

*Electronic Supplementary Information*

*for*

**Mechanistic Insights on Platinum- and Palladium-Pincer  
Catalyzed Coupling and Cyclopropanation Reactions between  
Olefins**

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**Table S1.** The relative free energies (in kcal mol<sup>-1</sup>) of the transition states and intermediates calculated at the B3LYP/LANL2DZ (Pt),6-31+G\*\* level of theory for the platinum pincer catalyzed coupling of ethene and butene

	Series 1	Series 2	Series 3	Series 4
<b>TS<sub>add</sub></b>	11.7	12.1	13.4	24.7
<b>c</b>	6.5	10.2	5.7	22.7
<b>TS(c-e)</b>	24.3	27.1	25.5	47.4
<b>TS(c-d)</b>	15.6	18.9	21.2	37.5
<b>d</b>	9.1	10.8	7.6	22.1
<b>TS(d-e)</b>	17.8	25.7	19.9	40.5
<b>TS(d-g)</b>	20.9	26.4	30.9	42.3
<b>e</b>	1.9	0.5	7.0	16.0
<b>e'</b>	-0.8	5.6	4.2	21.8
<b>g</b>	- <sup>a</sup> -	- <sup>a</sup> -	- <sup>a</sup> -	39.3

<sup>a</sup>- All attempts to optimize of these geometries reverted back to the corresponding intermediate 'd'. See Table S6 in Supporting Information for more details.

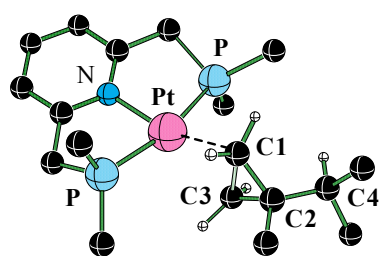
**Table S2.** Comparison of experimentally reported Pt-CNC and Pt-PCP compounds with optimized structural parameters of pincers under study

	Pt(CNC) <sup>1</sup>	Pt-PCP <sup>2</sup>	B3LYP	mPW1K	M06-2X
Pt-C(ethene)	2.17	2.30	2.26	2.21	2.22
Pt-C(ethene)	2.17	2.30	2.26	2.21	2.22
C-C	1.37	1.30	1.38	1.37	1.38

1) D. Serra, P. Cao, J. Cabrera, R. Padilla, F. Rominger and M. Limbach,

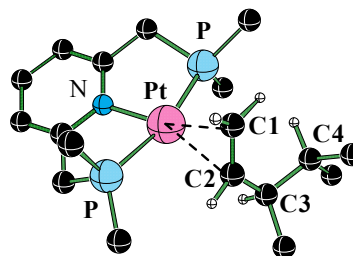
*Organometallics*. 2011, **30**, 1885.

2) J. J. Adams, N. Arulsamy and D. M. Roddick, *Organometallics* 2009, **28**, 1148.



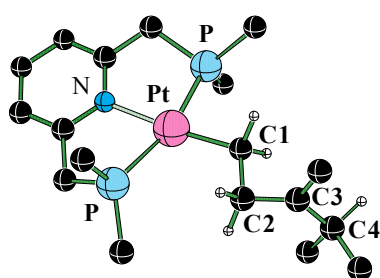
Pt-C1	2.39
C1-C3	1.49
Pt-C1-C3	126.08

**1g**



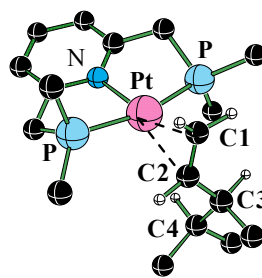
Pt-C1	2.19
Pt-C2	2.31
C1-C2	1.38

**1e**



Pt-C1	2.07
C1-C2	1.57
C2-C3	1.44

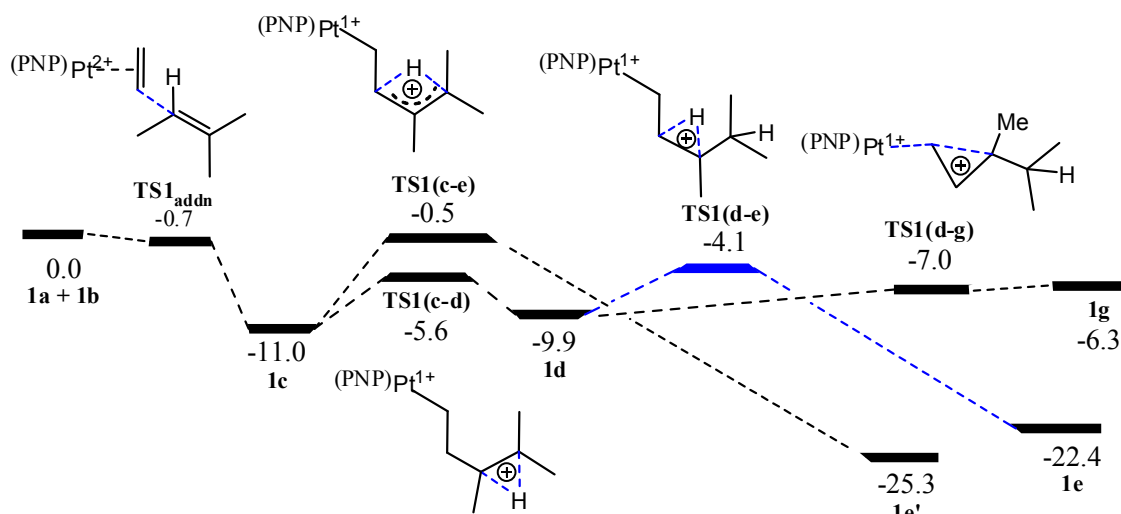
**1d**



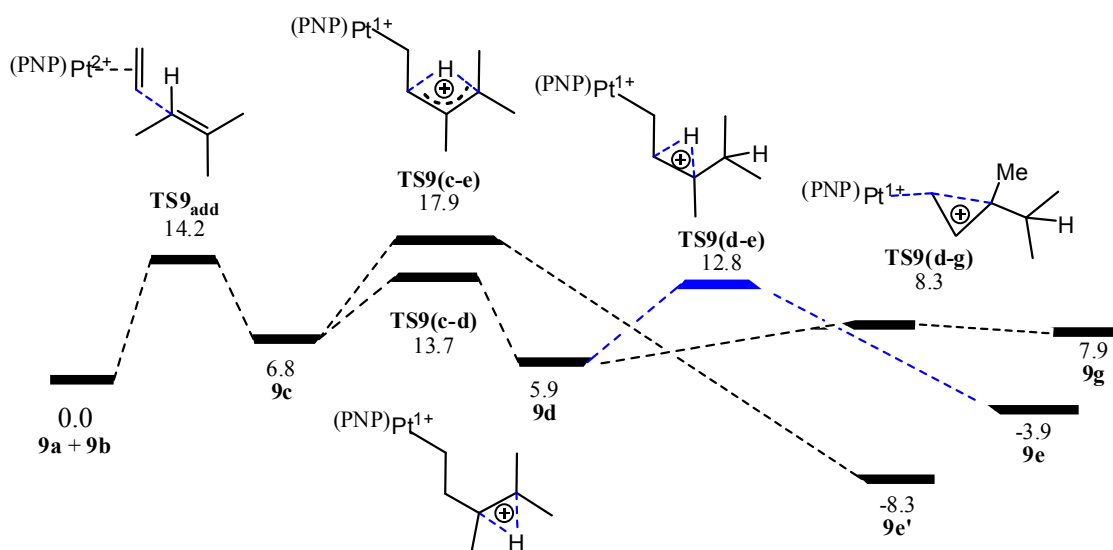
Pt-C1	2.18
Pt-C2	2.30
C1-C2	1.38

**1e'**

**Fig. S1** Optimized geometries of intermediate and products at the mPW1K /LANL2DZ (Pt),6-31+G\*\* level of theory. (Distances are given in Å and angles in °).



**Fig. S2** Enthalpy profile for platinum PNP-pincer catalyzed reaction between ethene and 2-methylbut-2-ene (Series 1) generated at the mPW1K/LANL2DZ (Pt),6-31+G\*\* level of theory. The relative energies (kcal mol<sup>-1</sup>) are with respect to the  $\pi$ -complex and the free olefin.



**Fig. S3** Free energy profile for platinum PNP-pincer (real system where the substituents on phosphorous are phenyls) catalyzed reaction between ethene and 2-methylbut-2-ene (Series 1) generated at the mPW1K/LANL2DZ (Pt),6-31G\* level of theory. The relative energies (kcal mol<sup>-1</sup>) are with respect to the  $\pi$ -complex and the free olefin.

**Table S3.** The relative free energies (in kcal mol<sup>-1</sup>) of the transition states and intermediates calculated at the B3LYP/LANL2DZ (Pd),6-31+G\*\* level of theory for the palladium pincer catalyzed coupling of ethene and butene

	Series 5	Series 6	Series 7	Series 8
<b>TS<sub>add</sub></b>	11.5	13.0	12.6	25.0
<b>c</b>	8.7	11.8	7.1	24.2
<b>TS(c-e')</b>	27.2	29.4	27.7	49.9
<b>TS(c-d)</b>	18.8	21.3	24.0	39.5
<b>d</b>	10.8	13.5	8.8	24.6
<b>TS(d-e)</b>	19.6	27.0	20.9	42.5
<b>TS(d-g)</b>	<i>-b-</i>	21.2	25.7	38.1
<b>e</b>	1.1	-0.3	3.6	14.7
<b>e'</b>	-1.9	4.0	2.6	20.1
<b>g</b>	<i>-a-</i>	<i>-a-</i>	<i>-a-</i>	37.5

<sup>-a,b-</sup> All attempts to optimize of these geometries reverted back to the corresponding intermediate 'd'. See Table S6 in Supporting Information for more details.

**Table S4.** Differences in relative energies (in kcal mol<sup>-1</sup>) of transition states leads to dimer and cyclopropane [ETS(d-e)-E(TS(d-g))]

		Series 1/5		Series 2/6		Series 3/7		Series 4/8	
		Pt	Pd	Pt	Pd	Pt	Pd	Pt	Pd
mPW1K	E	4.5	10.3	6.1	11.9	-3.2	3.0	2.3	8.2
	G	1.3	7.9	3.1	10.8	-7.1	-0.8	-0.1	6.0
	H	2.8	8.6	4.3	10.2	-5.3	1.0	1.0	6.8
	E <sub>sol</sub>	8.5	11.7	10.7	14.3	2.9	8.3	12.2	16.9
M06-2X	E	7.6	11.0	9.0	<i>-b-</i>	1.4	<i>-b-</i>	5.13	14.2
	G	6.3	7.4	7.6	<i>-b-</i>	-2.0	<i>-b-</i>	2.3	13.0
	H	6.5	9.4	7.6	<i>-b-</i>	-0.7	<i>-b-</i>	3.7	12.9
	E <sub>sol</sub>	10.5	15.9	11.6	<i>-b-</i>	9.2	<i>-b-</i>	14.5	22.7
B3LYP	E	0.3	4.61	2.0	8.7	-7.4	-0.7	0.2	6.5
	G	-3.0	0.6	-0.7	5.7	-10.9	-4.7	-1.7	4.4
	H	-1.4	2.6	0.2	6.9	-9.5	-2.8	-1.0	5.08
	E <sub>sol</sub>	4.7	9.1	7.1	14.7	-0.6	6.4	11.7	16.5

<sup>-b-</sup> All attempts to optimize of these geometries reverted back to the corresponding intermediate 'd'. See Table S6 in Supporting Information for more details.



## Details about optimization of intermediate 'g'

Attempts to optimize the geometry of 'g' revert backed to 'd' for a few cases. We believe that the nature of potential energy surface where the energy of product 'g' is very near to the transition state **TS(d-g)** causes this reversal. Energies of these missing geometries at the other level of theories studied also convey their thermodynamic instability. Various attempts to optimize missing geometries and the outcome are summarized in Table S6. However, these missing entries will not affect the final conclusions as the corresponding values are obtained with other levels of theory and different series.

**Table S5.** Details of the attempts and outcome of geometry optimization of 'g'

Increasing the Metal – C1 distance	M – C1 distance decreased and C1-C2 bond cleaved and converted to 'd'
Changing dihedral angles around Metal – C1 bond	Geometries collapsed to 'd'
Freezing C1 – C3 distance	Optimized geometries were higher order saddle points.

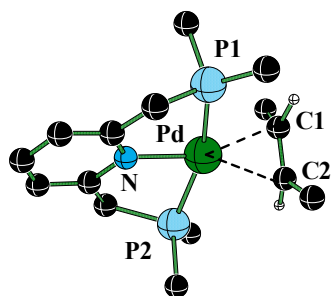
**Table S6.** Relative thermodynamic parameters (in kcal mol<sup>-1</sup>) of intermediates **d** and **g** at the MP2/LANL2DZ,6-31G\* level of theory<sup>i</sup>

Intermediate	$\Delta G$	$\Delta H$
<b>1d</b>	0.0	0.0
<b>1g</b>	-1.4	-1.3
<b>5d</b>	0.0	0.0
<b>5g</b>	-10.9	-12.3

<sup>i</sup> relative energies are defined with respect to the energies of '**d**'.

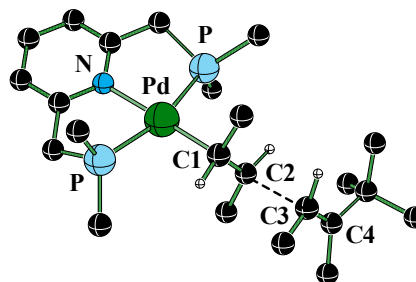
**Table S7.** Natural charges on platinum and palladium atom in the intermediates and **TS(d-g)** in Scheme 2

	Pt	Pd
<b>TS1(d-g)/TS5(d-g)</b>	0.02	0.08
<b>TS2(d-g)/TS6(d-g)</b>	0.04	0.09
<b>TS3(d-g)/TS7(d-g)</b>	0.04	0.11
<b>TS4(d-g)/TS8(d-g)</b>	0.06	0.13
<b>1c / 5c</b>	-0.08	-0.01
<b>2c / 6c</b>	-0.08	-0.01
<b>3c / 7c</b>	-0.08	-0.01
<b>4c / 8c</b>	-0.09	-0.03
<b>1d / 5d</b>	-0.05	0.03
<b>2d / 6d</b>	-0.06	0.02
<b>3d / 7d</b>	-0.08	0.02
<b>4d / 8d</b>	-0.08	-0.01



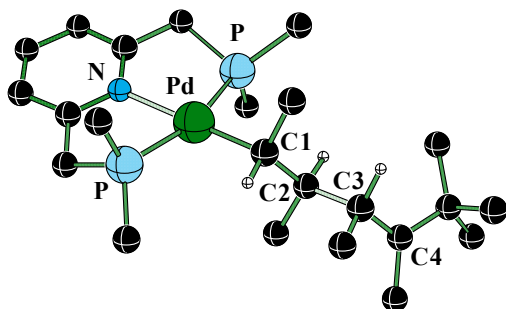
Pd-C1	2.27,	2.34,	2.33
Pd-C2	2.27,	2.34,	2.33
Pd-N	2.09,	2.13,	2.13
C1-C2	1.37,	1.37,	1.38
P1-Pd-C1-C2	-57.95,	-60.92,	-61.65

**8a**



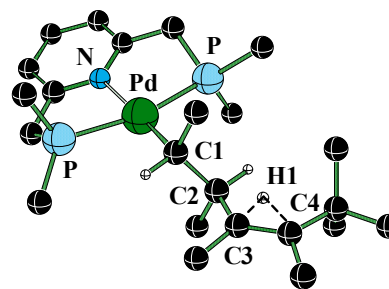
C2-C3	2.20	2.18,	2.10
Pd-C1	2.14	2.15,	2.18
C1-C2-C3	100.02,	99.34,	102.54
C2-C3-C4	97.74,	94.44,	101.62

**TS8<sub>add</sub>**



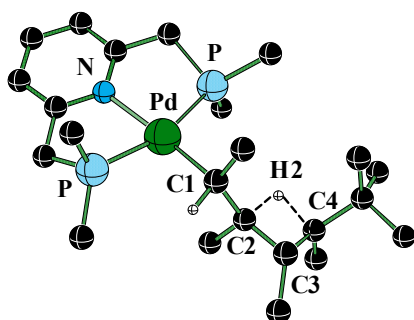
Pd-C1	2.07,	2.07,	2.13
C1-C2	1.52,	1.52,	1.52
C2-C3	1.61,	1.65,	1.69
C3-C4	1.45,	1.45,	1.45
Pd-C1-C2	112.16,	111.07,	111.55

**8c**



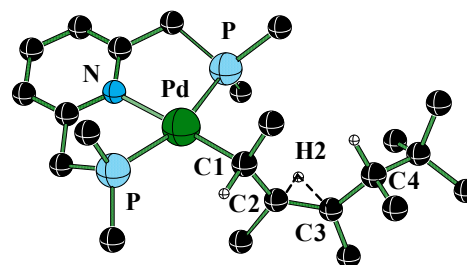
C3-H1	1.34,	1.42,	1.33
C4-H1	1.28,	1.24,	1.31
C3-H1-C4	65.10,	64.20,	65.30
C2-C3-C4	126.38,	125.82,	126.33

**TS8(c-d)**



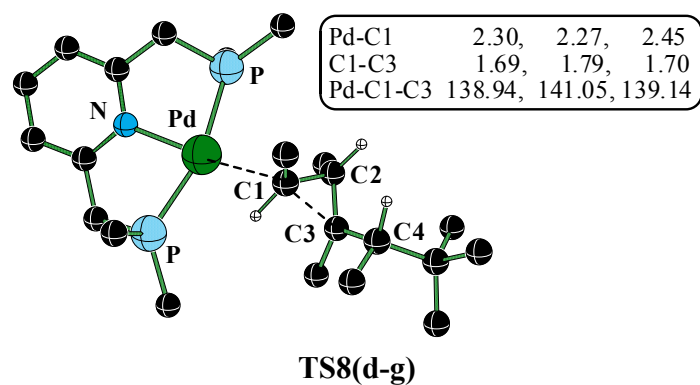
C2-H2	1.34,	1.34,	1.36
C4-H2	1.32,	1.32,	1.35
C2-H2-C4	93.43,	92.39,	95.72
C2-C3-C4	80.10,	78.90,	82.54

**TS8(c-e)**



C2-H2	1.23,	1.22,	1.26
C3-H2	1.42,	1.47,	1.40
C2-H2-C3	64.35,	63.54,	65.07

**TS8(d-e)**



**Fig. S4.** The optimized geometries of the key transition states obtained at the mPW1K/LANL2DZ(Pd),6-31+G\*\* level of theory for the palladium-PNP pincer catalyzed coupling between *trans*-butene and *tert*-butylbutene. Parameters are given as in the order mPW1K, M06-2X and B3LYP levels of theory. (Distances are given in Å and angles in °).

Total electronic energy (in a.u) and Cartesian coordinates of geometries optimized at the mPW1K/6-31+G\*\* level of theory. Gsol indicates the single-point energies at the PCM<sub>(CH<sub>3</sub>NO<sub>2</sub>)</sub>/mPW1K/6-311++G\*\* level of theory.

<b>TS1<sub>add</sub></b> Et = -1561.8570 Gsol = -1562.2470				<b>TS1(c-d)</b> Et = -1561.8634 Gsol = -1562.2447			
6	-3.069247	-1.001738	0.144761	6	-5.140280	-0.566442	-0.172403
6	-4.403270	-0.957207	0.505981	6	-4.615498	0.677359	0.129188
6	-4.942313	0.228265	0.971689	6	-3.242484	0.835113	0.195177
6	-4.130380	1.343720	1.072425	7	-2.411125	-0.192603	-0.057024
6	-2.796008	1.246659	0.724335	6	-2.912664	-1.402114	-0.361614
7	-2.280333	0.085740	0.268438	6	-4.278118	-1.620744	-0.412858
6	-1.872917	2.415972	0.881015	6	-2.636249	2.143730	0.602401
15	-0.457112	2.288286	-0.275251	15	-0.932749	2.321360	-0.053991
6	0.825039	3.389678	0.372783	6	-1.098367	3.051929	-1.705610
78	-0.257624	-0.021816	-0.273390	78	-0.287702	0.113241	0.024287
6	1.715783	-0.102357	-1.089180	6	1.713114	0.580975	0.135020
1	1.770509	-0.972497	-1.731231	1	1.955023	1.206903	-0.731199
6	-2.475405	-2.241478	-0.449100	6	-1.940246	-2.492099	-0.688463
15	-0.663934	-2.308709	-0.176879	15	-0.312029	-2.204280	0.109752
6	-0.010890	-3.448716	-1.421763	6	-0.453008	-2.914642	1.775152
6	-0.991361	3.006364	-1.849937	6	-0.142133	3.590329	0.967377
6	-0.420994	-3.112284	1.430018	6	0.802949	-3.324842	-0.784490
6	2.271842	-0.220073	0.201216	6	2.748458	-0.542925	0.204895
1	2.401335	0.655666	0.817541	1	2.521588	-1.208766	1.037392
6	4.574721	-0.626246	-0.298014	6	4.150480	-0.036831	0.485320
6	4.838304	0.048577	-1.596696	6	4.479129	0.150594	1.940059
6	4.739988	-0.109140	0.947150	6	5.132034	0.055562	-0.520184
6	5.099776	1.312477	1.217296	6	4.819185	-0.241076	-1.949505
6	4.635337	-0.981511	2.152729	6	6.551860	0.401736	-0.238005
1	6.149501	1.362811	1.511007	1	4.290164	1.068227	-0.089973
1	4.533375	1.708071	2.060194	1	-4.656130	-2.601746	-0.653457
1	-5.013472	-1.840684	0.404991	1	-6.208867	-0.712308	-0.218358
1	-5.984212	0.283578	1.248854	1	-5.261915	1.517347	0.328485
1	-4.521928	2.282403	1.431119	1	-1.761934	-2.494730	-1.766103
1	-2.629071	-2.221117	-1.530498	1	-2.346553	-3.468856	-0.431146
1	-2.975893	-3.132533	-0.074595	1	-2.554506	2.168656	1.691327
1	-1.456585	2.407088	1.890870	1	-3.273108	2.977434	0.312163
1	-2.411869	3.354792	0.767324	1	7.139225	-0.469909	-0.533831
1	1.911209	0.820050	-1.620582	1	6.771199	0.615276	0.799161
1	4.429035	-1.699628	-0.357635	1	6.887867	1.222711	-0.867012
1	4.972113	1.966343	0.361373	1	1.832793	1.218069	1.016460

1	2.265173	-1.162423	0.724767	1	2.729085	-1.143494	-0.699302
1	4.107891	-0.244263	-2.349930	1	-0.115538	3.179186	-2.152340
1	4.853761	1.131924	-1.530191	1	-1.679498	2.392590	-2.344882
1	5.810048	-0.269343	-1.975760	1	-1.587585	4.022417	-1.650476
1	-0.856053	-4.109919	1.425800	1	-0.676003	-3.978670	1.727081
1	0.639892	-3.200712	1.650267	1	0.477569	-2.775766	2.319814
1	-0.886638	-2.522237	2.215080	1	-1.242194	-2.407435	2.323975
1	-1.248013	4.056476	-1.724448	1	5.254284	0.882594	2.134354
1	-0.192298	2.925635	-2.582866	1	3.587679	0.445548	2.484933
1	-1.856279	2.468359	-2.229115	1	4.811245	-0.807312	2.339714
1	-0.492073	-4.421309	-1.336837	1	1.764578	-3.381836	-0.281990
1	-0.180550	-3.053953	-2.420147	1	0.379036	-4.327057	-0.814890
1	1.058465	-3.584647	-1.278009	1	0.954232	-2.975529	-1.802513
1	1.690654	3.379773	-0.285461	1	0.862046	3.783574	0.597916
1	0.452311	4.410965	0.426723	1	-0.705932	4.520388	0.931520
1	1.130916	3.075070	1.366968	1	-0.074818	3.252837	1.998144
1	5.576398	-0.962287	2.702908	1	5.077342	-1.287201	-2.125110
1	3.876741	-0.612260	2.845809	1	3.775371	-0.104994	-2.206933
1	4.420308	-2.017170	1.902732	1	5.435541	0.357413	-2.613276
NImag = 1 (-219.2495 cm <sup>-1</sup> )				NImag = 1 (-185.4331 cm <sup>-1</sup> )			
<b>TS1(c-e)</b>				<b>TS1(d-e)</b>			
Et = -1561.8568				Et = -1561.8615			
Gsol = -1562.2441				Gsol = -1562.2504			
6	4.051685	-1.220749	1.243232	6	4.341798	0.290324	-1.159968
6	2.732925	-1.171240	0.829282	6	3.044119	0.585123	-0.783216
7	2.209232	-0.046942	0.305069	7	2.230260	-0.367005	-0.287443
6	2.975831	1.051780	0.168357	6	2.678446	-1.629480	-0.147202
6	4.293012	1.061250	0.591168	6	3.959586	-1.979435	-0.534283
6	4.838662	-0.088320	1.133369	6	4.802678	-1.008797	-1.044181
6	1.830403	-2.358010	0.976393	6	2.486961	1.966068	-0.945786
15	0.479744	-2.306387	-0.263481	15	1.129599	2.267394	0.249802
6	1.166052	-3.001998	-1.791072	6	1.913085	2.780927	1.801928
78	0.176762	-0.005429	-0.331110	6	-2.516987	1.234124	-0.029928
15	0.551889	2.273302	-0.318943	6	-3.726875	0.805128	-0.599370
6	0.245434	3.161411	1.233044	6	-4.346175	-0.517871	-0.227213
6	2.375384	2.242609	-0.513685	6	-5.302214	-0.270918	0.945259
6	-1.750365	0.057087	-1.062885	6	1.768880	-2.628629	0.499060
6	-2.865280	-0.510002	-0.263938	15	0.006681	-2.177393	0.267219
6	-4.266800	-0.102770	-0.373727	6	-0.497031	-2.938852	-1.300567
6	-3.812430	0.466051	0.980232	6	-1.665520	0.572544	0.971108
6	-4.366759	-0.205676	2.219196	6	-0.894683	-3.062433	1.565138
1	-2.046780	1.035240	-1.437376	6	0.271600	3.742980	-0.364057
6	-0.061247	3.350342	-1.639447	6	-4.493976	1.741624	-1.477612

6	-0.731838	-3.529899	0.310037	6	-5.050518	-1.204476	-1.389387
1	-2.717944	-1.492428	0.174354	1	-2.557336	0.613919	-1.173260
6	-5.364794	-1.135124	-0.427328	1	4.294415	-2.998038	-0.418285
6	-3.735710	1.976876	1.021332	1	5.809140	-1.260490	-1.342564
1	-4.412151	0.695636	-1.093884	1	4.976414	1.070092	-1.550266
1	4.885677	1.955140	0.477895	1	1.952624	-2.623555	1.575941
1	5.867343	-0.103615	1.460385	1	1.979591	-3.636689	0.146361
1	4.450108	-2.133821	1.656387	1	2.054942	2.061338	-1.944414
1	2.575584	2.170520	-1.585143	1	3.272736	2.715155	-0.865507
1	2.834085	3.166850	-0.166835	1	-5.709180	-1.222282	1.278310
1	1.358371	-2.330310	1.960895	1	-6.142685	0.353231	0.650664
1	2.395584	-3.286715	0.919188	1	-4.804799	0.197058	1.792096
1	-3.881894	0.179019	3.111997	1	-1.525388	1.314028	1.760873
1	-4.252123	-1.285184	2.201634	1	-3.548469	-1.169466	0.128509
1	-5.429768	0.014604	2.288759	1	1.152097	2.961932	2.557169
1	-1.766710	-0.590634	-1.949802	1	2.569276	1.994013	2.164404
1	-2.665268	0.148071	1.010668	1	2.490398	3.692276	1.658651
1	0.409468	-2.998540	-2.571982	1	-0.367407	-4.018677	-1.260805
1	2.003842	-2.397699	-2.128818	1	-1.543116	-2.723990	-1.502968
1	1.502257	-4.024687	-1.631745	1	0.100073	-2.537563	-2.115308
1	0.659892	4.166634	1.185730	1	-5.412890	2.005839	-0.955294
1	-0.822634	3.235587	1.416887	1	-3.952324	2.659918	-1.682504
1	0.701705	2.626139	2.061728	1	-4.781703	1.276534	-2.415552
1	-6.320051	-0.693333	-0.156819	1	-0.681836	-4.128727	1.517782
1	-5.458647	-1.512577	-1.442368	1	-0.610227	-2.684406	2.543617
1	-5.182537	-1.980643	0.229935	1	-1.965643	-2.924536	1.439318
1	0.423973	4.323432	-1.593967	1	-0.511005	4.036643	0.332117
1	0.130922	2.900747	-2.610061	1	0.969014	4.574425	-0.449713
1	-1.132706	3.500979	-1.534087	1	-0.165244	3.555191	-1.341525
1	-1.535038	-3.631864	-0.416475	78	0.249455	0.120857	0.294836
1	-0.257794	-4.503935	0.418364	1	-2.215284	2.232324	-0.330218
1	-1.147498	-3.239836	1.271741	1	-2.162119	-0.280263	1.421616
1	-4.751556	2.366797	1.028501	1	-5.928391	-0.651408	-1.714940
1	-3.235676	2.321902	1.922066	1	-4.395625	-1.342481	-2.248788
1	-3.233600	2.385188	0.148377	1	-5.392561	-2.186862	-1.074274
NImag = 1 (-279.3503 cm <sup>-1</sup> )				NImag = 1 (-345.0394 cm <sup>-1</sup> )			
<b>TS1(d-g)</b> Et = -1561.8688 Gsol = -1562.2640				<b>TS2<sub>add</sub></b> Et = -1601.1683 Gsol = -1601.5646			
6	4.405610	0.537678	-0.487050	6	3.122318	1.171717	0.122628
6	3.041079	0.743097	-0.411645	6	4.462492	1.223355	0.459072
7	2.204228	-0.258313	-0.053820	6	5.099710	0.074628	0.891709
6	2.706933	-1.481420	0.231915	6	4.377711	-1.101528	0.985294

6	4.063305	-1.731723	0.144089	6	3.033214	-1.101276	0.663388
6	4.926475	-0.713499	-0.214791	7	2.421478	0.024608	0.239180
6	2.451512	2.071995	-0.758927	6	2.205904	-2.340679	0.815446
15	0.864546	2.305797	0.116180	15	0.759600	-2.300830	-0.308923
6	1.251709	2.941043	1.767172	6	-0.426782	-3.502599	0.342645
78	0.184619	0.076571	0.054905	78	0.385532	-0.012671	-0.257605
15	0.090873	-2.257640	0.021896	6	-1.609625	-0.075746	-1.032550
6	0.032380	-3.032897	-1.614035	1	-1.748446	0.800364	-1.653884
6	1.765750	-2.546476	0.692936	6	2.424193	2.372990	-0.435780
6	-2.004409	0.434783	0.682680	15	0.619483	2.297065	-0.125175
6	-3.300264	0.619168	-0.136234	6	-0.147569	3.404900	-1.333034
6	-3.921322	1.990337	-0.032607	6	1.311856	-2.949992	-1.907159
6	-2.107678	0.479815	-0.955713	6	0.353172	3.052231	1.501371
6	-4.248599	-0.575458	-0.097001	6	-2.109251	-0.023859	0.280978
6	-5.171177	-0.585547	-1.308947	1	-2.150864	-0.916816	0.884072
6	-5.038865	-0.643704	1.200948	6	-4.542624	0.304663	-0.210042
6	-1.040334	-3.195723	1.077865	6	-4.774892	-0.409359	-1.501540
6	-0.000911	3.637940	-0.750748	6	-4.499266	-0.328045	0.998135
1	-2.031074	-0.492038	1.234572	6	-4.653630	-1.811073	1.153548
1	-1.720526	1.359227	-1.445996	6	-4.453903	0.388310	2.310498
1	4.435009	-2.718032	0.372276	1	-5.695542	-2.046146	1.375816
1	5.989242	-0.891718	-0.278981	1	-4.075174	-2.172521	2.003152
1	5.048670	1.355396	-0.771358	1	5.001256	2.152852	0.364797
1	1.681418	-2.498123	1.781147	1	6.147930	0.094701	1.149149
1	2.145056	-3.536038	0.445552	1	4.846688	-2.013607	1.318842
1	2.230726	2.098197	-1.828512	1	2.557091	2.384171	-1.520042
1	3.156999	2.875651	-0.557123	1	2.863140	3.292628	-0.053248
1	-1.776820	1.321040	1.253665	1	1.812556	-2.382997	1.833620
1	-1.973715	-0.446546	-1.493395	1	2.812141	-3.233120	0.671159
1	-3.169800	2.774686	-0.092054	1	-1.742102	-1.003189	-1.574177
1	-4.623841	2.150859	-0.846581	1	-4.375955	-2.383515	0.275362
1	-4.456472	2.109887	0.905435	1	-2.177033	0.911891	0.812147
1	0.221751	-4.101800	-1.534457	1	-4.048688	-0.095945	-2.253221
1	-0.948629	-2.890100	-2.060999	1	-4.757235	-1.489764	-1.429927
1	0.776108	-2.584711	-2.267829	1	-5.752033	-0.125319	-1.894119
1	1.763256	3.899095	1.696122	1	0.713577	4.079193	1.505895
1	0.335899	3.077650	2.337370	1	-0.706221	3.058073	1.744575
1	1.883274	2.235300	2.300401	1	0.877736	2.485253	2.265981
1	-4.619746	-0.517959	-2.245824	1	1.651837	-3.978787	-1.805321
1	-5.749771	-1.505932	-1.330177	1	0.492407	-2.920641	-2.621211
1	-5.883225	0.236407	-1.276192	1	2.123681	-2.340705	-2.295689
1	-3.619382	-1.470508	-0.157152	1	0.264595	4.408414	-1.244836
1	-0.752014	-4.245486	1.091290	1	0.021300	3.037886	-2.342047
1	-1.021264	-2.812037	2.094824	1	-1.219158	3.461224	-1.156493
1	-2.055484	-3.128964	0.694577	1	-1.302933	-3.543158	-0.300394
1	-0.933697	3.872356	-0.243970	1	0.018206	-4.495543	0.372110



1	0.614529	4.536151	-0.754243	1	-0.737051	-3.226582	1.346961
1	-0.215165	3.357852	-1.778903	1	-5.355874	0.152406	2.876265
1	-4.396231	-0.615154	2.080358	1	-3.621019	0.031866	2.919943
1	-5.748657	0.177325	1.277852	1	-4.395194	1.467508	2.236820
1	-5.614758	-1.565087	1.241897	6	-4.557191	1.794492	-0.367194
NImag = 1 (-46.2700 cm <sup>-1</sup> )				1	-5.573330	2.127859	-0.580935
				1	-4.216098	2.344504	0.502811
				1	-3.957287	2.091367	-1.227978
				NImag = 1 (-179.3100 cm <sup>-1</sup> )			
<b>TS2(c-d)</b>				<b>TS2(c-e)</b>			
Et = -1601.1731				Et = -1601.1647			
Gsol = -1601.5596				Gsol = -1601.5571			
6	5.185366	0.006447	0.996494	6	-4.263520	1.126562	1.142019
6	4.434152	-1.149877	1.107012	6	-2.933586	1.115082	0.762165
6	3.096232	-1.123255	0.755014	7	-2.359044	0.000396	0.271832
7	2.523229	0.000124	0.287041	6	-3.084324	-1.125968	0.135789
6	3.250965	1.123319	0.154019	6	-4.410853	-1.173258	0.525609
6	4.585643	1.157471	0.518206	6	-5.008639	-0.033865	1.033235
6	2.227975	-2.334174	0.922496	6	-2.076147	2.334732	0.910878
15	0.784370	-2.283396	-0.211792	15	-0.688549	2.305926	-0.288186
6	1.344273	-3.011876	-1.775759	6	-1.350074	2.953089	-1.847733
78	0.452709	-0.000887	-0.264020	78	-0.308620	0.016194	-0.307646
6	-1.522890	-0.016461	-0.867369	15	-0.608423	-2.273172	-0.270234
1	-1.750375	0.917575	-1.388751	6	-0.312755	-3.130535	1.301137
6	2.587457	2.318892	-0.460463	6	-2.426796	-2.306660	-0.510123
15	0.765411	2.280291	-0.230797	6	1.643500	0.018986	-0.977443
6	0.454767	3.140397	1.337906	6	2.696691	0.610299	-0.116381
6	-0.395761	-3.478293	0.474223	6	4.138269	0.338364	-0.161421
6	0.106118	3.370282	-1.520340	6	3.629577	-0.372999	1.134627
6	-2.517326	-0.224861	0.269391	6	4.071215	0.234594	2.453667
1	-2.340992	-1.190841	0.749064	1	1.974623	-0.942868	-1.359451
6	-3.992388	-0.253373	-0.113429	6	0.069802	-3.348778	-1.560019
6	-4.299122	-0.977866	-1.391828	6	0.468075	3.576000	0.297496
6	-4.988775	-0.001784	0.849501	1	2.445521	1.544493	0.376452
6	-4.655805	0.345035	2.271487	6	5.048714	1.534071	0.051697
6	-6.426703	-0.385856	0.670818	6	3.650979	-1.888520	1.099870
1	5.148721	2.070909	0.409692	1	-4.970074	-2.088651	0.413898
1	6.228056	0.009315	1.275936	1	-6.045240	-0.048158	1.334252
1	4.874503	-2.063040	1.474979	1	-4.702927	2.032499	1.528472
1	2.764183	2.298383	-1.538226	1	-2.602219	-2.259074	-1.587259
1	3.023003	3.243905	-0.086570	1	-2.862821	-3.240131	-0.158803
1	1.826777	-2.342962	1.938336	1	-1.632423	2.342260	1.908800
1	2.807460	-3.247984	0.802420	1	-2.670586	3.242159	0.819192

1	-6.586182	-1.304781	1.235743	1	3.582359	-0.271173	3.281699
1	-6.728404	-0.567208	-0.352128	1	3.857455	1.295507	2.529186
1	-7.079026	0.368667	1.102266	1	5.144970	0.101338	2.563487
1	-1.637245	-0.802213	-1.613448	1	1.675025	0.683681	-1.851477
1	-2.351627	0.515243	1.046827	1	2.475320	-0.142665	1.132212
1	0.534422	-2.993411	-2.500927	1	-0.571001	2.958379	-2.606199
1	2.169250	-2.429063	-2.176942	1	-2.159204	2.317747	-2.198136
1	1.667028	-4.041159	-1.632580	1	-1.720813	3.967884	-1.717431
1	0.831749	4.160631	1.301402	1	-0.698498	-4.147369	1.259587
1	-0.612677	3.170803	1.540656	1	0.752454	-3.172802	1.509821
1	0.941344	2.608304	2.151204	1	-0.802005	-2.596185	2.111387
1	-5.348913	-0.990320	-1.653669	1	6.022976	1.216305	0.414604
1	-3.740143	-0.555240	-2.220575	1	5.207897	2.035531	-0.900015
1	-3.974649	-2.010994	-1.271450	1	4.649587	2.265111	0.748261
1	-0.967082	3.488165	-1.393796	1	-0.385255	-4.336191	-1.511725
1	0.566116	4.354989	-1.466128	1	-0.113762	-2.918951	-2.541212
1	0.292479	2.941527	-2.501435	1	1.142650	-3.463649	-1.427595
1	-1.264775	-3.548825	-0.175622	1	1.296318	3.680115	-0.400023
1	0.055704	-4.466051	0.545498	1	-0.034796	4.539447	0.361693
1	-0.717986	-3.165880	1.464046	1	0.854190	3.322807	1.281745
1	-3.712977	0.860163	2.402971	1	4.681847	-2.228186	1.034099
1	-5.448717	0.937774	2.718635	1	3.223831	-2.286974	2.016053
1	-4.602339	-0.591755	2.826761	1	3.111142	-2.301461	0.253974
6	-4.654865	1.383762	-0.288459	6	4.681243	-0.554012	-1.258996
1	-4.812689	2.089048	0.521291	1	4.789144	0.026769	-2.171846
1	-5.467784	1.386094	-0.999957	1	5.671323	-0.912258	-0.987254
1	-3.722695	1.677533	-0.765944	1	4.064989	-1.415647	-1.487014
NImag = 1 (-247.0783 cm <sup>-1</sup> )				NImag = 1 (-257.6856 cm <sup>-1</sup> )			
<p style="text-align: center;"><b>TS2(d-e)</b>                      Et = -1601.1628                      Gsol = -1601.5555</p>				<p style="text-align: center;"><b>TS2(d-g)</b>                      Et = -1601.1726                      Gsol = -1601.5727</p>			
6	4.410984	0.630454	-1.214845	6	4.507059	0.671623	-0.542720
6	3.098241	0.801681	-0.814532	6	3.137130	0.825967	-0.446549
7	2.386295	-0.220787	-0.303652	7	2.342545	-0.201039	-0.065787
6	2.956676	-1.433448	-0.164877	6	2.897688	-1.400690	0.221556
6	4.258480	-1.661493	-0.572867	6	4.260984	-1.601066	0.114717
6	4.995528	-0.618254	-1.103553	6	5.080028	-0.555603	-0.267372
6	2.410971	2.123599	-0.958109	6	2.494022	2.127463	-0.793265
15	1.072919	2.291078	0.284384	15	0.923456	2.318248	0.118232
6	1.874443	2.808402	1.826721	6	1.338024	2.942139	1.767457
6	-2.454961	1.135360	0.166257	78	0.308095	0.057490	0.064342
6	-3.704900	0.912406	-0.442728	15	0.313196	-2.278185	0.049411

6	-4.488112	-0.400626	-0.367559	6	0.270438	-3.059076	-1.584146
6	-4.975635	-0.536550	1.081951	6	2.004882	-2.494718	0.702563
6	2.153552	-2.508169	0.498622	6	-1.916966	0.287701	0.728735
15	0.359179	-2.239683	0.235782	6	-3.171226	0.688123	-0.064850
6	-0.012673	-3.026410	-1.355877	6	-3.533894	2.145721	0.115355
6	-1.573188	0.312072	1.005018	6	-2.002011	0.429071	-0.900824
6	-0.471060	-3.233251	1.501980	6	-4.366980	-0.290259	-0.121584
6	0.119486	3.738433	-0.256016	6	-3.954750	-1.754331	-0.010093
6	-4.382092	2.114846	-1.032305	6	-5.336032	0.009561	1.021508
6	-5.704775	-0.379532	-1.293132	6	-0.736340	-3.280055	1.129653
1	-2.583429	0.751860	-1.091044	6	0.052452	3.665920	-0.721335
1	4.691070	-2.642659	-0.457826	1	-1.991371	-0.691395	1.169523
1	6.015627	-0.774927	-1.420094	1	-1.547621	1.273888	-1.393807
1	4.961191	1.465632	-1.618381	1	4.671788	-2.570943	0.346139
1	2.325640	-2.462553	1.576305	1	6.147594	-0.694360	-0.347238
1	2.467397	-3.495885	0.166222	1	5.113019	1.510710	-0.845579
1	1.939625	2.180644	-1.941686	1	1.929330	-2.439684	1.791119
1	3.125582	2.942576	-0.897216	1	2.416997	-3.472168	0.459615
1	-5.583791	-1.434000	1.169409	1	2.244762	2.134498	-1.856925
1	-5.600880	0.305999	1.371854	1	3.174449	2.958314	-0.617008
1	-4.158514	-0.613077	1.794685	1	-1.602057	1.084580	1.386434
1	-1.439792	0.911435	1.911341	1	-1.962212	-0.497532	-1.450822
1	1.130561	2.916816	2.612253	1	-2.656126	2.779751	0.018484
1	2.591640	2.055067	2.141802	1	-4.247656	2.467940	-0.637504
1	2.387287	3.759051	1.694044	1	-3.969511	2.326474	1.093708
1	0.234862	-4.085720	-1.321610	1	0.503821	-4.119217	-1.504405
1	-1.067539	-2.922010	-1.592014	1	-0.719682	-2.956700	-2.021658
1	0.564555	-2.550376	-2.144363	1	0.988797	-2.581898	-2.245724
1	-5.225527	2.362573	-0.388012	1	1.834136	3.908190	1.695177
1	-3.731144	2.982850	-1.070359	1	0.432628	3.060071	2.358146
1	-4.781770	1.922199	-2.021964	1	1.990759	2.240513	2.280173
1	-0.145362	-4.270062	1.443121	1	-4.822335	-2.382927	-0.195239
1	-0.245349	-2.844086	2.491344	1	-3.204616	-2.044695	-0.747264
1	-1.548021	-3.207780	1.356313	1	-3.601005	-2.003307	0.989562
1	-0.635528	3.991397	0.485224	1	-0.349414	-4.297249	1.167131
1	0.779914	4.597745	-0.359720	1	-0.749702	-2.871863	2.137128
1	-0.358429	3.553271	-1.214632	1	-1.751740	-3.317081	0.746998
78	0.370375	0.072583	0.297062	1	-0.827621	3.962099	-0.157658
1	-2.113689	2.157033	0.039557	1	0.711854	4.529979	-0.790141
1	-2.035358	-0.617935	1.305773	1	-0.246623	3.376640	-1.725394
1	-6.413365	0.403787	-1.037930	1	-4.840763	-0.030066	1.991690
1	-5.427485	-0.273029	-2.340382	1	-5.808026	0.983045	0.917270
1	-6.230484	-1.326041	-1.194705	1	-6.133631	-0.730061	1.030620
6	-3.626287	-1.595651	-0.776243	6	-5.075323	-0.093345	-1.463978
1	-3.324063	-1.516783	-1.820805	1	-5.949060	-0.739000	-1.518960
1	-2.736758	-1.706467	-0.164845	1	-5.425946	0.926291	-1.602280

1	-4.211535	-2.506667	-0.676832	1	-4.427312	-0.345626	-2.303061
NImag = 1 (-417.8273 cm <sup>-1</sup> )				NImag = 1 (-44.1704 cm <sup>-1</sup> )			
<b>TS3<sub>add</sub></b> Et = -1679.7801 Gsol = -1680.2125				<b>TS3(c-d)</b> Et = -1679.7826 Gsol = -1680.1979			
6	-3.381753	-1.247331	0.332441	6	-5.515367	-0.728017	-0.687213
6	-4.640279	-1.375984	0.890817	6	-5.078659	0.543419	-0.361007
6	-5.202154	-0.301095	1.555504	6	-3.734178	0.754165	-0.110937
6	-4.487384	0.879273	1.653307	7	-2.843350	-0.249828	-0.207437
6	-3.221736	0.954736	1.102126	6	-3.257653	-1.486203	-0.533948
7	-2.683949	-0.099219	0.453167	6	-4.594533	-1.756815	-0.766995
6	-2.391909	2.194073	1.242503	6	-3.231984	2.096628	0.327805
15	-1.179938	2.321207	-0.126191	15	-1.460701	2.315003	-0.093317
6	0.084619	3.496129	0.418031	6	-1.416560	2.979809	-1.779754
78	-0.769882	0.054260	-0.389333	78	-0.763217	0.136932	0.158923
6	1.047108	0.244566	-1.499872	6	1.183786	0.690660	0.534018
1	1.081815	-0.568480	-2.213981	1	1.498362	1.368138	-0.265130
6	-2.780201	-2.357776	-0.472165	6	-2.213435	-2.548470	-0.680312
15	-0.949566	-2.262056	-0.475020	15	-0.729256	-2.175834	0.334743
6	-0.398819	-3.210508	-1.914726	6	-1.097880	-2.828255	1.988620
6	-2.033560	3.105880	-1.518026	6	-0.859585	3.646870	0.976228
6	-0.392049	-3.183904	0.983428	6	0.535651	-3.290839	-0.339569
6	1.791838	0.096561	-0.313062	6	2.259955	-0.391166	0.672954
1	1.938977	0.937608	0.345047	1	1.992273	-1.071416	1.483683
6	4.027740	0.007023	-1.141869	6	3.595751	0.160696	1.099321
6	3.960191	0.852898	-2.368701	6	3.645522	0.539638	2.553891
6	4.431894	0.417329	0.090912	6	4.747620	0.277575	0.288836
6	4.670539	1.869664	0.363245	6	4.838454	-0.190878	-1.180839
6	4.788615	-0.557844	1.203469	6	4.844912	-1.725062	-1.168880
6	4.638153	-2.019705	0.794954	6	6.040028	0.679271	0.939584
6	6.264634	-0.317954	1.560271	6	6.147538	0.279055	-1.824021
6	3.936024	-0.309369	2.454165	6	3.712757	0.363714	-2.060324
1	5.681746	2.136646	0.052436	1	3.914247	1.246223	0.360657
1	4.590248	2.117780	1.416696	1	-4.903024	-2.758313	-1.021881
1	-5.177762	-2.305305	0.787988	1	-6.561687	-0.914790	-0.875880
1	-6.187617	-0.380881	1.989011	1	-5.773691	1.364503	-0.284294
1	-4.899256	1.734866	2.164569	1	-1.880119	-2.575048	-1.720139
1	-3.101821	-2.252996	-1.510964	1	-2.619978	-3.531946	-0.450495
1	-3.135366	-3.326959	-0.126830	1	-3.301339	2.157973	1.416135
1	-1.815743	2.133287	2.168560	1	-3.848995	2.897101	-0.076422
1	-3.022218	3.078341	1.316438	1	6.683334	-0.200721	0.933691
1	1.067820	1.217497	-1.973021	1	5.939231	0.997961	1.967319
1	3.986822	-1.058328	-1.324319	1	6.554630	1.451032	0.378324

1	3.997522	2.514003	-0.195964	1	1.159241	1.288096	1.448979
1	1.955999	-0.874385	0.122769	1	2.338641	-0.981027	-0.229317
1	4.916454	-2.657230	1.630851	1	-0.385270	3.130644	-2.088873
1	3.613208	-2.279572	0.525525	1	-1.877640	2.274730	-2.466382
1	5.286112	-2.281017	-0.039178	1	-1.942213	3.931146	-1.834194
1	6.571687	-1.028750	2.324937	1	-1.293036	-3.898119	1.949427
1	6.909154	-0.460616	0.694855	1	-0.259395	-2.648280	2.656569
1	6.436498	0.680102	1.955199	1	-1.967484	-2.319533	2.396525
1	3.211353	0.482198	-3.066169	1	4.130751	1.490658	2.747018
1	3.759286	1.901528	-2.168934	1	2.643864	0.582660	2.966226
1	4.915928	0.803774	-2.892005	1	4.202318	-0.228467	3.091534
1	-0.726331	-4.218176	0.927143	1	4.981263	-2.087014	-2.185375
1	0.693426	-3.175323	1.041610	1	5.670154	-2.114531	-0.575157
1	-0.788176	-2.728635	1.887417	1	3.922480	-2.152908	-0.785288
1	-2.364129	4.107350	-1.249375	1	6.169789	-0.078211	-2.850385
1	-1.362369	3.174825	-2.370629	1	6.224266	1.364162	-1.862082
1	-2.894475	2.510429	-1.810594	1	7.032031	-0.117328	-1.333933
1	4.260596	-0.977506	3.249115	1	3.883801	0.040149	-3.084087
1	4.032886	0.704618	2.834192	1	2.716678	0.036153	-1.785919
1	2.878681	-0.508475	2.279333	1	3.726878	1.453845	-2.067765
1	-0.784101	-4.227460	-1.869033	1	1.422302	-3.281799	0.288388
1	-0.743320	-2.740142	-2.831992	1	0.155475	-4.310405	-0.371454
1	0.687386	-3.259472	-1.934518	1	0.809422	-2.985852	-1.346200
1	0.825644	3.629141	-0.366757	1	0.179561	3.863308	0.740543
1	-0.364205	4.465235	0.628197	1	-1.441777	4.553903	0.826193
1	0.579568	3.135494	1.315856	1	-0.924471	3.349115	2.019407
NImag = 1 (-243.3073 cm <sup>-1</sup> )				NImag = 1 (-282.0931 cm <sup>-1</sup> )			
<b>TS3(c-e)</b>				<b>TS3(d-e)</b>			
Et = -1679.7807				Et = -1679.7846			
Gsol = -1680.2099				Gsol = -1680.2095			
6	-4.125104	1.623747	1.476770	6	-4.582483	0.073630	1.623641
6	-2.865954	1.406506	0.946826	6	-3.361471	0.439742	1.086956
7	-2.541972	0.232385	0.375410	7	-2.606347	-0.444142	0.407226
6	-3.455319	-0.754954	0.306162	6	-3.041935	-1.706784	0.232213
6	-4.719966	-0.597650	0.844398	6	-4.244288	-2.128146	0.771000
6	-5.060666	0.605891	1.435033	6	-5.024932	-1.228394	1.474118
6	-1.804142	2.458713	1.014350	6	-2.820537	1.824503	1.264969
15	-0.586722	2.246657	-0.342319	15	-1.678232	2.251896	-0.104700
6	-1.334782	3.021547	-1.802561	6	-2.725094	2.772437	-1.491091
78	-0.583694	-0.080021	-0.418180	6	1.947532	1.533877	-0.512982
15	-1.266573	-2.283440	-0.370579	6	3.248338	1.323457	-0.022410
6	-0.950522	-3.220950	1.148718	6	3.979270	0.027302	-0.285102
6	-3.077437	-2.005928	-0.425062	6	4.919011	0.282005	-1.467486

6	1.242056	-0.522333	-1.269351	6	-2.212373	-2.620573	-0.615637
6	2.451312	0.322886	-1.079327	15	-0.444342	-2.138224	-0.571898
6	3.839383	-0.174047	-1.104255	6	0.265893	-3.004435	0.854111
6	3.677427	0.362120	0.314947	6	1.068105	0.663421	-1.302233
6	4.267030	1.738899	0.540782	6	0.308534	-2.887181	-2.038115
1	1.523419	-1.561498	-1.127497	6	-0.838458	3.764349	0.444300
6	-0.894890	-3.410848	-1.736794	6	3.958734	2.500410	0.576791
6	0.776905	3.353367	0.122993	6	4.649145	-0.656220	0.944910
1	2.352350	1.365895	-1.362245	6	3.709152	-0.586141	2.146973
6	4.856504	0.421893	-2.046895	6	6.013128	-0.075793	1.314189
6	3.793286	-0.651514	1.483933	6	4.850938	-2.130473	0.588372
6	5.251133	-1.113359	1.531051	1	2.208067	1.090627	0.711032
6	2.884381	-1.861803	1.299298	1	-4.569388	-3.145814	0.623546
6	3.421334	0.021423	2.803775	1	-5.970146	-1.536534	1.894765
1	3.874207	-1.257302	-1.114572	1	-5.170759	0.800306	2.161194
1	-5.432336	-1.405076	0.783453	1	-2.537751	-2.526090	-1.654164
1	-6.045524	0.750599	1.852695	1	-2.356671	-3.660898	-0.329943
1	-4.361106	2.575422	1.925944	1	-2.239156	1.868005	2.188526
1	-3.343899	-1.889954	-1.477997	1	-3.627639	2.548866	1.359787
1	-3.630984	-2.864169	-0.048735	1	5.395473	-0.645758	-1.769621
1	-1.254324	2.355672	1.952352	1	5.706204	0.989561	-1.223666
1	-2.241819	3.455640	1.007634	1	4.375230	0.663108	-2.330055
1	3.890148	2.198706	1.447160	1	0.763326	1.275801	-2.155599
1	4.078859	2.411584	-0.289629	1	3.224321	-0.682021	-0.625011
1	5.346160	1.643655	0.633272	1	-2.105298	3.032557	-2.345704
1	1.075203	-0.403769	-2.349449	1	-3.381468	1.957382	-1.784480
1	2.471870	0.581672	0.300476	1	-3.326513	3.636820	-1.216335
1	-0.668397	2.928158	-2.656506	1	0.144358	-4.080457	0.744362
1	-2.267449	2.519837	-2.046960	1	1.326133	-2.781367	0.935936
1	-1.531626	4.076536	-1.622125	1	-0.224908	-2.680449	1.768193
1	-1.509144	-4.155028	1.141176	1	4.771539	2.777751	-0.091676
1	0.108397	-3.450937	1.230426	1	3.306726	3.362971	0.680374
1	-1.244204	-2.635043	2.015738	1	4.397532	2.272515	1.541025
1	5.865862	0.200913	-1.709795	1	5.303820	-2.659081	1.424326
1	4.738990	-0.020875	-3.032602	1	3.904615	-2.623756	0.362844
1	4.762150	1.498302	-2.154671	1	5.510385	-2.261526	-0.266519
1	3.438918	-0.716242	3.602448	1	4.090079	-1.196731	2.962750
1	4.118320	0.805881	3.085471	1	3.602779	0.423887	2.544448
1	2.415028	0.442465	2.774138	1	2.714454	-0.967355	1.903013
1	5.376104	-1.812831	2.354834	1	6.410457	-0.610647	2.174473
1	5.547058	-1.626792	0.618204	1	6.732344	-0.194425	0.507333
1	5.940305	-0.290256	1.703780	1	5.983946	0.976483	1.583758
1	3.022309	-2.531495	2.144931	1	0.128172	-3.960352	-2.052598
1	1.834689	-1.569907	1.276579	1	-0.103892	-2.442854	-2.940105
1	3.114140	-2.437659	0.405163	1	1.383315	-2.723283	-2.031625
1	-1.467782	-4.330793	-1.637515	1	-0.222575	4.164401	-0.358193



1	-1.134447	-2.941502	-2.687166	1	-1.573872	4.523510	0.705268
1	0.162131	-3.665282	-1.732565	1	-0.218335	3.569604	1.315423
1	1.474713	3.465094	-0.703097	78	-0.733840	0.146483	-0.399124
1	0.385883	4.341824	0.358666	1	1.567363	2.530631	-0.315807
1	1.305394	2.973627	0.993471	1	1.603056	-0.193105	-1.696129
NImag = 1 (-301.2108 cm <sup>-1</sup> )				NImag = 1 (-336.3576 cm <sup>-1</sup> )			
<b>TS3(d-g)</b> Et = -1679.7795 Gsol = -1680.2142				<b>TS4<sub>add</sub></b> Et = -1758.4001 Gsol = -1758.8435			
6	4.911816	0.633666	-0.190763	6	4.516365	-2.235275	-0.296716
6	3.540735	0.800582	-0.237564	6	5.448598	-1.350187	-0.806040
7	2.701621	-0.218453	0.058425	6	5.076948	-0.036567	-1.027337
6	3.212226	-1.423254	0.401397	6	3.780731	0.358943	-0.751111
6	4.577302	-1.636320	0.437261	7	2.880717	-0.509732	-0.248063
6	5.441336	-0.598661	0.142627	6	3.239605	-1.786629	-0.010648
6	2.947673	2.107232	-0.647557	6	3.327249	1.755871	-1.042066
15	1.299265	2.313418	0.112224	15	1.912391	2.221661	0.024616
6	1.571301	2.904474	1.802833	78	0.919291	0.144316	0.199924
78	0.666420	0.058623	-0.026409	15	0.520391	-2.150580	0.242406
15	0.654878	-2.274860	-0.050483	6	0.118291	-2.893960	-1.364094
6	0.788498	-3.055613	-1.679121	6	2.230316	-2.691370	0.621527
6	2.262806	-2.508694	0.784366	6	2.610493	2.880775	1.561861
6	-1.612892	0.312292	0.371514	6	-0.952143	0.968599	0.844512
6	-2.767967	0.718517	-0.563516	6	-1.809020	0.409814	-0.164487
6	-3.071071	2.200185	-0.524242	6	-1.765165	0.884372	-1.579521
6	-1.514401	0.412488	-1.256340	6	-1.167257	0.574940	2.288361
6	-3.968878	-0.242484	-0.705014	6	-3.811336	1.169698	0.564614
6	-3.544092	-1.704934	-0.792542	6	-4.581412	0.551197	-0.383357
6	-5.119077	-0.052758	0.344331	6	-5.076930	-0.875983	-0.240983
6	-6.081968	-1.244272	0.270660	6	-6.611200	-0.847813	-0.347267
6	-4.576406	0.028740	1.769090	6	-3.612941	2.654097	0.635335
6	-5.976446	1.180290	0.040022	6	-5.062543	1.320269	-1.565610
6	-0.521742	-3.265131	0.901201	6	-4.524697	-1.751260	-1.374131
6	0.535685	3.692994	-0.777855	6	-4.713343	-1.510197	1.097282
1	-1.766576	-0.656618	0.815188	1	-6.008650	1.800518	-1.303889
1	-0.994575	1.241990	-1.709311	1	-5.258365	0.695951	-2.431877
1	4.952949	-2.609712	0.709962	1	4.776662	-3.263936	-0.103773
1	6.510074	-0.747386	0.174387	1	6.453217	-1.679084	-1.024901
1	5.553777	1.466786	-0.429028	1	5.780182	0.678306	-1.424260
1	2.070824	-2.452696	1.858403	1	2.341344	-2.638893	1.707024
1	2.688847	-3.490064	0.585345	1	2.399919	-3.727684	0.334587
1	2.802367	2.114530	-1.730334	1	2.972691	1.806364	-2.073997
1	3.616541	2.931517	-0.407476	1	4.153035	2.459600	-0.955009

1	-1.367288	1.114593	1.051767	1	-0.863702	2.045348	0.729927
1	-1.410455	-0.523789	-1.776317	1	-3.678873	0.639253	1.496434
1	-2.161336	2.781131	-0.653521	1	-4.384613	2.118435	-1.850833
1	-3.745326	2.469325	-1.333385	1	-2.114427	-0.616975	-0.014466
1	-3.525973	2.502084	0.412720	1	-5.098134	-2.526849	1.130348
1	0.996999	-4.118653	-1.573372	1	-3.636754	-1.567634	1.258254
1	-0.143461	-2.940817	-2.227313	1	-5.151308	-0.971936	1.935529
1	1.584541	-2.589290	-2.253772	1	-6.997848	-1.853182	-0.193966
1	2.086114	3.863365	1.791593	1	-7.050578	-0.204413	0.412798
1	0.617949	3.027453	2.311146	1	-6.952750	-0.511844	-1.322539
1	2.164674	2.184569	2.360370	6	-0.506055	-3.024993	1.453683
1	-4.346631	-2.304872	-1.205996	6	1.121271	3.625617	-0.801100
1	-2.692136	-1.865180	-1.450052	1	-0.816727	0.580124	-2.022784
1	-3.315540	-2.120188	0.188310	1	-2.558961	0.455362	-2.179645
1	-4.397839	0.019067	-1.676913	1	-1.817400	1.968837	-1.640418
1	-6.938560	-1.052026	0.912544	1	-2.892596	2.917922	1.404548
1	-6.464458	-1.392378	-0.738959	1	-3.286634	3.096686	-0.303186
1	-5.636118	-2.175754	0.610627	1	-4.549694	3.142594	0.903580
1	-3.953618	0.907411	1.932150	1	-1.981736	1.144583	2.736949
1	-5.400787	0.088794	2.476832	1	-1.408614	-0.480425	2.390061
1	-3.996967	-0.855705	2.036709	1	-0.282396	0.770079	2.888950
1	-5.471916	2.126529	0.194669	1	0.187369	-3.978862	-1.312974
1	-6.345612	1.156747	-0.984893	1	-0.891953	-2.624132	-1.661316
1	-6.847189	1.185028	0.692415	1	0.805214	-2.527604	-2.122750
1	-0.146629	-4.282979	0.996055	1	3.217387	3.761528	1.360896
1	-0.660752	-2.846422	1.894676	1	1.808323	3.156638	2.242183
1	-1.480655	-3.303440	0.393103	1	3.223745	2.125269	2.045997
1	-0.379336	4.004305	-0.281841	1	-4.948236	-2.750409	-1.296434
1	1.220498	4.539865	-0.779246	1	-4.778860	-1.371301	-2.360276
1	0.312704	3.425039	-1.807203	1	-3.440500	-1.852601	-1.319725
NImag = 1 (-45.3083 cm <sup>-1</sup> )				1	-0.323964	-4.096395	1.388989
				1	-0.276147	-2.687376	2.460622
				1	-1.560301	-2.848080	1.257564
				1	0.309910	4.011991	-0.189173
				1	1.843016	4.426582	-0.950749
				1	0.722275	3.323172	-1.765490
				NImag = 1 (-282.7654 cm <sup>-1</sup> )			
<b>TS4(c-d)</b> Et = -1758.3936 Gsol = -1758.8215				<b>TS4(d-e)</b> Et = -1758.3879 Gsol = -1758.8222			
6	5.145228	0.011503	-0.864056	6	5.148357	0.430515	0.702386
6	3.838020	0.393364	-0.618561	6	3.889927	-0.104660	0.492411



7	2.922806	-0.492662	-0.186978	7	2.851005	0.675100	0.138249
6	3.271572	-1.775927	0.006787	6	3.029763	1.999467	-0.014077
6	4.557766	-2.217288	-0.250686	6	4.261191	2.588506	0.211775
6	5.507744	-1.311500	-0.686260	6	5.335217	1.794547	0.570375
6	3.386621	1.800514	-0.867156	6	3.634669	-1.567535	0.692441
15	1.917811	2.213697	0.150078	15	2.182796	-2.117052	-0.280803
6	1.193272	3.677888	-0.634774	6	2.793800	-2.488013	-1.947481
78	0.896656	0.151138	0.189730	6	-1.873596	-1.125914	0.708438
15	0.528494	-2.140586	0.174157	6	-3.282383	-0.934519	0.767935
6	-0.482695	-3.060541	1.368049	6	-4.133207	-0.460916	-0.375858
6	2.234569	-2.698138	0.566077	6	-4.854790	-1.710783	-0.898340
6	-1.007728	0.893414	0.593495	6	1.867691	2.807046	-0.498378
6	-2.082897	0.465096	-0.424158	15	0.257947	2.034011	-0.069934
6	-3.406916	1.194692	-0.247265	6	-0.182540	2.721919	1.553054
6	-4.686524	0.600793	-0.122106	6	-0.930811	-1.142561	-0.481591
6	-5.886172	1.504673	-0.135109	6	-0.890108	2.794779	-1.250736
6	-1.407334	0.573661	2.026401	6	1.701055	-3.716612	0.421214
6	0.145021	-2.888989	-1.437120	6	-3.985730	-1.313231	2.037387
6	2.552004	2.790348	1.748526	6	-5.083645	0.758766	-0.103506
6	-1.662306	0.733772	-1.873956	6	-4.411065	1.758541	0.832854
6	-3.322217	2.697795	-0.340223	6	-6.464303	0.403817	0.448788
6	-4.977436	-0.920622	-0.155700	6	-5.294870	1.437653	-1.459758
6	-6.476951	-1.207123	-0.018742	1	-2.287616	0.017103	1.005303
6	-4.298607	-1.649545	1.007064	1	4.376560	3.653800	0.089267
6	-4.537495	-1.476643	-1.515383	1	6.306898	2.232710	0.741121
1	-3.974082	0.869528	0.919316	1	5.965707	-0.216182	0.979726
1	4.811450	-3.253724	-0.093686	1	1.906978	2.852823	-1.589068
1	6.519690	-1.632158	-0.882309	1	1.925076	3.832793	-0.138150
1	5.862955	0.741501	-1.203449	1	3.395649	-1.746623	1.743026
1	2.316410	-2.695348	1.655411	1	4.523605	-2.153053	0.464218
1	2.403873	-3.722891	0.239420	1	-5.454846	-1.446879	-1.764815
1	3.080089	1.894696	-1.911211	1	-5.518898	-2.149025	-0.158226
1	4.201544	2.505106	-0.710190	1	-4.148121	-2.476152	-1.212545
1	-6.337750	1.425107	-1.124717	1	-0.681880	-2.208385	-0.469424
1	-5.660262	2.547090	0.037345	1	-3.465664	-0.126203	-1.158745
1	-6.634535	1.188452	0.581271	1	1.969837	-2.813348	-2.577842
1	-0.922680	1.977804	0.522210	1	3.229071	-1.595550	-2.389262
1	-2.247635	-0.601959	-0.319652	1	3.543826	-3.275945	-1.916020
1	1.721275	3.038658	2.404486	1	-0.230706	3.808301	1.511305
1	3.132536	2.001986	2.220424	1	-1.150849	2.347182	1.875041
1	3.177814	3.671698	1.622576	1	0.559345	2.424791	2.289896
1	0.232042	-3.972826	-1.391657	1	-5.048602	-1.144674	1.950322
1	-0.868194	-2.633473	-1.737459	1	-3.816937	-2.369018	2.243603
1	0.828906	-2.507400	-2.191084	1	-3.630689	-0.758627	2.902017
1	-2.333564	1.074296	2.332734	1	-5.950021	2.299253	-1.351316
1	-1.546650	-0.493137	2.190408	1	-4.355789	1.789978	-1.887195

1	-0.645889	0.904480	2.728966	1	-5.760615	0.770060	-2.181949
1	-2.437843	0.469552	-2.590438	1	-4.999613	2.671287	0.896670
1	-1.400278	1.777019	-2.031812	1	-4.312742	1.379263	1.850112
1	-0.776848	0.141721	-2.091927	1	-3.422502	2.049069	0.470891
1	-3.740407	3.197596	0.529111	1	-7.072542	1.305698	0.478326
1	-2.293422	3.017183	-0.431999	1	-6.988988	-0.307936	-0.183190
1	-3.867383	3.044336	-1.215850	1	-6.451033	0.015370	1.463900
1	-4.839467	-2.519220	-1.584853	1	-0.848948	3.879613	-1.169900
1	-5.022736	-0.947321	-2.333995	1	-0.624473	2.504646	-2.263969
1	-3.464919	-1.432513	-1.673966	1	-1.910309	2.476809	-1.057318
1	-6.618692	-2.283134	-0.081395	1	0.867154	-4.133465	-0.138664
1	-6.881108	-0.892410	0.940565	1	2.531321	-4.417823	0.361772
1	-7.070238	-0.763685	-0.813806	1	1.406617	-3.606993	1.461165
1	-4.523953	-2.711386	0.939322	78	0.910632	-0.192104	-0.147763
1	-3.220336	-1.537577	1.019979	6	-1.230097	-1.726863	1.939721
1	-4.682476	-1.299779	1.964782	6	-1.417842	-0.844918	-1.890618
1	-1.538353	-2.942573	1.142879	1	-1.678394	0.198350	-2.050300
1	-0.242197	-4.121293	1.321592	1	-0.608353	-1.064158	-2.583536
1	-0.297715	-2.699583	2.376203	1	-2.261590	-1.462607	-2.196420
1	0.365926	4.048921	-0.034695	1	-1.594940	-1.315165	2.873798
1	1.934049	4.471193	-0.715177	1	-1.431921	-2.797855	1.955073
1	0.828425	3.431519	-1.628181	1	-0.157665	-1.573361	1.899474
NImag = 1 (-287.4553 cm <sup>-1</sup> )				NImag = 1 (-479.3162 cm <sup>-1</sup> )			
<b>TS4(c-e)</b> Et = -1758.3783 Gsol = -1758.8194				<b>TS4(d-g)</b> Et = -1758.3916 Gsol = -1758.8418			
6	3.764340	0.266562	-0.591108	6	5.051648	-0.804380	0.269532
7	2.794094	-0.579956	-0.199339	6	5.646717	0.350395	-0.203818
6	3.061337	-1.891767	-0.074537	6	4.844361	1.406319	-0.597000
6	4.315092	-2.400694	-0.363867	6	3.470020	1.281928	-0.525900
6	5.320059	-1.536840	-0.759630	7	2.898192	0.147073	-0.065430
6	5.042710	-0.185958	-0.865666	6	3.673317	-0.881630	0.342711
78	0.814451	0.165816	0.194829	6	2.567750	2.386888	-0.969187
6	-1.039455	1.020591	0.614919	15	1.016427	2.333872	-0.001457
6	-1.384058	0.828371	2.079778	6	1.370101	3.097955	1.602235
6	1.970944	-2.773983	0.444705	78	0.844801	-0.000881	0.054967
15	0.302058	-2.094735	0.088389	15	1.358323	-2.280620	0.090669
6	-0.754473	-2.978954	1.268220	6	1.752645	-3.032764	-1.512517
6	3.407713	1.711626	-0.761634	6	2.989529	-2.085517	0.901773
15	1.974494	2.161379	0.287548	6	-1.408741	-0.294427	0.520763
6	1.359246	3.729583	-0.381145	6	-2.830595	0.000281	-0.293370
6	-0.142704	-2.759655	-1.543521	6	-2.676315	0.857017	-1.523030

6	2.648319	2.567330	1.921523	6	-2.177867	-1.308178	-0.316065
6	-2.123467	0.957327	-0.466042	6	-1.691357	-1.941120	-1.591732
6	-1.521968	1.163738	-1.836548	6	-1.390775	-0.367864	2.028164
6	-3.499408	1.527440	-0.220148	6	-4.041684	0.250917	0.593955
6	-3.980335	2.741554	-0.978952	6	-3.987544	1.640719	1.217488
6	-3.876516	0.127327	-0.639061	6	-5.420672	-0.067814	-0.081239
6	-4.653635	-0.793963	0.329871	6	-5.946210	1.064235	-0.961935
6	-4.138187	-0.816601	1.758881	6	-5.341440	-1.352234	-0.902382
6	-4.230491	-0.101207	-2.094386	6	-6.434875	-0.300855	1.042250
6	-4.684431	-2.227771	-0.197176	1	5.647741	-1.641427	0.596550
6	-6.079919	-0.217139	0.369740	1	6.721904	0.428898	-0.261060
1	-3.670893	1.660236	0.842494	1	5.276211	2.322326	-0.967647
1	4.501791	-3.458020	-0.261972	1	2.810840	-1.936988	1.968797
1	6.308276	-1.911320	-0.979864	1	3.610273	-2.972983	0.796457
1	5.804605	0.513299	-1.171898	1	2.296206	2.240421	-2.016875
1	2.054846	-2.829069	1.532497	1	3.065465	3.351764	-0.894926
1	2.074957	-3.790416	0.068588	1	-1.013785	0.635130	0.052111
1	3.106314	1.884151	-1.797122	1	-2.643071	-2.021778	0.355354
1	4.267883	2.350803	-0.569992	6	0.473791	-3.523101	1.063123
1	-3.695754	-0.939401	-2.531659	6	-0.147519	3.436622	-0.838258
1	-4.099655	0.771602	-2.718046	1	-1.201254	-2.889796	-1.389914
1	-5.286209	-0.349665	-2.138535	1	-2.538689	-2.165801	-2.236324
1	-0.881326	2.102509	0.503404	1	-1.005642	-1.307345	-2.147099
1	-2.616833	-0.289071	-0.536391	1	-1.664819	0.822361	-1.925813
1	1.841391	2.843430	2.595677	1	-3.332843	0.491982	-2.309427
1	3.157553	1.701498	2.336412	1	-2.939664	1.892929	-1.332262
1	3.347987	3.398067	1.853419	1	-2.378976	-0.542005	2.443962
1	-0.132309	-3.847842	-1.535390	1	-0.758001	-1.178624	2.381603
1	-1.136857	-2.424343	-1.828943	1	-1.016064	0.553315	2.467800
1	0.562725	-2.401967	-2.289368	1	2.229095	-3.999425	-1.359756
1	-2.283921	1.355915	2.393247	1	0.858785	-3.172761	-2.110795
1	-1.485591	-0.214605	2.360009	1	2.431708	-2.384985	-2.061381
1	-0.569154	1.229213	2.678358	1	1.677638	4.133348	1.467424
1	-2.212806	1.084715	-2.662503	1	0.478972	3.077686	2.224758
1	-1.123327	2.176870	-1.849392	1	2.158657	2.552704	2.114153
1	-0.691301	0.481468	-1.991642	1	-4.817727	1.797460	1.899534
1	-5.058271	2.844330	-0.881391	1	-3.073546	1.777559	1.793529
1	-3.533747	3.638160	-0.555664	1	-4.036572	2.429839	0.470946
1	-3.739856	2.724014	-2.037070	1	-3.980980	-0.479891	1.400778
1	-5.210917	-2.862633	0.511104	1	-7.408732	-0.538047	0.618536
1	-5.198096	-2.321896	-1.149390	1	-6.143028	-1.135915	1.678739
1	-3.680170	-2.636331	-0.315627	1	-6.567248	0.575952	1.672074
1	-6.673743	-0.823620	1.049970	1	-5.291171	1.301267	-1.796494
1	-6.092307	0.802922	0.748533	1	-6.905138	0.772713	-1.386074
1	-6.582149	-0.234623	-0.593392	1	-6.116440	1.976042	-0.393790
1	-4.783674	-1.463030	2.348147	1	-4.701111	-1.250656	-1.777485

1	-3.133479	-1.221319	1.822928	1	-4.983542	-2.192410	-0.307078
1	-4.153710	0.159152	2.234437	1	-6.331730	-1.618522	-1.265888
1	-0.585786	-4.051571	1.189063	1	1.024937	-4.461728	1.043638
1	-0.531838	-2.660125	2.283140	1	0.373310	-3.196643	2.094389
1	-1.802667	-2.784771	1.064109	1	-0.516780	-3.695830	0.653384
1	0.532798	4.096331	0.223250	1	-1.078771	3.485664	-0.279225
1	2.147467	4.479996	-0.363851	1	0.272087	4.439822	-0.892054
1	1.019348	3.601804	-1.405324	1	-0.357296	3.084416	-1.844132
NImag = 1 (-638.2308 cm <sup>-1</sup> )				NImag = 1 (-393.7308 cm <sup>-1</sup> )			
<b>TS5<sub>add</sub></b> Et = -1569.4180 Gsol = -1569.8062				<b>TS5(c-d)</b> Et = -1569.4197 Gsol = -1569.8010			
7	2.324100	-0.085548	0.223577	6	5.130024	-0.653710	-0.378881
6	3.115224	0.994114	0.078842	6	4.604128	0.614693	-0.549972
6	4.451318	0.951847	0.436104	6	3.240293	0.803316	-0.405362
6	4.984902	-0.229391	0.919776	7	2.429169	-0.216430	-0.079083
6	4.168813	-1.340076	1.042512	6	2.933120	-1.446450	0.109174
6	2.833269	-1.239046	0.696440	6	4.284929	-1.699042	-0.050368
6	2.516404	2.223041	-0.532758	6	2.609815	2.142579	-0.646543
15	0.712059	2.319795	-0.211474	15	1.037177	2.319276	0.288373
6	0.536548	3.101649	1.416837	6	1.510655	2.877767	1.950092
6	1.897799	-2.396441	0.869665	46	0.320224	0.125414	0.143975
15	0.500361	-2.290225	-0.314599	6	-1.676552	0.525404	0.414867
6	1.091495	-2.988750	-1.879835	1	-1.909023	0.194107	1.430366
46	0.286218	0.025420	-0.313056	6	1.986940	-2.521172	0.551860
6	-1.706126	0.108894	-1.090632	15	0.269162	-2.203882	-0.025475
6	-2.285894	0.226998	0.183304	6	0.207908	-2.889998	-1.708323
1	-2.408123	-0.650394	0.799753	6	0.193928	3.735572	-0.469204
6	-0.760460	-3.437293	0.299814	6	-0.740477	-3.334770	0.977131
1	-1.724190	0.980681	-1.732168	6	-2.634516	-0.126867	-0.581911
6	0.060778	3.507309	-1.414784	1	-2.300317	0.048805	-1.603683
6	-4.542793	0.635004	-0.338648	6	-4.035742	0.461039	-0.519115
6	-4.742112	0.108590	0.900286	6	-4.254521	1.661688	-1.397903
6	-4.655570	0.969684	2.114093	6	-5.103573	-0.198016	0.121687
6	-4.795018	-0.027028	-1.646053	6	-4.892746	-1.455935	0.893938
6	-5.117061	-1.312176	1.148128	6	-6.508807	0.283506	0.060138
1	-6.176940	-1.357263	1.404691	1	-4.260666	0.797333	0.653576
1	-4.582832	-1.716100	2.007616	1	4.669008	-2.695903	0.098055
1	5.066332	1.830064	0.319159	1	6.189163	-0.825469	-0.497883
1	6.027483	-0.285192	1.194437	1	5.239679	1.447561	-0.806293
1	4.558025	-2.274356	1.415119	1	1.952039	-2.529738	1.643674
1	2.640564	2.174347	-1.617065	1	2.336939	-3.504038	0.239648
1	3.032393	3.120923	-0.196459	1	2.357091	2.230470	-1.705507

1	1.466808	-2.361481	1.872757	1	3.305549	2.948944	-0.419591
1	2.427688	-3.343972	0.785814	1	-7.076880	-0.509256	-0.431580
1	-1.870585	-0.817656	-1.624463	1	-6.654483	1.195946	-0.501521
1	-4.395838	1.708639	-0.385978	1	-6.932037	0.385597	1.056910
1	-4.964244	-1.960980	0.292550	1	-1.825649	1.604907	0.391206
1	-2.266328	1.166300	0.712981	1	-2.664129	-1.205189	-0.449216
1	-4.061266	0.278099	-2.390817	1	0.622402	3.004628	2.563976
1	-4.804614	-1.111065	-1.591383	1	2.146332	2.133735	2.423026
1	-5.766417	0.290259	-2.026410	1	2.043686	3.825534	1.903804
1	0.995574	4.088692	1.417490	1	0.446817	-3.951767	-1.705114
1	-0.514871	3.211365	1.670697	1	-0.784376	-2.755804	-2.131715
1	1.011415	2.488309	2.178291	1	0.918998	-2.367952	-2.343602
1	1.379844	-4.030248	-1.749752	1	-5.056886	2.314976	-1.075779
1	0.306355	-2.934482	-2.630025	1	-3.341577	2.246450	-1.453797
1	1.947243	-2.423948	-2.240396	1	-4.484051	1.310622	-2.403485
1	0.570763	4.464544	-1.321220	1	-1.766109	-3.337865	0.616624
1	0.195288	3.132332	-2.426151	1	-0.358774	-4.352157	0.912737
1	-1.000728	3.669176	-1.242710	1	-0.736812	-3.021370	2.017845
1	-1.611743	-3.451230	-0.376758	1	-0.715863	3.960409	0.082362
1	-0.357475	-4.446973	0.358150	1	0.829386	4.618966	-0.448868
1	-1.099212	-3.138672	1.288335	1	-0.067334	3.511579	-1.500117
1	-4.431176	2.006457	1.878119	1	-3.881171	-1.573883	1.264097
1	-5.607053	0.948622	2.646154	1	-5.591459	-1.527071	1.721913
1	-3.912255	0.589592	2.817712	1	-5.107916	-2.285667	0.217340
NImag = 1 (-182.6768 cm <sup>-1</sup> )				NImag = 1 (-205.7161 cm <sup>-1</sup> )			
<b>TS5(c-e)</b> Et = -1569.4132 Gsol = -1569.8001				<b>TS5(d-e)</b> Et = -1569.4192 Gsol = -1569.8070			
6	4.855772	-0.283305	1.033362	6	4.371770	0.365129	-1.112354
6	4.014849	-1.375023	1.159767	6	3.066726	0.635609	-0.739835
6	2.694390	-1.257656	0.762775	7	2.273373	-0.326917	-0.238121
7	2.223985	-0.111834	0.240731	6	2.742897	-1.577865	-0.087110
6	3.040661	0.945654	0.089380	6	4.031407	-1.909014	-0.468719
6	4.363061	0.891884	0.494202	6	4.855944	-0.924773	-0.984331
6	1.728942	-2.392700	0.922994	6	2.476763	2.002386	-0.911964
15	0.388837	-2.299209	-0.330480	15	1.128792	2.299504	0.300161
6	-0.831737	-3.530079	0.214996	6	1.946107	2.789145	1.845292
46	0.184358	0.032306	-0.374610	6	-2.499261	1.234797	0.034352
6	-1.730100	0.218560	-1.114098	6	-3.730713	0.832913	-0.518544
1	-1.981565	1.240907	-1.382331	6	-4.316030	-0.517738	-0.224681
6	2.484174	2.161822	-0.586732	6	-5.246300	-0.348157	0.985545
15	0.671159	2.299682	-0.330696	6	1.843861	-2.584827	0.563398

6	0.091073	3.463164	-1.593489	15	0.072416	-2.185726	0.288420
6	1.095824	-2.991450	-1.853198	6	-0.351739	-2.941967	-1.307866
6	0.476122	3.155472	1.259061	6	-1.645877	0.535894	1.012059
6	-2.869037	-0.403813	-0.397484	6	-0.829516	-3.137781	1.540265
1	-2.786488	-1.457578	-0.149147	6	0.295917	3.801975	-0.288794
6	-4.252586	0.097702	-0.426422	6	-4.503592	1.794578	-1.353827
6	-5.403373	-0.852324	-0.643694	6	-5.041180	-1.147088	-1.405842
6	-3.763772	0.409253	0.987643	1	-2.482200	0.711620	-1.102184
6	-3.553145	1.878228	1.275648	1	4.386427	-2.919929	-0.345269
6	-4.338679	-0.417913	2.116671	1	5.867741	-1.159468	-1.278731
1	-4.350332	1.006491	-1.010952	1	4.993153	1.153007	-1.507775
1	4.999555	1.753746	0.370500	1	2.007013	-2.555936	1.643225
1	5.886852	-0.349683	1.346352	1	2.082433	-3.595360	0.235572
1	4.373298	-2.305131	1.571669	1	2.031926	2.077953	-1.906700
1	2.643658	2.070293	-1.663559	1	3.246666	2.770095	-0.850850
1	3.003857	3.063322	-0.266113	1	-5.629430	-1.324007	1.272789
1	1.254365	-2.326748	1.904487	1	-6.102871	0.277691	0.746359
1	2.244447	-3.351154	0.883865	1	-4.734209	0.079107	1.844868
1	-3.808669	-0.225480	3.045232	1	-1.479368	1.233109	1.832996
1	-4.314479	-1.484415	1.915443	1	-3.501245	-1.175131	0.077264
1	-5.379232	-0.131504	2.255035	1	1.201095	2.984791	2.612703
1	-1.693793	-0.339641	-2.056228	1	2.590652	1.986978	2.195144
1	-2.630346	-0.002041	0.929364	1	2.542448	3.687760	1.698613
1	0.351862	-2.982382	-2.646093	1	-0.182834	-4.016905	-1.281152
1	1.942029	-2.390328	-2.175619	1	-1.397909	-2.762901	-1.542869
1	1.426380	-4.016233	-1.694580	1	0.256423	-2.507166	-2.097005
1	0.956458	4.131798	1.230004	1	-5.432768	2.009112	-0.824871
1	-0.577901	3.295217	1.483046	1	-3.981712	2.734086	-1.505090
1	0.921956	2.564592	2.055105	1	-4.780203	1.370921	-2.315100
1	-6.334758	-0.411762	-0.297857	1	-0.572439	-4.193672	1.478935
1	-5.513996	-1.051807	-1.706423	1	-0.591050	-2.771417	2.535412
1	-5.268264	-1.803834	-0.137075	1	-1.901218	-3.040100	1.385304
1	0.634647	4.403881	-1.528277	1	-0.474205	4.103048	0.418074
1	0.229194	3.041255	-2.585639	1	1.007704	4.621295	-0.374312
1	-0.966611	3.672423	-1.452597	1	-0.156800	3.634747	-1.262878
1	-1.617481	-3.635189	-0.529975	46	0.271859	0.126179	0.336139
1	-0.358143	-4.503058	0.335184	1	-2.230597	2.262706	-0.185797
1	-1.273185	-3.242820	1.166100	1	-2.121000	-0.349011	1.419215
1	-3.045540	2.384320	0.459112	1	-5.933559	-0.589093	-1.679514
1	-4.532362	2.339133	1.390594	1	-4.405313	-1.229966	-2.286100
1	-2.998363	2.028208	2.197639	1	-5.363085	-2.149743	-1.136821
NImag = 1 (-278.0701 cm <sup>-1</sup> )				NImag = 1 (-398.0367 cm <sup>-1</sup> )			
<b>TS5(d-g)</b> Et = -1569.4357				<b>TS6<sub>add</sub></b> Et = -1608.7294			



Gsol = -1569.8257				Gsol = -1609.1240			
6	4.462474	0.566884	-0.593421	7	2.479607	0.013283	0.197508
6	3.099457	0.763081	-0.462705	6	3.188191	1.150419	0.064850
7	2.287533	-0.238620	-0.069820	6	4.528855	1.198466	0.403660
6	2.800243	-1.454639	0.203229	6	5.153707	0.049961	0.855877
6	4.153401	-1.705783	0.062766	6	4.422112	-1.119180	0.966814
6	4.995297	-0.683532	-0.336585	6	3.077735	-1.108979	0.640629
6	2.475299	2.085070	-0.783425	6	2.493024	2.344824	-0.512369
15	0.932864	2.315052	0.179203	15	0.692656	2.304560	-0.158654
6	1.427371	2.901511	1.822001	6	0.492353	3.039895	1.488326
46	0.230863	0.093312	0.114985	6	2.231346	-2.334244	0.804818
15	0.169575	-2.246073	0.074996	15	0.809405	-2.305871	-0.354366
6	0.118256	-3.020429	-1.565030	6	1.422141	-2.932127	-1.941798
6	1.868463	-2.508923	0.711410	46	0.429360	-0.011763	-0.300848
6	-1.887732	0.458688	0.409151	6	-1.586546	-0.061513	-1.031131
6	-3.500042	0.638661	-0.313469	6	-2.106059	-0.023689	0.269508
6	-4.083986	1.980394	-0.009048	1	-2.135052	-0.923555	0.864055
6	-2.323125	0.534008	-1.102817	6	-0.361647	-3.546456	0.255588
6	-4.363959	-0.584320	-0.110042	1	-1.691538	0.825589	-1.643094
6	-5.419183	-0.624554	-1.218350	6	-0.067669	3.463786	-1.324522
6	-5.008130	-0.661991	1.265594	6	-4.497481	0.319706	-0.237874
6	-0.908230	-3.242958	1.137388	6	-4.471499	-0.337892	0.960193
6	0.060468	3.697223	-0.602807	6	-4.438567	0.353157	2.285457
1	-2.112447	-0.423374	0.989906	6	-4.722776	-0.370009	-1.543064
1	-1.953977	1.418208	-1.601961	6	-4.637182	-1.822281	1.082084
1	4.540529	-2.688587	0.280430	1	-5.686998	-2.054482	1.267491
1	6.055280	-0.858445	-0.443060	1	-4.086706	-2.203043	1.941373
1	5.093152	1.384308	-0.905205	1	5.076877	2.121255	0.297120
1	1.812039	-2.437731	1.800120	1	6.201459	0.064885	1.115742
1	2.238471	-3.505938	0.478135	1	4.883165	-2.029644	1.315636
1	2.197925	2.105991	-1.839767	1	2.602502	2.326555	-1.599176
1	3.179056	2.900183	-0.623155	1	2.949001	3.270646	-0.165268
1	-1.866747	1.372005	0.982524	1	1.817170	-2.350975	1.815421
1	-2.153805	-0.383069	-1.648615	1	2.826252	-3.239183	0.691620
1	-3.385550	2.786650	-0.213853	1	-1.691944	-0.984844	-1.584998
1	-4.950009	2.128322	-0.654090	1	-4.336307	-2.378875	0.201383
1	-4.427752	2.056341	1.018580	1	-2.156069	0.905021	0.815895
1	0.347025	-4.082219	-1.492196	1	-3.996542	-0.037273	-2.286091
1	-0.871298	-2.911584	-2.002175	1	-4.698633	-1.451411	-1.492553
1	0.839407	-2.545896	-2.225601	1	-5.700961	-0.083325	-1.931070
1	1.959206	3.848221	1.746092	1	0.878125	4.057700	1.500180
1	0.548098	3.044571	2.445496	1	-0.559164	3.067106	1.762730
1	2.070223	2.168436	2.302227	1	1.025102	2.448841	2.228806
1	-4.977776	-0.556160	-2.210703	1	1.788844	-3.951385	-1.834810
1	-5.964331	-1.563469	-1.160418	1	0.621887	-2.924175	-2.677787

1	-6.146808	0.176454	-1.109478	1	2.227414	-2.299775	-2.306479
1	-3.719518	-1.456651	-0.247638	1	0.373033	4.453909	-1.221656
1	-0.585420	-4.282743	1.134715	1	0.071647	3.118445	-2.345685
1	-0.886319	-2.869824	2.158123	1	-1.134022	3.544234	-1.126815
1	-1.932032	-3.205498	0.773395	1	-1.219524	-3.604506	-0.410329
1	-0.848343	3.924813	-0.051086	1	0.107770	-4.528131	0.290188
1	0.687702	4.587259	-0.601038	1	-0.707063	-3.288377	1.253326
1	-0.198923	3.456696	-1.630390	1	-4.369340	1.432820	2.232992
1	-4.277011	-0.601303	2.070831	1	-5.350752	0.113770	2.833262
1	-5.737724	0.131532	1.412013	1	-3.617857	-0.022937	2.899285
1	-5.539372	-1.604514	1.371276	6	-4.510673	1.811965	-0.365434
NImag = 1 (-125.7354 cm <sup>-1</sup> )				1	-5.525278	2.147532	-0.582948
				1	-4.179036	2.345029	0.518469
				1	-3.902388	2.125477	-1.214140
				NImag = 1 (-131.5969 cm <sup>-1</sup> )			
<b>TS6(c-d)</b>				<b>TS6(c-e)</b>			
Et = -1608.7301				Et = -1608.7211			
Gsol = -1609.1157				Gsol = -1609.1130			
6	5.237676	-0.051379	0.945581	6	-5.046386	0.080478	0.938852
6	4.467491	-1.193833	1.073840	6	-4.268894	1.218264	1.064803
6	3.128889	-1.145761	0.724049	6	-2.934500	1.165905	0.702015
7	2.576975	-0.020083	0.242845	7	-2.389911	0.038246	0.213590
6	3.321865	1.087034	0.092545	6	-3.144466	-1.064253	0.062299
6	4.658514	1.104770	0.453176	6	-4.477721	-1.075384	0.433761
6	2.234060	-2.335987	0.904493	6	-2.036508	2.354899	0.862945
15	0.812198	-2.293054	-0.261749	15	-0.662392	2.310203	-0.355674
6	1.437743	-2.997957	-1.814726	6	0.480807	3.611231	0.194711
46	0.498078	0.010904	-0.302049	46	-0.329505	-0.006768	-0.349157
6	-1.468804	0.030248	-0.905730	6	1.612296	-0.088734	-1.039085
1	-1.667762	0.989475	-1.387285	1	1.910143	-1.089120	-1.334056
6	2.670843	2.283054	-0.535588	6	-2.506323	-2.259425	-0.577730
15	0.852852	2.303087	-0.255669	15	-0.695260	-2.296171	-0.274192
6	0.630658	3.146458	1.339437	6	-0.027495	-3.452841	-1.499691
6	-0.344412	-3.537479	0.381401	6	-1.365377	2.936694	-1.908405
6	0.209872	3.458620	-1.498547	6	-0.501390	-3.113709	1.335904
6	-2.453616	-0.217022	0.225969	6	2.687460	0.570857	-0.263317
1	-2.275722	-1.198763	0.671930	1	2.503539	1.598659	0.034179
6	-3.931615	-0.239008	-0.150877	6	4.118910	0.202913	-0.238693
6	-4.241052	-0.930930	-1.445923	6	5.098645	1.362238	-0.232235
6	-4.924670	-0.006632	0.819852	6	3.563076	-0.235870	1.140806
6	-4.586588	0.308421	2.248642	6	3.437191	-1.726961	1.373143
6	-6.361984	-0.394668	0.640012	6	4.016864	0.558473	2.350324



1	5.238315	2.006138	0.332047	1	-5.063666	-1.972483	0.310779
1	6.280983	-0.063205	1.222768	1	-6.087093	0.096311	1.225515
1	4.893700	-2.109271	1.452798	1	-4.686972	2.134740	1.450198
1	2.817850	2.232579	-1.616882	1	-2.643283	-2.194746	-1.659598
1	3.138266	3.206748	-0.197728	1	-2.984734	-3.182396	-0.253904
1	1.814402	-2.314998	1.912692	1	-1.583761	2.333550	1.856636
1	2.797478	-3.263778	0.816371	1	-2.601726	3.283012	0.791988
1	-6.515604	-1.324192	1.188818	1	3.461425	0.255872	3.233617
1	-6.666913	-0.558556	-0.384966	1	3.907651	1.630309	2.224819
1	-7.015779	0.349444	1.087022	1	5.070051	0.350450	2.526951
1	-1.557721	-0.730859	-1.678116	1	1.577787	0.500436	-1.962379
1	-2.288334	0.497641	1.026752	1	2.418049	0.090832	1.053499
1	0.647198	-3.009039	-2.561035	1	-0.601959	2.952451	-2.682481
1	2.251940	-2.386365	-2.194730	1	-2.170801	2.286433	-2.239824
1	1.794841	-4.015144	-1.665473	1	-1.752297	3.945508	-1.777434
1	1.058730	4.146793	1.313157	1	-0.933405	-4.112509	1.312686
1	-0.427582	3.228638	1.573874	1	0.551458	-3.198293	1.590553
1	1.111722	2.574983	2.129099	1	-0.996477	-2.531041	2.108575
1	-5.291560	-0.939243	-1.704755	1	6.050338	1.058613	0.196945
1	-3.685107	-0.486495	-2.265386	1	5.291603	1.673530	-1.256097
1	-3.913771	-1.966028	-1.352387	1	4.741920	2.230087	0.314321
1	-0.855545	3.612689	-1.345995	1	-0.528804	-4.416532	-1.431242
1	0.707432	4.423903	-1.426802	1	-0.158825	-3.054884	-2.502594
1	0.358893	3.054953	-2.496664	1	1.034436	-3.610424	-1.327553
1	-1.195865	-3.629106	-0.288888	1	1.286453	3.733116	-0.526133
1	0.136539	-4.511395	0.452378	1	-0.040551	4.563929	0.272576
1	-0.701530	-3.251217	1.367365	1	0.902486	3.369818	1.167359
1	-3.647861	0.829292	2.387459	1	2.876469	-2.229568	0.592001
1	-5.381774	0.884889	2.712715	1	4.432952	-2.163629	1.402310
1	-4.522932	-0.640023	2.782416	1	2.956283	-1.918528	2.328391
6	-4.603645	1.403404	-0.281526	6	4.603889	-0.893662	-1.165113
1	-4.760319	2.092001	0.542697	1	4.713620	-0.493086	-2.169945
1	-5.417455	1.419342	-0.991772	1	5.585449	-1.235661	-0.845679
1	-3.672636	1.708550	-0.754361	1	3.953137	-1.758275	-1.222686
NImag = 1 (-246.7135 cm <sup>-1</sup> )				NImag = 1 (-266.7653 cm <sup>-1</sup> )			
<b>TS6(d-e)</b> Et = -1608.7209 Gsol = -1609.1125				<b>TS6(d-g)</b> Et = -1608.7400 Gsol = -1609.1354			
6	4.460360	0.660911	-1.156588	6	4.579841	0.691879	-0.638086
6	3.141764	0.820961	-0.768368	6	3.213034	0.841486	-0.488121
7	2.439115	-0.201854	-0.251826	7	2.440915	-0.184891	-0.078386
6	3.017418	-1.406025	-0.095894	6	3.000325	-1.380583	0.192339

6	4.325067	-1.628082	-0.490762	6	4.359353	-1.585566	0.034025
6	5.055123	-0.581568	-1.025913	6	5.159828	-0.537635	-0.382749
6	2.436271	2.132062	-0.930960	6	2.540086	2.139964	-0.801673
15	1.103713	2.316485	0.319763	15	1.017884	2.321903	0.200355
6	1.935604	2.818634	1.853772	6	1.546574	2.877614	1.843668
6	-2.415648	1.140921	0.227835	46	0.373113	0.074880	0.126899
6	-3.682728	0.930494	-0.357342	15	0.399387	-2.266362	0.094434
6	-4.432693	-0.397090	-0.349492	6	0.367351	-3.034217	-1.549202
6	-4.908325	-0.609226	1.096984	6	2.112516	-2.463024	0.715074
6	2.212771	-2.478658	0.571162	6	-1.775647	0.366831	0.418476
15	0.417012	-2.243190	0.269327	6	-3.328008	0.709434	-0.321968
6	0.105855	-3.021855	-1.341589	6	-3.669938	2.161347	-0.146580
6	-1.530653	0.300509	1.049603	6	-2.179792	0.390470	-1.101710
6	-0.415962	-3.283264	1.498198	6	-4.445259	-0.301001	-0.055216
6	0.183380	3.790870	-0.211167	6	-3.973604	-1.747748	0.046745
6	-4.367775	2.137089	-0.914367	6	-5.207611	0.049052	1.221141
6	-5.655583	-0.363795	-1.266363	6	-0.607684	-3.325526	1.164344
1	-2.485428	0.823663	-1.000723	6	0.118764	3.717742	-0.525606
1	4.767357	-2.603423	-0.363237	1	-2.010367	-0.506601	1.004014
1	6.079459	-0.731306	-1.332185	1	-1.715570	1.180475	-1.674006
1	5.006726	1.496341	-1.564949	1	4.782517	-2.553442	0.251358
1	2.364313	-2.414910	1.651025	1	6.223605	-0.676357	-0.503696
1	2.543295	-3.469030	0.262318	1	5.176695	1.529217	-0.963285
1	1.959903	2.167442	-1.913184	1	2.063083	-2.388234	1.803920
1	3.140854	2.961380	-0.889762	1	2.514132	-3.448099	0.483312
1	-5.488869	-1.527732	1.144415	1	2.236260	2.146920	-1.850879
1	-5.557754	0.200063	1.425418	1	3.220110	2.978483	-0.660797
1	-4.086270	-0.692454	1.802786	1	-1.692565	1.284173	0.979293
1	-1.353546	0.871497	1.963149	1	-2.111896	-0.580617	-1.566482
1	1.203847	2.950350	2.647102	1	-2.845879	2.802866	-0.445274
1	2.636959	2.048617	2.164308	1	-4.515873	2.407929	-0.785124
1	2.472827	3.754736	1.713391	1	-3.953279	2.398835	0.874522
1	0.381548	-4.074537	-1.314520	1	0.637994	-4.086588	-1.483341
1	-0.945698	-2.943810	-1.602514	1	-0.628891	-2.962299	-1.978721
1	0.688434	-2.522261	-2.111430	1	1.064400	-2.528440	-2.212436
1	-5.222569	2.343809	-0.268948	1	2.059932	3.835133	1.776328
1	-3.734001	3.018118	-0.913017	1	0.682146	2.990478	2.493590
1	-4.759849	1.971240	-1.912378	1	2.214521	2.144952	2.289015
1	-0.062811	-4.310675	1.431335	1	-4.844492	-2.397644	0.077018
1	-0.225778	-2.907063	2.500031	1	-3.379396	-2.067644	-0.808229
1	-1.489553	-3.282024	1.326557	1	-3.421169	-1.932324	0.966765
1	-0.564545	4.055540	0.533205	1	-0.194171	-4.332677	1.184279
1	0.860359	4.637308	-0.314561	1	-0.629634	-2.933702	2.178005
1	-0.304190	3.621263	-1.167896	1	-1.624391	-3.383447	0.786574
46	0.408023	0.077681	0.334892	1	-0.752229	3.956444	0.079354
1	-2.103500	2.177468	0.165059	1	0.760022	4.597461	-0.553482

1	-1.973326	-0.644876	1.327735	1	-0.201652	3.489505	-1.538595
1	-6.379614	0.392497	-0.975241	1	-4.549310	0.074358	2.089363
1	-5.387652	-0.208799	-2.309917	1	-5.718975	1.005268	1.148873
1	-6.160047	-1.324755	-1.204101	1	-5.968879	-0.704282	1.409076
6	-3.542824	-1.551071	-0.814653	6	-5.388167	-0.197920	-1.267494
1	-3.247351	-1.417924	-1.855524	1	-6.218143	-0.886905	-1.127921
1	-2.648371	-1.668023	-0.211963	1	-5.814512	0.794755	-1.382712
1	-4.107423	-2.478368	-0.754960	1	-4.884614	-0.466885	-2.194623
NImag = 1 (-448.8324 cm <sup>-1</sup> )				NImag = 1 (-156.1797 cm <sup>-1</sup> )			
<b>TS7<sub>add</sub></b> Et = -1687.3413 Gsol = -1687.7724				<b>TS7(c-d)</b> Et = -1687.3385 Gsol = -1687.7519			
7	2.794906	-0.080379	-0.387285	6	5.579331	-1.157290	-0.176216
6	3.502700	-1.217551	-0.252611	6	5.226158	0.172166	-0.325173
6	4.764924	-1.340821	-0.806026	6	3.889083	0.524979	-0.259772
6	5.315680	-0.265536	-1.480183	7	2.937628	-0.395191	-0.030417
6	4.589143	0.906721	-1.592705	6	3.273346	-1.684322	0.135898
6	3.320642	0.970848	-1.044402	6	4.591548	-2.098828	0.052146
6	2.903138	-2.322197	0.561823	6	3.447481	1.940326	-0.482292
15	1.069144	-2.266496	0.517135	15	1.849220	2.278904	0.359199
6	0.581094	-3.170738	-0.978929	6	2.275190	2.701555	2.072981
6	2.471782	2.196613	-1.192322	46	0.873649	0.203097	0.066884
15	1.280027	2.333382	0.196159	6	-1.059933	0.884247	0.214219
6	2.180949	3.085056	1.578852	1	-1.348900	0.730419	1.255953
46	0.862544	0.058999	0.449092	6	2.174488	-2.645786	0.470085
6	-0.982414	0.231357	1.526313	15	0.550750	-2.099940	-0.201234
6	-1.731264	0.100996	0.348385	6	0.526831	-2.718356	-1.911645
1	-1.871252	0.951770	-0.299500	6	1.245074	3.822433	-0.377362
6	0.044460	3.553706	-0.319143	6	-0.640328	-3.148057	0.686233
1	-0.983546	-0.597596	2.222083	6	-2.093262	0.230454	-0.708582
6	0.509487	-3.272022	1.916418	1	-1.728545	0.228368	-1.737547
6	-3.941809	-0.005707	1.171110	6	-3.380815	1.011898	-0.794101
6	-4.360542	0.417076	-0.054712	6	-3.257756	2.256432	-1.628708
6	-4.716740	-0.546465	-1.176159	6	-4.626694	0.647746	-0.235009
6	-3.871755	-0.276606	-2.427814	6	-4.891726	-0.667611	0.531496
6	-3.881915	0.825814	2.408040	6	-4.852589	-1.808115	-0.494006
6	-4.608760	1.870839	-0.305830	6	-5.836388	1.465349	-0.588618
6	-4.555946	-2.012391	-0.786571	6	-6.284792	-0.660063	1.169100
6	-6.196299	-0.310092	-1.521900	6	-3.903438	-0.896727	1.678936
1	-5.614851	2.129751	0.028048	1	-3.816141	1.360463	0.443941
1	-4.549423	2.131660	-1.357441	1	4.838655	-3.140657	0.181655
1	5.313035	-2.262804	-0.693215	1	6.614986	-1.456382	-0.234653

1	6.303155	-0.338898	-1.910346	1	5.975088	0.927442	-0.503846
1	4.994007	1.761326	-2.111272	1	2.064013	-2.688705	1.556038
1	3.198043	-2.191849	1.605636	1	2.420634	-3.653404	0.138336
1	3.281915	-3.293037	0.246388	1	3.280650	2.097272	-1.550262
1	1.883768	2.117061	-2.109438	1	4.220425	2.643748	-0.176364
1	3.086935	3.090042	-1.286854	1	-6.453645	0.849887	-1.243008
1	-0.973387	1.199279	2.008954	1	-5.615939	2.380241	-1.120062
1	-3.896267	-1.072912	1.340640	1	-6.435591	1.700310	0.283823
1	-3.927507	2.510636	0.248688	1	-1.056405	1.959347	0.041421
1	-1.880815	-0.863285	-0.107796	1	-2.266060	-0.801367	-0.435004
1	-4.836215	-2.640694	-1.628729	1	1.370513	2.915985	2.636377
1	-3.528141	-2.270407	-0.527063	1	2.779153	1.862807	2.546095
1	-5.197761	-2.287548	0.047889	1	2.925052	3.573966	2.106883
1	-6.502510	-1.012954	-2.294162	1	0.649341	-3.799565	-1.934910
1	-6.835631	-0.468253	-0.655346	1	-0.415607	-2.464156	-2.390110
1	-6.376314	0.691871	-1.902937	1	1.330028	-2.257792	-2.481282
1	-3.130396	0.451898	3.100875	1	-3.735815	3.129019	-1.196294
1	-3.688265	1.878144	2.221065	1	-2.213662	2.491116	-1.801625
1	-4.837823	0.762595	2.929390	1	-3.726937	2.068701	-2.595072
1	0.946668	-4.195295	-0.938708	1	-5.101179	-2.743036	0.003296
1	-0.502079	-3.194777	-1.067572	1	-5.588755	-1.658301	-1.281956
1	0.987449	-2.682809	-1.861139	1	-3.880503	-1.927659	-0.965566
1	2.539594	4.076552	1.308436	1	-6.425172	-1.603113	1.691238
1	1.526948	3.173410	2.442929	1	-6.398921	0.132428	1.906262
1	3.028001	2.462326	1.854769	1	-7.087777	-0.580719	0.441990
1	-4.196463	-0.936786	-3.229284	1	-4.172377	-1.817527	2.190893
1	-3.976511	0.741507	-2.794335	1	-2.868197	-0.989933	1.372070
1	-2.812593	-0.471855	-2.260329	1	-3.969064	-0.095369	2.414886
1	0.922556	-4.277274	1.852893	1	-1.632363	-3.041426	0.255193
1	0.819381	-2.820819	2.855475	1	-0.353124	-4.195679	0.614056
1	-0.575240	-3.349161	1.909211	1	-0.683830	-2.864837	1.734623
1	-0.682171	3.701866	0.476268	1	0.335075	4.140226	0.126087
1	0.519374	4.511009	-0.527080	1	1.985115	4.613421	-0.271334
1	-0.473931	3.218319	-1.213550	1	1.030102	3.679298	-1.433084
NImag = 1 (-212.1265 cm <sup>-1</sup> )				NImag = 1 (-295.8139 cm <sup>-1</sup> )			
<b>TS7(c-e)</b> Et = -1687.3376 Gsol = -1687.7653				<b>TS7(d-e)</b> Et = -1687.3426 Gsol = -1687.7653			
6	5.134627	-0.583165	1.339650	6	-4.688410	0.161228	1.534322
6	4.197102	-1.598500	1.406789	6	-3.452493	0.499707	1.011658
6	2.932625	-1.382343	0.887307	7	-2.713019	-0.397624	0.337587
7	2.608528	-0.216420	0.304276	6	-3.171903	-1.648020	0.153262

6	3.521793	0.766030	0.210118	6	-4.389132	-2.047336	0.677152
6	4.793041	0.614113	0.735898	6	-5.156669	-1.130944	1.374161
6	1.864778	-2.428559	0.976149	6	-2.876747	1.870242	1.198194
15	0.652913	-2.253771	-0.395142	15	-1.730148	2.293186	-0.173926
6	-0.672665	-3.415784	0.050862	6	-2.792738	2.795222	-1.558513
46	0.637550	0.093132	-0.472736	6	1.877442	1.522948	-0.578532
6	-1.181674	0.523983	-1.337438	6	3.200264	1.330762	-0.130323
1	-1.447357	1.569179	-1.223457	6	3.901811	0.015407	-0.323571
6	3.132429	2.005664	-0.535679	6	4.865870	0.215122	-1.500609
15	1.323928	2.304412	-0.436030	6	-2.346695	-2.572659	-0.688538
6	0.945319	3.467544	-1.772322	15	-0.563449	-2.143660	-0.601399
6	1.456192	-3.009600	-1.839192	6	0.067140	-3.008693	0.865112
6	1.068254	3.226138	1.106589	6	0.994923	0.633663	-1.353022
6	-2.387337	-0.318494	-1.119252	6	0.201375	-2.965213	-2.024311
1	-2.298255	-1.358368	-1.416991	6	-0.919292	3.826757	0.367072
6	-3.779936	0.185900	-1.135376	6	3.912961	2.511647	0.441440
6	-4.800285	-0.405692	-2.077080	6	4.539833	-0.637128	0.941080
6	-3.610027	-0.348750	0.276801	6	3.579665	-0.507339	2.122010
6	-3.684436	0.657994	1.452228	6	5.909206	-0.072202	1.313155
6	-3.279067	-0.019838	2.759573	6	4.715728	-2.125992	0.635986
6	-4.190100	-1.726340	0.512791	1	2.062105	1.149467	0.611218
6	-5.140089	1.123266	1.539231	1	-4.735951	-3.057022	0.523979
6	-2.778939	1.867384	1.245819	1	-6.113275	-1.419312	1.783072
1	-3.808699	1.269262	-1.149126	1	-5.267597	0.898072	2.068007
1	5.508342	1.417378	0.656275	1	-2.646826	-2.459375	-1.732826
1	6.123701	-0.725579	1.748218	1	-2.522998	-3.613107	-0.420196
1	4.436581	-2.544376	1.866383	1	-2.293546	1.894102	2.121348
1	3.370675	1.869303	-1.592961	1	-3.665698	2.613702	1.301581
1	3.700994	2.868110	-0.191745	1	5.315731	-0.735923	-1.769550
1	1.312289	-2.303066	1.909841	1	5.670722	0.904258	-1.262394
1	2.298920	-3.427236	0.995659	1	4.346222	0.588055	-2.381329
1	-3.795183	-2.187658	1.410593	1	0.666762	1.209526	-2.219538
1	-4.020135	-2.396359	-0.323483	1	3.140404	-0.690118	-0.654834
1	-5.267294	-1.630055	0.627340	1	-2.181986	3.067495	-2.415830
1	-0.969733	0.361964	-2.400971	1	-3.436352	1.969101	-1.849561
1	-2.388975	-0.578691	0.227969	1	-3.409950	3.648171	-1.282517
1	0.799104	-2.955132	-2.703669	1	-0.089369	-4.081823	0.771837
1	2.370170	-2.470900	-2.075722	1	1.131500	-2.822691	0.980541
1	1.697613	-4.053200	-1.646408	1	-0.442328	-2.651456	1.756382
1	1.643380	4.150268	1.097181	1	4.728144	2.761088	-0.236836
1	0.016689	3.474148	1.223385	1	3.269884	3.382893	0.520499
1	1.377171	2.623611	1.956892	1	4.356758	2.304171	1.408461
1	-5.808343	-0.174193	-1.742882	1	5.145082	-2.635216	1.495991
1	-4.677408	0.030855	-3.064888	1	3.762562	-2.606567	0.412593
1	-4.715474	-1.483467	-2.179249	1	5.385195	-2.298315	-0.203608
1	-3.272580	0.715494	3.560511	1	3.937774	-1.090176	2.967845

1	-3.970454	-0.803059	3.057976	1	3.479599	0.518909	2.477795
1	-2.275381	-0.444310	2.701669	1	2.585039	-0.886261	1.874292
1	-5.239530	1.824781	2.364727	1	6.281217	-0.586403	2.196952
1	-5.459840	1.635206	0.633661	1	6.638556	-0.232261	0.522749
1	-5.825961	0.302232	1.733297	1	5.898649	0.988629	1.548407
1	-2.892497	2.534556	2.097004	1	-0.017495	-4.031420	-2.014570
1	-1.730477	1.575127	1.193042	1	-0.168038	-2.534657	-2.951380
1	-3.031925	2.446142	0.360019	1	1.280894	-2.839688	-1.992046
1	1.542353	4.372157	-1.672953	1	-0.305410	4.229340	-0.435716
1	1.148220	3.011830	-2.737837	1	-1.666202	4.577316	0.620434
1	-0.104856	3.747046	-1.736404	1	-0.297364	3.650117	1.240935
1	-1.369291	-3.530274	-0.776078	46	-0.810683	0.155724	-0.452498
1	-0.253236	-4.396980	0.267257	1	1.519677	2.538643	-0.449570
1	-1.212539	-3.070201	0.928654	1	1.511604	-0.247156	-1.714029
NImag = 1 (-293.6542 cm <sup>-1</sup> )				NImag = 1 (-353.6212 cm <sup>-1</sup> )			
<b>TS7(d-g)</b> Et = -1687.3475 Gsol = -1687.7791				<b>TS8<sub>add</sub></b> Et = -1765.9619 Gsol = -1766.4024			
6	5.534651	-0.656599	0.005882	6	3.348180	-1.758520	0.030064
6	5.015577	0.589010	-0.297034	6	4.624529	-2.210594	-0.256440
6	3.644926	0.774354	-0.286479	6	5.553055	-1.326704	-0.775920
7	2.808054	-0.232960	0.034675	6	5.180589	-0.014582	-1.007423
6	3.306449	-1.444838	0.351595	6	3.883260	0.378769	-0.729232
6	4.668658	-1.684802	0.330356	7	2.989287	-0.486235	-0.216475
6	3.044092	2.091983	-0.658873	6	3.417944	1.771061	-1.026919
15	1.430556	2.313382	0.178859	15	2.024235	2.250250	0.066446
6	0.658868	3.743284	-0.623414	6	1.268340	3.695624	-0.724002
6	-1.440131	0.388478	0.082020	46	1.014875	0.171067	0.232607
6	-1.598520	0.556938	-1.470350	6	-0.863783	0.988687	0.853327
6	-2.832147	0.845260	-0.801280	6	-1.037276	0.606011	2.302652
6	-3.998281	-0.145567	-0.795166	6	2.336444	-2.654578	0.672750
6	-4.957407	-0.112980	0.448005	15	0.621051	-2.145018	0.261129
6	-5.875334	1.113709	0.418331	6	-0.405802	-3.069269	1.438129
6	2.345266	-2.507066	0.776535	6	2.770561	2.865000	1.601881
15	0.702800	-2.258810	0.003546	6	0.280230	-2.888114	-1.362049
6	-0.437339	-3.251211	1.001803	6	-1.728103	0.413355	-0.135521
6	1.800173	2.841415	1.874086	6	-1.653431	0.845405	-1.565884
6	0.776265	-3.050965	-1.626013	6	-3.669706	1.187708	0.555123
6	-3.135650	2.306400	-0.606927	6	-3.475341	2.674387	0.607739
6	-3.572601	-1.556235	-1.184001	6	-4.460152	0.565353	-0.379658
6	-5.890250	-1.328032	0.408877	6	-4.936199	1.324780	-1.568324
6	-4.195753	-0.149510	1.769781	6	-4.970823	-0.852426	-0.213996
1	-1.744408	-0.537447	0.539639	6	-4.616298	-1.469330	1.134976



1	-1.055532	1.386016	-1.898289	6	-6.505093	-0.807843	-0.322899
1	5.042081	-2.664825	0.581811	6	-4.427401	-1.751096	-1.333767
1	6.601246	-0.823019	-0.007175	1	-5.874403	1.820251	-1.304829
1	5.663721	1.412096	-0.553061	1	-5.146991	0.692622	-2.425226
1	2.197997	-2.441132	1.857088	1	4.888163	-3.237237	-0.057069
1	2.740317	-3.500571	0.571249	1	6.557384	-1.656193	-0.995549
1	2.853029	2.112772	-1.734203	1	5.882680	0.697039	-1.412278
1	3.728809	2.910108	-0.441408	1	2.434844	-2.577548	1.758035
1	-1.365419	1.235665	0.745953	1	2.514950	-3.696936	0.413209
1	-1.473219	-0.367763	-2.007625	1	3.043653	1.810979	-2.052342
1	-2.272978	2.919786	-0.853174	1	4.241286	2.480780	-0.963712
1	-3.943147	2.592856	-1.278116	1	-0.755996	2.060252	0.717259
1	-3.450291	2.542364	0.403736	1	-3.557956	0.674363	1.499525
1	1.001314	-4.111175	-1.524038	1	-4.250161	2.111129	-1.866332
1	-0.179595	-2.949946	-2.134169	1	-2.023810	-0.613204	0.033198
1	1.542821	-2.581192	-2.236959	1	-5.014886	-2.479966	1.183637
1	2.346619	3.782846	1.869786	1	-3.541148	-1.539481	1.298946
1	0.876115	2.977183	2.430813	1	-5.049014	-0.912222	1.963653
1	2.395176	2.085550	2.379887	1	-6.902144	-1.806098	-0.151218
1	-4.442778	-2.173536	-1.370229	1	-6.938260	-0.146299	0.425059
1	-2.997608	-1.573747	-2.105734	1	-6.842184	-0.486628	-1.304587
1	-2.999448	-2.049747	-0.399068	1	-0.705452	0.513910	-1.989882
1	-4.600055	0.225754	-1.633810	1	-2.445562	0.413874	-2.166863
1	-6.631964	-1.234021	1.198667	1	-1.687225	1.928406	-1.659786
1	-6.432937	-1.394086	-0.533654	1	-2.774210	2.949124	1.390586
1	-5.369141	-2.268109	0.574190	1	-3.124731	3.102682	-0.328649
1	-3.571848	0.730622	1.919567	1	-4.418901	3.165231	0.845090
1	-4.900719	-0.183636	2.597956	1	-1.850935	1.168204	2.764755
1	-3.568688	-1.037974	1.855685	1	-1.260644	-0.451715	2.421364
1	-5.365291	2.055978	0.582587	1	-0.144664	0.822855	2.884869
1	-6.413635	1.179677	-0.526687	1	0.384706	-3.970761	-1.320316
1	-6.621576	1.025954	1.205059	1	-0.731569	-2.649384	-1.680228
1	-0.068285	-4.272708	1.080699	1	0.971686	-2.493349	-2.102275
1	-0.533541	-2.832256	2.000063	1	3.401077	3.729789	1.403314
1	-1.418469	-3.283320	0.536559	1	1.991286	3.155539	2.302399
1	-0.260143	4.010958	-0.108392	1	3.370914	2.084926	2.062956
1	1.331069	4.598983	-0.578529	1	-4.863297	-2.743465	-1.240024
1	0.435398	3.532621	-1.665893	1	-4.677260	-1.383312	-2.325573
46	0.741287	0.078183	0.021174	1	-3.344744	-1.864413	-1.276850
				1	-0.191937	-4.134487	1.367111
				1	-0.209301	-2.738441	2.454526
				1	-1.460491	-2.920155	1.221570
				1	0.479353	4.097436	-0.092820
				1	2.012023	4.476286	-0.874323
				1	0.842961	3.423168	-1.686190

NImag = 1 (-140.1019 cm<sup>-1</sup>)

				NImag = 1 (-293.9292 cm <sup>-1</sup> )			
<b>TS8(c-d)</b> Et = -1765.9516 Gsol = -1766.3779				<b>TS8(d-e)</b> Et = -1765.9462 Gsol = -1766.3788			
6	5.616139	-1.262944	-0.610046	6	-5.240915	0.387499	-0.721580
6	5.245657	0.054511	-0.814202	6	-3.982356	-0.142736	-0.495567
6	3.932117	0.427142	-0.585148	7	-2.954060	0.637555	-0.120974
7	3.023298	-0.458770	-0.146865	6	-3.138525	1.958013	0.039649
6	3.379118	-1.733748	0.072787	6	-4.368072	2.546801	-0.200768
6	4.671117	-2.170652	-0.166216	6	-5.433021	1.750411	-0.582242
6	3.463561	1.825419	-0.855310	6	-3.713453	-1.603831	-0.695609
15	2.007849	2.251361	0.180896	15	-2.285482	-2.155628	0.316148
6	2.684342	2.799716	1.774734	6	-2.946224	-2.467738	1.978394
46	0.982254	0.176486	0.213206	6	1.753735	-1.149800	-0.683983
6	-0.915823	0.908057	0.625149	6	3.164251	-0.959291	-0.759983
6	-1.279597	0.547545	2.053740	6	4.020962	-0.483445	0.374467
6	2.339220	-2.651422	0.636970	6	4.743066	-1.737966	0.888458
15	0.633862	-2.148001	0.163385	6	-1.984040	2.760919	0.551260
6	0.388208	-2.886020	-1.482331	15	-0.357356	2.033341	0.095528
6	1.318209	3.748068	-0.578731	6	0.025805	2.745934	-1.534330
6	-0.399489	-3.151951	1.271932	6	0.835139	-1.168348	0.517716
6	-1.973672	0.477221	-0.402402	6	0.780274	2.851212	1.252596
6	-1.534220	0.740088	-1.847541	6	-1.842567	-3.790988	-0.332366
6	-3.296587	1.211892	-0.238536	6	3.850050	-1.328816	-2.038889
6	-3.209493	2.712970	-0.342494	6	4.971394	0.735004	0.098276
6	-4.575270	0.618897	-0.098060	6	4.295561	1.732577	-0.838195
6	-4.865906	-0.903670	-0.126949	6	6.350958	0.377848	-0.454923
6	-4.430747	-1.462556	-1.486979	6	5.184777	1.415524	1.453305
6	-5.775245	1.523755	-0.116855	1	2.130003	-0.010519	-0.990052
6	-6.365353	-1.187954	0.015256	1	-4.490531	3.610608	-0.071915
6	-4.184947	-1.631724	1.035296	1	-6.403556	2.186592	-0.764603
1	-3.872552	0.890069	0.938314	1	-6.052612	-0.259247	-1.015175
1	4.933487	-3.201825	0.010350	1	-2.022946	2.768996	1.642989
1	6.632358	-1.578425	-0.792335	1	-2.053684	3.798611	0.228355
1	5.961151	0.783874	-1.159781	1	-3.449954	-1.780147	-1.740817
1	2.384839	-2.606248	1.727501	1	-4.604104	-2.196060	-0.490759
1	2.535603	-3.685220	0.356519	1	5.347706	-1.476489	1.752549
1	3.141426	1.898369	-1.896396	1	5.402702	-2.174038	0.143097
1	4.273727	2.541195	-0.724211	1	4.036357	-2.502580	1.204628
1	-6.225948	1.442576	-1.106586	1	0.558257	-2.224808	0.523831
1	-5.548647	2.566436	0.053937	1	3.359531	-0.151169	1.163465
1	-6.524200	1.210492	0.600111	1	-2.148211	-2.801277	2.637296
1	-0.819225	1.990813	0.567764	1	-3.366997	-1.553024	2.387772
1	-2.143398	-0.588169	-0.295627	1	-3.718629	-3.234062	1.949154



1	1.873171	3.065731	2.448061	1	0.026766	3.833434	-1.490854
1	3.253153	1.993578	2.230934	1	1.004505	2.416409	-1.874818
1	3.331816	3.664960	1.645501	1	-0.714656	2.420511	-2.260796
1	0.534629	-3.964130	-1.450596	1	4.908658	-1.124918	-1.981913
1	-0.617728	-2.682797	-1.841328	1	3.710286	-2.393216	-2.224657
1	1.093714	-2.453736	-2.187573	1	3.452343	-0.802190	-2.902353
1	-2.210820	1.022221	2.387824	1	5.841754	2.275503	1.343124
1	-1.395433	-0.524787	2.196515	1	4.246591	1.770543	1.880413
1	-0.513749	0.881535	2.750338	1	5.649525	0.747923	2.176230
1	-2.303999	0.481278	-2.572147	1	4.881160	2.647161	-0.902562
1	-1.259938	1.780156	-2.004873	1	4.197099	1.352707	-1.855152
1	-0.653609	0.136878	-2.055514	1	3.306180	2.019166	-0.475298
1	-3.623837	3.219620	0.524845	1	6.957139	1.280723	-0.494303
1	-2.180881	3.031294	-0.441492	1	6.878706	-0.327042	0.182196
1	-3.759571	3.053341	-1.217606	1	6.336759	-0.020541	-1.466185
1	-4.734181	-2.504863	-1.554160	1	0.694732	3.933180	1.167618
1	-4.917709	-0.933929	-2.305048	1	0.545989	2.559290	2.273186
1	-3.358452	-1.420842	-1.649007	1	1.809602	2.574429	1.043900
1	-6.508722	-2.263902	-0.044421	1	-1.027864	-4.215100	0.250097
1	-6.765951	-0.870398	0.975149	1	-2.692880	-4.467255	-0.265720
1	-6.960545	-0.745543	-0.778933	1	-1.530988	-3.722332	-1.370993
1	-4.417227	-2.692398	0.972713	6	1.099199	-1.778165	-1.897338
1	-3.105687	-1.528136	1.044198	6	1.303084	-0.822287	1.917914
1	-4.562882	-1.276620	1.993449	1	1.568073	0.224402	2.043150
1	-1.446217	-3.070156	0.993021	1	0.486598	-1.016379	2.610552
1	-0.113201	-4.200487	1.209095	1	2.141218	-1.433230	2.254996
1	-0.286208	-2.818104	2.300071	1	1.422258	-1.354536	-2.841554
1	0.501958	4.130279	0.029798	1	1.335503	-2.841719	-1.918328
1	2.076494	4.525511	-0.652059	1	0.023346	-1.663106	-1.829919
1	0.942532	3.527317	-1.574323	46	-1.000766	-0.223343	0.174439
NImag = 1 (-293.3629 cm <sup>-1</sup> )				NImag = 1 (-493.3713 cm <sup>-1</sup> )			
<p style="text-align: center;"><b>TS8(c-e)</b>                      Et = -1765.9362                      Gsol = -1766.3759</p>				<p style="text-align: center;"><b>TS8(d-g)</b>                      Et = -1765.9594                      Gsol = -1766.4059</p>			
6	5.122413	-0.140008	-0.862139	6	5.143662	-0.887455	0.385266
6	3.841337	0.304123	-0.583150	6	5.774886	0.252166	-0.079645
7	2.882773	-0.544032	-0.174151	6	5.008199	1.320945	-0.509431
6	3.159691	-1.849986	-0.032585	6	3.629383	1.220825	-0.479700
6	4.415065	-2.355382	-0.324394	7	3.023805	0.104957	-0.026622
6	5.409534	-1.487874	-0.739766	6	3.761322	-0.933826	0.413699
6	3.466584	1.744216	-0.762524	6	2.755199	2.333256	-0.960891

15	2.056531	2.199052	0.320210	15	1.186638	2.339786	-0.015454
6	2.780182	2.562441	1.945655	6	1.556641	3.080207	1.597639
46	0.890522	0.190690	0.227643	15	1.433674	-2.296716	0.065232
15	0.394341	-2.101479	0.109068	6	1.908045	-3.003196	-1.539600
6	0.035574	-2.775577	-1.543171	6	3.027699	-2.117888	0.954654
6	2.076508	-2.729395	0.508323	6	-1.315770	-0.165876	0.482039
6	-0.956182	1.032671	0.670025	6	-2.793532	0.103892	-0.303701
6	-2.023039	0.995583	-0.419671	6	-2.696332	1.074950	-1.447375
6	-3.403963	1.551826	-0.170780	6	-2.061306	-1.146775	-0.425458
6	-3.765434	0.159173	-0.628738	6	-1.541774	-1.655070	-1.743462
6	-4.107797	-0.032939	-2.091927	6	-1.276611	-0.354775	1.980630
6	-1.278502	0.778762	2.126506	6	-3.985134	0.220963	0.629310
6	-0.657541	-3.058422	1.240110	6	-4.002911	1.570198	1.339135
6	1.476900	3.800506	-0.306424	6	-5.359803	-0.140394	-0.038871
6	-1.404165	1.235440	-1.776958	6	-5.973952	1.011633	-0.831859
6	-3.888312	2.781149	-0.901896	6	-5.220442	-1.360109	-0.946059
6	-4.544438	-0.791407	0.310660	6	-6.329244	-0.509642	1.086601
6	-5.967631	-0.210460	0.374995	1	5.713709	-1.732415	0.737578
6	-4.020591	-0.866151	1.734622	1	6.852770	0.308936	-0.102992
6	-4.582722	-2.206036	-0.265811	1	5.471298	2.223757	-0.874842
1	-3.583266	1.656166	0.894000	1	2.802004	-1.955468	2.010679
1	4.612089	-3.409566	-0.209582	1	3.632848	-3.020328	0.888946
1	6.399040	-1.857793	-0.962243	1	2.498887	2.172424	-2.010307
1	5.877641	0.560215	-1.182557	1	3.267202	3.291982	-0.898592
1	2.149527	-2.745422	1.598263	1	-0.957684	0.796335	0.093471
1	2.200558	-3.757541	0.171151	1	-2.469845	-1.935610	0.197522
1	3.140640	1.904248	-1.792576	6	0.519064	-3.585652	0.948595
1	4.324568	2.394379	-0.598095	6	0.096551	3.511636	-0.863474
1	-3.581028	-0.869889	-2.540836	1	-0.970685	-2.567616	-1.598852
1	-3.959277	0.849775	-2.697157	1	-2.373633	-1.907530	-2.398088
1	-5.166955	-0.264470	-2.149866	1	-0.911830	-0.936432	-2.259794
1	-0.770606	2.110748	0.589502	1	-1.697004	1.107545	-1.877164
1	-2.509990	-0.253423	-0.527561	1	-3.365839	0.762354	-2.245963
1	1.998223	2.852166	2.643357	1	-2.982618	2.080445	-1.154299
1	3.274967	1.677237	2.336666	1	-2.257063	-0.291828	2.445510
1	3.502439	3.373539	1.874322	1	-0.865846	-1.324748	2.250138
1	0.095222	-3.862306	-1.541830	1	-0.658777	0.405860	2.453861
1	-0.962554	-2.485088	-1.862257	1	2.413057	-3.955929	-1.389535
1	0.749244	-2.383054	-2.263409	1	1.039494	-3.165301	-2.169805
1	-2.172611	1.297495	2.473145	1	2.580927	-2.323551	-2.056256
1	-1.383735	-0.274210	2.363571	1	1.916237	4.100119	1.472394
1	-0.454985	1.153328	2.730536	1	0.657791	3.101688	2.209082
1	-2.092205	1.220705	-2.608830	1	2.312023	2.496378	2.117051
1	-0.964724	2.230912	-1.743182	1	-4.802242	1.615367	2.072633
1	-0.602721	0.525623	-1.961126	1	-3.069739	1.749038	1.871603
1	-4.967759	2.872805	-0.810061	1	-4.155693	2.396436	0.649608

1	-3.452030	3.670087	-0.452638	1	-3.856918	-0.556962	1.383241
1	-3.639909	2.791813	-1.958196	1	-7.297477	-0.776059	0.667449
1	-5.100642	-2.864702	0.426872	1	-5.972552	-1.366637	1.657332
1	-5.109136	-2.266690	-1.213815	1	-6.497545	0.313215	1.777571
1	-3.580395	-2.610512	-0.411645	1	-5.352800	1.348285	-1.658376
1	-6.566570	-0.845849	1.023636	1	-6.919687	0.685701	-1.260583
1	-5.976088	0.790343	0.802144	1	-6.192685	1.869915	-0.200655
1	-6.466875	-0.179061	-0.589409	1	-4.606838	-1.162930	-1.824511
1	-4.668567	-1.525070	2.307073	1	-4.799842	-2.213764	-0.414231
1	-3.019668	-1.283691	1.776294	1	-6.200520	-1.662964	-1.308640
1	-4.022863	0.093438	2.241927	1	1.082939	-4.516902	0.928434
1	-0.438524	-4.121079	1.149399	1	0.356377	-3.298017	1.983558
1	-0.482798	-2.750923	2.268009	1	-0.444840	-3.757642	0.477841
1	-1.707269	-2.908256	1.007144	1	-0.842543	3.606236	-0.323937
1	0.662600	4.172601	0.311272	1	0.569017	4.492050	-0.901249
1	2.282166	4.532408	-0.277576	1	-0.111861	3.181109	-1.877189
1	1.127465	3.707937	-1.331329	46	0.940297	-0.002116	0.043735
NImag = 1 (-625.8991 cm <sup>-1</sup> )				NImag = 1 (-360.1231 cm <sup>-1</sup> )			
<b>1a</b>				<b>1c</b>			
Et = -1365.3425				Et = -1561.8745			
Gsol = -1365.7388				Gsol = -1562.2566			
7	0.000000	-1.416630	0.000000	6	-3.065533	1.130576	-0.168683
6	-1.131398	-2.093037	0.308063	6	-4.395104	1.171831	-0.550391
6	-1.154334	-3.474215	0.301533	6	-4.990629	0.028241	-1.051048
6	0.000000	-4.174610	0.000000	6	-4.240451	-1.128379	-1.166294
6	1.154334	-3.474215	-0.301533	6	-2.907165	-1.109533	-0.797100
6	1.131398	-2.093037	-0.308063	7	-2.338381	0.007384	-0.307643
6	-2.344386	-1.310209	0.704622	6	-2.039983	-2.321056	-0.969808
15	-2.319638	0.359041	-0.044915	15	-0.607033	-2.286290	0.178677
6	-3.054511	0.225402	-1.693442	6	0.604394	-3.437995	-0.523596
6	2.344386	-1.310209	-0.704622	78	-0.283222	-0.008473	0.277261
15	2.319638	0.359041	0.044915	6	1.672959	-0.040678	0.945387
6	3.054511	0.225403	1.693442	1	1.831357	0.786595	1.638119
78	0.000000	0.650543	0.000000	6	-2.409993	2.317005	0.472110
6	0.097562	2.760262	0.681539	15	-0.583805	2.278222	0.276345
6	-0.097562	2.760262	-0.681539	6	0.058570	3.341766	1.595491
6	3.415947	1.403490	-0.942276	6	-1.169151	-3.056647	1.720959
6	-3.415947	1.403489	0.942276	6	-0.243889	3.162434	-1.273223
1	-2.067699	-3.993018	0.545906	6	2.683706	0.048332	-0.188327
1	0.000000	-5.254324	0.000000	1	2.595713	-0.798935	-0.866598
1	2.067699	-3.993018	-0.545906	6	4.184947	0.054342	0.407500
1	-2.339168	-1.171378	1.788295	6	4.512093	-1.225788	1.151807
1	-3.255144	-1.852865	0.458253	6	4.941244	0.328695	-0.790142

1	2.339168	-1.171378	-1.788295	6	5.516743	-0.751128	-1.591159
1	3.255145	-1.852864	-0.458253	6	5.148362	1.707880	-1.231993
1	1.078795	2.927148	1.100144	1	6.458633	-1.017579	-1.091336
1	-1.078796	2.927148	-1.100144	1	5.753808	-0.460231	-2.608800
1	-4.088188	-0.107313	-1.617958	1	-4.957951	2.084875	-0.437390
1	-3.038259	1.192554	-2.190366	1	-6.029638	0.036813	-1.343787
1	-2.494445	-0.481546	-2.300011	1	-4.678150	-2.035872	-1.551055
1	4.088188	-0.107313	1.617958	1	-2.607171	2.283958	1.546016
1	3.038259	1.192554	2.190366	1	-2.837231	3.247286	0.101695
1	2.494445	-0.481545	2.300011	1	-1.629647	-2.319349	-1.981997
1	-4.423167	0.990104	0.944733	1	-2.623123	-3.234449	-0.865664
1	-3.060569	1.471734	1.967250	1	1.839956	-0.952234	1.515332
1	-3.463702	2.403691	0.517104	1	4.217129	0.921642	1.066581
1	3.463702	2.403691	-0.517103	1	4.918194	-1.658183	-1.564798
1	4.423167	0.990104	-0.944733	1	2.523719	0.954089	-0.769841
1	3.060569	1.471734	-1.967250	1	3.950660	-1.261526	2.079372
1	-0.728435	2.903131	1.363328	1	4.265641	-2.116088	0.577146
1	0.728434	2.903131	-1.363328	1	5.566865	-1.268997	1.413643
				1	-0.618544	4.183109	-1.226279
				1	0.826858	3.193493	-1.457939
				1	-0.718176	2.645394	-2.103340
				1	-1.475773	-4.087057	1.552701
				1	-0.365362	-3.042352	2.452963
				1	-2.005713	-2.494501	2.127711
				1	-0.384452	4.334314	1.543139
				1	-0.158951	2.903402	2.565875
				1	1.136706	3.441605	1.497920
				1	1.466788	-3.502317	0.135674
				1	0.177726	-4.433946	-0.625520
				1	0.930516	-3.090049	-1.500182
				1	6.225846	1.896641	-1.138051
				1	4.936876	1.827437	-2.294249
				1	4.622730	2.443816	-0.634200
<b>4a</b>				<b>4c</b>			
Et = -1443.9770				Et = -1758.4142			
Gsol = -1444.3818				Gsol = -1758.8516			
6	-2.310058	1.127700	0.303105	6	4.534737	-2.250478	-0.345469
6	-3.691723	1.150783	0.297657	6	5.472486	-1.357912	-0.832244
6	-4.392625	-0.004043	0.001779	6	5.110408	-0.036517	-1.022538
6	-3.689800	-1.157431	-0.295214	6	3.814633	0.357573	-0.737990
6	-2.308208	-1.131543	-0.302620	7	2.912220	-0.516160	-0.257616
7	-1.630138	-0.001253	-0.000147	6	3.260746	-1.797611	-0.050339
6	-1.525499	-2.345777	-0.687491	6	3.360653	1.762271	-0.997551

15	0.136490	-2.313746	0.073347	15	1.928992	2.210013	0.060223
6	1.133284	-3.492778	-0.870038	78	0.916814	0.149014	0.208560
78	0.452320	0.000403	0.000108	15	0.526887	-2.134817	0.229629
6	2.593628	-0.348538	0.599452	6	0.088338	-2.882438	-1.367762
6	2.853591	0.253105	1.939748	6	2.240678	-2.704252	0.566205
6	-1.529322	2.343700	0.686482	6	2.621799	2.861384	1.605152
15	0.132046	2.313980	-0.075734	6	-0.950657	0.899975	0.766338
6	1.127096	3.497170	0.864277	6	-2.085132	0.423076	-0.140099
6	-0.021101	-2.998709	1.741977	6	-1.830868	0.720354	-1.608386
6	-0.028728	2.995260	-1.745570	6	-1.174083	0.593083	2.238183
6	2.594371	0.353374	-0.594367	6	-3.481301	1.076599	0.385787
6	2.859594	-0.247871	-1.933832	6	-4.544644	0.525157	-0.435170
1	-4.209274	2.065827	0.538299	6	-5.153425	-0.810496	-0.170423
1	-5.472258	-0.005146	0.002582	6	-6.690217	-0.650210	-0.175288
1	-4.205854	-2.073485	-0.535223	6	-3.429519	2.597305	0.448194
1	-1.380085	2.346181	1.768708	6	-5.072024	1.325116	-1.543165
1	-2.074538	3.252238	0.437623	6	-4.755330	-1.747341	-1.335936
1	-1.377055	-2.347057	-1.769835	6	-4.739844	-1.440454	1.155271
1	-2.068791	-3.255561	-0.439011	1	-5.835283	1.972471	-1.088470
1	2.762309	-1.416226	0.529706	1	-5.568764	0.750143	-2.315309
1	2.760550	1.421410	-0.524303	1	4.789558	-3.284875	-0.177170
1	2.238674	0.189593	-2.711477	1	6.475361	-1.687626	-1.057688
1	3.896859	-0.041651	-2.202170	1	5.819423	0.682797	-1.400852
1	2.725691	-1.324857	-1.935650	1	2.365737	-2.682459	1.651201
1	3.890023	0.047667	2.211877	1	2.391794	-3.735405	0.250930
1	2.718887	1.330002	1.940947	1	3.018831	1.836692	-2.032232
1	2.230169	-0.184741	2.715185	1	4.184291	2.465102	-0.884633
1	-0.393899	4.019678	-1.700833	1	-0.890733	1.982200	0.648744
1	0.938557	2.995005	-2.242555	1	-3.584915	0.667077	1.388210
1	-0.717704	2.394766	-2.333711	1	-4.333495	1.998817	-1.964402
1	-0.381884	-4.024602	1.695470	1	-2.200521	-0.653709	-0.011178
1	0.946204	-2.995204	2.238918	1	-5.211200	-2.415969	1.242558
1	-0.712621	-2.402243	2.331242	1	-3.666460	-1.590940	1.235979
1	0.666587	4.482376	0.808397	1	-5.070480	-0.849281	2.007157
1	1.194111	3.199955	1.907290	1	-7.124536	-1.619265	0.058024
1	2.129972	3.572611	0.451052	1	-7.023536	0.051450	0.586546
1	2.136029	-3.568388	-0.456515	1	-7.082139	-0.338391	-1.138210
1	0.673859	-4.478680	-0.817580	6	-0.467936	-3.029920	1.455676
1	1.200487	-3.192069	-1.912037	6	1.159876	3.631964	-0.758695
				1	-0.864919	0.307137	-1.890645
				1	-2.579079	0.286482	-2.269656
				1	-1.786133	1.790514	-1.804214
				1	-2.764360	2.903097	1.249057
				1	-3.074984	3.055911	-0.470662
				1	-4.408022	3.014098	0.675747
				1	-2.005247	1.155079	2.671842

	1	-1.373994	-0.464515	2.405749
	1	-0.297248	0.848223	2.829466
	1	0.151225	-3.967772	-1.319433
	1	-0.924186	-2.602186	-1.646640
	1	0.763118	-2.519417	-2.138853
	1	3.234746	3.740161	1.414422
	1	1.816218	3.135458	2.282068
	1	3.227495	2.099438	2.088656
	1	-5.246520	-2.703185	-1.169654
	1	-5.076215	-1.375541	-2.304560
	1	-3.682651	-1.922882	-1.366627
	1	-0.284231	-4.100333	1.382325
	1	-0.218887	-2.695204	2.459055
	1	-1.526204	-2.852638	1.284365
	1	0.342128	4.010758	-0.150576
	1	1.884870	4.432698	-0.891435
	1	0.768719	3.340455	-1.729658
<b>5a</b>				
Et = -1372.9018				
Gsol = -1373.2954				
7	0.000000	1.297959	0.000000	
6	-1.118318	1.971328	-0.344168	
6	-1.144565	3.353567	-0.339815	
6	0.000000	4.053138	0.000000	
6	1.144565	3.353567	0.339815	
6	1.118318	1.971328	0.344168	
6	-2.312222	1.175765	-0.770338	
15	-2.319323	-0.462362	0.049536	
6	-3.030511	-0.230258	1.698828	
6	2.312222	1.175765	0.770338	
15	2.319323	-0.462362	-0.049536	
6	3.030511	-0.230258	-1.698828	
46	0.000000	-0.782485	0.000000	
6	0.123375	-2.932617	-0.670456	
6	-0.123375	-2.932617	0.670455	
6	3.460410	-1.515126	0.878696	
6	-3.460410	-1.515126	-0.878696	
1	-2.049378	3.872792	-0.613519	
1	0.000000	5.132846	0.000000	
1	2.049378	3.872792	0.613518	
1	-2.259834	0.995398	-1.846557	
1	-3.235686	1.722073	-0.585257	
1	2.259834	0.995398	1.846557	
1	3.235686	1.722073	0.585257	
<b>5c</b>				
Et = -1569.4320				
Gsol = -1569.8127				
7	-2.367324	-0.130319	-0.258080	
6	-3.197096	0.915810	-0.112518	
6	-4.528688	0.828241	-0.481572	
6	-5.012610	-0.369802	-0.976489	
6	-4.155058	-1.449078	-1.098497	
6	-2.826579	-1.296640	-0.740617	
6	-2.646440	2.159234	0.519844	
15	-0.833892	2.320330	0.253987	
6	-0.660528	3.180430	-1.337821	
6	-1.840194	-2.413696	-0.911855	
15	-0.438680	-2.259734	0.269290	
6	-1.022461	-3.002680	1.820498	
46	-0.306638	0.061848	0.302581	
6	1.639825	0.258882	0.954947	
6	2.643405	0.101715	-0.166608	
1	2.611765	-0.900953	-0.589717	
6	0.815338	-3.414576	-0.357356	
1	1.751889	1.232048	1.429061	
6	-0.279167	3.509742	1.505924	
6	4.142670	0.362019	0.396940	
6	4.907361	0.275700	-0.822185	
6	5.033678	1.440846	-1.698236	
6	4.508508	-0.595747	1.513274	
6	5.564802	-0.967909	-1.222703	

1	1.123426	-3.068252	-1.054360	1	6.515222	-0.988961	-0.671050
1	-1.123426	-3.068253	1.054360	1	5.798482	-1.015333	-2.280935
1	-4.052516	0.136200	1.617209	1	-5.177996	1.681459	-0.364519
1	-3.043841	-1.173579	2.239329	1	-6.050074	-0.463087	-1.260077
1	-2.440397	0.484199	2.266955	1	-4.506645	-2.395264	-1.478505
1	4.052516	0.136200	-1.617209	1	-2.796769	2.096659	1.600046
1	3.043841	-1.173579	-2.239329	1	-3.182827	3.043198	0.178373
1	2.440398	0.484199	-2.266955	1	-1.412384	-2.358535	-1.915349
1	-4.454234	-1.069964	-0.890522	1	-2.331245	-3.382303	-0.830661
1	-3.120353	-1.640106	-1.903577	1	1.787078	-0.495270	1.724226
1	-3.535392	-2.494046	-0.410299	1	4.123966	1.395257	0.742795
1	3.535392	-2.494046	0.410299	1	5.027724	-1.852972	-0.891425
1	4.454234	-1.069964	0.890522	1	2.446728	0.810474	-0.967632
1	3.120353	-1.640106	1.903577	1	3.934614	-0.355373	2.402208
1	-0.677973	-3.036783	-1.388390	1	4.304391	-1.633299	1.257296
1	0.677973	-3.036784	1.388390	1	5.560364	-0.508864	1.775939
				1	-1.161275	4.146491	-1.312642
				1	0.390897	3.341320	-1.562046
				1	-1.091655	2.577651	-2.132992
				1	-1.296461	-4.045814	1.674839
				1	-0.240915	-2.946552	2.574239
				1	-1.886164	-2.455045	2.188624
				1	-0.836156	4.441776	1.431647
				1	-0.411589	3.094094	2.501475
				1	0.776218	3.729910	1.364408
				1	1.664699	-3.437008	0.321379
				1	0.410116	-4.422437	-0.426823
				1	1.156255	-3.105822	-1.342149
				1	4.475371	2.306673	-1.361125
				1	6.099551	1.700547	-1.718903
				1	4.791438	1.188697	-2.731118
<b>8a</b>				<b>8c</b>			
Et = -1451.5378				Et = -1765.9732			
Gsol = -1451.9396				Gsol = -1766.4076			
7	-1.553718	-0.002099	-0.000104	6	5.245408	0.056612	-0.977186
6	-2.227412	-1.121450	-0.336410	6	3.939758	0.423010	-0.697284
6	-3.609900	-1.151004	-0.331209	7	3.054820	-0.467724	-0.221702
6	-4.312025	-0.006296	0.001215	6	3.424583	-1.740997	-0.015557
6	-3.613071	1.140544	0.332932	6	4.708336	-2.171258	-0.305949
6	-2.230486	1.115202	0.336821	6	5.630372	-1.258664	-0.786593
6	-1.431937	-2.317464	-0.751437	6	3.453285	1.817918	-0.955860
15	0.208305	-2.315432	0.062598	15	2.028570	2.249448	0.122758
6	-0.028980	-2.987737	1.728250	6	2.754268	2.856410	1.673688



6	-1.438304	2.313717	0.750986	46	1.035164	0.161264	0.238026
15	0.201307	2.316168	-0.064239	15	0.687005	-2.154961	0.225092
6	-0.039779	2.985209	-1.730678	6	0.327350	-2.895685	-1.398095
46	0.538137	0.000776	0.000002	6	2.415476	-2.666398	0.593844
6	2.711621	0.387134	-0.568701	6	-0.844371	0.862285	0.785777
6	2.711592	-0.379621	0.572659	6	-1.937082	0.377629	-0.159938
6	2.918942	0.147775	1.952188	6	-3.352064	0.977918	0.342679
6	1.196070	3.531703	0.836437	6	-4.410053	0.466243	-0.523354
6	2.923994	-0.139557	-1.947757	6	-4.802854	1.222637	-1.718166
6	1.206520	-3.526087	-0.840817	6	-1.057327	0.497242	2.241601
1	-4.126542	-2.059119	-0.598740	6	-0.295106	-3.130366	1.403197
1	-5.391681	-0.007941	0.001749	6	1.285065	3.711554	-0.653286
1	-4.132210	2.047094	0.600943	6	-1.638759	0.711932	-1.612546
1	-1.253384	-2.276379	-1.828421	6	-3.338010	2.499838	0.464374
1	-1.976153	-3.239870	-0.555088	6	-5.184012	-0.746685	-0.170786
1	-1.258926	2.273532	1.827867	6	-6.231060	-0.124403	0.817575
1	-1.985462	3.234402	0.554704	6	-4.400444	-1.824567	0.577721
1	2.859920	1.452390	-0.440790	6	-5.934369	-1.379335	-1.339824
1	2.863612	-1.444408	0.445156	1	-3.481329	0.539294	1.329487
1	2.274520	-0.337168	2.681645	1	4.983133	-3.200935	-0.139702
1	3.946359	-0.065894	2.251280	1	6.640389	-1.568895	-1.008138
1	2.775142	1.222510	2.008702	1	5.943103	0.789137	-1.351325
1	3.950872	0.079083	-2.245077	1	2.522726	-2.633034	1.680510
1	2.785611	-1.215004	-2.004296	1	2.598148	-3.696748	0.292034
1	2.278520	0.342043	-2.678504	1	3.096666	1.882770	-1.986242
1	-0.422360	-4.001318	1.671884	1	4.264096	2.538196	-0.857584
1	0.919587	-3.014905	2.259050	1	-4.807732	0.571996	-2.593036
1	-0.722080	-2.367504	2.290649	1	-4.199104	2.100663	-1.900031
1	-0.436256	3.997647	-1.675478	1	-5.845232	1.535830	-1.603597
1	0.908138	3.014464	-2.262511	1	-0.785364	1.946063	0.695890
1	-0.731544	2.361930	-2.291354	1	-2.028937	-0.703174	-0.057001
1	0.713773	-4.497053	-0.815513	1	1.964043	3.128946	2.369079
1	1.331628	-3.225374	-1.877579	1	3.355109	2.075013	2.131898
1	2.186804	-3.636257	-0.383426	1	3.379973	3.728917	1.495150
1	2.175485	3.644718	0.377876	1	0.450535	-3.976744	-1.370989
1	0.699787	4.500837	0.810112	1	-0.693272	-2.667973	-1.695822
1	1.323300	3.233103	1.873546	1	0.997614	-2.481005	-2.146918
				1	-1.906677	1.021690	2.689388
				1	-1.228035	-0.570152	2.374471
				1	-0.191893	0.761878	2.845859
				1	-2.350505	0.272375	-2.308418
				1	-1.615424	1.786266	-1.787338
				1	-0.655170	0.326176	-1.871941
				1	-4.340544	2.895965	0.609879
				1	-2.757031	2.783940	1.336298
				1	-2.902482	2.994277	-0.399267



	1	-6.503038	-2.230362	-0.974701
	1	-6.643075	-0.701189	-1.806992
	1	-5.250976	-1.748742	-2.102771
	1	-6.884500	-0.943352	1.112094
	1	-5.770194	0.282156	1.713299
	1	-6.848026	0.638478	0.350420
	1	-5.102719	-2.577517	0.925963
	1	-3.694936	-2.321124	-0.084889
	1	-3.871498	-1.451182	1.450177
	1	-0.078036	-4.191830	1.297329
	1	-0.071235	-2.824736	2.421929
	1	-1.356391	-2.978026	1.224789
	1	0.471631	4.083973	-0.035162
	1	2.021010	4.506043	-0.761872
	1	0.889943	3.458078	-1.633437