Kinetic Studies on the Thermal *Cis-to-Trans* Isomerization of 1-Phenyltriazenes Derived from Cyclic Amines

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1. Full citation for reference 20: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A. Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, Revision C.02; Gaussian, Inc.: Wallingford CT, 2004.

2. General synthesis method.

The appropriate aromatic amine (3 mmol), dissolved in 1 N HCl (9 mL, 9 mmol), was diazotized at *ca.* 0 °C by slowly adding to it a (pre-chilled) 0.2 M NaNO₂ solution (1.5 mL, 3 mmol) under constant stirring on an ice bath. The resulting aryldiazonium ion mixture was then slowly added to a cyclic amine solution, prepared by mixing appropriate cyclic amine (3.3 mmol) and 1 N NaOH (3 mL, 3 mmol), on an ice bath under constant stirring and maintaining the pH of the reaction mixture at *ca.* 8-9 with 1 N NaOH. Once the coupling reaction was completed, the product was filtered out and purified by recrystallization from petroleum ether (unless indicated otherwise).

3. Analytical data for known triazenes.

N-(4-Methoxyphenylazo)pyrrolidine (**1b**). Crude product was purified by recrystallization from ethanol to afford light brown needles; mp 54-56 °C (lit.¹ 55.5-57 °C); ¹H NMR (300 MHz, DMSO-*d*₆) δ 7.28-7.26, 6.90-6.88 (AA'XX', 4H), 3.75 (s, 3H), 3.68 (br, 4H), 1.96 (m, 4H).

N-(4-Methoxyphenylazo)piperidine (**1c**). Brown solid; mp 32-33.5 °C (lit.² 29-31 °C); ¹H NMR (300 MHz, CDCl₃) δ 7.38-7.36, 6.87-6.85 (AA'XX', 4H), 3.78 (s, 3H), 3.69 (m, 4H), 1.67 (m, 6H).

N-(4-Methoxyphenylazo)morpholine (**1d**). Shiny beige flakes; mp 69-70 °C (lit.³ 69-70 °C); ¹H NMR (300 MHz, CDCl₃) δ 7.41-7.38, 6.88-6.85 (AA'XX', 4H), 3.84 (t, *J* = 4.9 Hz, 4H), 3.80 (s, 3H), 3.70 (t, *J* = 4.9 Hz, 4H).

N-(4-Methylphenylazo)pyrrolidine (**2b**). Crude product was purified by recrystallization (ethanol) to afford pale yellow crystals; mp 79-80 °C (lit.¹ 78.5-80 °C); ¹H NMR (300 MHz, CDCl₃) δ 7.30-7.27, 7.12-7.09 (AA'BB', 4H), 3.76 (br, 4H), 2.31 (s, 3H), 2.00 (m, 4H).

N-(Phenylazo)pyrrolidine (**3b**). Golden yellow crystals; mp 52-53 °C (lit.¹ 51-53 °C); ¹H NMR (300 MHz, DMSO-*d*₆) δ 7.37 (d, *J* = 6.9 Hz, 2H), 7.30 (t, *J* = 6.9 Hz, 2H), 7.10 (t, *J* = 6.9 Hz, 1H), 3.77 (br, 4H), 1.96 (m, 4H).

(1) Foster, N. I.; Heindel, N. D.; Burns, H. D.; Muhr, W. *Synthesis*, **1980**, 7, 572.

(2) Patrick, T. B.; Willaredt, R. P.; DeGonia, D. J. *J. Org. Chem.*, **1985**, 50, 2232.

N-(Phenylazo)piperidine (**3c**). Brown solid; mp 43-44 °C (lit.⁴ 38-40 °C); ¹H NMR (300 MHz, CDCl₃) δ 7.41 (d, *J* = 7.6 Hz, 2H), 7.31 (t, *J* = 7.6 Hz, 2H), 7.13 (t, *J* = 7.6 Hz, 1H), 3.75 (m, 4H), 1.70 (m, 6H).

N-(Phenylazo)morpholine (**3d**). Bright yellow granules; mp 26-27 °C (lit.³ 29-30 °C); ¹H NMR (300 MHz, CDCl₃) δ 7.43 (d, *J* = 7.5 Hz, 2H), 7.33 (t, *J* = 7.5 Hz, 2H), 7.18 (t, *J* = 7.5 Hz, 1H), 3.84 (t, *J* = 4.8 Hz, 4H), 3.76 (t, *J* = 4.8 Hz, 4H).

N-(Phenylazo)perhydroazepine (**3e**). Product was isolated from reaction medium by solvent extraction (with diethyl ether) to afford a viscous dark-brown oil (mp lit.⁴ 19-21 °C); ¹H NMR (300 MHz, CDCl₃) δ 7.39 (d, *J* = 7.6 Hz, 2H), 7.30 (t, *J* = 7.6 Hz, 2H), 7.10 (t, *J* = 7.6 Hz, 1H), 3.96 (br, 2H), 3.78 (br, 2H), 1.81 (m, 4H), 1.60 (br, 4H).

4. UV-visible absorption spectra for compounds synthesized.⁵

(3) Henry, R. A., Dehn, W. M. *J. Am. Chem. Soc.* **1943**, 65, 479.

(4) Ludwig, M., Bednářová, I., Pařík, P. *Collect. Czech. Chem. Commun.* **1999**, 64, 1654.

(5) Spectra for *trans* forms dissolved in MeCN. Spectra for *cis*-isomers (transient species) are not available.

N-(4-Methoxyphenylazo)piperidine (**1c**)

N-(4-Methoxyphenylazo)morpholine (**1d**)

N-(4-Methoxyphenylazo)perhydroazepine (**1e**)

N-(4-Methylphenylazo)pyrrolidine (**2b**)

N-(Phenylazo)azetidine (**3a**)

N-(Phenylazo)pyrrolidine (**3b**)

N-(Phenylazo)piperidine (**3c**)

N-(Phenylazo)morpholine (**3d**)

N-(Phenylazo)perhydroazepine (**3e**)

N-(4-Chlorophenylazo)azetidine (**4a**)

N-(4-Trifluoromethylphenylazo)azetidine (**5a**)

N-(4-Trifluoromethylphenylazo)pyrrolidine (**5b**)

5. ^1H and ^{13}C NMR spectra for new compounds

N-(4-Methoxyphenylazo)azetidine (**1a**)

N-(4-Methoxyphenylazo)perhydroazepine (**1e**)

N-(Phenylazo)azetidine (**3a**)

N-(4-Chlorophenylazo)azetidine (**4a**)

Fc1ccc(cc1)/N=N/N2CCN2

N-(4-Trifluoromethylphenylazo)pyrrolidine (**5b**)

Table S1. Percent photolytic decomposition for compounds **1-2**

Solvent	Percent decomposition ^a					
	1a	1b	1c	1d	1e	2b
c-HexH	(31)	14 (9)	24 (18)	(33)	(3)	6
PhH	> 30	12 (10)	12 (8)	24 (23)	3	2
MeCN	(6)	5	4 (6)	(6)	(1)	0.9
DMF	2	(1)	(1)	(5)	(1)	1
DMSO	(11)	4 (2)	5 (2)	(5)	(0.2)	0.9
MeOH	45	(12)	(21)	(43)		2
2-PrOH	43	(23)	(25)	(47)		4
1-BuOH	48	(29)	(26)	(49)		5
1-OctOH	48	(27)	63	(67)		19

^a Relative errors are typically ± 10 %. Values correspond to solutions having an absorbance of 0.5 (7×7 mm² cell) @ 350 nm (before irradiation), except for those given in brackets which correspond to solutions having a triazene concentration of 1.05×10^{-4} M. In all cases, observed rate constants for *cis*-to-*trans* isomerization are independent of triazene concentration.

Table S3. Percent photolytic decomposition for compounds **3-5**

Solvent	Percent decomposition ^a							
	3a	3b	3c	3d	3e	4a	5a	5b
c-HexH	16	0.9 (2)	0.7 (1)	4 (6)	0	2	0.2	0.2
PhH	1	0.9 (2)	0.2 (0)	1 (3)		2	0.2	
MeCN	0.4	0.9 (0.8)	< 0.1 (< 0.1)	0.5 (1)	0	0.6	0.1	1
DMF	0.2	0.3 (0.6)	(0.2)	(0.9)		0.3	0.2	
DMSO	2	0.5 (0.3)	< 0.1 (0)	0.4 (0.5)		0.6	0	
MeOH	14	0.5	0.7	1		9	0.1	0.1
2-PrOH	5	0.5	0.2	0.7		1	0.3	
1-BuOH	10	0.7	0.2	2			0.4	
1-OctOH	11	4	0	11		4	0.4	

^a Relative errors are typically ± 10 %. Values correspond to solutions having an absorbance of 0.5 (7×7 mm² cell) @ 350 nm (before irradiation), except for those given in brackets which correspond to solutions having a triazene concentration of 1.05×10^{-4} M. In all cases, observed rate constants for *cis*-to-*trans* isomerization are independent of triazene concentration.

Figure S1. Potential energy curves for the rotation (filled circles) and inversion (open circles) pathways for *cis*-to-*trans* isomerization of **3b**.

The potential energy curve for rotation was obtained by relax scanning of the C-N=N-N torsional angle, from 12° to 182° at a 10° interval. The transition state structure found is fully consistent with that obtained using the QST2 option. The potential energy curve for inversion was obtained by relaxed scanning of the C-N=N bending angle, from 116° to 255° at 2° interval. Attempts to obtain a similar curve by relaxed scanning of the N=N-N bending angle were unsuccessful. Nonetheless, inversion is expected to involve N(1) rather than N(2), since the later would be hindered by the so-called hetero effect (see: Kessler, H. *Angew. Chem., Int. Ed. Engl.* **1970** *9*, 219).

8. Calculated geometries (coordinates), imaginary frequencies (where applicable) and energies of all stationary points

cis-1a

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	-2.383022	1.343348	0.332518
7	-1.216721	1.790288	0.194521
6	-0.038717	0.986457	0.165058
6	0.230792	-0.049373	1.081299
6	0.988942	1.404289	-0.689341
6	1.480727	-0.653029	1.114657
1	-0.537991	-0.361653	1.780599
6	2.234668	0.778201	-0.687229
1	0.797222	2.235164	-1.361977
6	2.488289	-0.256513	0.222602
1	1.701982	-1.441905	1.827184
1	2.999461	1.115645	-1.377440
6	-4.058106	-0.377186	0.065087
6	-2.128700	-1.002079	-0.655292
6	-3.550287	-1.610595	-0.723819
1	-4.581616	0.365727	-0.547494
1	-4.635626	-0.567622	0.975479
1	-1.792155	-0.530305	-1.586288
1	-1.324920	-1.632329	-0.266524
1	-3.965287	-1.735053	-1.726100
1	-3.643578	-2.550869	-0.175694
7	-2.652293	0.005185	0.318720
8	3.671727	-0.930169	0.327301
6	4.735285	-0.555069	-0.532624
1	4.471865	-0.699019	-1.589099
1	5.032429	0.490374	-0.375646
1	5.571301	-1.209169	-0.278111

E = -628.25416898; ZPE = 0.223238

Number of imaginary freq = 0

trans-1a

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	1.891745	0.533740	-0.209966
7	1.117834	-0.467501	-0.243363
6	-0.257215	-0.143634	-0.153872
6	-0.789416	1.160947	-0.131259
6	-1.138152	-1.226898	-0.090824
6	-2.156836	1.358241	-0.039333
1	-0.114712	2.008029	-0.188088
6	-2.518158	-1.038138	0.004127
1	-0.721873	-2.229633	-0.114559
6	-3.034333	0.261715	0.031062
1	-2.580067	2.358163	-0.022867
1	-3.171203	-1.901927	0.053486
6	4.261806	0.991662	0.256926
6	3.792711	-1.099125	-0.018023
6	5.081656	-0.324998	0.370107
1	3.975807	1.424008	1.223577
1	4.665002	1.779588	-0.387896
1	3.272268	-1.582647	0.818364
1	3.851229	-1.802192	-0.853923
1	5.484866	-0.543835	1.360580
1	5.879712	-0.405648	-0.371271
7	3.180777	0.202870	-0.356208
8	-4.361543	0.573114	0.119869
6	-5.294972	-0.491207	0.194969
1	-5.257655	-1.126372	-0.700309
1	-5.127094	-1.114167	1.083818
1	-6.278979	-0.023430	0.263611

E = -628.27317003; ZPE = 0.223466

Number of imaginary freq = 0

ts-1a

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	2.026178	0.112834	-0.903927
7	1.013215	0.854891	-0.750690
6	-0.214654	0.416478	-0.363738
6	-0.578150	-0.942746	-0.289859
6	-1.221251	1.382674	-0.245874
6	-1.901431	-1.307888	-0.081413
1	0.179065	-1.709213	-0.419163
6	-2.546024	1.024797	0.000549
1	-0.949491	2.428880	-0.351461
6	-2.894132	-0.329888	0.080540
1	-2.193018	-2.352897	-0.037736
1	-3.294769	1.801561	0.106317
6	4.005005	-1.028839	-0.234008
6	3.734632	0.838914	0.800613
6	4.884941	-0.194442	0.730898
1	4.297150	-0.955868	-1.287842
1	3.836846	-2.079644	0.023170
1	3.900596	1.743063	0.202652
1	3.372718	1.129694	1.789998
1	5.826594	0.171090	0.316220
1	5.079111	-0.688403	1.685655
7	2.863334	-0.145410	0.086907
8	-4.157852	-0.798548	0.301152
6	-5.206849	0.144582	0.447572
1	-5.042430	0.802269	1.311669
1	-5.326319	0.759477	-0.454380
1	-6.114845	-0.439680	0.607971

E = -628.21238314; ZPE = 0.221054

Number of imaginary freq = 1 (-621.559 Hz)

cis-1b

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	2.006538	1.551740	0.178648
7	0.825644	1.885422	-0.092226
6	-0.324251	1.051169	0.003865
6	-0.600168	0.233100	1.117542
6	-1.331841	1.236189	-0.950495
6	-1.834209	-0.390417	1.246942
1	0.151355	0.107072	1.890682
6	-2.560657	0.585129	-0.845199
1	-1.139446	1.903849	-1.785269
6	-2.819975	-0.233302	0.261426
1	-2.058684	-1.011181	2.109120
1	-3.308716	0.738469	-1.614722
6	1.851324	-0.880824	-0.405773
6	3.833338	0.107004	0.593757
6	3.066861	-1.804630	-0.611301
1	1.472672	-0.485049	-1.356512
1	1.019477	-1.385560	0.092941
6	4.276481	-0.862327	-0.506505
1	4.032225	-0.312453	1.589406
1	4.286261	1.099170	0.541591
1	3.105690	-2.555571	0.186938
1	3.011975	-2.338900	-1.564890
1	5.209120	-1.383497	-0.269346
1	4.419422	-0.317797	-1.447878
7	2.377210	0.249440	0.400197
8	-3.989127	-0.907473	0.477118
6	-5.027218	-0.768880	-0.478680
1	-5.854855	-1.379647	-0.113070
1	-5.358885	0.274278	-0.567754
10	-4.718450	-1.132886	-1.467991

E = -667.59346250; ZPE = 0.253187

Number of imaginary freq = 0

trans-1b

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	-1.500596	0.509691	-0.105808
7	-0.725311	-0.498831	-0.068067
6	0.648843	-0.162529	-0.045613
6	1.174883	1.144963	-0.067177
6	1.542052	-1.237179	0.002888
6	2.544110	1.352940	-0.039606
1	0.493822	1.987944	-0.105370
6	2.923844	-1.037656	0.031536
1	1.133699	-2.243422	0.018658
6	3.432267	0.264911	0.010614
1	2.959288	2.356384	-0.055689
1	3.583961	-1.896787	0.069642
6	-3.318990	-1.167845	-0.030145
6	-3.801520	1.240124	-0.089756
6	-4.837869	-0.940540	-0.115311
1	-3.003012	-1.623891	0.918586
1	-2.917479	-1.793816	-0.834047
6	-5.034099	0.487652	0.433892
1	-3.979511	1.648717	-1.096051
1	-3.477526	2.061539	0.555840
1	-5.164943	-0.988400	-1.160847
1	-5.402238	-1.693081	0.443050
1	-5.973619	0.946128	0.111907
1	-5.022737	0.474514	1.530213
7	-2.785012	0.192503	-0.124173
8	4.761624	0.586812	0.035669
6	5.702864	-0.470623	0.090426
1	5.579250	-1.076548	0.998371
1	5.629406	-1.125165	-0.788791
1	6.686767	0.002526	0.105019

E = -667.61744102; ZPE = 0.253319

Number of imaginary freq = 0

ts-1b

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	1.804781	-1.284885	0.450665
7	0.737688	-0.801438	0.945838
6	-0.519255	-0.552360	0.490498
6	-0.886535	-0.794309	-0.858667
6	-1.502415	-0.039069	1.370317
6	-2.184835	-0.532577	-1.288566
1	-0.146296	-1.198332	-1.543770
6	-2.788615	0.217493	0.912869
1	-1.231885	0.145712	2.405647
6	-3.150181	-0.022968	-0.417950
1	-2.441102	-0.733024	-2.327025
1	-3.524241	0.611847	1.610648
6	2.422049	1.051393	-0.048067
6	4.031744	-0.778190	-0.340106
6	3.807563	1.619823	-0.400100
1	2.079012	1.302786	0.965282
1	1.628501	1.345108	-0.740774
6	4.791753	0.506851	0.017347
1	4.154818	-1.030859	-1.401369
1	4.287630	-1.653824	0.259310
1	3.878156	1.799661	-1.479179
1	4.000679	2.570004	0.105732
1	5.757752	0.577154	-0.490304
1	4.972244	0.543418	1.097955
7	2.633417	-0.407241	-0.078815
8	-4.478669	0.244623	-0.874474
6	-5.262065	0.753451	0.208246
1	-6.285815	0.824375	-0.094747
1	-5.183152	0.093323	1.046639
1	-4.903405	1.723388	0.482994

E = -667.55838103; ZPE = 0.251351

Number of imaginary freq = 1 (-573.729 Hz)

cis-1c

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-4.127713	-0.743036	-0.665639
6	-3.762014	-1.755157	0.429453
6	-2.253507	-1.720959	0.711989
6	-1.769141	-0.294651	0.995483
6	-3.593397	0.649574	-0.322061
1	-2.005393	-2.358142	1.570011
1	-4.307761	-1.503737	1.350628
1	-4.076275	-2.765977	0.142603
1	-3.697902	-1.061710	-1.624556
1	-5.215279	-0.690348	-0.798534
1	-2.235281	0.085478	1.921575
1	-0.690887	-0.284299	1.139613
1	-4.091099	1.031354	0.587066
1	-3.787642	1.361172	-1.127484
1	-1.701971	-2.114063	-0.152010
7	-1.628606	1.898741	-0.158896
7	-0.403747	2.141829	-0.067789
6	0.657386	1.190600	-0.085961
6	0.733093	0.115531	-0.995506
6	1.781581	1.487953	0.692565
6	1.892541	-0.638147	-1.094940
1	-0.120171	-0.116654	-1.622991
6	2.937356	0.709170	0.625717
1	1.739956	2.345799	1.357253
6	2.999920	-0.359094	-0.276974
1	1.966394	-1.459673	-1.801071
1	3.781562	0.957707	1.258705
7	-2.136801	0.593496	-0.125764
8	4.079574	-1.177104	-0.443633
6	5.231477	-0.937330	0.348936
1	5.652425	0.058845	0.158808
1	5.012542	-1.036771	1.420503
1	5.958786	-1.697335	0.057717

E = -706.90877052; ZPE = 0.282198

Number of imaginary freq = 0

trans-1c

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-4.694646	1.154065	-0.191166
6	-5.293497	-0.240257	0.042218
6	-4.330959	-1.324298	-0.462512
6	-2.937336	-1.188525	0.162289
6	-3.311446	1.264152	0.455861
1	-4.721722	-2.325099	-0.241718
1	-5.475811	-0.382889	1.117735
1	-6.265780	-0.329526	-0.457107
1	-4.602708	1.340959	-1.269211
1	-5.346713	1.933747	0.220915
1	-2.962957	-1.450821	1.234353
1	-2.216184	-1.854752	-0.312677
1	-3.414566	1.231213	1.555151
1	-2.812964	2.202283	0.199374
1	-4.237544	-1.248775	-1.553919
7	-1.131373	0.477773	0.057192
7	-0.353023	-0.519647	0.051744
6	1.020304	-0.177074	0.008794
6	1.533243	1.125918	-0.147964
6	1.921032	-1.239542	0.125720
6	2.900737	1.343144	-0.174719
1	0.843588	1.956514	-0.249031
6	3.301302	-1.030506	0.101315
1	1.520697	-2.242557	0.240309
6	3.798046	0.268341	-0.049196
1	3.308097	2.342356	-0.297126
1	3.969631	-1.878587	0.197578
7	-2.443349	0.180556	0.003288
8	5.123854	0.597982	-0.090902
6	6.075990	-0.445217	0.027281
1	5.986176	-0.968057	0.989074
1	5.980173	-1.175448	-0.787647
1	7.055352	0.033599	-0.031925

E = -706.93632119; ZPE = 0.282889

Number of imaginary freq = 0

ts-1c

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-4.431039	-1.067433	-0.437115
6	-4.822291	-0.421281	0.899582
6	-3.569269	-0.038248	1.699464
6	-2.604550	0.805490	0.858775
6	-3.452450	-0.177686	-1.207580
1	-3.841952	0.525043	2.600636
1	-5.416092	0.483451	0.703431
1	-5.459475	-1.096232	1.483739
1	-3.957424	-2.041165	-0.254503
1	-5.318650	-1.248720	-1.055596
1	-3.075023	1.769952	0.598201
1	-1.700624	1.020640	1.424586
1	-3.945374	0.769495	-1.490156
1	-3.114021	-0.660072	-2.127134
1	-3.045744	-0.944315	2.031397
7	-1.300221	0.569939	-1.170256
7	-0.280551	1.158535	-0.705686
6	0.895452	0.581352	-0.340342
6	1.152956	-0.802215	-0.430954
6	1.965666	1.444879	-0.080917
6	2.437481	-1.289754	-0.245110
1	0.340488	-1.485123	-0.652851
6	3.253108	0.957300	0.146122
1	1.776036	2.514007	-0.059758
6	3.496645	-0.418580	0.058952
1	2.649442	-2.351625	-0.325633
1	4.053585	1.655054	0.364078
7	-2.261958	0.087530	-0.385547
8	4.713602	-1.008367	0.242626
6	5.823326	-0.177190	0.542948
1	6.022223	0.538804	-0.265448
1	5.673978	0.372678	1.481786
1	6.678701	-0.846768	0.649687

E = -706.87675152; ZPE = 0.280767

Number of imaginary freq = 1 (-566.87 Hz)

cis-1d

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	4.118695	-0.790277	0.577644
6	2.384691	-1.713702	-0.692478
6	1.779829	-0.333763	-0.954755
6	3.589567	0.620596	0.339744
1	2.215018	-2.367058	-1.553549
1	3.706685	-1.188236	1.519909
1	5.210253	-0.782780	0.648350
1	2.181118	0.075380	-1.896123
1	0.698668	-0.423885	-1.050221
1	4.075422	1.053138	-0.549588
1	3.805469	1.264255	1.196414
1	1.900276	-2.163121	0.190097
7	1.630459	1.876144	0.166530
7	0.408804	2.120983	0.061694
6	-0.658407	1.177280	0.086654
6	-0.745472	0.106672	1.000382
6	-1.776728	1.480380	-0.698255
6	-1.910688	-0.638406	1.096650
1	0.102635	-0.128774	1.633628
6	-2.937606	0.709748	-0.635102
1	-1.725474	2.336052	-1.364961
6	-3.011926	-0.354938	0.271457
1	-1.994126	-1.456445	1.805663
1	-3.776888	0.961613	-1.273172
7	2.131124	0.561144	0.165302
8	-4.096924	-1.164376	0.435145
6	-5.244655	-0.919754	-0.363179
1	-5.659979	0.079356	-0.176939
1	-5.021478	-1.023648	-1.433292
1	-5.977285	-1.674736	-0.072671
8	3.789820	-1.652128	-0.503995

E = -742.79755669; ZPE = 0.258235

Number of imaginary freq = 0

trans-1d

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-4.733623	1.037342	-0.137892
6	-4.370768	-1.259458	-0.399396
6	-2.937455	-1.170879	0.125103
6	-3.332719	1.252333	0.430980
1	-4.810406	-2.225634	-0.135735
1	-4.720435	1.188828	-1.229893
1	-5.439800	1.744194	0.307085
1	-2.894126	-1.450347	1.190183
1	-2.277837	-1.846566	-0.422854
1	-3.381062	1.238904	1.532147
1	-2.916841	2.213267	0.115396
1	-4.366785	-1.163376	-1.497588
7	-1.138586	0.501175	0.012302
7	-0.364836	-0.497847	0.005163
6	1.011033	-0.163837	-0.018922
6	1.532663	1.137358	-0.160174
6	1.902822	-1.233225	0.101495
6	2.901386	1.346294	-0.168357
1	0.849234	1.972763	-0.263940
6	3.284314	-1.032448	0.096400
1	1.494847	-2.234418	0.204000
6	3.790485	0.264709	-0.038519
1	3.316552	2.343615	-0.278651
1	3.946418	-1.885030	0.195125
7	-2.451990	0.196829	-0.057420
8	5.117557	0.586444	-0.060507
6	6.063069	-0.462422	0.067135
1	5.955090	-0.989384	1.024635
1	5.976409	-1.187412	-0.753301
1	7.045256	0.012234	0.025965
8	-5.212042	-0.264862	0.170507

E = -742.82460388; ZPE = 0.258834

Number of imaginary freq = 0

ts-1d

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-4.378997	-0.607523	-0.705475
6	-2.871201	-1.557631	0.826120
6	-2.206183	-0.208966	1.122346
6	-3.809477	0.797815	-0.486722
1	-2.856345	-2.192203	1.716283
1	-3.866684	-1.088160	-1.554690
1	-5.449542	-0.557440	-0.922245
1	-2.650624	0.242999	2.020223
1	-1.130828	-0.311664	1.272536
1	-4.411767	1.323595	0.267943
1	-3.795436	1.386051	-1.407780
1	-2.322042	-2.068344	0.019015
7	-1.528937	1.505079	-0.555601
7	-0.399027	1.565048	-0.000735
6	0.808455	0.930974	-0.079193
6	1.013328	-0.171100	-0.948521
6	1.897805	1.363074	0.702585
6	2.253629	-0.791992	-1.022505
1	0.193604	-0.516863	-1.572019
6	3.136815	0.727232	0.624433
1	1.763141	2.208087	1.370543
6	3.328420	-0.356700	-0.239003
1	2.407956	-1.630119	-1.696362
1	3.947074	1.094802	1.244827
7	-2.435210	0.680007	-0.018718
8	4.508466	-1.051115	-0.390103
6	5.621390	-0.622642	0.367459
1	5.901525	0.414337	0.132217
1	5.435946	-0.701592	1.448602
1	6.446482	-1.285829	0.097803
8	-4.237734	-1.396866	0.467520

E = -742.76403319; ZPE = 0.256669

Number of imaginary freq = 1 (-575.621 Hz)

cis-1e

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	-1.533702	-0.990220	1.177590
7	-0.459462	-0.595181	1.699911
6	0.749744	-0.282313	1.022631
6	1.478152	0.835256	1.470703
6	1.362475	-1.154850	0.111539
6	2.746650	1.102876	0.978912
1	1.028518	1.485101	2.215797
6	2.653458	-0.909199	-0.363641
1	0.832522	-2.044509	-0.215666
6	3.347814	0.230625	0.057815
1	3.305007	1.973759	1.308169
1	3.101223	-1.610768	-1.058537
8	4.604266	0.576094	-0.354017
6	5.269906	-0.282059	-1.265058
1	5.415647	-1.285630	-0.843236
1	4.723383	-0.367741	-2.214109
1	6.243645	0.174979	-1.451124
6	-3.155231	-1.480162	-0.421625
6	-1.304338	0.024811	-1.122094
6	-4.281524	-0.496376	-0.072149
1	-3.198971	-1.752610	-1.482692
1	-3.281649	-2.399590	0.156032
6	-1.606011	1.487248	-0.740322
1	-1.810761	-0.217067	-2.061298
1	-0.234921	-0.096407	-1.304505
6	-4.157572	0.916481	-0.671007
1	-4.330503	-0.407923	1.020664
1	-5.228665	-0.951829	-0.393626
6	-2.983078	1.732953	-0.093864
1	-1.518766	2.071021	-1.667192
1	-0.825247	1.863837	-0.069938
1	-4.089460	0.865919	-1.768327
1	-5.091768	1.450261	-0.454802
1	-3.206509	2.803935	-0.179489
1	-2.917248	1.524680	0.981921
7	-1.788589	-0.991730	-0.168493

E = -746.21562084; ZPE = 0.311917
Number of imaginary freq = 0

trans-1e

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	-1.050820	-0.674876	-0.566592
7	-0.288395	0.337010	-0.641262
6	1.071008	0.053855	-0.368079
6	1.611291	-1.228181	-0.143228
6	1.932200	1.154638	-0.332618
6	2.962848	-1.385454	0.116306
1	0.956004	-2.091483	-0.176782
6	3.295937	1.006222	-0.072101
1	1.513475	2.140376	-0.513098
6	3.818380	-0.271045	0.155298
1	3.389999	-2.368769	0.289751
1	3.931744	1.884038	-0.052040
8	5.132703	-0.543304	0.416935
6	6.042232	0.542192	0.465752
1	6.090879	1.073823	-0.494303
1	5.778227	1.256508	1.257367
1	7.018987	0.106625	0.685431
6	-3.271032	-1.491343	-0.566631
6	-2.816712	0.893765	-1.240721
6	-3.887713	-1.360960	0.835255
1	-4.061292	-1.473679	-1.328104
1	-2.740687	-2.443728	-0.657357
6	-3.033180	1.840194	-0.037802
1	-3.762575	0.728474	-1.766605
1	-2.110035	1.342329	-1.944627
6	-4.483400	0.019602	1.168032
1	-3.114576	-1.596712	1.578831
1	-4.663339	-2.133485	0.932903
6	-3.432271	1.145475	1.277925
1	-3.810203	2.560943	-0.326890
1	-2.117423	2.413192	0.137331
1	-5.258291	0.287996	0.434020
1	-5.003025	-0.068873	2.130572
1	-3.799940	1.918669	1.964400
1	-2.530454	0.730989	1.747787
7	-2.321730	-0.438500	-0.903347

E = -746.24378386; ZPE = 0.311917
Number of imaginary freq = 0

ts-1e

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	-1.134761	-0.971711	-0.003801
7	-0.290932	-0.514508	0.818216
6	1.052848	-0.298909	0.420044
6	1.409474	0.763724	-0.432339
6	2.074183	-1.075428	0.980700
6	2.738828	1.010810	-0.736378
1	0.625944	1.390261	-0.846171
6	3.417493	-0.822325	0.693172
1	1.808125	-1.882515	1.656953
6	3.756115	0.220812	-0.175739
1	3.021672	1.822879	-1.399380
1	4.181894	-1.440892	1.149744
8	5.032003	0.555702	-0.534605
6	6.100036	-0.198771	0.012010
1	6.127230	-0.127455	1.107771
1	6.037971	-1.256806	-0.276735
1	7.014421	0.233116	-0.399359
6	-2.937457	-0.791850	-1.503255
6	-2.140841	1.285004	-0.351519
6	-4.200542	-1.168255	-0.713546
1	-3.193539	-0.124859	-2.335648
1	-2.484884	-1.691691	-1.928977
6	-2.904195	1.500659	0.972314
1	-2.718338	1.700133	-1.183365
1	-1.186269	1.815743	-0.320535
6	-4.842836	-0.032328	0.104103
1	-3.947582	-1.989151	-0.029818
1	-4.932029	-1.569156	-1.429156
6	-3.979492	0.444365	1.291721
1	-3.366102	2.495744	0.912310
1	-2.191364	1.538681	1.802762
1	-5.099032	0.814697	-0.550266
1	-5.797799	-0.406041	0.494920
1	-4.631111	0.857574	2.072047
1	-3.495314	-0.433955	1.738442
7	-1.901679	-0.116205	-0.718191

E = -746.18352745; ZPE = 0.310031
Number of imaginary freq = 1 (-600.441 Hz)

cis-2b

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	-1.551554	1.564315	-0.297593
7	-0.367892	1.867741	-0.002323
6	0.747108	0.983409	0.006408
6	1.061305	0.143626	-1.074537
6	1.684437	1.125332	1.041906
6	2.272976	-0.547264	-1.096428
1	0.363088	0.047100	-1.900700
6	2.874655	0.406822	1.020652
1	1.459043	1.804152	1.859401
6	3.197521	-0.440606	-0.050638
1	2.501242	-1.186526	-1.946900
1	3.576147	0.516345	1.845321
6	-1.497672	-0.847463	0.407337
6	-3.429888	0.170760	-0.662394
6	-2.747975	-1.721678	0.623867
1	-1.115660	-0.436398	1.349924
1	-0.678208	-1.393648	-0.067446
6	-3.924544	-0.745553	0.460975
1	-3.619497	-0.278333	-1.647035
1	-3.853308	1.177068	-0.655885
1	-2.797671	-2.501098	-0.145885
1	-2.728660	-2.220402	1.597776
1	-4.868143	-1.245492	0.221833
1	-4.069326	-0.164416	1.379850
7	-1.975850	0.274630	-0.437163
6	4.512827	-1.183190	-0.085176
1	5.342012	-0.519061	-0.364114
1	4.759934	-1.609814	0.894081
1	4.491581	-2.001454	-0.812503

E = -592.38939443; ZPE = 0.247827

Number of imaginary freq = 0

trans-2b

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	1.049196	-0.491724	-0.106956
7	0.307150	0.541836	-0.058739
6	-1.077600	0.248186	-0.033487
6	-1.643457	-1.039535	-0.064514
6	-1.934603	1.354402	0.024767
6	-3.023775	-1.196415	-0.035154
1	-0.990153	-1.903751	-0.114454
6	-3.317611	1.183948	0.054239
1	-1.492998	2.346531	0.043771
6	-3.890600	-0.092375	0.027658
1	-3.443564	-2.200500	-0.062610
1	-3.962535	2.059106	0.097735
6	2.920658	1.124657	-0.025138
6	3.323884	-1.297777	-0.107739
6	4.431044	0.847876	-0.115858
1	2.621375	1.583622	0.927284
1	2.537107	1.768093	-0.823810
6	4.581615	-0.591087	0.419489
1	3.484398	-1.698867	-1.119771
1	2.975001	-2.115586	0.529106
1	4.757828	0.895142	-1.161487
1	5.020733	1.576073	0.448474
1	5.504590	-1.077074	0.090252
1	4.573680	-0.588223	1.515885
7	2.341123	-0.217336	-0.126022
6	-5.387993	-0.284914	0.083510
1	-5.725437	-1.033155	-0.643627
1	-5.712383	-0.632123	1.073990
1	-5.919299	0.649482	-0.125355

E = -592.41305066; ZPE = 0.248097

Number of imaginary freq = 0

ts-2b

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	1.355574	-1.148547	-0.727008
7	0.324985	-1.233527	0.013445
6	-0.932005	-0.715033	-0.007027
6	-1.347048	0.198112	-1.010814
6	-1.866735	-1.084423	0.989960
6	-2.644073	0.704641	-1.003505
1	-0.644676	0.483209	-1.789240
6	-3.152672	-0.559494	0.975576
1	-1.559577	-1.785646	1.760140
6	-3.561432	0.340116	-0.016013
1	-2.937764	1.398569	-1.788654
1	-3.850508	-0.860556	1.753999
6	2.060779	0.683996	0.767119
6	3.579734	-0.225399	-0.932750
6	3.459581	1.304761	0.924263
1	1.757518	0.044432	1.607797
1	1.261898	1.414265	0.611156
6	4.405161	0.283657	0.257312
1	3.661938	0.452201	-1.792616
1	3.813504	-1.239092	-1.263338
1	3.507889	2.263904	0.395634
1	3.708304	1.493208	1.972417
1	5.358783	0.721159	-0.050915
1	4.617152	-0.544278	0.943759
7	2.206893	-0.194278	-0.407835
6	-4.991217	0.912221	-0.019207
1	-5.657314	0.205111	-0.467771
1	-5.300464	1.105058	0.986815
1	-5.009295	1.823997	-0.578884

E = -592.35709730; ZPE = 0.246325

Number of imaginary freq = 1 (-539.018 Hz)

cis-3a

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	-1.348591	1.423351	-0.470368
7	-0.134083	1.699714	-0.301339
6	0.896857	0.725484	-0.145340
6	1.086484	-0.328227	-1.055861
6	1.869481	0.966229	0.837300
6	2.220878	-1.134741	-0.962439
1	0.354194	-0.497600	-1.839352
6	2.983246	0.136916	0.942218
1	1.733630	1.809567	1.508102
6	3.166481	-0.916343	0.041558
1	2.363852	-1.940120	-1.678569
1	3.719885	0.322901	1.719528
1	4.043813	-1.552933	0.114722
6	-1.476821	-0.882186	0.647995
6	-3.275656	-0.008196	-0.159685
6	-2.977171	-1.261820	0.702732
1	-1.086613	-0.435147	1.569607
1	-0.773925	-1.641616	0.296526
1	-3.710588	0.830970	0.394834
1	-3.840767	-0.162421	-1.084585
1	-3.426496	-1.265881	1.697787
1	-3.204312	-2.205223	0.201253
7	-1.822376	0.156192	-0.369825

E = -513.73192901; ZPE = 0.190379

Number of imaginary freq = 0

trans-3a

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	-0.953618	0.539033	-0.170026
7	-0.196987	-0.476225	-0.216302
6	1.183005	-0.174882	-0.094045
6	1.732661	1.119121	-0.095805
6	2.035233	-1.281798	0.020698
6	3.108290	1.288583	0.027986
1	1.072521	1.973599	-0.196461
6	3.412133	-1.104755	0.146378
1	1.592600	-2.273429	0.011796
6	3.954888	0.181267	0.151238
1	3.526511	2.292196	0.024088
1	4.061229	-1.971789	0.237524
1	5.028275	0.322523	0.244892
6	-2.893036	-1.059696	-0.090514
6	-3.331367	1.034479	0.232963
6	-4.177973	-0.269929	0.281321
1	-2.413943	-1.590579	0.741478
1	-2.936758	-1.724475	-0.957971
1	-3.078436	1.443255	1.218576
1	-3.693619	1.841287	-0.412701
1	-4.613243	-0.509316	1.253179
1	-4.955637	-0.313373	-0.484229
7	-2.239753	0.239443	-0.351028

E = -513.75052249; ZPE = 0.190705

Number of imaginary freq = 0

ts-3a

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	-1.082073	0.486132	0.971277
7	-0.152096	-0.354971	1.113903
6	1.095532	-0.124167	0.470983
6	1.544062	1.142637	0.059007
6	1.947704	-1.230354	0.340396
6	2.821931	1.286997	-0.477100
1	0.889776	2.001101	0.170223
6	3.218830	-1.079972	-0.209842
1	1.592643	-2.199190	0.679189
6	3.662900	0.179484	-0.619851
1	3.162866	2.271176	-0.788862
1	3.866641	-1.946668	-0.312746
1	4.656214	0.298636	-1.043792
6	-2.438689	-1.012956	-0.568273
6	-3.307802	0.868550	0.042057
6	-3.830042	-0.354739	-0.760073
1	-2.403007	-1.803254	0.191123
1	-1.910910	-1.355512	-1.462382
1	-3.683301	0.927946	1.070236
1	-3.395007	1.851156	-0.433015
1	-4.669463	-0.887447	-0.309237
1	-4.064596	-0.127280	-1.802256
7	-1.955603	0.285476	-0.031224

E = -513.69418214; ZPE = 0.188438

Number of imaginary freq = 1 (-568.502 Hz)

cis-3b

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	0.974024	1.587453	0.238298
7	-0.238462	1.739200	-0.057483
6	-1.242498	0.731719	-0.021248
6	-1.448180	-0.086787	1.103678
6	-2.190564	0.720626	-1.056717
6	-2.571046	-0.911696	1.171287
1	-0.737784	-0.056028	1.924392
6	-3.292617	-0.128023	-0.993569
1	-2.045593	1.387254	-1.901854
6	-3.491050	-0.947608	0.121481
1	-2.725019	-1.531671	2.051060
1	-4.008797	-0.138974	-1.811221
1	-4.359339	-1.598227	0.176320
6	1.197159	-0.838625	-0.378796
6	3.003461	0.435060	0.636758
6	2.540043	-1.568260	-0.579284
1	0.761562	-0.511648	-1.330978
1	0.451376	-1.458418	0.126441
6	3.597004	-0.457809	-0.456668
1	3.244766	0.046209	1.635514
1	3.308220	1.482438	0.591918
1	2.683309	-2.312892	0.212899
1	2.574037	-2.095745	-1.537433
1	4.591961	-0.838024	-0.205793
1	3.673112	0.103361	-1.395972
7	1.546998	0.363459	0.416784

E = -553.07152668; ZPE = 0.220344

Number of imaginary freq = 0

trans-3b

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	-0.580935	0.506075	-0.093705
7	0.182826	-0.511502	-0.036826
6	1.561553	-0.187571	-0.012375
6	2.094838	1.114010	-0.027093
6	2.437887	-1.281583	0.033149
6	3.473375	1.302163	0.002614
1	1.419149	1.961478	-0.061335
6	3.817600	-1.086025	0.062781
1	2.010419	-2.279921	0.044393
6	4.343083	0.207084	0.047675
1	3.875301	2.312557	-0.008874
1	4.482693	-1.945202	0.097757
1	5.418285	0.363006	0.071171
6	-2.418509	-1.148568	-0.015768
6	-2.871669	1.264270	-0.125901
6	-3.932659	-0.904413	-0.135344
1	-2.126965	-1.599733	0.942542
1	-2.005773	-1.783916	-0.806334
6	-4.123907	0.535846	0.383823
1	-3.018928	1.648053	-1.146584
1	-2.554415	2.097754	0.507102
1	-4.239635	-0.967906	-1.186084
1	-4.516889	-1.639930	0.425071
1	-5.050283	0.999124	0.032320
1	-4.136963	0.543070	1.480122
7	-1.865542	0.205467	-0.108416

E = -553.09522392; ZPE = 0.220629

Number of imaginary freq = 0

ts-3b

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	0.718222	-0.651925	0.984629
7	-0.228930	0.153780	1.219172
6	-1.448938	0.039408	0.502299
6	-1.916607	-1.157659	-0.068913
6	-2.270884	1.176235	0.473827
6	-3.176224	-1.201031	-0.662824
1	-1.291675	-2.044036	-0.032170
6	-3.523052	1.128287	-0.134871
1	-1.906531	2.088466	0.937164
6	-3.983557	-0.060721	-0.705756
1	-3.530231	-2.133256	-1.096370
1	-4.144479	2.019923	-0.156929
1	-4.963232	-0.101102	-1.173929
6	1.985241	1.113819	-0.263811
6	2.813830	-1.182444	-0.064904
6	3.402996	1.009669	-0.857781
1	1.944316	1.757212	0.624715
1	1.244338	1.495433	-0.972853
6	4.011233	-0.229195	-0.171488
1	2.681068	-1.761499	-0.990067
1	2.867193	-1.883383	0.771636
1	3.344037	0.847357	-1.940656
1	3.983887	1.921739	-0.691633
1	4.847639	-0.661791	-0.728429
1	4.369403	0.031680	0.831609
7	1.680713	-0.272561	0.130948

E = -553.04027000; ZPE = 0.218751

Number of imaginary freq = 1 (-521.091 Hz)

cis-3c

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	3.490103	-0.249015	0.639811
6	3.259426	-1.383493	-0.368519
6	1.757719	-1.617133	-0.583834
6	1.032909	-0.314630	-0.943766
6	2.724710	1.010926	0.227565
1	1.590111	-2.348962	-1.383708
1	3.724522	-1.113956	-1.328115
1	3.746456	-2.305971	-0.030283
1	3.149403	-0.561620	1.635751
1	4.558025	-0.012204	0.720779
1	1.399354	0.065664	-1.913198
1	-0.034659	-0.491110	-1.039366
1	3.125912	1.400146	-0.724812
1	2.818456	1.801171	0.974878
1	1.307267	-2.027380	0.329312
7	0.553186	1.869493	0.194788
7	-0.697161	1.899885	0.114976
6	-1.568510	0.773345	0.087045
6	-1.548641	-0.195120	1.106607
6	-2.607145	0.760185	-0.855447
6	-2.541556	-1.171292	1.156626
1	-0.759459	-0.170612	1.851419
6	-3.580275	-0.236992	-0.811631
1	-2.635501	1.536979	-1.613942
6	-3.554699	-1.205711	0.194398
1	-2.523032	-1.911075	1.953023
1	-4.370928	-0.247044	-1.557407
1	-4.322418	-1.973204	0.235425
7	1.292867	0.706731	0.089824

E = -592.38659946; ZPE = 0.249620

Number of imaginary freq = 0

trans-3c

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-3.775862	1.183339	-0.199030
6	-4.393072	-0.206311	0.012463
6	-3.432334	-1.296599	-0.481959
6	-2.051150	-1.182502	0.173997
6	-2.405670	1.276367	0.478402
1	-3.838462	-2.294902	-0.278770
1	-4.598060	-0.354971	1.083028
1	-5.356062	-0.281491	-0.506588
1	-3.659339	1.376274	-1.273624
1	-4.428592	1.966970	0.204227
1	-2.102983	-1.454505	1.242193
1	-1.325309	-1.849386	-0.292448
1	-2.532452	1.239943	1.574655
1	-1.890193	2.208909	0.236048
1	-3.314806	-1.212413	-1.570376
7	-0.230123	0.469163	0.083828
7	0.542113	-0.534145	0.061305
6	1.918024	-0.196170	0.006417
6	2.428935	1.101001	-0.175592
6	2.809489	-1.270377	0.135749
6	3.804804	1.306741	-0.213523
1	1.738772	1.929976	-0.286414
6	4.186409	-1.057224	0.097318
1	2.397144	-2.266279	0.268388
6	4.690875	0.232616	-0.076853
1	4.191628	2.313000	-0.355450
1	4.865327	-1.899707	0.201172
1	5.763788	0.401722	-0.110863
7	-1.539575	0.183780	0.043508

E = -592.41384079; ZPE = 0.250169

Number of imaginary freq = 0

ts-3c

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	3.421713	-0.976573	-0.702844
6	3.837429	0.490965	-0.878820
6	2.601789	1.401765	-0.880930
6	1.729402	1.178660	0.360278
6	2.554167	-1.150117	0.546592
1	2.897229	2.457382	-0.920162
1	4.502960	0.781304	-0.052515
1	4.409841	0.620369	-1.805152
1	2.853129	-1.308548	-1.581552
1	4.302926	-1.624422	-0.621128
1	2.260791	1.512199	1.268346
1	0.804657	1.748921	0.295367
1	3.155751	-0.944018	1.449335
1	2.164600	-2.166816	0.633074
1	1.997750	1.202239	-1.775706
7	0.359466	-0.699296	1.247953
7	-0.634749	0.050848	1.437291
6	-1.751731	-0.012703	0.560907
6	-2.070972	-1.146552	-0.206895
6	-2.622322	1.086433	0.558579
6	-3.239047	-1.165274	-0.964705
1	-1.400904	-1.999737	-0.198877
6	-3.782969	1.063809	-0.213075
1	-2.370652	1.948442	1.169388
6	-4.098095	-0.061795	-0.977155
1	-3.480474	-2.047340	-1.552731
1	-4.445883	1.925201	-0.211905
1	-5.005418	-0.082049	-1.574534
7	1.400642	-0.247957	0.495778

E = -592.35859073; ZPE = 0.248260

Number of imaginary freq = 1 (-516.945 Hz)

cis-3d

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	3.469444	-0.328071	0.565201
6	1.860643	-1.596301	-0.567515
6	1.041061	-0.348880	-0.902966
6	2.724003	0.966114	0.251594
1	1.769864	-2.331435	-1.372596
1	3.149444	-0.711763	1.548007
1	4.548549	-0.151377	0.591531
1	1.348448	0.044880	-1.884994
1	-0.013763	-0.609429	-0.948612
1	3.113790	1.398835	-0.683588
1	2.856198	1.697078	1.052802
1	1.476334	-2.044080	0.363556
7	0.565831	1.855620	0.194755
7	-0.680950	1.896677	0.097318
6	-1.562190	0.776468	0.079504
6	-1.568003	-0.168972	1.120067
6	-2.580354	0.750034	-0.884120
6	-2.566919	-1.139139	1.169463
1	-0.793695	-0.132992	1.879789
6	-3.559156	-0.241640	-0.840120
1	-2.588705	1.510888	-1.658990
6	-3.559309	-1.188831	0.186478
1	-2.569174	-1.862057	1.981273
1	-4.333888	-0.263906	-1.602007
7	1.289316	0.672530	0.132212
8	3.244170	-1.306416	-0.441120

E = -628.27514288; ZPE = 0.225540

Number of imaginary freq = 0

trans-3d

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	3.813616	1.076102	0.147532
6	3.475722	-1.220258	0.447316
6	2.057430	-1.166219	-0.121893
6	2.427863	1.260472	-0.468139
1	3.937646	-2.184972	0.219117
1	3.764937	1.248704	1.235334
1	4.523448	1.783912	-0.289874
1	2.050629	-1.471448	-1.180281
1	1.388996	-1.835484	0.422936
1	2.509960	1.228334	-1.566518
1	1.986742	2.219119	-0.181847
1	3.437116	-1.099421	1.542323
7	0.237288	0.487088	-0.057190
7	-0.528276	-0.519022	-0.025297
6	-1.907773	-0.190685	0.006232
6	-2.427891	1.102286	0.189611
6	-2.789350	-1.269732	-0.145122
6	-3.805299	1.299943	0.206145
1	-1.744257	1.934004	0.318929
6	-4.167937	-1.064392	-0.129149
1	-2.369023	-2.262262	-0.277550
6	-4.682114	0.221429	0.046083
1	-4.200558	2.302527	0.349963
1	-4.840366	-1.909564	-0.250729
1	-5.756370	0.384113	0.063550
7	1.548385	0.199131	0.008997
8	4.317967	-0.225202	-0.120327

E = -628.30190136; ZPE = 0.226106

Number of imaginary freq = 0

ts-3d

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	3.432456	1.176521	-0.112305
6	2.993839	-0.575665	1.376705
6	1.956449	-1.185287	0.431991
6	2.431324	0.619800	-1.120642
1	3.505040	-1.367373	1.932305
1	2.933948	1.915991	0.535925
1	4.263622	1.665596	-0.628396
1	2.440203	-1.929078	-0.221210
1	1.185063	-1.684353	1.013815
1	2.951716	-0.045234	-1.828222
1	1.958063	1.425489	-1.686864
1	2.485369	0.087468	2.095596
7	0.339761	-0.311409	-1.204314
7	-0.697823	-0.934368	-0.844103
6	-1.800240	-0.391192	-0.261663
6	-1.885595	0.986620	0.004816
6	-2.943553	-1.192415	-0.132025
6	-3.095390	1.538356	0.421323
1	-1.006482	1.610918	-0.119430
6	-4.141718	-0.634562	0.311381
1	-2.875410	-2.247341	-0.380779
6	-4.224877	0.732078	0.587885
1	-3.155582	2.605733	0.618136
1	-5.017655	-1.267734	0.425424
1	-5.163343	1.167477	0.919129
7	1.380857	-0.108732	-0.396396
8	3.999963	0.137309	0.674182

E = -628.24572841; ZPE = 0.224073

Number of imaginary freq = 1 (-524.356 Hz)

cis-3e

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	-0.635079	-1.112125	1.066807
7	0.499885	-0.745028	1.467567
6	1.594358	-0.331987	0.663138
6	2.300411	0.820454	1.044350
6	2.124575	-1.156717	-0.345829
6	3.482346	1.169161	0.393715
1	1.910803	1.425429	1.858026
6	3.320869	-0.812369	-0.973718
1	1.600570	-2.068105	-0.619157
6	4.000144	0.355206	-0.617079
1	4.009138	2.073339	0.687864
1	3.723476	-1.461052	-1.747710
6	-2.480251	-1.457985	-0.312459
6	-0.722250	0.090374	-1.157437
6	-3.542880	-0.505890	0.254624
1	-2.667445	-1.655017	-1.374473
1	-2.530018	-2.415940	0.211334
6	-0.976440	1.528149	-0.660479
1	-1.338993	-0.103493	-2.039796
1	0.316125	-0.017196	-1.474081
6	-3.494236	0.944999	-0.256989
1	-3.440893	-0.493386	1.347422
1	-4.527356	-0.942488	0.035827
6	-2.241092	1.720719	0.197980
1	-1.036177	2.158662	-1.558423
1	-0.106616	1.883633	-0.096937
1	-3.586299	0.971086	-1.353384
1	-4.382466	1.461074	0.128900
1	-2.465952	2.794481	0.223353
1	-2.018392	1.435608	1.234570
7	-1.090808	-0.978944	-0.209943
1	4.929189	0.621359	-1.113241

E = -631.69378845; ZPE = 0.279822

Number of imaginary freq = 0

trans-3e

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	-0.175132	-0.664735	-0.498456
7	0.566833	0.365445	-0.538844
6	1.916415	0.110922	-0.190770
6	2.479052	-1.163707	-0.000332
6	2.730506	1.243947	-0.049365
6	3.823649	-1.287421	0.337118
1	1.853381	-2.041027	-0.121760
6	4.076266	1.112902	0.288792
1	2.282696	2.220550	-0.208517
6	4.629784	-0.153595	0.484705
1	4.249924	-2.277319	0.481445
1	4.693472	2.001139	0.396977
6	-2.369671	-1.536692	-0.618820
6	-1.930970	0.851605	-1.299435
6	-3.071457	-1.405741	0.742293
1	-3.111975	-1.543728	-1.426992
1	-1.812190	-2.476459	-0.667226
6	-2.250045	1.806901	-0.126513
1	-2.835190	0.654215	-1.883845
1	-1.189222	1.306680	-1.961459
6	-3.717793	-0.036180	1.021554
1	-2.338232	-1.614609	1.532765
1	-3.832864	-2.195802	0.803190
6	-2.701158	1.116378	1.174081
1	-3.033293	2.495584	-0.471294
1	-1.366717	2.414528	0.092776
1	-4.455512	0.203757	0.241012
1	-4.288905	-0.125338	1.954255
1	-3.123535	1.887771	1.830351
1	-1.815554	0.730067	1.695959
7	-1.426481	-0.463098	-0.907244
1	5.679700	-0.259208	0.744320

E = -631.72149815; ZPE = 0.279622

Number of imaginary freq = 0

ts-3e

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	0.424761	-0.982751	-0.913954
7	-0.537910	-0.159104	-0.967730
6	-1.814719	-0.080269	-0.508983
6	-2.377475	-1.087546	0.318003
6	-2.624712	1.027756	-0.858860
6	-3.693246	-0.976203	0.760427
1	-1.774916	-1.951804	0.583850
6	-3.931582	1.115739	-0.397010
1	-2.206284	1.799963	-1.497485
6	-4.485813	0.120607	0.416881
1	-4.101354	-1.766987	1.386720
1	-4.530846	1.977916	-0.681680
6	2.529012	-1.584641	-0.007683
6	1.067281	0.090299	1.209701
6	3.669254	-0.709716	-0.550315
1	2.779846	-1.975108	0.985478
1	2.350874	-2.432773	-0.673359
6	1.510098	1.531264	0.874611
1	1.656029	-0.304550	2.042400
1	0.016560	0.070628	1.506527
6	3.867209	0.648122	0.149051
1	3.485961	-0.528952	-1.617566
1	4.593094	-1.300039	-0.485325
6	2.710428	1.643935	-0.084118
1	1.750003	2.016350	1.829906
1	0.665589	2.079769	0.447532
1	4.041247	0.504164	1.225863
1	4.791464	1.087066	-0.246206
1	3.094432	2.669042	-0.015263
1	2.354243	1.525988	-1.116233
7	1.254452	-0.873203	0.113726
1	-5.509480	0.198652	0.770317

E = -631.66542896; ZPE = 0.277375

Number of imaginary freq = 1 (-545.549 Hz)

cis-4a

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	-2.375264	1.298784	-0.429226
7	-1.233243	1.799326	-0.263047
6	-0.032004	1.043474	-0.143043
6	0.335881	0.036589	-1.052184
6	0.909569	1.482845	0.800950
6	1.607677	-0.532117	-1.001072
1	-0.369115	-0.286926	-1.811335
6	2.169511	0.897800	0.877873
1	0.637191	2.291927	1.471867
6	2.511245	-0.107960	-0.027740
1	1.894688	-1.301363	-1.710526
1	2.887918	1.227561	1.620961
6	-2.052473	-1.014580	0.634309
6	-3.993668	-0.478605	-0.141385
6	-3.453896	-1.670798	0.690480
1	-1.738844	-0.525219	1.563815
1	-1.225405	-1.620714	0.255879
1	-4.576065	0.250118	0.433076
1	-4.524545	-0.717869	-1.068232
1	-3.882820	-1.779675	1.688427
1	-3.504134	-2.629461	0.169757
7	-2.599956	-0.033986	-0.352220
17	4.108784	-0.841008	0.051096

E = -973.32792939; ZPE = 0.180700

Number of imaginary freq = 0

trans-4a

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	1.836832	-0.520927	-0.181227
7	1.112788	0.520246	-0.220058
6	-0.275205	0.257001	-0.135821
6	-0.863329	-1.019863	-0.163185
6	-1.101848	1.384054	-0.031565
6	-2.243883	-1.160535	-0.076408
1	-0.228801	-1.894269	-0.254519
6	-2.485658	1.252699	0.057664
1	-0.637124	2.365095	-0.019114
6	-3.046849	-0.022678	0.035262
1	-2.700299	-2.144780	-0.098915
1	-3.121750	2.127469	0.140968
6	3.829879	1.008165	-0.036450
6	4.193153	-1.109958	0.238160
6	5.081451	0.164401	0.332207
1	3.362410	1.543724	0.798952
1	3.906524	1.683437	-0.893429
1	3.920705	-1.543718	1.207528
1	4.532815	-1.905217	-0.433428
1	5.507842	0.363405	1.316920
1	5.872826	0.201702	-0.419293
7	3.131938	-0.261030	-0.324469
17	-4.794843	-0.204975	0.142084

E = -973.34718415; ZPE = 0.181047

Number of imaginary freq = 0

ts-4a

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	-2.009850	-0.325845	-1.040192
7	-1.121854	0.567597	-1.136503
6	0.187838	0.295895	-0.660406
6	0.713784	-0.995439	-0.481711
6	1.022720	1.404574	-0.457553
6	2.042241	-1.169366	-0.103156
1	0.079089	-1.859040	-0.649423
6	2.347969	1.239336	-0.064707
1	0.613854	2.397834	-0.615707
6	2.849373	-0.050606	0.108942
1	2.450677	-2.165789	0.030344
1	2.988558	2.099445	0.098878
6	-3.249647	0.852566	0.841192
6	-4.116016	-0.954335	0.028113
6	-4.592304	0.106529	1.058243
1	-3.315790	1.755682	0.222693
1	-2.642522	1.070350	1.724047
1	-4.596451	-0.879909	-0.954120
1	-4.114781	-1.999579	0.353605
1	-5.488979	0.661849	0.777185
1	-4.713431	-0.287616	2.069451
7	-2.785915	-0.318813	0.053675
17	4.525138	-0.272278	0.599438

E = -973.29151555; ZPE = 0.178996

Number of imaginary freq = 1 (-564.046 Hz)

cis-5a

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	3.054288	-1.255066	-0.431419
7	1.942665	-1.820885	-0.264012
6	0.702387	-1.136341	-0.142112
6	0.264827	-0.188656	-1.084894
6	-0.193305	-1.585399	0.841799
6	-1.032639	0.311061	-1.023558
1	0.940032	0.140824	-1.868180
6	-1.479312	-1.063856	0.915704
1	0.139366	-2.344645	1.542829
6	-1.905947	-0.112589	-0.017489
1	-1.365713	1.041511	-1.754143
1	-2.157572	-1.397784	1.694087
6	2.586333	1.043881	0.618332
6	4.564800	0.617677	-0.138292
6	3.947209	1.780461	0.681924
1	2.287423	0.550804	1.550502
1	1.732153	1.596359	0.218574
1	5.193571	-0.066841	0.441379
1	5.078520	0.883793	-1.067412
1	4.359605	1.917344	1.683310
1	3.947282	2.738502	0.157854
7	3.203228	0.082755	-0.345305
6	-3.316499	0.402127	0.016877
9	-4.147323	-0.339662	-0.754286
9	-3.829819	0.385822	1.268252
9	-3.398754	1.674097	-0.438788

E = -850.7701749; ZPE = 0.195107

Number of imaginary freq = 0

trans-5a

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	2.526304	-0.511536	-0.173985
7	1.815799	0.540309	-0.229217
6	0.424721	0.291146	-0.167584
6	-0.175341	-0.979834	-0.224744
6	-0.390773	1.427210	-0.061461
6	-1.557282	-1.100660	-0.160454
1	0.451820	-1.858362	-0.323946
6	-1.774764	1.304109	0.004226
1	0.085749	2.402014	-0.032227
6	-2.364389	0.038097	-0.044406
1	-2.018376	-2.081838	-0.212554
1	-2.397889	2.188994	0.083070
6	4.542592	0.989472	-0.024824
6	4.874067	-1.135427	0.259309
6	5.779207	0.127578	0.354479
1	4.084130	1.545993	0.801551
1	4.631622	1.649678	-0.892272
1	4.598929	-1.571799	1.226519
1	5.201105	-1.930515	-0.418637
1	6.200006	0.323487	1.342128
1	6.577196	0.151404	-0.390390
7	3.822470	-0.270478	-0.295063
6	-3.853414	-0.107437	0.083846
9	-4.239369	-0.239427	1.377214
9	-4.512780	0.966303	-0.408498
9	-4.313856	-1.199392	-0.569350

E = -850.78934391; ZPE = 0.195475

Number of imaginary freq = 0

ts-5a

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	-2.849015	0.669363	-1.044694
7	-1.820659	1.152379	-0.468463
6	-0.528269	0.777900	-0.323402
6	-0.033263	-0.436707	-0.870867
6	0.374722	1.609971	0.385621
6	1.299683	-0.784614	-0.710506
1	-0.709381	-1.085273	-1.419722
6	1.699684	1.239475	0.536941
1	0.007974	2.539877	0.808226
6	2.183120	0.038410	-0.002995
1	1.658428	-1.717746	-1.135006
1	2.373338	1.886967	1.090048
6	-3.508273	-0.438927	1.131430
6	-5.002753	-0.446656	-0.459265
6	-5.007029	-0.847445	1.046375
1	-3.271419	0.467495	1.701048
1	-2.791576	-1.222979	1.389955
1	-5.591557	0.435919	-0.726139
1	-5.200742	-1.251417	-1.173188
1	-5.674850	-0.250976	1.669995
1	-5.193832	-1.907335	1.226191
7	-3.568367	-0.139032	-0.313159
6	3.626518	-0.321734	0.117755
9	4.382254	0.168411	-0.901714
9	3.820323	-1.664786	0.115035
9	4.179098	0.161760	1.258488

E = -850.73705231; ZPE = 0.193498

Number of imaginary freq = 1 (-521.504 Hz)

cis-5b

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	2.678794	-1.516258	-0.346413
7	1.540612	-1.958272	-0.039281
6	0.335655	-1.214408	0.005068
6	-0.088052	-0.404651	-1.065662
6	-0.560181	-1.478413	1.054852
6	-1.367614	0.141908	-1.067043
1	0.584181	-0.221678	-1.898084
6	-1.827638	-0.909332	1.061479
1	-0.241488	-2.133267	1.859924
6	-2.239183	-0.095431	0.000002
1	-1.687991	0.765012	-1.896159
1	-2.503678	-1.099014	1.888884
6	2.357221	0.854377	0.429927
6	4.387891	0.090341	-0.677517
6	3.495966	1.869996	0.645611
1	2.034982	0.388821	1.369630
1	1.475114	1.304199	-0.033617
6	4.781313	1.048351	0.450512
1	4.500678	0.569925	-1.659152
1	4.931834	-0.855902	-0.690812
1	3.437163	2.661809	-0.110398
1	3.430539	2.346474	1.628282
1	5.650214	1.665189	0.202684
1	5.014313	0.479704	1.358787
7	2.961440	-0.193832	-0.428379
6	-3.631536	0.464957	-0.029912
9	-4.496815	-0.353274	-0.676588
9	-4.129240	0.650567	1.214361
9	-3.680038	1.658383	-0.667256

E = -890.11022779; ZPE = 0.225215

Number of imaginary freq = 0

trans-5b

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	2.150459	-0.465978	-0.101509
7	1.431269	0.587383	-0.053881
6	0.043839	0.319938	-0.052096
6	-0.542768	-0.958875	-0.096760
6	-0.790189	1.447430	-0.003012
6	-1.924642	-1.093842	-0.088680
1	0.095686	-1.833642	-0.140327
6	-2.174177	1.310287	0.005504
1	-0.326329	2.428407	0.025664
6	-2.749140	0.037278	-0.037510
1	-2.372232	-2.081933	-0.129868
1	-2.808787	2.189987	0.038172
6	4.060239	1.100569	-0.000583
6	4.400015	-1.332796	-0.106459
6	5.561723	0.783962	-0.106770
1	3.781380	1.564764	0.954808
1	3.682833	1.751614	-0.795629
6	5.680140	-0.663426	0.414001
1	4.534823	-1.718653	-1.127460
1	4.037648	-2.150795	0.521918
1	5.880990	0.833190	-1.154467
1	6.174564	1.490925	0.459452
1	6.585991	-1.169981	0.069395
1	5.684401	-0.671767	1.510259
7	3.442746	-0.227090	-0.095483
6	-4.239381	-0.123858	0.034645
9	-4.676654	-0.242900	1.313425
9	-4.892188	0.934592	-0.498774
9	-4.661852	-1.230838	-0.620150

E = -890.13468829; ZPE = 0.225518

Number of imaginary freq = 0

ts-5b

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	2.472720	-1.115169	-0.813576
7	1.458598	-1.367328	-0.077933
6	0.179668	-0.926885	-0.063867
6	-0.287870	0.064500	-0.969807
6	-0.740242	-1.455912	0.878085
6	-1.607909	0.488767	-0.926635
1	0.398544	0.478387	-1.702682
6	-2.050961	-1.013698	0.906200
1	-0.395945	-2.212311	1.576176
6	-2.506132	-0.034136	0.010014
1	-1.944223	1.247344	-1.627471
1	-2.736423	-1.427300	1.639835
6	3.039569	0.616585	0.848330
6	4.598898	0.017711	-0.954841
6	4.367262	1.372442	1.025160
1	2.833302	-0.117707	1.639010
1	2.162131	1.263855	0.766788
6	5.397076	0.517777	0.256659
1	4.578356	0.766684	-1.756718
1	4.930053	-0.934380	-1.373030
1	4.294672	2.369325	0.575542
1	4.625543	1.503344	2.079438
1	6.287320	1.081428	-0.034913
1	5.719240	-0.333482	0.867485
7	3.244921	-0.143446	-0.400482
6	-3.936484	0.390763	0.011353
9	-4.719414	-0.379274	-0.792112
9	-4.488985	0.320945	1.248554
9	-4.091989	1.665989	-0.426380

E = -890.08344126; ZPE = 0.223856

Number of imaginary freq = 1 (-473.436 Hz)