.04730000	-0.41390000	7.74580000
O	1.30500000	0.99010000	3.66030000
O	4.02880000	2.88820000	6.39220000
O	1.24920000	0.62760000	10.69630000
O	-1.44280000	3.73710000	11.97500000
O	-3.02870000	1.10940000	8.69830000
C	2.79890000	5.67870000	7.79890000
C	3.02350000	3.14770000	9.34570000
C	1.71440000	5.32120000	10.38770000
C	-1.01820000	2.49220000	6.16460000
C	0.99700000	0.65600000	7.33410000
C	1.16680000	1.52130000	4.66410000
C	2.89950000	2.72840000	6.49780000
C	0.62890000	1.40410000	10.11800000
C	-1.08770000	3.34310000	10.95230000
C	-2.08940000	1.73800000	8.90440000
Te	-0.89720000	5.28090000	8.24050000
Te	0.90740000	4.82120000	4.96340000

C	-1.46170000	6.42780000	9.99020000
H	-0.81000000	6.22820000	10.84600000
H	-1.40580000	7.48910000	9.72430000
H	-2.49570000	6.17250000	10.24890000
C	0.33300000	4.08070000	3.01080000
H	0.10800000	4.96560000	2.40370000
H	1.14210000	3.51940000	2.53300000
H	-0.57330000	3.46710000	3.07890000

Species TSCD
SCF Done: E(RM06) = -1501.07830268
One imaginary frequency (50*i*)
Zero-point correction = 0.161274 (Hartree/Particle)
Thermal correction to Energy = 0.196764
Thermal correction to Enthalpy = 0.197708
Thermal correction to Gibbs Free Energy = 0.088853
Sum of electronic and zero-point Energies = -1500.917029
Sum of electronic and thermal Energies = -1500.881539
Sum of electronic and thermal Enthalpies = -1500.880595
Sum of electronic and thermal Free Energies = -1500.989449

Coordinates: **TSCD**

Os	1.75680000	4.46480000	8.74380000
Os	0.99390000	2.03720000	6.39310000
Os	-0.39400000	2.76490000	9.11300000
O	3.43020000	6.86740000	7.69800000
O	4.00750000	2.72370000	9.89870000
O	1.40140000	5.62370000	11.50380000
O	-1.88030000	2.94090000	5.56660000
O	-0.02450000	-0.66270000	7.47390000
O	1.57550000	0.97560000	3.55560000
O	3.97500000	1.49740000	7.14700000
O	1.43840000	0.59880000	10.28210000
O	-1.38070000	3.69930000	11.84180000
O	-2.95280000	1.16550000	8.41640000
C	2.81470000	5.95420000	8.01860000
C	3.17340000	3.34800000	9.41290000
C	1.55730000	5.18820000	10.44670000
C	-0.84210000	2.63280000	5.94000000
C	0.34810000	0.36600000	7.13040000
C	1.38190000	1.37660000	4.61000000
C	2.87280000	1.72670000	6.94740000
C	0.73830000	1.39990000	9.83850000
C	-1.01270000	3.34420000	10.80930000
C	-2.01260000	1.77810000	8.67110000
Te	-0.78660000	5.29210000	8.03880000

Te	1.95900000	4.47930000	5.18460000
C	-1.52920000	6.44760000	9.70930000
H	-2.53060000	6.08400000	9.96420000
H	-0.87500000	6.36390000	10.58240000
H	-1.58860000	7.49420000	9.39200000
C	0.48170000	4.54030000	3.60090000
H	0.81190000	5.32140000	2.90640000
H	0.43220000	3.58530000	3.06510000
H	-0.50420000	4.80900000	3.99540000

Species D
SCF Done: E(RM06) = -1501.11916260
No imaginary frequency
Zero-point correction = 0.161908 (Hartree/Particle)
Thermal correction to Energy = 0.197841
Thermal correction to Enthalpy = 0.198785
Thermal correction to Gibbs Free Energy = 0.089291
Sum of electronic and zero-point Energies = -1500.957255
Sum of electronic and thermal Energies = -1500.921322
Sum of electronic and thermal Enthalpies = -1500.920378
Sum of electronic and thermal Free Energies = -1501.029872

Coordinates: **D**

Os	1.72400000	5.05870000	8.34480000
Os	0.76290000	1.43490000	6.28460000
Os	0.00600000	2.73050000	8.98280000
O	2.86570000	7.63950000	7.09450000
O	4.22090000	3.49750000	9.22700000
O	1.30150000	6.30490000	11.11060000
O	-2.02180000	2.62860000	5.55540000
O	-0.48930000	-1.14030000	7.43420000
O	1.36290000	0.41090000	3.42290000
O	3.58620000	0.77580000	7.45300000
O	2.01620000	0.70800000	10.11260000
O	-0.49990000	3.85170000	11.77690000
O	-2.55330000	1.01680000	8.95260000
C	2.41710000	6.68500000	7.55700000
C	3.28940000	4.08420000	8.88890000
C	1.46150000	5.81860000	10.07960000
C	-1.00120000	2.20670000	5.86720000
C	-0.03600000	-0.17910000	7.00550000
C	1.16620000	0.80590000	4.48120000
C	2.53670000	0.99630000	7.05570000
C	1.27690000	1.46590000	9.65520000
C	-0.29570000	3.46250000	10.71110000
C	-1.58600000	1.64200000	8.94330000

Te	-0.98400000	5.06580000	7.86910000
Te	2.05930000	3.87480000	5.83270000
C	-1.87800000	6.14490000	9.51020000
H	-2.88500000	5.74430000	9.66880000
H	-1.29200000	6.04780000	10.42860000
H	-1.94320000	7.19950000	9.22170000
C	0.71840000	4.92470000	4.51310000
H	1.08430000	5.95500000	4.42880000
H	0.75310000	4.43570000	3.53290000
H	-0.30750000	4.93030000	4.89540000

Species TSDA2
SCF Done: E(RM06) = -1501.08508025
One imaginary frequency (85*i*)
Zero-point correction = 0.162260 (Hartree/Particle)
Thermal correction to Energy = 0.196812
Thermal correction to Enthalpy = 0.197756
Thermal correction to Gibbs Free Energy = 0.092589
Sum of electronic and zero-point Energies = -1500.922820
Sum of electronic and thermal Energies = -1500.888269
Sum of electronic and thermal Enthalpies = -1500.887325
Sum of electronic and thermal Free Energies = -1500.992491

Coordinates: **TSDA2**

Os	1.79530000	4.89470000	8.27740000
Os	-0.08700000	1.97030000	6.20030000
Os	0.51810000	2.40730000	9.28840000
O	2.30920000	7.61450000	6.91960000
O	4.69700000	4.11550000	8.94740000
O	1.19010000	6.08110000	11.03510000
O	-1.67030000	3.24910000	3.83430000
O	-2.37210000	0.17520000	7.20070000
O	1.20750000	-0.26250000	4.57320000
O	2.40160000	0.69640000	7.58120000
O	3.11490000	1.98690000	10.83120000
O	-0.81830000	3.65770000	11.82820000
O	-0.79830000	-0.26590000	10.06790000
C	2.11420000	6.59310000	7.41140000
C	3.61170000	4.40150000	8.70640000
C	1.42350000	5.62120000	10.00630000
C	-1.14830000	2.82350000	4.76350000
C	-1.51300000	0.83640000	6.82250000
C	0.71530000	0.56990000	5.18910000
C	1.43220000	1.36390000	7.73710000
C	2.14210000	2.17910000	10.24940000
C	-0.40310000	3.29840000	10.81900000

C	-0.35240000	0.74570000	9.75290000
Te	-0.83480000	4.56080000	7.56320000
Te	2.14760000	3.62320000	5.76050000
C	-2.18410000	5.09210000	9.18070000
H	-2.72760000	4.20390000	9.51640000
H	-1.62500000	5.53660000	10.01000000
H	-2.88610000	5.82460000	8.76580000
C	1.40520000	5.17020000	4.44920000
H	2.15610000	5.96690000	4.39890000
H	1.25850000	4.74070000	3.45180000
H	0.45990000	5.57900000	4.82380000

Species TSA2A1
SCF Done: E(RM06) = -1501.09557026
One imaginary frequency (185*i*)
Zero-point correction = 0.161181 (Hartree/Particle)
Thermal correction to Energy = 0.196814
Thermal correction to Enthalpy = 0.197758
Thermal correction to Gibbs Free Energy = 0.088705
Sum of electronic and zero-point Energies = -1500.934389
Sum of electronic and thermal Energies = -1500.898756
Sum of electronic and thermal Enthalpies = -1500.897812
Sum of electronic and thermal Free Energies = -1501.006866

Coordinates: **TSA2A1**

Os	1.79530000	4.89470000	8.27740000
Os	-0.08700000	1.97030000	6.20030000
Os	0.51810000	2.40730000	9.28840000
O	2.30920000	7.61450000	6.91960000
O	4.69700000	4.11550000	8.94740000
O	1.19010000	6.08110000	11.03510000
O	-1.67030000	3.24910000	3.83430000
O	-2.37210000	0.17520000	7.20070000
O	1.20750000	-0.26250000	4.57320000
O	2.40160000	0.69640000	7.58120000
O	3.11490000	1.98690000	10.83120000
O	-0.81830000	3.65770000	11.82820000
O	-0.79830000	-0.26590000	10.06790000
C	2.11420000	6.59310000	7.41140000
C	3.61170000	4.40150000	8.70640000
C	1.42350000	5.62120000	10.00630000
C	-1.14830000	2.82350000	4.76350000
C	-1.51300000	0.83640000	6.82250000
C	0.71530000	0.56990000	5.18910000
C	1.43220000	1.36390000	7.73710000
C	2.14210000	2.17910000	10.24940000

C	-0.40310000	3.29840000	10.81900000
C	-0.35240000	0.74570000	9.75290000
Te	-0.83480000	4.56080000	7.56320000
Te	2.14760000	3.62320000	5.76050000
C	-2.18410000	5.09210000	9.18070000
H	-2.72760000	4.20390000	9.51640000
H	-1.62500000	5.53660000	10.01000000
H	-2.88610000	5.82460000	8.76580000
C	1.40520000	5.17020000	4.44920000
H	2.15610000	5.96690000	4.39890000
H	1.25850000	4.74070000	3.45180000
H	0.45990000	5.57900000	4.82380000

Species TSBA3
SCF Done: E(RM06) = -1501.07435777
One imaginary frequency (86*i*)
Zero-point correction = 0.160641 (Hartree/Particle)
Thermal correction to Energy = 0.196071
Thermal correction to Enthalpy = 0.197015
Thermal correction to Gibbs Free Energy = 0.088614
Sum of electronic and zero-point Energies = -1500.913717
Sum of electronic and thermal Energies = -1500.878287
Sum of electronic and thermal Enthalpies = -1500.877343
Sum of electronic and thermal Free Energies = -1500.985744

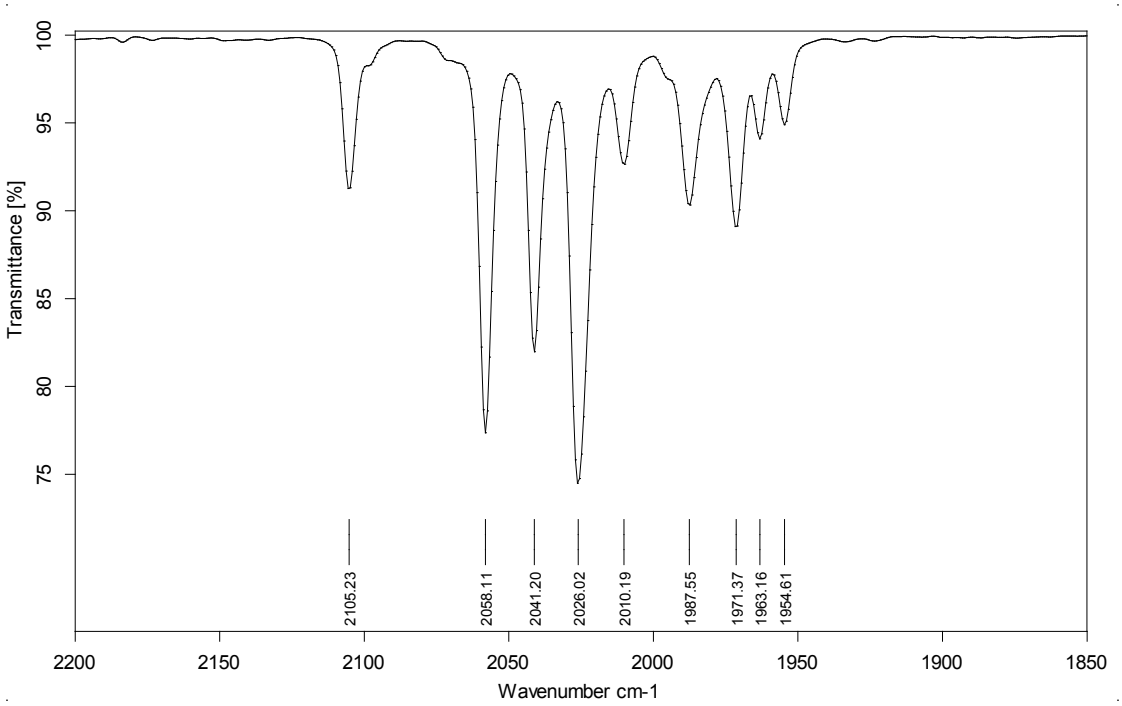
Coordinates: **TSBA3**

Os	1.57070000	5.15770000	8.53620000
Os	-0.43590000	2.41620000	6.37840000
Os	1.51770000	1.97320000	8.58700000
O	2.26700000	7.61440000	6.73070000
O	4.38990000	4.82730000	9.71980000
O	0.48700000	6.82600000	10.84660000
O	-1.78390000	3.27810000	3.73940000
O	-2.93560000	1.33240000	7.79990000
O	0.50100000	-0.27890000	5.26470000
O	2.92680000	-0.47430000	7.24570000
O	3.60100000	1.69560000	10.83910000
O	0.13090000	3.57270000	10.78980000
O	-0.61530000	0.18230000	9.82260000
C	2.02880000	6.66370000	7.32440000
C	3.33690000	4.96300000	9.28330000
C	0.91740000	6.20620000	9.98300000
C	-1.27950000	2.98450000	4.72860000
C	-1.98810000	1.71620000	7.27420000
C	0.14810000	0.72550000	5.70100000
C	2.43790000	0.50330000	7.60240000

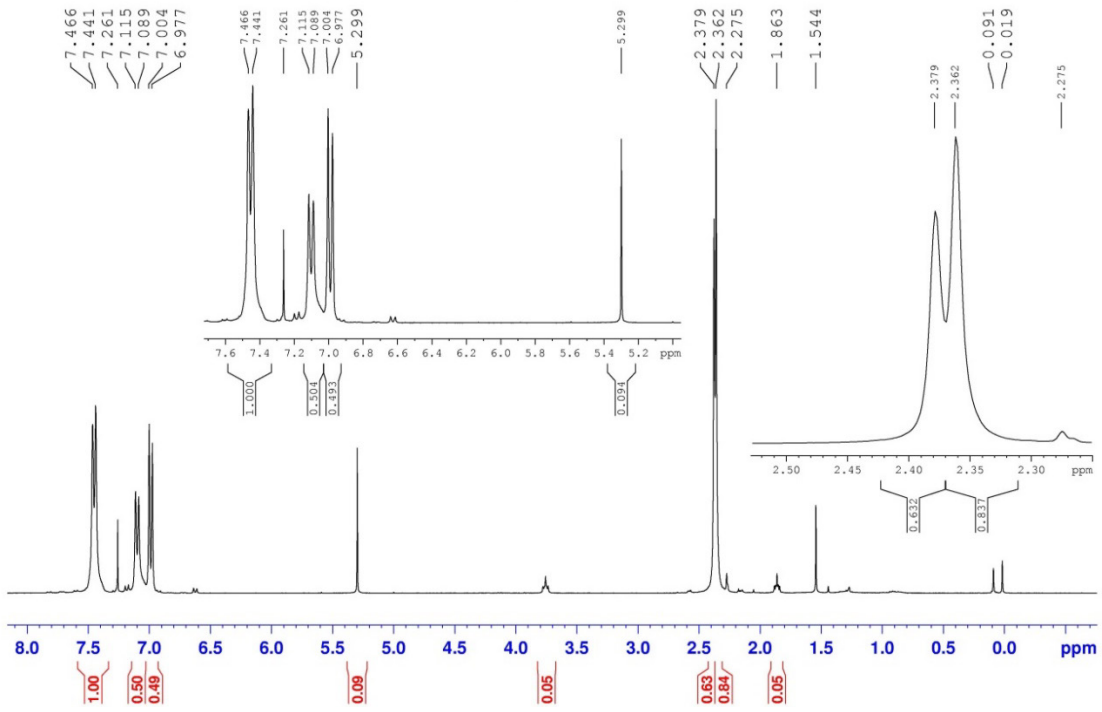
C	2.85630000	1.83140000	9.97380000
C	0.73780000	3.48510000	9.77290000
C	0.16810000	0.85100000	9.30780000
Te	-1.02440000	4.98310000	7.44790000
Te	1.99000000	3.66770000	5.98120000
C	-2.28120000	4.55170000	9.15060000
H	-2.00900000	3.59550000	9.60590000
H	-2.15990000	5.35640000	9.88450000
H	-3.31400000	4.52680000	8.78600000
C	3.50680000	2.23270000	5.38250000
H	3.03980000	1.26550000	5.17170000
H	3.96900000	2.63690000	4.47450000
H	4.25550000	2.13290000	6.17380000

IR and ^{1}H NMR spectra of **3-Tol-*p***

IR spectrum (cyclohexane)

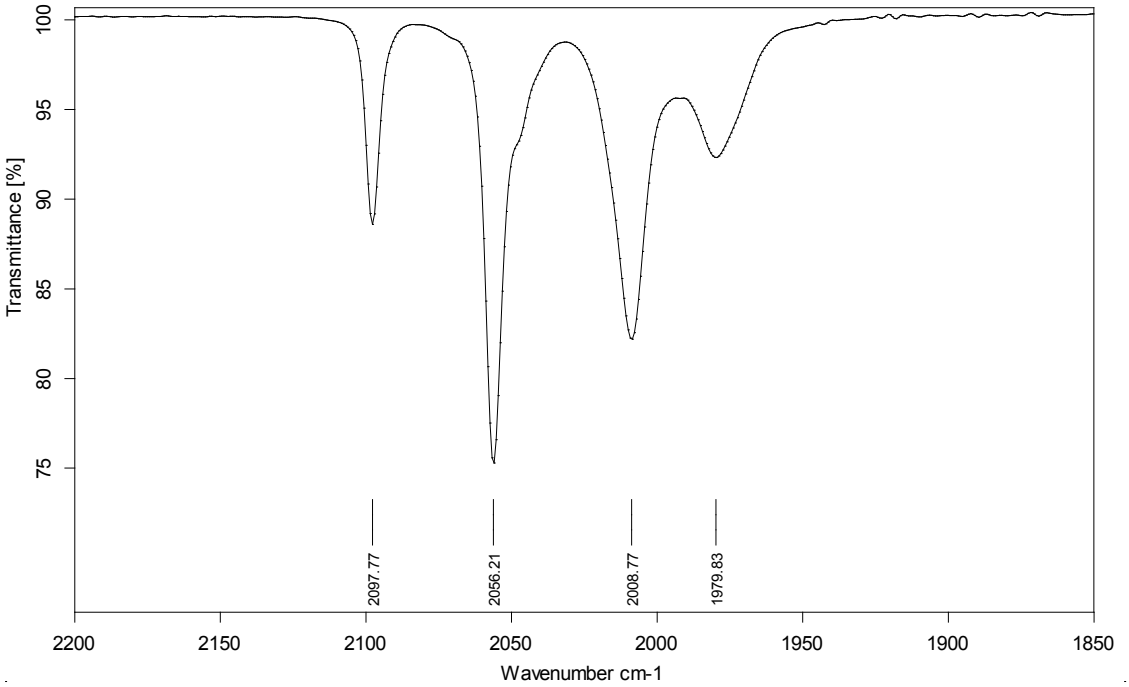


^{1}H NMR spectrum ($CDCl_3$)

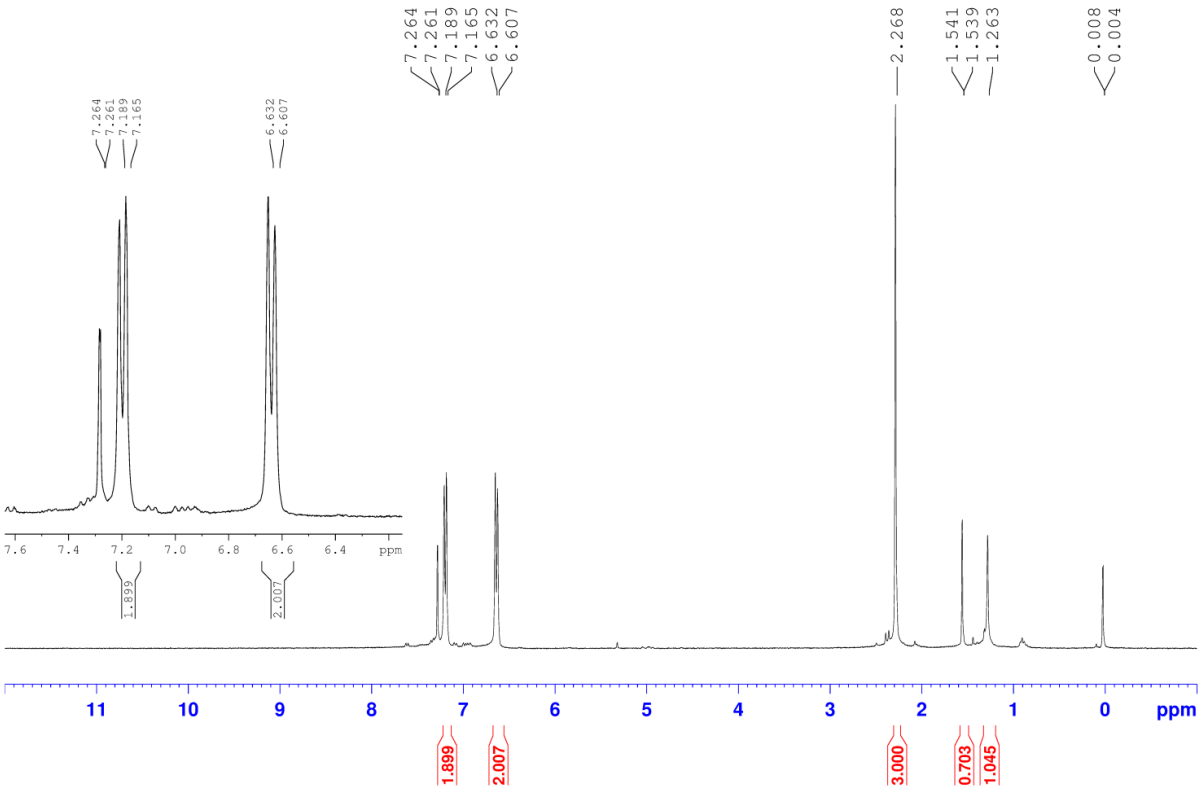


IR and ^{1}H NMR spectra of **4-Tol-*p***

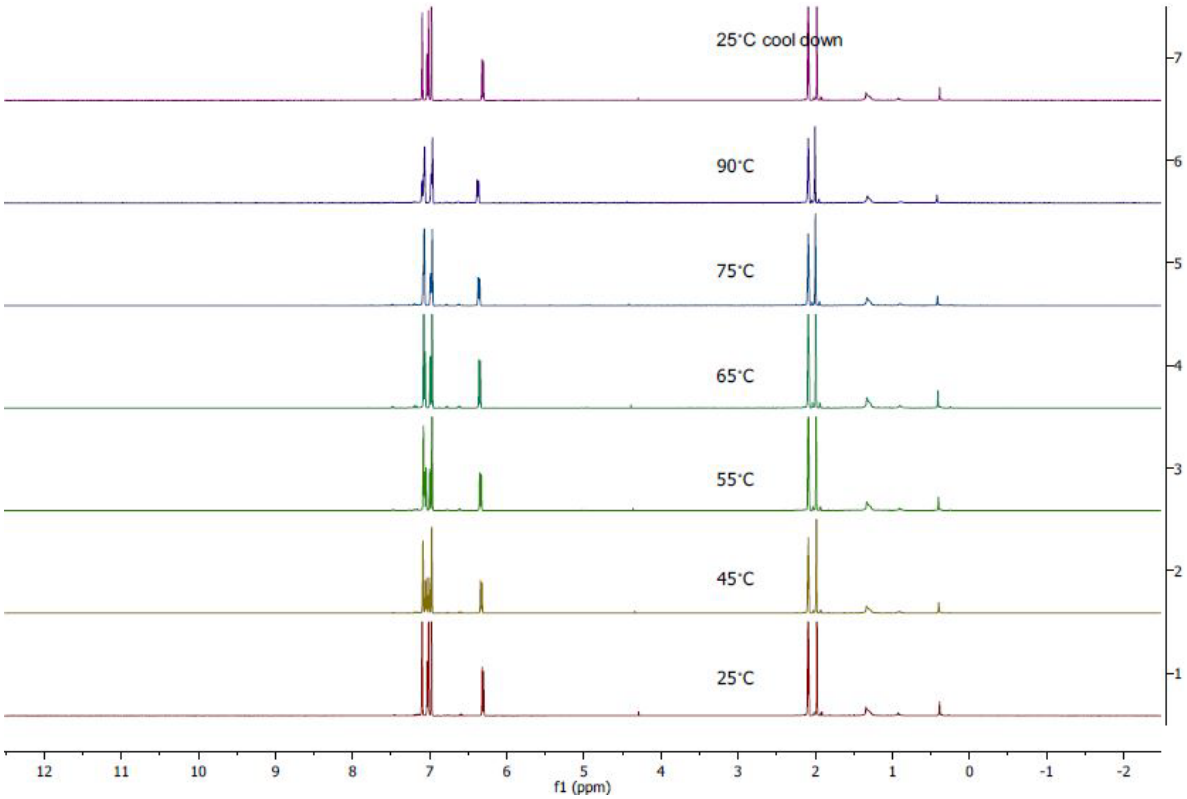
IR spectrum (hexane)



^{1}H NMR spectrum ($CDCl_3$)



Variable-temperature ^{1}H NMR spectrum of **4-Tol-*p*** from 25˚C to 90˚C in toluene-d_8



Methyl region only.