Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Electronic Supplementary Information
for

Ni, Pd, or Pt Catalyzed Ethylene Dimerization: A Mechanistic Description of the Catalytic Cycle and the Active Species

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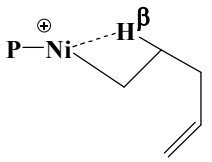
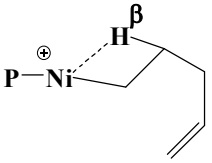
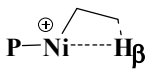
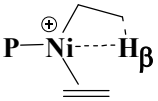
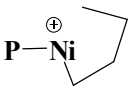
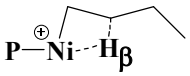
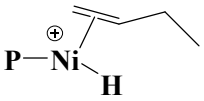
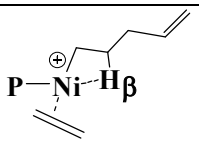
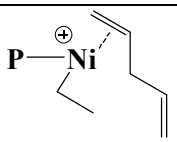
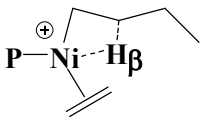
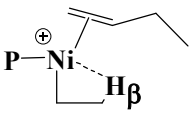
Table S1: Relative energies[a] (in kcal/mol) obtained at the mPW1K level of theory for the stationary points involved in pathway-1 and pathway-2 for ethylene dimerization[b]

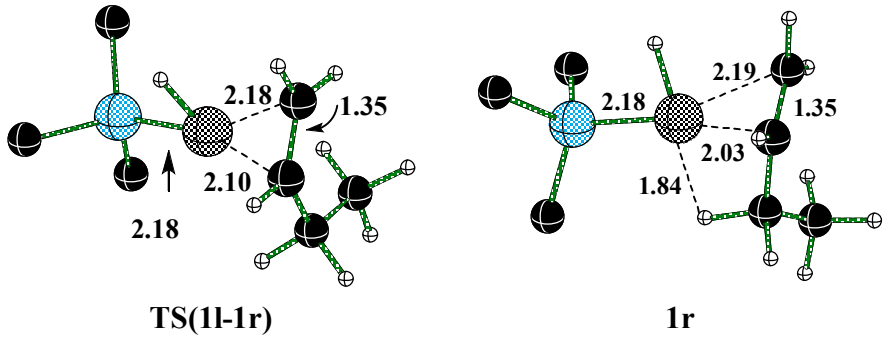
Species	ΔH			ΔG		
	Ni(II)	Pd(II)	Pt(II)	Ni(II)	Pd(II)	Pt(II)
b	-25.8	-24.6	-37.2	-13.2	-11.3	-23.5
b-c	-17.0	-5.3	-8.9	-3.4	9.1	4.6
c	-26.7	-29.4	-32.5	-13.8	-15.0	-19.5
c-d	-4.6	-12.0	-9.8	6.8	1.31	2.7
d	-9.4	-11.6	-10.5	1.1	0.2	0.6
d-d′	3.2	–[c]	–[c]	13.9	–[c]	–[c]
d′	0.5	–[c]	–[c]	11.0	–[c]	–[c]
d-e	1.2	0.4	3.9	12.1	12.8	14.1
e	-17.7	-20.3	-14.9	-4.8	-6.7	-4.1
e′	-1.2	–[c]	–[c]	8.3	–[c]	–[c]
e-f′	–[d]	-5.2	-13.9	–[c]	7.1	-2.3
f′	–[d]	-6.1	-31.9	–[d]	4.7	-18.6
f	55.2	60.2	78.4	53.8	60.1	76.9
g	3.0	-4.0	-12.3	11.7	5.9	-2.9
g-h	3.2	2.0	5.5	13.3	13.4	15.3
h	-0.1	2.6	-10.9	11.4	13.4	-0.9
i	-30.6	-27.1	-32.9	-8.4	-3.6	-9.9
i-j	-28.0	-16.3	-16.1	-4.8	7.5	7.3
j	-40.0	-42.5	-44.5	-16.8	-18.1	-20.7
j-k	-37.2	-39.3	-37.1	-14.3	-15.6	-14.2
k	-39.4	-40.4	-39.5	-17.7	-17.6	-17.6
k-l	-29.0	-23.9	-26.0	-7.1	-0.4	-2.4
l	-33.6	-37.1	-46.6	-11.6	-14.2	-24.1
m	-33.6	-31.5	-36.7	-10.2	-7.4	-12.7
m-n	-28.3	-22.2	-32.0	-4.0	2.6	-7.7
n	-36.6	-33.4	-38.5	-13.8	-9.6	-14.4
o	-62.6	-60.4	-65.9	-28.3	-25.5	-31.0
o-p	-57.6	-51.6	-61.4	-22.4	-15.8	-26.3
p	-66.1	-63.2	-67.6	-31.9	-28.1	-32.6
m′	–[d]	-39.7	-52.8	–[d]	-13.4	-26.2
m′-n′	–[d]	6.9	2.2	–[d]	33.6	28.8
n′	–[d]	-38.3	-48.6	–[d]	-12.1	-23.6

[a]Relative energies are with respect to **1** and appropriate number of ethylene and pentadiene molecule(s). [b]LANL2DZ ECP basis set for transition metals and 6-311+G** basis set for all other atoms are used for all calculations. [c]Feature of Ni-catalyzed reactions only. [d]Feature of Pd and Pt catalyzed reactions only.

Table S2: Summary of the topological analysis of the Ni···H_β interaction present in various key intermediates involved in pathway-1 and pathway-2 for ethylene dimerization[a,b]

Molecule			
	1d	**1d′**	
ρ	0.0643	0.1003	
$\nabla^2\rho$	-0.0862	-0.0773	
Molecule			
	1h	**1i**	**1j**
ρ	0.0914	0.0837	0.0473
$\nabla^2\rho$	-0.0839	-0.0903	-0.0649
Molecule			
	1k	**1l**	**1m**
ρ	0.0640	0.0318	0.0994
$\nabla^2\rho$	-0.0848	-0.0463	-0.0776
Molecule			
	1n	**1o**	**1p**
ρ	0.0700	0.0762	0.0700
$\nabla^2\rho$	-0.0885	-0.0881	-0.0885

[a]Topologaical properties at the Ni···H_β bond critical point are in a.u. [b]The mPW1K/LANL2DZ, 6-311+G** level of theory is used for all calculations



TS(1l-1r) **1r**

Figure S1: The mPW1K/LANL2DZ, 6-311+G** optimized geometries of important transition state and intermediate (bond length in Å). Color Code: Gray-Ni; Cyan-P; Black-C; Ivory-H.

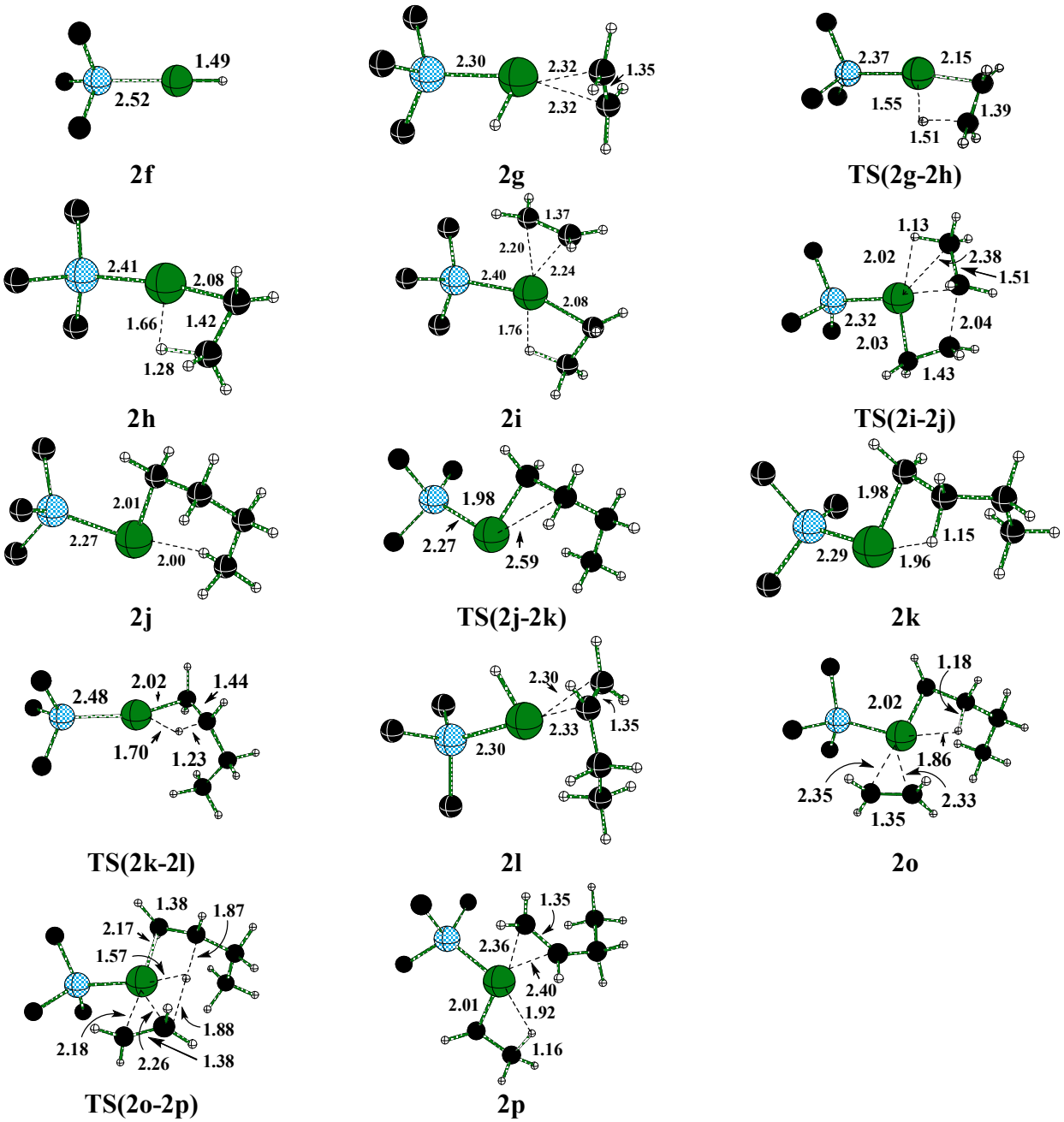


Figure S2: The mPW1K/LANL2DZ,6-311+G** optimized geometries of key intermediates and interconnecting transition states (bond length in Å). Color Code: Green-Pd; Cyan-P; Black-C; Ivory-H.

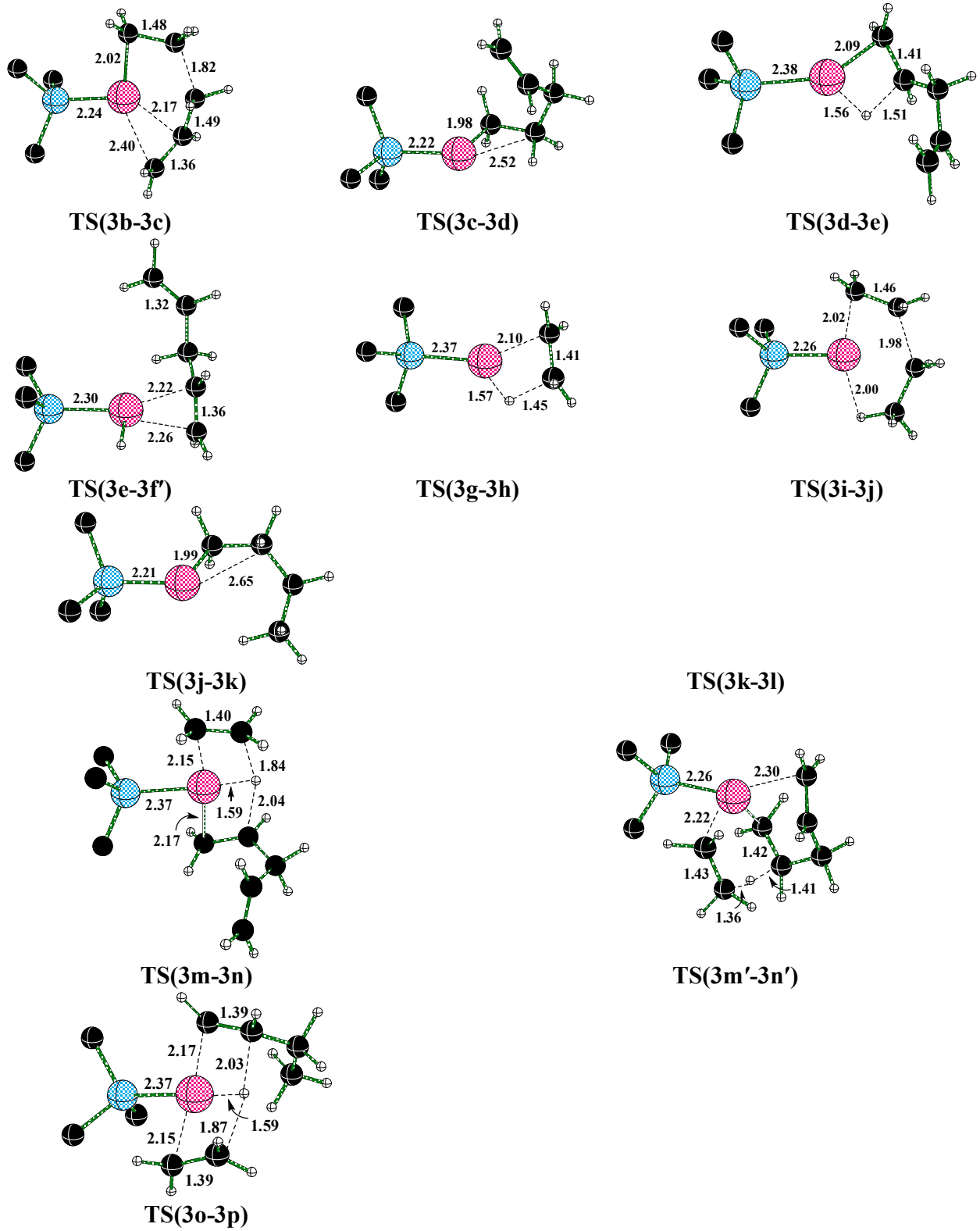


Figure S3: The mPW1K/LANL2DZ,6-311+G** optimized geometries of key transition states (bond length in Å). Color Code: Pink-Pt; Cyan-P; Black-C; Ivory-H.

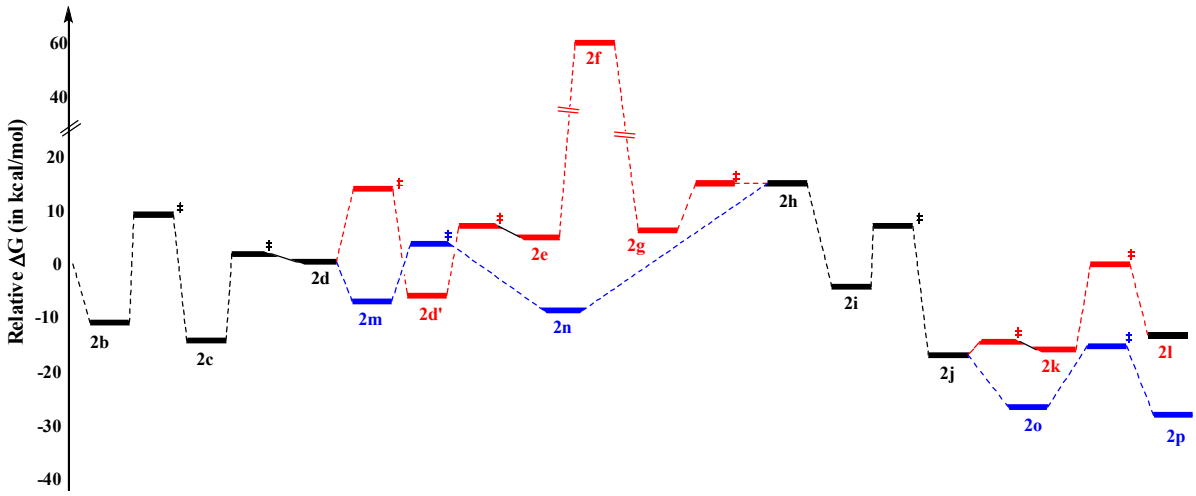


Figure S4: The reaction profile constructed using the Gibbs free energies obtained at the mPW1K level of theory for Pd(II) catalyzed ethylene dimerization. (Elementary steps common to both the pathways are in black while that associated exclusively with pathway-1 and pathway-2 are respectively in red and blue colours.)

Full Citation of Reference 20:

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

mPW1K/LANL2DZ ECP, 6-311+G Optimized coordinates, energy (in a.u.), and number and magnitude (in cm^{-1}) of imaginary frequency (NImag) of all stationary points reported in the manuscript**

C_2H_4
E= -78.5852066
NImag= 0

6	0.000000	0.659901	0.000000
6	0.000000	-0.659901	0.000000
1	-0.919047	1.226843	0.000000
1	0.919047	1.226843	0.000000
1	0.919047	-1.226843	0.000000
1	-0.919047	-1.226843	0.000000

1,4-Pentadiene
E= -195.2942678
NImag= 0

6	-2.352491	-0.173338	0.147933
6	-1.163376	-0.178028	-0.429533
1	-3.153506	-0.805363	-0.203441
1	-2.567224	0.466093	0.992714
1	-0.983783	-0.836426	-1.270703
6	-0.000002	0.659115	-0.000198
1	-0.310433	1.306014	0.821041
1	0.310409	1.305499	-0.821850
6	1.163392	-0.177724	0.429669
6	2.352480	-0.173437	-0.147854
1	0.983837	-0.835540	1.271304
1	3.153508	-0.805225	0.203917
1	2.567176	0.465412	-0.993084

Ni(II)-Catalyzed Dimerization:

1a
E= -747.483945
NImag=0

28	0.842632	-0.469081	0.039901
6	1.521780	1.318069	-0.249274
6	2.559146	0.581184	0.371633
6	2.907177	-0.609968	-0.211692
1	1.079906	2.152597	0.273554
1	1.508565	1.391326	-1.331139
1	2.837317	0.786813	1.395949
1	2.811757	-0.746106	-1.283884
1	3.515831	-1.328875	0.314457
15	-1.350459	-0.015180	0.005442
6	-1.883014	0.990814	-1.405097
1	-1.633057	0.489550	-2.335860
1	-2.957331	1.154493	-1.370996
1	-1.380854	1.953514	-1.386894
6	-1.932924	0.871763	1.475710
1	-3.004614	1.045298	1.415983

1	-1.719518	0.291416	2.368826
1	-1.426033	1.828412	1.560040
6	-2.373907	-1.514833	-0.073104
1	-2.179760	-2.149678	0.787258
1	-3.429236	-1.251971	-0.079761
1	-2.149347	-2.076994	-0.975444

1b

E= -826.1137003

NImag=0

28	-0.766970	0.061968	-0.027442
6	-0.739988	-1.925890	-0.209819
1	-0.707671	-1.991181	-1.291079
1	-0.044202	-2.560104	0.315788
6	-1.934822	-1.555951	0.409461
1	-2.090841	-1.769651	1.457879
6	-0.643084	2.169526	-0.029268
1	-0.062586	2.398294	0.850618
1	-0.209617	2.426522	-0.983657
6	-1.964163	1.900244	0.078984
1	-2.447928	1.869228	1.042959
1	-2.608112	1.921595	-0.785693
6	-2.733425	-0.624206	-0.228936
1	-3.593101	-0.211022	0.271299
1	-2.746633	-0.581040	-1.311065
15	1.476498	-0.025310	0.002919
6	2.199961	-1.075589	-1.291300
1	1.926386	-0.694354	-2.271535
1	3.283982	-1.074291	-1.207797
1	1.845236	-2.097217	-1.207502
6	2.435211	1.510234	-0.169774
1	2.217303	1.992415	-1.118292
1	2.212649	2.204515	0.634305
1	3.496824	1.277719	-0.138105
6	2.085025	-0.715439	1.569775
1	1.766563	-0.087361	2.397285
1	1.689801	-1.713538	1.729107
1	3.171347	-0.763547	1.565342

TS(1b-1c)

E= -826.0992375

NImag=1(-243.15)

28	0.628228	-0.009984	-0.011019
6	1.135492	2.066133	-0.273632
1	1.070541	2.013048	-1.352744
1	0.599495	2.870617	0.203162
6	2.058337	1.346657	0.414971
1	2.214851	1.545390	1.466610
6	0.726652	-1.884995	-0.103485
1	0.217393	-2.356833	0.726774
1	0.435559	-2.264057	-1.074410
6	2.125041	-1.579174	0.088385
1	2.506887	-1.756961	1.083056
1	2.794251	-1.934217	-0.682057
6	2.732066	0.196773	-0.182473

1	3.669831	-0.037430	0.297089
1	2.846923	0.269720	-1.257609
15	-1.553784	0.018145	0.006084
6	-2.306406	1.624064	-0.382988
1	-2.008143	1.946367	-1.376691
1	-3.391019	1.550718	-0.351097
1	-1.985728	2.372294	0.335718
6	-2.361873	-1.132971	-1.138010
1	-2.056012	-0.919143	-2.158278
1	-2.083053	-2.155022	-0.901365
1	-3.442630	-1.037787	-1.067808
6	-2.214250	-0.406060	1.641516
1	-1.900978	-1.407088	1.921554
1	-1.841264	0.291621	2.385753
1	-3.300886	-0.366423	1.633920

1c
E= -826.1162856
NImag=0

28	0.379256	-0.505859	0.010076
6	2.155826	-1.682002	0.372590
1	2.337574	-1.590054	1.434389
1	1.782507	-2.636501	0.018962
6	2.567646	-0.740876	-0.497629
1	2.489477	-0.937282	-1.561854
6	0.830858	1.229748	0.574675
1	0.036886	1.964631	0.487191
1	1.038108	1.058279	1.634034
6	2.058611	1.633127	-0.205448
1	1.808437	1.797364	-1.253273
1	2.433655	2.587029	0.171418
6	3.146121	0.568521	-0.086892
1	3.999623	0.817154	-0.712688
1	3.492894	0.512352	0.943212
15	-1.763885	0.020955	-0.038616
6	-2.768409	-1.439346	-0.443366
1	-2.616875	-2.218128	0.299154
1	-3.823892	-1.177273	-0.461520
1	-2.491316	-1.829679	-1.418921
6	-2.434671	0.627171	1.530941
1	-2.305060	-0.127426	2.301433
1	-1.915206	1.528369	1.841502
1	-3.494219	0.848365	1.427853
6	-2.221173	1.256853	-1.282779
1	-1.709723	2.195153	-1.091060
1	-1.938381	0.906887	-2.271487
1	-3.294237	1.431328	-1.263783

TS(1c-1d)
E= -826.0795954
NImag=1 (-95.58)

28	0.340174	-0.996805	-0.170605
6	-4.402643	1.543199	-0.043133
1	-4.428666	1.781866	1.010791
1	-4.810946	2.277311	-0.719901
6	-3.918304	0.395293	-0.483319

1	-3.928416	0.188661	-1.547371
6	-0.951248	0.165629	0.380341
1	-0.874627	0.434431	1.430040
1	-1.092041	1.037677	-0.249640
6	-1.885014	-0.980606	0.092076
1	-1.828104	-1.265625	-0.968174
1	-1.615469	-1.857581	0.698372
6	-3.370050	-0.680387	0.391283
1	-3.928768	-1.603315	0.240741
1	-3.469541	-0.407833	1.439541
15	2.070769	0.304686	0.000907
6	3.613587	-0.572528	-0.381154
1	3.584755	-0.963166	-1.394607
1	4.460255	0.104577	-0.292831
1	3.756595	-1.401087	0.306946
6	2.024892	1.719691	-1.127682
1	1.951513	1.374924	-2.154900
1	1.161429	2.340647	-0.909577
1	2.926923	2.317041	-1.017569
6	2.304658	1.001112	1.655301
1	1.450525	1.615437	1.923154
1	2.400643	0.203391	2.385947
1	3.202253	1.614488	1.680079

1d

E= -826.0876544

NImag=0

28	-0.222696	-0.945600	-0.174033
6	4.250820	1.566661	-0.224971
1	3.782478	2.020724	-1.087081
1	4.977614	2.162029	0.304751
6	3.969189	0.331349	0.149812
1	4.476321	-0.091506	1.008792
6	0.926208	0.068503	0.835835
1	1.118181	1.062099	0.446191
1	0.646424	0.077957	1.883167
6	1.877998	-0.991642	0.407050
1	2.252712	-1.574645	1.244946
1	1.290207	-1.812102	-0.153712
6	2.991149	-0.559209	-0.542077
1	3.500887	-1.446480	-0.917320
1	2.567155	-0.045142	-1.403533
15	-2.028503	0.293165	-0.030001
6	-3.451206	-0.474168	-0.858013
1	-3.675981	-1.436708	-0.406787
1	-4.326647	0.165115	-0.769028
1	-3.237634	-0.626036	-1.912522
6	-2.573556	0.602578	1.669087
1	-2.758645	-0.338565	2.178566
1	-1.805532	1.144696	2.212207
1	-3.487674	1.191409	1.669611
6	-1.857064	1.927906	-0.791571
1	-1.069883	2.487492	-0.295530
1	-1.599052	1.825223	-1.841593
1	-2.789130	2.481886	-0.709090

TS(1d-1d')
E = -826.0653394
Nimag = 1 (-101.91)

28	-0.102287	-0.307020	0.122138
15	-2.407290	0.167476	-0.030470
6	-3.362797	-1.247192	-0.657018
1	-4.418912	-0.993340	-0.711199
1	-3.017751	-1.523439	-1.649395
1	-3.240829	-2.102634	0.001307
6	-2.831294	1.539012	-1.142245
1	-2.363952	2.456392	-0.796135
1	-2.471883	1.328877	-2.145505
1	-3.908779	1.682482	-1.175480
6	-3.191237	0.587372	1.553074
1	-3.057712	-0.225178	2.261358
1	-2.736122	1.482109	1.967876
1	-4.255099	0.764615	1.413780
6	1.412723	-1.352163	-0.139711
1	1.308397	-2.277737	0.415739
1	1.583977	-1.484055	-1.203584
6	2.013326	-0.206741	0.517281
1	2.361722	-0.403384	1.527777
1	1.096577	0.523628	0.783485
6	2.962734	0.683854	-0.274203
1	3.052333	1.654981	0.206551
1	2.548314	0.849345	-1.269526
6	4.308328	0.042473	-0.372978
6	5.415061	0.566262	0.122566
1	4.352070	-0.908923	-0.888902
1	6.366049	0.068318	0.018470
1	5.413913	1.515091	0.639972

1d'
E = -826.0702107
Nimag=0

28	-0.211848	-0.860999	-0.038955
15	-2.190014	0.312241	0.000364
6	-3.601399	-0.618610	-0.667348
1	-4.507314	-0.018903	-0.621042
1	-3.415856	-0.890815	-1.702816
1	-3.756168	-1.528850	-0.094448
6	-2.160197	1.851392	-0.961903
1	-1.400450	2.521458	-0.569870
1	-1.924235	1.636204	-2.000284
1	-3.125667	2.349532	-0.916590
6	-2.713319	0.809289	1.666138
1	-2.835497	-0.068392	2.294641
1	-1.960928	1.449936	2.117137
1	-3.657110	1.347703	1.626721
6	1.507374	-1.647284	0.015050
1	1.508158	-2.454720	0.738700
1	1.814466	-1.930727	-0.986534
6	1.805561	-0.315442	0.466205
1	2.038007	-0.226928	1.523883
1	0.702446	0.273555	0.497261

6	2.639754	0.609132	-0.407324
1	2.466697	1.647483	-0.134318
1	2.335066	0.486840	-1.447351
6	4.089578	0.281788	-0.250522
6	4.991074	1.125112	0.219583
1	4.391808	-0.714159	-0.549336
1	6.028989	0.844779	0.305167
1	4.728989	2.128095	0.525076

TS(1d-1e)

E= -826.0665116

NImag=1 (-489.67)

28	-0.238457	-0.841113	-0.030063
15	-2.143870	0.326941	0.001765
6	-3.567107	-0.618372	-0.618504
1	-4.469416	-0.012510	-0.578947
1	-3.397018	-0.922822	-1.647656
1	-3.719271	-1.509252	-0.015223
6	-2.107212	1.830213	-1.011394
1	-1.339677	2.505452	-0.645027
1	-1.878079	1.578183	-2.042902
1	-3.069112	2.335986	-0.977157
6	-2.634047	0.875266	1.658855
1	-2.747671	0.017275	2.315388
1	-1.870366	1.525468	2.075224
1	-3.576566	1.415766	1.618648
6	1.522954	-1.737110	0.031751
1	1.393011	-2.520868	0.768158
1	1.729917	-2.050121	-0.985391
6	1.875369	-0.463905	0.438535
1	1.983902	-0.282238	1.501096
1	0.409744	0.311263	0.479061
6	2.598878	0.509536	-0.450359
1	2.326523	1.532716	-0.203738
1	2.328447	0.330429	-1.490466
6	4.073742	0.322130	-0.256429
6	4.873477	1.241595	0.253290
1	4.477325	-0.635039	-0.560294
1	5.930969	1.062064	0.365894
1	4.505871	2.209173	0.564158

1e

E= -826.0992589

Nimag= 0

28	-0.463066	-0.280087	-0.057832
6	-0.966331	1.826664	0.462518
1	-1.016517	1.670284	1.532839
1	-0.204993	2.496092	0.099085
6	-1.951070	1.411661	-0.352105
1	-1.918046	1.691259	-1.397957
6	-2.022291	-1.743303	0.415581
1	-1.756618	-2.711467	0.025117
1	-2.017952	-1.635463	1.492455
6	-2.571227	-0.807251	-0.387458

1	0.139466	-1.551652	-0.028792
1	-2.663464	-1.021640	-1.445210
6	-3.080730	0.525025	0.072149
1	-4.014533	0.792339	-0.413315
1	-3.222356	0.548945	1.149034
15	1.706136	-0.025534	-0.016276
6	2.385573	1.660810	-0.057315
1	2.079891	2.217256	0.823870
1	3.472260	1.617887	-0.077988
1	2.044184	2.186630	-0.944659
6	2.477952	-0.763985	1.448208
1	2.084273	-0.302439	2.349432
1	2.260336	-1.826788	1.484801
1	3.555050	-0.618876	1.421591
6	2.493976	-0.832103	-1.436886
1	2.274633	-1.895059	-1.429145
1	2.112078	-0.410111	-2.362396
1	3.570982	-0.686859	-1.403473

1e′
E= -826.0714456
NImag=0

28	0.123507	-0.532121	-0.005186
15	2.156686	0.296916	0.003890
6	2.494996	1.306100	1.476858
1	3.510642	1.693985	1.440048
1	1.804325	2.143295	1.527659
1	2.383575	0.708324	2.377347
6	2.498374	1.378582	-1.406937
1	2.400550	0.819608	-2.332602
1	1.788845	2.200710	-1.425913
1	3.505703	1.782029	-1.338261
6	3.447440	-0.971610	-0.015137
1	3.335179	-1.629238	0.842007
1	3.364358	-1.567895	-0.918625
1	4.431155	-0.509815	0.019464
6	-1.504164	-1.917975	0.062394
1	-1.210920	-2.710228	-0.609236
1	-1.550883	-2.162846	1.117208
6	-1.987324	-0.745440	-0.401026
1	-2.062507	-0.593598	-1.471084
1	0.642316	-1.039707	-1.186807
6	-2.610030	0.311300	0.459892
1	-2.188707	1.289720	0.223244
1	-2.415155	0.100803	1.513289
6	-4.092292	0.359043	0.222424
6	-4.729753	1.405517	-0.268693
1	-4.638414	-0.539092	0.478799
1	-5.798157	1.389024	-0.414827
1	-4.213893	2.317466	-0.533502

1f
E= -630.6851943
NImag=0

28	1.697044	-0.005071	0.000224
15	-0.713720	-0.002372	-0.000061

6	-1.409929	1.670042	-0.109537
1	-1.087828	2.151961	-1.028585
1	-2.496450	1.627048	-0.100997
1	-1.078741	2.272611	0.731804
6	-1.438280	-0.920955	-1.385908
1	-1.098252	-0.507806	-2.331510
1	-1.144040	-1.965804	-1.338618
1	-2.523273	-0.861978	-1.348058
6	-1.437457	-0.731394	1.494892
1	-1.137500	-1.771338	1.589920
1	-1.102623	-0.192526	2.377004
1	-2.522662	-0.683604	1.447043
1	3.093937	0.002849	-0.000035

1g
E= -709.355805
NImag=0

28	-0.902760	0.186651	0.000005
15	1.264887	-0.026881	0.000003
6	2.073308	1.600784	-0.000876
1	1.787467	2.166185	0.881928
1	3.154422	1.479831	-0.000806
1	1.787469	2.165209	-0.884306
6	1.919290	-0.891606	-1.447517
1	3.005694	-0.915560	-1.414081
1	1.541482	-1.909213	-1.472991
1	1.604855	-0.385978	-2.355999
6	1.919417	-0.890114	1.448356
1	1.541608	-1.907693	1.474917
1	3.005819	-0.914106	1.414845
1	1.605069	-0.383547	2.356346
6	-2.918635	-0.791970	-0.000055
1	-2.959703	-1.357969	-0.918487
1	-2.959835	-1.358075	0.918303
6	-2.977023	0.553435	0.000021
1	-3.097134	1.102885	0.925376
1	-3.097019	1.102986	-0.925293
1	-0.714353	-1.191137	0.000501

TS(1g-1h)
E= -709.3543292
NImag=1 (-447.05)

28	-0.938049	0.302960	0.000001
15	1.258261	-0.030671	0.000011
6	2.189692	1.529958	-0.001389
1	1.945862	2.116149	0.880521
1	3.258821	1.330048	-0.001309
1	1.945712	2.114629	-0.884259
6	1.861640	-0.942861	-1.443879
1	2.943380	-1.044392	-1.404499
1	1.414320	-1.932021	-1.471469
1	1.589631	-0.418481	-2.355449
6	1.861930	-0.940491	1.445261
1	1.414450	-1.929531	1.474681
1	2.943630	-1.042272	1.405741
1	1.590271	-0.414521	2.356021

6	-2.749640	-0.895109	-0.000029
1	-2.819340	-1.465829	-0.914509
1	-2.819420	-1.465889	0.914411
6	-2.940709	0.460701	0.000001
1	-3.165239	0.978601	0.923811
1	-3.165199	0.978651	-0.923799
1	-1.022900	-1.101130	0.000111

1h

E= -709.3614509

28	-0.991390	0.352294	0.000939
15	1.284196	-0.030798	0.000483
6	2.264662	1.493053	-0.140483
1	2.050410	2.157105	0.692523
1	3.327201	1.261839	-0.137549
1	2.023238	2.010990	-1.064670
6	1.858837	-1.076958	-1.366819
1	2.938130	-1.201451	-1.324445
1	1.389967	-2.055233	-1.310889
1	1.594341	-0.624548	-2.318421
6	1.897919	-0.838837	1.505272
1	1.422768	-1.807899	1.628568
1	2.974723	-0.979630	1.451757
1	1.665750	-0.231142	2.375345
6	-2.667935	-0.969476	-0.000491
1	-2.932570	-1.509402	-0.902027
1	-2.936504	-1.508855	0.900216
6	-2.872964	0.457656	-0.001298
1	-3.221381	0.928286	0.910875
1	-3.218993	0.928034	-0.914510
1	-1.464216	-1.162982	0.002602

1i

E= -788.0006997

NImag=0

28	-0.820754	0.054298	-0.022383
15	1.454597	0.086348	-0.002438
6	2.298331	-1.082882	-1.104854
1	1.988538	-0.915174	-2.132742
1	3.375073	-0.948198	-1.038129
1	2.060353	-2.106719	-0.833370
6	2.129291	-0.259788	1.647462
1	3.214964	-0.200941	1.637014
1	1.745109	0.460722	2.364068
1	1.837129	-1.253374	1.974187
6	2.178429	1.692640	-0.452409
1	1.838518	2.464776	0.232572
1	3.264035	1.646742	-0.412424
1	1.878779	1.967664	-1.460183
6	-0.738909	-1.984026	-0.076311
1	-0.355254	-2.235510	-1.053980
1	-0.145424	-2.287714	0.773276
6	-2.060803	-1.686907	0.083536
1	-2.514607	-1.703545	1.061506
1	-2.733872	-1.700399	-0.757200

1	-0.637802	1.667594	0.002300
6	-1.785425	1.940196	0.006699
1	-1.831475	2.570759	-0.873857
1	-1.854334	2.517691	0.921017
6	-2.620921	0.738416	-0.038936
1	-3.144405	0.556113	-0.966591
1	-3.223132	0.538054	0.834705

TS(1i-1j)
E= -787.9963516
NImag=1 (-231.21)

28	-0.724067	0.078458	-0.026668
15	1.491893	0.073680	-0.005773
6	2.263871	-1.073569	-1.178549
1	1.945005	-0.840281	-2.190501
1	3.347051	-0.997433	-1.124495
1	1.972884	-2.094673	-0.952037
6	2.182645	-0.371955	1.611502
1	3.269290	-0.348828	1.582204
1	1.835637	0.324939	2.369009
1	1.860828	-1.370196	1.892240
6	2.246427	1.681036	-0.394572
1	1.927879	2.430119	0.325417
1	3.331263	1.611454	-0.366707
1	1.943853	2.004506	-1.386899
6	-0.861461	-1.822202	-0.025271
1	-0.571603	-2.229146	-0.984642
1	-0.333125	-2.228054	0.826386
6	-2.207715	-1.426158	0.155448
1	-2.615678	-1.478010	1.153133
1	-2.918998	-1.649950	-0.623621
1	-0.785155	1.797115	0.033525
6	-1.923829	1.821671	0.138274
1	-2.153405	2.611456	-0.570519
1	-2.107981	2.155886	1.151830
6	-2.641044	0.545491	-0.212127
1	-2.886463	0.477141	-1.264763
1	-3.519163	0.396050	0.395518

1j
E= -788.0178752
NImag=0

28	0.433910	-0.592676	-0.053883
15	-1.657298	0.020612	0.026859
6	-2.081587	1.066979	1.443039
1	-3.144640	1.295830	1.435147
1	-1.837892	0.553384	2.368565
1	-1.522127	1.996633	1.407776
6	-2.737834	-1.432726	0.171140
1	-2.506438	-1.987712	1.076223
1	-3.779375	-1.121762	0.211818
1	-2.603734	-2.088852	-0.684423
6	-2.235964	0.906232	-1.441508
1	-3.288748	1.157519	-1.338164
1	-1.666418	1.820480	-1.576801
1	-2.104760	0.284586	-2.322344

6	3.313628	0.188379	-0.024155
6	2.657732	-1.175251	0.052347
1	2.165258	-1.327740	1.024022
1	1.972921	-1.324078	-0.815424
1	3.340824	-2.011832	-0.060731
6	2.320154	1.278353	0.344973
6	1.013362	1.148460	-0.405590
1	1.137033	1.137948	-1.491658
1	0.308581	1.927986	-0.134218
1	3.691542	0.349260	-1.032487
1	4.171524	0.221265	0.642144
1	2.133325	1.258709	1.419818
1	2.746177	2.261576	0.135090

TS(1j-1k)
E= -788.0116485
NImag=1 (-127.39)

28	-0.434672	-0.275996	-0.446898
15	1.669252	-0.039346	0.055450
6	2.467542	1.382878	-0.733296
1	3.520499	1.421050	-0.464312
1	2.380935	1.306914	-1.813251
1	1.989327	2.303692	-0.413361
6	2.644165	-1.481134	-0.463637
1	2.572238	-1.618394	-1.539146
1	3.690030	-1.339788	-0.200159
1	2.279106	-2.379325	0.026628
6	1.989663	0.144668	1.827724
1	3.058775	0.222357	2.010650
1	1.502387	1.040129	2.201391
1	1.599318	-0.712895	2.367744
6	-3.287040	0.065660	0.327066
6	-2.694051	-1.329949	0.299101
1	-2.472013	-1.641917	-0.729783
1	-1.789247	-1.401149	0.917129
1	-3.367804	-2.085038	0.694348
6	-2.354655	1.073054	-0.326883
6	-1.023223	1.254508	0.366097
1	-1.053763	1.156318	1.448680
1	-0.489538	2.151166	0.067440
1	-3.490528	0.366286	1.353488
1	-4.240827	0.065922	-0.194791
1	-2.180549	0.758392	-1.377020
1	-2.830720	2.046271	-0.451299

1k
E= -788.0165089
NImag=0

28	0.329742	-0.324027	-0.668259
15	-1.691271	0.123434	0.061723
6	-2.548052	-1.303302	0.776909
1	-3.547449	-1.020815	1.098923
1	-2.625077	-2.098694	0.041330
1	-1.994636	-1.677593	1.632888
6	-2.779458	0.721499	-1.264081
1	-2.867607	-0.028178	-2.045688

1	-3.771013	0.931975	-0.869872
1	-2.377586	1.632041	-1.700055
6	-1.740894	1.410034	1.336109
1	-2.767675	1.604439	1.636646
1	-1.174023	1.093386	2.206549
1	-1.304739	2.328629	0.954418
6	3.388184	0.095574	0.234758
6	2.894769	1.515247	0.043423
1	2.511892	1.664256	-0.968132
1	2.106543	1.776253	0.747296
1	3.700220	2.229578	0.185948
6	2.306323	-0.950130	0.020133
6	1.106010	-0.879576	0.898918
1	1.124454	-0.133066	1.684580
1	0.703408	-1.828414	1.235776
1	3.786724	-0.036113	1.239532
1	4.209628	-0.103653	-0.450006
1	1.960410	-0.808337	-1.074316
1	2.701515	-1.960518	-0.047424

TS(1k-1l)
E= -787.995456
NImag=1 (-522.84)

28	-0.316879	-0.687712	-0.247615
15	1.735526	0.158439	0.030800
6	2.569013	-0.451227	1.521195
1	2.644966	-1.534367	1.487467
1	3.568328	-0.029910	1.598951
1	1.999231	-0.175932	2.403808
6	2.861463	-0.253730	-1.335658
1	2.956735	-1.331846	-1.433000
1	2.478389	0.144678	-2.271229
1	3.847634	0.167626	-1.155021
6	1.797470	1.966468	0.153568
1	1.379527	2.415137	-0.743069
1	1.215310	2.299976	1.007519
1	2.823890	2.305307	0.271326
6	-2.154187	-1.402392	-0.306522
6	-2.268390	-0.523923	0.757081
1	-2.036851	-2.460635	-0.107856
1	-2.535028	-1.129737	-1.282577
6	-2.916439	0.826213	0.671765
1	-2.215385	-0.944187	1.754448
1	-0.718449	-0.010828	0.934093
1	-2.505655	1.469561	1.447392
1	-3.960614	0.666067	0.949707
6	-2.833530	1.500676	-0.679491
1	-3.278365	2.489969	-0.635678
1	-1.796154	1.621023	-0.995897
1	-3.360175	0.944927	-1.450800

1l
E= -788.0043775
NImag=0

28	-0.478605	-0.378777	-0.038889
15	1.669259	0.054286	0.025687

6	2.621924	-0.975842	-1.118769
1	2.269896	-0.825482	-2.135334
1	3.677268	-0.719005	-1.068823
1	2.495990	-2.023468	-0.863546
6	2.111745	1.763207	-0.406188
1	1.780313	1.994594	-1.414759
1	1.643042	2.459620	0.283566
1	3.190181	1.895388	-0.355039
6	2.400327	-0.215647	1.660071
1	1.905363	0.409798	2.397427
1	2.276840	-1.253848	1.952379
1	3.459751	0.028577	1.643982
6	-2.327796	-1.341305	-0.580127
6	-2.532723	-0.632272	0.548338
1	-2.239454	-2.415089	-0.544000
1	-2.390692	-0.896247	-1.564768
6	-2.756244	0.849573	0.598797
1	-2.600397	-1.168861	1.485339
1	0.088409	-1.587973	0.351422
1	-2.396936	1.226665	1.554714
1	-3.827272	1.055015	0.586761
6	-2.075510	1.585349	-0.545824
1	-2.134886	2.660459	-0.406389
1	-0.980240	1.403843	-0.623372
1	-2.505445	1.349107	-1.513750

1m

E = -787.9989832

NImag= 0

28	-0.351284	-0.739046	-0.256962
15	1.749292	0.156322	0.033787
6	2.489877	-0.222925	1.647222
1	2.565307	-1.298782	1.777809
1	3.483695	0.211615	1.722954
1	1.869449	0.175358	2.444967
6	2.964603	-0.440293	-1.179587
1	3.058870	-1.520982	-1.116399
1	2.649069	-0.180566	-2.186428
1	3.938465	0.006033	-0.992805
6	1.819992	1.965452	-0.099038
1	1.471316	2.280787	-1.078446
1	1.182462	2.419326	0.654271
1	2.838321	2.319679	0.042247
6	-2.123217	-1.396333	-0.300667
6	-2.216263	-0.457944	0.784892
1	-2.111594	-2.453911	-0.061043
1	-2.587384	-1.151080	-1.248475
6	-2.983571	0.841708	0.629913
1	-2.325156	-0.910593	1.766633
1	-1.045782	-0.047409	0.951659
1	-2.748926	1.489923	1.471727
1	-4.040736	0.595156	0.722736
6	-2.723800	1.564403	-0.674354
1	-3.225037	2.527549	-0.683100
1	-1.657249	1.753385	-0.814537
1	-3.084242	1.008557	-1.535912

TS(1m-1n)
E= -904.7022618
NImag= 1 (-968.97)

28	-0.069391	0.639691	-0.213410
6	-3.291608	-1.851411	1.203110
1	-3.901655	-2.438177	0.531296
1	-3.089362	-2.275026	2.174453
6	-2.836537	-0.658578	0.862536
1	-2.243698	-0.097819	1.577904
6	-0.863551	-0.754626	-1.375663
1	-0.267178	-0.816959	-2.274831
1	-0.974346	-1.660661	-0.798645
6	-1.857476	0.218930	-1.286003
1	-1.292103	1.435698	-0.479245
1	-1.984622	0.874013	-2.140608
6	-3.099285	0.012324	-0.443926
1	-3.588483	0.972044	-0.277083
1	-3.790814	-0.583111	-1.039657
15	1.793357	-0.536424	0.055685
6	1.650090	-2.342071	-0.073235
1	1.283094	-2.626727	-1.054406
1	2.621577	-2.804492	0.083136
1	0.959393	-2.716147	0.677616
6	3.011331	-0.091850	-1.216611
1	2.609376	-0.295405	-2.204919
1	3.246504	0.966797	-1.155309
1	3.926518	-0.663980	-1.084756
6	2.678773	-0.310483	1.625884
1	2.975590	0.725927	1.753000
1	2.039640	-0.592916	2.458187
1	3.570294	-0.932497	1.645015
6	0.650363	2.134692	0.887858
1	0.748609	1.779925	1.902425
1	1.548377	2.513166	0.422029
6	-0.588200	2.564256	0.432423
1	-0.643616	3.276092	-0.379499
1	-1.433923	2.568193	1.105869

1n
E= -904.718992
Nimag= 0

28	-0.011160	0.750799	-0.194856
6	-3.310141	-1.932325	1.068971
1	-4.118759	-2.256119	0.429320
1	-3.039459	-2.587861	1.881963
6	-2.697939	-0.776855	0.880391
1	-1.902111	-0.484720	1.558193
6	-1.063199	-0.581628	-1.564681
1	-0.467412	-0.489987	-2.461459
1	-1.074808	-1.533935	-1.058405
6	-1.975692	0.358771	-1.249991
1	-0.961695	2.163782	-0.177308
1	-2.072974	1.220161	-1.900535
6	-3.035015	0.199530	-0.197298
1	-3.259076	1.173292	0.239630

1	-3.948096	-0.106163	-0.711615
15	1.668945	-0.655932	0.027194
6	1.336214	-2.411209	-0.308389
1	1.020806	-2.553536	-1.337196
1	2.240145	-2.992056	-0.140914
1	0.556707	-2.781461	0.351941
6	3.004707	-0.239438	-1.130367
1	2.636599	-0.271971	-2.151846
1	3.374977	0.761484	-0.931351
1	3.825082	-0.946028	-1.030037
6	2.469680	-0.708673	1.655139
1	2.890883	0.258849	1.907078
1	1.745503	-0.982090	2.417601
1	3.267411	-1.447331	1.649751
6	0.933569	1.970348	0.865188
1	0.980376	1.679747	1.906948
1	1.891865	2.295646	0.480397
6	-0.231124	2.786984	0.480479
1	-0.013435	3.626511	-0.169392
1	-0.880581	3.077380	1.298658

1o

E= -866.6413392

NImag= 0

28	0.319190	0.480345	-0.334912
15	-1.662848	-0.403744	0.080412
6	-2.229266	-1.703409	-1.052826
1	-1.545813	-2.545734	-1.045485
1	-3.215175	-2.049607	-0.752687
1	-2.289517	-1.313389	-2.065202
6	-1.662157	-1.187596	1.718327
1	-0.914857	-1.974242	1.755499
1	-1.425070	-0.454623	2.484161
1	-2.637769	-1.617142	1.932632
6	-3.096998	0.713621	0.132823
1	-2.975340	1.472273	0.899141
1	-3.229236	1.203074	-0.828348
1	-3.994841	0.141600	0.354435
6	0.882595	-1.223214	-0.892283
6	2.149695	-0.484065	-0.964050
1	0.446130	-1.503537	-1.842559
1	0.821707	-2.012957	-0.153744
6	3.254397	-0.829415	0.023267
1	2.514889	-0.382564	-1.982696
1	1.922834	0.655967	-0.749614
1	4.081584	-0.137431	-0.122328
1	3.633038	-1.816023	-0.239197
6	2.816586	-0.806455	1.473265
1	2.060110	-1.557662	1.688009
1	3.658158	-1.004024	2.130737
1	2.411539	0.167613	1.750381
6	-0.392717	2.431495	0.325883
1	-0.655554	2.283095	1.362904
1	-1.194176	2.663256	-0.357822
6	0.892887	2.578276	-0.045464
1	1.150164	2.912903	-1.040280

1	1.692453	2.540217	0.679751

TS(1o-1p)
E= -866.6299246
NImag= 1(-958.28)

28	0.322714	0.458132	-0.303375
15	-1.719165	-0.325185	0.074769
6	-2.304434	-1.626540	-1.048856
1	-1.648053	-2.490061	-1.012093
1	-3.307182	-1.938458	-0.767213
1	-2.330132	-1.253155	-2.069023
6	-1.814889	-1.076088	1.726511
1	-1.093269	-1.882961	1.813414
1	-1.589945	-0.333765	2.487029
1	-2.810825	-1.473239	1.907308
6	-3.087811	0.868868	0.052033
1	-2.934731	1.643322	0.797095
1	-3.159642	1.336896	-0.926085
1	-4.026352	0.362659	0.264056
6	0.944731	-1.291683	-0.990274
6	2.102653	-0.512502	-0.976430
1	0.442449	-1.458834	-1.931509
1	0.803412	-2.051101	-0.235523
6	3.205079	-0.687353	0.039243
1	2.424656	-0.119007	-1.934472
1	1.705132	0.934098	-0.548511
1	3.806146	0.219588	0.077369
1	3.866216	-1.459212	-0.357289
6	2.743235	-1.065368	1.430899
1	2.256189	-2.036879	1.452253
1	3.590444	-1.117359	2.107988
1	2.046111	-0.329472	1.833328
6	-0.172988	2.275725	0.347630
1	-0.451041	2.199125	1.388615
1	-0.917445	2.682272	-0.319500
6	1.168026	2.352861	0.001681
1	1.454085	2.833158	-0.923767
1	1.923649	2.354934	0.774874

1p
E= -866.646974
NImag= 0

28	0.291714	0.589258	-0.279712
15	-1.647065	-0.400694	0.062927
6	-2.168776	-1.565649	-1.231636
1	-1.451598	-2.371629	-1.345471
1	-3.134127	-1.993847	-0.972482
1	-2.263201	-1.046833	-2.181779
6	-1.602368	-1.393411	1.583282
1	-0.816148	-2.140318	1.525315
1	-1.402746	-0.751787	2.436841
1	-2.554529	-1.895875	1.736114
6	-3.115084	0.646192	0.262501
1	-2.994094	1.324277	1.100975
1	-3.280650	1.231823	-0.637433
1	-3.988944	0.023743	0.438639

6	1.098943	-1.216972	-1.186013
6	2.195710	-0.457586	-0.988531
1	0.589749	-1.199748	-2.137969
1	0.845265	-2.012970	-0.502455
6	3.150869	-0.574829	0.155536
1	2.508310	0.191871	-1.798583
1	1.565244	1.714851	-0.377237
1	3.450788	0.421774	0.478689
1	4.061284	-1.014742	-0.258851
6	2.673965	-1.391175	1.337336
1	2.481378	-2.425998	1.064461
1	3.429725	-1.399666	2.116600
1	1.763639	-0.976581	1.769739
6	-0.396052	2.174887	0.430177
1	-0.641570	2.118639	1.483881
1	-1.183675	2.628566	-0.156578
6	0.978292	2.595458	0.106202
1	1.057876	3.350945	-0.667049
1	1.603026	2.833214	0.959543

TS(1l-1r)
E= -788.0012551
NImag= 1(-167.96)

28	0.439611	-0.430083	-0.013332
15	-1.684036	0.083005	-0.005967
6	-2.515599	-0.361473	1.539597
1	-2.039899	0.141440	2.376622
1	-3.562709	-0.070948	1.501330
1	-2.447870	-1.433086	1.700018
6	-2.001867	1.859586	-0.219330
1	-1.522955	2.425358	0.574946
1	-1.610723	2.200196	-1.173935
1	-3.071451	2.055403	-0.190608
6	-2.621706	-0.729238	-1.324291
1	-2.212090	-0.459410	-2.293452
1	-2.555079	-1.807103	-1.212178
1	-3.666124	-0.429579	-1.285475
6	2.321514	-1.343916	0.610025
6	2.452075	-0.688212	-0.560538
1	2.287845	-2.420913	0.633800
1	2.387587	-0.841154	1.565213
6	2.544792	0.798744	-0.707472
1	2.512840	-1.264065	-1.475296
1	-0.155308	-1.677976	0.116258
1	1.742103	1.122494	-1.391685
1	3.450714	1.033343	-1.267302
6	2.487552	1.596077	0.582556
1	2.535317	2.659333	0.370685
1	1.564619	1.428475	1.148627
1	3.314043	1.346035	1.241935

1r
E= -788.0054994
NImag= 0

28	0.434644	-0.451592	-0.072543
15	-1.668513	0.102843	0.018003

6	-2.368111	-0.014237	1.683365
1	-1.825605	0.637581	2.362050
1	-3.415078	0.278713	1.673836
1	-2.284644	-1.033758	2.046806
6	-2.033614	1.798168	-0.524099
1	-1.507703	2.513437	0.102152
1	-1.718251	1.939026	-1.554194
1	-3.101471	1.993896	-0.456313
6	-2.698585	-0.956013	-1.028508
1	-2.366514	-0.894158	-2.060926
1	-2.616073	-1.988359	-0.703015
1	-3.738777	-0.644335	-0.972816
6	2.296603	-1.393328	0.585185
6	2.393563	-0.692253	-0.565153
1	2.344939	-2.469858	0.572137
1	2.319865	-0.922717	1.557742
6	2.268437	0.793778	-0.646506
1	2.498012	-1.230697	-1.497819
1	-0.164594	-1.601533	0.445909
1	1.165704	1.061669	-0.810230
1	2.682914	1.143494	-1.588194
6	2.780232	1.607038	0.526153
1	2.605690	2.664936	0.356446
1	2.298496	1.339377	1.462583
1	3.849602	1.456284	0.642388

Pd(II)-Catalyzed Dimerization:

2a
E= -705.0044294
NImag=0

46	0.718847	-0.419613	0.029839
6	1.501114	1.470849	-0.229450
6	2.550439	0.729780	0.386592
6	2.992270	-0.399908	-0.251150
1	1.027137	2.266018	0.325461
1	1.504200	1.594905	-1.305053
1	2.803173	0.907138	1.421873
1	2.912875	-0.501809	-1.325700
1	3.623204	-1.109694	0.260780
15	-1.580187	0.044744	-0.001846
6	-2.109674	1.258348	-1.240416
1	-1.828233	0.921988	-2.234062
1	-3.188701	1.389396	-1.204490
1	-1.634820	2.216840	-1.052286
6	-2.223402	0.670590	1.574256
1	-3.296063	0.837928	1.508140
1	-2.025977	-0.046878	2.365513
1	-1.735991	1.606341	1.831635
6	-2.574796	-1.434486	-0.351047
1	-2.386498	-2.199488	0.397173
1	-3.634237	-1.187545	-0.338491
1	-2.319916	-1.835140	-1.328126

2b

E= -783.631851

NImag= 0

46	-0.673712	0.075101	-0.014563
6	-0.798553	-2.048026	-0.208298
1	-0.774258	-2.147612	-1.285651
1	-0.118474	-2.684390	0.335666
6	-1.980082	-1.621740	0.420141
1	-2.131024	-1.824342	1.470857
6	-0.484264	2.330867	-0.019932
1	0.087708	2.565123	0.863998
1	-0.037015	2.575567	-0.971028
6	-1.813258	2.068967	0.071560
1	-2.313195	2.060505	1.027942
1	-2.441647	2.082393	-0.805382
6	-2.772624	-0.680359	-0.218750
1	-3.595283	-0.221918	0.305062
1	-2.807512	-0.638933	-1.299036
15	1.678138	-0.069862	0.005580
6	2.345812	-1.106164	-1.327809
1	2.065082	-0.694239	-2.293104
1	3.430814	-1.146915	-1.265664
1	1.953485	-2.115643	-1.257005
6	2.651757	1.456313	-0.135934
1	2.425746	1.965500	-1.068127
1	2.438232	2.127528	0.690123
1	3.712432	1.216375	-0.120524
6	2.295467	-0.828650	1.535315
1	2.004592	-0.225236	2.390447
1	1.873446	-1.821278	1.659255
1	3.380032	-0.906468	1.510617

TS(2b-2c)

E= -783.6007434

NIMAG=1 (-261.07)

46	0.492517	0.002156	0.008696
6	1.482838	2.180868	-0.274600
1	1.416637	2.146146	-1.352685
1	1.094566	3.061669	0.211288
6	2.231119	1.288390	0.421086
1	2.399413	1.450381	1.476933
6	0.716162	-1.999192	-0.108819
1	0.220711	-2.476995	0.725567
1	0.411024	-2.371909	-1.077350
6	2.125975	-1.685092	0.072145
1	2.504679	-1.894157	1.061840
1	2.771840	-2.063059	-0.708117
6	2.790990	0.064388	-0.181708
1	3.718671	-0.216745	0.294996
1	2.911569	0.136841	-1.255140
15	-1.787663	0.046407	0.003757
6	-2.463013	1.589349	-0.668331
1	-2.155977	1.708640	-1.703301
1	-3.549837	1.580793	-0.620249
1	-2.089585	2.433856	-0.096938

6	-2.613728	-1.260638	-0.941986
1	-2.309837	-1.210478	-1.983611
1	-2.341868	-2.235584	-0.548503
1	-3.693662	-1.145701	-0.883396
6	-2.483526	-0.076731	1.673414
1	-2.201395	-1.023452	2.124225
1	-2.100032	0.727371	2.294299
1	-3.568648	-0.010941	1.636576

2c

E= -783.641217

NImag= 0

46	0.327859	-0.497666	-0.011758
6	2.344181	-1.587873	0.357642
1	2.500951	-1.516620	1.424611
1	2.097990	-2.565262	-0.036687
6	2.660372	-0.569518	-0.468333
1	2.634051	-0.734312	-1.539603
6	0.768198	1.404982	0.506528
1	-0.052344	2.083609	0.303759
1	0.906649	1.300259	1.581979
6	2.024490	1.793392	-0.225914
1	1.826401	1.909840	-1.290294
1	2.340684	2.775051	0.137119
6	3.128053	0.769048	-0.002718
1	4.025984	1.053865	-0.546924
1	3.384369	0.724936	1.054547
15	-1.899187	0.082032	-0.024734
6	-2.899611	-1.413172	-0.267097
1	-2.725613	-2.115344	0.543355
1	-3.956776	-1.157384	-0.288518
1	-2.637566	-1.891930	-1.206508
6	-2.533209	0.828795	1.498954
1	-2.374852	0.151498	2.333093
1	-2.017631	1.760985	1.709730
1	-3.597413	1.031498	1.403518
6	-2.399849	1.200869	-1.359277
1	-1.892044	2.156025	-1.264542
1	-2.138544	0.766615	-2.319793
1	-3.473721	1.369705	-1.325657

TS(2c-2d)

E= -783.6112225

NImag=1 (-50.24)

46	-0.123064	-0.494693	-0.608943
6	-2.606734	2.201027	0.063684
1	-2.682366	2.455332	1.111607
1	-2.337205	2.996461	-0.613630
6	-2.877658	0.981988	-0.375478
1	-2.837037	0.789032	-1.443683
6	-0.916022	-0.853039	1.169667
1	-0.369901	-1.652978	1.656145
1	-0.950805	0.052855	1.763967
6	-2.193528	-1.248699	0.502226
1	-1.971461	-1.527673	-0.569482

1	-2.549870	-2.201398	0.893836
6	-3.275687	-0.174946	0.478965
1	-4.196019	-0.612846	0.095833
1	-3.479374	0.152470	1.496653
15	1.897550	0.236410	0.156659
6	3.127746	0.247505	-1.176339
1	2.794670	0.886965	-1.989033
1	4.079081	0.622001	-0.804322
1	3.271451	-0.758329	-1.560372
6	1.857276	1.933110	0.788708
1	1.504428	2.607333	0.014103
1	1.178931	1.997207	1.634164
1	2.850629	2.242256	1.106384
6	2.638218	-0.750234	1.482220
1	2.000437	-0.735024	2.361088
1	2.758860	-1.779166	1.156735
1	3.611591	-0.345065	1.749583

2d
E= -783.6114957
NImag=0

46	-0.023306	-0.702706	-0.487926
6	-3.042012	2.195878	-0.139718
1	-3.337384	2.481623	0.860112
1	-2.809706	2.994566	-0.826774
6	-3.007158	0.928648	-0.516394
1	-2.741002	0.691862	-1.541895
6	-0.966137	-0.516040	1.246509
1	-0.457272	-1.103068	2.001606
1	-1.072843	0.529158	1.511849
6	-2.145369	-1.149339	0.593855
1	-1.831358	-1.538842	-0.434847
1	-2.419889	-2.079679	1.086546
6	-3.342275	-0.232049	0.357404
1	-4.141535	-0.816963	-0.095902
1	-3.710530	0.113071	1.321666
15	1.923097	0.339825	0.111367
6	3.201666	0.128323	-1.158172
1	2.862056	0.538508	-2.105148
1	4.112449	0.643617	-0.860431
1	3.423359	-0.926387	-1.293970
6	1.752229	2.129815	0.326724
1	1.379134	2.578707	-0.588895
1	1.047208	2.342183	1.124810
1	2.713822	2.573145	0.575904
6	2.671659	-0.259423	1.647483
1	1.996713	-0.091128	2.481463
1	2.872257	-1.323984	1.572138
1	3.604498	0.265823	1.839709

TS(2d-2e)
E= -783.5875275
NImag=1 (-378.42)

46	0.044676	-0.660779	-0.302045
6	3.839377	1.665212	-0.746390

1	4.818093	1.240125	-0.574885
1	3.754132	2.385407	-1.544886
6	2.798962	1.338286	-0.000328
1	1.837552	1.801644	-0.195493
6	1.984941	-1.514236	-0.343159
1	1.801189	-2.579262	-0.396997
1	2.486551	-1.053665	-1.184554
6	2.039523	-0.887458	0.907456
1	0.686017	-0.376644	1.100429
1	1.929805	-1.529426	1.775557
6	2.840757	0.376131	1.137803
1	2.498292	0.855099	2.054121
1	3.865902	0.055069	1.324704
15	-2.082289	0.351729	0.068069
6	-2.548371	1.556384	-1.210507
1	-2.575497	1.076929	-2.185153
1	-3.529074	1.977011	-1.000284
1	-1.819699	2.361212	-1.244884
6	-3.457708	-0.835122	0.094376
1	-3.504786	-1.374521	-0.847579
1	-3.309408	-1.555075	0.894081
1	-4.403515	-0.321704	0.251852
6	-2.249692	1.266696	1.627172
1	-2.082493	0.599302	2.467644
1	-1.515642	2.066186	1.669204
1	-3.244905	1.696838	1.711632

2e

E= -783.6234758

NImag=0

46	-0.375847	-0.315957	-0.037086
6	-1.023659	1.961723	0.482516
1	-1.121712	1.835059	1.552068
1	-0.245328	2.620138	0.133471
6	-1.963166	1.513939	-0.367420
1	-1.883822	1.767345	-1.417234
6	-2.223447	-1.670936	0.450659
1	-1.988580	-2.657778	0.085661
1	-2.263450	-1.541987	1.523473
6	-2.677674	-0.720047	-0.393544
1	0.265751	-1.691526	-0.050943
1	-2.745618	-0.949094	-1.449697
6	-3.121872	0.648974	0.030678
1	-4.035236	0.946462	-0.477108
1	-3.289477	0.690429	1.103579
15	1.896013	0.012423	-0.012332
6	2.449224	1.740690	-0.009138
1	2.104528	2.246019	0.888042
1	3.536477	1.775603	-0.031720
1	2.067053	2.262453	-0.881695
6	2.711368	-0.720387	1.429015
1	2.298437	-0.300460	2.341542
1	2.545524	-1.793085	1.439482
1	3.780058	-0.521521	1.398500
6	2.714207	-0.712912	-1.456395
1	2.546663	-1.785185	-1.475787

1	2.304479	-0.285642	-2.367070
1	3.783123	-0.515844	-1.421835

TS(2e-2f')
E= -783.5967622
NImag=1(-93.39)

46	0.086940	-0.583148	0.056184
6	2.959848	2.499670	0.081813
1	2.127570	2.792269	-0.543878
1	3.458387	3.286127	0.625415
6	3.366055	1.246190	0.159688
1	4.217167	0.997171	0.780877
6	1.765165	-2.176937	-0.126729
1	1.553278	-2.984757	0.555438
1	1.689216	-2.398958	-1.182863
6	2.298494	-1.018036	0.319571
1	-0.724331	-1.541259	0.856576
1	2.500555	-0.909448	1.377506
6	2.748057	0.105902	-0.579849
1	3.448320	-0.297066	-1.314682
1	1.909798	0.485829	-1.191176
15	-2.016178	0.343146	-0.011408
6	-1.980418	1.942331	-0.867760
1	-1.619148	1.816377	-1.884519
1	-2.980998	2.368327	-0.902831
1	-1.325127	2.632405	-0.343870
6	-3.234397	-0.654691	-0.902300
1	-2.887995	-0.846986	-1.913454
1	-3.371564	-1.606792	-0.398755
1	-4.187533	-0.132730	-0.945814
6	-2.740470	0.682961	1.611139
1	-2.881326	-0.246570	2.154375
1	-2.075576	1.319835	2.187074
1	-3.701247	1.179516	1.497777

2f'
E= -783.5997622
NImag=0

46	0.124874	-0.427214	0.011333
6	-4.979270	1.425638	-0.277975
1	-4.493507	2.353728	-0.543692
1	-6.045811	1.372052	-0.429055
6	-4.307625	0.404123	0.220736
1	-4.824773	-0.510977	0.477812
6	-1.707350	-1.810101	0.019449
1	-1.430769	-2.588243	-0.675340
1	-1.787967	-2.094010	1.061149
6	-2.167436	-0.612978	-0.413124
1	0.629772	-0.953126	-1.282151
1	-2.226419	-0.429687	-1.478852
6	-2.825417	0.409268	0.462474
1	-2.623686	0.188976	1.512171
1	-2.436950	1.403237	0.241603
15	2.294364	0.348392	-0.009466
6	2.626283	1.308370	1.494276
1	2.484038	0.688753	2.375266

1	3.652099	1.671076	1.484046
1	1.955108	2.160585	1.553064
6	3.553126	-0.950664	-0.040519
1	3.408009	-1.626963	0.796655
1	3.473895	-1.520911	-0.961087
1	4.546129	-0.511921	0.023692
6	2.686173	1.455549	-1.385956
1	2.595032	0.922180	-2.327340
1	1.994184	2.292381	-1.396562
1	3.701061	1.833611	-1.286846

2g
E= -666.8872896
NImag =0

46	-0.774581	-0.000051	0.068203
15	1.524652	0.000014	-0.027150
6	2.195797	-0.000945	1.657838
1	1.865319	-0.885162	2.195567
1	3.283273	-0.000724	1.620368
1	1.865005	0.882434	2.196753
6	2.245471	1.447214	-0.837251
1	3.330161	1.413376	-0.765757
1	1.957792	1.468894	-1.884001
1	1.886092	2.355224	-0.362157
6	2.245668	-1.446149	-0.838920
1	1.958052	-1.466624	-1.885711
1	3.330352	-1.412286	-0.767334
1	1.886356	-2.354756	-0.364917
6	-2.993999	-0.674147	-0.075208
1	-3.019662	-1.238071	-0.995588
1	-3.130972	-1.234315	0.839838
6	-2.993954	0.674253	-0.075055
1	-3.130879	1.234228	0.840115
1	-3.019576	1.238382	-0.995310
1	-0.494254	0.000206	-1.390382

TS(2g-2h)
E= -666.8764209
NImag=1 (-509.81)

46	-0.820784	-0.279964	0.000224
15	1.525399	0.069366	0.000173
6	2.465433	-1.485028	-0.064410
1	2.218149	-2.035919	-0.967700
1	3.533829	-1.280704	-0.061773
1	2.227219	-2.104733	0.795758
6	2.156935	0.925025	1.469465
1	3.238625	1.024396	1.417606
1	1.714887	1.914533	1.540855
1	1.895682	0.367683	2.364353
6	2.142535	1.034831	-1.405796
1	1.703371	2.028115	-1.394679
1	3.225078	1.126901	-1.359144
1	1.868818	0.549426	-2.338086
6	-2.701553	1.058656	-0.000338
1	-2.812374	1.624452	0.914571
1	-2.810875	1.624399	-0.915455

6	-2.970519	-0.304141	-0.000517
1	-3.243035	-0.800123	-0.921995
1	-3.243934	-0.800120	0.920696
1	-1.197346	1.223500	0.001653

2h

E = -666.8772444

NImag = 0

46	-0.840670	-0.284605	0.000702
15	1.543481	0.068904	0.000165
6	2.501679	-1.472512	-0.114742
1	2.254466	-1.999769	-1.032042
1	3.568077	-1.258626	-0.111465
1	2.273493	-2.119921	0.727563
6	2.186228	0.885517	1.489178
1	3.266819	0.993111	1.430905
1	1.739898	1.870184	1.594504
1	1.937337	0.300968	2.370253
6	2.157857	1.080824	-1.376610
1	1.712560	2.070803	-1.337217
1	3.239712	1.179032	-1.326414
1	1.889210	0.621888	-2.323787
6	-2.698737	1.080559	0.000136
1	-2.923916	1.623743	0.909608
1	-2.921055	1.626132	-0.908607
6	-2.921676	-0.322725	-0.002028
1	-3.219694	-0.811160	-0.920827
1	-3.222348	-0.813450	0.914691
1	-1.428062	1.265360	0.002475

2i

E= -745.5145129

NImag=0

46	0.726532	-0.039024	-0.011440
15	-1.674647	-0.136035	-0.000142
6	-2.337969	-1.785283	-0.382323
1	-1.976616	-2.510498	0.341623
1	-3.425170	-1.776773	-0.355075
1	-2.015783	-2.094348	-1.372890
6	-2.536972	0.950153	-1.172847
1	-3.610160	0.781677	-1.122737
1	-2.339654	1.992718	-0.942040
1	-2.197336	0.748903	-2.185047
6	-2.402594	0.268666	1.613812
1	-2.149023	1.286296	1.896364
1	-3.485530	0.174400	1.580675
1	-2.012785	-0.402980	2.373341
6	0.520134	2.147454	-0.043587
1	0.074868	2.387134	-0.996967
1	-0.042420	2.415596	0.837707
6	1.861844	1.894582	0.044587
1	2.367637	1.931791	0.996575
1	2.483987	1.922788	-0.835612
1	0.788110	-1.802155	-0.009002

6	1.978324	-1.974223	-0.000622
1	2.082625	-2.570641	-0.899234
1	2.076300	-2.561928	0.904285
6	2.694136	-0.706891	-0.004271
1	3.207498	-0.428591	-0.912798
1	3.211293	-0.424515	0.900682

TS(2i-2j)
E= -745.4978217
NImag=1(-267.48)

46	0.580069	0.095201	0.029726
15	-1.734699	0.087302	-0.001542
6	-2.468067	1.744825	-0.115564
1	-2.147101	2.230783	-1.032673
1	-3.554039	1.682851	-0.112365
1	-2.149493	2.351160	0.727754
6	-2.485461	-0.638281	1.482178
1	-3.570350	-0.591667	1.422051
1	-2.182555	-1.676382	1.581528
1	-2.156754	-0.098964	2.365778
6	-2.474706	-0.827546	-1.382493
1	-2.186247	-1.873522	-1.334515
1	-3.559624	-0.762141	-1.343640
1	-2.129521	-0.417420	-2.327107
6	0.842999	-1.914085	-0.034914
1	0.527743	-2.365224	0.895912
1	0.354017	-2.298546	-0.918819
6	2.208155	-1.505211	-0.155967
1	2.645307	-1.566982	-1.140359
1	2.875297	-1.784510	0.644622
1	1.170119	2.026618	0.008168
6	2.249605	1.783300	-0.200359
1	2.748381	2.547922	0.393707
1	2.424515	1.971213	-1.252698
6	2.741788	0.425508	0.247452
1	2.896681	0.360659	1.317191
1	3.645065	0.164332	-0.280794

2j
E= -745.542185
NImag= 0

46	0.360307	-0.582156	-0.046544
15	-1.797618	0.113791	0.031198
6	-2.875729	-1.336746	0.183295
1	-2.642490	-1.884708	1.091909
1	-3.916786	-1.022845	0.222267
1	-2.740277	-1.996424	-0.668999
6	-2.374443	0.998942	-1.437183
1	-3.423820	1.262959	-1.327906
1	-1.796241	1.907213	-1.578981
1	-2.254018	0.371856	-2.315492
6	-2.217995	1.170065	1.440230
1	-1.662850	2.102027	1.395323
1	-3.282043	1.395808	1.431927
1	-1.968953	0.664462	2.368417

6	0.973949	1.300675	-0.388233
1	1.074561	1.305202	-1.473474
1	0.241958	2.037259	-0.077651
6	2.280716	1.443089	0.348662
1	2.112210	1.398091	1.424760
1	2.644473	2.454955	0.146560
1	2.122693	-1.277847	-0.671165
6	2.860828	-0.995403	0.118038
1	3.640630	-1.733919	-0.049559
1	2.479922	-1.172588	1.126879
6	3.337028	0.432662	-0.063652
1	3.617566	0.592065	-1.104141
1	4.237470	0.589037	0.525453

TS(2j-2k)

E= -745.5357912

NImag=1 (-84.92)

46	-0.304248	-0.435146	-0.469936
15	1.812736	0.068986	0.180332
6	2.609778	1.376967	-0.785199
1	3.635335	1.516477	-0.450355
1	2.611867	1.112198	-1.838258
1	2.071444	2.312332	-0.664865
6	2.878207	-1.386264	-0.007605
1	2.889795	-1.712259	-1.043846
1	3.894995	-1.143138	0.294135
1	2.513292	-2.200693	0.611599
6	1.984978	0.574459	1.909608
1	3.034043	0.735627	2.147770
1	1.441236	1.497801	2.085613
1	1.585823	-0.195296	2.563161
6	-3.372308	0.388477	0.507368
6	-2.969139	-1.039655	0.816056
1	-2.935065	-1.642777	-0.094380
1	-1.995841	-1.088180	1.313979
1	-3.674727	-1.526867	1.483474
6	-2.411406	1.075040	-0.448811
6	-1.028901	1.327341	0.085138
1	-0.960892	1.426120	1.164188
1	-0.487461	2.116618	-0.424910
1	-3.440222	0.968549	1.426931
1	-4.366663	0.396338	0.066660
1	-2.346281	0.483948	-1.384176
1	-2.813572	2.026919	-0.803974

2k

E= -745.5382919

NImag= 0

46	0.243646	-0.544390	-0.454730
15	-1.841166	0.234328	0.090906
6	-2.561476	-0.514719	1.574155
1	-3.564404	-0.128109	1.740848
1	-2.611180	-1.593388	1.459060
1	-1.949343	-0.286359	2.441642

6	-3.030991	-0.097018	-1.238047
1	-3.107268	-1.166126	-1.415134
1	-4.012370	0.284063	-0.963505
1	-2.712298	0.387415	-2.156764
6	-1.925008	2.022151	0.369487
1	-2.947787	2.320131	0.589150
1	-1.290930	2.299069	1.206460
1	-1.583118	2.552396	-0.514416
6	3.520697	0.296196	0.348830
6	3.128920	1.429863	-0.576282
1	2.805581	1.051482	-1.546610
1	2.325602	2.039555	-0.167197
1	3.972610	2.090386	-0.753621
6	2.394449	-0.690227	0.621625
6	1.162984	-0.148648	1.258289
1	1.150841	0.913240	1.472838
1	0.726100	-0.743552	2.051099
1	3.863490	0.687969	1.305585
1	4.359554	-0.251354	-0.075018
1	2.110396	-1.128981	-0.402736
1	2.736838	-1.586393	1.133973

TS(2k-2l)
E= -745.5092128
NImag=1 (-102.66)

46	0.328863	-0.367074	-0.011393
15	-2.087199	0.178569	-0.026276
6	-2.489944	1.805410	-0.730576
1	-2.170711	1.849280	-1.767729
1	-3.561472	1.986133	-0.682720
1	-1.973669	2.585625	-0.179049
6	-3.137686	-0.984764	-0.944748
1	-2.831465	-1.016836	-1.986314
1	-3.037044	-1.983078	-0.528660
1	-4.181312	-0.683086	-0.891374
6	-2.819544	0.221219	1.638929
1	-2.707142	-0.745091	2.122344
1	-2.320536	0.970545	2.246728
1	-3.878564	0.462500	1.581497
6	2.030180	-1.171214	0.726248
6	2.587778	-0.659088	-0.496244
1	1.835308	-2.233791	0.809131
1	2.234797	-0.665622	1.661809
6	3.551200	0.516033	-0.478763
1	2.849871	-1.436746	-1.209207
1	1.614108	-0.224685	-1.115200
1	3.696278	0.852127	-1.502604
1	4.513599	0.126505	-0.148198
6	3.120513	1.674090	0.394788
1	3.827314	2.493605	0.306590
1	2.142612	2.052425	0.095488
1	3.073320	1.406955	1.447863

2l
E= -745.5300192

NImag= 0

46	-0.365605	-0.345228	-0.024050
15	1.886574	0.118131	0.029171
6	2.667465	-0.113210	1.644903
1	2.603311	-1.156059	1.940302
1	3.713050	0.182862	1.602148
1	2.158030	0.487722	2.392368
6	2.865031	-0.857947	-1.138819
1	2.804134	-1.911142	-0.882096
1	2.479319	-0.726775	-2.145494
1	3.905539	-0.542762	-1.112226
6	2.200169	1.849802	-0.411895
1	1.827817	2.055774	-1.411451
1	1.702971	2.511778	0.291371
1	3.268978	2.052168	-0.387975
6	-2.384057	-1.298957	-0.582282
6	-2.613668	-0.593990	0.548557
1	-2.261600	-2.369861	-0.543560
1	-2.494928	-0.862729	-1.565455
6	-2.967326	0.861938	0.603964
1	-2.650984	-1.134439	1.485402
1	0.239210	-1.639716	0.396090
1	-2.658536	1.260068	1.568474
1	-4.054346	0.954409	0.583673
6	-2.355503	1.683487	-0.517749
1	-2.573640	2.739554	-0.389193
1	-1.249954	1.631689	-0.533599
1	-2.711788	1.389273	-1.500139

2m

E= -862.2309475

NImag= 0

46	-0.035867	0.601723	-0.236663
6	-3.318511	-1.602907	1.582206
1	-3.699843	-2.480998	1.080292
1	-3.143361	-1.685122	2.643576
6	-3.110736	-0.469664	0.933705
1	-2.753562	0.393941	1.485038
6	-0.977353	-0.903933	-1.195777
1	-0.473263	-1.160465	-2.118867
1	-1.152015	-1.750722	-0.545324
6	-2.084115	0.065844	-1.300572
1	-1.730856	1.097908	-0.871000
1	-2.283086	0.357243	-2.328659
6	-3.356927	-0.262231	-0.521905
1	-4.069444	0.549736	-0.663464
1	-3.801890	-1.153573	-0.959703
15	1.803197	-0.767603	0.066525
6	1.546330	-2.554702	-0.101482
1	1.170870	-2.797718	-1.090405
1	2.487777	-3.076983	0.052487
1	0.829706	-2.898983	0.638751
6	3.118896	-0.391856	-1.125139
1	2.763371	-0.568840	-2.135983
1	3.412608	0.650219	-1.044150
1	3.987129	-1.020124	-0.939470

6	2.594998	-0.619040	1.692914
1	2.986047	0.382514	1.838482
1	1.875770	-0.832540	2.478410
1	3.417490	-1.326897	1.767430
6	1.087585	2.321064	0.911583
1	1.142779	1.966288	1.929161
1	2.019456	2.445555	0.380959
6	-0.060094	2.832082	0.420654
1	-0.078382	3.360214	-0.521680
1	-0.945822	2.896186	1.035641

TS(2m-2n)

E=

NImag=

46	-0.057418	0.643163	-0.205064
6	-3.490384	-1.885189	1.298891
1	-4.151356	-2.443933	0.651664
1	-3.287095	-2.307995	2.270371
6	-2.974228	-0.726121	0.930127
1	-2.327225	-0.190531	1.616079
6	-1.047373	-0.917194	-1.340711
1	-0.460939	-1.018760	-2.241809
1	-1.127809	-1.782074	-0.699420
6	-2.031946	0.051551	-1.278808
1	-1.303312	1.569448	-0.445392
1	-2.144300	0.706862	-2.132646
6	-3.235107	-0.059071	-0.378295
1	-3.660534	0.930483	-0.216671
1	-3.982818	-0.621321	-0.940331
15	1.855025	-0.749907	0.069952
6	1.570320	-2.540549	-0.032460
1	1.156689	-2.804750	-1.000876
1	2.506492	-3.076790	0.103875
1	0.872607	-2.851535	0.740202
6	3.107912	-0.431077	-1.206736
1	2.689254	-0.613942	-2.192190
1	3.431684	0.604670	-1.161637
1	3.971218	-1.076960	-1.064784
6	2.760147	-0.570467	1.634693
1	3.140714	0.440758	1.740130
1	2.102359	-0.784233	2.472599
1	3.599060	-1.261737	1.663802
6	0.958344	2.228946	0.883750
1	1.093931	1.876008	1.894406
1	1.851926	2.473370	0.329725
6	-0.250007	2.781486	0.508870
1	-0.305022	3.443044	-0.342137
1	-1.055731	2.859135	1.222775

2n

E= -862.2338761

NImag= 0

46	-0.061165	0.701769	0.181049
6	3.691312	-1.856451	-1.068624

1	4.543038	-2.031710	-0.426906
1	3.513461	-2.578578	-1.850240
6	2.916825	-0.796752	-0.917368
1	2.080737	-0.651669	-1.592314
6	1.258681	-0.710497	1.525724
1	0.694524	-0.686772	2.446053
1	1.334580	-1.651101	1.002712
6	2.071706	0.313493	1.189918
1	0.714821	2.447195	0.050891
1	2.115148	1.172053	1.850503
6	3.121375	0.259430	0.117011
1	3.199970	1.237318	-0.359918
1	4.076947	0.106053	0.622663
15	-1.677835	-0.919180	-0.056011
6	-1.070137	-2.628314	-0.043097
1	-0.637154	-2.868284	0.922621
1	-1.895298	-3.311050	-0.233428
1	-0.313692	-2.765542	-0.810288
6	-2.883688	-0.854200	1.297298
1	-2.379832	-0.980114	2.250860
1	-3.386461	0.108258	1.300099
1	-3.625178	-1.641514	1.181349
6	-2.680324	-0.840687	-1.565512
1	-3.208679	0.105517	-1.624123
1	-2.044497	-0.940455	-2.440671
1	-3.408783	-1.648259	-1.567288
6	-1.242423	2.002827	-0.805208
1	-1.378247	1.719452	-1.840310
1	-2.178497	2.190551	-0.294907
6	-0.146767	2.958265	-0.529448
1	-0.416883	3.770457	0.135856
1	0.361728	3.321836	-1.415478

2m'

E= -862.2459774

NImag=0

46	0.329072	0.322829	-0.122695
6	2.556310	1.023167	-0.656777
1	2.731422	0.689995	-1.669796
1	2.460645	2.086541	-0.507960
6	2.706016	0.179529	0.382995
1	2.654315	0.572686	1.392064
6	0.728020	-1.651196	-0.501022
1	-0.122931	-2.321817	-0.464771
1	1.068252	-1.607178	-1.536950
6	1.820317	-2.118736	0.434439
1	1.491710	-2.063575	1.471988
1	2.048850	-3.169099	0.241295
6	3.059458	-1.263693	0.237468
1	3.833304	-1.521686	0.957374
1	3.468195	-1.438600	-0.756128
15	-1.852684	-0.427947	0.014840
6	-2.478466	-1.257437	-1.471930
1	-1.872564	-2.120913	-1.723125
1	-3.504788	-1.579689	-1.312233
1	-2.452294	-0.565142	-2.308629

6	-2.127468	-1.583588	1.386741
1	-1.473525	-2.445103	1.303833
1	-1.917550	-1.083249	2.328037
1	-3.161187	-1.921434	1.390702
6	-3.103298	0.858626	0.308340
1	-2.862595	1.447868	1.187856
1	-3.183057	1.518095	-0.550513
1	-4.072075	0.389553	0.465582
6	-0.250758	2.679026	-0.346973
1	0.474164	3.005453	-1.076348
1	-1.277335	2.663977	-0.673748
6	0.076141	2.481856	0.938419
1	-0.674006	2.295059	1.691216
1	1.078381	2.652001	1.301445

TS(2m'-2n')
E= -862.1641433
NImag=1 (-1561.42)

46	0.198769	-0.185313	-0.417701
6	2.102730	-1.222883	-1.446408
1	1.998762	-2.228890	-1.066996
1	1.872647	-1.074644	-2.491299
6	2.677724	-0.244512	-0.726877
1	2.884576	0.690197	-1.229299
6	0.857665	-0.971782	1.529805
1	0.105243	-0.943438	2.303880
1	1.001975	-1.948546	1.080470
6	1.948271	-0.087288	1.628014
1	1.515910	1.130023	1.078499
1	2.151731	0.347187	2.601567
6	3.125807	-0.357787	0.705308
1	3.924570	0.353295	0.894256
1	3.527590	-1.350420	0.901710
15	-2.007862	-0.112372	0.091873
6	-2.674095	-1.739961	0.534409
1	-2.175313	-2.121210	1.420234
1	-3.741627	-1.669894	0.731849
1	-2.510331	-2.438402	-0.281014
6	-2.492032	0.970226	1.464461
1	-1.980251	0.671021	2.374142
1	-2.229798	2.000834	1.244139
1	-3.565625	0.911315	1.628726
6	-3.024291	0.431661	-1.308291
1	-2.748337	1.438383	-1.607550
1	-2.867630	-0.232040	-2.153597
1	-4.078133	0.419848	-1.038251
6	0.359415	2.022591	-0.694474
1	0.756713	2.005896	-1.701202
1	-0.655949	2.380110	-0.621550
6	1.234671	2.282740	0.381082
1	0.832309	2.834325	1.222378
1	2.260308	2.536989	0.142894

2n'
E= -862.243934
NIMAG=0

46	-0.373299	0.091216	0.147661
6	-2.498133	0.925854	0.927848
1	-2.611791	0.374034	1.850695
1	-2.354769	1.989865	1.012410
6	-2.737575	0.352160	-0.264405
1	-2.743050	0.959945	-1.159616
6	-0.979456	-2.318489	0.275409
1	-0.083563	-2.862771	0.032590
1	-1.316412	-2.362173	1.301702
6	-1.742970	-1.787774	-0.689765
1	-1.333479	2.848261	-0.894637
1	-1.423841	-1.856459	-1.721583
6	-3.051538	-1.108096	-0.412112
1	-3.758166	-1.275445	-1.219598
1	-3.486519	-1.493422	0.506014
15	1.894908	-0.314793	-0.017016
6	2.379589	-2.033796	-0.357137
1	1.906644	-2.395153	-1.265764
1	3.458475	-2.084089	-0.486937
1	2.104474	-2.679172	0.471543
6	2.704655	0.596809	-1.361496
1	2.274942	0.294609	-2.312487
1	2.568897	1.666813	-1.247054
1	3.769447	0.375679	-1.370743
6	2.835168	0.078461	1.484559
1	2.705990	1.118194	1.765308
1	2.483077	-0.542948	2.302925
1	3.892863	-0.115710	1.322475
6	0.238057	2.037097	0.375865
1	-0.204253	2.337145	1.322628
1	1.310935	2.143527	0.486620
6	-0.251789	2.864006	-0.787788
1	0.177034	2.540344	-1.733634
1	0.035184	3.907476	-0.645884

2o
E= -824.157929
NIMAG=0

46	0.263502	0.444519	-0.265613
15	-1.782239	-0.566075	0.117625
6	-2.100286	-2.123505	-0.755995
1	-1.357597	-2.869986	-0.493381
1	-3.084706	-2.501900	-0.490360
1	-2.066467	-1.961205	-1.829673
6	-1.996906	-0.977793	1.871300
1	-1.226367	-1.676315	2.183628
1	-1.911748	-0.081907	2.478866
1	-2.972832	-1.428028	2.037937
6	-3.234715	0.439125	-0.299858
1	-3.270241	1.335656	0.310365
1	-3.200696	0.727958	-1.346529
1	-4.140843	-0.136369	-0.124301

6	1.033122	-1.348712	-0.784812
6	2.289222	-0.587581	-0.927047
1	0.585469	-1.710650	-1.700795
1	0.995484	-2.073001	0.019170
6	3.429146	-0.905610	0.031206
1	2.613316	-0.537405	-1.963421
1	2.064079	0.551697	-0.741309
1	4.269249	-0.256448	-0.206411
1	3.760066	-1.922236	-0.176295
6	3.067667	-0.759686	1.494463
1	2.273509	-1.440067	1.794092
1	3.926797	-0.973656	2.123662
1	2.743280	0.255981	1.720999
6	-0.674402	2.524712	0.305224
1	-1.043898	2.395793	1.311551
1	-1.404108	2.703706	-0.469126
6	0.640001	2.716389	0.070789
1	0.988784	3.046718	-0.896913
1	1.354864	2.730860	0.880463

TS(2o-2p)
E= -824.1401805
NImag=1 (-650.64)

46	0.315116	0.486974	-0.247025
15	-1.829121	-0.492839	0.093664
6	-2.312074	-1.756526	-1.118813
1	-1.602790	-2.578314	-1.116132
1	-3.298802	-2.147170	-0.881689
1	-2.337411	-1.324118	-2.115294
6	-1.938076	-1.342893	1.695466
1	-1.181090	-2.119092	1.758085
1	-1.767700	-0.636057	2.502506
1	-2.918921	-1.794863	1.823002
6	-3.256027	0.631862	0.097489
1	-3.153675	1.375048	0.882415
1	-3.330780	1.143226	-0.858361
1	-4.173736	0.073166	0.265794
6	1.063287	-1.406752	-0.988175
6	2.227385	-0.659274	-0.940039
1	0.565277	-1.540087	-1.936602
1	0.877127	-2.156630	-0.234352
6	3.293685	-0.815646	0.105257
1	2.551004	-0.203900	-1.867269
1	1.746112	1.090166	-0.477722
1	3.858635	0.110304	0.185025
1	3.994539	-1.547158	-0.304198
6	2.822760	-1.264695	1.471716
1	2.357419	-2.246876	1.443408
1	3.664536	-1.329670	2.154504
1	2.105923	-0.561068	1.893917
6	-0.435999	2.407658	0.444150
1	-0.737947	2.279316	1.472705
1	-1.202171	2.709252	-0.253030
6	0.891047	2.639499	0.145252
1	1.163098	3.112838	-0.785793

1	1.626914	2.684090	0.933479

2p
E= -824.1624246
NIMAg=0

46	0.252464	0.573188	-0.219804
15	-1.713351	-0.581233	0.082812
6	-2.188517	-1.597700	-1.342996
1	-1.427645	-2.342195	-1.552521
1	-3.128547	-2.105108	-1.138034
1	-2.311882	-0.970014	-2.220840
6	-1.607586	-1.741424	1.472936
1	-0.785558	-2.434099	1.322582
1	-1.432819	-1.196128	2.395865
1	-2.533593	-2.304642	1.564592
6	-3.208946	0.385394	0.424308
1	-3.081969	0.983305	1.321434
1	-3.424415	1.048258	-0.408790
1	-4.055015	-0.283129	0.566274
6	1.233135	-1.311996	-1.236384
6	2.277160	-0.516572	-0.918439
1	0.780665	-1.254885	-2.214670
1	0.976366	-2.161374	-0.621909
6	3.176435	-0.675824	0.266760
1	2.606805	0.198316	-1.664253
1	1.468274	2.053016	-0.212231
1	3.368092	0.302794	0.707103
1	4.144015	-0.993211	-0.129543
6	2.711680	-1.649311	1.328563
1	2.624739	-2.660629	0.938239
1	3.424962	-1.680482	2.146598
1	1.748113	-1.358063	1.744531
6	-0.584419	2.257929	0.494688
1	-0.867639	2.163181	1.534942
1	-1.393765	2.612779	-0.128959
6	0.749202	2.843086	0.232327
1	0.757894	3.610203	-0.533788
1	1.280988	3.162475	1.121583

Pt(II)-Catalyzed Dimerization:

3a
E= -697.4200942
NImag= 0

78	-0.539504	-0.253007	-0.036080
6	-1.464790	1.551985	0.209859
6	-2.464919	0.691297	-0.368780
6	-2.787815	-0.441224	0.338929
1	-1.072803	2.355483	-0.396223
1	-1.508726	1.763225	1.271180
1	-2.754593	0.801002	-1.403161
1	-2.722367	-0.467876	1.417717
1	-3.342089	-1.236262	-0.135541

15	1.748705	0.071703	0.016024
6	2.339190	0.812725	1.557626
1	2.077168	0.176323	2.397617
1	3.419083	0.937438	1.527615
1	1.875222	1.783867	1.702278
6	2.340635	1.154018	-1.308409
1	3.421067	1.262779	-1.248712
1	2.076234	0.734212	-2.274186
1	1.881277	2.133980	-1.219382
6	2.682944	-1.471726	-0.169518
1	2.436690	-1.946968	-1.114862
1	3.750479	-1.264707	-0.148065
1	2.442635	-2.155959	0.639340

TS(3b-3c)
E= -776.0219711
NImag= 1 (-195.71)

78	0.366267	0.006837	0.003946
6	1.341598	2.176612	-0.313896
1	1.359892	2.147614	-1.393092
1	0.916982	3.055088	0.144979
6	2.061118	1.295012	0.439606
1	2.190724	1.478889	1.496740
6	0.689658	-1.977907	-0.151872
1	0.234732	-2.549277	0.647221
1	0.457679	-2.372952	-1.133199
6	2.110105	-1.619691	0.081945
1	2.443052	-1.846079	1.084646
1	2.784262	-2.021781	-0.663103
6	2.709173	0.083527	-0.139815
1	3.636157	-0.116640	0.380017
1	2.883404	0.183478	-1.203417
15	-1.868296	0.034312	0.009299
6	-2.544879	-0.407772	1.627324
1	-2.177917	0.281980	2.381182
1	-3.631430	-0.366972	1.603519
1	-2.231793	-1.412221	1.895512
6	-2.566385	1.655420	-0.385113
1	-2.215710	2.389515	0.334155
1	-2.248473	1.960207	-1.377799
1	-3.653115	1.617764	-0.355549
6	-2.626535	-1.111097	-1.167824
1	-2.297669	-0.874139	-2.175308
1	-2.327736	-2.128867	-0.935738
1	-3.710539	-1.038197	-1.120152

TS(3c-3d)
E= -776.0233027
NImag = 1 (-82.31)

78	-0.087878	-0.278817	-0.425101
6	-2.614378	2.217028	0.234089
1	-2.670953	2.406466	1.296752
1	-2.334506	3.046691	-0.396282
6	-2.914917	1.032403	-0.276328
1	-2.891156	0.905237	-1.354621

6	-0.977391	-0.921765	1.224858
1	-0.465355	-1.786191	1.634470
1	-1.077502	-0.128313	1.958679
6	-2.238886	-1.244013	0.461500
1	-1.977073	-1.416582	-0.619872
1	-2.605558	-2.230409	0.745063
6	-3.319073	-0.170352	0.509530
1	-4.241686	-0.579686	0.101388
1	-3.519916	0.096345	1.545395
15	1.962689	0.259542	0.235055
6	2.964697	0.838394	-1.156813
1	2.512616	1.718946	-1.604103
1	3.962700	1.094283	-0.807246
1	3.045232	0.060461	-1.910594
6	1.988410	1.586355	1.460172
1	1.500708	2.469074	1.058504
1	1.460078	1.273423	2.355624
1	3.015797	1.829205	1.722474
6	2.868719	-1.120364	0.967926
1	2.344897	-1.480563	1.848144
1	2.946171	-1.932644	0.252048
1	3.866534	-0.797282	1.256653

TS(3d-3e)
E = -775.9980411
NImag = 1 (-666.38)

78	-0.061537	-0.383141	-0.060590
6	-3.244244	2.417096	0.171239
1	-2.786685	2.560818	1.139929
1	-3.485448	3.304282	-0.392723
6	-3.521357	1.211261	-0.293091
1	-4.001897	1.108679	-1.258628
6	-1.444940	-1.893742	0.345774
1	-1.121218	-2.772724	-0.194298
1	-1.514607	-1.998220	1.420828
6	-2.247811	-0.936024	-0.305952
1	-1.308484	0.112067	-0.861047
1	-2.516099	-1.159628	-1.333832
6	-3.220144	-0.056663	0.437291
1	-4.135512	-0.642653	0.549633
1	-2.848034	0.154763	1.436324
15	2.183779	0.407657	0.038160
6	2.892231	0.441231	1.705636
1	2.923296	-0.562732	2.118800
1	3.903186	0.841082	1.675010
1	2.280831	1.063261	2.352351
6	3.350273	-0.536061	-0.974206
1	3.395091	-1.564208	-0.627294
1	3.021099	-0.536284	-2.008931
1	4.343570	-0.097379	-0.913672
6	2.272903	2.114943	-0.566516
1	1.929801	2.161875	-1.595425
1	1.642420	2.756601	0.041088
1	3.300433	2.468315	-0.515548

TS(3e-3f')

E = -776.0268393
NImag = 1 (-108.43)

78	0.090026	-0.533301	0.049376
6	2.597623	2.766066	0.069442
1	1.788470	2.973542	-0.617517
1	2.978629	3.599506	0.637536
6	3.116184	1.558372	0.189719
1	3.941743	1.395752	0.871064
6	1.806113	-1.982368	-0.215717
1	1.667214	-2.836325	0.427936
1	1.781510	-2.171430	-1.280289
6	2.274631	-0.805105	0.290889
1	-0.620006	-1.522127	0.932449
1	2.511325	-0.737639	1.344041
6	2.668711	0.360902	-0.580550
1	3.452181	0.029829	-1.266653
1	1.838124	0.647162	-1.254415
15	-1.976135	0.472035	-0.029774
6	-1.944727	2.048784	-0.921014
1	-1.600525	1.895461	-1.939965
1	-2.942150	2.481670	-0.949645
1	-1.275599	2.744212	-0.422448
6	-3.217790	-0.540828	-0.868314
1	-2.900432	-0.748542	-1.885803
1	-3.338907	-1.484785	-0.345600
1	-4.172184	-0.019995	-0.890437
6	-2.654028	0.845852	1.604014
1	-2.782517	-0.072769	2.168619
1	-1.970684	1.490959	2.148055
1	-3.616543	1.342386	1.507562

TS(3g-3h)
E = -659.2866965
NImag = 1 (-642.72)

78	0.622490	-0.046033	-0.003831
15	-1.750299	0.014206	0.007794
6	-2.488658	-0.420676	1.600918
1	-2.135281	0.261186	2.368491
1	-3.573119	-0.364109	1.541829
1	-2.199149	-1.430011	1.877501
6	-2.486132	-1.102558	-1.212389
1	-3.570744	-1.029264	-1.177047
1	-2.139830	-0.839532	-2.207168
1	-2.191895	-2.126435	-1.002685
6	-2.379545	1.667175	-0.396085
1	-2.032591	1.967927	-1.380082
1	-3.467151	1.655775	-0.391598
1	-2.032301	2.391111	0.335146
6	2.825669	-0.494093	0.011657
1	3.196186	-0.940977	0.924735
1	3.175848	-0.947662	-0.905225
6	2.508715	0.877271	0.012409
1	2.595273	1.444171	-0.904093
1	2.591513	1.443468	0.929488

1	1.603221	-1.270893	0.073556

TS(3i-3j)
E = -737.9129471
NImag = 1 (-261.54)

78	0.428567	0.061596	0.011289
15	-1.829947	0.069898	-0.000531
6	-2.544886	-0.840742	-1.392030
1	-2.236179	-1.880970	-1.350987
1	-3.630709	-0.793380	-1.356762
1	-2.199624	-0.414113	-2.328977
6	-2.568528	1.722080	-0.093919
1	-3.653888	1.653455	-0.085704
1	-2.247442	2.319678	0.754587
1	-2.253803	2.216729	-1.008458
6	-2.546325	-0.680576	1.482881
1	-2.208550	-0.146945	2.366209
1	-3.632247	-0.645067	1.437983
1	-2.228203	-1.715594	1.563078
6	2.060085	1.791164	-0.173745
1	2.232724	2.026209	-1.216183
1	2.498001	2.559142	0.461452
6	2.629563	0.440857	0.235255
1	0.955663	1.989749	0.026517
6	0.793944	-1.919899	-0.012397
6	2.164310	-1.447504	-0.152393
1	2.825095	0.384883	1.297644
1	3.533224	0.255359	-0.324504
1	0.363297	-2.397987	-0.882220
1	0.539325	-2.404073	0.921615
1	2.586353	-1.522142	-1.142478
1	2.848957	-1.730149	0.632731

TS(3j-3k)
E = -737.9477885
NImag = 1(-104.90)

78	-0.196298	-0.308553	-0.324143
15	1.894043	0.129276	0.246101
6	2.583335	1.569859	-0.594803
1	3.619840	1.708933	-0.295020
1	2.534940	1.429349	-1.670020
1	2.018474	2.459015	-0.331611
6	2.964225	-1.268168	-0.169072
1	2.936420	-1.456710	-1.238418
1	3.987857	-1.041722	0.122249
1	2.638558	-2.160713	0.357441
6	2.097398	0.427500	2.014625
1	3.144892	0.618376	2.238147
1	1.509321	1.289471	2.314948
1	1.761076	-0.437984	2.576896
6	-3.409554	0.430404	0.550205
6	-3.000411	-0.979675	0.923846
1	-2.981675	-1.627093	0.044811
1	-2.014673	-1.003050	1.398981
1	-3.691387	-1.430795	1.631028
6	-2.453311	1.077472	-0.436889

6	-1.080932	1.421126	0.103841
1	-1.060362	1.610573	1.173989
1	-0.592295	2.222673	-0.441900
1	-3.480745	1.053289	1.441274
1	-4.404000	0.412742	0.109616
1	-2.352283	0.423184	-1.325541
1	-2.877861	1.987364	-0.865764

TS(3k-3l)
E = -737.9256974
NImag = 1(-625.19)

78	-0.233477	-0.246559	0.030816
15	2.098083	0.227875	-0.010992
6	2.629710	1.282484	-1.385569
1	2.098137	2.228682	-1.350889
1	3.699068	1.469917	-1.321005
1	2.414046	0.798630	-2.333755
6	2.596132	1.103101	1.496982
1	2.053752	2.039795	1.579498
1	2.376127	0.493773	2.368062
1	3.663899	1.308502	1.464849
6	3.143645	-1.247779	-0.090777
1	2.923561	-1.898693	0.749966
1	2.946576	-1.793072	-1.009090
1	4.194272	-0.968020	-0.063128
6	-1.930622	-1.084204	-0.851317
6	-2.454558	-0.661769	0.389809
1	-1.719372	-2.133867	-1.002434
1	-2.144584	-0.514570	-1.744886
6	-3.348817	0.539544	0.555830
1	-2.625127	-1.454899	1.111675
1	-1.267870	-0.300675	1.205188
1	-3.257857	0.908040	1.575721
1	-4.367550	0.155855	0.474146
6	-3.134107	1.665287	-0.431384
1	-3.801072	2.490571	-0.201645
1	-2.113081	2.041887	-0.387967
1	-3.341225	1.361610	-1.454519

TS(3m-3n)
E = -854.64413
NImag= 1 (-357.46)

78	0.031144	-0.568142	-0.152326
6	3.536291	1.994247	1.245922
1	4.212618	2.488066	0.562673
1	3.359241	2.480334	2.192672
6	2.971556	0.837066	0.949167
1	2.309822	0.366709	1.667213
6	1.029939	0.978296	-1.309650
1	0.473800	1.085683	-2.229138
1	1.148645	1.859239	-0.697672
6	1.997229	-0.010728	-1.222626
1	1.184896	-1.649840	-0.329597
1	2.093489	-0.694293	-2.054826
6	3.196545	0.087449	-0.320771

1	3.571682	-0.912172	-0.106360
1	3.971226	0.580549	-0.911713
15	-1.774223	0.949769	0.073227
6	-1.393614	2.713826	-0.105190
1	-0.999544	2.924109	-1.094176
1	-2.298955	3.298385	0.039212
1	-0.659468	3.015125	0.636856
6	-3.045254	0.634351	-1.181451
1	-2.619710	0.744539	-2.174554
1	-3.420775	-0.379808	-1.082980
1	-3.872306	1.331345	-1.069928
6	-2.661744	0.884827	1.654296
1	-3.115127	-0.090132	1.800254
1	-1.976268	1.079595	2.474317
1	-3.446236	1.637533	1.666579
6	-1.155947	-1.967136	0.973444
1	-1.264083	-1.610546	1.985862
1	-2.069649	-2.181099	0.439502
6	-0.001031	-2.670472	0.631502
1	-0.018250	-3.375737	-0.184744
1	0.775241	-2.819388	1.365718

TS(3m'-3n')
E = -854.5873706
NImag = 1 (-1494.57)

78	0.153869	-0.263849	-0.294841
6	1.965681	-1.484019	-1.007231
1	1.933757	-2.364385	-0.383074
1	1.737434	-1.629305	-2.053277
6	2.553758	-0.333685	-0.590617
1	2.749330	0.422970	-1.336357
6	0.846147	-0.488853	1.759441
1	0.097904	-0.276664	2.509931
1	1.036447	-1.552497	1.634892
6	1.950796	0.395308	1.678966
1	1.512573	1.474455	0.882006
1	2.188272	1.001837	2.546090
6	3.088482	-0.078308	0.795345
1	3.874663	0.669291	0.748885
1	3.530357	-0.985029	1.206391
15	-2.040314	-0.009969	0.179031
6	-2.719979	-1.448711	1.041894
1	-2.208276	-1.588633	1.989360
1	-3.782704	-1.311546	1.228374
1	-2.576174	-2.338999	0.436950
6	-2.456055	1.409886	1.224441
1	-1.945753	1.330571	2.179750
1	-2.149304	2.334224	0.744281
1	-3.528823	1.445279	1.399289
6	-3.048930	0.177641	-1.312013
1	-2.748630	1.067430	-1.857209
1	-2.909665	-0.684640	-1.957381
1	-4.100904	0.260289	-1.048645
6	0.375835	1.798728	-1.083495
1	0.807482	1.602842	-2.057583

1	-0.631034	2.186725	-1.139503
6	1.225422	2.373985	-0.093507
1	0.785909	3.130486	0.545868
1	2.243122	2.603188	-0.386265

TS(3o-3p)
E = -816.572102
NImag = 1 (-243.16)

78	0.268867	0.445424	-0.191380
15	-1.828007	-0.625012	0.108868
6	-2.297596	-1.804221	-1.187229
1	-1.587426	-2.622696	-1.239954
1	-3.282616	-2.212353	-0.974594
1	-2.325951	-1.303832	-2.151193
6	-1.861381	-1.584801	1.647369
1	-1.076783	-2.335594	1.636234
1	-1.690640	-0.927199	2.494813
1	-2.822711	-2.078209	1.768736
6	-3.284337	0.451226	0.219132
1	-3.195334	1.136724	1.055722
1	-3.393338	1.026764	-0.695880
1	-4.177454	-0.153073	0.358571
6	0.943435	-1.453584	-0.999741
6	2.131897	-0.744434	-0.897119
1	0.481582	-1.547829	-1.970705
1	0.741249	-2.243528	-0.292574
6	3.173724	-0.967141	0.155644
1	2.479285	-0.246826	-1.792249
1	1.672778	1.162017	-0.385009
1	3.728741	-0.045037	0.311194
1	3.887737	-1.660648	-0.296754
6	2.687132	-1.520687	1.477200
1	2.228504	-2.500392	1.367170
1	3.521415	-1.634384	2.162824
1	1.961951	-0.853836	1.941018
6	-0.633185	2.241427	0.584660
1	-0.936265	2.077831	1.607712
1	-1.401742	2.571349	-0.096584
6	0.689523	2.587721	0.321705
1	0.935267	3.142239	-0.570390
1	1.404942	2.647613	1.126823

B3LYP/LANL2DZ ECP, 6-311+G** Optimized coordinates, energy (in a.u.), and number and magnitude (in cm^{-1}) of imaginary frequency (NImag) of transition states involved in the NI(II) catalyzed ethylene dimerization discussed in this manuscript

C_2H_4
E= -78.6155126

NImag= 0

6	0.000000	0.000000	0.664514
6	0.000000	0.000000	-0.664514
1	0.000000	0.922735	1.235297
1	0.000000	-0.922735	1.235297
1	0.000000	-0.922735	-1.235297
1	0.000000	0.922735	-1.235297

1,4-Pentadiene

E= -195.357985

NImag= 0

6	-2.373365	-0.175935	0.149910
6	-1.176370	-0.177544	-0.432326
1	-3.179612	-0.806896	-0.206866
1	-2.590296	0.460640	1.002912
1	-0.997647	-0.833790	-1.282225
6	-0.000001	0.662315	-0.000049
1	-0.310315	1.313853	0.825708
1	0.310310	1.313726	-0.825908
6	1.176374	-0.177471	0.432358
6	2.373363	-0.175960	-0.149889
1	0.997658	-0.833574	1.282369
1	3.179612	-0.806862	0.206985
1	2.590286	0.460473	-1.002999

1a

E= -747.6125846

NImag= 0

28	-0.837214	-0.435823	-0.048455
6	-1.615600	1.337951	0.241854
6	-2.620421	0.534283	-0.381568
6	-2.967319	-0.650057	0.233147
1	-1.189838	2.173423	-0.302506
1	-1.607780	1.436414	1.326000
1	-2.899338	0.715635	-1.415234
1	-2.866686	-0.776049	1.309267
1	-3.545201	-1.401630	-0.292144
15	1.376314	-0.012021	-0.002454
6	1.961490	0.843636	1.510408
1	1.717967	0.249353	2.392797
1	3.042982	0.993142	1.470927
1	1.474235	1.815804	1.602121
6	1.979411	1.013089	-1.399168
1	3.062738	1.140752	-1.338034
1	1.731428	0.534008	-2.347831
1	1.506101	1.995846	-1.374238
6	2.370225	-1.557317	-0.090061
1	2.146349	-2.098043	-1.011623
1	3.437169	-1.321042	-0.072731
1	2.140451	-2.203750	0.759089

TS(1b-1c)

E= -826.2459513

NImag= 1 (-206.84)

28	0.603394	-0.008142	-0.010730
6	1.242873	2.109486	-0.281170

1	1.201849	2.076428	-1.365955
1	0.732070	2.935977	0.197096
6	2.098491	1.317093	0.429705
1	2.239004	1.499645	1.491740
6	0.770753	-1.897779	-0.123964
1	0.260759	-2.402501	0.692798
1	0.495675	-2.269771	-1.108196
6	2.186910	-1.576411	0.094049
1	2.540181	-1.776956	1.100658
1	2.856452	-1.982343	-0.659374
6	2.793288	0.158152	-0.172745
1	3.744007	-0.039478	0.311745
1	2.919911	0.244530	-1.250165
15	-1.593792	0.017128	0.007891
6	-2.328920	1.644202	-0.421475
1	-2.021111	1.939623	-1.425978
1	-3.419767	1.586826	-0.389691
1	-1.994505	2.405310	0.284870
6	-2.419326	-1.160118	-1.130251
1	-2.116873	-0.956501	-2.158953
1	-2.138597	-2.184307	-0.881929
1	-3.504672	-1.061965	-1.054351
6	-2.271055	-0.374424	1.667812
1	-1.965115	-1.377252	1.968922
1	-1.892915	0.338321	2.402512
1	-3.362586	-0.325755	1.654570

TS(1c-1d)
E= -826.2371922
NImag= 1 (-60.82)

28	-0.213146	-0.401570	-0.618675
6	-2.422318	2.103206	0.347987
1	-2.431428	2.113376	1.433703
1	-2.140053	3.025708	-0.146452
6	-2.787337	1.024450	-0.346192
1	-2.813020	1.084582	-1.435041
6	-0.902078	-1.266548	0.878759
1	-0.383668	-2.201593	1.088363
1	-0.966742	-0.615564	1.749079
6	-2.140756	-1.378230	0.022402
1	-1.827315	-1.321703	-1.072308
1	-2.540585	-2.397064	0.051706
6	-3.214696	-0.294777	0.242155
1	-4.147639	-0.618898	-0.228184
1	-3.412332	-0.196553	1.312887
15	1.809660	0.133769	0.049054
6	2.914552	-1.294566	0.364680
1	3.000471	-1.906402	-0.534690
1	3.908776	-0.948247	0.657343
1	2.504137	-1.911325	1.165632
6	2.677112	1.148034	-1.214865
1	2.763779	0.593387	-2.151021
1	2.123216	2.069507	-1.402795
1	3.680214	1.404821	-0.864802
6	1.859571	1.133737	1.583631

1	1.276588	2.046251	1.450998
1	1.433783	0.566076	2.412461
1	2.890696	1.399242	1.828868

TS(1d-1e)
E= -826.2165315
NImag= 1(-581.70)

28	-0.231351	-0.814730	-0.021103
15	-2.189082	0.319599	0.002271
6	-3.594088	-0.681899	-0.636919
1	-4.519406	-0.101453	-0.603427
1	-3.404872	-0.980754	-1.669733
1	-3.722729	-1.581487	-0.031922
6	-2.201081	1.842423	-1.021727
1	-1.452883	2.545047	-0.651341
1	-1.960973	1.596556	-2.057616
1	-3.183618	2.319046	-0.988578
6	-2.723942	0.861108	1.671974
1	-2.819137	-0.004049	2.330465
1	-1.982382	1.538495	2.098557
1	-3.686694	1.374805	1.619323
6	1.546528	-1.731312	0.020801
1	1.422853	-2.523242	0.756668
1	1.747035	-2.044286	-1.002610
6	1.900913	-0.440510	0.435785
1	2.043990	-0.284091	1.504227
1	0.536633	0.299659	0.487017
6	2.665621	0.529069	-0.454538
1	2.413050	1.562036	-0.203833
1	2.390343	0.360883	-1.500853
6	4.147500	0.308115	-0.257427
6	4.974969	1.213138	0.257858
1	4.529759	-0.661662	-0.567080
1	6.033827	1.010073	0.365718
1	4.630744	2.192078	0.577003

1f
E= -630.7684569
NIMag= 0

28	1.709749	-0.001511	0.000078
15	-0.715942	-0.000134	-0.000254
6	-1.436346	1.680850	-0.154695
1	-1.117526	2.143274	-1.090780
1	-2.527364	1.626901	-0.142454
1	-1.105853	2.308793	0.674776
6	-1.444382	-0.972207	-1.376258
1	-1.111062	-0.574652	-2.336705
1	-1.133731	-2.016259	-1.304280
1	-2.535071	-0.925325	-1.334800
6	-1.443910	-0.704092	1.530871
1	-1.128214	-1.741768	1.654717
1	-1.115300	-0.133261	2.401436
1	-2.534779	-0.672011	1.479925
1	3.122901	0.001329	0.000290

TS(1g-1h)

E= -709.4715931
NImag= 1 (-634.85)

28	0.952490	0.286407	-0.000024
15	-1.276607	-0.032094	0.000004
6	-2.193621	1.562964	-0.001817
1	-1.938943	2.145263	-0.889471
1	-3.270711	1.377699	-0.001542
1	-1.938866	2.147409	0.884406
6	-1.910837	-0.940477	1.460558
1	-2.999030	-1.025484	1.414920
1	-1.477766	-1.941487	1.493757
1	-1.633818	-0.414217	2.375610
6	-1.910713	-0.943636	-1.458637
1	-1.477764	-1.944769	-1.489579
1	-2.998919	-1.028409	-1.412940
1	-1.633525	-0.419431	-2.374813
6	2.786047	-0.893309	-0.000067
1	2.901909	-1.462414	0.917255
1	2.901749	-1.462274	-0.917478
6	2.972977	0.482686	0.000024
1	3.199198	1.004554	-0.926603
1	3.199286	1.004406	0.926715
1	1.183457	-1.128199	0.000013

TS(1i-1j)
E= -788.1299471
NImag= 1(-240.72)

28	-0.703421	0.076650	-0.015998
15	1.522238	0.073592	-0.004798
6	2.278021	1.749503	-0.039730
1	1.966661	2.321051	0.836683
1	3.368150	1.675750	-0.041205
1	1.961860	2.285101	-0.936896
6	2.268134	-0.786434	-1.444523
1	3.358476	-0.735804	-1.396823
1	1.962695	-1.833631	-1.456024
1	1.932327	-0.318341	-2.371547
6	2.273744	-0.727262	1.465961
1	1.972423	-1.774353	1.520575
1	3.363733	-0.676299	1.411480
1	1.941163	-0.223574	2.375286
6	-0.918074	-1.829874	0.008582
1	-0.631459	-2.279929	-0.938292
1	-0.414202	-2.238259	0.879644
6	-2.278156	-1.391241	0.163947
1	-2.697202	-1.433140	1.163071
1	-2.979789	-1.670676	-0.613717
1	-0.872173	1.855917	0.077576
6	-2.005593	1.817934	0.182946
1	-2.288540	2.641655	-0.476751
1	-2.224435	2.074544	1.217800
6	-2.685366	0.533751	-0.272821
1	-2.821044	0.484907	-1.351617
1	-3.632677	0.396732	0.234507

TS(1j-1k)

E= -788.1438363
NImag= 1 (-118.64)

28	-0.396407	-0.244786	-0.455212
15	1.715537	-0.046835	0.066054
6	2.559093	1.397297	-0.682311
1	3.618832	1.395258	-0.415727
1	2.464546	1.362743	-1.768736
1	2.106268	2.322484	-0.323166
6	2.661877	-1.512849	-0.509450
1	2.585757	-1.610628	-1.593959
1	3.715640	-1.403509	-0.239928
1	2.272666	-2.421165	-0.046215
6	2.039838	0.070328	1.864659
1	3.115353	0.117561	2.051846
1	1.570070	0.967490	2.270364
1	1.626076	-0.800626	2.375043
6	-3.352784	0.082755	0.398455
6	-2.892362	-1.368996	0.250287
1	-2.969859	-1.708722	-0.787977
1	-1.846198	-1.498446	0.592762
1	-3.478613	-2.058784	0.860900
6	-2.421212	1.056054	-0.338178
6	-1.071081	1.305950	0.321458
1	-1.062488	1.243317	1.411292
1	-0.553500	2.195851	-0.037780
1	-3.403088	0.360628	1.455621
1	-4.366099	0.181991	0.001936
1	-2.270981	0.696065	-1.380987
1	-2.898254	2.031797	-0.499683

TS(1k-1l)
E= -788.1283311
NImag= 1(-576.34)

28	-0.304840	-0.677888	-0.229846
15	1.779894	0.168237	0.031401
6	2.656397	-0.457905	1.517298
1	2.728444	-1.546157	1.475689
1	3.663098	-0.037291	1.574629
1	2.104851	-0.183675	2.418081
6	2.887683	-0.254297	-1.376108
1	2.967487	-1.338035	-1.481739
1	2.489053	0.157517	-2.305262
1	3.887048	0.155527	-1.210435
6	1.872392	1.996644	0.159969
1	1.444458	2.455354	-0.733036
1	1.307187	2.337891	1.028773
1	2.910608	2.321066	0.262524
6	-2.153728	-1.423260	-0.332635
6	-2.292088	-0.538478	0.747683
1	-2.016066	-2.484836	-0.137099
1	-2.533498	-1.156547	-1.315633
6	-3.029020	0.786723	0.677404
1	-2.262365	-0.982181	1.742377
1	-0.857357	-0.010650	0.932125
1	-2.659158	1.443848	1.469575
1	-4.066139	0.553848	0.952135