

Electronic Supplimentary Information
for

Mechanism and Electronic Effects in Nitrogen Ylide-Promoted
Asymmetric Aziridination Reaction

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Table S1. The Relative Energies (in kcal mol⁻¹) Obtained at the mPW1K/6-31G* level of theory for the Transition States for the Addition of g-ylide to Benzaldehyde with Substituents (X) at the para Position ⁱ

Substituents (X)	TS1 _{re-re}	TS2 _{re-si}	TS3 _{si-si}	TS4 _{si-re}
NO ₂	-ii-	-ii-	-ii-	-ii-
CN	0.00	1.01	4.53	5.04
COOMe	0.00	1.16	5.50	5.34
Cl	0.00	0.78	4.53	4.85
H	0.00	1.25	5.30	5.23
Me	0.00	1.69	5.31	5.31
OMe	0.00	1.28	4.77	5.08
OH	0.00	1.51	4.81	4.85

ⁱ The relative energies are with respect to the lowest energy transition state in each set of substituents. ⁱⁱ Transition state, TS1_{re-re}(NO₂) could not be optimized as all the attempts led to a saddle point with an undesired low imaginary frequency.

Table S2. The Relative Energies (in kcal mol⁻¹) Obtained at the mPW1PW91/6-31G* level of theory for the Transition States for the Addition of g-ylide to Benzaldehyde with Substituents (X) at the para Position ⁱ

Substituents (X)	TS1 _{re-re}	TS2 _{re-si}	TS3 _{si-si}	TS4 _{si-re}
NO ₂	0.00	0.89	-ii-	4.82
CN	0.00	0.76	4.59	5.33
COOMe	0.00	1.41	5.84	5.37
Cl	0.00	0.61	4.69	5.17
H	0.00	1.55	5.57	5.36
Me	0.00	0.90	4.46	4.37
OMe	0.00	0.97	4.84	4.75
OH	0.00	0.91	3.95	4.53

ⁱ The relative energies are with respect to the lowest energy transition state in each set of substituents. ⁱⁱ Transition state, TS3_{si-re}(NO₂) could not be optimized as all the attempts led to a saddle point with an undesired low imaginary frequency.

Table S3. The Relative Energies (in kcal mol⁻¹) Obtained at the PCM_(THF)/mPW1PW91//6-311++G**//mPW1PW91/6-31G* level of theory for the Transition States for the Addition of g-ylide to Benzaldehyde with Substituents (X) at the para Positionⁱ

Substituents (X)	TS1 _{re-re}	TS2 _{re-si}	TS3 _{si-si}	TS4 _{si-re}
NO ₂	0.00	0.99	-ii-	7.06
CN	0.00	1.67	6.78	6.66
COOMe	0.00	1.67	5.90	6.10
Cl	0.00	1.93	5.87	5.52
H	0.00	1.55	4.87	4.55
Me	0.00	1.36	4.76	4.61
OMe	0.00	0.33	3.78	3.27
OH	0.00	1.06	4.53	3.96

ⁱ The relative energies are with respect to the lowest energy transition state in each set of substituents. ⁱⁱ Transition state, TS3_{si-si}(NO₂) could not be optimized as all the attempts led to a saddle point with an undesired low imaginary frequency.

Table S4. The Relative Energies (in kcal mol⁻¹) Obtained at the B3LYP/6-31G* level of theory for the Transition States for the Addition of g-ylide to Benzaldehyde with Substituents (X) at the para Position ⁱ

Substituents (X)	TS1 _{re-re}	TS2 _{re-si}	TS3 _{si-si}	TS4 _{si-re}
NO ₂	0.00	1.64	-ii-	5.56
CN	0.00	1.06	5.27	5.22
COOMe	0.00	1.05	4.11	5.38
Cl	0.00	1.25	5.01	5.29
H	0.00	1.25	4.30	5.39
Me	0.00	0.49	3.29	5.01
OMe	0.00	0.42	4.46	4.59
OH	0.00	0.68	3.70	4.93

ⁱ The relative energies are with respect to the lowest energy transition state in each set of substituents. ⁱⁱ Transition state, TS3_{si-si}(NO₂) could not be optimized as all the attempts led to a saddle point with an undesired low imaginary frequency.

Table S5. The Relative Energies (in kcal mol⁻¹) of Transition States Obtained at the PCM_(THF)/B3LYP/6-311++G**//B3LYP/6-31G* level of theory for the Addition of glylide to Benzaldehyde with Various Substituents (X) at the para Position ^{i,ii}

Substituents (X)	TS1 _{re-re}	TS2 _{re-si}	TS3 _{si-si}	TS4 _{si-re}
NO ₂	0.00	0.60	-ii-	2.72
CN	0.00	0.64	2.26	2.77
COOMe	0.00	0.12	2.32	1.79
Cl	0.00	0.28	2.24	1.98
H	0.00	0.08	1.92	1.84
Me	0.00	0.31	1.85	1.48
OMe	0.00	0.02	1.63	1.20
OH	0.00	0.03	2.73	1.19

ⁱ For each substituents relative energy is calculated with respect to the lowest energy transition state. ⁱⁱ Transition state, TS3_{si-si}(NO₂) is not able to optimized as all the attempt to optimize leads to a saddle point with low imaginary frequency.

Table S6. The Relative Energies (in kcal mol⁻¹) of Transition States for the Addition of g-ylide to Benzaldehyde with Various Substituents (X) at the para Position Obtained at the mPW1K/6-31+G** level of theoryⁱ

X ⁱⁱ	TS1 _{re-re}	TS2 _{re-si}	TS3 _{si-si}	TS4 _{si-re}
COOMe	0.00	0.94	5.51	5.56
Cl	0.00	0.88	5.26	5.31
H	0.00	0.81	5.20	5.18
Me	0.00	0.78	5.18	5.10

ⁱ For each substituent, the relative energy is calculated with respect to the lowest energy transition state.

Table S7. The Relative Energies (in kcal mol⁻¹) of Transition States for the Addition of g-ylide to Benzaldehyde with Various Substituents (X) at the para Position Obtained at the PCM_(THF)/mPW1K/6-311++G**//mPW1K/6-31+G** level of theoryⁱ

X ⁱⁱ	TS1 _{re-re}	TS2 _{re-si}	TS3 _{si-si}	TS4 _{si-re}
COOMe	0.00	0.82	4.92	4.95
Cl	0.00	0.87	4.87	4.91
H	0.00	0.80	4.61	4.67
Me	0.00	1.05	4.77	4.70

ⁱ For each substituent, the relative energy is calculated with respect to the lowest energy transition state.

Table S8. Relative Gibbs Free Energies (in kcal mol⁻¹) of Transition States for the Addition of g-ylide to Benzaldehyde with Various Substituents (X) at the para Position Obtained at the mPW1K/6-31G* level of theoryⁱ

X^{ii}	TS1 _{re-re}	TS2 _{re-si}	TS3 _{si-si}	TS4 _{si-re}
CN	0.00	1.01	4.53	5.04
COOMe	0.00	1.16	5.50	5.34
Cl	0.00	0.78	4.53	4.85
H	0.00	1.25	5.30	5.23
Me	0.00	1.69	5.31	5.31
OMe	0.00	1.28	4.77	5.08
OH	0.00	1.51	4.81	4.85

ⁱ For each substituent, the relative free energy is calculated with respect to the lowest energy transition state. ⁱⁱ Transition state, TS1_{re-re}(NO₂) could not be successfully optimized, as all attempts led to a saddle point with low imaginary frequency not pertaining to the reaction coordinate.

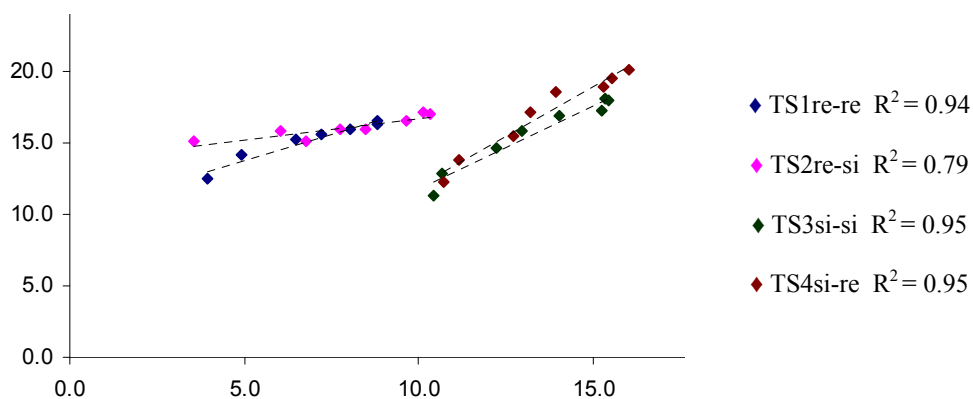


Figure S1. Correlation diagram for activation energies with degree of pyramidalization around the carbon atoms involved in the C-C bond formation. Activation energies (in kcal mol⁻¹) in X-axis are computed at the mPW1K /6-31G* level of theory

Table S9. Deformation Energies (in kcal mol⁻¹) around the Carbonyl Carbon of Electrophile (A) and Carbon Atom of Ylide (G) ⁱ Computed at the mPW1K/6-31G* Level of Theory

Substituents (X)	TS1 _{re-re}		TS2 _{re-si}		TS3 _{si-si}		TS4 _{si-re}	
	G	A	G	A	G	A	G	A
NO ₂	-ii-	-ii-	4.31	4.46	11.56	1.95	12.05	2.27
CN	3.90	3.36	5.65	5.82	12.53	2.61	12.84	2.73
COOMe	5.18	5.26	6.59	5.53	13.43	3.25	13.85	3.35
Cl	5.45	6.36	6.81	6.57	14.18	4.15	14.39	4.31
H	6.06	7.01	7.90	6.76	14.59	4.63	15.14	5.06
Me	6.34	7.45	8.16	7.33	14.96	5.03	15.33	5.41
OMe	6.50	8.30	8.48	8.15	15.07	5.60	15.74	6.27
OH	6.55	8.06	8.37	8.07	15.20	5.68	15.59	5.99

ⁱ Deformation energies are calculated by fragmenting both nucleophile and electrophile of respective pre-reacting complexes and the transition states followed by calculating the difference in energies of each fragments. ⁱⁱ Transition state, TS1_{re-re}(NO₂) could not be successfully optimized, as all attempts led to a saddle point with low imaginary frequency.

Table S10. Gibbs Free Energies of Activation (in kcal mol⁻¹) Obtained at the PCM_(THF)/mPW1K/6-311++G**//mPW1K/6-31G* Level of Theory for the Addition of g-ylide to Benzaldehyde with Various Substituents at para Position ⁱ

Substituents (X)	TS5 _{re-re}	TS6 _{re-si}
NO ₂	3.21	-ii-
CN	3.20	-ii-
COOH	4.95	5.99
COOMe	5.56	6.06
Cl	6.52	7.01
F	7.44	7.51
H	6.82	7.01
Me	7.81	7.54
OMe	9.46	9.1
OH	8.62	8.48

ⁱ Absolute energies are with respect to the corresponding PRCs. PRCs are optimized and verified as true minima by frequency analysis. ⁱⁱ Transition state, TS6_{re-si}(NO₂) and (CN) could not be optimized as all attempts led to a saddle point with an undesired low imaginary frequency.

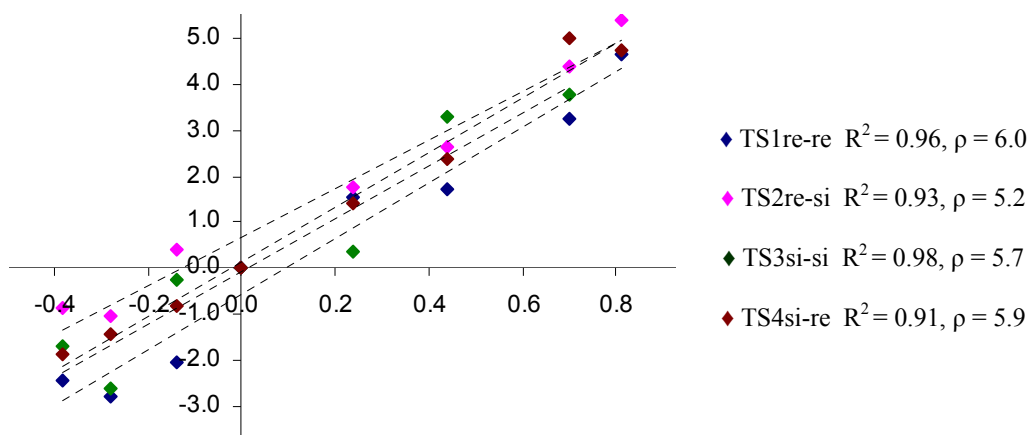


Figure S2. Hammett plots for the four stereochemical modes of addition of g-ylide (when R= *tert*-butyl) to para-substituted benzaldehydes. The $-(\Delta G_x^\ddagger - \Delta G_H^\ddagger)$ term is in the Y-axis and substituent constant (σ) is in the X-axis. Activation energies (in kcal mol⁻¹) in the Y-axis are computed at the B3LYP/6-31G* level of theory

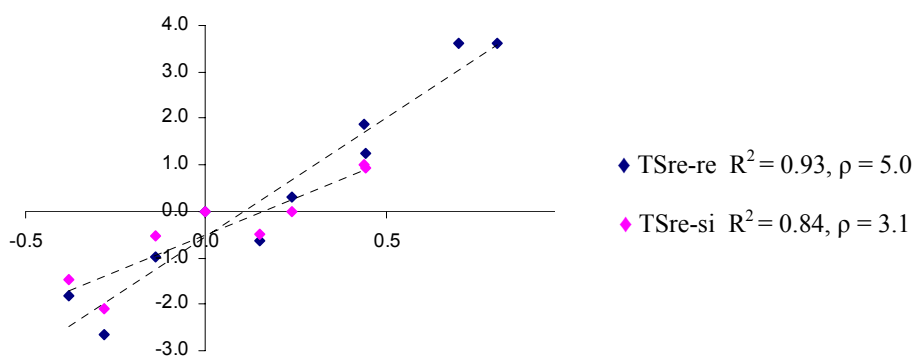


Figure S3. Hammett plots for the two stereochemical modes of addition of g-ylide (when R= Me) to para-substituted benzaldehydes. The $-(\Delta G_x^\ddagger - \Delta G_H^\ddagger)$ term is in the Y-axis and substituent constant (σ) is in the X-axis. Activation energies (in kcal mol⁻¹) in the Y-axis are computed at the mPW1K/6-31G* level of theory.

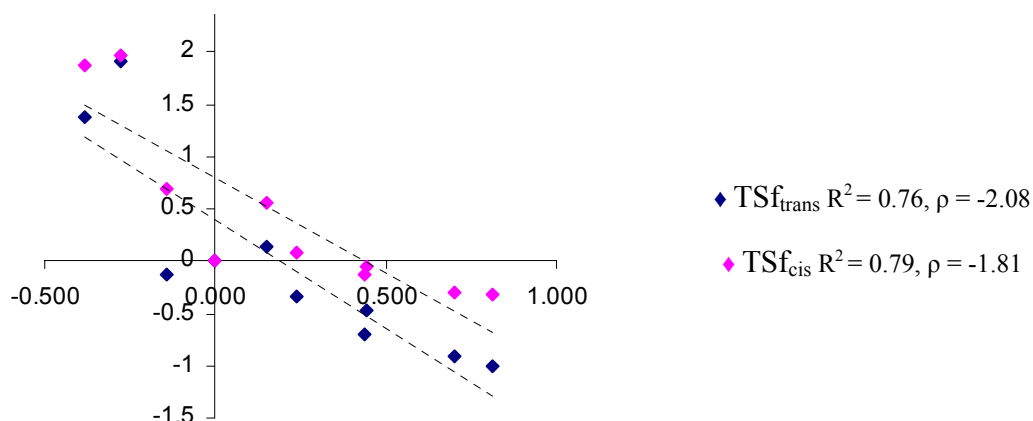


Figure S4. Hammett plot for the fragmentation of *cis* and *trans* oxaspirocyclic intermediates of a simplified model. The $-(\Delta G_{\text{x}}^{\ddagger} - \Delta G_{\text{H}}^{\ddagger})$ term is in the Y-axis and substituent constant (σ) is in the X-axis. Activation energies (in kcal mol^{-1}) in the Y-axis are computed at the B3LYP/6-31G* level of theory

Table S11. Stereoselectivity Calculated on the Basis of the Relative Energies of Pertinent Transition States Involved in the Most Preferred Pathwayⁱ

Substituents	Selectivity determining transition states	Difference in energy (kcal mol^{-1})	<i>de</i>
OH	Addition	1.2	76
OMe	Addition	1.2	76
Me	Rotation	9.5	>99
H	Rotation	8.3	>99
Cl	Rotation	7.2	>99
COOMe	Rotation	7.2	>99

ⁱ *ee* of the reaction is determined by the difference in energies of the addition step TS1_{re-re} and TS3_{si-si} . Energy differences for the substituents considered is found to be $> 4.5 \text{ kcal mol}^{-1}$. These differences lead to an *ee* >99 . Lower stereoselectivity noticed in experimental studies might be due to the likely involvement of competitive pathways ($\text{S}_{\text{N}1}$ vs $\text{S}_{\text{N}2}$). Low stereoselectivity noticed in the case of CN and NO_2 is due to energetically closer transition states (TS_{cis} and TSf3) as described in the text.

Full citation for Gaussian 03

Reference 26) Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

Total electronic energy (in a.u) and Cartesian coordinates of geometries optimized at the mPW1K/6-31G* level of theory. Gsol indicates the single-point energies at the PCM_(THF)/mPW1K/6-311++G** level of theory. *Pre-reacting complex for each transition states are denoted by 'PRC' followed by substituent and mode of addition*

TS1(CN)re-re				TS1(COOMe)re-re			
Et = -1341.175765				Et = -1476.7722707			
Gsol = -1341.492903				Gsol = -1477.125372			
7	3.474093	-0.975296	-0.339580	7	3.850355	-1.300275	-0.332019
6	2.456745	-0.186981	0.050474	6	2.930858	-0.413610	0.087301
7	2.459500	-0.045079	1.387762	7	2.872183	-0.399632	1.431211
6	3.448390	-0.917755	1.995806	6	3.684341	-1.464429	1.992649
6	4.329533	-1.297937	0.793489	6	4.581231	-1.846368	0.803057
7	1.570763	0.380271	-0.744125	7	2.186040	0.355864	-0.681084
6	1.921418	0.821697	-2.097086	6	2.661488	0.843511	-1.978108
6	3.135300	1.723467	-2.117362	6	3.994588	1.550577	-1.877459
6	1.856103	1.065527	2.081070	6	2.386931	0.713658	2.206918
6	2.813105	-2.105536	2.691788	6	2.841622	-2.609553	2.519246
6	5.651026	-0.557306	0.741668	6	5.989928	-1.293874	0.893303
6	3.495536	-1.743068	-1.562589	6	3.835246	-1.952730	-1.621286
6	0.206123	0.471213	-0.329421	6	0.816462	0.582191	-0.332527
6	-0.316825	1.793029	-0.220013	6	0.453321	1.954162	-0.146199
8	-1.530605	1.798771	0.370007	8	-0.767205	2.067878	0.412445
6	-2.257043	3.021757	0.572180	6	-1.362137	3.352303	0.658357
6	-2.605099	3.667297	-0.758744	6	-1.591912	4.096995	-0.646143
8	0.232658	2.805956	-0.634101	8	1.132673	2.915318	-0.478833
6	-3.517854	2.562752	1.282025	6	-2.688985	2.999659	1.305884
6	-1.474626	3.970785	1.466419	6	-0.511896	4.163763	1.623231
6	-0.603218	-1.026623	-1.923633	6	-0.067695	-0.642612	-1.993065
8	0.344288	-1.796811	-2.044191	8	0.765870	-1.541882	-2.121242
6	-1.830049	-1.418305	-1.182252	6	-1.390808	-0.906151	-1.364501
6	-2.983451	-0.644981	-1.236941	6	-2.436134	0.001975	-1.479702
6	-4.134097	-1.057144	-0.596523	6	-3.676917	-0.285143	-0.944791
6	-4.137291	-2.256714	0.113842	6	-3.882476	-1.489463	-0.278635
6	-2.984838	-3.040812	0.166644	6	-2.839317	-2.404460	-0.167484
6	-1.844556	-2.622451	-0.485678	6	-1.606626	-2.117540	-0.714734
1	2.476494	-1.926769	-1.895218	6	-5.183887	-1.849192	0.317373
1	4.057071	-1.239440	-2.349373	8	-5.404924	-2.872876	0.910831
1	3.976229	-2.697310	-1.359224	8	-6.114566	-0.909813	0.133033
1	1.752715	1.908747	1.403261	1	2.821023	-1.951246	-2.014727
1	0.873296	0.818952	2.477673	1	4.512717	-1.472175	-2.327159
1	2.508675	1.353041	2.902995	1	4.158609	-2.982479	-1.486653
1	4.509297	-2.372965	0.789917	1	2.437852	1.623055	1.614017
1	4.028509	-0.336171	2.712495	1	1.358746	0.572487	2.534375
1	2.129676	-1.777060	3.472537	1	3.024719	0.828169	3.081106
1	2.249364	-2.706299	1.979410	1	4.616131	-2.930361	0.696943

1	3.574691	-2.735073	3.150778	1	4.290447	-1.048738	2.797845
1	6.278925	-0.832432	1.588433	1	2.162405	-2.265434	3.296952
1	6.193293	-0.794442	-0.171905	1	2.245481	-3.041860	1.716878
1	5.486185	0.519015	0.769288	1	3.473514	-3.389865	2.942235
1	-0.074345	-0.246839	0.421971	1	6.522634	-1.733739	1.735774
1	1.062335	1.393744	-2.424296	1	6.550763	-1.513646	-0.013339
1	2.022391	-0.030311	-2.763529	1	5.967431	-0.212846	1.024935
1	-0.743846	-0.183540	-2.611409	1	0.428108	-0.128245	0.377162
1	-2.973809	0.287056	-1.782583	1	1.914084	1.563906	-2.285493
1	-5.033479	-0.462227	-0.640941	1	2.666253	0.040512	-2.709725
1	-3.000938	-3.974279	0.708482	1	-0.063520	0.230151	-2.660372
1	-0.946135	-3.220576	-0.484825	1	-2.270984	0.937794	-1.994297
1	3.316820	2.066674	-3.134575	1	-4.491689	0.415137	-1.041001
1	2.952268	2.592429	-1.489674	1	-3.024915	-3.337885	0.341920
1	4.037362	1.219055	-1.772928	1	-0.790447	-2.822588	-0.668681
1	-3.240706	4.536497	-0.592639	1	4.274487	1.940450	-2.854747
1	-1.707013	3.979142	-1.281206	1	3.911486	2.386400	-1.186499
1	-3.154050	2.965416	-1.385757	1	4.794744	0.891542	-1.542694
1	-4.165331	3.412330	1.492269	1	-2.131017	5.023737	-0.452199
1	-4.065804	1.851790	0.667397	1	-0.648086	4.331029	-1.127038
1	-3.269953	2.074365	2.222549	1	-2.194705	3.492723	-1.322868
1	-2.092734	4.831231	1.720410	1	-3.252762	3.903828	1.529842
1	-1.200840	3.468484	2.393955	1	-3.281205	2.371557	0.644177
1	-0.573683	4.315517	0.970671	1	-2.526773	2.452977	2.233043
6	-5.323231	-2.687299	0.782161	1	-1.044512	5.070334	1.908718
7	-6.278678	-3.035432	1.324219	1	-0.321314	3.586968	2.527961
NImag = 1 (-59.9945 cm ⁻¹)				1	0.435599	4.436568	1.171377
				6	-7.381799	-1.204494	0.684056
				1	-8.012686	-0.355378	0.447669
				1	-7.788713	-2.112306	0.247164
				1	-7.311295	-1.336285	1.760322
				NImag = 1 (-107.7282 cm ⁻¹)			
TS1(Cl)re-re				TS1(H)re-re			
Et = -1708.5743495				Et = -1248.9676894			
Gsol = -1708.893711				Gsol = -1249.262789			
6	-2.904413	-0.482853	-1.262474	6	1.571413	3.081238	0.234326
6	-1.764864	-1.267527	-1.153127	6	1.773427	2.078539	-0.706186
6	-1.834332	-2.462497	-0.448016	6	3.066086	1.645762	-0.969071
6	-3.010389	-2.860888	0.159245	6	4.142333	2.197225	-0.294439
6	-4.132680	-2.057097	0.043491	6	3.932829	3.184852	0.656366
6	-4.092737	-0.870771	-0.669429	6	2.643409	3.625798	0.918438
6	-0.494806	-0.901817	-1.839980	6	0.612307	1.545458	-1.472603
8	0.421085	-1.724138	-1.950051	8	-0.481016	2.125691	-1.457434
17	-5.617500	-2.551898	0.792906	6	0.178626	-0.236352	-0.285575
6	0.317290	0.500402	-0.339890	6	1.027629	-1.393104	-0.282714

6	-0.185084	1.837497	-0.215701	8	0.812813	-2.429691	-0.894003
8	0.367799	2.840734	-0.642776	7	-1.145126	-0.461647	-0.788907
7	1.689656	0.407357	-0.740528	6	-1.292464	-0.787578	-2.208084
6	2.046955	0.844149	-2.092015	6	-2.269339	-1.917674	-2.445175
6	3.291893	1.702663	-2.112130	6	-2.182125	-0.162930	-0.033717
6	2.550347	-0.217183	0.037812	7	-3.334371	0.396496	-0.445435
7	2.551210	-0.109434	1.378789	6	-4.302081	0.412078	0.643272
6	3.503384	-1.033147	1.968793	6	-3.417638	0.176889	1.878262
6	4.379489	-1.408897	0.761462	7	-2.229963	-0.413721	1.288096
7	3.544668	-1.025713	-0.368428	6	-3.457668	1.267216	-1.593359
6	1.979440	1.000179	2.098266	6	-1.429510	-1.410940	1.950694
6	3.535007	-1.774976	-1.604555	6	-3.100646	1.440251	2.654516
6	5.725833	-0.712820	0.739547	6	-5.386074	-0.631092	0.457050
6	2.820590	-2.217541	2.624577	8	2.133011	-1.183682	0.455000
8	-1.381330	1.857549	0.401910	6	3.172875	-2.169829	0.549410
6	-2.098578	3.086099	0.607887	6	3.789596	-2.433616	-0.814022
6	-3.344583	2.637803	1.349789	6	4.186682	-1.512486	1.468437
6	-1.291853	4.040262	1.474492	6	2.646042	-3.448153	1.182545
6	-2.472736	3.719110	-0.721775	1	-2.490071	1.718427	-1.804771
1	2.507110	-1.909950	-1.935127	1	-3.829833	0.733996	-2.468277
1	4.118955	-1.282006	-2.381691	1	-4.166611	2.055048	-1.349175
1	3.975656	-2.751360	-1.415783	1	-1.078767	-2.138317	1.223686
1	1.890764	1.857467	1.436424	1	-0.564829	-0.982168	2.453850
1	0.994095	0.769817	2.498860	1	-2.049978	-1.920898	2.685164
1	2.644437	1.258568	2.920057	1	-4.748794	1.404732	0.689249
1	4.522615	-2.488758	0.728467	1	-3.880869	-0.558724	2.536073
1	4.097606	-0.493085	2.706339	1	-2.400799	1.233271	3.461994
1	2.145187	-1.888375	3.412060	1	-2.649919	2.183482	1.998308
1	2.239010	-2.774003	1.890915	1	-4.005850	1.862367	3.090002
1	3.555776	-2.888813	3.067280	1	-6.111150	-0.582659	1.268882
1	6.338857	-1.034704	1.580776	1	-5.916367	-0.474254	-0.480465
1	6.264901	-0.940504	-0.178281	1	-4.953977	-1.630815	0.439190
1	5.597542	0.367181	0.799149	1	0.199518	0.373532	0.601477
1	0.051735	-0.190409	0.442587	1	-0.307609	-1.116633	-2.514244
1	1.207515	1.448772	-2.411355	1	-1.538323	0.102638	-2.780933
1	2.112957	-0.006963	-2.763626	1	0.912217	0.940451	-2.340823
1	-0.613243	-0.090764	-2.572074	1	3.225993	0.877156	-1.712971
1	-2.862939	0.441867	-1.820184	1	5.146326	1.861597	-0.513058
1	-4.982230	-0.266560	-0.759448	1	4.771851	3.616419	1.183138
1	-3.068210	-3.789139	0.706579	1	2.478580	4.405561	1.648775
1	-0.948493	-3.078234	-0.403842	1	0.561693	3.428629	0.396229
1	3.483026	2.043386	-3.128413	1	-2.305007	-2.151333	-3.508002
1	3.142266	2.575481	-1.480712	1	-1.935712	-2.804564	-1.911246
1	4.176402	1.165715	-1.771455	1	-3.281100	-1.671797	-2.125495
1	-3.095778	4.596320	-0.550210	1	4.640430	-3.106155	-0.709736
1	-1.584984	4.017321	-1.269482	1	3.064890	-2.882650	-1.485035

1	-3.043166	3.015406	-1.326768	1	4.146879	-1.501590	-1.249415
1	-3.989367	3.490309	1.556901	1	5.049013	-2.162705	1.607609
1	-3.900692	1.913171	0.759223	1	4.521365	-0.566205	1.049288
1	-3.077158	2.167565	2.294288	1	3.742869	-1.311769	2.441983
1	-1.902181	4.903737	1.736969	1	3.472975	-4.130559	1.376667
1	-0.995939	3.544683	2.398832	1	2.166127	-3.222397	2.134550
1	-0.402735	4.379593	0.954235	1	1.928332	-3.936853	0.532530
NImag = 1 (-133.5993 cm ⁻¹)				NImag = 1 (-152.4467 cm ⁻¹)			
TS1(Me)re-re				TS1(OMe)re-re			
Et = -1288.2779118				Et = -1363.4530108			
Gsol = -1288.577667				Gsol = -1363.776441			
7	2.422264	0.093776	1.350089	6	-2.850965	-0.380673	-1.427595
6	2.400432	-0.022088	0.008757	6	-1.757952	-1.192687	-1.142580
7	3.486815	-0.691246	-0.419596	6	-1.958717	-2.319116	-0.362421
6	4.393789	-0.936574	0.694014	6	-3.209445	-2.629409	0.148683
6	3.486645	-0.716576	1.914454	6	-4.289868	-1.804576	-0.139594
7	1.448154	0.486194	-0.745327	6	-4.104431	-0.678815	-0.938035
6	1.698658	0.906180	-2.124463	6	-0.414744	-0.922281	-1.724144
6	2.824507	1.910794	-2.228535	8	0.471706	-1.791986	-1.708299
6	3.542221	-1.469530	-1.637628	8	-5.551748	-2.016549	0.296201
6	5.602079	-0.022108	0.655298	6	0.352371	0.500097	-0.315775
6	2.960727	-2.000512	2.526144	6	-0.175915	1.830250	-0.178415
6	1.730728	1.119629	2.087003	8	0.337645	2.844242	-0.626577
6	0.085193	0.397185	-0.308144	7	1.728683	0.442320	-0.719647
6	-0.606882	1.652693	-0.231755	6	2.064253	0.890257	-2.071175
8	-1.757623	1.531352	0.454046	6	3.313098	1.742995	-2.104103
6	-2.661551	2.636796	0.608468	6	2.589851	-0.218722	0.026414
6	-1.995547	3.773097	1.368265	7	2.598413	-0.159544	1.371023
8	-0.236758	2.697523	-0.746459	6	3.541051	-1.116896	1.920271
6	-3.183686	3.098452	-0.741900	6	4.424948	-1.427234	0.701207
6	-3.788462	2.045026	1.435759	7	3.586594	-1.007764	-0.413761
6	-0.524548	-1.200677	-1.640458	6	2.028006	0.918007	2.136798
8	0.476627	-1.931241	-1.625907	6	3.559763	-1.731745	-1.666039
6	-1.787561	-1.619375	-0.971807	6	5.759945	-0.709340	0.712276
6	-1.781162	-2.702679	-0.102215	6	2.845640	-2.333887	2.498961
6	-2.953064	-3.137647	0.487142	8	-1.348031	1.821226	0.480116
6	-4.168192	-2.514348	0.215682	6	-2.103402	3.025473	0.690987
6	-4.170414	-1.445239	-0.673553	6	-3.310352	2.540864	1.473548
6	-2.996143	-1.000985	-1.256614	6	-1.306308	4.019577	1.520893
1	2.533883	-1.772863	-1.914025	6	-2.539395	3.625424	-0.634979
1	4.012028	-0.915859	-2.450742	1	2.524144	-1.876955	-1.969892
1	4.136636	-2.359662	-1.445547	1	4.120512	-1.214038	-2.444364
1	1.512511	1.956389	1.429056	1	4.019008	-2.704722	-1.507080
1	0.794897	0.764631	2.514819	1	1.920941	1.795652	1.505303
1	2.378729	1.465553	2.890115	1	1.050819	0.665800	2.544729

1	4.715323	-1.976556	0.650437	1	2.703303	1.156359	2.956420
1	4.008526	-0.128507	2.669355	1	4.585003	-2.502024	0.622176
1	2.250835	-1.786818	3.322979	1	4.129167	-0.620653	2.692634
1	2.451745	-2.597143	1.770414	1	2.166426	-2.047214	3.299726
1	3.775365	-2.589805	2.946070	1	2.265648	-2.839324	1.728022
1	6.276814	-0.239329	1.482740	1	3.572843	-3.035960	2.905768
1	6.153522	-0.150065	-0.274352	1	6.378493	-1.058386	1.538575
1	5.293031	1.020029	0.725615	1	6.301697	-0.886767	-0.214987
1	-0.051692	-0.271150	0.524684	1	5.614177	0.364749	0.819770
1	0.779581	1.386985	-2.434142	1	0.117503	-0.183662	0.482290
1	1.851865	0.041449	-2.764499	1	1.223081	1.501732	-2.371965
1	-0.693465	-0.503236	-2.474653	1	2.119621	0.045099	-2.752335
1	-3.017676	-0.170968	-1.949991	1	-0.447678	-0.177941	-2.534547
1	-5.106300	-0.959559	-0.916873	1	-2.714501	0.492576	-2.050927
6	-5.434081	-2.975145	0.873332	1	-4.961407	-0.061739	-1.163296
1	-2.932254	-3.985027	1.160051	1	-3.333265	-3.515933	0.750826
1	-0.841342	-3.203069	0.079432	1	-1.112443	-2.964347	-0.177637
1	2.937133	2.225971	-3.264611	1	3.490613	2.091333	-3.120268
1	2.586951	2.786489	-1.628801	1	3.176610	2.611524	-1.463749
1	3.780087	1.504892	-1.899218	1	4.199742	1.199938	-1.779579
1	-3.942033	3.868093	-0.601094	1	-3.183846	4.485603	-0.456047
1	-2.379650	3.502219	-1.348293	1	-1.679715	3.943483	-1.215618
1	-3.642916	2.264610	-1.270629	1	-3.105652	2.893398	-1.208761
1	-4.564435	2.789652	1.606787	1	-3.983543	3.370575	1.683766
1	-4.225165	1.189978	0.924402	1	-3.849630	1.783065	0.909591
1	-3.414268	1.706501	2.400431	1	-2.998208	2.100224	2.418881
1	-2.731925	4.542643	1.597762	1	-1.938638	4.865556	1.788490
1	-1.589012	3.404652	2.309814	1	-0.967529	3.548232	2.443252
1	-1.193608	4.212389	0.784750	1	-0.443999	4.381064	0.971091
1	-5.436536	-4.053939	1.021090	6	-5.791662	-3.141558	1.087841
1	-5.559402	-2.513850	1.854476	1	-6.850423	-3.126431	1.324987
1	-6.308485	-2.716083	0.279118	1	-5.558204	-4.065606	0.556006
				1	-5.217709	-3.110853	2.015767
NImag = 1 (-161.5503 cm ⁻¹)				NImag = 1 (-179.1476 cm ⁻¹)			
TS1(OH)re-re				TS2(NO₂)re-si			
Et = -1324.157527				Et = -1453.3863078			
Gsol = -1324.488075				Gsol = -1453.741944			
7	2.430329	0.128740	1.337370	7	-3.483483	0.598114	-0.138728
6	2.396880	-0.010268	-0.001589	6	-2.699994	-0.461748	0.132031
7	3.483316	-0.680328	-0.428585	7	-3.428392	-1.591949	0.148997
6	4.400997	-0.902456	0.681166	6	-4.845402	-1.282452	0.016290
6	3.503224	-0.667338	1.905648	6	-4.823201	0.166195	-0.499182
7	1.435606	0.481317	-0.755145	7	-1.403022	-0.376092	0.349817
6	1.671243	0.875857	-2.144077	6	-0.717872	-1.287295	1.268750
6	2.789302	1.885783	-2.277127	6	-1.330758	-1.281832	2.651212

6	3.529035	-1.482802	-1.631496	6	-2.902958	-2.909562	-0.124641
6	5.603838	0.017786	0.617208	6	-5.593507	-1.458811	1.322571
6	2.988189	-1.943916	2.541558	6	-5.082634	0.291688	-1.987626
6	1.740240	1.163460	2.062951	6	-3.172571	1.950224	0.252313
6	0.076033	0.386714	-0.306267	6	-0.612908	0.541746	-0.408109
6	-0.625735	1.639253	-0.246952	6	0.082394	1.532834	0.353481
8	-1.766809	1.522777	0.454921	8	0.674250	2.439467	-0.454011
6	-2.674279	2.626795	0.605195	6	1.358503	3.584582	0.085011
6	-2.000658	3.779798	1.332368	6	1.816201	4.327944	-1.157032
8	-0.270292	2.675633	-0.787742	8	0.170604	1.559715	1.571293
6	-3.221492	3.061343	-0.744163	6	0.396145	4.448148	0.884740
6	-3.783562	2.044783	1.462454	6	2.557057	3.166606	0.919825
6	-0.527771	-1.237646	-1.582927	6	0.396827	-0.974102	-1.814455
8	0.473410	-1.970360	-1.539959	8	-0.420142	-1.891111	-1.826566
6	-1.798239	-1.645112	-0.923847	6	1.739110	-1.121692	-1.186717
6	-1.803996	-2.722696	-0.049946	6	2.685028	-0.104006	-1.275684
6	-2.978796	-3.154697	0.537934	6	3.954305	-0.279296	-0.764924
6	-4.175775	-2.515711	0.240969	6	4.268905	-1.489540	-0.168201
6	-4.188512	-1.447926	-0.646994	6	3.353660	-2.524444	-0.080240
6	-3.004856	-1.021688	-1.217338	6	2.089972	-2.334132	-0.600885
1	2.518795	-1.797078	-1.888844	1	-2.677011	-3.455373	0.791294
1	3.986820	-0.943125	-2.460707	1	-3.654638	-3.468833	-0.676596
1	4.130506	-2.365727	-1.428407	1	-2.009858	-2.822330	-0.739200
1	1.508804	1.986100	1.391858	1	-2.782923	2.539627	-0.575646
1	0.811665	0.810523	2.508026	1	-4.081035	2.420857	0.623092
1	2.394722	1.528938	2.852034	1	-2.432793	1.940768	1.048117
1	4.728014	-1.941201	0.651810	1	-5.268777	-1.940045	-0.742556
1	4.028564	-0.064888	2.646645	1	-5.541507	0.770452	0.055025
1	2.284667	-1.720762	3.341480	1	-4.964468	1.322740	-2.315569
1	2.474769	-2.553540	1.799288	1	-4.381496	-0.325164	-2.547993
1	3.808896	-2.523655	2.962976	1	-6.096075	-0.026775	-2.229481
1	6.287062	-0.182290	1.442025	1	-6.653285	-1.243530	1.190432
1	6.147817	-0.122089	-0.315119	1	-5.498979	-2.479677	1.688193
1	5.289604	1.059230	0.673471	1	-5.197052	-0.787695	2.083359
1	-0.044823	-0.261488	0.544797	1	-1.103626	0.884496	-1.303412
1	0.746251	1.343935	-2.455677	1	0.294883	-0.909642	1.326814
1	1.826169	0.000306	-2.768946	1	-0.665313	-2.287338	0.848996
1	-0.689835	-0.567697	-2.440930	1	0.358661	-0.174113	-2.564289
1	-3.016633	-0.192259	-1.911312	1	1.356009	-3.124773	-0.581929
1	-5.130754	-0.974968	-0.879483	1	3.648103	-3.454379	0.377305
8	-5.357654	-2.898747	0.778390	7	5.600706	-1.682502	0.368994
1	-2.971976	-3.998404	1.217159	1	4.702903	0.493512	-0.820184
1	-0.867616	-3.224861	0.143216	1	2.409200	0.834301	-1.733460
1	2.891912	2.180904	-3.320120	1	-0.754699	-1.931438	3.308155
1	2.550418	2.771688	-1.693152	1	-1.303981	-0.272965	3.055600
1	3.749987	1.492740	-1.947056	1	-2.359781	-1.640222	2.650274

1	-3.980170	3.830766	-0.604260	1	3.123873	4.049448	1.213957
1	-2.429912	3.456772	-1.372087	1	2.242128	2.633058	1.809705
1	-3.687446	2.216597	-1.249095	1	3.213963	2.520294	0.340713
1	-4.559860	2.788954	1.633766	1	2.341700	5.240123	-0.880019
1	-4.226277	1.178923	0.975114	1	2.490276	3.709874	-1.747685
1	-3.391047	1.725719	2.426492	1	0.963836	4.594179	-1.779646
1	-2.737341	4.548934	1.562117	1	0.891051	5.371191	1.184006
1	-1.574711	3.430233	2.272545	1	-0.468245	4.711794	0.275537
1	-1.212284	4.213328	0.726457	1	0.059039	3.927264	1.774914
1	-5.210609	-3.648987	1.355179	8	6.390369	-0.771753	0.260047
NImag = 1 (-176.4583 cm ⁻¹)				NImag = 1 (-70.7933 cm ⁻¹)			
TS2(CN)re-si				TS2(COOMe)re-si			
Et = -1341.1740859				Et = -1476.7707297			
Gsol = -1341.493027				Gsol = -1477.123185			
7	-3.180535	0.720561	-0.149347	7	-3.759790	0.302316	-0.085909
6	-2.451192	-0.371716	0.143034	6	-2.822342	-0.610911	0.233443
7	-3.233437	-1.465219	0.169489	7	-3.370901	-1.840438	0.294677
6	-4.632362	-1.088879	0.016425	6	-4.815577	-1.748740	0.115156
6	-4.533773	0.347605	-0.523648	6	-4.981800	-0.356389	-0.510887
7	-1.154375	-0.342469	0.374726	7	-1.561601	-0.306624	0.458376
6	-0.518939	-1.277271	1.304678	6	-0.725441	-1.100579	1.360101
6	-1.142706	-1.235324	2.681678	6	-1.302218	-1.178395	2.755746
6	-2.768856	-2.808552	-0.089836	6	-2.650398	-3.068137	0.041924
6	-5.399498	-1.204444	1.318459	6	-5.562540	-1.927866	1.421642
6	-4.763275	0.457697	-2.018280	6	-5.111185	-0.379917	-2.021813
6	-2.810172	2.061351	0.227012	6	-3.690373	1.696387	0.265450
6	-0.314640	0.518901	-0.397704	6	-0.929765	0.697866	-0.337819
6	0.433855	1.482331	0.351586	6	-0.284208	1.752286	0.380178
8	1.071168	2.344790	-0.470006	8	0.143272	2.715941	-0.467637
6	1.816683	3.459729	0.050249	6	0.756735	3.919958	0.020674
6	2.307313	4.160430	-1.203968	6	1.015503	4.713153	-1.247779
8	0.528100	1.520610	1.568094	8	-0.092973	1.788120	1.585644
6	0.904331	4.383424	0.841274	6	-0.204033	4.678252	0.923025
6	2.994849	2.990348	0.886770	6	2.066614	3.618713	0.729594
6	0.594295	-1.028419	-1.779279	6	0.050343	-0.647656	-1.876864
8	-0.302053	-1.869786	-1.836367	8	-0.793082	-1.539989	-1.971074
6	1.904720	-1.321817	-1.131624	6	1.400045	-0.891644	-1.295541
6	2.936674	-0.388813	-1.143750	6	2.341367	0.130626	-1.225028
6	4.169544	-0.699807	-0.609332	6	3.611253	-0.117311	-0.745057
6	4.387062	-1.963808	-0.060550	6	3.960688	-1.402555	-0.337609
6	3.363191	-2.909467	-0.061151	6	3.028757	-2.431051	-0.424320
6	2.134960	-2.585953	-0.600552	6	1.760014	-2.176895	-0.905223
1	-2.574817	-3.356390	0.832227	1	-2.289225	-3.523629	0.963688
1	-3.542380	-3.336736	-0.642223	1	-3.329635	-3.769018	-0.436561

1	-1.869348	-2.767242	-0.700281	1	-1.822536	-2.866659	-0.634984
1	-2.395341	2.624512	-0.607062	1	-3.432389	2.326874	-0.584092
1	-3.696345	2.576069	0.593374	1	-4.659006	2.007474	0.653191
1	-2.071044	2.027025	1.022697	1	-2.942864	1.839146	1.040312
1	-5.080334	-1.738476	-0.735000	1	-5.121175	-2.515689	-0.595095
1	-5.230546	0.995357	0.008501	1	-5.831359	0.160529	-0.065321
1	-4.592919	1.476188	-2.362223	1	-5.137659	0.631475	-2.423172
1	-4.081582	-0.200209	-2.555482	1	-4.259376	-0.896394	-2.462836
1	-5.786167	0.181255	-2.271846	1	-6.026014	-0.888701	-2.324227
1	-6.446696	-0.941556	1.172751	1	-6.639045	-1.881615	1.260017
1	-5.356549	-2.221392	1.704138	1	-5.327903	-2.890830	1.871443
1	-4.977536	-0.538499	2.070041	1	-5.285620	-1.147306	2.129140
1	-0.794898	0.884212	-1.289712	1	-1.520862	0.997368	-1.185198
1	0.509423	-0.946044	1.369658	1	0.222651	-0.580386	1.393483
1	-0.507702	-2.281605	0.891842	1	-0.537373	-2.084571	0.941669
1	0.656531	-0.220993	-2.519778	1	0.021699	0.223839	-2.542811
1	1.335104	-3.309497	-0.639350	1	1.031282	-2.967090	-1.005158
1	3.544895	-3.890893	0.349996	1	3.325433	-3.422851	-0.118410
1	4.971006	0.023123	-0.613362	1	4.338941	0.676301	-0.682160
1	2.756201	0.590730	-1.561736	1	2.057160	1.127101	-1.531763
1	-0.602289	-1.906108	3.347525	1	-0.626560	-1.739002	3.399594
1	-1.073654	-0.226287	3.080772	1	-1.408124	-0.174682	3.160276
1	-2.187024	-1.546056	2.674096	1	-2.271534	-1.675729	2.776389
1	3.606012	3.846366	1.171345	1	2.557833	4.551766	1.004427
1	2.655125	2.481559	1.782015	1	1.893475	3.030142	1.623688
1	3.617583	2.306720	0.312443	1	2.735517	3.066595	0.071259
1	2.882836	5.046666	-0.942522	1	1.485859	5.665754	-1.009875
1	2.943263	3.498486	-1.789368	1	1.673710	4.160842	-1.916182
1	1.467242	4.463612	-1.826313	1	0.082534	4.908414	-1.773562
1	1.447581	5.283942	1.124939	1	0.215105	5.652242	1.172857
1	0.052090	4.682581	0.231431	1	-1.150968	4.840397	0.408597
1	0.544547	3.893771	1.740209	1	-0.388716	4.128921	1.840153
6	5.662027	-2.292833	0.491395	6	5.303442	-1.727894	0.183066
7	6.690557	-2.559640	0.937301	8	6.117892	-0.671028	0.206209
				8	5.646964	-2.820751	0.552275
				6	7.417760	-0.925251	0.698870
				1	7.941924	0.022421	0.654874
				1	7.376033	-1.288316	1.722098
				1	7.922389	-1.666551	0.085336
NImag = 1 (-96.9097 cm ⁻¹)				NImag = 1 (-106.0811 cm ⁻¹)			
TS2(Cl)re-si Et = -1708.5728343 Gsol = -1708.891670				TS2(H)re-si Et = -1248.9664854 Gsol = -1249.260167			
6	1.974825	-2.489254	-0.816372	6	-2.804258	1.727510	-0.734263
6	1.775149	-1.158745	-1.159086	6	-1.488799	2.138254	-0.918342

6	2.815008	-0.254090	-0.980669	6	-1.116000	3.414462	-0.516364
6	4.021906	-0.657963	-0.442099	6	-2.034801	4.257405	0.086701
6	4.191469	-1.988279	-0.091247	6	-3.339622	3.834093	0.285579
6	3.177620	-2.911791	-0.278011	6	-3.723187	2.566294	-0.130473
6	0.491641	-0.746708	-1.796707	6	-0.503229	1.268546	-1.623205
8	-0.439654	-1.542182	-1.948486	8	0.672241	1.616373	-1.783447
6	-0.409184	0.681051	-0.336543	6	-0.229219	-0.468581	-0.269816
6	0.301568	1.695494	0.381311	6	-1.272973	-1.172954	0.412241
8	0.452823	1.747203	1.591311	8	-1.436234	-1.232623	1.620080
7	-1.153894	-0.240703	0.464719	7	0.825816	0.040513	0.551298
6	-0.418342	-1.088492	1.403833	6	0.481301	1.015628	1.587345
6	-1.044491	-1.095702	2.780283	6	1.110340	0.677050	2.920047
6	-2.429729	-0.436693	0.205370	6	2.073612	-0.195995	0.206883
7	-3.275557	0.550240	-0.145448	7	3.114359	0.656257	0.321915
6	-4.538452	-0.003132	-0.599687	6	4.348741	-0.024872	-0.058927
6	-4.508244	-1.401615	0.034768	6	3.827649	-1.231522	-0.850600
7	-3.083026	-1.613815	0.261538	7	2.490960	-1.371158	-0.303508
6	-3.085679	1.938933	0.179582	6	2.991243	2.095284	0.236365
6	-2.460002	-2.898122	0.030300	6	1.841044	-2.636284	-0.094153
6	-5.309291	-1.511955	1.316656	6	3.792774	-1.007798	-2.350589
6	-4.631537	-0.022351	-2.113367	6	5.182172	-0.399893	1.150049
8	0.844852	2.592594	-0.473073	8	-2.116332	-1.743903	-0.478544
6	1.540387	3.754971	0.007257	6	-3.212010	-2.566785	-0.048585
6	2.794045	3.365865	0.773223	6	-2.700590	-3.768495	0.730292
6	1.911877	4.485875	-1.270502	6	-4.216182	-1.763536	0.761586
6	0.616162	4.617059	0.852324	6	-3.835880	-3.020100	-1.356363
1	-2.164249	-3.378868	0.962410	1	2.890227	2.552379	1.220211
1	-3.181702	-3.541728	-0.466214	1	3.894502	2.486752	-0.223888
1	-1.600275	-2.766218	-0.624184	1	2.139790	2.343470	-0.394834
1	-2.748273	2.523399	-0.675190	1	1.287782	-2.972080	-0.970431
1	-4.030293	2.347285	0.534841	1	2.595692	-3.381698	0.151991
1	-2.347321	2.027728	0.971183	1	1.149046	-2.553887	0.738537
1	-4.854035	-2.143672	-0.683507	1	4.916447	0.634804	-0.713034
1	-5.351287	0.586858	-0.176754	1	4.403179	-2.124410	-0.608091
1	-4.565772	0.986168	-2.517471	1	3.348298	-1.862864	-2.856765
1	-3.813620	-0.607990	-2.531563	1	3.190814	-0.129498	-2.581890
1	-5.576970	-0.456262	-2.437525	1	4.798014	-0.865065	-2.746147
1	-6.372472	-1.377415	1.120034	1	6.111174	-0.880876	0.845407
1	-5.170244	-2.488913	1.775962	1	5.432209	0.483326	1.734889
1	-4.991619	-0.753774	2.031303	1	4.631949	-1.086259	1.792457
1	-0.953340	1.016758	-1.201902	1	0.131558	-0.937852	-1.167457
1	0.569113	-0.649951	1.462703	1	-0.595641	0.964725	1.675525
1	-0.300448	-2.091609	1.005274	1	0.728169	2.021924	1.263815
1	0.605186	0.116886	-2.464115	1	-0.977523	0.566548	-2.320913
1	1.174396	-3.191371	-0.995905	1	-0.102112	3.735645	-0.704446
1	3.336891	-3.946103	-0.014503	1	-1.736996	5.250341	0.393087

17	5.703831	-2.505287	0.582275	1	-4.058159	4.490754	0.754667
1	4.827067	0.044549	-0.292614	1	-4.741099	2.234693	0.017197
1	2.662945	0.781251	-1.250445	1	-3.092492	0.736311	-1.055420
1	-0.440448	-1.701876	3.453368	1	0.799478	1.405725	3.666962
1	-1.077408	-0.080747	3.169104	1	0.775081	-0.306422	3.240926
1	-2.052887	-1.508331	2.774578	1	2.199106	0.685329	2.877829
1	3.349517	4.262548	1.046476	1	-5.083535	-2.382904	0.988701
1	2.542436	2.815840	1.673283	1	-3.774108	-1.415828	1.688706
1	3.440508	2.747186	0.152496	1	-4.558579	-0.901465	0.191056
1	2.454528	5.401073	-1.039798	1	-4.693507	-3.662875	-1.164762
1	2.542688	3.859903	-1.899152	1	-4.169792	-2.162332	-1.937429
1	1.018466	4.745123	-1.835782	1	-3.113058	-3.574334	-1.952521
1	1.112043	5.554350	1.101843	1	-3.523571	-4.451022	0.939422
1	-0.289945	4.853083	0.294759	1	-1.957254	-4.306644	0.142562
1	0.344649	4.107612	1.770937	1	-2.253191	-3.458735	1.668979
NImag = 1 (-131.9859 cm ⁻¹)				NImag = 1 (-148.6753 cm ⁻¹)			
TS2(Me)re-si				TS2(OMe)re-si			
Et = -1288.2768028				Et = -1363.4519898			
Gsol = -1288.575057				Gsol = -1363.774490			
7	-2.941922	0.936152	-0.222847	6	1.999874	-2.329511	-0.873388
6	-2.261940	-0.137724	0.224410	6	1.763729	-0.994302	-1.151792
7	-3.086838	-1.201941	0.321168	6	2.795969	-0.082105	-0.941221
6	-4.450940	-0.795680	-0.005213	6	4.010964	-0.488956	-0.438812
6	-4.231369	0.528963	-0.748084	6	4.229597	-1.834119	-0.144410
7	-0.983345	-0.105899	0.534437	6	3.219040	-2.759164	-0.367509
6	-0.406772	-1.018174	1.523512	6	0.463689	-0.573318	-1.746850
6	-1.034249	-0.844873	2.888532	8	-0.460659	-1.382819	-1.918078
6	-2.655316	-2.574456	0.168769	8	5.451859	-2.138223	0.343392
6	-5.313626	-0.667443	1.234140	6	-0.430448	0.760230	-0.280801
6	-4.195266	0.382698	-2.257666	6	0.249945	1.808496	0.425118
6	-2.580393	2.303912	0.031406	8	0.444032	1.862743	1.627877
6	-0.088062	0.651765	-0.285857	7	-1.116263	-0.196201	0.534964
6	0.798478	1.539029	0.408145	6	-0.325690	-0.984763	1.480817
8	1.476196	2.311118	-0.471489	6	-0.961203	-1.030956	2.852214
6	2.382649	3.332305	-0.025183	6	-2.359022	-0.510932	0.236762
6	2.864075	3.955799	-1.323098	7	-3.274066	0.392680	-0.165002
8	0.975611	1.587434	1.614235	6	-4.446505	-0.281694	-0.689565
6	1.646001	4.367812	0.809986	6	-4.344219	-1.643807	0.009157
6	3.553573	2.732548	0.735475	7	-2.917993	-1.737397	0.308418
6	0.513080	-0.912981	-1.706144	6	-3.224663	1.799511	0.124716
8	-0.561883	-1.507973	-1.858677	6	-2.186513	-2.968757	0.102682
6	1.686720	-1.571670	-1.064611	6	-5.191174	-1.756432	1.260901
6	2.891411	-0.896458	-0.897733	6	-4.405674	-0.368554	-2.203714
6	3.986687	-1.535426	-0.352012	8	0.709422	2.737897	-0.442752
6	3.919414	-2.873322	0.034596	6	1.364332	3.931485	0.017328

6	2.719996	-3.547457	-0.154394	6	2.667004	3.602781	0.727425
6	1.618993	-2.908148	-0.701085	6	1.643606	4.687401	-1.269355
1	-2.435727	-3.038793	1.129631	6	0.432728	4.739515	0.906784
1	-3.461471	-3.134373	-0.297807	1	-1.841478	-3.396375	1.043582
1	-1.784749	-2.603099	-0.484158	1	-2.854501	-3.686089	-0.366694
1	-2.160864	2.794426	-0.846205	1	-1.349951	-2.776146	-0.567161
1	-3.468269	2.849312	0.347960	1	-2.932063	2.394153	-0.739979
1	-1.846302	2.340246	0.830397	1	-4.209312	2.124466	0.457415
1	-4.876514	-1.536565	-0.679921	1	-2.510936	1.978576	0.923232
1	-4.980758	1.262039	-0.450613	1	-4.601019	-2.440307	-0.687150
1	-3.963928	1.335204	-2.731154	1	-5.337531	0.250874	-0.358210
1	-3.424040	-0.331652	-2.544300	1	-4.414182	0.625704	-2.646938
1	-5.157262	0.040195	-2.637984	1	-3.493243	-0.871452	-2.522955
1	-6.333927	-0.392583	0.968315	1	-5.267237	-0.916024	-2.585048
1	-5.346087	-1.608428	1.780182	1	-6.251967	-1.712043	1.015965
1	-4.912373	0.095806	1.899773	1	-4.999404	-2.697837	1.772470
1	-0.572526	1.073612	-1.148367	1	-4.960975	-0.944676	1.949783
1	0.641836	-0.757370	1.572232	1	-1.023414	1.090167	-1.115230
1	-0.463526	-2.045481	1.178234	1	0.627433	-0.477073	1.544096
1	0.802575	-0.104620	-2.390419	1	-0.133067	-1.977472	1.086462
1	0.695625	-3.441533	-0.872886	1	0.564792	0.298681	-2.406792
1	2.650743	-4.591733	0.120341	1	1.213921	-3.041843	-1.077190
1	4.913538	-0.992270	-0.221986	1	3.371800	-3.807909	-0.166537
1	2.953484	0.143324	-1.187414	1	4.813174	0.211763	-0.262901
1	-0.553379	-1.513741	3.600603	1	2.625403	0.961871	-1.163785
1	-0.889807	0.178169	3.227199	1	-0.323378	-1.592686	3.532800
1	-2.099992	-1.072184	2.884470	1	-1.066908	-0.019801	3.238213
1	4.272953	3.514789	0.976633	1	-1.939559	-1.510475	2.838895
1	3.216900	2.262625	1.652860	1	3.182275	4.525550	0.992683
1	4.059624	1.986843	0.124235	1	2.480536	3.028223	1.627992
1	3.566480	4.762129	-1.118741	1	3.321814	3.029006	0.073285
1	3.362084	3.211736	-1.942210	1	2.152100	5.625937	-1.055055
1	2.025246	4.360790	-1.886400	1	2.274366	4.095164	-1.929771
1	2.308685	5.203933	1.030252	1	0.714735	4.907264	-1.792646
1	0.789137	4.752536	0.257486	1	0.884929	5.704088	1.134554
1	1.300392	3.936983	1.743892	1	-0.510462	4.922069	0.392377
6	5.111990	-3.555330	0.634135	1	0.233364	4.215929	1.835844
1	4.925336	-4.615630	0.791147	6	5.721852	-3.473338	0.652137
1	5.987752	-3.462638	-0.008067	1	6.739435	-3.498661	1.027783
1	5.373635	-3.118945	1.598759	1	5.047522	-3.852434	1.422145
				1	5.650698	-4.112792	-0.229457
NImag = 1 (-156.4183 cm ⁻¹)				NImag = 1 (-175.7323 cm ⁻¹)			
TS2(OH)re-si Et = -1324.1563352 Gsol = -1324.486087				TS3(NO2)si-si Et = -1453.3790274 Gsol = -1453.732059			

7	-2.923359	0.965123	-0.235749	6	2.917926	0.014934	-1.180132
6	-2.258035	-0.113807	0.220680	6	2.121117	-1.118550	-1.296446
7	-3.095105	-1.168305	0.317358	6	2.510976	-2.306258	-0.685332
6	-4.452252	-0.749245	-0.021809	6	3.678210	-2.364460	0.048789
6	-4.212943	0.569514	-0.769166	6	4.449688	-1.219639	0.153482
7	-0.981304	-0.093488	0.539557	6	4.089299	-0.027401	-0.452148
6	-0.420197	-1.007398	1.535452	6	0.889684	-1.102263	-2.127611
6	-1.057522	-0.825713	2.894843	8	0.163215	-2.073002	-2.236338
6	-2.676816	-2.545912	0.174583	7	5.679474	-1.272190	0.921904
6	-5.323431	-0.606129	1.209946	6	-0.472652	0.254782	-0.528698
6	-4.166356	0.415639	-2.277722	6	-0.466142	1.660382	-0.374582
6	-2.546579	2.330122	0.010479	8	0.706776	2.105872	0.140801
6	-0.071822	0.644100	-0.284596	6	0.934832	3.500953	0.376391
6	0.819887	1.528898	0.409115	6	0.907874	4.282079	-0.927588
8	1.513723	2.283928	-0.471920	7	-1.760116	-0.272741	-0.914485
6	2.426364	3.301584	-0.028109	6	-2.228468	-0.048172	-2.280130
6	2.923818	3.907425	-1.328279	6	-3.086664	-1.179129	-2.804868
8	0.986898	1.586453	1.615884	6	-2.622330	-0.576752	0.052929
6	1.692138	4.351727	0.790589	7	-3.876865	-0.128290	0.170106
6	3.585231	2.698756	0.748207	6	-4.559198	-0.798299	1.270240
6	0.523240	-0.923453	-1.673983	6	-3.391587	-1.445865	2.037492
8	-0.555407	-1.514884	-1.831898	7	-2.333510	-1.423018	1.043340
6	1.689165	-1.594110	-1.032483	6	-4.346791	1.115881	-0.397635
6	2.901512	-0.933441	-0.856307	6	-1.214049	-2.325342	1.056312
6	3.994359	-1.576537	-0.313754	6	-3.001136	-0.709947	3.304068
6	3.892962	-2.913663	0.053993	6	-5.596549	-1.787220	0.778594
6	2.697059	-3.592258	-0.132366	8	-1.371454	2.425869	-0.708021
6	1.608701	-2.931994	-0.677293	6	-0.068591	4.049662	1.379167
1	-2.470367	-3.007961	1.139526	6	2.330136	3.530241	0.974970
1	-3.484920	-3.099431	-0.296288	1	-4.904868	0.954968	-1.319281
1	-1.801022	-2.585526	-0.470990	1	-5.004914	1.593536	0.324572
1	-2.116887	2.809266	-0.868537	1	-3.493996	1.767421	-0.580683
1	-3.429240	2.888507	0.318830	1	-1.551852	-3.300676	1.402936
1	-1.815932	2.362957	0.812820	1	-0.825343	-2.422013	0.045432
1	-4.880161	-1.488850	-0.696440	1	-0.418676	-1.973997	1.712046
1	-4.956729	1.311901	-0.480879	1	-5.034791	-0.039050	1.890384
1	-3.921342	1.363405	-2.753838	1	-3.625891	-2.485609	2.267202
1	-3.400227	-0.307990	-2.554688	1	-2.122653	-1.160177	3.762181
1	-5.128784	0.081354	-2.664197	1	-2.772065	0.331559	3.083414
1	-6.338602	-0.321781	0.934642	1	-3.813094	-0.742094	4.029468
1	-5.370331	-1.544144	1.760051	1	-6.100993	-2.262078	1.619222
1	-4.919498	0.155954	1.875285	1	-6.349511	-1.289547	0.170272
1	-0.550713	1.070296	-1.148298	1	-5.128404	-2.562659	0.173907
1	0.629826	-0.753937	1.592645	1	0.113401	-0.340951	0.147095
1	-0.481721	-2.035256	1.192240	1	-1.321695	0.012499	-2.868275
1	0.824267	-0.126714	-2.367110	1	-2.720064	0.917323	-2.375282

1	0.680385	-3.454776	-0.853917	1	-3.360426	-0.979103	-3.839746
1	2.622710	-4.639162	0.135084	1	-2.526308	-2.110259	-2.771877
1	4.934605	-1.066962	-0.167167	1	-4.011341	-1.298645	-2.240607
1	2.974810	0.107455	-1.138644	1	0.811112	-0.242009	-2.802773
1	-0.587507	-1.495910	3.612889	1	1.888998	-3.178854	-0.813865
1	-0.908252	0.197191	3.231877	1	4.006632	-3.271195	0.529038
1	-2.124889	-1.044842	2.882745	1	4.722161	0.836894	-0.340002
1	4.308131	3.477451	0.990088	1	2.598047	0.937876	-1.639055
1	3.236812	2.238741	1.666222	1	2.620421	4.552228	1.213047
1	4.092262	1.944729	0.148130	1	2.367076	2.937003	1.886681
1	3.632876	4.708462	-1.126239	1	3.055844	3.121005	0.274561
1	3.419046	3.152393	-1.936203	1	1.191577	5.318502	-0.746082
1	2.093512	4.315397	-1.901953	1	1.620514	3.856877	-1.633902
1	2.360309	5.184457	1.006922	1	-0.082281	4.253761	-1.369246
1	0.842616	4.737791	0.227769	1	0.193816	5.073468	1.644168
1	1.336207	3.933791	1.726468	1	-1.070846	4.035209	0.964944
8	4.991597	-3.502823	0.579209	1	-0.051528	3.449808	2.288734
1	4.791736	-4.417566	0.780670	8	6.351391	-0.267910	0.978723
				8	5.960767	-2.317710	1.462550
NImag = 1 (-171.3199 cm ⁻¹)				NImag = 1 (-59.9980 cm ⁻¹)			
TS3(CN)si-si Et = -1341.1670491 Gsol = -1341.483717				TS3(COOMe)si-si Et = -1476.7637336 Gsol = -1477.116683			
7	-3.612605	-0.028343	0.146934	6	-2.557392	0.458006	1.370570
6	-2.368069	-0.506430	0.036316	6	-1.798427	-0.697393	1.520589
7	-2.116054	-1.388392	1.005676	6	-2.293442	-1.909328	1.051094
6	-3.195109	-1.420593	1.976976	6	-3.521282	-1.966518	0.421096
6	-4.331018	-0.712812	1.214702	6	-4.272929	-0.806078	0.264173
7	-1.486042	-0.193275	-0.907234	6	-3.785672	0.405640	0.745029
6	-1.924494	0.080916	-2.274466	6	-0.501420	-0.672675	2.247008
6	-2.813690	-1.004936	-2.840876	8	0.171125	-1.680257	2.417490
6	-1.033157	-2.335374	0.993688	6	-5.594851	-0.805227	-0.394794
6	-2.812081	-0.746983	3.279853	8	-6.284407	0.169875	-0.541025
6	-5.390443	-1.653131	0.676848	8	-5.959640	-2.015910	-0.822722
6	-4.031532	1.250333	-0.382290	6	-7.221828	-2.072603	-1.455962
6	-0.177759	0.265168	-0.499932	6	0.781182	0.375371	0.515928
6	-0.110377	1.673034	-0.350637	6	0.856376	1.763937	0.224766
8	-0.972795	2.476305	-0.703931	8	-0.300935	2.229848	-0.298819
8	1.071922	2.067205	0.183731	6	-0.467618	3.614041	-0.631666
6	1.358197	3.451974	0.418727	6	-0.360216	4.485410	0.609330
6	0.365465	4.047130	1.405314	7	2.067152	-0.179429	0.875368
6	2.744777	3.421154	1.037572	6	2.639365	0.175431	2.172985
6	1.385635	4.229442	-0.887362	6	3.403858	-0.963031	2.813730
6	1.125824	-1.103300	-2.054021	6	2.827580	-0.708218	-0.074285
8	0.339694	-2.017061	-2.243738	7	4.113369	-0.414004	-0.307012

6	2.318302	-1.259601	-1.179398	6	4.664122	-1.299742	-1.324572
6	2.601582	-2.511419	-0.643952	6	3.397406	-1.922519	-1.940893
6	3.726018	-2.702076	0.132874	7	2.399405	-1.645363	-0.922909
6	4.584460	-1.630943	0.375586	6	4.716970	0.854764	0.033192
6	4.310565	-0.375743	-0.167608	6	1.217283	-2.445713	-0.737400
6	3.184045	-0.197899	-0.943409	6	3.017289	-1.341406	-3.288455
6	5.748257	-1.820937	1.181367	6	5.624689	-2.314446	-0.738074
1	-4.587698	1.140843	-1.312485	8	1.818195	2.494314	0.457370
1	-4.676400	1.729946	0.350631	6	0.529819	4.036060	-1.699665
1	-3.154199	1.875008	-0.540972	6	-1.878002	3.669387	-1.191417
1	-1.414962	-3.311125	1.290257	1	5.330135	0.784009	0.930764
1	-0.632188	-2.401702	-0.015264	1	5.350844	1.166953	-0.793899
1	-0.235778	-2.047113	1.677033	1	3.933643	1.597222	0.175119
1	-4.792780	0.040184	1.852805	1	1.463651	-3.487385	-0.938161
1	-3.461126	-2.461917	2.160558	1	0.880874	-2.351400	0.293483
1	-1.954028	-1.237505	3.735327	1	0.413586	-2.139676	-1.405404
1	-2.553516	0.296704	3.107299	1	5.177450	-0.689555	-2.067279
1	-3.638821	-0.788161	3.987948	1	3.514402	-3.003536	-2.021413
1	-5.920750	-2.139753	1.494559	1	2.072409	-1.752749	-3.638224
1	-6.119442	-1.113340	0.075337	1	2.910853	-0.259757	-3.220047
1	-4.937027	-2.422209	0.053121	1	3.780395	-1.569686	-4.031602
1	0.339472	-0.344149	0.219013	1	6.029610	-2.955087	-1.520618
1	-1.006257	0.121170	-2.846552	1	6.457451	-1.819438	-0.241892
1	-2.378962	1.065649	-2.352108	1	5.116782	-2.941412	-0.006668
1	-3.062967	-0.767789	-3.874131	1	0.168571	-0.232055	-0.125890
1	-2.286438	-1.955422	-2.824492	1	1.781053	0.420162	2.785711
1	-3.751337	-1.105708	-2.294665	1	3.233824	1.082921	2.106544
1	1.152943	-0.220333	-2.703234	1	3.762170	-0.653568	3.794641
1	1.930564	-3.327434	-0.865562	1	2.744634	-1.817844	2.940443
1	3.954185	-3.672260	0.547325	1	4.273763	-1.262499	2.229058
1	4.980780	0.447037	0.027840	1	-0.350382	0.226685	2.857201
1	2.948616	0.776417	-1.343622	1	-1.704426	-2.799990	1.210752
1	3.073514	4.429509	1.283564	1	-3.910308	-2.905376	0.059433
1	2.743729	2.823897	1.947419	1	-4.388011	1.291629	0.615456
1	3.463209	2.985552	0.345265	1	-2.165846	1.398803	1.728070
1	1.719100	5.250686	-0.704495	1	-2.128815	4.686099	-1.489765
1	2.084043	3.766675	-1.584148	1	-1.968970	3.019423	-2.059671
1	0.400738	4.249900	-1.340986	1	-2.599060	3.339054	-0.446454
1	0.668792	5.059098	1.671973	1	-0.594627	5.519516	0.357906
1	-0.630232	4.076198	0.976256	1	-1.072174	4.152699	1.364070
1	0.342141	3.449627	2.316248	1	0.640400	4.437172	1.025325
7	6.684720	-1.975935	1.834514	1	0.305801	5.048035	-2.036112
				1	1.542530	4.005866	-1.312634
				1	0.458101	3.370286	-2.559276
				1	-7.365710	-3.109210	-1.738066
				1	-8.006674	-1.752448	-0.776224

NImag = 1 (-74.5295 cm⁻¹)

	1	-7.239270	-1.434155	-2.334981			
		NImag = 1 (-82.0848 cm ⁻¹)					
	TS3(Cl)si-si Et = -1708.5662024 Gsol = -1708.885027			TS3(H)si-si Et = -1248.959832 Gsol = -1249.254991			
6	-2.486794	-2.398828	0.707302	7	2.190634	-0.936345	-1.019150
6	-2.190745	-1.131602	1.193278	6	2.140120	-0.130743	0.044947
6	-3.078145	-0.090093	0.953687	7	3.275187	0.577096	0.155984
6	-4.233194	-0.300323	0.224214	6	4.246766	0.139544	-0.837949
6	-4.501639	-1.569893	-0.262026	6	3.375512	-0.669525	-1.816303
6	-3.638340	-2.625963	-0.024693	7	1.113949	-0.065495	0.876313
6	-0.969095	-0.939383	2.020064	6	1.330033	0.149732	2.307785
8	-0.181004	-1.855786	2.226593	6	2.306289	-0.835485	2.914355
6	0.274094	0.340651	0.481165	6	3.337800	1.875788	0.787342
6	0.202698	1.751318	0.306550	6	5.376416	-0.658259	-0.218768
8	-0.973871	2.129314	-0.246907	6	3.046215	0.063694	-3.101609
6	-1.269695	3.509107	-0.499594	6	1.357042	-2.095234	-1.217035
6	-2.648502	3.458866	-1.134263	6	-0.232992	0.062635	0.363526
7	1.596727	-0.084989	0.882435	6	-0.664583	1.421215	0.365064
6	2.048160	0.248430	2.233445	8	-0.108271	2.348283	0.947728
6	2.885949	-0.841921	2.865817	8	-1.821886	1.578069	-0.315767
6	2.456162	-0.504920	-0.033120	6	-2.468131	2.853492	-0.407696
7	2.166744	-1.429707	-0.952088	6	-2.897035	3.342744	0.966193
6	3.253259	-1.573488	-1.905197	6	-1.573624	3.865152	-1.108048
6	4.417265	-0.878664	-1.174307	6	-3.687138	2.562499	-1.265380
7	3.724719	-0.092526	-0.161440	6	-1.213340	-1.684177	1.525433
6	1.064511	-2.353360	-0.867964	8	-0.248284	-2.438034	1.629741
6	4.184042	1.208265	0.269808	6	-2.338279	-1.966789	0.593444
6	5.420264	-1.837292	-0.564889	6	-3.459699	-1.147707	0.554496
6	2.917565	-0.963667	-3.251793	6	-4.524323	-1.458199	-0.272606
8	1.058079	2.561680	0.654546	6	-4.478346	-2.593709	-1.068545
6	-1.319403	4.299186	0.798216	6	-3.365851	-3.420712	-1.026166
6	-0.270621	4.103351	-1.480315	6	-2.303665	-3.111090	-0.194233
1	4.744452	1.151859	1.202182	1	3.792454	1.825679	1.775947
1	4.834584	1.618064	-0.499822	1	3.938498	2.535594	0.164807
1	3.327280	1.868080	0.393235	1	2.333205	2.286851	0.866115
1	1.427800	-3.354626	-1.095504	1	1.987593	-2.932117	-1.514463
1	0.666105	-2.341494	0.145389	1	0.855946	-2.342041	-0.281420
1	0.270944	-2.100857	-1.569481	1	0.610335	-1.926776	-1.991595
1	4.924879	-0.192604	-1.851907	1	4.646156	1.021693	-1.337657
1	3.467603	-2.636046	-2.022087	1	3.855655	-1.621386	-2.044206
1	2.036010	-1.433852	-3.683127	1	2.357966	-0.515277	-3.714240
1	2.716363	0.101626	-3.148181	1	2.579466	1.023182	-2.883505
1	3.745220	-1.094927	-3.947865	1	3.950022	0.240744	-3.683497
1	5.933390	-2.401042	-1.343165	1	6.092461	-0.964015	-0.980788

1	6.169661	-1.299349	0.012773	1	5.906328	-0.067238	0.525938
1	4.920011	-2.541112	0.098738	1	4.988463	-1.551294	0.269004
1	-0.202766	-0.266005	-0.267952	1	-0.444098	-0.505763	-0.524838
1	1.132331	0.367305	2.798797	1	0.352332	0.007607	2.750512
1	2.546314	1.214180	2.254194	1	1.605580	1.180342	2.513016
1	3.141218	-0.556374	3.885453	1	2.382571	-0.656774	3.986261
1	2.314184	-1.765537	2.898651	1	1.943188	-1.847124	2.754486
1	3.820648	-1.013667	2.332083	1	3.308131	-0.738597	2.496053
1	-1.005991	-0.059454	2.674028	1	-1.478563	-0.990447	2.334199
1	-1.805873	-3.206193	0.931951	1	-1.441132	-3.756865	-0.120092
1	-3.875489	-3.609791	-0.399160	1	-3.334331	-4.314722	-1.632953
17	-5.949103	-1.842382	-1.177907	1	-5.310988	-2.837141	-1.712868
1	-4.921039	0.507304	0.028134	1	-5.393231	-0.816178	-0.298111
1	-2.844854	0.899323	1.317436	1	-3.484502	-0.256948	1.165571
1	-2.984387	4.461988	-1.392047	1	-4.277197	3.466760	-1.406576
1	-2.630193	2.854318	-2.039066	1	-3.384558	2.187564	-2.241374
1	-3.370071	3.019989	-0.447583	1	-4.312659	1.807400	-0.793828
1	-1.659544	5.315512	0.600808	1	-3.476194	4.260721	0.868922
1	-2.021911	3.837353	1.491397	1	-3.526429	2.596858	1.450635
1	-0.340230	4.333853	1.263363	1	-2.031554	3.531803	1.592197
1	-0.580449	5.109670	-1.760665	1	-2.130530	4.782701	-1.296512
1	0.719776	4.146237	-1.040316	1	-0.703348	4.095381	-0.503200
1	-0.230973	3.496979	-2.384774	1	-1.243016	3.467281	-2.067066
NImag = 1 (-100.4451 cm ⁻¹)				NImag = 1 (-114.4085 cm ⁻¹)			
TS3(Me)si-si				TS3(OMe)si-si			
Et = -1288.2700715				Et = -1363.4453923			
Gsol = -1288.570121				Gsol = -1363.769089			
6	2.410690	-2.719925	-0.321349	6	2.519634	-2.257250	-0.574784
6	2.270337	-1.494603	-0.958217	6	2.172521	-1.053557	-1.165827
6	3.298278	-0.565341	-0.854847	6	3.079093	0.001800	-1.106021
6	4.429948	-0.850264	-0.115614	6	4.286747	-0.138727	-0.460124
6	4.570116	-2.070144	0.542062	6	4.617738	-1.349266	0.145452
6	3.543768	-3.000026	0.422822	6	3.729053	-2.414911	0.085757
6	1.073653	-1.235855	-1.802497	6	0.896983	-0.939116	-1.918688
8	0.193595	-2.081551	-1.958509	8	0.131207	-1.895986	-2.050977
6	-0.024184	0.241567	-0.419223	6	-0.294485	0.328217	-0.448913
6	0.246381	1.638220	-0.315365	6	-0.176142	1.740758	-0.273840
8	1.418758	1.873415	0.315820	8	0.978405	2.068826	0.346053
6	1.920389	3.204238	0.489590	6	1.333493	3.435100	0.594252
6	3.218078	2.988141	1.248087	6	2.663440	3.320801	1.318034
7	-1.379135	-0.001169	-0.864428	7	-1.633586	-0.036450	-0.859691
6	-1.717122	0.326853	-2.250867	6	-2.054876	0.311315	-2.218203
6	-2.610378	-0.705854	-2.904345	6	-2.820044	-0.801223	-2.902771
6	-2.327106	-0.302489	0.005400	6	-2.510618	-0.483630	0.020201
7	-2.196197	-1.214236	0.973161	7	-2.245073	-1.410725	0.945399

6	-3.353376	-1.207825	1.851434	6	-3.366567	-1.571396	1.854433
6	-4.388817	-0.430600	1.017867	6	-4.510843	-0.889772	1.082926
7	-3.553390	0.243367	0.032914	7	-3.791446	-0.086403	0.103028
6	-1.208226	-2.264011	0.988596	6	-1.147627	-2.344384	0.888896
6	-3.833754	1.578174	-0.443876	6	-4.236205	1.228012	-0.300873
6	-5.439246	-1.309601	0.369459	6	-5.474730	-1.859234	0.429042
6	-3.046505	-0.579969	3.196656	6	-3.090801	-0.963308	3.215417
8	-0.449136	2.538299	-0.777290	8	-0.978394	2.580335	-0.670537
6	2.200525	3.856763	-0.854641	6	1.509337	4.194097	-0.711034
6	0.963786	4.038496	1.327643	6	0.308310	4.104141	1.496980
1	-4.341667	1.568149	-1.407497	1	-4.764805	1.203948	-1.252996
1	-4.475474	2.077862	0.278826	1	-4.912051	1.615043	0.458808
1	-2.902307	2.134289	-0.528160	1	-3.377731	1.892213	-0.377124
1	-1.703559	-3.205340	1.223192	1	-1.530324	-3.344176	1.090851
1	-0.748296	-2.340166	0.003384	1	-0.708288	-2.327180	-0.108881
1	-0.436019	-2.080082	1.733993	1	-0.381138	-2.108439	1.625626
1	-4.870119	0.327572	1.635173	1	-5.055286	-0.216226	1.744296
1	-3.683320	-2.237671	1.989656	1	-3.570498	-2.637171	1.959479
1	-2.246658	-1.117041	3.702677	1	-2.218754	-1.422795	3.676538
1	-2.731778	0.455058	3.070896	1	-2.900913	0.105189	3.123745
1	-3.926533	-0.600108	3.838596	1	-3.941642	-1.109529	3.879938
1	-6.057891	-1.790209	1.126558	1	-6.008942	-2.436760	1.182736
1	-6.089818	-0.723850	-0.277371	1	-6.209027	-1.328060	-0.173750
1	-4.967913	-2.083969	-0.234056	1	-4.938492	-2.550171	-0.219852
1	0.304453	-0.368591	0.403346	1	0.121842	-0.277833	0.336136
1	-0.761973	0.349621	-2.760117	1	-1.128718	0.493210	-2.748467
1	-2.123789	1.331149	-2.328287	1	-2.597129	1.252453	-2.232744
1	-2.777887	-0.432026	-3.945337	1	-3.052359	-0.505497	-3.925223
1	-2.121040	-1.675560	-2.873557	1	-2.204396	-1.696268	-2.928549
1	-3.586498	-0.775212	-2.424399	1	-3.764064	-1.022333	-2.404595
1	1.220904	-0.432800	-2.536980	1	0.893507	-0.113528	-2.643404
1	1.628052	-3.454200	-0.443888	1	1.831896	-3.085701	-0.660793
1	3.641995	-3.962285	0.907842	1	3.972743	-3.367094	0.530166
6	5.790902	-2.361672	1.361583	8	5.822136	-1.391697	0.755249
1	5.222519	-0.116955	-0.046086	1	4.997908	0.671816	-0.408152
1	3.197897	0.390610	-1.348236	1	2.822609	0.945862	-1.564681
1	3.710241	3.940717	1.438512	1	3.051278	4.309520	1.558546
1	3.024502	2.498982	2.200956	1	2.545995	2.758240	2.242391
1	3.892650	2.354956	0.675435	1	3.391278	2.800846	0.698738
1	2.681010	4.823365	-0.705170	1	1.880648	5.198415	-0.508556
1	2.873618	3.232963	-1.441948	1	2.236779	3.687720	-1.344633
1	1.279949	3.999316	-1.410272	1	0.567592	4.264556	-1.244763
1	1.421538	4.998257	1.566168	1	0.658484	5.095780	1.782459
1	0.034807	4.209934	0.794983	1	-0.647248	4.195693	0.992298
1	0.745752	3.525559	2.263936	1	0.174649	3.518093	2.405792
1	5.886022	-3.425765	1.568326	6	6.207542	-2.587213	1.366067

1	6.698204	-2.036348	0.854260	1	7.190326	-2.408926	1.789863
1	5.754934	-1.842861	2.320813	1	5.520304	-2.870632	2.165230
NImag = 1 (-120.9786 cm ⁻¹)				NImag = 1 (-128.8882 cm ⁻¹)			
TS3(OH)si-si				TS4(NO₂)si-re			
Et = -1324.1497739				Et = -1453.3789531			
Gsol = -1324.480902				Gsol = -1453.732304			
6	-2.419621	-2.736290	0.293031	6	2.881882	0.134278	1.143459
6	-2.278728	-1.504208	0.915579	6	2.167723	-1.049906	1.299132
6	-3.308841	-0.576828	0.797959	6	2.671340	-2.238876	0.781163
6	-4.442701	-0.860320	0.065045	6	3.872038	-2.250123	0.099460
6	-4.563732	-2.092766	-0.565837	6	4.558969	-1.057774	-0.047025
6	-3.548969	-3.033041	-0.449414	6	4.082751	0.138668	0.465210
6	-1.081538	-1.239497	1.755161	6	0.913294	-1.077077	2.093178
8	-0.200849	-2.087804	1.910673	8	0.218570	-2.071062	2.196911
6	0.012714	0.241936	0.408136	6	-0.598263	0.325489	0.654321
6	-0.270084	1.638915	0.318740	6	-0.270403	1.422374	-0.175235
8	-1.438153	1.870642	-0.320547	8	0.271669	2.440388	0.542987
6	-1.945438	3.200244	-0.493233	6	0.632042	3.680971	-0.077370
6	-3.232088	2.981582	-1.269337	6	-0.586517	4.341471	-0.703243
7	1.367761	0.011223	0.860366	7	-1.305407	-0.724919	-0.036657
6	1.690416	0.330050	2.253041	6	-0.552613	-1.571447	-0.958902
6	2.571853	-0.709980	2.911045	6	-1.023968	-3.010118	-0.959763
6	2.324474	-0.288272	0.000872	6	-2.631642	-0.664956	-0.105790
7	2.204135	-1.193280	-0.975178	7	-3.369503	-0.750035	-1.219076
6	3.373758	-1.184414	-1.836931	6	-4.788016	-0.807976	-0.887976
6	4.399489	-0.414591	-0.984886	6	-4.802613	-0.354001	0.582677
7	3.552508	0.255336	-0.007176	7	-3.414809	-0.542418	0.967935
6	1.220142	-2.246704	-1.005352	6	-2.889759	-0.375731	-2.531370
6	3.827221	1.588617	0.476895	6	-2.997486	-0.762280	2.327202
6	5.439477	-1.299737	-0.328039	6	-5.262244	1.076471	0.784389
6	3.087357	-0.548627	-3.182968	6	-5.367438	-2.190179	-1.110840
8	0.412509	2.538611	0.798819	8	-0.389485	1.467885	-1.398469
6	-2.245454	3.843293	0.851181	6	1.133909	4.517875	1.086594
6	-0.982565	4.043967	-1.314369	6	1.742801	3.481086	-1.095622
1	4.323651	1.575921	1.446431	1	-2.620865	-1.246791	-3.127527
1	4.477198	2.090952	-0.236559	1	-3.683671	0.161267	-3.045513
1	2.894975	2.144498	0.552349	1	-2.032182	0.286034	-2.422008
1	1.722053	-3.185705	-1.235683	1	-3.747025	-1.370357	2.831331
1	0.747808	-2.326955	-0.025921	1	-2.048238	-1.293828	2.332788
1	0.457510	-2.063839	-1.760905	1	-2.885401	0.175763	2.869581
1	4.890675	0.346241	-1.591051	1	-5.313422	-0.081282	-1.506896
1	3.703175	-2.214278	-1.976304	1	-5.418530	-1.030107	1.176228
1	2.293144	-1.080862	-3.702797	1	-5.171536	1.370854	1.828147
1	2.773579	0.486579	-3.056245	1	-4.659574	1.758362	0.186198

1	3.976115	-0.567752	-3.812800	1	-6.305905	1.186951	0.492597
1	6.067105	-1.777112	-1.079783	1	-6.429880	-2.203628	-0.870568
1	6.082627	-0.719221	0.330821	1	-5.251679	-2.496382	-2.148811
1	4.958696	-2.076662	0.264640	1	-4.861681	-2.921176	-0.481592
1	-0.294977	-0.355031	-0.432206	1	-0.911713	0.532042	1.661295
1	0.729481	0.353962	2.751163	1	0.465635	-1.519950	-0.593939
1	2.099789	1.332279	2.340926	1	-0.535546	-1.150046	-1.961229
1	2.727286	-0.443071	3.955725	1	-0.389507	-3.601569	-1.618541
1	2.078836	-1.677326	2.867566	1	-0.958050	-3.422407	0.044573
1	3.553619	-0.779553	2.442731	1	-2.048898	-3.112840	-1.316415
1	-1.236610	-0.446854	2.499304	1	0.791319	-0.217830	2.762138
1	-1.635332	-3.467501	0.421851	1	2.468728	1.055294	1.527863
1	-3.651798	-4.000681	-0.924958	1	4.653543	1.040890	0.321972
8	-5.693490	-2.325457	-1.272430	7	5.824362	-1.061530	-0.757262
1	-5.246031	-0.145919	-0.032072	1	4.287960	-3.155916	-0.309380
1	-3.207814	0.385984	1.277032	1	2.108813	-3.147162	0.934875
1	-3.726219	3.932815	-1.461140	1	1.433511	5.506603	0.742936
1	-3.024452	2.498208	-2.222128	1	0.354714	4.632828	1.838158
1	-3.911703	2.342703	-0.709210	1	1.993383	4.043215	1.557437
1	-2.727806	4.808829	0.701054	1	2.082116	4.447134	-1.468795
1	-2.924009	3.213791	1.426010	1	2.591908	2.980598	-0.632111
1	-1.332758	3.986133	1.419591	1	1.395768	2.877404	-1.926857
1	-1.443210	5.001842	-1.554718	1	-0.326720	5.337146	-1.061323
1	-0.061824	4.219071	-0.768721	1	-0.955316	3.750714	-1.534941
1	-0.748973	3.536767	-2.250024	1	-1.378099	4.444052	0.038741
1	-5.657620	-3.209102	-1.640093	8	6.415269	-0.010925	-0.859341
				8	6.215080	-2.115414	-1.205449
NImag = 1 (-133.4371 cm ⁻¹)				NImag = 1 (-56.4634 cm ⁻¹)			
TS4(CN)si-re Et = -1341.1670071 Gsol = -1341.484006				TS4(COOMe)si-re Et = -1476.7636777 Gsol = -1477.116713			
6	3.157325	-0.120983	1.048239	7	-3.678203	-0.644851	0.912275
6	2.363463	-1.258271	1.153047	6	-2.859601	-0.756355	-0.137026
6	2.787198	-2.452126	0.579819	7	-3.559400	-0.974067	-1.259922
6	3.984700	-2.511289	-0.104554	6	-4.972610	-1.153720	-0.951615
6	4.773008	-1.367347	-0.212759	6	-5.066573	-0.611213	0.486088
6	4.354962	-0.168565	0.366850	7	-1.539422	-0.685294	-0.052429
6	1.111558	-1.236951	1.951564	6	-0.694716	-1.510874	-0.914299
8	0.361136	-2.195403	2.027815	6	-1.029406	-2.984905	-0.828485
6	-0.304786	0.283246	0.622250	6	-3.090200	-0.594340	-2.573935
6	0.086100	1.376746	-0.189354	6	-5.406342	-2.598758	-1.092727
8	0.708127	2.337253	0.541519	6	-5.661123	0.779880	0.582797
6	1.147392	3.562137	-0.059501	6	-3.285483	-0.786437	2.290931
6	-0.031734	4.323724	-0.644936	6	-0.919679	0.417768	0.644176
7	-1.100107	-0.689344	-0.088878	6	-0.586854	1.489370	-0.226126

6	-0.427280	-1.543267	-1.065118	8	-0.616317	1.459175	-1.453449
6	-0.965404	-2.958174	-1.081393	8	-0.159955	2.572394	0.469163
6	-2.421884	-0.564860	-0.099427	6	0.205392	3.789113	-0.194626
7	-3.204207	-0.576779	-1.186124	6	1.405446	3.578314	-1.103322
6	-4.610482	-0.579398	-0.802372	6	-0.980422	4.360288	-0.956864
6	-4.547959	-0.175710	0.682152	6	0.575347	4.711833	0.953536
7	-3.157243	-0.440138	1.007644	6	0.521173	-0.796284	2.161873
6	-2.754838	-0.169209	-2.499163	8	-0.130649	-1.824515	2.277839
6	-2.705453	-0.742501	2.340470	6	1.830767	-0.751131	1.462534
6	-4.933542	1.266355	0.946662	6	2.531610	0.445085	1.343276
6	-5.264381	-1.924125	-1.047283	6	3.778749	0.461849	0.755351
8	-0.048511	1.458245	-1.408204	6	4.344118	-0.720179	0.284012
6	1.731458	4.333286	1.111323	6	3.650707	-1.919387	0.410324
6	2.220477	3.304584	-1.104755	6	2.402237	-1.932381	1.002252
1	-2.559147	-1.024878	-3.144029	6	5.684088	-0.644699	-0.333552
1	-3.535013	0.435194	-2.956604	1	-2.736773	-1.453735	-3.142312
1	-1.856057	0.436534	-2.397112	1	-3.915455	-0.138202	-3.116546
1	-3.466135	-1.338449	2.842542	1	-2.290742	0.137501	-2.471900
1	-1.782387	-1.317092	2.289257	1	-3.990062	-1.450737	2.789471
1	-2.532945	0.163416	2.920333	1	-2.289107	-1.223537	2.344640
1	-5.122757	0.192145	-1.376412	1	-3.286835	0.172631	2.807598
1	-5.172243	-0.842784	1.277101	1	-5.552881	-0.524804	-1.626159
1	-4.792113	1.522202	1.994952	1	-5.633310	-1.302297	1.110359
1	-4.322493	1.940202	0.347844	1	-5.622777	1.150027	1.605467
1	-5.980866	1.432760	0.697689	1	-5.109647	1.474109	-0.049603
1	-6.316450	-1.895438	-0.766156	1	-6.703176	0.772855	0.265341
1	-5.202690	-2.199601	-2.098415	1	-6.468289	-2.703954	-0.873616
1	-4.771640	-2.699679	-0.462656	1	-5.232135	-2.958110	-2.105189
1	-0.615152	0.501518	1.628152	1	-4.847580	-3.232864	-0.405895
1	0.606869	-1.547243	-0.744044	1	-1.368298	0.682028	1.585041
1	-0.433863	-1.095728	-2.055855	1	0.308933	-1.340854	-0.544800
1	-0.387246	-3.560086	-1.781349	1	-0.702836	-1.151342	-1.939952
1	-0.877352	-3.398437	-0.090924	1	-0.325763	-3.553704	-1.435107
1	-2.007749	-3.003290	-1.397296	1	-0.949263	-3.320048	0.202801
1	1.057679	-0.408052	2.666443	1	-2.031233	-3.205731	-1.197275
1	2.809015	0.806919	1.477994	1	0.338372	0.070947	2.807093
1	4.973138	0.711163	0.274576	1	2.074452	1.360576	1.690388
1	4.322255	-3.435195	-0.548786	1	4.337115	1.379153	0.648071
1	2.165259	-3.327021	0.694821	1	4.098630	-2.833224	0.053023
1	2.094592	5.305783	0.783024	1	1.852684	-2.852783	1.131402
1	0.977606	4.486198	1.881688	1	0.864754	5.691239	0.576067
1	2.563541	3.787149	1.552888	1	-0.268515	4.835525	1.630115
1	2.625195	4.251512	-1.461454	1	1.409351	4.301005	1.519939
1	3.036856	2.729278	-0.670215	1	1.741016	4.536054	-1.500758
1	1.813541	2.749253	-1.942471	1	2.228181	3.136748	-0.543063
1	0.292862	5.306187	-0.986263	1	1.153759	2.918341	-1.925986

1	-0.459491	3.781774	-1.481696	1	-0.727566	5.342629	-1.354783
1	-0.799140	4.465759	0.115700	1	-1.258812	3.707279	-1.777171
6	6.015486	-1.423550	-0.914740	1	-1.833955	4.475055	-0.289002
7	7.018156	-1.470201	-1.480418	8	6.121650	-1.829461	-0.764468
NImag = 1 (-67.5352 cm ⁻¹)				8	6.327700	0.365676	-0.445504
				6	7.401861	-1.814172	-1.363038
				1	7.604707	-2.838069	-1.655032
				1	7.410854	-1.162718	-2.232546
				1	8.151031	-1.465657	-0.657455
				NImag = 1 (-74.9482 cm ⁻¹)			
TS4(Cl)si-re				TS4(H)si-re			
Et = -1708.5661986				Et = -1248.9599661			
Gsol = -1708.885509				Gsol = -1249.255247			
6	3.048455	-0.051022	1.060272	7	-3.029692	-0.120462	-1.066114
6	2.216212	-1.160549	1.147604	6	-2.151174	-0.236499	-0.055665
6	2.629705	-2.365289	0.593582	7	-2.758759	-0.043415	1.119713
6	3.847483	-2.463393	-0.056161	6	-4.128105	0.403439	0.925159
6	4.656234	-1.343101	-0.139502	6	-4.382299	0.032810	-0.546263
6	4.267781	-0.133439	0.415600	7	-0.869173	-0.519145	-0.196603
6	0.940252	-1.101140	1.906821	6	-0.415771	-1.413146	-1.263906
8	0.187608	-2.065161	1.998444	6	-1.133846	-2.745892	-1.260690
6	-0.404946	0.343478	0.614731	6	-2.262837	-0.493404	2.396891
6	0.019911	1.425080	-0.207925	6	-4.295232	1.878919	1.229400
8	0.622481	2.392701	0.525629	6	-5.208595	-1.224503	-0.727809
6	1.098344	3.601038	-0.082434	6	-2.651733	0.317899	-2.390740
6	-0.051632	4.367064	-0.717628	6	0.142152	0.203065	0.540439
7	-1.199609	-0.613661	-0.120371	6	0.741671	1.224222	-0.255283
6	-0.512907	-1.460499	-1.095751	8	0.608147	1.367023	-1.465224
6	-0.985995	-2.898199	-1.061878	8	1.548997	2.014673	0.491689
6	-2.520970	-0.546791	-0.100271	6	2.241374	3.129632	-0.085449
7	-3.317389	-0.613685	-1.178038	6	2.985784	3.723742	1.097612
6	-4.716314	-0.672156	-0.773685	6	3.227510	2.672813	-1.148296
6	-4.651974	-0.231481	0.699818	6	1.253076	4.143732	-0.639869
7	-3.246847	-0.426107	1.014683	6	1.225052	-1.530529	1.637431
6	-2.905053	-0.177532	-2.493677	8	0.298327	-2.332477	1.738533
6	-2.778675	-0.718443	2.345997	6	2.420583	-1.804173	0.795408
6	-5.098651	1.197505	0.937751	6	2.533325	-3.023168	0.137811
6	-5.311022	-2.050932	-0.977004	6	3.671067	-3.320080	-0.593755
8	-0.077798	1.484250	-1.429297	6	4.709807	-2.404687	-0.664101
6	1.656004	4.383894	1.093465	6	4.607798	-1.191533	0.003148
6	2.199657	3.310829	-1.089024	6	3.470267	-0.894718	0.731730
1	-2.687727	-1.018606	-3.150630	1	-2.622203	-0.508234	-3.100034
1	-3.712351	0.403863	-2.934048	1	-3.383407	1.044267	-2.738221
1	-2.025313	0.456961	-2.402977	1	-1.675883	0.797351	-2.347829
1	-3.514701	-1.347041	2.845472	1	-3.066969	-1.007821	2.921574

1	-1.832312	-1.256755	2.292366	1	-1.437512	-1.190655	2.246651
1	-2.645145	0.191004	2.930815	1	-1.927023	0.341346	3.011315
1	-5.272258	0.060811	-1.357645	1	-4.856571	0.865629	-1.064634
1	-5.238043	-0.911332	1.318572	1	-4.775015	-0.185302	1.575683
1	-4.949886	1.483777	1.977092	1	-4.015601	2.096793	2.258264
1	-4.529273	1.883909	0.312610	1	-3.664002	2.476719	0.573438
1	-6.156630	1.311344	0.704389	1	-5.331340	2.184559	1.088291
1	-6.359357	-2.064014	-0.680922	1	-6.218409	-1.078924	-0.345672
1	-5.250661	-2.348759	-2.022106	1	-5.279758	-1.492694	-1.780243
1	-4.774680	-2.788420	-0.381599	1	-4.754678	-2.058670	-0.194725
1	-0.794593	0.611930	1.580948	1	-0.153455	0.505080	1.529983
1	0.529133	-1.409364	-0.805410	1	0.636697	-1.562765	-1.057107
1	-0.567859	-1.038426	-2.095477	1	-0.465973	-0.926108	-2.233380
1	-0.394441	-3.492038	-1.757739	1	-0.701590	-3.391431	-2.024435
1	-0.857064	-3.302227	-0.060853	1	-1.013011	-3.222106	-0.291003
1	-2.031332	-2.998123	-1.354811	1	-2.196990	-2.645822	-1.480243
1	0.905793	-0.281872	2.634739	1	1.409404	-0.779335	2.415452
1	2.720130	0.889042	1.480096	1	3.374590	0.054407	1.240207
1	4.916006	0.725625	0.339240	1	5.418675	-0.478781	-0.046472
17	6.187107	-1.455298	-0.945826	1	5.599662	-2.636697	-1.231488
1	4.175571	-3.397417	-0.485343	1	3.753707	-4.270595	-1.101565
1	1.984793	-3.225449	0.695068	1	1.721487	-3.729825	0.227612
1	2.041234	5.346450	0.760985	1	3.552282	4.600835	0.788734
1	0.880857	4.558534	1.837626	1	2.287010	4.018682	1.878533
1	2.466918	3.834831	1.569331	1	3.678435	2.996337	1.517629
1	2.633354	4.246319	-1.441973	1	3.833826	3.517370	-1.475667
1	2.989968	2.724369	-0.622921	1	3.892700	1.912600	-0.742015
1	1.809842	2.754213	-1.933991	1	2.705928	2.254231	-2.001774
1	0.297274	5.338040	-1.067725	1	1.782955	5.038636	-0.964923
1	-0.461330	3.814917	-1.556799	1	0.711384	3.727781	-1.482719
1	-0.839542	4.534308	0.016339	1	0.541001	4.432890	0.132607
NImag = 1 (-95.2476 cm ⁻¹)				NImag = 1 (-112.6867 cm ⁻¹)			
TS4(Me)si-re				TS4(OMe)si-re			
Et = -1288.2702656				Et = -1363.4457062			
Gsol = -1288.570452				Gsol = -1363.769777			
6	3.275596	-0.395534	0.980579	7	-3.237304	-0.416447	1.017838
6	2.322674	-1.408099	1.001998	6	-2.515035	-0.566423	-0.097926
6	2.609783	-2.611205	0.372287	7	-3.319490	-0.742655	-1.161006
6	3.814286	-2.787993	-0.287756	6	-4.707117	-0.860294	-0.732984
6	4.765299	-1.775655	-0.327117	6	-4.653127	-0.315171	0.704817
6	4.476834	-0.577606	0.323996	7	-1.196908	-0.555456	-0.146385
6	1.061260	-1.255820	1.773319	6	-0.475888	-1.410600	-1.092213
8	0.229514	-2.159647	1.855126	6	-0.884033	-2.865466	-0.999768
6	-0.144139	0.299600	0.580275	6	-2.951195	-0.341299	-2.499488
6	0.380826	1.347123	-0.235196	6	-5.216108	-2.284401	-0.829779

8	1.073886	2.243411	0.506067	6	-5.168744	1.103127	0.847789
6	1.678052	3.397530	-0.092976	6	-2.755416	-0.641668	2.359079
6	0.618193	4.288391	-0.722498	6	-0.421877	0.417055	0.590076
7	-1.044136	-0.550492	-0.165097	6	0.025981	1.474955	-0.262176
6	-0.460852	-1.430381	-1.179964	8	-0.027143	1.485929	-1.485365
6	-1.039258	-2.829064	-1.147902	8	0.585307	2.475232	0.457493
6	-2.353240	-0.396913	-0.082223	6	1.074027	3.666454	-0.175133
7	-3.195809	-0.395133	-1.128769	6	2.212565	3.353298	-1.132158
6	-4.577700	-0.367692	-0.668076	6	-0.060064	4.398252	-0.875631
6	-4.424483	0.053109	0.804825	6	1.583419	4.492945	0.992785
7	-3.025130	-0.240501	1.062802	6	0.882910	-0.913984	1.886821
6	-2.807649	0.043453	-2.450349	8	0.150082	-1.899666	2.005860
6	-2.535592	-0.603935	2.369838	6	2.184982	-0.986381	1.174611
6	-4.761975	1.507041	1.069857	6	3.029018	0.119598	1.096728
6	-5.267833	-1.703627	-0.855740	6	4.265477	0.023237	0.499776
8	0.281642	1.429476	-1.454007	6	4.691885	-1.193271	-0.031613
6	2.315946	4.106420	1.088905	6	3.866911	-2.307225	0.048823
6	2.742769	2.997888	-1.101521	6	2.624902	-2.193443	0.656665
1	-2.672297	-0.793995	-3.133549	8	5.919115	-1.190152	-0.594462
1	-3.589679	0.688231	-2.846047	1	-2.682736	-1.194366	-3.121362
1	-1.883335	0.613996	-2.384037	1	-3.798607	0.165237	-2.956722
1	-3.299978	-1.190888	2.877609	1	-2.114010	0.351798	-2.451168
1	-1.633781	-1.210021	2.269483	1	-3.464431	-1.283871	2.880256
1	-2.318207	0.276963	2.972991	1	-1.786083	-1.142689	2.323911
1	-5.108822	0.405127	-1.223103	1	-2.664785	0.292709	2.912129
1	-5.031301	-0.590406	1.442021	1	-5.315104	-0.206436	-1.357705
1	-4.550878	1.773108	2.103800	1	-5.199141	-0.977707	1.376464
1	-4.172689	2.158301	0.425814	1	-5.019624	1.469334	1.861636
1	-5.818305	1.695453	0.881414	1	-4.642330	1.770080	0.166416
1	-6.301809	-1.652663	-0.516338	1	-6.234123	1.148696	0.624605
1	-5.269271	-1.995145	-1.904391	1	-6.258677	-2.341529	-0.518704
1	-4.755660	-2.479313	-0.288286	1	-5.146916	-2.652200	-1.851840
1	-0.515817	0.609506	1.541573	1	-4.628728	-2.942648	-0.191280
1	0.593003	-1.464220	-0.932382	1	-0.881372	0.743539	1.507070
1	-0.524422	-0.986801	-2.169518	1	0.563812	-1.303696	-0.808348
1	-0.518498	-3.452712	-1.873756	1	-0.552699	-1.028311	-2.105912
1	-0.902832	-3.256051	-0.157594	1	-0.260745	-3.458881	-1.667894
1	-2.099001	-2.846120	-1.403235	1	-0.740366	-3.216844	0.018714
1	1.121187	-0.474988	2.542186	1	-1.921895	-3.025312	-1.292259
1	3.056853	0.543247	1.470155	1	0.840807	-0.092491	2.613754
1	5.208892	0.219218	0.315144	1	2.693061	1.066163	1.496080
6	6.062207	-1.955818	-1.056479	1	4.927776	0.873003	0.429847
1	4.025962	-3.732516	-0.771091	1	4.182285	-3.261929	-0.341601
1	1.880653	-3.406237	0.427712	1	1.980330	-3.054901	0.752405
1	2.806182	5.022481	0.763310	1	1.970484	5.448338	0.642194
1	1.562714	4.360872	1.832513	1	0.781484	4.683092	1.704048

1	3.059077	3.466790	1.561954	1	2.382639	3.967940	1.513290
1	3.276331	3.884201	-1.444925	1	2.657182	4.281461	-1.491023
1	3.461991	2.322721	-0.640840	1	2.985079	2.779427	-0.623228
1	2.295830	2.496024	-1.952431	1	1.856014	2.775715	-1.977689
1	1.070609	5.219283	-1.063225	1	0.293209	5.358119	-1.251102
1	0.152597	3.791817	-1.567277	1	-0.437386	3.811342	-1.706480
1	-0.148679	4.533107	0.011996	1	-0.873170	4.586167	-0.174964
1	6.059906	-1.413286	-2.003044	6	6.392867	-2.383902	-1.144048
1	6.902558	-1.581378	-0.473171	1	7.378081	-2.164929	-1.542311
1	6.250086	-3.004012	-1.279964	1	6.478816	-3.168032	-0.389840
				1	5.750847	-2.736569	-1.953042
NImag = 1 (-117.5871 cm ⁻¹)				NImag = 1 (-130.6027 cm ⁻¹)			
TS4(OH)si-re				TSf1- trans(NO₂)			
Et = -1324.150044				Et = -1453.3277043			
Gsol = -1324.481270				Gsol = -1453.676557			
6	3.287682	-0.409499	0.943807	7	2.590298	-1.824220	1.337487
6	2.323565	-1.413014	0.972766	6	1.768738	-1.950544	0.273315
6	2.601915	-2.621965	0.350953	7	2.488622	-2.262772	-0.823171
6	3.802968	-2.821500	-0.307212	6	3.885231	-2.431074	-0.485719
6	4.749736	-1.806919	-0.337856	6	3.958099	-1.718801	0.867626
6	4.490137	-0.595997	0.294400	8	0.525802	-1.891586	0.314610
6	1.062291	-1.247545	1.739070	6	1.902144	-2.857126	-1.985897
8	0.226906	-2.150691	1.823395	6	4.832531	-1.878935	-1.526572
6	-0.131756	0.306594	0.570547	6	4.974467	-2.312613	1.815143
6	0.404796	1.350312	-0.245020	6	2.168783	-1.056129	2.475786
8	1.108184	2.237119	0.497109	6	-0.379805	-0.281874	-0.589829
6	1.716305	3.391567	-0.098920	6	0.236191	0.843230	0.167122
6	0.658100	4.289879	-0.720411	7	1.629110	0.694292	0.019019
7	-1.042847	-0.528879	-0.178144	6	2.218306	1.394850	-1.084973
6	-0.468578	-1.406317	-1.200576	6	3.229734	2.435347	-0.611847
6	-1.046210	-2.805342	-1.167140	6	-1.677305	-0.852641	-0.321429
6	-2.350493	-0.380361	-0.078275	6	-2.218549	-0.929336	0.966437
7	-3.204900	-0.383051	-1.116044	6	-3.516764	-1.346377	1.157589
6	-4.581571	-0.360725	-0.639630	6	-4.279133	-1.688521	0.052475
6	-4.413283	0.066193	0.829635	6	-3.772798	-1.633174	-1.234490
7	-3.010511	-0.223541	1.073935	6	-2.469235	-1.223579	-1.412637
6	-2.833405	0.060886	-2.440468	6	-0.423825	2.149228	-0.281960
6	-2.509747	-0.591129	2.375980	8	-1.195047	2.222217	-1.204498
6	-4.750849	1.520439	1.092707	8	-0.014261	3.160863	0.463567
6	-5.266893	-1.700954	-0.813965	6	-0.471106	4.517257	0.228211
8	0.305434	1.434752	-1.463088	6	0.258188	5.310602	1.295016
6	2.361286	4.091770	1.084221	6	-1.972805	4.601153	0.435094
6	2.775551	2.991998	-1.113051	6	-0.059134	4.979432	-1.157634
1	-2.700965	-0.773857	-3.127574	1	5.020864	-1.756730	2.749267
1	-3.622502	0.702993	-2.826337	1	5.968103	-2.280881	1.370248

1	-1.911145	0.635493	-2.383306	1	4.729260	-3.348712	2.042446
1	-3.270426	-1.178972	2.888316	1	4.172817	-0.657476	0.697384
1	-1.609218	-1.198163	2.266396	1	4.088232	-3.500803	-0.342610
1	-2.287365	0.287999	2.979907	1	5.862932	-1.980599	-1.188985
1	-5.123077	0.407179	-1.191400	1	4.744546	-2.417622	-2.468589
1	-5.011754	-0.575957	1.475956	1	4.629539	-0.825652	-1.709184
1	-4.527898	1.791001	2.122981	1	2.165957	-2.307452	-2.887932
1	-4.170674	2.170404	0.439138	1	0.823934	-2.848544	-1.864986
1	-5.809740	1.705964	0.916093	1	2.230902	-3.892620	-2.100049
1	-6.297157	-1.654028	-0.462888	1	2.280663	0.009178	2.262234
1	-5.278760	-1.996829	-1.861336	1	1.123688	-1.275399	2.667012
1	-4.744133	-2.471555	-0.249219	1	2.747286	-1.345121	3.349316
1	-0.508039	0.626270	1.527001	1	1.335455	5.220558	1.170838
1	0.587397	-1.440162	-0.961999	1	-0.003584	4.947636	2.286944
1	-0.540829	-0.959737	-2.188082	1	-0.011483	6.362944	1.228850
1	-0.530882	-3.427054	-1.898623	1	-2.240146	4.218703	1.419043
1	-0.901997	-3.233633	-0.178518	1	-2.288553	5.641902	0.379868
1	-2.107789	-2.822142	-1.414428	1	-2.506311	4.034490	-0.320917
1	1.132228	-0.473335	2.513785	1	-0.293121	6.037164	-1.269875
1	3.075478	0.535308	1.424205	1	-0.580993	4.423174	-1.929227
1	5.242614	0.177396	0.264315	1	1.013610	4.853514	-1.294991
8	5.942937	-1.943860	-0.959078	1	-0.031184	0.721478	1.223322
1	4.012038	-3.770266	-0.785688	1	2.751879	0.693641	-1.743088
1	1.864633	-3.409113	0.407966	1	1.489969	1.897216	-1.738117
1	2.854662	5.007014	0.761189	1	3.720639	2.929233	-1.452571
1	1.611779	4.346148	1.831610	1	2.737870	3.186704	0.002263
1	3.103379	3.446785	1.551578	1	3.995175	1.960402	0.001045
1	3.310521	3.877926	-1.455093	1	-2.060743	-1.163243	-2.410331
1	3.495341	2.313264	-0.658683	1	-1.603539	-0.692442	1.819431
1	2.324064	2.495097	-1.964427	1	-4.398356	-1.913619	-2.065215
1	1.113620	5.220270	-1.058235	1	-3.949300	-1.419025	2.141424
1	0.187532	3.799703	-1.566200	1	-0.001432	-0.394109	-1.593996
1	-0.105250	4.534601	0.017750	7	-5.644939	-2.129818	0.250991
1	5.995159	-2.816488	-1.350434	8	-6.063574	-2.168916	1.385657
				8	-6.285160	-2.432893	-0.730026
NImag = 1 (-128.5153 cm ⁻¹)				NImag = 1 (-331.9691 cm ⁻¹)			
TSfl- trans(CN) Et = -1341.1158491 Gsol = -1341.428391				TSfl- trans(COOMe) Et = -1476.717031 Gsol = -1477.065774			
6	-2.371103	-1.939979	-1.373678	7	2.898912	-1.535553	1.463038
6	-1.689943	-1.367585	-0.295966	6	2.017909	-1.805501	0.482610
6	-2.200938	-1.541105	0.993990	7	2.643271	-2.448416	-0.530270
6	-3.364977	-2.247014	1.197512	6	4.001023	-2.772253	-0.144600
6	-4.046019	-2.796078	0.110458	6	4.246517	-1.756352	0.972515
6	-3.542740	-2.638213	-1.179608	8	0.793845	-1.583109	0.530836

6	-0.559343	-0.518779	-0.579994	6	1.920638	-3.238366	-1.483309
6	-0.197422	0.717557	0.166908	6	4.993842	-2.710579	-1.282003
6	-1.138537	1.844512	-0.267137	6	5.208350	-2.239580	2.033093
8	-0.921743	2.931313	0.453610	6	2.625589	-0.508647	2.431665
6	-1.660762	4.157562	0.228778	6	-0.004772	-0.134439	-0.629592
6	-1.406382	4.676234	-1.174956	6	0.598962	1.033109	0.070807
6	-5.252447	-3.528607	0.321243	7	1.995406	0.935673	-0.138564
7	1.189841	0.896713	0.006444	6	2.378757	1.577838	-1.348643
6	1.588955	1.693923	-1.116693	6	3.836433	1.325270	-1.668801
6	2.464006	2.863143	-0.678376	6	-1.343514	-0.637479	-0.428247
8	-1.944043	1.738931	-1.156503	6	-2.019552	-0.514308	0.788884
6	-1.074713	5.101571	1.260692	6	-3.338781	-0.897021	0.897431
6	-3.138330	3.929683	0.493640	6	-4.010961	-1.409764	-0.209270
8	0.703133	-1.878314	0.317357	6	-3.345865	-1.541555	-1.422779
6	1.925547	-1.646046	0.278254	6	-2.023520	-1.167423	-1.527895
7	2.692855	-1.323653	1.342468	6	-0.104055	2.325808	-0.351712
6	3.998666	-0.904596	0.871650	8	-0.829128	2.422961	-1.307126
6	4.098053	-1.622468	-0.477011	8	0.223975	3.312676	0.470600
7	2.702356	-1.794219	-0.813710	6	-0.271778	4.658558	0.282667
6	2.101481	-0.661871	2.472040	6	0.367901	5.418289	1.428995
6	2.272614	-2.511902	-1.974746	6	-1.785183	4.678251	0.408206
6	4.885248	-0.863224	-1.520955	6	0.194931	5.216092	-1.050126
6	5.123683	-1.237883	1.824037	1	5.386530	-1.477053	2.788287
1	5.035207	-0.682340	2.755351	1	6.171149	-2.481241	1.585109
1	6.083460	-0.975702	1.380848	1	4.821874	-3.130137	2.526042
1	5.128067	-2.301446	2.056740	1	4.607173	-0.820533	0.532030
1	3.958558	0.176187	0.694505	1	4.011530	-3.782991	0.286437
1	4.551346	-2.611567	-0.328364	1	5.998375	-2.915839	-0.915146
1	5.905983	-0.701247	-1.177424	1	4.768162	-3.455092	-2.043582
1	4.941029	-1.415966	-2.457326	1	4.989954	-1.728034	-1.747774
1	4.426848	0.104217	-1.715707	1	2.243983	-3.019135	-2.499014
1	2.400599	-1.918033	-2.878445	1	0.864804	-3.007812	-1.387586
1	1.222352	-2.755971	-1.853413	1	2.062189	-4.305365	-1.293917
1	2.834947	-3.441806	-2.086516	1	2.789423	0.473280	1.981776
1	1.957427	0.396472	2.243079	1	1.585802	-0.592569	2.730916
1	1.139046	-1.121250	2.671466	1	3.248678	-0.661712	3.308737
1	2.733457	-0.792932	3.346551	1	1.452562	5.361173	1.364252
1	-0.007628	5.235334	1.095123	1	0.059702	4.998542	2.384684
1	-1.218512	4.706965	2.264584	1	0.071420	6.465238	1.398188
1	-1.560137	6.073697	1.197432	1	-2.090560	4.228242	1.351847
1	-3.283810	3.515722	1.490386	1	-2.138353	5.708451	0.394734
1	-3.666792	4.880556	0.442498	1	-2.253182	4.137077	-0.407568
1	-3.568805	3.251879	-0.236111	1	-0.091774	6.264391	-1.124312
1	-1.863911	5.658402	-1.286116	1	-0.247019	4.673155	-1.878889
1	-1.825085	4.010175	-1.922163	1	1.279294	5.154597	-1.125911
1	-0.336874	4.778866	-1.351729	1	0.385071	0.913693	1.137963

1	-0.418967	0.542031	1.226583	1	1.765575	1.243765	-2.215509
1	2.170680	1.097111	-1.836928	1	2.212866	2.670838	-1.326787
1	0.751443	2.099757	-1.702407	1	4.147849	1.845673	-2.574345
1	2.823179	3.440437	-1.532389	1	4.464109	1.662403	-0.844524
1	1.903854	3.520519	-0.016293	1	4.006987	0.258941	-1.808065
1	3.328198	2.498471	-0.123834	1	-1.510413	-1.259910	-2.474301
1	-1.986012	-1.810122	-2.374241	1	-1.495328	-0.143166	1.655484
1	-1.661622	-1.145799	1.839681	1	-3.882835	-1.944093	-2.267599
1	-4.070340	-3.068764	-2.016359	1	-3.857099	-0.806664	1.838610
1	-3.754084	-2.385857	2.194224	1	0.461089	-0.372848	-1.574014
1	-0.172389	-0.553645	-1.586858	6	-5.424830	-1.837344	-0.148160
7	-6.226064	-4.120670	0.491565	8	-5.964040	-1.660940	1.057422
NImag = 1 (-333.0222 cm ⁻¹)				8	-6.034536	-2.296835	-1.077642
				6	-7.318545	-2.051986	1.173352
				1	-7.598669	-1.847317	2.199944
				1	-7.940545	-1.482045	0.488949
				1	-7.431416	-3.109574	0.952164
				NImag = 1 (-320.2375 cm ⁻¹)			
TSf1- trans(Cl)				TSf1- trans(H)			
Et = -1708.5162919				Et = -1248.9143699			
Gsol = -1708.831358				Gsol = -1249.205508			
6	-2.494208	-1.654365	-1.371600	7	-2.711806	-0.410968	1.406695
6	-1.791109	-1.083163	-0.308606	6	-2.315555	0.513861	0.511424
6	-2.363609	-1.120579	0.965631	7	-3.198492	0.562732	-0.514100
6	-3.603576	-1.688841	1.167536	6	-4.344936	-0.269876	-0.217676
6	-4.287933	-2.228333	0.088470	6	-3.759226	-1.226757	0.822208
6	-3.741211	-2.214670	-1.184469	8	-1.345279	1.280535	0.645561
6	-0.563782	-0.386344	-0.590451	6	-3.301207	1.711741	-1.363895
6	-0.019386	0.773032	0.169537	6	-4.945208	-0.943758	-1.429658
6	-0.792866	2.023795	-0.260190	6	-4.772341	-1.725936	1.826211
8	-0.431527	3.068742	0.465900	6	-1.770126	-0.979475	2.333357
6	-0.981919	4.387398	0.231278	6	0.322696	1.020715	-0.484051
6	-0.643465	4.860024	-1.171194	6	0.748838	-0.283645	0.094404
17	-5.843192	-2.938469	0.338228	7	-0.250643	-1.228745	-0.243863
7	1.381509	0.766569	0.018382	6	-0.001516	-1.804649	-1.520504
6	1.887002	1.498928	-1.105908	6	-1.156954	-2.678343	-1.960429
6	2.886868	2.564791	-0.670113	6	0.841970	2.317494	-0.123511
8	-1.600021	2.037954	-1.154908	6	1.408620	2.578236	1.126843
6	-0.273613	5.240356	1.266099	6	2.000408	3.798290	1.383915
6	-2.479284	4.378467	0.484048	6	2.040518	4.777341	0.400101
8	0.533265	-1.942157	0.237956	6	1.476672	4.533251	-0.842658
6	1.773120	-1.844926	0.238442	6	0.872788	3.316875	-1.098144
7	2.541563	-1.657893	1.336353	6	2.189020	-0.593394	-0.322310
6	3.899067	-1.372344	0.915863	8	2.767650	-0.047719	-1.225723

6	3.957730	-2.044767	-0.458640	8	2.685032	-1.564895	0.432747
7	2.562850	-2.046164	-0.835891	6	4.014536	-2.091157	0.220115
6	1.995904	-0.961302	2.467969	6	4.127539	-3.167804	1.282726
6	2.087550	-2.648245	-2.042629	6	5.049008	-1.003436	0.451549
6	4.855277	-1.339199	-1.450161	6	4.131754	-2.699439	-1.166191
6	4.949849	-1.868925	1.882032	1	-4.326878	-2.428703	2.526965
1	4.893354	-1.346195	2.834663	1	-5.581527	-2.247298	1.316739
1	5.946676	-1.697685	1.477597	1	-5.195161	-0.896588	2.390942
1	4.828775	-2.935098	2.066811	1	-3.288681	-2.071167	0.307059
1	3.986606	-0.288100	0.782777	1	-5.113605	0.349831	0.265143
1	4.295488	-3.083213	-0.340063	1	-5.772392	-1.586100	-1.131247
1	5.877033	-1.306401	-1.074356	1	-5.339781	-0.211701	-2.132358
1	4.877139	-1.859028	-2.406697	1	-4.203842	-1.550890	-1.943527
1	4.513427	-0.319767	-1.616866	1	-3.346927	1.420858	-2.411603
1	2.305384	-2.026684	-2.910050	1	-2.426159	2.332869	-1.203988
1	1.013422	-2.775858	-1.956052	1	-4.192414	2.297852	-1.124624
1	2.543975	-3.629371	-2.193569	1	-1.138266	-1.704175	1.813705
1	2.004600	0.114000	2.275236	1	-1.148448	-0.177792	2.719128
1	0.972821	-1.293563	2.610045	1	-2.305720	-1.428950	3.165439
1	2.565747	-1.205395	3.361082	1	3.356354	-3.922554	1.142769
1	0.802389	5.222764	1.105325	1	4.009041	-2.738239	2.275738
1	-0.475554	4.869375	2.269027	1	5.101826	-3.650273	1.227470
1	-0.617660	6.271033	1.201730	1	4.912062	-0.556835	1.435484
1	-2.690853	3.992919	1.480416	1	6.047884	-1.436025	0.412204
1	-2.863841	5.395807	0.426702	1	4.973799	-0.226052	-0.301681
1	-2.996951	3.767267	-0.247921	1	5.099474	-3.189887	-1.265634
1	-0.943031	5.901174	-1.283997	1	4.043166	-1.940466	-1.936349
1	-1.155679	4.266302	-1.921102	1	3.354708	-3.446935	-1.316829
1	0.429943	4.795287	-1.341790	1	0.774727	-0.161404	1.182142
1	-0.267046	0.628110	1.228032	1	0.175366	-1.037396	-2.307720
1	2.404526	0.833219	-1.815811	1	0.921570	-2.414235	-1.549673
1	1.109865	1.993066	-1.708295	1	-0.962384	-3.156792	-2.920366
1	3.321315	3.087934	-1.524596	1	-1.340352	-3.455017	-1.218525
1	2.399731	3.289328	-0.020306	1	-2.061310	-2.078429	-2.050269
1	3.696723	2.108980	-0.100631	1	0.440113	3.121315	-2.069159
1	-2.064485	-1.635754	-2.362547	1	1.361123	1.828598	1.901423
1	-1.821805	-0.724322	1.809732	1	1.504660	5.292684	-1.610002
1	-4.286142	-2.642566	-2.010893	1	2.430953	3.992006	2.355323
1	-4.041848	-1.722588	2.152447	1	-0.146327	0.942713	-1.453601
1	-0.183402	-0.469640	-1.597115	1	2.506914	5.729868	0.604725
NImag = 1 (-332.3647 cm ⁻¹)				NImag = 1 (-316.5466 cm ⁻¹)			
TSfl- trans(Me) Et = -1288.2254452 Gsol = -1288.521731				TSfl- trans(OMe) Et = -1363.4019512 Gsol = -1363.722228			

7	-2.878740	0.015648	1.421916	6	-1.979378	-2.196338	-1.085682
6	-2.298625	0.804654	0.497646	6	-1.514606	-1.266674	-0.156989
7	-3.155312	1.005390	-0.532226	6	-2.228937	-1.119054	1.040419
6	-4.449700	0.440797	-0.214330	6	-3.359342	-1.857019	1.282417
6	-4.075039	-0.581698	0.859747	6	-3.820953	-2.768784	0.330178
8	-1.188445	1.353353	0.610562	6	-3.124626	-2.936324	-0.862371
6	-3.018970	2.124135	-1.416573	6	-0.395421	-0.436957	-0.497039
6	-5.179737	-0.135131	-1.405420	6	-0.084202	0.906112	0.078607
6	-5.167422	-0.824159	1.875534	6	-1.173031	1.899890	-0.337795
6	-2.075875	-0.707313	2.371269	8	-1.116111	2.986887	0.421675
6	0.372215	0.714711	-0.527076	6	-1.996950	4.111793	0.207184
6	0.517830	-0.633112	0.093362	6	-1.785765	4.700631	-1.176360
7	-0.657386	-1.366592	-0.200422	8	-4.936944	-3.437007	0.656172
6	-0.552230	-2.020209	-1.459656	7	1.252221	1.235682	-0.252620
6	-1.860056	-2.677903	-1.846202	6	1.327613	1.845128	-1.535971
6	1.162722	1.878371	-0.221418	6	2.767355	2.048354	-1.958822
6	1.827766	2.038663	0.997370	8	-1.945008	1.725865	-1.245437
6	2.663313	3.114728	1.202595	6	-1.555978	5.095820	1.274148
6	2.874186	4.066151	0.205215	6	-3.440110	3.694433	0.432102
6	2.205416	3.910600	-1.004067	8	0.910115	-1.498663	0.646647
6	1.356144	2.841931	-1.211986	6	2.133647	-1.312118	0.522553
6	1.858158	-1.246294	-0.323467	7	2.930778	-0.706501	1.424047
8	2.532389	-0.848770	-1.238249	6	4.244553	-0.509556	0.841309
8	2.146149	-2.288734	0.445098	6	4.291468	-1.638622	-0.188844
6	3.334212	-3.083894	0.232796	7	2.885900	-1.799499	-0.493662
6	3.229465	-4.144938	1.311690	6	2.389354	0.258820	2.343135
6	4.575413	-2.233489	0.441585	6	2.414550	-2.853415	-1.340852
6	3.309717	-3.723407	-1.144160	6	5.154810	-1.355968	-1.396273
1	-4.875637	-1.579434	2.602162	6	5.369819	-0.557397	1.848736
1	-6.068724	-1.183207	1.380622	1	5.320189	0.279478	2.542035
1	-5.407135	0.094014	2.409542	1	6.331820	-0.499425	1.341366
1	-3.792360	-1.522571	0.375366	1	5.335138	-1.482575	2.421987
1	-5.071748	1.223372	0.242697	1	4.243677	0.452450	0.317539
1	-6.116351	-0.590292	-1.086775	1	4.651886	-2.552916	0.303588
1	-5.425296	0.639020	-2.130605	1	6.187468	-1.195973	-1.089759
1	-4.577694	-0.893343	-1.900260	1	5.148445	-2.194204	-2.091178
1	-3.124330	1.817987	-2.455685	1	4.808622	-0.469228	-1.921483
1	-2.034433	2.555933	-1.269539	1	2.601867	-2.628145	-2.389163
1	-3.770082	2.888376	-1.199993	1	1.346459	-2.962626	-1.184452
1	-1.614968	-1.567818	1.880189	1	2.900768	-3.801361	-1.095239
1	-1.296433	-0.043183	2.730867	1	2.202906	1.197558	1.815258
1	-2.692236	-1.003082	3.216215	1	1.451337	-0.128420	2.728281
1	2.314750	-4.721259	1.189277	1	3.074654	0.388542	3.176710
1	3.214680	-3.686027	2.298515	1	-0.507710	5.354995	1.140629
1	4.079342	-4.823101	1.257088	1	-1.677491	4.663795	2.265762
1	4.541001	-1.751477	1.417762	1	-2.150880	6.005737	1.216639

1	5.461345	-2.866364	0.407850	1	-3.550475	3.237021	1.414503
1	4.660517	-1.470258	-0.324923	1	-4.084622	4.571716	0.393317
1	4.154279	-4.404560	-1.242465	1	-3.764642	2.987036	-0.323953
1	3.371547	-2.973473	-1.925613	1	-2.373177	5.612917	-1.274858
1	2.393407	-4.296022	-1.277085	1	-2.089118	4.002913	-1.949668
1	0.585083	-0.482637	1.175999	1	-0.736862	4.953125	-1.321697
1	-0.255178	-1.327293	-2.279562	1	-0.170978	0.813189	1.166387
1	0.238457	-2.794160	-1.484334	1	0.814339	1.252820	-2.327813
1	-1.780592	-3.215389	-2.791296	1	0.818200	2.827125	-1.586194
1	-2.165317	-3.382277	-1.072909	1	2.841479	2.556193	-2.920736
1	-2.640945	-1.925239	-1.942356	1	3.293076	2.643319	-1.212417
1	0.850183	2.734193	-2.161158	1	3.271234	1.086160	-2.037057
1	1.666433	1.327026	1.792281	1	-1.444164	-2.324043	-2.016041
1	2.349639	4.639247	-1.789507	1	-1.878544	-0.426971	1.790356
1	3.162946	3.226820	2.154930	1	-3.462863	-3.633091	-1.611930
1	-0.128900	0.709570	-1.483775	1	-3.913493	-1.754119	2.202459
6	3.811402	5.211916	0.428744	1	0.077331	-0.630423	-1.448720
1	3.618940	6.025986	-0.266681	6	-5.449770	-4.366924	-0.257703
1	3.726192	5.603553	1.440967	1	-6.340922	-4.779690	0.201682
1	4.847125	4.898788	0.288862	1	-5.719499	-3.890927	-1.200921
				1	-4.738742	-5.171355	-0.448551
NImag = 1 (-315.4680 cm ⁻¹)				NImag = 1 (-316.6104 cm ⁻¹)			
TSf1- trans(OH) Et = -1324.1060197 Gsol = -1324.434054				TSf2- cis(NO₂) Et = -1453.3198294 Gsol = -1453.669603			
6	1.317096	2.905444	-1.171730	6	2.430594	-1.265083	-1.346677
6	1.170256	1.900443	-0.214045	6	1.685661	-0.219734	-0.784038
6	1.883293	2.023094	0.985285	6	2.326067	0.671809	0.080457
6	2.716556	3.092229	1.210748	6	3.661000	0.507888	0.396545
6	2.864131	4.072623	0.232477	6	4.353659	-0.554925	-0.150333
6	2.161394	3.975254	-0.963295	6	3.757204	-1.446493	-1.027345
6	0.378188	0.746095	-0.526845	6	0.317310	-0.009423	-1.236075
6	0.515688	-0.609605	0.084342	6	-0.715480	0.743344	-0.464646
6	1.862700	-1.211775	-0.328816	6	-0.550191	2.250940	-0.678151
8	2.155960	-2.253802	0.438215	8	-1.551071	2.904092	-0.114730
6	3.347274	-3.043393	0.224836	6	-1.652044	4.348359	-0.169421
6	3.326277	-3.680367	-1.153345	6	-0.450547	4.991406	0.499612
8	3.696173	5.093145	0.502102	7	-0.831513	0.207152	0.836070
7	-0.648014	-1.356399	-0.219787	6	-0.169115	0.904509	1.886546
6	-0.533829	-1.991479	-1.487844	6	-0.946537	0.819837	3.191017
6	-1.832268	-2.664868	-1.879479	8	0.351379	2.752967	-1.301036
8	2.536886	-0.808790	-1.241791	6	-2.914129	4.627821	0.623523
6	3.246287	-4.107087	1.301523	6	-1.813414	4.803693	-1.608893
6	4.585054	-2.188555	0.436091	8	-0.375390	-1.829575	-1.223581
8	-1.201429	1.369351	0.595256				

6	-2.300310	0.795458	0.494500	6	-1.365744	-2.227519	-0.570124
7	-2.856596	-0.002063	1.426591	7	-2.638317	-2.152049	-1.007614
6	-4.042710	-0.627530	0.873252	6	-3.523470	-2.913440	-0.148524
6	-4.451986	0.388720	-0.193609	6	-2.665360	-3.069952	1.120741
7	-3.173043	0.979479	-0.525519	7	-1.322870	-2.890619	0.590842
6	-2.029944	-0.711109	2.366375	6	-2.996852	-1.729721	-2.327758
6	-3.068686	2.099453	-1.411789	6	-0.154373	-2.893674	1.424423
6	-5.184988	-0.199318	-1.376952	6	-3.004787	-2.050868	2.189623
6	-5.119382	-0.900821	1.897860	6	-3.925623	-4.245354	-0.757338
1	-4.803196	-1.652638	2.617781	1	-4.482522	-4.117152	-1.683570
1	-6.016479	-1.278816	1.409459	1	-4.563658	-4.791958	-0.064632
1	-5.376042	0.008610	2.438987	1	-3.045184	-4.852338	-0.964459
1	-3.739752	-1.558793	0.382641	1	-4.413586	-2.322893	0.069918
1	-5.084023	1.157651	0.272988	1	-2.761920	-4.083077	1.513490
1	-6.109514	-0.671487	-1.047995	1	-4.059015	-2.126473	2.454832
1	-5.452785	0.571020	-2.098368	1	-2.424394	-2.224164	3.093710
1	-4.575079	-0.946111	-1.879346	1	-2.776369	-1.048635	1.827525
1	-3.178770	1.790744	-2.449739	1	-0.148618	-2.038524	2.095583
1	-2.091332	2.550360	-1.274835	1	0.719929	-2.830796	0.785513
1	-3.832191	2.849297	-1.187888	1	-0.119023	-3.823116	1.989723
1	-1.555246	-1.558946	1.865901	1	-3.812219	-1.008960	-2.288818
1	-1.263516	-0.031021	2.724474	1	-2.131472	-1.261791	-2.783601
1	-2.633379	-1.024566	3.214259	1	-3.300718	-2.568936	-2.954569
1	2.333766	-4.686501	1.177481	1	-2.812618	4.259947	1.642412
1	3.229278	-3.650259	2.289291	1	-3.769933	4.135482	0.165865
1	4.098807	-4.781868	1.245982	1	-3.106686	5.698566	0.657002
1	4.548530	-1.708964	1.413413	1	-2.653033	4.289861	-2.074929
1	5.473596	-2.817714	0.401349	1	-2.018335	5.873051	-1.630506
1	4.667435	-1.423249	-0.328641	1	-0.915224	4.610232	-2.186393
1	4.173697	-4.357897	-1.252386	1	-0.603378	6.068277	0.556185
1	3.385416	-2.928609	-1.933246	1	0.461302	4.798928	-0.056002
1	2.412224	-4.256120	-1.287913	1	-0.335159	4.612952	1.514021
1	0.575733	-0.467236	1.168596	1	-1.655640	0.532843	-0.997757
1	-0.250304	-1.285787	-2.302044	1	0.845429	0.504247	2.092530
1	0.267387	-2.754682	-1.525506	1	-0.003606	1.974663	1.678457
1	-1.746692	-3.191968	-2.829992	1	-0.423887	1.341053	3.994201
1	-2.125343	-3.380936	-1.112185	1	-1.934293	1.262135	3.070204
1	-2.624541	-1.923050	-1.966729	1	-1.080160	-0.216630	3.496150
1	0.777201	2.829794	-2.104814	1	1.938100	-1.954832	-2.013307
1	1.766018	1.275201	1.753967	1	1.801202	1.530063	0.455461
1	2.275979	4.736345	-1.723666	1	4.335582	-2.256188	-1.439719
1	3.264563	3.194958	2.134333	1	4.169848	1.194603	1.051896
1	-0.127539	0.751436	-1.481165	1	0.181119	-0.136112	-2.300785
1	3.718376	5.698014	-0.240932	7	5.751619	-0.735736	0.192605
				8	6.336570	-1.667942	-0.310427
				8	6.248855	0.054700	0.961283

NImag = 1 (-314.3856 cm⁻¹)

				NImag = 1 (-351.9804 cm ⁻¹)			
TSf2- cis(CN) Et = -1341.1081237 Gsol = -1341.420875				TSf2- cis(COOMe) Et = -1476.7054774 Gsol = -1477.054256			
6	1.978339	-2.247277	-1.333146	6	2.315514	-0.891613	-1.340257
6	1.702975	-1.002787	-0.752317	6	1.432356	0.033048	-0.768247
6	2.634178	-0.458144	0.134729	6	1.945432	0.998092	0.101480
6	3.787912	-1.148073	0.452521	6	3.293250	1.017287	0.404852
6	4.029421	-2.399300	-0.105404	6	4.152026	0.074455	-0.141996
6	3.117973	-2.947019	-1.009103	6	3.655838	-0.882577	-1.024089
6	0.540036	-0.256151	-1.207627	6	0.048258	0.057300	-1.215305
6	-0.126337	0.834263	-0.433040	6	-1.090455	0.654364	-0.448160
6	0.625710	2.154562	-0.628417	6	-1.130985	2.169845	-0.673024
8	-0.053450	3.152217	-0.089919	8	-2.208316	2.689127	-0.108760
6	0.414941	4.521379	-0.154872	6	-2.501698	4.104702	-0.179755
6	1.754332	4.660629	0.545808	6	-1.395309	4.910523	0.477275
7	-0.468946	0.385868	0.859967	6	-1.166522	0.117976	0.853038
6	0.406774	0.752584	1.921618	6	-0.585465	0.887458	1.901449
6	-0.350668	0.966649	3.222903	6	-1.337957	0.702886	3.210194
8	1.670719	2.259037	-1.220543	8	-0.311199	2.784306	-1.308676
6	-0.660075	5.281105	0.598075	6	-3.788135	4.222814	0.614708
6	0.478942	4.978719	-1.601388	6	-2.725468	4.518298	-1.623691
8	-0.828376	-1.651389	-1.239209	8	-0.394244	-1.849782	-1.207247
6	-1.901404	-1.630677	-0.596043	6	-1.337411	-2.364494	-0.568119
7	-3.033941	-1.048056	-1.036735	7	-2.604969	-2.441005	-1.021038
6	-4.156549	-1.393178	-0.187957	6	-3.409593	-3.290073	-0.166455
6	-3.444151	-1.903072	1.079047	6	-2.548013	-3.356592	1.108749
7	-2.138135	-2.270778	0.554802	7	-1.230229	-3.021667	0.593147
6	-3.180263	-0.494560	-2.348585	6	-2.997038	-2.058190	-2.343024
6	-1.074673	-2.745437	1.394012	6	-0.083321	-2.870725	1.443266
6	-3.355064	-0.851451	2.166377	6	-3.012419	-2.391272	2.180619
6	-5.065256	-2.435833	-0.815397	6	-3.668961	-4.656296	-0.776889
1	-5.516632	-2.078062	-1.738919	1	-4.233899	-4.585902	-1.704589
1	-5.874419	-2.683296	-0.129980	1	-4.247851	-5.267480	-0.086083
1	-4.509206	-3.346944	-1.032870	1	-2.729363	-5.167569	-0.982807
1	-4.729146	-0.493584	0.039679	1	-4.357607	-2.795581	0.047696
1	-3.943597	-2.798290	1.452128	1	-2.531702	-4.377336	1.493869
1	-4.353520	-0.504336	2.431239	1	-4.053169	-2.590722	2.435220
1	-2.897575	-1.257588	3.066456	1	-2.423582	-2.502785	3.089112
1	-2.742850	-0.018162	1.821489	1	-2.896930	-1.367041	1.825255
1	-0.715729	-1.958918	2.053115	1	-0.185214	-1.999348	2.085179
1	-0.253411	-3.060874	0.759370	1	0.789935	-2.730864	0.815117
1	-1.427618	-3.598007	1.971167	1	0.043288	-3.773775	2.037553
1	-3.631612	0.495204	-2.296886	1	-3.886077	-1.429921	-2.310844
1	-2.195795	-0.412771	-2.795604				

1	-3.795293	-1.126934	-2.990058	1	-2.183398	-1.498642	-2.791032
1	-0.734260	4.920792	1.622003	1	-3.203175	-2.924627	-2.972879
1	-1.627960	5.149431	0.118381	1	-3.636066	3.883466	1.637196
1	-0.424492	6.343552	0.618412	1	-4.571181	3.614644	0.166024
1	-0.482770	4.823854	-2.088715	1	-4.122433	5.258522	0.636731
1	0.707532	6.042911	-1.636910	1	-3.491778	3.893276	-2.080205
1	1.244269	4.439749	-2.150433	1	-3.068121	5.551524	-1.657225
1	2.026697	5.714011	0.596109	1	-1.810426	4.434724	-2.200960
1	2.534812	4.124867	0.015828	1	-1.690499	5.957896	0.525148
1	1.689656	4.279324	1.563629	1	-0.468222	4.835075	-0.081186
1	-1.063194	1.015418	-0.982334	1	-1.225981	4.559977	1.494110
1	1.181049	-0.016063	2.126362	1	-1.983092	0.317079	-0.998444
1	0.981588	1.674432	1.728390	1	0.472990	0.620252	2.101172
1	0.328660	1.233307	4.033764	1	-0.558538	1.971767	1.697335
1	-1.085066	1.762046	3.104709	1	-0.880336	1.282981	4.012959
1	-0.882106	0.062599	3.515637	1	-2.374289	1.017879	3.096206
1	1.261661	-2.671530	-2.018358	1	-1.339368	-0.343232	3.512789
1	2.490097	0.531760	0.525272	1	1.921978	-1.639397	-2.010736
1	3.314106	-3.912981	-1.448025	1	1.305455	1.769620	0.486900
1	4.508565	-0.715417	1.128744	1	4.324998	-1.609191	-1.456509
1	0.377623	-0.303701	-2.275088	1	3.699076	1.767349	1.065698
6	5.214733	-3.118595	0.235889	1	-0.071244	-0.085533	-2.279977
7	6.169284	-3.701998	0.511046	6	5.581504	0.139908	0.232426
NImag = 1 (-353.5819 cm ⁻¹)				8	6.310562	-0.808681	-0.355524
				8	6.050376	0.953147	0.983941
				6	7.687817	-0.793091	-0.034399
				1	8.129554	-1.615342	-0.585010
				1	8.139206	0.149236	-0.331897
				1	7.833078	-0.929380	1.033575
				NImag = 1 (-353.9391 cm ⁻¹)			
TSf2- cis(Cl)				TSf2- cis(H)			
Et = -1708.5086467				Et = -1248.9031614			
Gsol = -1708.823521				Gsol = -1249.193762			
6	2.309962	-1.792906	-1.329308	7	2.649667	-1.348925	-1.121470
6	1.778995	-0.642603	-0.733963	6	2.423109	-0.135575	-0.578005
6	2.571302	0.056351	0.178122	7	3.066632	-0.038808	0.593543
6	3.841372	-0.388012	0.498923	6	3.547363	-1.345715	1.013980
6	4.325109	-1.545545	-0.082404	6	3.592341	-2.105527	-0.324611
6	3.566525	-2.254811	-1.002411	8	1.799308	0.782409	-1.149768
6	0.498585	-0.138676	-1.194578	6	-0.155999	1.051024	-1.094693
6	-0.385106	0.813931	-0.442533	6	-0.622238	-0.205828	-0.414088
6	0.121805	2.246045	-0.650581	7	-0.070435	-0.368895	0.869711
8	-0.719057	3.115023	-0.115906	6	-0.866055	0.064730	1.968309
6	-0.484882	4.541921	-0.175656	6	-0.638680	-0.803171	3.196773
6	0.811575	4.898699	0.529547	6	2.771801	1.010982	1.527453

7	-0.685005	0.347424	0.851408	6	2.631799	-1.999284	2.029409
6	0.109892	0.856362	1.917638	6	4.980993	-2.139386	-0.939104
6	-0.698305	0.987166	3.199545	6	2.295911	-1.693419	-2.463815
8	1.130720	2.528955	-1.247862	6	-0.244332	2.396474	-0.559594
6	-1.671945	5.110319	0.577963	6	-1.196763	2.756763	0.395635
6	-0.494372	5.011110	-1.619880	6	-1.333340	4.079478	0.781822
8	-0.577550	-1.784299	-1.206994	6	-0.519852	5.057232	0.235657
6	-1.648111	-1.949731	-0.583618	6	0.423679	4.714720	-0.724555
7	-2.861155	-1.602900	-1.058387	6	0.550153	3.401394	-1.125809
6	-3.916969	-2.127835	-0.217342	6	-2.132902	-0.354699	-0.633447
6	-3.147958	-2.473344	1.071912	8	-2.822159	0.465066	-1.188141
7	-1.785363	-2.597741	0.580077	8	-2.555996	-1.518290	-0.167835
6	-3.081336	-1.106255	-2.381870	6	-3.942088	-1.919642	-0.262172
6	-0.667205	-2.829839	1.449574	6	-3.946103	-3.280589	0.407486
6	-3.284868	-1.405173	2.138039	6	-4.353185	-2.041970	-1.719164
6	-4.611016	-3.330309	-0.832883	6	-4.829360	-0.951020	0.499435
1	-5.103851	-3.078502	-1.770153	1	4.981859	-2.625844	-1.912899
1	-5.373006	-3.707668	-0.152496	1	5.659995	-2.694906	-0.293827
1	-3.894962	-4.128871	-1.023124	1	5.369740	-1.128771	-1.057747
1	-4.646909	-1.342540	-0.017961	1	3.222192	-3.122634	-0.191575
1	-3.478739	-3.440212	1.454509	1	4.556222	-1.242490	1.416513
1	-4.337181	-1.249929	2.375524	1	2.939520	-3.030939	2.199630
1	-2.780059	-1.701336	3.055674	1	2.676307	-1.480242	2.985112
1	-2.833164	-0.477481	1.786116	1	1.602188	-1.960383	1.671046
1	-0.487766	-1.972101	2.092960	1	1.911925	0.755467	2.141755
1	0.213662	-2.984576	0.835630	1	2.535138	1.908832	0.966273
1	-0.852681	-3.723595	2.042507	1	3.647783	1.195843	2.146680
1	-3.703333	-0.212486	-2.356410	1	1.775988	-2.650255	-2.488183
1	-2.119403	-0.856569	-2.815736	1	1.638080	-0.922685	-2.849981
1	-3.561845	-1.848876	-3.020266	1	3.170510	-1.753987	-3.113141
1	-1.689626	4.733395	1.598438	1	-3.607564	-3.198051	1.438164
1	-2.603840	4.826336	0.092998	1	-3.281703	-3.965186	-0.116150
1	-1.612801	6.196809	0.608135	1	-4.950941	-3.699326	0.402263
1	-1.415485	4.699744	-2.110631	1	-3.670903	-2.706254	-2.247913
1	-0.446582	6.098805	-1.649808	1	-5.353970	-2.467285	-1.780483
1	0.351479	4.609368	-2.168283	1	-4.354109	-1.073788	-2.209105
1	0.908667	5.982415	0.580589	1	-5.847986	-1.336249	0.523845
1	1.670267	4.496454	0.002344	1	-4.837654	0.027369	0.030534
1	0.806472	4.511066	1.547032	1	-4.480784	-0.849094	1.525905
1	-1.321343	0.811329	-1.022602	1	-0.217037	-1.006341	-1.053157
1	0.985119	0.215860	2.156951	1	-0.658496	1.111474	2.275328
1	0.547842	1.849887	1.714792	1	-1.952054	0.051323	1.766121
1	-0.084795	1.368552	4.017377	1	-1.244280	-0.464019	4.038955
1	-1.538163	1.662870	3.044351	1	-0.891919	-1.838997	2.975380
1	-1.099770	0.022002	3.504428	1	0.405854	-0.774731	3.503400
1	1.703248	-2.343433	-2.031386	1	1.290726	3.124360	-1.860388

1	2.224492	0.984998	0.591396	1	-1.869649	2.016774	0.787540
1	3.962511	-3.151553	-1.452356	1	1.055463	5.474976	-1.159998
1	4.454672	0.165428	1.192138	1	-2.085068	4.344510	1.510415
1	0.349551	-0.232199	-2.260698	1	-0.017299	1.016397	-2.165715
17	5.905694	-2.112323	0.331000	1	-0.625858	6.086214	0.547458
NImag = 1 (-347.3273 cm ⁻¹)				NImag = 1 (-339.8790 cm ⁻¹)			
TSf2- cis(Me) Et = -1288.2142868 Gsol = -1288.510300				TSr_{cis}(H) Et = -1248.9173723 Gsol = -1249.210992			
6	0.262117	3.134844	-1.296333	6	2.080567	2.122251	-1.608121
6	-0.418564	2.081529	-0.671015	6	0.926031	2.111003	-0.829985
6	-1.373010	2.398893	0.295444	6	0.485939	3.300610	-0.254681
6	-1.619389	3.719022	0.630612	6	1.223250	4.461349	-0.424533
6	-0.921267	4.759751	0.034200	6	2.388213	4.463074	-1.175670
6	0.024837	4.443383	-0.941570	6	2.812613	3.288319	-1.772853
6	-0.223680	0.732620	-1.158437	6	0.089083	0.857963	-0.735966
6	-0.568566	-0.538736	-0.429375	6	-0.655063	0.447866	0.562221
6	-2.061599	-0.824907	-0.633816	6	-1.725407	-0.575404	0.085459
8	-2.378301	-2.010268	-0.139123	8	-2.807417	0.013446	-0.395101
6	-3.723625	-2.534480	-0.216101	6	-3.961285	-0.730882	-0.837356
6	-4.690039	-1.630004	0.527951	6	-4.534041	-1.545400	0.309274
7	-0.002808	-0.618542	0.855751	8	0.893492	-0.299551	-1.174845
6	-0.832123	-0.224088	1.944135	6	1.560750	-1.055324	-0.373103
6	-0.547592	-1.049078	3.190458	7	1.644485	-2.349025	-0.655817
8	-2.824463	-0.081526	-1.200134	6	2.584246	-3.006660	0.234165
6	-3.605278	-3.874400	0.484905	6	2.698458	-1.971171	1.361605
6	-4.127257	-2.726402	-1.667572	7	2.305416	-0.736242	0.680390
8	1.746153	0.613773	-1.247153	6	3.897909	-3.316511	-0.456934
6	2.469368	-0.178288	-0.608722	6	1.784832	-2.273857	2.533274
7	2.852835	-1.386714	-1.068342	6	0.852290	-3.039073	-1.635411
6	3.873401	-1.964353	-0.220036	6	2.456216	0.553541	1.333334
6	3.716231	-1.130557	1.065154	7	-1.064072	1.543702	1.289379
7	3.081218	0.074842	0.556530	6	-1.713138	1.139915	2.485796
6	2.548547	-1.868325	-2.380029	6	-2.013072	2.341549	3.361222
6	2.651773	1.141344	1.416001	8	-1.566191	-1.775252	0.151371
6	2.876071	-1.827651	2.115810	6	-4.932368	0.359517	-1.248759
6	5.262271	-1.862859	-0.826412	6	-3.603829	-1.602020	-2.029368
1	5.334342	-2.407387	-1.766194	1	4.372852	-2.400669	-0.805405
1	5.998611	-2.285562	-0.144349	1	4.576906	-3.816543	0.231894
1	5.522445	-0.821259	-1.010517	1	3.748286	-3.972244	-1.312430
1	3.632589	-3.009200	-0.021230	1	3.732519	-1.871481	1.687955
1	4.698582	-0.874886	1.465552	1	2.129062	-3.922464	0.609599
1	3.312196	-2.796192	2.360164	1	0.758396	-2.397474	2.190751
1	2.835946	-1.243256	3.033187	1	1.798209	-1.471066	3.267118
				1	2.107664	-3.189252	3.027742

1	1.856914	-1.947979	1.746328	1	1.485917	-3.478931	-2.403571
1	1.828730	0.824167	2.051684	1	0.170098	-2.333949	-2.091633
1	2.305067	1.960521	0.794711	1	0.268008	-3.817171	-1.149872
1	3.494770	1.479068	2.016406	1	1.499864	1.017041	1.577382
1	2.151579	-2.881597	-2.332121	1	3.030369	1.228269	0.707288
1	1.800631	-1.215104	-2.815811	1	3.006644	0.376229	2.252036
1	3.425572	-1.866643	-3.029012	1	0.003628	-0.261281	1.125874
1	-3.272631	-3.737935	1.511770	1	-2.670261	0.599231	2.322345
1	-2.884014	-4.509515	-0.025707	1	-1.101877	0.419243	3.079747
1	-4.569014	-4.380486	0.494083	1	-1.088953	2.866822	3.601747
1	-3.392338	-3.342488	-2.184003	1	-2.657114	3.037762	2.825036
1	-5.088364	-3.236801	-1.713996	1	-2.506815	2.059155	4.292414
1	-4.211791	-1.773392	-2.179556	1	-2.912159	-2.387178	-1.741698
1	-5.669687	-2.104365	0.571261	1	-3.151693	-0.997739	-2.815332
1	-4.788459	-0.669045	0.034092	1	-4.506285	-2.058908	-2.433480
1	-4.344944	-1.469992	1.548151	1	-4.508462	0.967063	-2.046051
1	-0.096705	-1.317633	-1.049142	1	-5.864792	-0.077820	-1.601989
1	-0.704429	0.841017	2.232867	1	-5.147504	1.010572	-0.404440
1	-1.913802	-0.321175	1.740414	1	-5.476066	-1.997130	0.000171
1	-1.184383	-0.743188	4.022498	1	-3.850162	-2.331242	0.612624
1	-0.717612	-2.105155	2.985911	1	-4.727817	-0.900484	1.164477
1	0.488969	-0.933794	3.503119	1	-0.407642	3.248670	0.352836
1	1.004945	2.901207	-2.043911	1	0.880243	5.375297	0.039198
1	-1.968551	1.621677	0.737211	1	2.955530	5.374034	-1.303149
1	0.573431	5.238046	-1.428545	1	3.708929	3.276254	-2.376718
1	-2.377153	3.941491	1.368615	1	2.414926	1.218014	-2.095062
1	-0.096725	0.669476	-2.229617	1	-0.643483	0.907244	-1.538117
6	-1.167810	6.184539	0.422293	NImag = 1 (-23.1899 cm ⁻¹)			
1	-1.288528	6.818713	-0.455128				
1	-2.061482	6.281662	1.034313	NImag = 1 (-332.8234 cm ⁻¹)			
1	-0.329421	6.583276	0.994938				
TSr_{trans}(NO₂) Et = -1453.341762 Gsol = -1453.690729				TSr_{trans}(CN) Et = -1341.1299907 Gsol = -1341.452217			
6	-2.038517	-0.663445	-1.697876	6	-2.160851	-1.003073	-1.757062
6	-1.124490	-0.941257	-0.688003	6	-1.248178	-1.157325	-0.721038
6	-1.550891	-1.616276	0.451171	6	-1.634264	-1.840690	0.426937
6	-2.861628	-2.032327	0.572321	6	-2.899246	-2.382701	0.529475
6	-3.744153	-1.753485	-0.455376	6	-3.803468	-2.234872	-0.520071
6	-3.356475	-1.064677	-1.589222	6	-3.433471	-1.532792	-1.663573
6	0.290290	-0.478702	-0.852815	6	0.117803	-0.561907	-0.869150
6	0.761468	0.789727	-0.090491	6	0.464949	0.740668	-0.099252
6	-0.369391	1.335093	0.813244	6	-0.718377	1.178285	0.794743
8	-1.198018	2.129177	0.160474	8	-1.614926	1.885576	0.132024

6	-2.283717	2.814968	0.822451	6	-2.766917	2.466121	0.782031
6	-3.277822	1.818296	1.391078	6	-3.657746	1.382770	1.363428
8	1.120838	-1.635377	-0.468274	8	1.050260	-1.639426	-0.480082
6	2.378516	-1.436951	-0.219195	6	2.279910	-1.325605	-0.212609
7	2.917787	-1.871600	0.921394	7	2.842836	-1.713736	0.933968
6	4.278221	-1.354000	1.023010	6	4.145498	-1.068521	1.056636
6	4.567442	-0.859249	-0.408911	6	4.408916	-0.549118	-0.371177
7	3.254039	-0.915572	-1.038577	7	3.114058	-0.720429	-1.017883
6	2.109418	-2.106853	2.094792	6	2.042940	-2.026417	2.094863
6	2.998616	-0.491266	-2.400605	6	2.838899	-0.316898	-2.382368
6	5.178652	0.523222	-0.452881	6	4.899088	0.881028	-0.406191
6	5.272562	-2.377060	1.521644	6	5.224885	-1.991861	1.572902
7	1.330032	1.632467	-1.033146	7	0.960596	1.636643	-1.034514
6	1.885566	2.789941	-0.425509	6	1.403641	2.836598	-0.417370
6	2.551731	3.673736	-1.462788	6	1.999737	3.780674	-1.444125
8	-0.453729	1.050572	1.984793	8	-0.782871	0.893720	1.967697
6	-1.739849	3.745901	1.891954	6	-2.322487	3.462527	1.838393
6	-2.915676	3.611807	-0.303064	6	-3.472703	3.178852	-0.355907
7	-5.122534	-2.197823	-0.338345	6	-5.110499	-2.803874	-0.422001
1	-3.210565	-2.559455	1.444408	1	-3.196687	-2.915389	1.419326
1	-0.855840	-1.806182	1.252213	1	-0.944985	-1.935626	1.249944
1	-1.713897	-0.123540	-2.574752	1	-1.871236	-0.457885	-2.643133
1	-4.076836	-0.863643	-2.364476	1	-4.137831	-1.415368	-2.472411
1	2.475147	0.476512	-2.344438	1	2.228717	0.598797	-2.331109
1	3.953407	-0.413656	-2.911836	1	3.789230	-0.151584	-2.881006
1	2.397969	-1.243215	-2.907230	1	2.315257	-1.118605	-2.898083
1	2.727861	-2.578007	2.851568	1	2.687391	-2.457279	2.854035
1	1.690922	-1.177118	2.484148	1	1.547617	-1.137342	2.489287
1	1.302864	-2.787047	1.844595	1	1.295249	-2.764056	1.825618
1	4.258580	-0.493527	1.698525	1	4.032801	-0.213641	1.730254
1	5.215593	-1.574078	-0.923074	1	5.124025	-1.204205	-0.876253
1	2.640034	2.546766	0.363423	1	2.168212	2.658671	0.379437
1	1.143557	3.411151	0.113738	1	0.603357	3.387274	0.115505
1	2.970589	4.579366	-1.022083	1	2.329758	4.718808	-0.995963
1	3.355313	3.135328	-1.967504	1	2.854586	3.318396	-1.939912
1	1.824605	3.959964	-2.221218	1	1.259046	4.002889	-2.210840
1	1.456997	0.418804	0.722045	1	1.186573	0.434885	0.717496
1	0.481357	-0.262204	-1.896535	1	0.298228	-0.325316	-1.910401
1	5.415688	0.823385	-1.470830	1	5.122973	1.202745	-1.420522
1	4.492573	1.255279	-0.032174	1	4.147985	1.551071	0.006792
1	6.106025	0.531883	0.118808	1	5.814721	0.967474	0.177782
1	5.052174	-2.688060	2.540695	1	5.020296	-2.319786	2.589926
1	5.270595	-3.258364	0.883147	1	5.314974	-2.870918	0.937705
1	6.274421	-1.950310	1.521542	1	6.182049	-1.472724	1.585243
1	-3.758110	4.190938	0.071291	1	-4.366936	3.680680	0.009784
1	-2.188334	4.292485	-0.740444	1	-2.813869	3.918558	-0.805667

1	-3.273121	2.945701	-1.086034	1	-3.763731	2.467548	-1.126434
1	-2.552204	4.349438	2.295170	1	-3.192967	3.981644	2.237846
1	-1.284103	3.186643	2.702509	1	-1.808032	2.965099	2.654142
1	-0.996423	4.416365	1.463994	1	-1.655148	4.202774	1.400028
1	-4.147851	2.351131	1.772957	1	-4.581801	1.829805	1.728197
1	-3.613730	1.136005	0.611991	1	-3.913966	0.653838	0.596501
1	-2.836662	1.242927	2.198038	1	-3.166999	0.871345	2.184659
8	-5.877509	-1.927521	-1.243115	7	-6.162765	-3.265727	-0.344423
8	-5.430719	-2.812705	0.655992				
NImag = 1 (-22.5434 cm ⁻¹)				NImag = 1 (-21.7134cm ⁻¹)			
TSr_{trans}(COOMe)				TSr_{trans}(Cl)			
Et = -1476.7277996				Et = -1708.5301982			
Gsol = -1477.085425				Gsol = -1708.853769			
7	3.405675	-1.146184	-1.072240	7	3.165421	-0.800491	-1.009393
6	2.511499	-1.569527	-0.216027	6	2.314158	-1.366141	-0.191841
7	3.045452	-2.015759	0.923590	7	2.866684	-1.744954	0.963485
6	4.443609	-1.603605	0.977067	6	4.184281	-1.129208	1.073964
6	4.735079	-1.180952	-0.477054	6	4.462847	-0.647463	-0.364277
8	1.237580	-1.670681	-0.429189	8	1.077063	-1.649487	-0.451679
6	0.489637	-0.455349	-0.817397	6	0.181859	-0.548080	-0.871425
6	1.097800	0.783629	-0.106295	6	0.581490	0.761239	-0.138989
7	1.700676	1.554662	-1.089853	7	1.053154	1.632004	-1.110069
6	2.371213	2.674957	-0.532188	6	1.529801	2.841070	-0.537951
6	3.083583	3.465892	-1.613081	6	2.108611	3.748918	-1.606534
6	2.251960	-2.147828	2.123013	6	2.052234	-1.996010	2.130282
6	5.367596	-2.684053	1.489884	6	5.239734	-2.067404	1.612512
6	5.458876	0.142789	-0.581475	6	4.987783	0.769335	-0.428903
6	3.147533	-0.741356	-2.439464	6	2.902850	-0.421063	-2.383740
6	-0.951651	-0.796482	-0.596388	6	-1.206089	-1.085731	-0.715462
6	-1.873075	-0.466600	-1.582800	6	-2.120234	-0.883289	-1.740340
6	-3.215161	-0.757331	-1.421082	6	-3.419268	-1.351206	-1.641367
6	-3.649461	-1.394309	-0.265012	6	-3.800602	-2.039019	-0.503222
6	-2.733729	-1.716351	0.729733	6	-2.909441	-2.245184	0.536149
6	-1.396738	-1.413726	0.567864	6	-1.618946	-1.760482	0.426755
6	-5.067920	-1.749460	-0.041320	17	-5.416680	-2.648829	-0.374403
6	0.056488	1.449382	0.821608	6	-0.558062	1.227461	0.794946
8	0.013234	1.230398	2.009154	8	-0.589817	0.941911	1.969588
8	-0.746115	2.271716	0.169510	8	-1.457675	1.960648	0.165952
6	-1.757635	3.048863	0.845417	6	-2.573967	2.563913	0.854462
6	-2.399282	3.825363	-0.289024	6	-3.299818	3.296769	-0.257932
6	-2.776959	2.140015	1.508995	6	-3.470877	1.499244	1.460525
6	-1.110407	3.996866	1.839687	6	-2.073178	3.546092	1.899120
1	-3.091776	-2.200237	1.625263	1	-3.227327	-2.772300	1.421862
1	-0.694677	-1.648497	1.351421	1	-0.931011	-1.900597	1.244887

1	-1.533234	0.027597	-2.481209	1	-1.815339	-0.344532	-2.625635
1	-3.925710	-0.502824	-2.191233	1	-4.125679	-1.193842	-2.441170
1	2.708278	0.267942	-2.400713	1	2.317991	0.512032	-2.358639
1	4.090455	-0.759523	-2.977928	1	3.858342	-0.294490	-2.884137
1	2.471215	-1.454166	-2.905675	1	2.358081	-1.220112	-2.881362
1	2.846948	-2.652483	2.877115	1	2.686759	-2.394386	2.915133
1	1.927048	-1.174916	2.495917	1	1.559551	-1.085399	2.475789
1	1.381937	-2.759315	1.911478	1	1.301506	-2.740503	1.889503
1	4.508035	-0.721765	1.621778	1	4.092020	-0.257098	1.728420
1	5.308352	-1.963454	-0.982002	1	5.163073	-1.330371	-0.853367
1	3.123800	2.389650	0.245059	1	2.316037	2.673101	0.239932
1	1.702504	3.375418	0.006706	1	0.753699	3.417201	0.003555
1	3.592313	4.343674	-1.212125	1	2.464779	4.693773	-1.193604
1	3.822167	2.842855	-2.119711	1	2.941852	3.260788	-2.114150
1	2.363779	3.792542	-2.362205	1	1.348879	3.961572	-2.357257
1	1.792303	0.376254	0.689657	1	1.332740	0.462003	0.654064
1	0.663632	-0.282745	-1.872364	1	0.374652	-0.346634	-1.917730
1	5.690381	0.391089	-1.614589	1	5.218527	1.064431	-1.449811
1	4.849211	0.942744	-0.166684	1	4.253139	1.465734	-0.029927
1	6.400064	0.090054	-0.035159	1	5.905497	0.846021	0.153234
1	5.149061	-2.941469	2.524182	1	5.023212	-2.370346	2.634858
1	5.280477	-3.583825	0.883914	1	5.310428	-2.960873	0.995201
1	6.399504	-2.338155	1.451920	1	6.209243	-1.571483	1.618508
1	-3.187857	4.471577	0.093187	1	-4.171030	3.816252	0.137761
1	-1.657208	4.439014	-0.795475	1	-2.639662	4.023948	-0.725912
1	-2.831733	3.142104	-1.017498	1	-3.629861	2.594604	-1.021018
1	-1.867408	4.660878	2.255789	1	-2.918190	4.082916	2.328884
1	-0.640594	3.449661	2.650451	1	-1.543484	3.033399	2.695477
1	-0.357345	4.606089	1.342455	1	-1.403902	4.272997	1.441655
1	-3.600707	2.739821	1.894951	1	-4.371937	1.967016	1.856023
1	-3.179449	1.433608	0.785118	1	-3.767125	0.778739	0.700263
1	-2.331772	1.586078	2.328528	1	-2.966272	0.973474	2.264116
8	-5.856964	-1.371204	-1.046269	NImag = 1 (-19.1262 cm ⁻¹)			
8	-5.479517	-2.318233	0.935056				
6	-7.227019	-1.683983	-0.885960	NImag = 1 (-21.3350 cm ⁻¹)			
1	-7.721069	-1.314385	-1.776807				
1	-7.365844	-2.757369	-0.791950	NImag = 1 (-21.3350 cm ⁻¹)			
1	-7.628478	-1.199586	-0.000327				
<p style="text-align: center;">TSr_{trans}(H) Et = -1248.9250258 Gsol = -1249.224276</p>				<p style="text-align: center;">TSr_{trans}(Me) Et = -1288.2354846 Gsol = -1288.539493</p>			
7	2.836672	-1.324460	0.925218	7	3.053737	-0.575994	-1.003156
6	2.233967	-1.040705	-0.233127				

7	2.935957	-0.240950	-0.995665	6	2.254845	-1.231609	-0.198734
6	4.137428	0.198167	-0.299033	7	2.829798	-1.555657	0.963099
6	3.940144	-0.388901	1.112425	6	4.069005	-0.798225	1.094700
8	1.115031	-1.609631	-0.549795	6	4.318626	-0.291108	-0.339808
6	-0.018126	-0.740276	-0.945001	8	1.059368	-1.641391	-0.476876
6	0.032518	0.582900	-0.134006	6	0.059386	-0.631751	-0.899389
7	0.301270	1.597575	-1.040924	6	0.321055	0.704162	-0.151932
6	0.454289	2.850410	-0.391285	7	0.694710	1.632648	-1.112065
6	0.819580	3.931839	-1.390528	6	1.033486	2.880829	-0.526956
6	2.620314	0.124205	-2.362208	6	1.527535	3.851506	-1.583055
6	4.303917	1.701207	-0.304288	6	2.026374	-1.889792	2.117264
6	5.184340	-1.032447	1.678890	6	5.211783	-1.612360	1.656180
6	2.081218	-1.828444	2.049283	6	4.696974	1.172082	-0.398663
6	-1.235312	-1.608626	-0.869343	6	2.771373	-0.220313	-2.379720
6	-1.482362	-2.457237	0.203007	6	-1.268819	-1.308215	-0.770237
6	-2.624966	-3.238090	0.229094	6	-2.200296	-1.149624	-1.786686
6	-3.541778	-3.168925	-0.808538	6	-3.446804	-1.746532	-1.703784
6	-3.311653	-2.310182	-1.871208	6	-3.793904	-2.530442	-0.610228
6	-2.161651	-1.538802	-1.901991	6	-2.859133	-2.676669	0.409838
6	-1.204722	0.702908	0.783717	6	-1.618251	-2.071015	0.337149
8	-1.190631	0.343742	1.938325	6	-5.124832	-3.215932	-0.538930
8	-2.241833	1.240920	0.168584	6	-0.857062	1.032415	0.792042
6	-3.484919	1.502815	0.852877	8	-0.853147	0.728267	1.962548
6	-3.261000	2.492617	1.983040	8	-1.833262	1.676649	0.178820
6	-4.343700	2.123098	-0.233145	6	-3.010931	2.127956	0.878980
6	-4.107280	0.208803	1.346607	6	-3.818781	2.796730	-0.217474
1	-4.432768	-3.779498	-0.786585	6	-3.775667	0.949917	1.455919
1	-2.803773	-3.897472	1.065910	6	-2.629326	3.136681	1.948300
1	-0.783189	-2.499333	1.022878	1	-3.110623	-3.268371	1.279542
1	-1.981613	-0.866651	-2.728682	1	-0.920144	-2.183914	1.151407
1	-4.022630	-2.246560	-2.682029	1	-1.949998	-0.541359	-2.644179
1	1.826450	0.885403	-2.321476	1	-4.157273	-1.607355	-2.507126
1	3.527318	0.500038	-2.826635	1	2.098403	0.650314	-2.363096
1	2.296234	-0.759876	-2.906326	1	3.715832	-0.000439	-2.868922
1	2.774765	-2.084360	2.843565	1	2.312322	-1.067186	-2.884504
1	1.358908	-1.092386	2.406919	1	2.687365	-2.207354	2.917065
1	1.556065	-2.729496	1.752535	1	1.425502	-1.039307	2.444428
1	3.593449	0.406183	1.779965	1	1.370067	-2.716575	1.869303
1	4.997483	-0.276863	-0.779949	1	3.869526	0.060134	1.743655
1	1.239179	2.833725	0.406436	1	5.092986	-0.898616	-0.816841
1	-0.451229	3.189647	0.149640	1	1.823923	2.792163	0.260363
1	0.925842	4.909332	-0.917750	1	0.194558	3.368676	0.007586
1	1.757817	3.689490	-1.891825	1	1.776884	4.826158	-1.160885
1	0.048415	3.997841	-2.156734	1	2.413977	3.456111	-2.081164
1	0.815274	0.429625	0.670436	1	0.759764	3.987757	-2.343416
1	0.144114	-0.437279	-1.971881	1	1.103890	0.479801	0.635986

1	4.490216	2.079259	-1.306817	1	0.245658	-0.401705	-1.940923
1	3.408670	2.184091	0.081816	1	4.918458	1.487797	-1.415517
1	5.155453	1.977741	0.316579	1	3.885748	1.789437	-0.018483
1	5.016478	-1.415279	2.683373	1	5.588978	1.344033	0.202808
1	5.513711	-1.854566	1.046370	1	5.010797	-1.935090	2.675660
1	5.986449	-0.298437	1.740324	1	5.392612	-2.494160	1.044480
1	-5.324912	2.381159	0.162184	1	6.120268	-1.012222	1.677901
1	-3.872984	3.024414	-0.620195	1	-4.746238	3.198767	0.187386
1	-4.472312	1.424641	-1.057689	1	-3.249985	3.608983	-0.665126
1	-4.220603	2.778516	2.412673	1	-4.060814	2.078894	-0.998705
1	-2.642263	2.060483	2.762753	1	-3.531486	3.559782	2.389123
1	-2.774780	3.390525	1.604904	1	-2.042120	2.670307	2.732681
1	-5.101931	0.413381	1.742191	1	-2.050198	3.948033	1.510217
1	-4.203246	-0.500449	0.526550	1	-4.730530	1.296207	1.850929
1	-3.503352	-0.240389	2.127833	1	-3.971742	0.213047	0.679121
NImag = 1 (-18.2252 cm ⁻¹)				1	-3.215924	0.474137	2.254088
				1	-5.867331	-2.706758	-1.149966
				1	-5.056023	-4.244076	-0.897483
				1	-5.498303	-3.253372	0.482874
				NImag = 1 (-18.6661 cm ⁻¹)			
TSr_{trans}(OMe)				TSr_{trans}(OH)			
Et = -1363.4107779				Et = -1324.1150318			
Gsol = -1363.737124				Gsol = -1324.449044			
7	3.165563	-0.842455	-1.023465	7	3.053393	-0.556137	-0.995042
6	2.343316	-1.365474	-0.147053	6	2.259720	-1.211677	-0.184391
7	2.931870	-1.661556	1.014058	7	2.833773	-1.513395	0.983003
6	4.245451	-1.029660	1.047456	6	4.066194	-0.743930	1.108287
6	4.474804	-0.625197	-0.423684	6	4.311720	-0.245778	-0.330487
8	1.104893	-1.678735	-0.350704	8	1.069804	-1.638957	-0.459325
6	0.191118	-0.614749	-0.828965	6	0.062933	-0.645513	-0.903449
6	0.596828	0.745291	-0.198483	6	0.306313	0.704598	-0.176099
7	0.954131	1.575349	-1.250347	7	0.635046	1.628616	-1.156264
6	1.418562	2.836215	-0.791271	6	0.954568	2.894250	-0.597803
6	1.883415	3.691079	-1.955211	6	1.411379	3.856305	-1.678307
6	2.146451	-1.836850	2.216061	6	2.027929	-1.841385	2.138279
6	5.325841	-1.928863	1.603248	6	5.215882	-1.543940	1.675975
6	4.964819	0.797188	-0.581711	6	4.667384	1.222665	-0.401410
6	2.861102	-0.548859	-2.410495	6	2.770756	-0.218539	-2.376317
6	-1.191225	-1.145627	-0.622332	6	-1.259930	-1.330907	-0.778328
6	-2.146596	-0.908058	-1.596108	6	-2.194943	-1.163599	-1.789099
6	-3.450855	-1.360496	-1.458323	6	-3.439075	-1.766635	-1.719706
6	-3.808506	-2.079751	-0.325858	6	-3.758973	-2.564361	-0.630311
6	-2.858116	-2.318514	0.663372	6	-2.835512	-2.734552	0.393118
6	-1.571365	-1.848232	0.518321				

8	-5.037828	-2.583821	-0.096740	6	-1.604772	-2.114201	0.318381
6	-0.482919	1.208900	0.803949	8	-4.946014	-3.197783	-0.513225
8	-0.427762	0.941539	1.982731	6	-0.860791	1.006504	0.789971
8	-1.437247	1.919290	0.232185	8	-0.833583	0.686033	1.956247
6	-2.517465	2.502257	0.989852	8	-1.855741	1.646208	0.203239
6	-3.333185	3.209625	-0.076149	6	-3.023122	2.079115	0.931908
6	-3.347032	1.421740	1.660202	6	-3.857865	2.753638	-0.140715
6	-1.972014	3.503805	1.993046	6	-3.766668	0.888618	1.510505
1	-3.157467	-2.870163	1.541359	6	-2.629051	3.079191	2.004850
1	-0.851806	-2.027644	1.301172	1	-3.102958	-3.348850	1.239037
1	-1.873025	-0.346061	-2.477629	1	-0.901837	-2.239920	1.126377
1	-4.165625	-1.156412	-2.239360	1	-1.951253	-0.542130	-2.638718
1	2.261892	0.374348	-2.433097	1	-4.154564	-1.625336	-2.519377
1	3.801863	-0.438819	-2.942120	1	2.083526	0.640808	-2.374492
1	2.317672	-1.384376	-2.845685	1	3.713609	0.012530	-2.863449
1	2.817496	-2.096397	3.028224	1	2.328960	-1.078093	-2.875089
1	1.592516	-0.930140	2.464691	1	2.691502	-2.095599	2.958230
1	1.449637	-2.656191	2.076040	1	1.383696	-1.007993	2.423784
1	4.166348	-0.123649	1.655711	1	1.415365	-2.708261	1.915553
1	5.179009	-1.318492	-0.892100	1	3.859400	0.117596	1.750530
1	2.265246	2.749057	-0.065209	1	5.097113	-0.844959	-0.799859
1	0.660083	3.418619	-0.232170	1	1.759064	2.836247	0.177762
1	2.229667	4.673635	-1.630919	1	0.113552	3.373090	-0.058802
1	2.697382	3.199334	-2.489700	1	1.645491	4.843611	-1.277291
1	1.064591	3.826087	-2.660572	1	2.298720	3.471048	-2.182606
1	1.421567	0.520222	0.545406	1	0.629617	3.962284	-2.429220
1	0.368984	-0.482071	-1.888677	1	1.110840	0.512085	0.598427
1	5.157739	1.040968	-1.623887	1	0.255624	-0.427088	-1.946293
1	4.226565	1.498683	-0.198381	1	4.885188	1.533293	-1.420646
1	5.897480	0.926094	-0.033456	1	3.846431	1.830888	-0.027333
1	5.138475	-2.182804	2.644622	1	5.555829	1.413645	0.199600
1	5.389911	-2.851587	1.029792	1	5.016097	-1.863092	2.696838
1	6.289827	-1.424078	1.558918	1	5.405870	-2.427505	1.069616
1	-4.189780	3.709961	0.372924	1	6.118661	-0.935155	1.695718
1	-2.724232	3.949994	-0.590670	1	-4.781376	3.141418	0.286444
1	-3.693135	2.493648	-0.812443	1	-3.305530	3.576828	-0.588994
1	-2.798935	4.025610	2.473771	1	-4.107665	2.043166	-0.926303
1	-1.380082	3.008444	2.755823	1	-3.525903	3.490847	2.466749
1	-1.349873	4.241264	1.488287	1	-2.024419	2.608933	2.773502
1	-4.231348	1.871171	2.111502	1	-2.063876	3.899390	1.565023
1	-3.671786	0.687531	0.925290	1	-4.716053	1.222052	1.928833
1	-2.778118	0.913727	2.431467	1	-3.973173	0.159081	0.729619
6	-6.034557	-2.346183	-1.048147	1	-3.187488	0.407474	2.291255
1	-6.934139	-2.818995	-0.668893	1	-5.493733	-2.989133	-1.270893
1	-6.218752	-1.278571	-1.177520				
1	-5.780479	-2.784996	-2.014314				

NImag = 1 (-22.0013 cm ⁻¹)				NImag = 1 (-17.6374 cm ⁻¹)			
TSr_{cis}(NO₂)				TSr_{cis}(CN)			
Et = -1453.336615				Et = -1341.1247115			
Gsol = -1453.690729				Gsol = -1341.441490			
7	0.024475	2.423439	0.763125	7	-0.527346	2.335293	0.731515
6	0.573033	1.949999	-0.349929	6	0.094779	1.945333	-0.375170
7	1.568933	2.714433	-0.770209	7	0.983743	2.840163	-0.780228
6	1.737804	3.862385	0.105612	6	0.973963	4.001462	0.094353
6	0.920790	3.431386	1.333484	6	0.215491	3.455567	1.312906
8	0.200810	0.960867	-1.092531	8	-0.124835	0.917990	-1.124991
6	-0.209249	-0.354827	-0.568872	6	-0.397529	-0.433534	-0.609342
6	0.689315	-0.701236	0.643829	6	0.505787	-0.678097	0.626755
7	0.126688	-1.691707	1.418969	7	0.023279	-1.707410	1.404917
6	0.955330	-1.997286	2.532366	6	0.845500	-1.907498	2.546625
6	0.256332	-2.965340	3.466917	6	0.222052	-2.926113	3.480877
6	2.475351	2.390600	-1.838000	6	1.952872	2.637883	-1.823034
6	1.249092	5.142974	-0.541939	6	0.310700	5.195561	-0.563319
6	1.777983	2.850626	2.440752	6	1.138187	2.992980	2.423281
6	-1.070797	1.868900	1.536630	6	-1.548573	1.639007	1.494429
6	-1.714406	-0.413506	-0.489741	6	-1.888495	-0.659661	-0.565743
6	-2.487289	0.512544	-1.188398	6	-2.745318	0.179374	-1.273606
6	-3.866489	0.420520	-1.201799	6	-4.104685	-0.068547	-1.318742
6	-4.464393	-0.620727	-0.518525	6	-4.623458	-1.178356	-0.660169
6	-3.720382	-1.569620	0.159350	6	-3.767105	-2.036303	0.026880
6	-2.341081	-1.472962	0.165469	6	-2.408392	-1.788027	0.066234
6	2.096513	-0.954169	0.030971	6	1.941673	-0.792183	0.039915
8	2.987188	-0.132714	0.064619	8	2.727939	0.130456	0.043815
8	2.197681	-2.153422	-0.513532	8	2.189685	-1.991590	-0.454307
6	3.432059	-2.652703	-1.072996	6	3.478637	-2.359319	-0.991864
6	3.849338	-1.810458	-2.266124	6	3.800372	-1.518493	-2.215114
6	4.510693	-2.700167	-0.005641	6	4.548580	-2.237236	0.078517
6	3.061159	-4.055019	-1.516097	6	3.281531	-3.811788	-1.381782
1	0.188443	5.072663	-0.778175	1	-0.726760	4.972119	-0.807067
1	1.396961	5.984722	0.132578	1	0.330518	6.053243	0.107035
1	1.791606	5.354553	-1.461181	1	0.824755	5.477543	-1.480003
1	0.317684	4.260399	1.700431	1	-0.499770	4.190256	1.679306
1	2.791460	3.947575	0.368469	1	2.000559	4.240967	0.368761
1	2.393079	2.037388	2.058017	1	1.866811	2.280401	2.039027
1	1.169043	2.458755	3.252728	1	0.585910	2.508567	3.225656
1	2.426182	3.624489	2.850095	1	1.665335	3.847634	2.845421
1	2.563345	3.234412	-2.518519	1	1.969559	3.501619	-2.483531
1	2.089175	1.536977	-2.380141	1	1.677578	1.760584	-2.394450
1	3.451019	2.133891	-1.432314	1	2.937857	2.477279	-1.390982
1	-0.904252	0.828138	1.812918	1	-1.268558	0.613508	1.736027
1	-2.002470	1.950564	0.986761	1	-2.490063	1.637882	0.954898

1	-1.151300	2.462827	2.441392	1	-1.681215	2.190681	2.419617
1	0.914026	0.248209	1.189954	1	0.626872	0.294464	1.165372
1	1.933439	-2.445669	2.256791	1	1.872065	-2.257100	2.306999
1	1.235358	-1.089411	3.115321	1	1.013170	-0.965298	3.118793
1	-0.682062	-2.535270	3.816258	1	-0.767134	-2.590592	3.791615
1	0.019212	-3.886946	2.936488	1	0.100184	-3.877459	2.964124
1	0.869805	-3.213348	4.334185	1	0.829635	-3.091535	4.371656
1	4.126518	-0.807906	-1.956609	1	3.950559	-0.478540	-1.943817
1	3.035544	-1.750504	-2.988258	1	2.991613	-1.585117	-2.942267
1	4.702840	-2.272957	-2.759943	1	4.708042	-1.892178	-2.686981
1	2.265937	-4.023725	-2.258582	1	2.489387	-3.904618	-2.122293
1	3.924598	-4.554111	-1.952488	1	4.199886	-4.218191	-1.802073
1	2.710480	-4.637782	-0.667405	1	3.003000	-4.401200	-0.511148
1	5.395824	-3.194014	-0.404924	1	5.486978	-2.643239	-0.297354
1	4.783101	-1.702442	0.322518	1	4.703749	-1.201810	0.363237
1	4.160417	-3.268315	0.854120	1	4.260111	-2.804426	0.961559
1	-1.698615	-2.157069	0.706606	1	-1.707203	-2.401912	0.617884
1	-4.224344	-2.370737	0.674446	1	-4.171987	-2.900279	0.531548
7	-5.912410	-0.720340	-0.524204	6	-6.028330	-1.435025	-0.698501
1	-4.476428	1.130811	-1.734621	1	-4.762901	0.587364	-1.867707
1	-2.013256	1.313115	-1.734843	1	-2.353314	1.034256	-1.803014
1	0.081519	-1.005425	-1.390378	1	-0.016357	-1.046116	-1.423151
8	-6.532945	0.136183	-1.113728	7	-7.162620	-1.634555	-0.729797
8	-6.415473	-1.650429	0.061500				
NImag = 1 (-16.7674 cm ⁻¹)				NImag = 1 (-12.9993 cm ⁻¹)			
TSr_{cis}(COOMe)				TSr_{cis}(Cl)			
Et = -1476.7214933				Et = -1708.5240001			
Gsol = -1477.073875				Gsol = -1708.842251			
6	-2.145515	-1.220639	0.162866	6	-2.338050	-1.709809	0.130025
6	-1.431440	-0.226340	-0.502202	6	-1.795602	-0.615097	-0.538706
6	-2.125838	0.749664	-1.215267	6	-2.641935	0.215275	-1.265628
6	-3.507623	0.763615	-1.228472	6	-4.010277	-0.003437	-1.293540
6	-4.218800	-0.210492	-0.540983	6	-4.531559	-1.078486	-0.598858
6	-3.528713	-1.201991	0.147644	6	-3.703935	-1.934311	0.106695
6	0.073860	-0.290446	-0.578224	6	-0.301020	-0.416302	-0.598971
6	0.949926	-0.690207	0.637168	6	0.615012	-0.663085	0.627905
6	2.310749	-1.115317	0.016031	6	2.039421	-0.811003	0.021612
8	2.274240	-2.338962	-0.483966	8	2.264057	-2.025972	-0.447180
6	3.435645	-2.978568	-1.053500	6	3.537730	-2.420207	-0.999852
6	2.912470	-4.347628	-1.444319	6	3.317317	-3.878911	-1.352757
6	-5.694360	-0.146616	-0.584397	17	-6.243452	-1.360868	-0.624746
8	0.592720	0.983519	-1.110762	8	-0.012411	0.932611	-1.119536
6	1.017991	1.950667	-0.370681	6	0.204468	1.961012	-0.372866
7	0.495789	2.462883	0.738044	7	-0.412796	2.353689	0.736146

6	1.449206	3.418802	1.304081	6	0.327723	3.481023	1.305943
6	2.291677	3.795142	0.075895	6	1.071696	4.026748	0.079027
7	2.062864	2.650699	-0.789447	7	1.091016	2.857675	-0.783285
6	-0.621872	1.967622	1.523115	6	-1.419193	1.653787	1.516927
6	2.952400	2.263151	-1.850013	6	2.042840	2.662873	-1.842050
6	1.873272	5.094528	-0.583668	6	0.388980	5.206819	-0.584500
6	2.271577	2.794899	2.414773	6	1.264015	3.029322	2.409621
7	0.300157	-1.576855	1.467590	7	0.127086	-1.670215	1.431676
6	1.115728	-1.916546	2.579822	6	0.962423	-1.861526	2.564544
6	0.338421	-2.759261	3.572510	6	0.336463	-2.850980	3.528238
8	3.284109	-0.393791	0.002444	8	2.837721	0.100444	-0.012430
6	3.908003	-2.220320	-2.282381	6	3.846374	-1.611646	-2.248135
6	4.530615	-3.106941	-0.009448	6	4.629450	-2.286415	0.047083
1	0.810797	5.078391	-0.821495	1	-0.646811	4.967620	-0.820406
1	2.064654	5.933307	0.083661	1	0.401024	6.070181	0.078777
1	2.427758	5.268184	-1.503771	1	0.894372	5.487830	-1.506303
1	0.895653	4.283188	1.667650	1	-0.388924	4.212373	1.676419
1	3.347673	3.827077	0.341602	1	2.096751	4.282485	0.344753
1	2.842379	1.948480	2.035451	1	1.994072	2.320497	2.021243
1	1.640890	2.436868	3.225624	1	0.722667	2.543078	3.218234
1	2.960199	3.533146	2.824024	1	1.789026	3.889036	2.824156
1	3.091886	3.091625	-2.540948	1	1.965923	3.466501	-2.571493
1	2.519228	1.426212	-2.382401	1	1.836908	1.718082	-2.327893
1	3.910908	1.954981	-1.438684	1	3.049701	2.628198	-1.432459
1	-0.509358	0.918470	1.799294	1	-1.127930	0.631965	1.761513
1	-1.551252	2.097220	0.978978	1	-2.366526	1.640072	0.988190
1	-0.662188	2.568422	2.426189	1	-1.544464	2.212420	2.439141
1	1.288024	0.251488	1.138761	1	0.763309	0.315711	1.150128
1	2.035487	-2.479320	2.311610	1	1.979958	-2.233080	2.317951
1	1.503510	-1.017070	3.113603	1	1.154667	-0.911010	3.115973
1	-0.543877	-2.216483	3.910969	1	-0.641690	-2.492076	3.847851
1	-0.003120	-3.675886	3.092743	1	0.189342	-3.809356	3.031402
1	0.939028	-3.027077	4.443117	1	0.955337	-3.010569	4.412442
1	4.292784	-1.242110	-2.012592	1	4.013314	-0.567629	-2.003613
1	3.087087	-2.098981	-2.988575	1	3.023201	-1.685295	-2.958255
1	4.697597	-2.782895	-2.778910	1	4.740693	-2.006928	-2.728017
1	2.105685	-4.255711	-2.169117	1	2.509510	-3.979077	-2.075178
1	3.708984	-4.945276	-1.884510	1	4.222653	-4.305404	-1.781464
1	2.525707	-4.866683	-0.570263	1	3.049089	-4.445296	-0.463764
1	5.351155	-3.698932	-0.413421	1	5.555332	-2.714345	-0.335625
1	4.910552	-2.133601	0.282894	1	4.803121	-1.246411	0.302995
1	4.146116	-3.612897	0.874237	1	4.349800	-2.827473	0.949188
1	-1.568628	-1.948876	0.717456	1	-1.649866	-2.324998	0.696216
1	-4.080069	-1.962901	0.677390	1	-4.125562	-2.773789	0.637697
1	-4.052580	1.518896	-1.773940	1	-4.661504	0.647408	-1.856000
1	-1.586619	1.503323	-1.768897	1	-2.240180	1.046768	-1.825122

1	0.312590	-0.965412	-1.396833	1	0.066258	-1.031300	-1.417128
8	-6.273955	-1.140414	0.088453				
8	-6.322978	0.704430	-1.158916				
6	-7.687162	-1.129285	0.081211				
1	-7.992872	-1.989751	0.664881				
1	-8.065853	-0.213983	0.527768				
1	-8.065995	-1.205746	-0.934253				
	NImag = 1 (-15.7331 cm ⁻¹)				NImag = 1 (-19.5636 cm ⁻¹)		
	TSr_{cis}(Me)				TSr_{cis}(OMe)		
	Et = -1288.2277244				Et = -1363.4036212		
	Gsol = -1288.524233				Gsol = -1363.724918		
6	-2.133259	-2.274340	0.039437	6	-2.438408	-1.482189	0.052374
6	-1.816382	-1.089087	-0.621700	6	-1.795514	-0.451329	-0.621239
6	-2.799096	-0.470350	-1.385290	6	-2.566712	0.416712	-1.392214
6	-4.082183	-0.993244	-1.452838	6	-3.941089	0.295171	-1.449135
6	-4.415347	-2.157644	-0.776674	6	-4.578672	-0.722283	-0.748481
6	-3.416128	-2.785181	-0.038117	6	-3.818310	-1.613192	-0.003309
6	-0.401617	-0.565775	-0.636747	6	-0.290798	-0.356313	-0.644376
6	0.514842	-0.603010	0.613387	6	0.579543	-0.650469	0.606593
6	1.954878	-0.442488	0.048355	6	1.994890	-0.944518	0.036387
8	2.433219	-1.575988	-0.437561	8	2.110027	-2.184035	-0.411640
6	3.775240	-1.693139	-0.952765	6	3.348920	-2.704854	-0.934854
6	3.861821	-3.155897	-1.345262	6	2.996903	-4.140376	-1.276642
6	-5.800272	-2.727892	-0.838395	8	-5.924190	-0.764597	-0.859008
8	-0.402115	0.821784	-1.148297	8	0.101730	0.973988	-1.155557
6	-0.434409	1.864658	-0.392679	6	0.353184	1.986794	-0.400900
7	-1.163709	2.109399	0.691139	7	-0.275106	2.417383	0.687673
6	-0.690755	3.354548	1.298393	6	0.508793	3.501348	1.281316
6	-0.025374	4.058095	0.106565	6	1.332819	3.995332	0.083607
7	0.259406	2.932367	-0.765640	7	1.306256	2.828868	-0.780943
6	-2.019213	1.198163	1.432138	6	-1.337110	1.770787	1.442056
6	1.276766	2.948313	-1.780463	6	2.286613	2.567585	-1.798752
6	-0.906722	5.089169	-0.570916	6	0.753855	5.218185	-0.600991
6	0.273455	3.087695	2.437711	6	1.371086	3.004806	2.425537
7	0.244138	-1.686341	1.420862	7	-0.005240	-1.580955	1.439188
6	1.080419	-1.678707	2.567961	6	0.797998	-1.799915	2.589148
6	0.666672	-2.770219	3.536278	6	0.078508	-2.694607	3.580178
8	2.557632	0.608936	0.061531	8	2.880399	-0.117947	0.009492
6	3.954033	-0.804740	-2.172148	6	3.756126	-1.945727	-2.186220
6	4.786468	-1.374211	0.134218	6	4.429759	-2.663280	0.131000
1	-1.862228	4.649329	-0.852327	1	-0.285423	5.045781	-0.876501
1	-1.095803	5.923498	0.102704	1	0.796290	6.078421	0.065234
1	-0.434501	5.485410	-1.467713	1	1.310312	5.467173	-1.502466
1	-1.554864	3.920506	1.643107	1	-0.176475	4.277285	1.619350

1	0.916906	4.509107	0.415767	1	2.361899	4.183597	0.387919
1	1.145896	2.544973	2.076534	1	2.072829	2.249913	2.073786
1	-0.189866	2.492618	3.221706	1	0.769740	2.559111	3.214802
1	0.597507	4.030696	2.876513	1	1.929479	3.835774	2.855002
1	1.096599	3.763357	-2.478209	1	2.332241	3.400494	-2.497063
1	1.250777	2.008659	-2.317010	1	2.004953	1.669671	-2.333494
1	2.257494	3.058543	-1.323383	1	3.262324	2.408296	-1.345075
1	-1.504173	0.282954	1.725632	1	-1.101161	0.737034	1.699868
1	-2.893760	0.941028	0.844567	1	-2.266913	1.797492	0.883700
1	-2.340956	1.726942	2.324049	1	-1.462957	2.343303	2.355878
1	0.433295	0.388183	1.128266	1	0.807310	0.328309	1.100996
1	2.159786	-1.822542	2.344364	1	1.782912	-2.266875	2.372306
1	1.052288	-0.702967	3.109217	1	1.066536	-0.849049	3.108577
1	-0.371721	-2.628134	3.835231	1	-0.868795	-2.241094	3.871494
1	0.738642	-3.742569	3.050067	1	-0.145391	-3.654875	3.116654
1	1.289531	-2.783504	4.432136	1	0.671091	-2.873253	4.478821
1	3.905334	0.244312	-1.898848	1	4.018644	-0.919559	-1.950345
1	3.180833	-1.018155	-2.909660	1	2.941127	-1.948332	-2.909430
1	4.921401	-1.003057	-2.632069	1	4.615686	-2.431359	-2.646624
1	3.115353	-3.392899	-2.101079	1	2.199000	-4.171668	-2.016173
1	4.848167	-3.382598	-1.746701	1	3.866143	-4.657540	-1.679690
1	3.680510	-3.789327	-0.479857	1	2.656082	-4.666344	-0.387654
1	5.791378	-1.586873	-0.229127	1	5.320008	-3.175675	-0.232370
1	4.731828	-0.330676	0.426351	1	4.690938	-1.641074	0.384251
1	4.600838	-1.993124	1.010163	1	4.086026	-3.170381	1.030766
1	-1.351973	-2.727534	0.634589	1	-1.818893	-2.136286	0.651410
1	-3.646565	-3.699761	0.492488	1	-4.284352	-2.417671	0.543592
1	-4.829652	-0.489130	-2.050840	1	-4.539354	0.971546	-2.040781
1	-2.570388	0.427772	-1.940106	1	-2.093062	1.204580	-1.959415
1	0.117269	-1.074845	-1.445361	1	0.061970	-0.988430	-1.455782
1	-6.282599	-2.702564	0.139309	6	-6.605150	-1.778797	-0.179131
1	-6.429025	-2.173129	-1.532009	1	-7.658223	-1.636845	-0.398638
1	-5.785322	-3.768627	-1.161057	1	-6.298607	-2.768274	-0.521593
				1	-6.452438	-1.712775	0.899244
	NImag = 1 (-19.3401 cm ⁻¹)				NImag = 1 (-12.1593 cm ⁻¹)		
	TSr_{cis}(OH) Et = -1324.1082491 Gsol = -1324.436972				TSf3-(NO₂) Et = -1453.3406178 Gsol = -1453.693049		
6	-1.988932	-2.397464	0.026349	6	1.216578	-1.993872	-0.649372
6	-1.739643	-1.201941	-0.641607	6	1.000306	-1.036075	0.340317
6	-2.755583	-0.651401	-1.417725	6	2.061576	-0.666352	1.172914
6	-4.006332	-1.238803	-1.492065	6	3.306671	-1.238877	1.011075
6	-4.251550	-2.415287	-0.800590	6	3.488847	-2.195618	0.026741
6	-3.236827	-2.990661	-0.048819	6	2.458454	-2.578671	-0.809067

6	-0.360500	-0.592189	-0.650831	6	-0.339658	-0.404157	0.545705
6	0.549911	-0.581897	0.604607	6	-0.384958	1.115598	0.767955
6	1.978288	-0.326767	0.046632	7	0.027408	1.235964	2.092841
8	2.539312	-1.428870	-0.422573	6	-1.070074	1.127348	2.995273
6	3.886730	-1.453411	-0.936297	6	-1.916448	2.397634	3.108873
6	4.080628	-2.910454	-1.311623	8	-1.194641	-0.854206	-0.720537
8	-5.486872	-2.957839	-0.897915	6	-2.460744	-0.846128	-0.606584
8	-0.448948	0.797808	-1.148458	7	-3.152086	-1.543231	0.300460
6	-0.562876	1.828935	-0.385045	6	-4.581226	-1.377729	0.082848
7	-1.311337	2.010457	0.697941	6	-4.638435	-0.236561	-0.948041
6	-0.946690	3.289561	1.308389	7	-3.259892	-0.138634	-1.397308
6	-0.329005	4.046007	0.123630	6	-2.633369	-2.689637	1.003025
7	0.051464	2.948187	-0.746917	6	-2.803810	0.911015	-2.274986
6	-2.102071	1.036096	1.431117	6	-5.619337	-0.474630	-2.073584
6	1.054627	3.052277	-1.769896	6	-5.342716	-1.089924	1.357306
6	-1.281755	5.007729	-0.559615	6	0.460222	1.819128	-0.286099
6	0.024016	3.102100	2.458097	8	1.533322	2.394762	0.201406
7	0.342942	-1.685358	1.405331	6	2.469482	3.110168	-0.637284
6	1.164494	-1.625917	2.561554	6	3.512328	3.583424	0.357376
6	0.815856	-2.746702	3.522020	8	0.144811	1.821319	-1.456126
8	2.502326	0.765946	0.046766	6	3.091469	2.172078	-1.656174
6	4.001825	-0.568968	-2.166160	6	1.785861	4.296762	-1.293601
6	4.871014	-1.048848	0.146876	7	4.789938	-2.813155	-0.133036
1	-2.198002	4.496980	-0.851852	1	2.637501	-3.319452	-1.570368
1	-1.541326	5.822592	0.114397	1	0.416573	-2.275706	-1.312873
1	-0.832872	5.442808	-1.450387	1	1.856869	0.085047	1.925291
1	-1.857433	3.783133	1.644173	1	4.134125	-0.961425	1.643054
1	0.572217	4.569097	0.441848	1	-2.669641	-2.538966	2.078917
1	0.943251	2.635837	2.106477	1	-3.220912	-3.571597	0.745982
1	-0.396136	2.468252	3.235895	1	-1.604765	-2.864316	0.705435
1	0.262791	4.067903	2.901870	1	-3.059727	0.681220	-3.306902
1	0.761226	3.786487	-2.517768	1	-3.279514	1.849652	-1.991549
1	1.172180	2.086193	-2.242982	1	-1.727924	1.028003	-2.171385
1	2.005903	3.336375	-1.325845	1	-4.890292	0.698768	-0.438163
1	-1.526191	0.154263	1.713392	1	-4.961420	-2.298511	-0.372230
1	-2.960523	0.728015	0.844009	1	-0.685926	0.890048	3.991345
1	-2.454551	1.532926	2.329761	1	-1.778821	0.293452	2.760015
1	0.403250	0.398400	1.125806	1	-2.742220	2.278149	3.814632
1	2.253260	-1.695479	2.349000	1	-1.291597	3.224439	3.441613
1	1.064363	-0.656351	3.105409	1	-2.343167	2.679614	2.144423
1	-0.232880	-2.676731	3.810576	1	-1.419419	1.438944	0.526339
1	0.959224	-3.710085	3.033691	1	-0.896551	-0.843330	1.364516
1	1.428624	-2.720979	4.424505	1	-5.297576	-1.931969	2.045174
1	3.879343	0.477240	-1.905434	1	-4.932193	-0.214559	1.856818
1	3.245408	-0.845154	-2.900211	1	-6.392188	-0.905136	1.132672
1	4.980559	-0.704310	-2.624848	1	-5.634439	0.363636	-2.766859

1	3.353636	-3.210524	-2.063986	1	-5.361270	-1.376103	-2.626626
1	5.081012	-3.068580	-1.711197	1	-6.625706	-0.589351	-1.673924
1	3.946414	-3.545404	-0.438771	1	4.286204	4.155232	-0.151746
1	5.889079	-1.193209	-0.213293	1	3.053566	4.212034	1.117576
1	4.741056	-0.008273	0.425153	1	3.975865	2.733978	0.854292
1	4.729301	-1.668091	1.030764	1	2.529891	4.905538	-1.805625
1	-1.183772	-2.796771	0.629648	1	1.042853	3.973689	-2.015314
1	-3.420607	-3.913899	0.486888	1	1.302328	4.915573	-0.539236
1	-4.794088	-0.805759	-2.089574	1	3.887460	2.691706	-2.188105
1	-2.577456	0.254892	-1.977682	1	3.524965	1.308146	-1.155574
1	0.194364	-1.055198	-1.463281	1	2.355462	1.828775	-2.375473
1	-5.512410	-3.767924	-0.387190	8	4.915675	-3.647660	-1.001584
				8	5.676823	-2.459388	0.610023
NImag = 1 (-25.3303 cm ⁻¹)				NImag = 1 (-196.0943 cm ⁻¹)			
TSf3-(CN)				TSf3-(COOMe)			
Et = -1341.1284062				Et = -1476.7244059			
Gsol = -1341.444553				Gsol = -1477.076406			
7	3.067030	-0.136136	-1.392191	7	-3.408814	-0.578388	-1.440855
6	2.345130	0.675131	-0.627895	6	-2.534076	-1.105413	-0.590254
7	3.104247	1.328174	0.257431	7	-3.137659	-1.847820	0.343694
6	4.508931	1.010739	0.048960	6	-4.568009	-1.915619	0.088614
6	4.448985	-0.163234	-0.944220	6	-4.768146	-0.858572	-1.011511
8	1.086155	0.809145	-0.747159	8	-1.279731	-0.923728	-0.676016
6	0.189961	0.503902	0.524961	6	-0.544646	-0.286510	0.582358
6	0.056993	-1.004816	0.791606	6	-0.842732	1.216186	0.713016
6	-0.861014	-1.632745	-0.248445	6	-0.072021	1.988172	-0.348849
8	-0.524094	-1.750588	-1.406769	8	-0.380684	1.943936	-1.520333
6	2.707408	2.544719	0.920193	6	-2.470545	-2.863690	1.118254
6	5.238635	0.689789	1.333842	6	-5.400446	-1.674630	1.327919
6	5.446490	-0.059219	-2.075717	6	-5.670434	-1.310339	-2.137527
6	2.506021	-1.161906	-2.236908	6	-3.092914	0.481785	-2.366452
6	-1.067152	1.284650	0.301307	6	0.882894	-0.715047	0.450971
6	-1.182095	2.219024	-0.725081	6	1.286839	-1.654031	-0.495205
6	-2.348702	2.940205	-0.897702	6	2.610467	-2.047480	-0.578881
6	-3.426012	2.734295	-0.043354	6	3.555152	-1.506596	0.282176
6	-3.322049	1.792532	0.979831	6	3.156677	-0.561626	1.222638
6	-2.153943	1.080519	1.156390	6	1.836574	-0.171318	1.316301
6	-4.628466	3.485115	-0.215484	6	4.978598	-1.895826	0.240257
7	-0.370436	-1.046115	2.117364	7	-0.517618	1.484490	2.041322
6	0.730456	-1.046753	3.021859	6	-1.621665	1.244652	2.908300
6	1.419049	-2.405780	3.171294	6	-2.674744	2.356478	2.906503
8	-2.022534	-2.005769	0.234269	8	0.939327	2.671526	0.132300
6	-3.040764	-2.609799	-0.595440	6	1.813449	3.449616	-0.714913
6	-2.541984	-3.930731	-1.154015	6	1.032357	4.566425	-1.384666

6	-4.174385	-2.841554	0.385403	6	2.814391	4.018830	0.272621
6	-3.473886	-1.651150	-1.690622	6	2.512756	2.554985	-1.723421
1	-2.428501	3.661454	-1.696581	1	2.912643	-2.773995	-1.316577
1	-0.362973	2.376317	-1.406703	1	0.568930	-2.070477	-1.182223
1	-2.032022	0.337358	1.934924	1	1.491766	0.563920	2.031511
1	-4.159226	1.628671	1.641233	1	3.900151	-0.145334	1.885360
1	2.732622	2.427776	2.000571	1	-2.556196	-2.663819	2.183278
1	3.381116	3.352676	0.632883	1	-2.912831	-3.836571	0.900675
1	1.700841	2.813514	0.617500	1	-1.420171	-2.895989	0.848198
1	2.775336	-0.987505	-3.276276	1	-3.263486	0.156201	-3.390301
1	2.892243	-2.132991	-1.928149	1	-3.726982	1.343108	-2.157426
1	1.424620	-1.172549	-2.124912	1	-2.056513	0.782721	-2.234364
1	4.606446	-1.102735	-0.405102	1	-5.172690	0.055712	-0.565723
1	4.980020	1.872438	-0.435858	1	-4.791659	-2.908361	-0.316629
1	0.375781	-0.740779	4.010347	1	-1.250423	1.137918	3.931800
1	1.535127	-0.309762	2.771322	1	-2.171289	0.289337	2.708286
1	2.250036	-2.369365	3.880261	1	-3.500401	2.142172	3.590158
1	0.698010	-3.143916	3.517876	1	-2.213028	3.296723	3.202752
1	1.813361	-2.759227	2.216601	1	-3.098444	2.501720	1.910806
1	1.047586	-1.451346	0.562772	1	-1.903208	1.351972	0.410697
1	0.792237	0.895887	1.335827	1	-1.052462	-0.761910	1.412776
1	5.281270	1.555111	1.992314	1	-5.246676	-2.458424	2.066988
1	4.740963	-0.121079	1.862169	1	-5.141641	-0.719417	1.780504
1	6.263100	0.390526	1.117385	1	-6.459141	-1.666605	1.072508
1	5.376900	-0.915103	-2.743775	1	-5.792799	-0.527832	-2.883463
1	5.278308	0.846643	-2.655535	1	-5.263486	-2.193695	-2.626559
1	6.460118	-0.033356	-1.678721	1	-6.658772	-1.552921	-1.750018
1	-5.016615	-3.314167	-0.116896	1	3.536488	4.649213	-0.243566
1	-3.845514	-3.482570	1.200421	1	2.305203	4.613016	1.028318
1	-4.506938	-1.896612	0.809654	1	3.348291	3.215298	0.775277
1	-3.357559	-4.440462	-1.665304	1	1.720131	5.223179	-1.916070
1	-1.729962	-3.777086	-1.857154	1	0.310272	4.170261	-2.091235
1	-2.194163	-4.572042	-0.345594	1	0.507587	5.158015	-0.636034
1	-4.339548	-2.062524	-2.208215	1	3.269760	3.131727	-2.253807
1	-3.759261	-0.692980	-1.259845	1	3.007690	1.730257	-1.213675
1	-2.678914	-1.489105	-2.410810	1	1.810232	2.150799	-2.444630
7	-5.597512	4.092504	-0.356309	8	5.238307	-2.804869	-0.703562
NImag = 1 (-167.8267 cm ⁻¹)				8	5.830040	-1.455151	0.967008
				6	6.589459	-3.209479	-0.788899
				1	6.631249	-3.936980	-1.591406
				1	7.230845	-2.361411	-1.012425
				1	6.916204	-3.656942	0.145823
				NImag = 1 (-175.1655 cm ⁻¹)			
TSf3-(Cl)				TSf3-(H)			

Et = -1708.5272321 Gsol = -1708.845828				Et = -1248.9207266 Gsol = -1249.215831			
7	-3.144650	0.078647	-1.392548	7	3.048943	0.976663	0.162036
6	-2.386720	-0.706482	-0.635050	6	2.186081	0.381420	-0.667266
7	-3.115238	-1.401894	0.242982	7	2.750507	-0.626393	-1.325255
6	-4.532285	-1.142594	0.041720	6	4.095755	-0.863036	-0.829663
6	-4.524925	0.042520	-0.940027	6	4.371669	0.389636	0.019839
8	-1.122986	-0.783143	-0.754845	8	0.975336	0.730551	-0.827714
6	-0.248867	-0.452961	0.516872	6	0.039147	0.725352	0.446238
6	-0.187005	1.058789	0.789652	6	-0.378494	-0.706154	0.821733
6	0.713640	1.724870	-0.240705	6	-1.412433	-1.204167	-0.176329
8	0.369750	1.862460	-1.395219	8	-1.106521	-1.541761	-1.300168
6	-2.660912	-2.603637	0.895717	6	2.008620	-1.628359	-2.050777
6	-5.270101	-0.863239	1.331915	6	5.106774	-1.093026	-1.930006
6	-5.521230	-0.090890	-2.069427	6	5.033772	0.096623	1.347357
6	-2.630334	1.142835	-2.219463	6	2.873665	2.309706	0.680415
6	1.043205	-1.177855	0.296669	6	-1.038847	1.720509	0.142708
6	1.226333	-2.066360	-0.756698	6	-2.088457	1.873234	1.051225
6	2.428486	-2.735950	-0.924365	6	-3.095733	2.787489	0.799976
6	3.457772	-2.512737	-0.031164	6	-3.074086	3.570876	-0.345024
6	3.301375	-1.624512	1.020017	6	-2.036024	3.421924	-1.247194
6	2.097911	-0.965191	1.186518	6	-1.025119	2.502621	-1.007454
17	4.961181	-3.356868	-0.228309	7	-0.793789	-0.589318	2.148581
7	0.223676	1.128956	2.121110	6	0.301012	-0.737233	3.047404
6	-0.887781	1.072533	3.010344	6	0.733568	-2.188520	3.278848
6	-1.652523	2.392437	3.145902	8	-2.638167	-1.200470	0.293389
8	1.873892	2.102891	0.242202	6	-3.771686	-1.569420	-0.520307
6	2.883588	2.722840	-0.584152	6	-3.898820	-0.633352	-1.709832
6	2.376122	4.049301	-1.121744	6	-3.662925	-3.023804	-0.943737
6	4.021959	2.945922	0.393428	6	-4.939169	-1.378543	0.429546
6	3.315920	1.781713	-1.694977	1	-3.859597	4.289231	-0.531450
1	2.563224	-3.422153	-1.745924	1	-2.008682	4.018363	-2.148007
1	0.434481	-2.233393	-1.468411	1	-0.233057	2.386397	-1.729292
1	1.932455	-0.250641	1.983537	1	-2.085485	1.230111	1.921266
1	4.114667	-1.455044	1.708695	1	-3.903351	2.891253	1.510724
1	-2.686820	-2.495086	1.976942	1	2.885689	2.310572	1.767349
1	-3.298438	-3.439284	0.604989	1	3.674763	2.952621	0.313580
1	-1.644114	-2.823342	0.587385	1	1.925579	2.710812	0.337405
1	-2.891553	0.973947	-3.261829	1	2.319796	-1.650057	-3.092876
1	-3.060216	2.090057	-1.894489	1	2.191323	-2.605941	-1.604739
1	-1.550408	1.202083	-2.106469	1	0.944275	-1.416249	-1.980637
1	-4.719693	0.968789	-0.390239	1	4.061402	-1.741832	-0.177626
1	-4.968984	-2.018770	-0.449349	1	4.990993	1.087742	-0.553908
1	-0.530816	0.790728	4.005535	1	0.021862	-0.315409	4.017894
1	-1.649164	0.291514	2.754921	1	1.225795	-0.175881	2.755334
1	-2.491006	2.312777	3.842859	1	1.567654	-2.263168	3.981896

1	-0.977933	3.169794	3.500432	1	-0.105340	-2.760195	3.672063
1	-2.051291	2.721809	2.184379	1	1.043045	-2.665369	2.346637
1	-1.194258	1.460965	0.548063	1	0.504160	-1.350812	0.622506
1	-0.832662	-0.873444	1.327381	1	0.704560	1.054492	1.236014
1	-5.274802	-1.735190	1.983022	1	5.233649	1.012329	1.900296
1	-4.803746	-0.037355	1.865531	1	4.397583	-0.541908	1.957169
1	-6.306843	-0.604303	1.121658	1	5.986493	-0.406293	1.187933
1	-5.488957	0.774239	-2.728393	1	4.877526	-1.995172	-2.493284
1	-5.317592	-0.982733	-2.659531	1	5.124825	-0.250535	-2.619184
1	-6.531637	-0.162804	-1.669823	1	6.101703	-1.214567	-1.504435
1	4.859125	3.430089	-0.106561	1	-5.873992	-1.639447	-0.063961
1	3.694364	3.573152	1.219661	1	-4.818023	-2.006777	1.309404
1	4.360542	1.996065	0.801612	1	-4.992467	-0.342446	0.756825
1	3.186552	4.570210	-1.630171	1	-4.583814	-3.328920	-1.439485
1	1.560907	3.901133	-1.822366	1	-2.831898	-3.171171	-1.625588
1	2.029043	4.677311	-0.302632	1	-3.520416	-3.658266	-0.070265
1	4.178569	2.203628	-2.209393	1	-4.836779	-0.832207	-2.227537
1	3.604684	0.818043	-1.279020	1	-3.905772	0.401970	-1.373165
1	2.518721	1.628212	-2.414540	1	-3.078423	-0.769154	-2.406659
NImag = 1 (-123.8707 cm ⁻¹)				NImag = 1 (-133.4704 cm ⁻¹)			
TSf3-(Me)				TSf4-(NO₂)			
Et = -1288.2309214				Et = -1453.3445396			
Gsol = -1288.530923				Gsol = -1453.703433			
7	2.972005	-0.332023	-1.372730	6	-2.820044	-1.226683	0.071503
6	2.289596	0.540660	-0.638436	6	-2.214461	0.029691	0.119573
7	3.079447	1.187817	0.223957	6	-3.000868	1.166364	-0.078066
6	4.465995	0.793003	0.033201	6	-4.349454	1.044592	-0.346535
6	4.349205	-0.411656	-0.917671	6	-4.920576	-0.215560	-0.391778
8	1.040580	0.732971	-0.766066	6	-4.171039	-1.357118	-0.180730
6	0.132977	0.538315	0.508242	6	-0.744414	0.152283	0.387859
6	-0.096615	-0.953987	0.805429	6	-0.094241	1.427759	-0.131022
6	-1.064503	-1.524101	-0.219723	7	-0.553036	2.446048	0.734677
8	-0.723134	-1.767512	-1.357686	6	0.087524	2.509375	2.009286
6	2.738740	2.445260	0.839925	6	-0.615608	3.551374	2.858395
6	5.174971	0.481744	1.332149	8	-0.171358	-1.136710	-0.283743
6	5.353719	-0.398321	-2.047725	6	0.905658	-1.754825	-0.005991
6	2.358317	-1.369703	-2.165038	7	1.330696	-2.197724	1.180911
6	-1.065688	1.403836	0.267795	6	2.690945	-2.705633	1.025981
6	-1.170171	2.242987	-0.833781	6	2.719776	-3.066819	-0.460640
6	-2.294962	3.035302	-1.015381	7	1.703015	-2.176635	-0.987468
6	-3.344173	3.015307	-0.110006	6	0.864751	-1.716771	2.456909
6	-3.234859	2.163256	0.987166	6	1.373986	-2.089839	-2.382297
6	-2.119233	1.373710	1.184676	6	4.072364	-2.894567	-1.110859
6	-4.551354	3.885216	-0.291266	6	3.012090	-3.870086	1.932894

7	-0.516986	-0.966178	2.136147	6	1.414164	1.323679	-0.170336
6	0.591663	-1.026586	3.027868	8	1.929849	2.260756	-0.946196
6	1.203553	-2.423058	3.177495	6	3.342559	2.552649	-0.996591
8	-2.281204	-1.689457	0.244714	6	3.850494	2.964098	0.373344
6	-3.364800	-2.149367	-0.589374	8	2.070299	0.549830	0.500737
6	-3.088352	-3.559452	-1.081092	6	4.104201	1.361660	-1.551478
6	-4.544062	-2.141607	0.365203	6	3.411967	3.722079	-1.960175
6	-3.603242	-1.179011	-1.733512	7	-6.337406	-0.346597	-0.660778
1	-2.352638	3.676947	-1.884444	1	-4.965421	1.913416	-0.509593
1	-0.381874	2.272109	-1.568653	1	-2.520227	2.130572	0.039550
1	-2.027998	0.686722	2.015607	1	-2.230174	-2.117251	0.218231
1	-4.041524	2.119497	1.707263	1	-4.647962	-2.322282	-0.218779
1	2.749989	2.365487	1.923985	1	2.214356	-1.687648	-2.942030
1	3.454496	3.207647	0.530280	1	1.116095	-3.071715	-2.781793
1	1.748512	2.751814	0.518770	1	0.524221	-1.427651	-2.497977
1	2.630508	-1.259382	-3.212485	1	1.186759	-2.414155	3.223380
1	2.698758	-2.342232	-1.809983	1	1.257673	-0.724584	2.671170
1	1.277578	-1.324563	-2.050955	1	-0.219915	-1.699746	2.471348
1	4.458905	-1.337770	-0.344465	1	3.382992	-1.877643	1.206280
1	4.982047	1.611766	-0.479800	1	2.379881	-4.101713	-0.589222
1	0.266417	-0.698554	4.020092	1	1.159719	2.782758	1.961699
1	1.437729	-0.338579	2.770775	1	0.091940	1.559671	2.589910
1	2.044710	-2.432842	3.876067	1	-0.142033	3.669053	3.834134
1	0.444892	-3.116642	3.536165	1	-0.602623	4.511100	2.344554
1	1.564135	-2.803285	2.219632	1	-1.657983	3.273100	3.007819
1	0.860172	-1.468500	0.571631	1	-0.445337	1.620136	-1.148880
1	0.760561	0.902957	1.313267	1	-0.498253	0.050911	1.434445
1	5.258865	1.367134	1.959317	1	4.051662	-3.190673	-2.157620
1	4.634461	-0.282861	1.886702	1	4.402828	-1.860315	-1.047603
1	6.183650	0.123259	1.131739	1	4.806448	-3.524317	-0.611192
1	5.240936	-1.272219	-2.685907	1	3.072308	-3.570485	2.976426
1	5.233262	0.494178	-2.659296	1	2.263439	-4.654494	1.836829
1	6.366608	-0.410777	-1.648038	1	3.982086	-4.285536	1.665095
1	-5.443552	-2.486250	-0.142540	1	4.883765	3.299619	0.291369
1	-4.347494	-2.792690	1.214334	1	3.252822	3.786115	0.761790
1	-4.715977	-1.135411	0.741401	1	3.804589	2.138902	1.076479
1	-3.968077	-3.944600	-1.595634	1	4.443127	4.047887	-2.084771
1	-2.246342	-3.577239	-1.765326	1	3.016240	3.439353	-2.933807
1	-2.873797	-4.214401	-0.238020	1	2.824373	4.556057	-1.583177
1	-4.518043	-1.454824	-2.257367	1	5.148668	1.630741	-1.702581
1	-3.719714	-0.167505	-1.348007	1	4.052047	0.522172	-0.865902
1	-2.778330	-1.191833	-2.438031	1	3.688546	1.064430	-2.513658
1	-4.558357	4.356689	-1.271919	8	-6.802423	-1.464486	-0.706117
1	-5.472521	3.312368	-0.189036	8	-6.976141	0.667156	-0.828278
1	-4.582487	4.678564	0.456709				
			NImag = 1 (-113.6507 cm ⁻¹)				NImag = 1 (-81.5629 cm ⁻¹)

TSf4-(CN)				TSf4-(COOMe)			
Et = -1341.1322102				Et = -1476.7280147			
Gsol = -1341.454254				Gsol = -1477.086788			
6	-3.082632	-1.309654	-0.043126	6	2.598941	0.998914	0.197548
6	-2.503965	-0.043324	0.027935	6	1.915465	-0.216395	0.201643
6	-3.309645	1.076284	-0.182866	6	2.635549	-1.393560	-0.003833
6	-4.647702	0.926326	-0.485638	6	3.995419	-1.341579	-0.236640
6	-5.216596	-0.343857	-0.559735	6	4.671372	-0.126362	-0.245511
6	-4.424219	-1.464078	-0.331542	6	3.962308	1.046715	-0.021579
6	-1.043986	0.111483	0.336565	6	0.434982	-0.254271	0.437215
6	-0.408022	1.399674	-0.164419	6	-0.287900	-1.471442	-0.115183
7	-0.909189	2.406572	0.692536	7	0.068733	-2.532657	0.749503
6	-0.297411	2.482351	1.980552	6	-0.595522	-2.556076	2.013513
6	-1.040135	3.509759	2.813716	6	0.016822	-3.653782	2.863335
8	-0.425736	-1.167295	-0.321914	8	-0.047779	1.083080	-0.233961
6	0.658782	-1.759805	-0.021363	6	-1.092718	1.757811	0.022931
7	1.069099	-2.192905	1.174685	7	-1.521823	2.215272	1.203864
6	2.444516	-2.666414	1.049013	6	-2.849112	2.794416	1.022076
6	2.513143	-3.028630	-0.435985	6	-2.821229	3.172149	-0.460288
7	1.487208	-2.163142	-0.985264	7	-1.845244	2.230372	-0.972534
6	0.565244	-1.721641	2.439799	6	-1.112577	1.696816	2.484383
6	1.185768	-2.085294	-2.386722	6	-1.485465	2.138486	-2.359027
6	3.874800	-2.825454	-1.057680	6	-4.164909	3.086009	-1.145224
6	2.775953	-3.821169	1.964568	6	-3.132407	3.964365	1.934627
6	1.102761	1.330856	-0.169332	6	-1.783598	-1.268450	-0.194141
8	1.613858	2.284185	-0.928795	8	-2.334985	-2.141172	-1.022009
6	3.020239	2.607273	-0.947295	6	-3.757774	-2.361695	-1.099657
6	3.491504	3.019184	0.435580	6	-4.299621	-2.812370	0.244782
8	1.762441	0.569577	0.512709	8	-2.412442	-0.484277	0.491346
6	3.818797	1.437236	-1.494905	6	-4.459651	-1.112871	-1.604905
6	3.083983	3.785361	-1.900725	6	-3.871743	-3.480275	-2.118224
6	-6.603125	-0.500769	-0.862279	6	6.126986	-0.135771	-0.488084
1	-5.262947	1.796771	-0.655126	1	4.557723	-2.247621	-0.403621
1	-2.852562	2.049863	-0.047686	1	2.097476	-2.329594	0.079578
1	-2.478933	-2.189443	0.113758	1	2.060446	1.921003	0.351652
1	-4.861421	-2.449500	-0.383442	1	4.479493	1.993249	-0.022105
1	2.025714	-1.658729	-2.928870	1	-2.333414	1.794043	-2.945282
1	0.965165	-3.074196	-2.791278	1	-1.157034	3.106465	-2.740787
1	0.319684	-1.448079	-2.520468	1	-0.675034	1.426267	-2.459558
1	0.887774	-2.410118	3.214105	1	-1.408454	2.405719	3.251010
1	0.929471	-0.719953	2.660385	1	-1.567602	0.727660	2.680501
1	-0.519578	-1.730575	2.431300	1	-0.031408	1.614752	2.519573
1	3.111688	-1.820946	1.241708	1	-3.587952	2.002174	1.175477
1	2.200426	-4.071448	-0.569854	1	-2.419625	4.187441	-0.567519
1	0.769807	2.778240	1.956714	1	-1.684577	-2.749588	1.950871

1	-0.286159	1.533400	2.562388	1	-0.538379	-1.613973	2.603167
1	-0.590704	3.637244	3.799646	1	-0.477766	-3.743724	3.831831
1	-1.035591	4.469517	2.299704	1	-0.059684	-4.605992	2.340917
1	-2.079626	3.209993	2.940185	1	1.074798	-3.454327	3.028090
1	-0.739321	1.587113	-1.189890	1	0.079245	-1.679297	-1.123942
1	-0.823784	0.011181	1.388878	1	0.171125	-0.143200	1.478296
1	3.883010	-3.121786	-2.104561	1	-4.100554	3.391419	-2.187602
1	4.179977	-1.783901	-0.987851	1	-4.556019	2.072006	-1.103079
1	4.612473	-3.438190	-0.542368	1	-4.873757	3.752084	-0.656225
1	2.807239	-3.518618	3.008526	1	-3.230605	3.657116	2.973087
1	2.049068	-4.624053	1.854796	1	-2.343545	4.711270	1.864223
1	3.761239	-4.212887	1.717584	1	-4.074287	4.430710	1.650612
1	4.518221	3.378942	0.376709	1	-5.346813	-3.094019	0.139070
1	2.867524	3.824143	0.818337	1	-3.744278	-3.678363	0.598823
1	3.450556	2.187549	1.131303	1	-4.221383	-2.023460	0.985774
1	4.110243	4.133797	-2.002588	1	-4.915674	-3.750948	-2.266995
1	2.713425	3.501878	-2.883989	1	-3.452718	-3.171013	-3.073960
1	2.471507	4.603783	-1.529259	1	-3.327595	-4.357604	-1.776049
1	4.860885	1.728497	-1.618928	1	-5.509639	-1.332212	-1.794205
1	3.767341	0.590570	-0.818139	1	-4.392764	-0.313832	-0.873810
1	3.431707	1.140570	-2.469104	1	-4.009128	-0.781105	-2.539810
7	-7.720880	-0.632889	-1.109575	8	6.661831	1.089162	-0.471836
NImag = 1 (-92.8004 cm ⁻¹)				8	6.782737	-1.125164	-0.683604
				6	8.055631	1.135284	-0.698268
				1	8.329132	2.183341	-0.654131
				1	8.587515	0.572540	0.064019
				1	8.300692	0.720292	-1.672134
				NImag = 1 (-112.1063 cm ⁻¹)			
TSf4-(Cl)				TSf4-(H)			
Et = -1708.5308128				Et = -1248.9239962			
Gsol = -1708.854724				Gsol = -1249.223766			
6	-2.994355	-1.280590	0.003593	7	0.866118	-2.153352	1.129086
6	-2.405141	-0.021160	0.061788	6	0.492422	-1.741715	-0.087978
6	-3.206775	1.098704	-0.152674	7	1.451138	-1.984945	-0.985607
6	-4.551051	0.957353	-0.445815	6	2.543928	-2.711074	-0.369882
6	-5.111650	-0.306457	-0.506711	6	2.301583	-2.413032	1.111187
6	-4.341575	-1.430769	-0.278688	8	-0.635774	-1.300757	-0.462652
6	-0.943010	0.130406	0.363657	6	-1.489576	-0.122552	0.167023
6	-0.297974	1.405015	-0.148638	6	-0.976093	1.238996	-0.256224
7	-0.783231	2.422461	0.708148	6	0.524119	1.367674	-0.132816
6	-0.159445	2.501630	1.990313	8	1.218190	0.711540	0.620773
6	-0.889830	3.539027	2.822326	6	1.250648	-1.911249	-2.404625
8	-0.331518	-1.162274	-0.301039	6	3.907250	-2.292359	-0.867982
6	0.751297	-1.758558	-0.011371	6	2.728652	-3.535874	2.027031

7	1.171604	-2.193700	1.181488	6	0.196113	-1.800322	2.354515
6	2.544150	-2.670393	1.044233	6	-2.879585	-0.466600	-0.281349
6	2.598224	-3.034724	-0.440827	6	-3.798810	0.537746	-0.579119
7	1.572709	-2.164597	-0.981954	6	-5.073972	0.208929	-1.005916
6	0.680671	-1.717010	2.449511	6	-5.463678	-1.116036	-1.124803
6	1.255114	-2.091390	-2.379822	6	-4.561020	-2.117751	-0.811540
6	3.955567	-2.839717	-1.074611	6	-3.280353	-1.795479	-0.393233
6	2.880930	-3.824902	1.958242	7	-1.663127	2.160218	0.572115
6	1.211715	1.326958	-0.164494	6	-1.190918	2.265182	1.915893
8	1.723226	2.270704	-0.937649	6	-2.124864	3.181486	2.684619
6	3.129930	2.587269	-0.966072	8	0.971450	2.375779	-0.866414
6	3.609688	3.013707	0.409603	6	2.303279	2.911066	-0.738454
8	1.874060	0.570323	0.520192	6	3.334280	1.874052	-1.149742
6	3.922328	1.408139	-1.503451	6	2.298686	4.068426	-1.719479
6	3.194728	3.753968	-1.933562	6	2.539341	3.415296	0.673809
17	-6.800858	-0.484652	-0.862253	1	-6.463266	-1.365410	-1.450968
1	-5.165124	1.828304	-0.614780	1	-5.773162	1.000196	-1.235944
1	-2.746957	2.072336	-0.028578	1	-3.492229	1.562403	-0.410453
1	-2.398236	-2.165739	0.162680	1	-2.583708	-2.589165	-0.169690
1	-4.788146	-2.411873	-0.323929	1	-4.850077	-3.155940	-0.893977
1	2.091532	-1.673896	-2.934453	1	2.063433	-1.360734	-2.871435
1	1.021558	-3.080280	-2.777541	1	1.197922	-2.909305	-2.842864
1	0.392373	-1.447878	-2.505406	1	0.318311	-1.392827	-2.595065
1	1.004700	-2.405927	3.222945	1	0.543104	-2.465683	3.138728
1	1.052298	-0.716909	2.665000	1	0.397001	-0.766402	2.629309
1	-0.404204	-1.718918	2.448409	1	-0.872101	-1.955868	2.246585
1	3.215783	-1.826755	1.229697	1	2.817218	-1.485622	1.377975
1	2.279431	-4.076460	-0.570168	1	2.401103	-3.783694	-0.551261
1	0.909368	2.792416	1.956783	1	-0.166910	2.678441	2.008843
1	-0.148525	1.557543	2.579490	1	-1.131845	1.309549	2.482860
1	-0.431846	3.671441	3.803838	1	-1.795291	3.330154	3.714294
1	-0.884590	4.494972	2.301084	1	-2.176006	4.149915	2.189379
1	-1.929834	3.245395	2.958782	1	-3.131351	2.765284	2.695731
1	-0.635998	1.591539	-1.172037	1	-1.245053	1.414435	-1.301409
1	-0.712402	0.024253	1.412764	1	-1.344534	-0.235833	1.230608
1	3.952708	-3.137262	-2.121217	1	4.044646	-2.550017	-1.916181
1	4.266524	-1.799604	-1.009108	1	4.047643	-1.220192	-0.751589
1	4.694764	-3.455599	-0.565180	1	4.682678	-2.807520	-0.303489
1	2.921036	-3.521116	3.001569	1	2.626903	-3.267411	3.075846
1	2.151216	-4.626166	1.855376	1	2.143751	-4.434405	1.838021
1	3.863335	-4.219140	1.703755	1	3.779132	-3.767047	1.858076
1	4.637756	3.368231	0.341884	1	3.500085	3.927040	0.722298
1	2.990558	3.825584	0.785539	1	1.758937	4.120180	0.952772
1	3.567870	2.190523	1.115256	1	2.539892	2.598499	1.388257
1	4.221925	4.097299	-2.043649	1	3.263661	4.572479	-1.714502
1	2.818982	3.460373	-2.911913	1	2.096647	3.713315	-2.728337

1	2.586720	4.578915	-1.569223	1	1.526938	4.785970	-1.450307
1	4.964781	1.694432	-1.636298	1	4.322029	2.331837	-1.186381
1	3.871122	0.570057	-0.816127	1	3.352801	1.051540	-0.442417
1	3.529156	1.100780	-2.471920	1	3.103282	1.487032	-2.141721
NImag = 1 (-127.5062 cm ⁻¹)				NImag = 1 (-157.9142 cm ⁻¹)			
TSf4-(Me)				TS5(NO₂)re-re			
Et = -1288.2343472				Et = -1223.2476304			
Gsol = -1288.539210							
6	-3.202689	-1.411906	-0.127562	7	2.226797	-0.407495	1.371714
6	-2.655276	-0.135989	-0.060012	6	2.166545	-0.147841	0.054106
6	-3.486921	0.953517	-0.317074	7	3.039061	-0.920309	-0.616967
6	-4.811575	0.754490	-0.655712	6	3.869471	-1.671628	0.313653
6	-5.364279	-0.520754	-0.733560	6	3.085032	-1.550394	1.631621
6	-4.535224	-1.598338	-0.460325	7	1.357123	0.744128	-0.481841
6	-1.213040	0.066698	0.297402	6	1.735375	1.513086	-1.671279
6	-0.589758	1.363035	-0.181018	6	3.078905	2.191350	-1.523292
7	-1.126400	2.361456	0.668971	6	2.903074	-1.292659	-2.005595
6	-0.560440	2.434397	1.978005	6	5.281235	-1.124823	0.388649
6	-1.345863	3.449559	2.787474	6	2.291999	-2.791154	1.992496
8	-0.525416	-1.200525	-0.358752	6	1.810083	0.516646	2.396560
6	0.567795	-1.756967	-0.038833	6	0.033146	0.894665	0.030887
7	0.968812	-2.183919	1.164318	6	-0.292814	2.182967	0.534980
6	2.363498	-2.601167	1.067842	8	-1.492213	2.198961	1.162314
6	2.478148	-2.955223	-0.416124	6	-1.904155	3.462615	1.625613
7	1.437164	-2.122870	-0.985034	8	0.368989	3.202983	0.407914
6	0.418979	-1.735818	2.418438	6	-1.048568	0.070353	-1.887473
6	1.157393	-2.058494	-2.391144	8	-0.244897	-0.763871	-2.288538
6	3.845817	-2.703902	-1.006444	6	-2.305014	-0.323221	-1.199780
6	2.720828	-3.745213	1.987253	6	-2.525891	-1.665092	-0.906589
6	0.920771	1.337660	-0.150700	6	-3.702638	-2.066554	-0.310547
8	1.422427	2.290348	-0.922237	6	-4.681924	-1.119686	-0.010346
6	2.810848	2.674984	-0.892121	6	-4.471917	0.224689	-0.314207
6	3.203620	3.147135	0.496293	6	-3.288471	0.614122	-0.906523
8	1.590481	0.618588	0.566842	6	-5.903573	-1.529241	0.604972
6	3.686079	1.529182	-1.370145	7	-6.888014	-1.861015	1.103676
6	2.864209	3.828046	-1.876791	1	3.516829	-0.669772	-2.656295
6	-6.808233	-0.713937	-1.086227	1	3.227403	-2.324843	-2.117483
1	-5.435843	1.615976	-0.853448	1	1.859126	-1.219101	-2.301764
1	-3.069249	1.944006	-0.187376	1	2.514712	0.452736	3.223152
1	-2.584572	-2.276579	0.062115	1	1.820014	1.530023	2.003876
1	-4.932890	-2.603302	-0.509241	1	0.809569	0.299378	2.765172
1	1.990509	-1.603464	-2.920815	1	3.893061	-2.711523	-0.011671
1	0.978094	-3.055181	-2.797826	1	3.763360	-1.294907	2.445807
1	0.271496	-1.452301	-2.539544	1	1.689124	-2.619929	2.882284

1	0.746070	-2.416178	3.198268	1	1.622824	-3.064678	1.177972
1	0.742267	-0.722701	2.650303	1	2.958499	-3.629777	2.191168
1	-0.664302	-1.781652	2.381761	1	5.887260	-1.717192	1.073328
1	2.993231	-1.731107	1.277071	1	5.757984	-1.146394	-0.589623
1	2.204828	-4.008216	-0.558961	1	5.271675	-0.093816	0.739756
1	0.503938	2.743078	1.998062	1	-0.345476	0.030847	0.549255
1	-0.560645	1.484345	2.557397	1	0.972298	2.277457	-1.750027
1	-0.936980	3.576410	3.791342	1	1.675123	0.893986	-2.562307
1	-1.331718	4.412236	2.278741	1	-1.054090	1.093299	-2.283874
1	-2.386176	3.137497	2.869824	1	-3.116793	1.655485	-1.134755
1	-0.902565	1.551425	-1.211725	1	-5.237240	0.949359	-0.082632
1	-1.015077	-0.047547	1.352137	1	-3.880059	-3.106436	-0.081761
1	3.887287	-2.995903	-2.053843	1	-1.758674	-2.377213	-1.169611
1	4.112627	-1.652497	-0.927512	1	-2.870329	3.307490	2.094661
1	4.592850	-3.292461	-0.476464	1	-1.199273	3.866241	2.348925
1	2.715483	-3.445364	3.032502	1	-1.995099	4.173629	0.807590
1	2.029249	-4.576085	1.858657	1	3.283254	2.789752	-2.409589
1	3.726531	-4.096276	1.762011	1	3.058697	2.853572	-0.660740
1	4.213397	3.555808	0.469863	1	3.897017	1.481388	-1.407869
1	2.524458	3.929036	0.829626	NImag = 1 (-50.6779 cm ⁻¹)			
1	3.172550	2.332897	1.212814				
1	3.877178	4.221116	-1.945150				
1	2.550468	3.500258	-2.866106				
1	2.199199	4.626781	-1.556224				
1	4.717409	1.866974	-1.463624				
1	3.646975	0.702281	-0.668682				
1	3.352164	1.183769	-2.348065				
1	-7.060427	-1.769464	-1.166400				
1	-7.461611	-0.273639	-0.332415				
1	-7.051307	-0.239896	-2.037193				
NImag = 1 (-146.5236 cm ⁻¹)							
TS5(COOH)re-re Et = -1319.5483509				TS5(COOMe)re-re Et = -1358.843973			
6	-2.252713	-1.394002	-0.998609	7	2.639687	-0.753376	1.345481
6	-1.956812	-0.059644	-1.257757	6	2.712301	-0.307256	0.078480
6	-2.912484	0.916851	-0.999278	7	3.533335	-1.086864	-0.647040
6	-4.139499	0.568107	-0.474365	6	4.190430	-2.062841	0.211046
6	-4.426583	-0.765786	-0.202176	6	3.322249	-2.028224	1.480243
6	-3.476524	-1.748508	-0.468535	7	2.065938	0.754584	-0.358267
6	-0.647899	0.287965	-1.872782	6	2.607666	1.606693	-1.420017
8	0.118731	-0.580664	-2.287466	6	4.013082	2.079644	-1.123230
6	-5.749972	-1.086968	0.357977	6	3.447229	-1.253771	-2.079987
6	0.384635	0.953739	0.045457	6	5.646357	-1.719021	0.455166

6	0.097123	2.230922	0.611166	6	2.352249	-3.188096	1.592545
8	0.795635	3.230588	0.542376	6	2.266577	0.065967	2.470765
7	1.722434	0.775659	-0.425461	6	0.727611	0.996118	0.083530
6	2.171490	1.589459	-1.558330	6	0.512507	2.251604	0.728630
6	3.543383	2.186300	-1.337822	8	-0.704817	2.321125	1.308193
6	2.459738	-0.200023	0.064795	6	-1.026372	3.568374	1.876294
7	3.317343	-0.967972	-0.630656	8	1.279742	3.201397	0.744592
6	4.067106	-1.830272	0.272689	6	-0.280599	0.538421	-1.878696
6	3.227495	-1.772327	1.559984	8	0.429548	-0.361598	-2.330392
7	2.453800	-0.559353	1.361078	6	-1.634253	0.255655	-1.329271
6	3.205864	-1.244023	-2.044774	6	-2.037379	-1.064833	-1.159789
6	2.057190	0.310981	2.439091	6	-3.301205	-1.355629	-0.687543
6	2.343500	-2.985602	1.772105	6	-4.185220	-0.321762	-0.389668
6	5.496979	-1.360829	0.453317	6	-3.790640	0.999523	-0.573766
8	-1.107582	2.255887	1.221373	6	-2.524032	1.284257	-1.040790
6	-1.498265	3.512442	1.721369	6	-5.550022	-0.569410	0.114449
1	3.869491	-0.612775	-2.635715	8	-6.348627	0.291355	0.379280
1	3.484399	-2.281737	-2.213499	8	-5.822427	-1.869405	0.254204
1	2.174927	-1.100649	-2.361587	1	4.173495	-0.633700	-2.605541
1	2.741459	0.162247	3.272121	1	3.654754	-2.295057	-2.316046
1	2.119400	1.346338	2.115118	1	2.439578	-1.011983	-2.412260
1	1.040946	0.115607	2.775845	1	2.900143	-0.198749	3.314916
1	4.058201	-2.841252	-0.133800	1	2.424111	1.113730	2.229257
1	3.877312	-1.630488	2.423641	1	1.224397	-0.069752	2.753263
1	1.704123	-2.851359	2.642545	1	4.116334	-3.040571	-0.264336
1	1.704804	-3.145542	0.904599	1	3.957184	-1.988532	2.365504
1	2.946921	-3.879091	1.929008	1	1.701791	-3.067066	2.456741
1	6.042408	-2.033559	1.114328	1	1.726178	-3.246740	0.703359
1	6.017926	-1.328813	-0.501814	1	2.889559	-4.129597	1.702056
1	5.517009	-0.361032	0.885037	1	6.120892	-2.475289	1.079570
1	-0.027171	0.087731	0.534378	1	6.193774	-1.663318	-0.483967
1	1.452061	2.396827	-1.611369	1	5.731143	-0.755194	0.955478
1	2.103076	1.024837	-2.484160	1	0.245715	0.132336	0.508157
1	-0.598686	1.315846	-2.256321	1	1.952116	2.468269	-1.435360
1	-2.685182	1.952471	-1.206837	1	2.525648	1.112725	-2.384247
1	-4.893502	1.311882	-0.267236	1	-0.145474	1.579702	-2.201768
1	-3.709511	-2.782624	-0.267594	1	-2.214373	2.310184	-1.179229
1	-1.505827	-2.135907	-1.237446	1	-4.494119	1.785166	-0.344600
1	-2.479143	3.365584	2.161104	1	-3.616565	-2.378803	-0.555550
1	-0.800156	3.870624	2.474631	1	-1.339932	-1.846351	-1.421140
1	-1.551507	4.253740	0.927387	1	-2.024962	3.459706	2.286106
1	3.801021	2.825183	-2.180925	1	-0.324847	3.834835	2.663541
1	3.534072	2.796406	-0.437411	1	-1.013318	4.357208	1.127711
1	4.321510	1.429596	-1.246324	1	4.345577	2.750434	-1.913677
8	-5.928156	-2.395594	0.583721	1	4.021398	2.627888	-0.183838
8	-6.611110	-0.282665	0.603082	1	4.727559	1.259672	-1.062178

1	-6.818083	-2.481532	0.941747	6	-7.119805	-2.161316	0.731298
				1	-7.179183	-3.242226	0.787118
	NImag = 1 (-87.6305 cm ⁻¹)			1	-7.276297	-1.721834	1.712667
				1	-7.874718	-1.775069	0.051922
				NImag = 1 (-95.2445 cm ⁻¹)			
TS5(Cl)re-re				TS5(F)re-re			
Et = -1590.6461899				Et = -1230.2420361			
6	-3.164334	0.693690	-0.929515	7	2.933922	-0.772673	-0.658581
6	-2.164899	-0.244643	-1.148442	6	2.026319	-0.053687	0.024631
6	-2.407829	-1.575724	-0.833536	7	2.123477	-0.306513	1.342516
6	-3.616783	-1.966167	-0.288771	6	3.042215	-1.404092	1.587778
6	-4.595000	-1.010058	-0.069530	6	3.820022	-1.470928	0.262502
6	-4.381838	0.319907	-0.390061	7	1.163732	0.800112	-0.488500
6	-0.867002	0.129507	-1.774988	6	1.453089	1.550134	-1.712532
8	-0.077308	-0.736040	-2.165600	6	2.762339	2.303469	-1.635629
17	-6.118883	-1.489408	0.608700	6	1.670635	0.591725	2.373460
6	0.153090	0.909941	0.030810	6	2.317417	-2.688355	1.939932
6	-0.188537	2.195440	0.554407	6	5.194021	-0.833787	0.324485
8	0.449397	3.227551	0.422702	6	2.785437	-1.174531	-2.039484
7	1.494395	0.786322	-0.453279	6	-0.173778	0.839379	0.022876
6	1.875765	1.570108	-1.630482	6	-0.604167	2.120161	0.495927
6	3.225420	2.234086	-1.473371	8	-1.766042	2.041340	1.178218
6	2.281126	-0.144372	0.047279	6	-2.304849	3.276650	1.584897
7	2.317692	-0.461429	1.354144	8	-0.059008	3.192291	0.291973
6	3.148719	-1.632000	1.574550	6	-1.169028	-0.096200	-1.677492
6	3.962046	-1.696110	0.270806	8	-0.326185	-0.921898	-2.052560
7	3.157607	-0.895432	-0.642331	6	-2.423652	-0.539782	-1.007146
6	1.904331	0.424644	2.412425	6	-3.491636	0.326711	-0.813752
6	3.025518	-1.225451	-2.043640	6	-4.666365	-0.113827	-0.230271
6	5.374536	-1.162422	0.403521	6	-4.755695	-1.435574	0.156368
6	2.324214	-2.874846	1.846640	6	-3.716861	-2.325791	-0.030376
8	-1.375356	2.180296	1.197799	6	-2.552874	-1.868358	-0.620541
6	-1.821503	3.433797	1.657686	1	3.351676	-0.530299	-2.712158
1	3.646749	-0.586331	-2.671064	1	3.162271	-2.189678	-2.142770
1	3.346753	-2.255041	-2.183781	1	1.729779	-1.162578	-2.304164
1	1.981167	-1.139199	-2.337142	1	2.398103	0.584076	3.182671
1	2.612587	0.335945	3.233870	1	1.601502	1.600061	1.974195
1	1.911018	1.450246	2.053404	1	0.696811	0.310159	2.769774
1	0.905993	0.193832	2.779292	1	3.907756	-2.506006	-0.066310
1	3.987108	-2.719157	-0.103398	1	3.711897	-1.120217	2.399781
1	3.810232	-1.432780	2.417784	1	1.711343	-2.558141	2.834532
1	1.700977	-2.740491	2.728714	1	1.658896	-2.987131	1.125628
1	1.672109	-3.089621	1.001224	1	3.028255	-3.492804	2.126062
1	2.969930	-3.735966	2.015645	1	5.845522	-1.387618	0.999684

1	5.962507	-1.790895	1.071613	1	5.658801	-0.820964	-0.659661
1	5.872115	-1.138998	-0.564235	1	5.122012	0.193527	0.679315
1	5.362351	-0.149553	0.803966	1	-0.424588	-0.009938	0.635343
1	-0.190217	0.050900	0.581704	1	0.648637	2.271393	-1.783926
1	1.119724	2.342350	-1.697013	1	1.392371	0.900232	-2.581036
1	1.807994	0.964460	-2.529883	1	-1.272992	0.870013	-2.192505
1	-0.874490	1.130003	-2.229876	1	-3.402165	1.359044	-1.120671
1	-2.988243	1.730014	-1.180189	1	-5.506972	0.544162	-0.073136
1	-5.160621	1.046751	-0.219101	1	-3.837980	-3.354314	0.273622
1	-3.810497	-2.999421	-0.044872	1	-1.723725	-2.533423	-0.810068
1	-1.631516	-2.296882	-1.041060	1	-3.230512	3.042159	2.099882
1	-2.780790	3.252623	2.130986	1	-1.626281	3.800519	2.254256
1	-1.124632	3.859978	2.375820	1	-2.504168	3.919932	0.730978
1	-1.936016	4.137405	0.836371	1	2.901935	2.882555	-2.546940
1	3.434934	2.843339	-2.351022	1	2.738622	2.992526	-0.794221
1	3.212707	2.884392	-0.601551	1	3.621859	1.643137	-1.527951
1	4.037094	1.515396	-1.367779	9	-5.885806	-1.868960	0.720767
NImag = 1 (-125.5409 cm ⁻¹)				NImag = 1 (-149.5615 cm ⁻¹)			
TS5(H)re-re Et = -1131.0393205				TS5(Me)re-re Et = -1170.3495188			
7	1.923363	-0.132026	1.325719	7	2.953220	-0.759582	-0.663083
6	1.773768	0.055146	0.001181	6	2.040171	-0.059949	0.033135
7	2.735576	-0.597506	-0.675237	7	2.114722	-0.364476	1.341957
6	3.699456	-1.175148	0.251660	6	3.014808	-1.482837	1.557865
6	2.945070	-1.128559	1.590659	6	3.814063	-1.506127	0.244219
7	0.818791	0.797079	-0.521180	7	1.194025	0.823408	-0.456198
6	0.997124	1.506185	-1.790104	6	1.499530	1.604578	-1.656199
6	2.213549	2.404604	-1.783475	6	2.811286	2.349069	-1.544076
6	2.600342	-1.073493	-2.034315	6	1.657741	0.498203	2.400664
6	5.010866	-0.415040	0.257868	6	2.267210	-2.770458	1.844431
6	2.350477	-2.460198	2.005591	6	5.195013	-0.890919	0.354912
6	1.414862	0.763434	2.332496	6	2.822346	-1.110027	-2.060213
6	-0.503514	0.726871	0.026422	6	-0.152077	0.849537	0.035320
6	-1.052112	1.983876	0.441547	6	-0.589285	2.120962	0.532163
8	-2.180139	1.827821	1.164338	8	-1.750685	2.023254	1.210540
6	-2.834405	3.023187	1.516478	6	-2.305113	3.248359	1.625877
8	-0.625199	3.091747	0.161599	8	-0.048961	3.199026	0.349179
6	-1.427877	-0.394551	-1.580553	6	-1.113973	-0.042539	-1.674045
8	-0.508452	-1.139624	-1.948365	8	-0.268908	-0.868601	-2.051234
6	-2.603680	-0.941902	-0.843726	6	-2.384567	-0.490779	-1.035955
6	-2.564179	-2.251032	-0.379437	6	-3.460477	0.369842	-0.868580
6	-3.655979	-2.796864	0.271749	6	-4.646352	-0.083895	-0.319342
6	-4.805093	-2.041123	0.455587	6	-4.790656	-1.408368	0.080117
6	-4.855357	-0.738830	-0.018256	6	-3.711802	-2.268509	-0.102389

6	-3.759445	-0.193331	-0.664738	6	-2.527574	-1.818982	-0.656383
1	1.544456	-1.197106	-2.267909	6	-6.065569	-1.890849	0.704124
1	3.070141	-0.397350	-2.748593	1	1.769113	-1.094239	-2.335244
1	3.093094	-2.040311	-2.107076	1	3.393043	-0.437743	-2.700930
1	1.208487	1.732236	1.886543	1	3.207427	-2.118051	-2.196444
1	0.500769	0.393287	2.793162	1	0.679618	0.207567	2.779631
1	2.174163	0.886979	3.102594	1	2.378834	0.458997	3.214831
1	3.875074	-2.210136	-0.040313	1	1.596031	1.520257	2.036809
1	3.600835	-0.752454	2.376222	1	3.894055	-2.528190	-0.124755
1	1.750156	-2.352637	2.907045	1	3.673732	-1.241252	2.392105
1	1.709123	-2.850140	1.216449	1	1.648256	-2.668914	2.733937
1	3.136865	-3.187140	2.206403	1	1.617963	-3.025205	1.007985
1	5.723214	-0.881561	0.937606	1	2.964027	-3.591964	2.007918
1	5.452516	-0.399053	-0.736849	1	5.827660	-1.480437	1.017781
1	4.853618	0.614842	0.575846	1	5.676650	-0.844735	-0.620095
1	-0.646721	-0.103094	0.697424	1	5.130556	0.122221	0.749764
1	0.113720	2.125290	-1.881320	1	-0.405559	-0.009433	0.633054
1	0.994539	0.806078	-2.620399	1	0.698858	2.330769	-1.717609
1	-1.661458	0.521736	-2.143142	1	1.445769	0.977815	-2.541813
1	-3.796563	0.822332	-1.033579	1	-1.210329	0.927367	-2.185215
1	-5.751552	-0.149586	0.114853	1	-3.368725	1.403022	-1.174727
1	-5.661081	-2.468056	0.958475	1	-5.477125	0.599210	-0.201352
1	-3.618744	-3.816952	0.627812	1	-3.809698	-3.307963	0.182746
1	-1.667087	-2.824627	-0.559965	1	-1.696835	-2.487655	-0.827726
1	-3.717455	2.725882	2.072224	1	-3.233343	2.999019	2.129066
1	-2.197712	3.653115	2.133662	1	-1.637925	3.771344	2.307395
1	-3.121130	3.590065	0.633814	1	-2.502949	3.898901	0.777170
1	2.272534	2.944381	-2.727178	1	2.965659	2.949977	-2.438750
1	2.125964	3.131729	-0.979201	1	2.780331	3.017040	-0.686044
1	3.143205	1.850467	-1.660086	1	3.665989	1.681655	-1.441490
	NImag = 1 (-153.9732 cm ⁻¹)			1	-6.227936	-2.949707	0.510169
				1	-6.049778	-1.758019	1.787352
				1	-6.927054	-1.344396	0.324009
					NImag = 1 (-162.2721 cm ⁻¹)		
	TS5(OMe)re-re Et = -1245.524757				TS5(OH)re-re Et = -1206.2292462		
6	-3.118756	0.869313	-0.948516	7	2.943823	-0.744707	-0.667542
6	-2.145306	-0.110724	-1.118384	6	2.030201	-0.047307	0.029856
6	-2.466841	-1.420940	-0.805612	7	2.109004	-0.349973	1.338885
6	-3.717761	-1.759681	-0.313173	6	3.010593	-1.467482	1.553331
6	-4.674998	-0.767798	-0.139525	6	3.808808	-1.487505	0.239224
6	-4.369385	0.550772	-0.465979	7	1.181183	0.835025	-0.456894
6	-0.804073	0.202317	-1.685427	6	1.477639	1.608794	-1.663740
8	-0.043039	-0.708404	-2.052555	6	2.787298	2.358652	-1.562967

8	-5.924819	-0.984537	0.328692	6	1.651822	0.511038	2.398556
6	-6.283507	-2.293106	0.657757	6	2.264456	-2.756348	1.838013
6	0.186459	0.935324	0.064064	6	5.187091	-0.866127	0.348392
6	-0.151152	2.213738	0.619741	6	2.809703	-1.100082	-2.063407
8	0.478001	3.251021	0.495791	6	-0.166320	0.851956	0.033533
7	1.537381	0.818371	-0.403164	6	-0.613625	2.125517	0.519938
6	1.931860	1.628255	-1.556756	8	-1.774333	2.024008	1.199440
6	3.299249	2.251691	-1.386561	6	-2.334176	3.248110	1.610613
6	2.288884	-0.166100	0.044730	8	-0.084128	3.206547	0.326366
7	2.304467	-0.555098	1.333359	6	-1.122300	-0.055573	-1.640178
6	3.085147	-1.768734	1.491273	8	-0.272001	-0.880360	-2.016417
6	3.922365	-1.774194	0.202196	6	-2.389878	-0.515928	-1.005434
7	3.154239	-0.901473	-0.676300	6	-3.475993	0.329488	-0.838234
6	1.906310	0.279423	2.437067	6	-4.658198	-0.131308	-0.285217
6	3.017348	-1.167384	-2.091928	6	-4.763985	-1.457508	0.110222
6	5.343302	-1.281972	0.392626	6	-3.687263	-2.318884	-0.060156
6	2.206354	-2.993317	1.656282	6	-2.517537	-1.845805	-0.618955
8	-1.325406	2.178106	1.280740	8	-5.893555	-1.965020	0.658286
6	-1.787153	3.422395	1.749561	1	3.376063	-0.427664	-2.707810
1	3.652718	-0.513700	-2.689592	1	3.198329	-2.107003	-2.197472
1	3.320060	-2.195637	-2.275682	1	1.755169	-1.089562	-2.333923
1	1.972950	-1.050958	-2.377157	1	2.378469	0.480344	3.208171
1	2.615616	0.141148	3.251017	1	1.579162	1.531476	2.032380
1	1.925655	1.321262	2.129767	1	0.678837	0.212917	2.785070
1	0.905811	0.044660	2.795996	1	3.892817	-2.509176	-0.129730
1	3.932016	-2.773193	-0.232160	1	3.669405	-1.225991	2.387666
1	3.733792	-1.654003	2.359827	1	1.645508	-2.657091	2.727769
1	1.566971	-2.895972	2.531694	1	1.615365	-3.010414	1.001237
1	1.567672	-3.119365	0.783153	1	2.962219	-3.577323	2.000026
1	2.813324	-3.890050	1.777256	1	5.823155	-1.452858	1.010455
1	5.904688	-1.962344	1.032224	1	5.667280	-0.817740	-0.627218
1	5.859375	-1.211869	-0.563109	1	5.118668	0.146717	0.743370
1	5.345562	-0.294573	0.852572	1	-0.405413	0.000863	0.648358
1	-0.149922	0.074382	0.616302	1	0.674300	2.331887	-1.726705
1	1.196300	2.421652	-1.595915	1	1.421663	0.975570	-2.544511
1	1.845412	1.051888	-2.473717	1	-1.234804	0.904407	-2.167730
1	-0.769453	1.186019	-2.178589	1	-3.399331	1.363876	-1.143416
1	-2.890791	1.895762	-1.201270	1	-5.500065	0.538611	-0.162291
1	-5.132334	1.302984	-0.333395	1	-3.795135	-3.350849	0.238510
1	-3.937939	-2.790468	-0.083339	1	-1.676238	-2.501920	-0.786484
1	-1.716305	-2.179255	-0.973660	1	-3.257671	2.995949	2.121166
1	-2.743631	3.225378	2.221890	1	-1.666433	3.779384	2.285034
1	-1.094551	3.852605	2.469591	1	-2.540964	3.892478	0.759273
1	-1.911861	4.129253	0.932657	1	2.935720	2.953424	-2.462730
1	3.520712	2.882521	-2.245851	1	2.758226	3.032900	-0.709769
1	3.308225	2.874888	-0.495029	1	3.644693	1.694935	-1.459124

1	4.092260	1.509406	-1.306816	1	-6.554938	-1.274164	0.707540
1	-7.309142	-2.248228	1.009354	NImag = 1 (-180.5649 cm ⁻¹)			
1	-6.232003	-2.955220	-0.208448				
1	-5.651744	-2.696733	1.451195	NImag = 1 (-173.9790 cm ⁻¹)			
TS6(COOH)re-si Et = -1319.5472439				TS6(COOMe)re-si Et = -1358.8428596			
6	2.781607	0.685054	-1.202877	7	-3.693912	0.784737	0.021965
6	1.914967	-0.404092	-1.206368	6	-2.801977	-0.209314	0.189634
6	2.360724	-1.629937	-0.723251	7	-3.416774	-1.404113	0.149242
6	3.635630	-1.757957	-0.211297	6	-4.860984	-1.225608	0.080408
6	4.490049	-0.660627	-0.187524	6	-4.996781	0.249472	-0.332513
6	4.058050	0.563496	-0.691547	7	-1.513285	-0.007275	0.374834
6	0.554040	-0.303211	-1.812388	6	-0.701206	-0.916459	1.186018
8	-0.185646	-1.286087	-1.910139	6	-1.245254	-1.073902	2.588169
6	5.840398	-0.846440	0.369453	6	-2.776826	-2.636595	-0.252550
6	-0.533218	0.973485	-0.357745	6	-5.539304	-1.560527	1.393860
6	0.150613	1.939195	0.446013	6	-5.315319	0.449131	-1.801347
8	0.345920	1.884902	1.646829	6	-3.498294	2.131693	0.493802
7	-1.242798	-0.037318	0.361752	6	-0.846695	1.014841	-0.369162
6	-0.473738	-0.973072	1.185108	6	-0.158381	1.998699	0.406898
6	-1.048908	-1.118415	2.576096	8	0.284649	3.020117	-0.363864
6	-2.533478	-0.200555	0.152419	6	1.054557	3.983491	0.317735
7	-3.179243	-1.377411	0.087345	8	0.075345	1.958357	1.601535
6	-4.616751	-1.160052	-0.003527	6	0.209613	-0.243443	-1.865427
6	-4.707251	0.324318	-0.395734	8	-0.546828	-1.212766	-1.969841
7	-3.394328	0.819437	-0.020043	6	1.578758	-0.375880	-1.284827
6	-2.565027	-2.622711	-0.315119	6	2.452971	0.706514	-1.251671
6	-3.168999	2.155524	0.469989	6	3.736283	0.557101	-0.765194
6	-5.006478	0.554357	-1.864155	6	4.168338	-0.687912	-0.315510
6	-5.327193	-1.497291	1.292214	6	3.305490	-1.777359	-0.368928
8	0.635309	2.957659	-0.301958	6	2.023451	-1.621724	-0.855820
6	1.407140	3.898019	0.409570	6	5.527773	-0.908326	0.215551
1	-2.291188	-3.235510	0.543524	8	5.942580	-1.965062	0.615582
1	-3.282079	-3.178486	-0.914857	8	6.270928	0.200755	0.211240
1	-1.687025	-2.411784	-0.922769	1	-2.462363	-3.228706	0.606725
1	-2.859618	2.838542	-0.319135	1	-3.492911	-3.221741	-0.824776
1	-4.092590	2.524005	0.912575	1	-1.922665	-2.408515	-0.887413
1	-2.397117	2.138736	1.234339	1	-3.224688	2.815286	-0.308011
1	-5.005194	-1.781587	-0.809863	1	-4.423108	2.477921	0.951675
1	-5.454444	0.827214	0.218489	1	-2.711035	2.145086	1.242266
1	-4.971169	1.615159	-2.105274	1	-5.247013	-1.869579	-0.709198
1	-4.274125	0.040894	-2.485527	1	-5.751232	0.741145	0.281886
1	-5.998852	0.182493	-2.117012	1	-5.309783	1.506803	-2.058178

1	-6.401859	-1.348975	1.191542	1	-4.574890	-0.054122	-2.421534
1	-5.153222	-2.535179	1.570021	1	-6.299814	0.047763	-2.039534
1	-4.965407	-0.864245	2.101432	1	-6.619234	-1.442835	1.310407
1	-1.089561	1.362355	-1.194179	1	-5.332254	-2.588680	1.684924
1	0.514489	-0.536565	1.251660	1	-5.180524	-0.904874	2.186257
1	-0.368524	-1.928884	0.681918	1	-1.433367	1.385567	-1.192674
1	0.470899	0.530792	-2.522658	1	0.274768	-0.451021	1.232397
1	1.689661	-2.473708	-0.776085	1	-0.577772	-1.871063	0.684415
1	3.996835	-2.701897	0.167931	1	0.124723	0.607680	-2.554600
1	4.727826	1.409141	-0.682572	1	1.346316	-2.459093	-0.930360
1	2.437622	1.633423	-1.589300	1	3.665655	-2.737597	-0.031998
1	1.721715	4.638253	-0.318860	1	4.411669	1.397458	-0.732709
1	0.822661	4.371965	1.194624	1	2.109333	1.671563	-1.595276
1	2.274459	3.426366	0.864486	1	1.332276	4.723905	-0.425387
1	-0.417595	-1.782754	3.163823	1	0.481881	4.451607	1.114966
1	-1.072053	-0.147196	3.064628	1	1.944666	3.535731	0.752582
1	-2.054487	-1.538468	2.567543	1	-0.584064	-1.718014	3.165423
8	6.585183	0.266567	0.339262	1	-1.286596	-0.102081	3.074389
8	6.267656	-1.878963	0.816640	1	-2.238642	-1.521880	2.600181
1	7.434084	0.025784	0.725127	6	7.582586	0.045164	0.712996
NImag = 1 (-112.5183 cm ⁻¹)				1	8.044496	1.023305	0.643844
				1	7.561036	-0.291695	1.745780
				1	8.136756	-0.678326	0.121287
				NImag = 1 (-115.3315 cm ⁻¹)			
TS6(Cl)re-si				TS6(F)re-si			
Et = -1590.6446867				Et = -1230.2409847			
6	2.626291	-1.679785	-0.380355	7	-2.625955	-1.340455	0.200536
6	2.157081	-0.563712	-1.060214	6	-2.010523	-0.143581	0.172802
6	3.026848	0.496481	-1.288569	7	-2.881330	0.822763	-0.174644
6	4.327270	0.463730	-0.818527	6	-4.132888	0.241210	-0.626390
6	4.763227	-0.650781	-0.121283	6	-4.056317	-1.170869	-0.024811
6	3.923181	-1.728800	0.099012	7	-0.745306	0.087378	0.455044
6	0.771392	-0.562676	-1.622305	6	-0.000294	-0.750129	1.396256
8	0.075586	-1.589282	-1.608423	6	-0.648213	-0.791229	2.762030
17	6.394627	-0.702833	0.468609	6	-2.733478	2.211538	0.173794
6	-0.280520	0.798792	-0.340119	6	-4.251220	0.256130	-2.138091
6	0.453307	1.722452	0.479830	6	-4.856491	-1.338194	1.251416
8	0.603466	1.665528	1.685523	6	-1.959695	-2.601463	-0.038986
7	-1.116683	-0.115708	0.377121	6	-0.012986	1.032422	-0.329950
6	-0.483451	-1.100256	1.259245	6	0.665648	2.056000	0.401728
6	-1.107307	-1.108892	2.636999	8	1.183007	2.995729	-0.427034
6	-2.407977	-0.153978	0.117136	6	1.930916	4.001876	0.215354
7	-3.157256	0.942837	-0.096344	8	0.842361	2.109194	1.605647
6	-4.498447	0.575879	-0.516473	6	1.037341	-0.333959	-1.696574

6	-4.565917	-0.909550	-0.120236	8	0.194290	-1.226009	-1.847198
7	-3.160874	-1.262725	0.030527	6	2.344650	-0.602380	-1.027927
6	-2.817258	2.257686	0.385021	6	2.650859	-1.894624	-0.621214
6	-2.649955	-2.561519	-0.349201	6	3.878358	-2.190999	-0.054545
6	-5.360424	-1.171739	1.143551	6	4.800538	-1.174958	0.089520
6	-4.725399	0.828687	-1.994033	6	4.536022	0.117393	-0.320427
8	1.035415	2.689623	-0.260531	6	3.304792	0.393986	-0.885705
6	1.883715	3.556750	0.458730	1	-1.695444	-3.102663	0.891981
1	-2.501333	-3.206129	0.516653	1	-2.639731	-3.247001	-0.589518
1	-3.375982	-3.035543	-1.006129	1	-1.072786	-2.428218	-0.646285
1	-1.712898	-2.433860	-0.889423	1	-2.400709	2.817349	-0.667595
1	-2.408800	2.892206	-0.399559	1	-3.693514	2.588835	0.521774
1	-3.715187	2.725470	0.784272	1	-2.008447	2.308997	0.976688
1	-2.081927	2.175722	1.180719	1	-4.375613	-1.907263	-0.761143
1	-4.977403	-1.494868	-0.942127	1	-4.956630	0.797240	-0.178871
1	-5.213496	1.151078	0.072094	1	-4.210727	1.274859	-2.519155
1	-4.578103	1.879816	-2.235297	1	-3.432014	-0.305357	-2.585362
1	-4.027891	0.242831	-2.590998	1	-5.194361	-0.187316	-2.455881
1	-5.740769	0.555549	-2.279380	1	-5.922880	-1.232155	1.054701
1	-6.410578	-0.921951	0.995816	1	-4.688056	-2.321421	1.686856
1	-5.298786	-2.220235	1.428890	1	-4.564543	-0.588154	1.985355
1	-4.975654	-0.572268	1.967588	1	-0.551641	1.357583	-1.203265
1	-0.785333	1.240274	-1.184354	1	0.971872	-0.282052	1.477106
1	0.548393	-0.781632	1.334983	1	0.154420	-1.743692	0.987273
1	-0.480681	-2.082898	0.800434	1	1.090263	0.505839	-2.402388
1	0.666524	0.162579	-2.443443	1	1.911334	-2.665976	-0.775303
1	1.957835	-2.518080	-0.253788	1	4.134845	-3.190133	0.262866
1	4.288751	-2.595647	0.627614	1	5.290082	0.879047	-0.195319
1	5.002966	1.286154	-0.996227	1	3.073725	1.398834	-1.210060
1	2.678226	1.360740	-1.835081	1	2.268078	4.670729	-0.569835
1	2.261373	4.272030	-0.264495	1	1.321933	4.546258	0.933367
1	1.339492	4.072601	1.245935	1	2.784175	3.580762	0.741551
1	2.706914	3.008214	0.908861	1	-0.037825	-1.388190	3.437621
1	-0.580103	-1.818953	3.272270	1	-0.715938	0.217254	3.163293
1	-1.023857	-0.121197	3.084013	1	-1.644299	-1.232227	2.736200
1	-2.156340	-1.404236	2.612878	9	5.988134	-1.449990	0.632866
NImag = 1 (-145.6391 cm ⁻¹)				NImag = 1 (-143.0359 cm ⁻¹)			
TS6(H)re-si Et = -1131.0385392				TS6(Me)re-si Et = -1170.3488474			
7	-2.536903	0.935534	-0.289361	6	3.228731	0.370921	-0.901716
6	-1.739737	-0.038979	0.191119	6	2.235401	-0.588830	-1.069566
7	-2.430363	-1.192866	0.303026	6	2.508003	-1.898367	-0.702779
6	-3.833805	-0.958023	-0.021442	6	3.733682	-2.236565	-0.153065
6	-3.775889	0.368799	-0.790430	6	4.722034	-1.279232	0.037436

7	-0.477550	0.148909	0.511695	6	4.448957	0.030939	-0.352278
6	0.184199	-0.659498	1.538250	6	0.934741	-0.252764	-1.715684
6	-0.477823	-0.511264	2.889728	8	0.044302	-1.097404	-1.867953
6	-1.836511	-2.506537	0.181315	6	6.043828	-1.634781	0.648274
6	-4.700720	-0.908829	1.220720	6	-0.041453	1.123331	-0.284353
6	-3.743390	0.199460	-2.297407	6	0.656923	2.159692	0.406782
6	-2.341311	2.341893	-0.059206	8	0.891357	2.232486	1.600041
6	0.331967	0.995826	-0.306541	7	-0.736594	0.173166	0.526574
6	1.099667	1.989231	0.372674	6	0.039694	-0.604745	1.494128
8	1.689840	2.837903	-0.506034	6	-0.609097	-0.622521	2.859910
6	2.528975	3.804254	0.080814	6	-1.979094	-0.137956	0.224460
8	1.292756	2.088549	1.571522	7	-2.541783	-1.361870	0.305248
6	1.234670	-0.538572	-1.637405	6	-3.967548	-1.267387	0.006679
8	0.281072	-1.310889	-1.780861	6	-4.066048	0.087552	-0.707046
6	2.478029	-0.946725	-0.921252	7	-2.886725	0.763567	-0.199297
6	3.541127	-0.063396	-0.766809	6	-1.814172	-2.599294	0.123716
6	4.708227	-0.472869	-0.147756	6	-2.834079	2.173884	0.076363
6	4.831121	-1.776197	0.313935	6	-4.040290	-0.017563	-2.220210
6	3.782586	-2.667093	0.145263	6	-4.814327	-1.363932	1.259960
6	2.614262	-2.254403	-0.473428	8	1.126732	3.092667	-0.459024
1	-1.607061	-2.939726	1.154559	6	1.895900	4.112340	0.133172
1	-2.550322	-3.157947	-0.316513	1	-1.495079	-3.024593	1.074843
1	-0.939580	-2.438506	-0.431876	1	-2.475210	-3.314372	-0.359009
1	-1.950900	2.857459	-0.935520	1	-0.958948	-2.418626	-0.525349
1	-3.295698	2.788228	0.215514	1	-2.524051	2.757177	-0.789712
1	-1.643421	2.481110	0.760775	1	-3.822240	2.507116	0.389548
1	-4.171382	-1.757209	-0.679374	1	-2.132263	2.358742	0.883890
1	-4.602055	1.015749	-0.496711	1	-4.227438	-2.070739	-0.680684
1	-3.619361	1.161643	-2.790959	1	-4.951860	0.628812	-0.375759
1	-2.906712	-0.436820	-2.584036	1	-4.035639	0.971157	-2.675545
1	-4.668654	-0.249431	-2.657540	1	-3.140751	-0.541108	-2.542549
1	-5.747386	-0.761877	0.956073	1	-4.914294	-0.555047	-2.587075
1	-4.618994	-1.836362	1.784177	1	-5.875028	-1.318810	1.014829
1	-4.390303	-0.090578	1.869393	1	-4.625468	-2.300481	1.781385
1	-0.167463	1.317586	-1.202950	1	-4.581453	-0.545595	1.940104
1	1.196689	-0.282163	1.587793	1	-0.605849	1.433304	-1.145516
1	0.245390	-1.697855	1.228860	1	0.995340	-0.102099	1.558239
1	1.403782	0.276712	-2.352959	1	0.228136	-1.605278	1.118438
1	1.795283	-2.939183	-0.637143	1	1.007249	0.606823	-2.394986
1	3.880948	-3.687526	0.488087	1	1.750059	-2.648460	-0.874778
1	5.743859	-2.096540	0.795433	1	3.931355	-3.263835	0.123390
1	5.525790	0.222917	-0.024120	1	5.207788	0.791288	-0.222797
1	3.436083	0.952348	-1.122346	1	3.028329	1.392385	-1.194927
1	2.920434	4.397447	-0.739325	1	2.193320	4.770728	-0.676679
1	1.976424	4.438979	0.769877	1	1.316814	4.664944	0.869602
1	3.344325	3.336437	0.627418	1	2.775035	3.704896	0.626650

1	0.061686	-1.101734	3.628548	1	0.017306	-1.179288	3.554961
1	-0.448187	0.531382	3.196781	1	-0.707761	0.395536	3.229487
1	-1.512722	-0.852550	2.880709	1	-1.591892	-1.092894	2.845641
NImag = 1 (-139.4587 cm ⁻¹)				1	6.171028	-2.713016	0.719704
				1	6.872660	-1.238385	0.062510
				1	6.136678	-1.224656	1.654871
				NImag = 1 (-145.8350 cm ⁻¹)			
TS6(OMe)re-si Et = -1245.5241639				TS6(OH)re-si Et = -1206.2284067			
6	2.229743	-1.813378	-0.798332	6	2.520292	-1.909025	-0.668339
6	1.935744	-0.495243	-1.134825	6	2.250950	-0.599344	-1.035962
6	2.925917	0.461610	-0.971980	6	3.250068	0.355819	-0.867715
6	4.169858	0.133526	-0.457209	6	4.471961	0.022786	-0.321422
6	4.439891	-1.184395	-0.106579	6	4.720849	-1.291410	0.058186
6	3.462071	-2.158704	-0.286422	6	3.742409	-2.259186	-0.120007
6	0.614136	-0.157594	-1.734635	6	0.950709	-0.262077	-1.680439
8	-0.268331	-1.015427	-1.882009	8	0.061528	-1.111511	-1.832124
8	5.614565	-1.613129	0.403638	6	-0.025777	1.116379	-0.284935
6	6.627480	-0.671694	0.603226	6	0.672781	2.156431	0.403693
6	-0.341926	1.166291	-0.281194	8	0.896216	2.238619	1.598022
6	0.360833	2.212281	0.392715	7	-0.733898	0.180553	0.532587
8	0.641039	2.283776	1.575787	6	0.031286	-0.593466	1.511720
7	-0.994686	0.198132	0.544433	6	-0.627061	-0.595625	2.873059
6	-0.177202	-0.558618	1.494778	6	-1.974090	-0.129713	0.220400
6	-0.804074	-0.606199	2.870086	7	-2.873754	0.770613	-0.222310
6	-2.227597	-0.159278	0.252823	6	-4.048144	0.092620	-0.738982
7	-3.170960	0.708601	-0.163562	6	-3.965521	-1.251900	-0.004278
6	-4.323788	-0.011106	-0.671494	7	-2.542946	-1.350341	0.309261
6	-4.176781	-1.357280	0.049455	6	-2.819337	2.183717	0.037686
7	-2.747050	-1.401893	0.343162	6	-1.818992	-2.592152	0.142955
6	-3.169406	2.120561	0.105475	6	-4.824291	-1.323505	1.242486
6	-1.978883	-2.613522	0.152352	6	-3.997920	-0.034226	-2.249861
6	-5.014372	-1.474311	1.307084	8	1.156286	3.077581	-0.466332
6	-4.287206	-0.122317	-2.184108	6	1.925736	4.099205	0.123203
8	0.780583	3.157979	-0.485499	1	-1.511408	-3.012577	1.100089
6	1.547401	4.192125	0.083841	1	-2.478287	-3.307559	-0.341690
1	-1.621600	-3.019173	1.098329	1	-0.956934	-2.418207	-0.499017
1	-2.625252	-3.355876	-0.308198	1	-2.502572	2.756493	-0.833009
1	-1.147616	-2.405772	-0.519368	1	-3.808417	2.523233	0.341118
1	-2.905130	2.712389	-0.770146	1	-2.121968	2.375610	0.847385
1	-4.162103	2.415514	0.442268	1	-4.223963	-2.064120	-0.681586
1	-2.455807	2.336991	0.894322	1	-4.936651	0.642295	-0.429518
1	-4.412099	-2.173026	-0.631955	1	-3.983746	0.947945	-2.718948
1	-5.229582	0.499075	-0.345025	1	-3.094004	-0.563611	-2.549708

1	-4.323955	0.863630	-2.644059	1	-4.866890	-0.575195	-2.623481
1	-3.363514	-0.606622	-2.499586	1	-5.882428	-1.276880	0.986866
1	-5.135488	-0.698930	-2.551996	1	-4.645019	-2.252322	1.780787
1	-6.077100	-1.466129	1.066677	1	-4.593238	-0.495301	1.911200
1	-4.791873	-2.400653	1.833462	1	-0.588423	1.427594	-1.146966
1	-4.805830	-0.644372	1.981052	1	0.989710	-0.096443	1.578134
1	-0.943323	1.476644	-1.116651	1	0.215795	-1.598408	1.145846
1	0.761605	-0.024259	1.548271	1	1.029958	0.586150	-2.373371
1	0.039060	-1.550043	1.110234	1	1.758748	-2.655933	-0.837167
1	0.663169	0.708102	-2.408539	1	3.942222	-3.286891	0.157354
1	1.472952	-2.565543	-0.965227	8	5.934344	-1.570420	0.586644
1	3.701018	-3.179219	-0.026826	1	5.247641	0.760165	-0.181247
1	4.913852	0.904595	-0.335053	1	3.053009	1.378047	-1.159929
1	2.714363	1.488052	-1.238873	1	2.234542	4.747587	-0.690357
1	1.805291	4.857693	-0.733669	1	1.342339	4.662095	0.848261
1	0.981094	4.731803	0.839576	1	2.797607	3.691704	0.629251
1	2.449869	3.802209	0.548599	1	-0.009422	-1.150534	3.577402
1	-0.148671	-1.145473	3.552020	1	-0.721581	0.426118	3.233356
1	-0.931631	0.405583	3.248143	1	-1.612868	-1.059520	2.855402
1	-1.770758	-1.108989	2.867786	1	5.977981	-2.503448	0.798398
1	7.469895	-1.215505	1.017770				
1	6.931951	-0.203156	-0.334231				
1	6.322199	0.104448	1.306996				
NImag = 1 (-169.2115 cm ⁻¹)				NImag = 1 (-161.3682 cm ⁻¹)			