

Supporting Information

Electronic Effect of Ligands vs. Reduction Potentials of Fischer Carbene Complexes of Chromium: A Molecular Electrostatic Potential Analysis

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1. Table S1. Bond distances in Å of oxidised and reduced complexes.

	Oxidised			Reduced		
	Cr-C	C-N	C-C	Cr-C	C-N	C-C
1a	2.160	1.323	1.497	2.252	1.417	1.451
1b	2.159	1.322	1.497	2.250	1.415	1.449
1c	2.158	1.322	1.497	2.251	1.412	1.449
1d	2.158	1.322	1.497	2.248	1.412	1.446
1e	2.157	1.321	1.495	2.241	1.390	1.438
1f	2.156	1.321	1.496	2.244	1.402	1.441
2a	2.106	1.324	1.487	2.226	1.425	1.439
2b	2.100	1.323	1.488	2.226	1.421	1.437
2c	2.098	1.322	1.488	2.225	1.419	1.437
2d	2.095	1.322	1.489	2.223	1.417	1.435
2e	2.097	1.321	1.486	2.218	1.391	1.430
2f	2.093	1.322	1.487	2.221	1.403	1.431

2. **Table S2.** Complexes **1-2** with corresponding V_{Cr} (in a. u) values in acetonitrile.

R	V_{Cr}	
	1a-1n	2a-2n
OCH₃	-103.4789	-103.4867
CH₃	-103.4784	-103.4857
H	-103.4758	-103.4836
Cl	-103.4679	-103.4759
COOCH₃	-103.4557	-103.4615
CF₃	-103.4594	-103.4664
F	-103.4709	-103.4787
Ph	-103.4683	-103.4731
Br	-103.4677	-103.4755
SH	-103.4675	-103.4749
CHCH₂	-103.4661	-103.4712
OCF₃	-103.4651	-103.4731
NC	-103.4542	-103.4605
CN	-103.4496	-103.4561

3. Table S3. Complexes **3-8** with corresponding V_{Cr} (in a. u) values in acetonitrile.

R	V_{Cr}					
	3a-3l	4a-4l	5a-5l	6a-6l	7a-7l	8a-8l
OCH ₃	-103.4827	-103.4750	-103.4805	-103.4875	-103.4861	-103.4991
CH ₃	-103.4844	-103.4763	-103.4854	-103.4820	-103.4800	-103.4924
H	-103.4826	-103.4745	-103.4845	-103.4793	-103.4773	-103.4901
CHCH ₂	-103.4806	-103.4720	-103.4810	-103.4785	-103.4765	-103.4877
SH	-103.4765	-103.4682	-103.4782	-103.4763	-103.4746	-103.4868
Br	-103.4744	-103.4653	-103.4772	-103.4767	-103.4756	-103.4871
COOCH ₃	-103.4744	-103.4670	-103.4762	-103.4835	-103.4832	-103.4904
Cl	-103.4743	-103.4653	-103.4770	-103.4772	-103.4766	-103.4876
OCF ₃	-103.4715	-103.4627	-103.4742	-103.4737	-103.4738	-103.4836
CF ₃	-103.4697	-103.4618	-103.4732	-103.4707	-103.4723	-103.4808
NC	-103.4671	-103.4588	-103.4700	-103.4695	-103.4700	-103.4785
CN	-103.4649	-103.4568	-103.4682	-103.4654	-103.4663	-103.4744

4. Cartesian coordinates of optimized structures in Å.

1a				1a'			
24	-1.690117000	-0.494794000	0.026337000	24	-1.772887000	-0.526572000	0.013205000
6	-2.941199000	0.366291000	-1.124729000	6	-3.156165000	0.642309000	-0.538686000
8	-3.728041000	0.809905000	-1.835746000	8	-4.098972000	1.215737000	-0.889371000
6	-2.924937000	-1.908868000	0.169821000	6	-3.090727000	-1.816127000	-0.145553000
8	-3.686373000	-2.766466000	0.259515000	8	-3.915342000	-2.628920000	-0.256075000
6	-0.507772000	-1.529773000	1.131000000	6	-0.706862000	-1.986969000	0.610954000
8	0.136945000	-2.211079000	1.788335000	8	-0.205119000	-2.949879000	1.002963000
6	-2.433120000	0.296912000	1.597251000	6	-2.074469000	-0.103403000	1.832034000
8	-2.879957000	0.750471000	2.553324000	8	-2.241352000	0.159601000	2.944755000
6	-0.952285000	-1.328869000	-1.526301000	6	-1.154410000	-0.580708000	-1.781106000
8	-0.558113000	-1.865275000	-2.461457000	8	-0.784314000	-0.566829000	-2.875334000
6	-0.221806000	1.084148000	-0.097250000	6	-0.085620000	0.964323000	0.075367000
7	-0.388722000	2.392234000	-0.200107000	7	-0.279132000	2.367918000	0.081493000
6	1.215248000	0.673194000	-0.007153000	6	1.322773000	0.615084000	0.061919000
6	1.896104000	0.797267000	1.216560000	6	2.305827000	1.495767000	0.616751000
6	1.909626000	0.135477000	-1.091222000	6	1.845663000	-0.598483000	-0.453536000
6	3.215162000	0.393612000	1.346560000	6	3.651586000	1.184054000	0.663898000
1	1.379097000	1.198224000	2.083252000	1	1.966168000	2.429012000	1.051867000
6	3.243503000	-0.262669000	-0.975230000	6	3.202017000	-0.916916000	-0.417313000
1	1.417506000	0.023592000	-2.050550000	1	1.177923000	-1.309797000	-0.918337000
6	3.903192000	-0.139746000	0.249408000	6	4.121226000	-0.028972000	0.143252000
1	3.732520000	0.475896000	2.296029000	1	4.364244000	1.866916000	1.118613000

1	3.744007000	-0.671578000	-1.843871000	1	3.521699000	-1.863329000	-0.839369000
6	0.693655000	3.386245000	-0.373498000	6	0.205920000	3.136828000	-1.060654000
1	0.416195000	4.060528000	-1.186718000	1	-0.535957000	3.154718000	-1.878625000
1	0.809702000	3.975027000	0.539796000	1	0.404105000	4.176374000	-0.768933000
1	1.633934000	2.902525000	-0.610604000	1	1.127894000	2.708225000	-1.448661000
6	-1.702999000	3.048661000	-0.195065000	6	-1.460834000	2.972463000	0.659357000
1	-2.447625000	2.407683000	0.256570000	1	-1.788765000	2.416228000	1.532759000
1	-1.631923000	3.972932000	0.381499000	1	-1.217812000	3.993392000	0.982706000
1	-2.005283000	3.297605000	-1.215328000	1	-2.301653000	3.046104000	-0.047153000
6	5.935079000	-1.089858000	-0.586136000	6	5.982808000	-1.480190000	-0.241450000
1	6.918381000	-1.313345000	-0.176799000	1	7.058437000	-1.465861000	-0.060606000
1	5.469070000	-2.016926000	-0.935293000	1	5.539360000	-2.329228000	0.293658000
1	6.042815000	-0.395289000	-1.425957000	1	5.802861000	-1.608549000	-1.316466000
8	5.195633000	-0.507506000	0.477597000	8	5.486639000	-0.247994000	0.230535000
E= -2130.32576674 Hartrees				E= -2130.35992286 Hartrees			
1b				1b'			
24	-1.456612000	-0.433165000	0.017679000	24	-1.559237000	-0.431446000	0.013737000
6	-2.612889000	0.572736000	-1.116506000	6	-2.802098000	0.890440000	-0.524328000
8	-3.342313000	1.112591000	-1.821736000	8	-3.671129000	1.572828000	-0.870140000
6	-2.798457000	-1.752639000	0.077564000	6	-3.013094000	-1.567119000	-0.136321000
8	-3.625703000	-2.550901000	0.116894000	8	-3.924196000	-2.282345000	-0.240218000
6	-0.378519000	-1.599474000	1.094415000	6	-0.646187000	-2.001283000	0.592516000
8	0.197970000	-2.355324000	1.734084000	8	-0.243584000	-3.012653000	0.974406000
6	-2.165715000	0.333311000	1.615583000	6	-1.809715000	-0.003321000	1.839306000
8	-2.593965000	0.765278000	2.590132000	8	-1.949908000	0.254766000	2.956862000
6	-0.749077000	-1.263097000	-1.554144000	6	-0.984384000	-0.555038000	-1.793012000
8	-0.376133000	-1.796682000	-2.498524000	8	-0.643265000	-0.583175000	-2.895709000
6	0.116125000	1.045305000	-0.032383000	6	0.277897000	0.867230000	0.069416000
7	0.046416000	2.365171000	-0.041668000	7	0.232078000	2.280277000	0.117597000
6	1.517428000	0.518853000	-0.038581000	6	1.637893000	0.370053000	0.026175000
6	2.216002000	0.372399000	1.167260000	6	2.719999000	1.124991000	0.579953000
6	2.156679000	0.141761000	-1.224702000	6	2.018745000	-0.883798000	-0.528610000
6	3.509093000	-0.141138000	1.180929000	6	4.025666000	0.662320000	0.588087000
1	1.741291000	0.650621000	2.103417000	1	2.493059000	2.079929000	1.041268000
6	3.454145000	-0.365178000	-1.200352000	6	3.332353000	-1.331101000	-0.525073000
1	1.643624000	0.244755000	-2.174863000	1	1.270151000	-1.505976000	-0.998720000
6	4.153800000	-0.523622000	-0.000406000	6	4.375501000	-0.579533000	0.033612000
1	4.023242000	-0.250176000	2.131927000	1	4.799073000	1.277711000	1.047092000
1	3.925906000	-0.648191000	-2.137181000	1	3.555154000	-2.295955000	-0.977904000
6	1.198859000	3.287864000	-0.142081000	6	0.808000000	3.036797000	-0.989785000
1	0.993514000	4.018934000	-0.927320000	1	0.068829000	3.193043000	-1.795265000
1	1.325386000	3.821793000	0.802988000	1	1.142126000	4.025724000	-0.649852000
1	2.111108000	2.752800000	-0.377581000	1	1.663101000	2.511931000	-1.410090000
6	-1.214935000	3.115994000	0.022311000	6	-0.867724000	2.996537000	0.728742000
1	-2.013410000	2.492145000	0.399352000	1	-1.248667000	2.456651000	1.590578000
1	-1.083306000	3.969842000	0.689650000	1	-0.505803000	3.972524000	1.078519000
1	-1.480521000	3.487958000	-0.970385000	1	-1.701118000	3.188315000	0.035782000
6	5.539781000	-1.118719000	0.026684000	6	5.792602000	-1.094356000	0.075856000
1	5.502933000	-2.194160000	0.231847000	1	6.021627000	-1.601944000	1.023181000
1	6.052653000	-0.988716000	-0.929117000	1	5.981274000	-1.816974000	-0.724634000

1	6.158599000	-0.663678000	0.804310000	1	6.522283000	-0.284489000	-0.033634000
E=-2055.09696511 Hartrees				E= -2055.13220997 Hartrees			
1c				1c'			
24	-1.240679000	-0.312917000	0.012042000	24	-1.322026000	-0.324788000	0.014798000
6	-2.160781000	0.815945000	-1.220087000	6	-2.433939000	1.134859000	-0.446035000
8	-2.747122000	1.443278000	-1.983505000	8	-3.241543000	1.911857000	-0.737521000
6	-2.771358000	-1.409149000	0.047269000	6	-2.904268000	-1.278409000	-0.105805000
8	-3.712748000	-2.069461000	0.069577000	8	-3.897058000	-1.877734000	-0.191724000
6	-0.396838000	-1.568428000	1.191361000	6	-0.597143000	-2.012615000	0.524899000
8	0.037131000	-2.362646000	1.894062000	8	-0.320928000	-3.079193000	0.866545000
6	-1.910660000	0.608704000	1.543605000	6	-1.433399000	0.103223000	1.854406000
8	-2.326723000	1.125578000	2.481385000	8	-1.478582000	0.370955000	2.977239000
6	-0.606350000	-1.327791000	-1.482213000	6	-0.804210000	-0.458546000	-1.807624000
8	-0.288219000	-1.970606000	-2.376964000	8	-0.484167000	-0.490686000	-2.916773000
6	0.534697000	0.913490000	-0.021986000	6	0.660015000	0.741498000	0.043457000
7	0.664484000	2.228983000	-0.032903000	7	0.793771000	2.146503000	0.088350000
6	1.842827000	0.184652000	-0.021844000	6	1.944138000	0.069849000	0.023678000
6	2.495580000	-0.083019000	1.189242000	6	3.092342000	0.661980000	0.640100000
6	2.429390000	-0.252262000	-1.216564000	6	2.169858000	-1.205707000	-0.567428000
6	3.706540000	-0.771181000	1.202666000	6	4.326581000	0.032439000	0.672520000
1	2.048618000	0.237085000	2.125416000	1	2.969728000	1.620846000	1.132131000
6	3.643388000	-0.936108000	-1.198495000	6	3.411400000	-1.825170000	-0.542286000
1	1.937392000	-0.058417000	-2.163764000	1	1.357178000	-1.702262000	-1.079394000
6	4.287049000	-1.198632000	0.009589000	6	4.511564000	-1.222175000	0.077440000
1	4.194441000	-0.976138000	2.150219000	1	5.158117000	0.518800000	1.179242000
1	4.082913000	-1.268157000	-2.133602000	1	3.524899000	-2.795871000	-1.019617000
1	5.227668000	-1.739066000	0.022021000	1	5.479558000	-1.714380000	0.099542000
6	1.943697000	2.969839000	-0.099935000	6	1.525839000	2.819968000	-0.980677000
1	1.870406000	3.724241000	-0.886322000	1	0.856121000	3.076891000	-1.819935000
1	2.122539000	3.477772000	0.851026000	1	1.973267000	3.752893000	-0.614464000
1	2.772901000	2.306469000	-0.314024000	1	2.321783000	2.184830000	-1.362065000
6	-0.469168000	3.162375000	0.005328000	6	-0.234556000	3.004947000	0.638139000
1	-1.375251000	2.653241000	0.301268000	1	-0.736347000	2.522324000	1.471293000
1	-0.252102000	3.955209000	0.724181000	1	0.231655000	3.925526000	1.013362000
1	-0.611252000	3.615123000	-0.979180000	1	-0.990825000	3.301350000	-0.104538000
E= -2015.77168313 Hartrees				E= -2015.80807423 Hartrees			
1d				1d'			
24	-1.686867000	-0.479269000	0.016807000	24	-1.801740000	-0.474979000	0.014474000
6	-2.881104000	0.456516000	-1.140206000	6	-3.103949000	0.783708000	-0.538359000
8	-3.626371000	0.955600000	-1.857966000	8	-4.000189000	1.424355000	-0.892048000
6	-2.956478000	-1.871014000	0.072971000	6	-3.198484000	-1.683627000	-0.126491000
8	-3.738297000	-2.712971000	0.109433000	8	-4.072543000	-2.443186000	-0.224491000
6	-0.558616000	-1.570771000	1.119240000	6	-0.808184000	-1.989340000	0.609899000
8	0.055586000	-2.281070000	1.775605000	8	-0.350219000	-2.972521000	1.001340000
6	-2.461027000	0.257310000	1.599677000	6	-2.088540000	-0.050573000	1.837536000
8	-2.927179000	0.668519000	2.565305000	8	-2.253407000	0.203803000	2.951903000
6	-0.919221000	-1.290075000	-1.536935000	6	-1.231105000	-0.600561000	-1.793774000
8	-0.506487000	-1.814848000	-2.469450000	8	-0.894629000	-0.631689000	-2.897258000
6	-0.202004000	1.085922000	-0.033101000	6	-0.037046000	0.917579000	0.061075000

7	-0.342490000	2.399955000	-0.042580000	7	-0.155582000	2.323825000	0.106088000
6	1.226489000	0.636741000	-0.038635000	6	1.344635000	0.491464000	0.024730000
6	1.928448000	0.524729000	1.168852000	6	2.383026000	1.303771000	0.585175000
6	1.882446000	0.296326000	-1.227797000	6	1.787357000	-0.746727000	-0.524759000
6	3.249173000	0.086108000	1.192430000	6	3.713607000	0.919371000	0.602259000
1	1.437331000	0.769785000	2.105223000	1	2.104005000	2.241162000	1.052892000
6	3.205690000	-0.137776000	-1.215445000	6	3.118861000	-1.134824000	-0.523971000
1	1.361973000	0.368339000	-2.176249000	1	1.071073000	-1.409355000	-0.988936000
6	3.880901000	-0.240045000	-0.003471000	6	4.084583000	-0.302430000	0.039558000
1	3.780752000	-0.004242000	2.132345000	1	4.462653000	1.556295000	1.062324000
1	3.705102000	-0.398631000	-2.141082000	1	3.408468000	-2.081985000	-0.966696000
6	0.757090000	3.385938000	-0.136510000	6	0.414592000	3.118925000	-0.978221000
1	0.508481000	4.112665000	-0.912818000	1	-0.321188000	3.271384000	-1.786642000
1	0.857538000	3.915979000	0.813813000	1	0.718530000	4.109156000	-0.615206000
1	1.697172000	2.906239000	-0.381251000	1	1.286884000	2.626545000	-1.401613000
6	-1.643377000	3.080228000	0.020702000	6	-1.297837000	2.988655000	0.698424000
1	-2.411198000	2.404776000	0.370815000	1	-1.680387000	2.421819000	1.541503000
1	-1.567203000	3.923868000	0.709397000	1	-0.982814000	3.972191000	1.071002000
1	-1.914584000	3.460421000	-0.967271000	1	-2.117941000	3.158538000	-0.015140000
17	5.548141000	-0.792889000	0.018101000	17	5.791785000	-0.792439000	0.035439000
E= -2475.39517754 Hartrees				E=-2475.43914816 Hartrees			
1e				1e'			
24	-2.141614000	-0.557206000	0.013140000	24	-2.241713000	-0.578728000	0.045077000
6	-3.330964000	0.200460000	-1.272079000	6	-3.681031000	0.475998000	-0.583785000
8	-4.064335000	0.591787000	-2.064933000	8	-4.637759000	0.995323000	-0.974128000
6	-3.302363000	-2.039117000	0.100454000	6	-3.493683000	-1.948244000	0.057175000
8	-4.019330000	-2.936137000	0.153546000	8	-4.278750000	-2.803388000	0.056313000
6	-0.996868000	-1.475786000	1.249227000	6	-1.048143000	-1.910958000	0.724844000
8	-0.368467000	-2.089109000	1.984736000	8	-0.463234000	-2.795990000	1.170574000
6	-3.064437000	0.212828000	1.497588000	6	-2.553094000	-0.046360000	1.838965000
8	-3.620201000	0.641374000	2.406484000	8	-2.735295000	0.276623000	2.931682000
6	-1.226499000	-1.414342000	-1.433009000	6	-1.720331000	-0.828343000	-1.766667000
8	-0.725932000	-1.974747000	-2.299219000	8	-1.429062000	-0.940909000	-2.876484000
6	-0.792154000	1.123115000	-0.075263000	6	-0.659553000	1.005308000	-0.056047000
7	-1.037658000	2.417674000	-0.170637000	7	-0.954074000	2.362122000	-0.129116000
6	0.663318000	0.791332000	0.000357000	6	0.751190000	0.725086000	-0.034994000
6	1.317121000	0.798473000	1.242114000	6	1.677375000	1.636582000	0.581132000
6	1.394015000	0.447028000	-1.145120000	6	1.342190000	-0.464878000	-0.562298000
6	2.663602000	0.473315000	1.332754000	6	3.026353000	1.384851000	0.657104000
1	0.764081000	1.048514000	2.141883000	1	1.284224000	2.531157000	1.052162000
6	2.743460000	0.124690000	-1.053387000	6	2.697627000	-0.704956000	-0.510796000
1	0.906611000	0.429965000	-2.113641000	1	0.713155000	-1.190793000	-1.058850000
6	3.391308000	0.135361000	0.186644000	6	3.588097000	0.210870000	0.099205000
1	3.167724000	0.475191000	2.292180000	1	3.685073000	2.082772000	1.163893000
1	3.296751000	-0.138573000	-1.946126000	1	3.092864000	-1.613712000	-0.949899000
6	-0.016276000	3.483157000	-0.276830000	6	-0.238662000	3.271139000	-1.021826000
1	-0.281319000	4.139372000	-1.108508000	1	-0.925484000	3.637954000	-1.799896000
1	-0.006142000	4.075005000	0.641728000	1	0.153497000	4.146687000	-0.487941000
1	0.969942000	3.068193000	-0.447336000	1	0.591094000	2.764258000	-1.505555000
6	-2.389898000	2.991447000	-0.203181000	6	-2.185209000	2.958763000	0.350158000

1	-3.118810000	2.274335000	0.147269000	1	-2.656657000	2.331549000	1.097591000
1	-2.415438000	3.871959000	0.441851000	1	-1.957660000	3.926354000	0.816679000
1	-2.640357000	3.298532000	-1.221574000	1	-2.902390000	3.146430000	-0.461466000
6	4.833139000	-0.201750000	0.342646000	6	5.022251000	-0.000612000	0.188352000
8	5.429825000	-0.185884000	1.395285000	8	5.839339000	0.753681000	0.699408000
8	5.416731000	-0.529550000	-0.830856000	8	5.426916000	-1.191045000	-0.380403000
6	6.810395000	-0.875162000	-0.763911000	6	6.823597000	-1.456141000	-0.316751000
1	6.957635000	-1.740615000	-0.117366000	1	7.170552000	-1.501544000	0.718368000
1	7.100714000	-1.107307000	-1.785906000	1	6.963200000	-2.422526000	-0.801513000
1	7.393217000	-0.037509000	-0.379721000	1	7.397080000	-0.686956000	-0.839920000
E=-2243.71642831 Hartrees				E=-2243.76806073 Hartrees			
1f				1f'			
24	-2.126201000	-0.522859000	0.013450000	24	-2.265236000	-0.515832000	0.022431000
6	-3.344868000	0.333452000	-1.181150000	6	-3.646913000	0.669976000	-0.495104000
8	-4.097336000	0.786284000	-1.921103000	8	-4.580799000	1.267352000	-0.824713000
6	-3.314240000	-1.986558000	0.056090000	6	-3.598850000	-1.800831000	-0.072135000
8	-4.046003000	-2.872193000	0.083039000	8	-4.434167000	-2.604553000	-0.140818000
6	-0.960989000	-1.533066000	1.153141000	6	-1.164612000	-1.973286000	0.581464000
8	-0.319332000	-2.196657000	1.831707000	8	-0.638916000	-2.929264000	0.950933000
6	-2.980853000	0.175338000	1.572986000	6	-2.527285000	-0.110971000	1.855850000
8	-3.494609000	0.559262000	2.525303000	8	-2.678284000	0.134045000	2.973599000
6	-1.279059000	-1.310345000	-1.511946000	6	-1.757456000	-0.627830000	-1.805988000
8	-0.816896000	-1.825718000	-2.425951000	8	-1.465576000	-0.652216000	-2.921558000
6	-0.744508000	1.131441000	-0.027333000	6	-0.586293000	0.973437000	0.021862000
7	-0.962211000	2.434499000	-0.034569000	7	-0.788534000	2.359945000	0.067544000
6	0.705976000	0.765312000	-0.031854000	6	0.808799000	0.615713000	-0.019458000
6	1.405440000	0.669491000	1.178225000	6	1.806477000	1.457094000	0.580164000
6	1.385006000	0.488177000	-1.226411000	6	1.313831000	-0.582943000	-0.608556000
6	2.747919000	0.306791000	1.196744000	6	3.146618000	1.134840000	0.588842000
1	0.895091000	0.868972000	2.114738000	1	1.480510000	2.360736000	1.082801000
6	2.728266000	0.131759000	-1.210254000	6	2.658601000	-0.898105000	-0.616745000
1	0.863375000	0.552036000	-2.174700000	1	0.630440000	-1.259090000	-1.102017000
6	3.415381000	0.041613000	0.001697000	6	3.607158000	-0.045052000	-0.026323000
1	3.273340000	0.236205000	2.141553000	1	3.852942000	1.797407000	1.080404000
1	3.240578000	-0.073056000	-2.143504000	1	2.985214000	-1.813067000	-1.099666000
6	0.078153000	3.484124000	-0.111317000	6	-0.159948000	3.237632000	-0.916690000
1	-0.209981000	4.206092000	-0.878056000	1	-0.876261000	3.492281000	-1.715111000
1	0.145307000	4.005429000	0.846754000	1	0.170047000	4.177550000	-0.455645000
1	1.045639000	3.064675000	-0.360262000	1	0.701544000	2.757555000	-1.372347000
6	-2.301216000	3.036718000	0.023694000	6	-1.970928000	2.975447000	0.635325000
1	-3.034582000	2.308099000	0.338858000	1	-2.400224000	2.349785000	1.410247000
1	-2.286529000	3.862616000	0.737667000	1	-1.690561000	3.933553000	1.092470000
1	-2.575718000	3.429676000	-0.958295000	1	-2.743693000	3.187459000	-0.118089000
6	4.855101000	-0.390693000	0.008718000	6	5.040596000	-0.407225000	0.026021000
9	5.552815000	0.155513000	-1.016062000	9	5.412393000	-1.278897000	-0.951004000
9	5.490236000	-0.044965000	1.150484000	9	5.871175000	0.672871000	-0.085500000
9	4.982296000	-1.735299000	-0.116169000	9	5.420721000	-1.011097000	1.204848000
E=-2352.92183976 Hartrees				E=-2352.97357412 Hartrees			
2a				2a'			

24	-1.851265000	-0.629356000	0.069996000	24	-1.979225000	-0.590816000	-0.002116000
6	-1.660867000	-1.585889000	-1.567853000	6	-1.689364000	-0.861670000	-1.853333000
8	-1.515047000	-2.189045000	-2.537298000	8	-1.464154000	-1.049876000	-2.973062000
6	-3.299020000	-1.725396000	0.576449000	6	-3.544978000	-1.574816000	0.044473000
8	-4.172617000	-2.405040000	0.898680000	8	-4.520818000	-2.213479000	0.073362000
6	-1.936172000	0.287277000	1.739050000	6	-1.905758000	-0.274987000	1.867478000
8	-1.951615000	0.798706000	2.770393000	8	-1.804127000	-0.149032000	3.012680000
6	-0.725257000	-1.887317000	0.877504000	6	-1.128080000	-2.194991000	0.374289000
8	-0.071769000	-2.687837000	1.384003000	8	-0.700302000	-3.240835000	0.635481000
6	-0.194052000	0.594208000	-0.367415000	6	-0.088630000	0.584244000	-0.047093000
7	-0.398399000	1.849610000	-0.736849000	7	-0.225278000	1.997381000	0.077975000
6	1.221006000	0.175632000	-0.187454000	6	1.263205000	0.094869000	0.021641000
6	1.983676000	0.628144000	0.903527000	6	2.308151000	0.806029000	0.695780000
6	1.806773000	-0.742809000	-1.062076000	6	1.662368000	-1.136700000	-0.563109000
6	3.280302000	0.180793000	1.102908000	6	3.604034000	0.326574000	0.773867000
1	1.548862000	1.322903000	1.614335000	1	2.063724000	1.733416000	1.200810000
6	3.120769000	-1.177573000	-0.886685000	6	2.965845000	-1.617711000	-0.495683000
1	1.235121000	-1.130931000	-1.898120000	1	0.929478000	-1.720163000	-1.104923000
6	3.864367000	-0.720486000	0.204096000	6	3.954234000	-0.888491000	0.173449000
1	3.860355000	0.514455000	1.956337000	1	4.366762000	0.878618000	1.316700000
1	3.538401000	-1.881516000	-1.595311000	1	3.194301000	-2.563789000	-0.973974000
6	0.667804000	4.000554000	-0.037186000	6	1.007806000	4.150682000	-0.132597000
1	-0.264901000	4.532184000	0.141996000	1	0.232935000	4.723242000	0.376306000
6	-2.650727000	1.098074000	-1.256866000	6	-2.542747000	1.591712000	-0.600470000
1	-2.523071000	0.774017000	-2.285123000	1	-2.384350000	1.654369000	-1.673500000
6	-1.808254000	2.271919000	-0.852960000	6	-1.611811000	2.424079000	0.242315000
1	-1.864326000	3.075404000	-1.596229000	1	-1.695143000	3.483276000	-0.036732000
1	-2.142818000	2.685120000	0.104584000	1	-1.909468000	2.356910000	1.294655000
6	0.624369000	2.881185000	-1.043449000	6	0.563063000	2.877494000	-0.805075000
1	1.592321000	2.392130000	-1.121500000	1	1.432598000	2.327458000	-1.159862000
1	0.373447000	3.282947000	-2.032655000	1	-0.030493000	3.133801000	-1.703221000
6	1.771393000	4.386321000	0.596837000	6	2.256995000	4.612770000	-0.127352000
1	2.723681000	3.885577000	0.447536000	1	3.068025000	4.068210000	-0.603772000
6	-3.747945000	0.667041000	-0.558371000	6	-3.706956000	1.036715000	-0.138099000
1	-4.073712000	1.165952000	0.347065000	1	-4.027928000	1.182181000	0.887717000
1	1.764192000	5.221207000	1.289505000	1	2.519963000	5.544795000	0.365182000
1	-4.481385000	0.023448000	-1.026876000	1	-4.473819000	0.694589000	-0.822526000
8	5.145649000	-1.092921000	0.481496000	8	5.281359000	-1.275658000	0.295773000
6	5.778107000	-2.039898000	-0.367736000	6	5.655020000	-2.513838000	-0.263154000
1	5.870970000	-1.660576000	-1.390845000	1	5.508567000	-2.532605000	-1.350946000
1	6.771414000	-2.195679000	0.048863000	1	6.716729000	-2.639546000	-0.045693000
1	5.236153000	-2.990941000	-0.377651000	1	5.096418000	-3.347586000	0.180906000

E=-2171.77206667 Hartrees

2b

24	-1.704409000	-0.417679000	0.075968000
6	-1.722849000	-1.326733000	-1.601365000
8	-1.708318000	-1.904135000	-2.596334000
6	-3.312153000	-1.261395000	0.586487000
8	-4.284295000	-1.788737000	0.911164000
6	-1.585799000	0.434222000	1.775977000

E=-2171.79916958 Hartrees

2b'

24	-1.848675000	-0.310264000	0.006993000
6	-1.689049000	-0.676958000	-1.844504000
8	-1.558130000	-0.933420000	-2.965293000
6	-3.583707000	-0.943132000	0.115807000
8	-4.671027000	-1.359369000	0.185775000
6	-1.679852000	0.014251000	1.869045000

8	-1.484532000	0.901836000	2.823329000	8	-1.541526000	0.132733000	3.011077000
6	-0.802045000	-1.888675000	0.801255000	6	-1.334224000	-2.050202000	0.400903000
8	-0.291399000	-2.814221000	1.255919000	8	-1.124425000	-3.156097000	0.676222000
6	0.124963000	0.511249000	-0.373012000	6	0.244870000	0.440852000	-0.091747000
7	0.142414000	1.790214000	-0.710201000	7	0.402452000	1.846487000	0.039464000
6	1.445830000	-0.162208000	-0.250171000	6	1.459103000	-0.326146000	-0.042959000
6	2.225886000	-0.013883000	0.904316000	6	2.640084000	0.128782000	0.623724000
6	1.907579000	-1.014481000	-1.260402000	6	1.572118000	-1.612146000	-0.649242000
6	3.431613000	-0.697010000	1.036289000	6	3.800413000	-0.632832000	0.672980000
1	1.883160000	0.628590000	1.709002000	1	2.611286000	1.077012000	1.148564000
6	3.123910000	-1.678449000	-1.124790000	6	2.739504000	-2.352170000	-0.603839000
1	1.313103000	-1.163030000	-2.156046000	1	0.720630000	-2.010654000	-1.186188000
6	3.905933000	-1.540503000	0.026321000	6	3.892370000	-1.888562000	0.058360000
1	4.011561000	-0.573109000	1.946841000	1	4.659423000	-0.244533000	1.219634000
1	3.462129000	-2.328008000	-1.927373000	1	2.763200000	-3.322664000	-1.097561000
6	1.566772000	3.699995000	0.041743000	6	2.072820000	3.690314000	-0.074248000
1	0.758349000	4.410475000	0.203651000	1	1.424233000	4.396848000	0.442823000
6	-2.221063000	1.470511000	-1.178281000	6	-1.949864000	1.924351000	-0.624398000
1	-2.185371000	1.161114000	-2.218206000	1	-1.786575000	1.935722000	-1.698488000
6	-1.170282000	2.462415000	-0.775846000	6	-0.862092000	2.559786000	0.200606000
1	-1.099142000	3.281786000	-1.500270000	1	-0.721973000	3.607026000	-0.100521000
1	-1.398509000	2.902982000	0.200283000	1	-1.161213000	2.578066000	1.254932000
6	1.332944000	2.631203000	-0.993083000	6	1.385755000	2.559316000	-0.795400000
1	2.199150000	1.979551000	-1.076105000	1	2.126920000	1.846187000	-1.150287000
1	1.165479000	3.092187000	-1.973897000	1	0.882786000	2.961607000	-1.694961000
6	2.700655000	3.834167000	0.723649000	6	3.390530000	3.880983000	-0.038446000
1	3.532973000	3.148709000	0.592617000	1	4.078983000	3.192980000	-0.522079000
6	-3.355744000	1.219329000	-0.452533000	6	-3.202519000	1.632202000	-0.150772000
1	-3.560969000	1.738604000	0.476544000	1	-3.483280000	1.861075000	0.871632000
1	2.839887000	4.637719000	1.439072000	1	3.832437000	4.722760000	0.487403000
1	-4.205682000	0.731145000	-0.911809000	1	-4.025743000	1.444754000	-0.829504000
6	5.194441000	-2.307512000	0.192288000	6	5.154208000	-2.713187000	0.105921000
1	5.016761000	-3.275910000	0.672719000	1	4.989951000	-3.692736000	0.573248000
1	5.671729000	-2.507004000	-0.770208000	1	5.560839000	-2.908571000	-0.895414000
1	5.909115000	-1.764410000	0.815670000	1	5.937188000	-2.207729000	0.679691000
E= -2096.54304675 Hartrees				E= -2096.57188183 Hartrees			

2c				2c'			
24	-1.554174000	-0.084974000	0.067861000	24	1.670461000	-0.023130000	0.005576000
6	-1.788499000	-1.022021000	-1.577834000	6	1.610153000	0.416775000	-1.835639000
8	-1.913273000	-1.623103000	-2.550680000	8	1.549041000	0.723021000	-2.949818000
6	-3.346402000	-0.424816000	0.550230000	6	3.512656000	0.113376000	0.111567000
8	-4.434783000	-0.646246000	0.857538000	8	4.672328000	0.217114000	0.179240000
6	-1.243612000	0.765183000	1.745576000	6	1.430644000	-0.340727000	1.861272000
8	-1.043335000	1.224638000	2.782094000	8	1.274589000	-0.451165000	3.001793000
6	-1.116933000	-1.719019000	0.869927000	6	1.642833000	1.781263000	0.446131000
8	-0.896000000	-2.730513000	1.371798000	8	1.736362000	2.895123000	0.750326000
6	0.468021000	0.275467000	-0.358727000	6	-0.547648000	-0.169647000	-0.094794000
7	0.854262000	1.484395000	-0.730095000	7	-1.082449000	-1.479580000	0.010801000
6	1.541879000	-0.742287000	-0.197558000	6	-1.503958000	0.900972000	-0.024438000
6	2.298140000	-0.806309000	0.981097000	6	-2.756223000	0.774237000	0.660516000

6	1.769606000	-1.691724000	-1.202695000	6	-1.264679000	2.173043000	-0.624073000
6	3.265174000	-1.795526000	1.144628000	6	-3.667895000	1.817510000	0.728975000
1	2.119640000	-0.088900000	1.775407000	1	-2.973716000	-0.152350000	1.179808000
6	2.748362000	-2.669589000	-1.039393000	6	-2.188054000	3.203363000	-0.563248000
1	1.175174000	-1.670116000	-2.110189000	1	-0.341414000	2.326432000	-1.168428000
6	3.498116000	-2.727167000	0.134209000	6	-3.408279000	3.047169000	0.111443000
1	3.834600000	-1.839713000	2.067664000	1	-4.593182000	1.676669000	1.284984000
1	2.915295000	-3.395678000	-1.828649000	1	-1.957373000	4.148288000	-1.050176000
6	2.751076000	2.920005000	0.029258000	6	-3.206374000	-2.778250000	-0.081234000
1	2.176699000	3.834443000	0.165083000	1	-2.775009000	-3.647944000	0.413699000
6	-1.491548000	1.827195000	-1.257265000	6	1.156191000	-2.181058000	-0.676739000
1	-1.520373000	1.481168000	-2.285870000	1	0.995410000	-2.123208000	-1.749697000
6	-0.213435000	2.497452000	-0.848961000	6	-0.063466000	-2.518170000	0.139765000
1	0.100866000	3.240348000	-1.590737000	1	-0.487087000	-3.476068000	-0.191825000
1	-0.329034000	3.014390000	0.109288000	1	0.220176000	-2.652197000	1.189988000
6	2.240148000	1.945343000	-0.998732000	6	-2.240817000	-1.878052000	-0.808550000
1	2.885762000	1.072454000	-1.056584000	1	-2.756887000	-0.981771000	-1.146590000
1	2.227737000	2.417558000	-1.988195000	1	-1.885900000	-2.397177000	-1.718692000
6	3.862641000	2.734643000	0.735412000	6	-4.522891000	-2.587385000	-0.015505000
1	4.465847000	1.837572000	0.629460000	1	-4.996920000	-1.724629000	-0.475974000
6	-2.667188000	1.928793000	-0.561542000	6	2.442027000	-2.254364000	-0.206387000
1	-2.739835000	2.516236000	0.346468000	1	2.651108000	-2.576064000	0.808203000
1	4.212946000	3.475759000	1.445986000	1	-5.174898000	-3.277015000	0.513336000
1	-3.608751000	1.679910000	-1.033890000	1	3.283948000	-2.284640000	-0.887442000
1	4.249611000	-3.498774000	0.264984000	1	-4.126048000	3.860791000	0.162662000

E=-2057.21763422 Hartrees

E=-2057.24778979 Hartrees

2d

24	-1.862431000	-0.582738000	0.076292000
6	-1.728247000	-1.503068000	-1.590514000
8	-1.614564000	-2.082271000	-2.577633000
6	-3.338174000	-1.648514000	0.578460000
8	-4.225920000	-2.309739000	0.897084000
6	-1.895173000	0.290952000	1.770398000
8	-1.880379000	0.775425000	2.814519000
6	-0.764013000	-1.897923000	0.828691000
8	-0.125047000	-2.730432000	1.300334000
6	-0.187509000	0.592773000	-0.373222000
7	-0.344819000	1.859151000	-0.719988000
6	1.215046000	0.107608000	-0.257890000
6	1.955873000	0.316136000	0.912887000
6	1.794910000	-0.630294000	-1.297797000
6	3.247091000	-0.188761000	1.039733000
1	1.519553000	0.866121000	1.739879000
6	3.090910000	-1.126795000	-1.185098000
1	1.230262000	-0.827943000	-2.202758000
6	3.808541000	-0.901217000	-0.015044000
1	3.810484000	-0.032413000	1.952131000
1	3.533933000	-1.692694000	-1.996059000
6	0.810578000	3.923992000	0.075881000
1	-0.087853000	4.509969000	0.259731000

2d'

24	-2.016260000	-0.508524000	0.009110000
6	-1.805366000	-0.855982000	-1.841450000
8	-1.637356000	-1.093834000	-2.960971000
6	-3.633823000	-1.402885000	0.119550000
8	-4.642551000	-1.982440000	0.189102000
6	-1.911099000	-0.151493000	1.870621000
8	-1.802948000	-0.004911000	3.012218000
6	-1.236896000	-2.144836000	0.415345000
8	-0.853589000	-3.200439000	0.699004000
6	-0.065001000	0.551457000	-0.100750000
7	-0.123580000	1.961724000	0.018748000
6	1.250220000	-0.020458000	-0.054766000
6	2.347891000	0.617043000	0.611329000
6	1.555408000	-1.277279000	-0.658021000
6	3.614977000	0.056740000	0.664474000
1	2.171584000	1.547895000	1.137370000
6	2.821950000	-1.834604000	-0.622079000
1	0.775147000	-1.805607000	-1.190278000
6	3.856271000	-1.166097000	0.038897000
1	4.412458000	0.558651000	1.203766000
1	3.012481000	-2.785743000	-1.107920000
6	1.270378000	4.025619000	-0.060103000
1	0.528649000	4.618895000	0.473689000

6	-2.634896000	1.205246000	-1.199086000	6	-2.462352000	1.681164000	-0.632750000
1	-2.546169000	0.895388000	-2.235790000	1	-2.309271000	1.711717000	-1.707883000
6	-1.739107000	2.339702000	-0.797138000	6	-1.479789000	2.480238000	0.180929000
1	-1.779485000	3.156020000	-1.527014000	1	-1.497407000	3.532944000	-0.132177000
1	-2.033350000	2.749882000	0.174645000	1	-1.774428000	2.466315000	1.236466000
6	0.719431000	2.860253000	-0.986152000	6	0.750374000	2.820688000	-0.801112000
1	1.665934000	2.334642000	-1.087268000	1	1.583727000	2.226171000	-1.170081000
1	0.486315000	3.317280000	-1.954980000	1	0.192614000	3.162723000	-1.692477000
6	1.920047000	4.196171000	0.756752000	6	2.546166000	4.406191000	-0.026811000
1	2.839440000	3.638568000	0.602764000	1	3.324191000	3.836943000	-0.528642000
6	-3.727457000	0.799276000	-0.479827000	6	-3.652624000	1.204148000	-0.149146000
1	-4.012180000	1.289868000	0.443759000	1	-3.958026000	1.392628000	0.874357000
1	1.951870000	4.992156000	1.493061000	1	2.864114000	5.293347000	0.513468000
1	-4.493933000	0.189502000	-0.940602000	1	-4.442307000	0.890535000	-0.821081000
17	5.441615000	-1.532457000	0.136870000	17	5.486072000	-1.874108000	0.077752000
E=-2516.84148927 Hartrees				E=-2516.87925951 Hartrees			
2e				2e'			
24	-2.205272000	-0.797065000	0.084581000	24	-2.321285000	-0.790840000	0.039825000
6	-1.897076000	-1.729610000	-1.551688000	6	-2.015766000	-1.410804000	-1.726330000
8	-1.676097000	-2.308308000	-2.520669000	8	-1.809584000	-1.808945000	-2.791467000
6	-3.491778000	-2.076421000	0.607324000	6	-3.699579000	-2.000665000	0.312918000
8	-4.262466000	-2.865790000	0.938670000	8	-4.554309000	-2.771520000	0.486135000
6	-2.404329000	0.115731000	1.747077000	6	-2.411793000	-0.132360000	1.819518000
8	-2.483846000	0.633595000	2.771797000	8	-2.429092000	0.206644000	2.923866000
6	-0.918701000	-1.894254000	0.888649000	6	-1.191189000	-2.111271000	0.715540000
8	-0.163187000	-2.601955000	1.390480000	8	-0.582201000	-2.980469000	1.172342000
6	-0.746398000	0.631452000	-0.391732000	6	-0.642881000	0.636634000	-0.218098000
7	-1.108917000	1.837794000	-0.791009000	7	-1.023952000	1.971720000	-0.300054000
6	0.711093000	0.390388000	-0.231999000	6	0.754202000	0.353169000	-0.104758000
6	1.373502000	0.759448000	0.948815000	6	1.681568000	1.232262000	0.556007000
6	1.431603000	-0.274073000	-1.234365000	6	1.323634000	-0.855295000	-0.617851000
6	2.723001000	0.478591000	1.114832000	6	3.021744000	0.943501000	0.659088000
1	0.825949000	1.257473000	1.741781000	1	1.301926000	2.122261000	1.044404000
6	2.784689000	-0.546923000	-1.069192000	6	2.669924000	-1.127341000	-0.542974000
1	0.928752000	-0.587177000	-2.143106000	1	0.675897000	-1.560702000	-1.123360000
6	3.443047000	-0.172583000	0.107316000	6	3.571036000	-0.232592000	0.091233000
1	3.235803000	0.757536000	2.028071000	1	3.683969000	1.613744000	1.197967000
1	3.331476000	-1.059173000	-1.850911000	1	3.053235000	-2.043188000	-0.977779000
6	-0.331221000	4.096797000	-0.063716000	6	-0.074417000	4.274343000	-0.103148000
1	-1.315053000	4.541474000	0.073142000	1	-0.987927000	4.671255000	0.338621000
6	-3.251493000	0.790710000	-1.262469000	6	-3.197122000	1.096529000	-0.949831000
1	-3.103384000	0.463012000	-2.286693000	1	-2.997092000	0.998078000	-2.012978000
6	-2.562856000	2.073069000	-0.899712000	6	-2.464408000	2.217357000	-0.268069000
1	-2.728382000	2.842908000	-1.661728000	1	-2.668573000	3.169565000	-0.776887000
1	-2.936434000	2.463554000	0.052788000	1	-2.822595000	2.330991000	0.762801000
6	-0.222326000	2.993399000	-1.082939000	6	-0.229928000	3.031791000	-0.942467000
1	0.800677000	2.630660000	-1.149492000	1	0.745063000	2.632508000	-1.211541000
1	-0.508851000	3.367307000	-2.072768000	1	-0.731424000	3.307375000	-1.886332000
6	0.700552000	4.562862000	0.634015000	6	1.076211000	4.909649000	0.109168000
1	1.699397000	4.149522000	0.527835000	1	2.015174000	4.541942000	-0.295365000

6	-4.267971000	0.236108000	-0.530933000	6	-4.281557000	0.446253000	-0.416862000
1	-4.637701000	0.707480000	0.372316000	1	-4.683029000	0.722937000	0.551879000
1	0.585178000	5.379778000	1.338342000	1	1.125538000	5.813842000	0.708797000
1	-4.918825000	-0.509038000	-0.969850000	1	-4.944028000	-0.135264000	-1.046290000
6	4.887864000	-0.446056000	0.340024000	6	4.996763000	-0.469571000	0.198802000
8	5.497854000	-0.111940000	1.330562000	8	5.822767000	0.263092000	0.730579000
8	5.458777000	-1.115420000	-0.685546000	8	5.390591000	-1.661517000	-0.381263000
6	6.852664000	-1.429359000	-0.531890000	6	6.781093000	-1.948364000	-0.302266000
1	7.007372000	-2.056018000	0.346841000	1	7.114118000	-2.013394000	0.736574000
1	7.130599000	-1.964496000	-1.436967000	1	6.913474000	-2.910232000	-0.798462000
1	7.440900000	-0.516918000	-0.429360000	1	7.374217000	-1.181236000	-0.806738000
E= -2285.16281559 Hartrees				E= -2285.20943975 Hartrees			
2f				2f'			
24	-2.237424000	-0.702530000	0.073631000	24	-2.378267000	-0.672977000	0.021624000
6	-2.009110000	-1.587053000	-1.603692000	6	-2.127369000	-1.174847000	-1.789301000
8	-1.833945000	-2.138158000	-2.597299000	8	-1.944696000	-1.503110000	-2.882631000
6	-3.596857000	-1.918036000	0.567890000	6	-3.853372000	-1.775920000	0.224907000
8	-4.411511000	-2.668877000	0.881669000	8	-4.770006000	-2.482401000	0.353663000
6	-2.354061000	0.152542000	1.773282000	6	-2.374338000	-0.142729000	1.845528000
8	-2.383817000	0.632445000	2.819039000	8	-2.329878000	0.112906000	2.971610000
6	-1.013286000	-1.910027000	0.812024000	6	-1.366451000	-2.133470000	0.576340000
8	-0.295663000	-2.681921000	1.273561000	8	-0.831828000	-3.086846000	0.954684000
6	-0.700464000	0.646303000	-0.374594000	6	-0.590435000	0.629841000	-0.173372000
7	-0.988568000	1.889029000	-0.719672000	7	-0.854043000	2.007278000	-0.144108000
6	0.743297000	0.305069000	-0.269720000	6	0.781872000	0.232985000	-0.096213000
6	1.434621000	0.478201000	0.937623000	6	1.784364000	1.012046000	0.577609000
6	1.416847000	-0.260972000	-1.359904000	6	1.248854000	-0.993458000	-0.664793000
6	2.770066000	0.109486000	1.045322000	6	3.102717000	0.613509000	0.652609000
1	0.922776000	0.891250000	1.799856000	1	1.484293000	1.915121000	1.095731000
6	2.755545000	-0.624429000	-1.254498000	6	2.571094000	-1.378177000	-0.611094000
1	0.890469000	-0.429425000	-2.293231000	1	0.543454000	-1.627096000	-1.186565000
6	3.436255000	-0.439169000	-0.051735000	6	3.531844000	-0.584847000	0.050706000
1	3.289998000	0.240665000	1.987443000	1	3.813219000	1.221860000	1.204230000
1	3.262478000	-1.063224000	-2.105739000	1	2.873168000	-2.309144000	-1.079593000
6	-0.041240000	4.038836000	0.121680000	6	0.270346000	4.230251000	-0.031893000
1	-0.989822000	4.534704000	0.318110000	1	-0.586623000	4.704609000	0.445235000
6	-3.201926000	1.003129000	-1.190329000	6	-3.105302000	1.356174000	-0.812194000
1	-3.089895000	0.709711000	-2.229491000	1	-2.926210000	1.319348000	-1.883006000
6	-2.425837000	2.222086000	-0.786715000	6	-2.271037000	2.355803000	-0.059532000
1	-2.554868000	3.034563000	-1.510435000	1	-2.412500000	3.360765000	-0.480294000
1	-2.755140000	2.592318000	0.189949000	1	-2.599977000	2.407002000	0.985524000
6	-0.033598000	2.999753000	-0.968317000	6	-0.022834000	2.997624000	-0.848612000
1	0.961025000	2.577135000	-1.089706000	1	0.906724000	2.526020000	-1.159200000
1	-0.320333000	3.453986000	-1.923659000	1	-0.545244000	3.301748000	-1.773265000
6	1.038055000	4.391274000	0.814055000	6	1.478025000	4.768427000	0.126414000
1	2.004773000	3.924517000	0.648188000	1	2.364435000	4.321864000	-0.316037000
6	-4.240588000	0.484137000	-0.464571000	6	-4.232788000	0.758846000	-0.308930000
1	-4.565283000	0.939372000	0.463909000	1	-4.595791000	0.991970000	0.686109000
1	0.996418000	5.165741000	1.572432000	1	1.628759000	5.668780000	0.714938000
1	-4.944307000	-0.199397000	-0.921822000	1	-4.949484000	0.281825000	-0.966301000

6	4.896299000	-0.777546000	0.056728000	6	4.961273000	-0.954524000	0.043403000
9	5.224463000	-1.242986000	1.282994000	9	5.635203000	-0.531928000	1.153332000
9	5.681799000	0.312755000	-0.160639000	9	5.674613000	-0.417161000	-1.013943000
9	5.278765000	-1.710192000	-0.842152000	9	5.173625000	-2.296885000	-0.048926000
E=-2394.36849658 Hartrees				E=-2394.41461355 Hartrees			
1g				1g'			
24	-1.447066000	-0.415971000	0.014474000	24	-1.546738000	-0.416353000	0.013309000
6	-2.544520000	0.598395000	-1.171636000	6	-2.762114000	0.923253000	-0.547060000
8	-3.233950000	1.148544000	-1.907678000	8	-3.614783000	1.618140000	-0.906939000
6	-2.818518000	-1.707541000	0.059659000	6	-3.019715000	-1.529001000	-0.133176000
8	-3.662969000	-2.487136000	0.089315000	8	-3.941907000	-2.229471000	-0.234490000
6	-0.419383000	-1.575459000	1.144494000	6	-0.661084000	-1.992556000	0.614679000
8	0.132562000	-2.321051000	1.817085000	8	-0.271664000	-3.004086000	1.009555000
6	-2.192836000	0.385888000	1.579082000	6	-1.806230000	0.031070000	1.833954000
8	-2.645872000	0.834157000	2.534515000	8	-1.952651000	0.298356000	2.948158000
6	-0.717302000	-1.298246000	-1.518078000	6	-0.969956000	-0.575926000	-1.789889000
8	-0.330980000	-1.863997000	-2.437913000	8	-0.624844000	-0.627724000	-2.890296000
6	0.151676000	1.032410000	-0.024930000	6	0.307927000	0.855540000	0.069055000
7	0.108400000	2.353603000	-0.034296000	7	0.286651000	2.270749000	0.114625000
6	1.545010000	0.479986000	-0.028834000	6	1.663007000	0.340307000	0.030406000
6	2.231419000	0.303283000	1.180282000	6	2.751040000	1.088572000	0.582758000
6	2.177763000	0.107528000	-1.221508000	6	2.021405000	-0.925851000	-0.514492000
6	3.516341000	-0.233127000	1.203216000	6	4.055993000	0.617187000	0.601063000
1	1.755205000	0.573643000	2.117159000	1	2.531806000	2.046621000	1.039537000
6	3.465238000	-0.424803000	-1.212290000	6	3.326302000	-1.402590000	-0.509092000
1	1.666278000	0.230534000	-2.169536000	1	1.261911000	-1.541041000	-0.974497000
6	4.111595000	-0.586386000	0.002683000	6	4.331268000	-0.626723000	0.048934000
1	4.048876000	-0.381508000	2.135550000	1	4.856331000	1.197695000	1.050564000
1	3.959930000	-0.717366000	-2.131289000	1	3.566840000	-2.369056000	-0.940615000
6	1.277939000	3.256641000	-0.117747000	6	0.857168000	3.009221000	-1.008325000
1	1.096418000	3.992331000	-0.904349000	1	0.114997000	3.152889000	-1.813069000
1	1.399691000	3.787055000	0.829875000	1	1.193293000	4.002850000	-0.685273000
1	2.185119000	2.708217000	-0.341307000	1	1.710259000	2.477489000	-1.424661000
6	-1.138909000	3.128915000	0.016296000	6	-0.802480000	3.003140000	0.726977000
1	-1.959474000	2.513482000	0.357275000	1	-1.179244000	2.476622000	1.598938000
1	-1.007302000	3.964717000	0.706163000	1	-0.429585000	3.980105000	1.061435000
1	-1.370101000	3.528259000	-0.974318000	1	-1.640932000	3.193114000	0.039986000
9	5.361416000	-1.108927000	0.017859000	9	5.624567000	-1.095072000	0.053690000
E=-2115.04087529 Hartrees				E=-2115.08167186 Hartrees			
1h				1h'			
24	-2.515282000	-0.590219000	-0.047308000	24	2.663275000	-0.578421000	-0.082215000
6	-3.884911000	0.328569000	-1.003754000	6	4.107637000	0.477969000	0.533714000
8	-4.735700000	0.809285000	-1.608677000	8	5.073200000	0.992714000	0.909108000
6	-3.609960000	-2.120632000	-0.128722000	6	3.929647000	-1.932079000	-0.124461000
8	-4.286934000	-3.049206000	-0.174375000	8	4.723264000	-2.780027000	-0.141013000
6	-1.206594000	-1.683482000	0.834588000	6	1.489844000	-1.919168000	-0.770426000
8	-0.482609000	-2.405311000	1.351495000	8	0.918259000	-2.808816000	-1.227378000
6	-3.265038000	-0.158636000	1.654473000	6	2.929732000	-0.005967000	-1.868997000
8	-3.711792000	0.076731000	2.686184000	8	3.080424000	0.343897000	-2.958840000
6	-1.757767000	-1.068329000	-1.737460000	6	2.147665000	-0.835865000	1.729297000

8	-1.348607000	-1.393688000	-2.758572000	8	1.851635000	-0.949926000	2.838424000
6	-1.217655000	1.129562000	0.071333000	6	1.062283000	0.986513000	0.077143000
7	-1.509792000	2.410878000	0.212671000	7	1.342697000	2.353161000	0.176932000
6	0.251886000	0.852273000	0.025903000	6	-0.349022000	0.699035000	0.085196000
6	0.974814000	0.746180000	1.222017000	6	-1.303323000	1.635191000	-0.434034000
6	0.936650000	0.662223000	-1.180275000	6	-0.921169000	-0.520046000	0.555614000
6	2.333925000	0.454833000	1.209483000	6	-2.656439000	1.373493000	-0.483449000
1	0.468112000	0.883940000	2.172595000	1	-0.937895000	2.571824000	-0.841251000
6	2.299305000	0.379948000	-1.186545000	6	-2.280078000	-0.762130000	0.532323000
1	0.405035000	0.725752000	-2.123259000	1	-0.275701000	-1.281776000	0.970554000
6	3.027984000	0.265254000	0.005729000	6	-3.208454000	0.168576000	0.011326000
1	2.868142000	0.393004000	2.151903000	1	-3.313165000	2.134112000	-0.897115000
1	2.796174000	0.213831000	-2.136677000	1	-2.633792000	-1.720760000	0.900424000
6	-0.531652000	3.521233000	0.208389000	6	0.718401000	3.185698000	1.201250000
1	-0.895899000	4.302467000	-0.462278000	1	1.446837000	3.418985000	1.994904000
1	-0.443533000	3.941155000	1.213460000	1	0.366798000	4.140001000	0.786457000
1	0.442332000	3.184405000	-0.126528000	1	-0.127702000	2.675376000	1.652566000
6	-2.877956000	2.922667000	0.371458000	6	2.552552000	2.966794000	-0.330344000
1	-3.543655000	2.138190000	0.704066000	1	2.971977000	2.384975000	-1.143448000
1	-2.869792000	3.721780000	1.115064000	1	2.313015000	3.965694000	-0.719192000
1	-3.239288000	3.331627000	-0.575291000	1	3.320013000	3.094704000	0.447240000
6	4.477398000	-0.053298000	-0.003282000	6	-4.650997000	-0.100945000	-0.019662000
6	5.025670000	-0.936782000	0.938865000	6	-5.498967000	0.491769000	-0.981849000
6	5.337027000	0.518005000	-0.953587000	6	-5.264111000	-0.968341000	0.912101000
6	6.385419000	-1.236520000	0.932362000	6	-6.865630000	0.237012000	-1.008159000
6	6.696843000	0.218590000	-0.960723000	6	-6.629899000	-1.226867000	0.881475000
6	7.227415000	-0.659932000	-0.017245000	6	-7.448422000	-0.626240000	-0.077599000
1	4.376793000	-1.415714000	1.664988000	1	-5.071225000	1.139740000	-1.739458000
1	4.941918000	1.222184000	-1.678855000	1	-4.660217000	-1.425342000	1.688657000
1	6.785758000	-1.930780000	1.664479000	1	-7.480632000	0.706332000	-1.771890000
1	7.344540000	0.678698000	-1.700407000	1	-7.062322000	-1.895482000	1.621510000
1	8.286988000	-0.894261000	-0.023058000	1	-8.515227000	-0.827581000	-0.100479000
E=-2246.87631662 Hartrees				E= -2246.91898264 Hartrees			
1i				1i'			
24	-2.185958000	-0.526164000	0.019142000	24	-2.322608000	-0.524194000	0.016454000
6	-3.429934000	0.335317000	-1.143552000	6	-3.710652000	0.658224000	-0.492746000
8	-4.200512000	0.789594000	-1.864288000	8	-4.652635000	1.246556000	-0.817277000
6	-3.374321000	-1.987448000	0.084757000	6	-3.651477000	-1.809451000	-0.108824000
8	-4.106967000	-2.872333000	0.126026000	8	-4.483618000	-2.615584000	-0.197195000
6	-0.994690000	-1.541310000	1.128173000	6	-1.235325000	-1.990093000	0.569940000
8	-0.337803000	-2.208004000	1.788866000	8	-0.718703000	-2.953532000	0.936313000
6	-3.002760000	0.172562000	1.597874000	6	-2.586303000	-0.129153000	1.849948000
8	-3.493943000	0.559144000	2.561275000	8	-2.733374000	0.113232000	2.969316000
6	-1.376496000	-1.306416000	-1.529415000	6	-1.777604000	-0.591929000	-1.802477000
8	-0.938236000	-1.817304000	-2.458001000	8	-1.455948000	-0.586867000	-2.910844000
6	-0.792709000	1.120202000	-0.041715000	6	-0.641051000	0.966498000	0.045822000
7	-1.008188000	2.424130000	-0.052804000	7	-0.837383000	2.361709000	0.093978000
6	0.659357000	0.754799000	-0.048770000	6	0.760546000	0.614286000	0.011210000
6	1.370996000	0.703493000	1.157211000	6	1.750941000	1.469239000	0.594779000
6	1.330015000	0.433965000	-1.235058000	6	1.270758000	-0.587743000	-0.559620000

6	2.715320000	0.342036000	1.182254000	6	3.099988000	1.155696000	0.614919000
1	0.869676000	0.933836000	2.092068000	1	1.420203000	2.380944000	1.079729000
6	2.677118000	0.078524000	-1.221557000	6	2.620818000	-0.905593000	-0.557837000
1	0.803268000	0.460144000	-2.182496000	1	0.592588000	-1.276797000	-1.042680000
6	3.362212000	0.033975000	-0.011034000	6	3.537396000	-0.034496000	0.030777000
1	3.249974000	0.298743000	2.123666000	1	3.808005000	1.824025000	1.094303000
1	3.183550000	-0.165957000	-2.147733000	1	2.958559000	-1.827365000	-1.019021000
6	0.033247000	3.470814000	-0.153206000	6	-0.278179000	3.202731000	-0.961174000
1	-0.272723000	4.194353000	-0.911588000	1	-1.009014000	3.350944000	-1.774582000
1	0.126710000	3.991064000	0.803282000	1	-0.012004000	4.193204000	-0.570101000
1	0.992443000	3.047929000	-0.427077000	1	0.614903000	2.750543000	-1.385278000
6	-2.344705000	3.029870000	0.019947000	6	-2.021481000	2.965284000	0.669539000
1	-3.073035000	2.308243000	0.361898000	1	-2.406148000	2.361314000	1.485017000
1	-2.314920000	3.867735000	0.719413000	1	-1.758223000	3.950868000	1.075655000
1	-2.637926000	3.406874000	-0.962937000	1	-2.825770000	3.120240000	-0.065188000
35	5.206202000	-0.461000000	0.014150000	35	5.421290000	-0.466019000	0.022896000
E=-4589.31815911 Hartrees				E=-4589.35972440 Hartrees			
1j				1j'			
24	-1.694378000	-0.482022000	0.019208000	24	-1.800038000	-0.482483000	0.016914000
6	-2.905168000	0.450048000	-1.122655000	6	-3.135033000	0.762365000	-0.483419000
8	-3.662070000	0.945043000	-1.831383000	8	-4.049514000	1.395440000	-0.802375000
6	-2.956948000	-1.878511000	0.086402000	6	-3.185490000	-1.707356000	-0.099503000
8	-3.735134000	-2.724019000	0.129706000	8	-4.053489000	-2.475365000	-0.182128000
6	-0.549922000	-1.572349000	1.106156000	6	-0.772409000	-1.995613000	0.560055000
8	0.073428000	-2.282837000	1.753846000	8	-0.296286000	-2.981266000	0.921366000
6	-2.452157000	0.250983000	1.610801000	6	-2.035293000	-0.082506000	1.853231000
8	-2.908062000	0.662025000	2.581686000	8	-2.165681000	0.160724000	2.974522000
6	-0.939887000	-1.282420000	-1.546472000	6	-1.276585000	-0.577193000	-1.807840000
8	-0.536191000	-1.800527000	-2.486718000	8	-0.970071000	-0.588585000	-2.920167000
6	-0.210859000	1.085227000	-0.038525000	6	-0.053329000	0.931371000	0.038842000
7	-0.356020000	2.399082000	-0.049792000	7	-0.187893000	2.330618000	0.094612000
6	1.219137000	0.641862000	-0.043633000	6	1.327815000	0.511747000	0.000027000
6	1.928448000	0.547759000	1.160229000	6	2.360433000	1.307377000	0.596334000
6	1.876490000	0.285980000	-1.227408000	6	1.779186000	-0.706041000	-0.589220000
6	3.250887000	0.116532000	1.183463000	6	3.687513000	0.918592000	0.613982000
1	1.441508000	0.803859000	2.096246000	1	2.076208000	2.229971000	1.090623000
6	3.198719000	-0.145380000	-1.209355000	6	3.110553000	-1.084738000	-0.589654000
1	1.354657000	0.340578000	-2.176440000	1	1.067834000	-1.349115000	-1.088157000
6	3.900756000	-0.235930000	-0.002997000	6	4.092756000	-0.289161000	0.021763000
1	3.769535000	0.054689000	2.134746000	1	4.426854000	1.545609000	1.104602000
1	3.679966000	-0.422910000	-2.141728000	1	3.401684000	-2.011925000	-1.074135000
6	0.740508000	3.387376000	-0.153440000	6	0.436788000	3.162080000	-0.930968000
1	0.483974000	4.112228000	-0.929032000	1	-0.275534000	3.376729000	-1.745683000
1	0.847560000	3.919517000	0.795059000	1	0.760589000	4.123356000	-0.511501000
1	1.679300000	2.908376000	-0.404538000	1	1.303723000	2.665107000	-1.358345000
6	-1.658328000	3.075760000	0.018019000	6	-1.344478000	2.988670000	0.666434000
1	-2.421737000	2.400012000	0.377245000	1	-1.773691000	2.392814000	1.465219000
1	-1.580301000	3.923525000	0.701526000	1	-1.032512000	3.950560000	1.094322000
1	-1.937657000	3.449820000	-0.970094000	1	-2.127808000	3.201469000	-0.076401000
16	5.597923000	-0.785061000	-0.060563000	16	5.822643000	-0.764539000	-0.006419000

1	5.767826000	-0.912850000	1.272963000	1	5.852274000	-1.551857000	1.103798000
E= -2413.98231925 Hartrees				E=-2414.02578167 Hartrees			
1k				1k'			
24	-1.648276000	-0.487938000	0.025259000	24	1.787509000	-0.442069000	-0.034735000
6	-2.868312000	0.478456000	-1.077245000	6	3.056543000	0.861940000	0.483277000
8	-3.627759000	0.999936000	-1.763902000	8	3.932359000	1.543153000	0.810844000
6	-2.912602000	-1.882865000	0.075360000	6	3.234749000	-1.598340000	0.038708000
8	-3.692685000	-2.727216000	0.108271000	8	4.141658000	-2.322057000	0.094822000
6	-0.489392000	-1.603067000	1.071597000	6	0.824075000	-1.992063000	-0.598971000
8	0.140703000	-2.328875000	1.695167000	8	0.391454000	-2.991626000	-0.974015000
6	-2.385511000	0.199980000	1.646243000	6	1.988060000	0.001025000	-1.865956000
8	-2.830750000	0.579072000	2.634955000	8	2.099885000	0.267969000	-2.983700000
6	-0.917552000	-1.258813000	-1.567097000	6	1.300899000	-0.613327000	1.795277000
8	-0.530861000	-1.763244000	-2.521607000	8	1.019692000	-0.671880000	2.912426000
6	-0.168921000	1.085219000	-0.023276000	6	-0.022909000	0.884710000	-0.005192000
7	-0.313764000	2.397871000	0.026442000	7	0.062882000	2.280195000	-0.023950000
6	1.256805000	0.641977000	-0.108268000	6	-1.376349000	0.402388000	0.049642000
6	2.011342000	0.473357000	1.063762000	6	-2.455782000	1.154125000	-0.530803000
6	1.869352000	0.366983000	-1.335251000	6	-1.768884000	-0.845055000	0.622236000
6	3.329460000	0.044632000	1.007731000	6	-3.758538000	0.712978000	-0.535336000
1	1.555926000	0.669446000	2.029688000	1	-2.217522000	2.085911000	-1.032983000
6	3.194241000	-0.055751000	-1.384035000	6	-3.081815000	-1.270260000	0.633997000
1	1.312542000	0.483454000	-2.258768000	1	-1.024440000	-1.468627000	1.097376000
6	3.955487000	-0.230941000	-0.219206000	6	-4.133684000	-0.516692000	0.064073000
1	3.876853000	-0.075385000	1.936380000	1	-4.512357000	1.319728000	-1.030494000
1	3.646270000	-0.261331000	-2.350062000	1	-3.318281000	-2.222428000	1.105498000
6	0.780583000	3.389876000	-0.063164000	6	-0.677063000	3.104573000	0.926685000
1	0.503058000	4.150877000	-0.795674000	1	0.011352000	3.520080000	1.680573000
1	0.915523000	3.876082000	0.906196000	1	-1.171594000	3.950465000	0.430229000
1	1.711025000	2.923374000	-0.363982000	1	-1.433946000	2.517905000	1.439294000
6	-1.611756000	3.071580000	0.165206000	6	1.169053000	3.013311000	-0.604345000
1	-2.372585000	2.374127000	0.485679000	1	1.671780000	2.423323000	-1.362391000
1	-1.519858000	3.867787000	0.906772000	1	0.784716000	3.922777000	-1.085794000
1	-1.904285000	3.516638000	-0.789109000	1	1.907291000	3.329066000	0.147478000
6	5.347772000	-0.689923000	-0.333018000	6	-5.492986000	-1.014862000	0.104054000
1	5.702866000	-0.808858000	-1.355344000	1	-5.598950000	-1.989854000	0.582394000
6	6.196380000	-0.974521000	0.659930000	6	-6.623020000	-0.440266000	-0.365334000
1	5.928052000	-0.896870000	1.708510000	1	-6.630547000	0.528218000	-0.855734000
1	7.206128000	-1.308366000	0.449722000	1	-7.582369000	-0.937859000	-0.269252000
E= -2093.18786654 Hartrees				E= -2093.23213336 Hartrees			
1l				1l'			
24	-2.245088000	-0.647388000	0.010368000	24	-2.472710000	-0.592726000	0.034458000
6	-3.552236000	0.023093000	-1.208425000	6	-3.987337000	0.508808000	-0.244903000
8	-4.345627000	0.369179000	-1.963215000	8	-4.996770000	1.041884000	-0.432693000
6	-3.192576000	-2.277168000	0.029043000	6	-3.711387000	-1.968315000	-0.057313000
8	-3.779794000	-3.265059000	0.041192000	8	-4.487490000	-2.830111000	-0.124768000
6	-0.957229000	-1.455577000	1.178541000	6	-1.228165000	-2.000890000	0.358495000
8	-0.231018000	-2.001664000	1.876415000	8	-0.604642000	-2.942166000	0.590861000
6	-3.233441000	-0.107332000	1.552796000	6	-2.572586000	-0.355492000	1.911619000

8	-3.824990000	0.174591000	2.495849000	8	-2.620212000	-0.210613000	3.055965000
6	-1.259241000	-1.301020000	-1.494636000	6	-2.122210000	-0.497461000	-1.830441000
8	-0.709989000	-1.748077000	-2.396326000	8	-1.922265000	-0.396381000	-2.962501000
6	-1.133573000	1.199696000	-0.011318000	6	-0.912288000	1.023912000	0.018798000
7	-1.551893000	2.453380000	0.004188000	7	-1.205951000	2.389370000	0.208552000
6	0.358128000	1.066126000	-0.040343000	6	0.500157000	0.792553000	-0.186264000
6	1.086790000	1.060468000	1.156780000	6	1.480904000	1.683520000	0.361880000
6	1.049291000	0.925735000	-1.250723000	6	1.032412000	-0.317608000	-0.906424000
6	2.471291000	0.916157000	1.148907000	6	2.842759000	1.479506000	0.219446000
1	0.570458000	1.163096000	2.105475000	1	1.135791000	2.530031000	0.943966000
6	2.433968000	0.782770000	-1.267448000	6	2.394433000	-0.522750000	-1.061844000
1	0.507037000	0.928199000	-2.189596000	1	0.358631000	-1.017001000	-1.379653000
6	3.128162000	0.772972000	-0.065651000	6	3.295729000	0.369477000	-0.489655000
1	3.035492000	0.914258000	2.073913000	1	3.556012000	2.165914000	0.664712000
1	2.971448000	0.678782000	-2.202595000	1	2.761398000	-1.368887000	-1.633450000
6	-0.689726000	3.654633000	-0.056119000	6	-0.829152000	3.355220000	-0.820051000
1	-1.077439000	4.326478000	-0.824839000	1	-1.650870000	3.502389000	-1.541518000
1	-0.719666000	4.174792000	0.904436000	1	-0.601618000	4.331458000	-0.373034000
1	0.335311000	3.394647000	-0.291333000	1	0.046872000	3.016384000	-1.367555000
6	-2.968193000	2.839288000	0.070292000	6	-2.361559000	2.844071000	0.954154000
1	-3.581100000	1.999154000	0.364181000	1	-2.604614000	2.149280000	1.751483000
1	-3.083052000	3.641241000	0.802282000	1	-2.130860000	3.814688000	1.412471000
1	-3.298312000	3.207616000	-0.904168000	1	-3.252380000	2.984813000	0.323971000
8	4.534989000	0.702924000	-0.090337000	8	4.695193000	0.205676000	-0.732638000
6	5.113483000	-0.513418000	0.020297000	6	5.417034000	-0.462054000	0.167606000
9	4.836565000	-1.117080000	1.195234000	9	5.441329000	0.124248000	1.391406000
9	6.433824000	-0.345941000	-0.062723000	9	6.690303000	-0.516530000	-0.271288000
9	4.730418000	-1.363458000	-0.954342000	9	5.004519000	-1.735555000	0.367365000

E=-2428.16062743 Hartrees

E= -2428.20804906 Hartrees

1m

24	-1.574421000	-0.474779000	0.014493000
6	-2.742887000	0.470822000	-1.162723000
8	-3.470515000	0.976975000	-1.892864000
6	-2.862223000	-1.851814000	0.059952000
8	-3.654515000	-2.683532000	0.089690000
6	-0.473208000	-1.574448000	1.134575000
8	0.126510000	-2.288311000	1.800534000
6	-2.360842000	0.273635000	1.586742000
8	-2.834062000	0.690451000	2.546116000
6	-0.796567000	-1.304912000	-1.524051000
8	-0.376439000	-1.841737000	-2.446148000
6	-0.080315000	1.079901000	-0.026434000
7	-0.207276000	2.394984000	-0.033423000
6	1.341635000	0.613365000	-0.032625000
6	2.036376000	0.470036000	1.177038000
6	1.996803000	0.283325000	-1.226625000
6	3.347294000	0.011874000	1.197945000
1	1.543890000	0.707505000	2.114215000
6	3.309891000	-0.171287000	-1.216842000
1	1.479368000	0.379956000	-2.174318000

1m'

24	-1.685724000	-0.464209000	0.019569000
6	-2.971811000	0.808541000	-0.537044000
8	-3.852990000	1.468381000	-0.890840000
6	-3.103586000	-1.656407000	-0.076917000
8	-3.990796000	-2.401891000	-0.146799000
6	-0.694137000	-1.983244000	0.615813000
8	-0.237832000	-2.965826000	1.006949000
6	-1.946255000	-0.020523000	1.844425000
8	-2.095913000	0.244621000	2.957677000
6	-1.164971000	-0.643181000	-1.800190000
8	-0.862776000	-0.708315000	-2.911217000
6	0.087718000	0.909762000	0.022630000
7	-0.028156000	2.303888000	0.048561000
6	1.455498000	0.461263000	-0.000803000
6	2.502464000	1.240322000	0.600475000
6	1.884502000	-0.778195000	-0.569029000
6	3.817784000	0.831067000	0.630511000
1	2.234402000	2.167525000	1.094232000
6	3.202274000	-1.185816000	-0.561227000
1	1.161231000	-1.414879000	-1.057987000

6	3.987884000	-0.307677000	-0.002433000	6	4.197114000	-0.389075000	0.036913000
1	3.878309000	-0.103176000	2.135571000	1	4.571870000	1.436255000	1.124758000
1	3.813249000	-0.425363000	-2.142296000	1	3.484955000	-2.126474000	-1.022868000
6	0.902414000	3.370426000	-0.116227000	6	0.699689000	3.144054000	-0.898727000
1	0.670584000	4.098470000	-0.896409000	1	0.014129000	3.518129000	-1.676120000
1	0.996280000	3.900832000	0.834505000	1	1.144610000	4.017266000	-0.403295000
1	1.841241000	2.882303000	-0.349270000	1	1.493300000	2.583369000	-1.384296000
6	-1.501995000	3.087889000	0.024132000	6	-1.167539000	3.006810000	0.602860000
1	-2.280641000	2.416222000	0.357047000	1	-1.664064000	2.408145000	1.358211000
1	-1.424978000	3.922324000	0.723818000	1	-0.819611000	3.931938000	1.081356000
1	-1.757567000	3.482501000	-0.962297000	1	-1.902427000	3.292520000	-0.163829000
7	5.296680000	-0.760898000	0.011989000	7	5.516382000	-0.793911000	0.045978000
6	6.407857000	-1.140508000	0.024743000	6	6.641898000	-1.135105000	0.055688000
E= -2108.00373878 Hartrees				E=-2108.05752207 Hartrees			
1n				1n'			
24	-1.577722000	-0.480821000	0.013915000	24	-1.691080000	-0.468541000	0.022404000
6	-2.747531000	0.457402000	-1.168708000	6	-2.982278000	0.792171000	-0.548673000
8	-3.474762000	0.958929000	-1.902153000	8	-3.862670000	1.447973000	-0.911163000
6	-2.859817000	-1.864075000	0.056562000	6	-3.101766000	-1.671905000	-0.053384000
8	-3.648258000	-2.699193000	0.084341000	8	-3.984759000	-2.422935000	-0.109688000
6	-0.475457000	-1.575615000	1.137738000	6	-0.679959000	-1.971770000	0.631668000
8	0.125061000	-2.286877000	1.805613000	8	-0.210260000	-2.943972000	1.030751000
6	-2.373075000	0.263636000	1.583972000	6	-1.957695000	-0.010530000	1.843820000
8	-2.851497000	0.677434000	2.541885000	8	-2.113630000	0.262704000	2.953987000
6	-0.791970000	-1.309948000	-1.521630000	6	-1.186758000	-0.674986000	-1.799513000
8	-0.367102000	-1.846448000	-2.441553000	8	-0.899596000	-0.758061000	-2.912937000
6	-0.096816000	1.085115000	-0.024102000	6	0.072085000	0.916582000	0.007905000
7	-0.230950000	2.399141000	-0.030143000	7	-0.056485000	2.304725000	0.022532000
6	1.325622000	0.624571000	-0.030705000	6	1.439628000	0.472861000	-0.011253000
6	2.018138000	0.476620000	1.180417000	6	2.480318000	1.248201000	0.608815000
6	1.982828000	0.305435000	-1.227382000	6	1.876420000	-0.760793000	-0.589184000
6	3.330452000	0.025313000	1.198290000	6	3.793942000	0.842888000	0.642860000
1	1.521814000	0.706242000	2.117466000	1	2.205536000	2.166898000	1.114967000
6	3.297035000	-0.142763000	-1.216961000	6	3.193913000	-1.160507000	-0.579492000
1	1.464571000	0.406373000	-2.174185000	1	1.157604000	-1.394492000	-1.088897000
6	3.983826000	-0.286148000	-0.002825000	6	4.197495000	-0.371681000	0.034258000
1	3.853760000	-0.088804000	2.140689000	1	4.534491000	1.451053000	1.154288000
1	3.795628000	-0.385209000	-2.148435000	1	3.473117000	-2.096053000	-1.054192000
6	0.873764000	3.380474000	-0.109199000	6	0.714376000	3.162662000	-0.874111000
1	0.642502000	4.105672000	-0.892146000	1	0.048056000	3.599471000	-1.634088000
1	0.959416000	3.913190000	0.840970000	1	1.189237000	3.993207000	-0.335175000
1	1.816762000	2.897433000	-0.336230000	1	1.488584000	2.595312000	-1.382366000
6	-1.529802000	3.084505000	0.025899000	6	-1.200378000	3.009206000	0.567158000
1	-2.305817000	2.406696000	0.352487000	1	-1.718429000	2.402022000	1.300399000
1	-1.460155000	3.915927000	0.729892000	1	-0.853419000	3.921838000	1.069498000
1	-1.783604000	3.482305000	-0.959676000	1	-1.914708000	3.315080000	-0.210469000
6	5.338827000	-0.742684000	0.010526000	6	5.552097000	-0.780359000	0.046261000
7	6.436202000	-1.105129000	0.021398000	7	6.667133000	-1.111475000	0.057173000
E= -2108.03864706 Hartrees				E= -2108.09690421 Hartrees			

2g				2g'			
24	-1.701742000	-0.376150000	0.074630000	24	-1.844575000	-0.266690000	0.003006000
6	-1.739799000	-1.302348000	-1.593754000	6	-1.684420000	-0.602792000	-1.854256000
8	-1.735133000	-1.889597000	-2.582764000	8	-1.551419000	-0.842629000	-2.978395000
6	-3.336776000	-1.167774000	0.588521000	6	-3.600711000	-0.844553000	0.088973000
8	-4.324285000	-1.663066000	0.915038000	8	-4.700611000	-1.227375000	0.144376000
6	-1.567371000	0.491599000	1.765636000	6	-1.677116000	0.017693000	1.872162000
8	-1.456324000	0.968681000	2.807510000	8	-1.541051000	0.111437000	3.016562000
6	-0.845926000	-1.864646000	0.819574000	6	-1.391555000	-2.028568000	0.368019000
8	-0.360388000	-2.797964000	1.285514000	8	-1.217829000	-3.145538000	0.624084000
6	0.153100000	0.494136000	-0.374690000	6	0.271076000	0.419512000	-0.073326000
7	0.211540000	1.768956000	-0.722334000	7	0.476973000	1.819164000	0.070456000
6	1.454965000	-0.217235000	-0.242131000	6	1.464233000	-0.382616000	-0.029075000
6	2.224770000	-0.094082000	0.922946000	6	2.655701000	0.044620000	0.641238000
6	1.895348000	-1.080274000	-1.254096000	6	1.537274000	-1.668313000	-0.641703000
6	3.411868000	-0.806841000	1.073110000	6	3.802143000	-0.738684000	0.693621000
1	1.889848000	0.552455000	1.726833000	1	2.647997000	0.993078000	1.165018000
6	3.089388000	-1.785292000	-1.121738000	6	2.681754000	-2.449959000	-0.601842000
1	1.300196000	-1.210249000	-2.151458000	1	0.675282000	-2.039868000	-1.179544000
6	3.825813000	-1.635661000	0.042459000	6	3.805552000	-1.975619000	0.065489000
1	4.006815000	-0.728164000	1.975814000	1	4.684980000	-0.403584000	1.230410000
1	3.439597000	-2.452360000	-1.901002000	1	2.711005000	-3.421086000	-1.085856000
6	1.692545000	3.627424000	0.046634000	6	2.198955000	3.612854000	-0.082730000
1	0.901654000	4.354510000	0.220771000	1	1.583920000	4.336227000	0.451561000
6	-2.157533000	1.513499000	-1.201223000	6	-1.873434000	1.986486000	-0.587551000
1	-2.123630000	1.193073000	-2.237875000	1	-1.709488000	2.011736000	-1.661331000
6	-1.081250000	2.478427000	-0.800128000	6	-0.764850000	2.567360000	0.250208000
1	-0.982279000	3.290431000	-1.529349000	1	-0.592378000	3.616791000	-0.024776000
1	-1.302208000	2.931461000	0.171992000	1	-1.061012000	2.568185000	1.305188000
6	1.427876000	2.575242000	-0.997785000	6	1.462035000	2.503501000	-0.787800000
1	2.274665000	1.899074000	-1.085883000	1	2.173606000	1.768826000	-1.159505000
1	1.275495000	3.048503000	-1.974963000	1	0.951689000	2.919513000	-1.676547000
6	2.833368000	3.728980000	0.722579000	6	3.521991000	3.766075000	-0.080462000
1	3.650440000	3.027828000	0.578861000	1	4.178354000	3.061193000	-0.584112000
6	-3.303389000	1.302674000	-0.480663000	6	-3.134490000	1.725947000	-0.119536000
1	-3.498965000	1.836761000	0.442056000	1	-3.407674000	1.942373000	0.907595000
1	2.994996000	4.521979000	1.444941000	1	4.000910000	4.594095000	0.434527000
1	-4.164130000	0.834015000	-0.940151000	1	-3.963226000	1.577192000	-0.801072000
9	4.982844000	-2.327314000	0.181193000	9	4.944387000	-2.749233000	0.103500000
E= -2156.48712258 Hartrees				E= -2156.52129860 Hartrees			
2h				2h'			
24	-2.558849000	-0.838192000	0.051541000	24	-2.700553000	-0.824562000	0.066840000
6	-2.296259000	-1.630984000	-1.664719000	6	-2.434942000	-1.346303000	-1.736287000
8	-2.102362000	-2.128892000	-2.683335000	8	-2.242677000	-1.682921000	-2.825474000
6	-3.793426000	-2.186248000	0.519031000	6	-4.060940000	-2.056225000	0.324861000
8	-4.533373000	-3.018225000	0.816229000	8	-4.904177000	-2.842877000	0.487376000
6	-2.704751000	-0.071863000	1.789490000	6	-2.711643000	-0.247173000	1.876436000
8	-2.748118000	0.354291000	2.858279000	8	-2.669804000	0.042897000	2.994331000
6	-1.214602000	-1.960383000	0.713465000	6	-1.548089000	-2.170194000	0.639099000
8	-0.423096000	-2.684079000	1.130313000	8	-0.923963000	-3.060691000	1.033014000
6	-1.146303000	0.658257000	-0.357184000	6	-1.045733000	0.632211000	-0.195683000

7	-1.553603000	1.886057000	-0.632578000	7	-1.438619000	1.976519000	-0.215807000
6	0.323982000	0.447482000	-0.282123000	6	0.359568000	0.370148000	-0.134803000
6	1.039911000	0.749213000	0.883880000	6	1.297358000	1.259727000	0.487652000
6	1.014826000	-0.122811000	-1.358949000	6	0.937090000	-0.823155000	-0.665794000
6	2.404683000	0.493768000	0.963363000	6	2.647320000	0.984062000	0.554704000
1	0.526414000	1.182750000	1.735820000	1	0.928461000	2.159017000	0.967357000
6	2.382863000	-0.360448000	-1.278074000	6	2.291940000	-1.071618000	-0.627548000
1	0.477732000	-0.397585000	-2.260848000	1	0.288975000	-1.548521000	-1.141620000
6	3.107562000	-0.061026000	-0.115723000	6	3.212429000	-0.180500000	-0.018254000
1	2.936543000	0.750202000	1.873875000	1	3.291497000	1.704926000	1.050783000
1	2.887863000	-0.821798000	-2.120443000	1	2.651055000	-2.005038000	-1.050506000
6	-0.794645000	4.092676000	0.255795000	6	-0.512790000	4.293686000	-0.191409000
1	-1.781608000	4.495343000	0.475475000	1	-1.395343000	4.700029000	0.301647000
6	-3.687443000	0.828779000	-1.114107000	6	-3.634464000	1.101725000	-0.805663000
1	-3.566861000	0.593613000	-2.167029000	1	-3.480158000	1.049204000	-1.879722000
6	-3.015301000	2.092889000	-0.665869000	6	-2.878715000	2.196797000	-0.105096000
1	-3.227730000	2.921013000	-1.351456000	1	-3.121355000	3.170829000	-0.551773000
1	-3.360492000	2.390608000	0.329766000	1	-3.186223000	2.250680000	0.946195000
6	-0.707333000	3.085057000	-0.859969000	6	-0.715571000	3.016429000	-0.965851000
1	0.319145000	2.756010000	-1.002394000	1	0.242968000	2.617719000	-1.290311000
1	-1.047406000	3.536261000	-1.799447000	1	-1.287280000	3.247708000	-1.882540000
6	0.256872000	4.526225000	0.944979000	6	0.643028000	4.946952000	-0.088949000
1	1.259194000	4.151674000	0.758204000	1	1.553484000	4.572046000	-0.548661000
6	-4.665310000	0.186440000	-0.401496000	6	-4.688418000	0.418881000	-0.254255000
1	-5.015505000	0.567419000	0.550934000	1	-5.045611000	0.648246000	0.743744000
1	0.154550000	5.275395000	1.722913000	1	0.726295000	5.874853000	0.469520000
1	-5.313360000	-0.534464000	-0.883068000	1	-5.374805000	-0.141493000	-0.877307000
6	4.563958000	-0.332233000	-0.026670000	6	4.651551000	-0.451994000	0.023344000
6	5.127995000	-0.861392000	1.143969000	6	5.492470000	0.112004000	1.011662000
6	5.414377000	-0.068818000	-1.111084000	6	5.278380000	-1.294369000	-0.925084000
6	6.494297000	-1.116707000	1.227746000	6	6.858013000	-0.144168000	1.045619000
6	6.780791000	-0.323647000	-1.027894000	6	6.643378000	-1.553392000	-0.886665000
6	7.327068000	-0.848588000	0.142355000	6	7.453006000	-0.980886000	0.097572000
1	4.486259000	-1.102424000	1.985213000	1	5.059450000	0.738738000	1.783830000
1	5.005486000	0.361733000	-2.019627000	1	4.685409000	-1.730959000	-1.721372000
1	6.907269000	-1.536468000	2.139640000	1	7.463819000	0.303405000	1.829742000
1	7.421141000	-0.104811000	-1.876723000	1	7.083108000	-2.201459000	-1.640818000
1	8.391682000	-1.048858000	0.207104000	1	8.519478000	-1.183209000	0.126674000

E= -2288.32245560 Hartrees

E=-2288.35979730 Hartrees

2i

24	-2.271445000	-0.728409000	0.081576000
6	-2.062616000	-1.598583000	-1.604064000
8	-1.899107000	-2.142151000	-2.604433000
6	-3.599143000	-1.968656000	0.595743000
8	-4.395331000	-2.734837000	0.921204000
6	-2.363995000	0.115532000	1.788136000
8	-2.377113000	0.589236000	2.837211000
6	-1.011341000	-1.917706000	0.789594000
8	-0.271635000	-2.678723000	1.233910000
6	-0.757719000	0.647236000	-0.381096000

2i'

24	-2.421356000	-0.700486000	0.013432000
6	-2.169436000	-1.056562000	-1.830523000
8	-1.976033000	-1.294665000	-2.945764000
6	-3.886274000	-1.824752000	0.150984000
8	-4.796526000	-2.547120000	0.238043000
6	-2.377422000	-0.297102000	1.867827000
8	-2.300454000	-0.117077000	3.007124000
6	-1.402633000	-2.191998000	0.449100000
8	-0.863334000	-3.171117000	0.751510000
6	-0.649356000	0.633273000	-0.123092000

7	-1.075778000	1.888851000	-0.706830000	7	-0.917342000	2.017748000	-0.015632000
6	0.694473000	0.336426000	-0.284625000	6	0.734313000	0.258207000	-0.074777000
6	1.424197000	0.664445000	0.865824000	6	1.728380000	1.044815000	0.595451000
6	1.341374000	-0.357010000	-1.315338000	6	1.217406000	-0.941394000	-0.678739000
6	2.767905000	0.317838000	0.982581000	6	3.063254000	0.673617000	0.648104000
1	0.938804000	1.184022000	1.685148000	1	1.419622000	1.938045000	1.125932000
6	2.689383000	-0.692724000	-1.214375000	6	2.551138000	-1.310222000	-0.646020000
1	0.790325000	-0.645400000	-2.204142000	1	0.520890000	-1.576767000	-1.210359000
6	3.394357000	-0.353109000	-0.063543000	6	3.478103000	-0.499969000	0.017600000
1	3.318295000	0.567023000	1.882054000	1	3.776307000	1.285557000	1.191382000
1	3.179576000	-1.224042000	-2.021449000	1	2.872446000	-2.223019000	-1.135881000
6	-0.158002000	4.074945000	0.079233000	6	0.162070000	4.263033000	-0.048315000
1	-1.116910000	4.542153000	0.295063000	1	-0.667807000	4.731817000	0.479485000
6	-3.281539000	0.968008000	-1.148531000	6	-3.184673000	1.383270000	-0.668307000
1	-3.182491000	0.686805000	-2.192371000	1	-3.032639000	1.416838000	-1.743535000
6	-2.519637000	2.196420000	-0.746678000	6	-2.336251000	2.335778000	0.131110000
1	-2.675568000	3.013219000	-1.460292000	1	-2.505187000	3.367232000	-0.207010000
1	-2.838941000	2.552088000	0.238670000	1	-2.632835000	2.302248000	1.185864000
6	-0.148043000	3.013704000	-0.989263000	6	-0.160900000	3.002452000	-0.808915000
1	0.852271000	2.608076000	-1.120698000	1	0.757616000	2.540005000	-1.164059000
1	-0.461035000	3.445030000	-1.947320000	1	-0.745125000	3.268522000	-1.709194000
6	0.928958000	4.481650000	0.728587000	6	1.365538000	4.830589000	0.008141000
1	1.905920000	4.044661000	0.542779000	1	2.227399000	4.390997000	-0.486959000
6	-4.300596000	0.425641000	-0.411206000	6	-4.293637000	0.743678000	-0.178225000
1	-4.618392000	0.867726000	0.526037000	1	-4.630007000	0.905049000	0.840230000
1	0.883248000	5.272146000	1.470061000	1	1.538588000	5.749127000	0.561600000
1	-5.000984000	-0.264200000	-0.864135000	1	-5.024139000	0.303679000	-0.846150000
35	5.239669000	-0.822343000	0.086616000	35	5.346053000	-0.998639000	0.046571000
E=-4630.76435370 Hartrees				E=-4630.79978786 Hartrees			
2j				2j			
24	-1.871376000	-0.584422000	0.080616000	24	-2.009034000	-0.522136000	0.015731000
6	-1.766937000	-1.492913000	-1.593123000	6	-1.822362000	-0.936872000	-1.824067000
8	-1.672879000	-2.067189000	-2.585773000	8	-1.676314000	-1.214812000	-2.937109000
6	-3.341964000	-1.647903000	0.597199000	6	-3.609977000	-1.439293000	0.175994000
8	-4.227804000	-2.308286000	0.924275000	8	-4.608407000	-2.031308000	0.277998000
6	-1.875566000	0.277814000	1.781227000	6	-1.906524000	-0.099462000	1.863815000
8	-1.844376000	0.754671000	2.828497000	8	-1.803983000	0.086924000	3.000033000
6	-0.766241000	-1.907925000	0.808824000	6	-1.190959000	-2.128173000	0.471869000
8	-0.124766000	-2.746595000	1.266028000	8	-0.782856000	-3.163821000	0.789760000
6	-0.192629000	0.590852000	-0.378030000	6	-0.074691000	0.561488000	-0.137927000
7	-0.355661000	1.861506000	-0.709503000	7	-0.159153000	1.966578000	-0.046278000
6	1.209911000	0.108819000	-0.266388000	6	1.243744000	0.002236000	-0.089336000
6	1.996730000	0.417430000	0.851886000	6	2.337746000	0.646342000	0.578919000
6	1.753081000	-0.729897000	-1.247277000	6	1.558713000	-1.254030000	-0.691686000
6	3.283029000	-0.093694000	0.984143000	6	3.603159000	0.089047000	0.633842000
1	1.594526000	1.046943000	1.638649000	1	2.155347000	1.575682000	1.106056000
6	3.050658000	-1.218229000	-1.133477000	6	2.829443000	-1.794924000	-0.657089000
1	1.159293000	-1.006156000	-2.112107000	1	0.781936000	-1.785377000	-1.226944000
6	3.827126000	-0.910908000	-0.012265000	6	3.880836000	-1.139898000	0.012701000
1	3.861341000	0.140441000	1.872361000	1	4.392230000	0.599500000	1.179343000

1	3.447301000	-1.851475000	-1.920490000	1	3.022875000	-2.740344000	-1.155110000
6	0.811908000	3.939190000	0.041392000	6	1.225174000	4.039509000	-0.032137000
1	-0.089301000	4.513048000	0.248696000	1	0.461106000	4.616166000	0.488286000
6	-2.652500000	1.213611000	-1.167849000	6	-2.488309000	1.632396000	-0.694527000
1	-2.576255000	0.914020000	-2.208566000	1	-2.332876000	1.630790000	-1.769742000
6	-1.750465000	2.342812000	-0.765422000	6	-1.521776000	2.475317000	0.092284000
1	-1.799385000	3.166469000	-1.486610000	1	-1.549728000	3.514191000	-0.263797000
1	-2.033331000	2.743734000	0.213679000	1	-1.822310000	2.500869000	1.146426000
6	0.701742000	2.861456000	-1.004536000	6	0.738881000	2.846383000	-0.814231000
1	1.646923000	2.336371000	-1.119491000	1	1.586738000	2.264063000	-1.168698000
1	0.447972000	3.307974000	-1.973378000	1	0.206837000	3.204671000	-1.714530000
6	1.939416000	4.239844000	0.679364000	6	2.495936000	4.429102000	0.049791000
1	2.862338000	3.695373000	0.501332000	1	3.294582000	3.875570000	-0.436808000
6	-3.738417000	0.803454000	-0.440305000	6	-3.672679000	1.152973000	-0.197500000
1	-4.012162000	1.286705000	0.490466000	1	-3.984385000	1.371532000	0.818116000
1	1.982838000	5.046853000	1.403008000	1	2.788515000	5.307762000	0.617544000
1	-4.511813000	0.200480000	-0.898508000	1	-4.455463000	0.805329000	-0.860643000
16	5.496745000	-1.500422000	0.208588000	16	5.536291000	-1.826321000	0.036925000
1	5.499776000	-2.362130000	-0.831109000	1	5.419166000	-2.662771000	1.106346000
E= -2455.42875948 Hartrees				E= -2455.46635313 Hartrees			
2k				2k'			
24	-1.818375000	-0.612688000	0.069192000	24	-1.934583000	-0.561337000	0.018726000
6	-1.619244000	-1.580412000	-1.563147000	6	-1.698085000	-1.123852000	-1.776153000
8	-1.469623000	-2.188441000	-2.528165000	8	-1.530840000	-1.490890000	-2.859607000
6	-3.288968000	-1.687893000	0.559964000	6	-3.504404000	-1.525298000	0.215187000
8	-4.175481000	-2.354437000	0.872595000	8	-4.482928000	-2.144597000	0.340086000
6	-1.914871000	0.311497000	1.732946000	6	-1.918415000	0.007778000	1.830291000
8	-1.939209000	0.827782000	2.761708000	8	-1.875251000	0.284279000	2.951674000
6	-0.720432000	-1.884715000	0.894703000	6	-1.067207000	-2.093218000	0.626801000
8	-0.084982000	-2.692354000	1.411973000	8	-0.631501000	-3.081880000	1.039055000
6	-0.148770000	0.583667000	-0.362705000	6	-0.031991000	0.573659000	-0.161242000
7	-0.322743000	1.835506000	-0.752240000	7	-0.178116000	1.966592000	-0.174432000
6	1.256251000	0.133737000	-0.181413000	6	1.297046000	0.060404000	-0.053548000
6	1.972453000	0.440977000	0.981514000	6	2.363563000	0.762493000	0.603691000
6	1.872799000	-0.673002000	-1.150696000	6	1.659372000	-1.220744000	-0.579348000
6	3.266064000	-0.038469000	1.159710000	6	3.636460000	0.239981000	0.698289000
1	1.512547000	1.045435000	1.756327000	1	2.148137000	1.704596000	1.094569000
6	3.170398000	-1.131218000	-0.973356000	6	2.938537000	-1.719364000	-0.506308000
1	1.327570000	-0.948708000	-2.047392000	1	0.902659000	-1.801675000	-1.091891000
6	3.900180000	-0.825510000	0.187253000	6	3.990026000	-1.008962000	0.134258000
1	3.796986000	0.203089000	2.076137000	1	4.396706000	0.801649000	1.239957000
1	3.613409000	-1.749371000	-1.746611000	1	3.143083000	-2.688095000	-0.953228000
6	0.769601000	3.955518000	-0.010661000	6	1.146612000	4.078491000	-0.057933000
1	-0.146774000	4.525908000	0.128862000	1	0.329795000	4.627760000	0.409325000
6	-2.583000000	1.119684000	-1.283593000	6	-2.465143000	1.500852000	-0.872442000
1	-2.454704000	0.781089000	-2.307032000	1	-2.272608000	1.424437000	-1.938862000
6	-1.723027000	2.283822000	-0.888204000	6	-1.559421000	2.441372000	-0.126869000
1	-1.756293000	3.077162000	-1.643473000	1	-1.602211000	3.443653000	-0.575218000
1	-2.057332000	2.716609000	0.060503000	1	-1.902292000	2.549415000	0.909380000
6	0.728427000	2.847280000	-1.029274000	6	0.754319000	2.869665000	-0.868601000

1	1.687395000	2.337611000	-1.084308000	1	1.639818000	2.309661000	-1.160271000
1	0.512337000	3.260216000	-2.021748000	1	0.276254000	3.213661000	-1.803273000
6	1.856090000	4.284048000	0.682288000	6	2.394545000	4.513865000	0.104473000
1	2.791568000	3.742988000	0.572899000	1	3.242391000	3.988846000	-0.327198000
6	-3.690375000	0.713845000	-0.586908000	6	-3.649659000	1.017261000	-0.377197000
1	-4.013135000	1.226785000	0.311705000	1	-4.006925000	1.305672000	0.605394000
1	1.851303000	5.110557000	1.384951000	1	2.617397000	5.403426000	0.686628000
1	-4.430697000	0.076175000	-1.052619000	1	-4.395624000	0.591303000	-1.037092000
6	5.273052000	-1.294479000	0.426941000	6	5.347378000	-1.496040000	0.239481000
1	5.682525000	-1.019123000	1.397507000	1	6.022458000	-0.829670000	0.779780000
6	6.049613000	-2.001572000	-0.400321000	6	5.879402000	-2.646756000	-0.235303000
1	5.728132000	-2.318759000	-1.387088000	1	5.297998000	-3.380135000	-0.784991000
1	7.052275000	-2.292900000	-0.108668000	1	6.926333000	-2.883374000	-0.076246000
E=-2134.63388895 Hartrees				E= -2134.67298854 Hartrees			
2l				2l'			
24	-2.272634000	-0.924279000	0.083190000	24	-2.504026000	-0.853708000	0.037566000
6	-1.992084000	-1.705161000	-1.636589000	6	-2.407669000	-1.044932000	-1.844823000
8	-1.784924000	-2.191109000	-2.657995000	8	-2.305655000	-1.177896000	-2.989322000
6	-3.336736000	-2.396141000	0.603377000	6	-3.814571000	-2.150040000	0.218386000
8	-3.969155000	-3.300987000	0.931176000	8	-4.625662000	-2.978950000	0.329783000
6	-2.448772000	-0.162133000	1.821608000	6	-2.313331000	-0.580157000	1.907219000
8	-2.509320000	0.267578000	2.887717000	8	-2.139497000	-0.471938000	3.044692000
6	-0.791093000	-1.886753000	0.701605000	6	-1.288417000	-2.242981000	0.249638000
8	0.092773000	-2.511963000	1.090585000	8	-0.616822000	-3.171341000	0.416379000
6	-1.049416000	0.708673000	-0.387215000	6	-0.914834000	0.687069000	-0.154867000
7	-1.591436000	1.885961000	-0.649560000	7	-1.323679000	2.020709000	0.078302000
6	0.438390000	0.651964000	-0.374465000	6	0.500168000	0.479605000	-0.268186000
6	1.161826000	1.021092000	0.767743000	6	1.461544000	1.345903000	0.351808000
6	1.134110000	0.163979000	-1.488621000	6	1.049580000	-0.615935000	-1.001751000
6	2.549564000	0.914583000	0.795542000	6	2.827052000	1.134994000	0.246849000
1	0.639092000	1.388022000	1.644200000	1	1.108245000	2.168297000	0.961946000
6	2.522549000	0.065191000	-1.471651000	6	2.412412000	-0.821851000	-1.120664000
1	0.590373000	-0.146392000	-2.374265000	1	0.376959000	-1.292856000	-1.511448000
6	3.212885000	0.436288000	-0.326306000	6	3.298426000	0.050689000	-0.488009000
1	3.111923000	1.199542000	1.676821000	1	3.528904000	1.797774000	0.743541000
1	3.065876000	-0.301954000	-2.334343000	1	2.795950000	-1.651241000	-1.705701000
6	-1.025867000	4.158192000	0.215014000	6	-0.514916000	4.378190000	0.077912000
1	-2.038888000	4.437322000	0.498215000	1	-1.327254000	4.719378000	0.718735000
6	-3.616588000	0.606243000	-1.046170000	6	-3.563495000	1.167650000	-0.395744000
1	-3.506145000	0.381528000	-2.102551000	1	-3.531854000	1.293834000	-1.474380000
6	-3.067123000	1.935747000	-0.620481000	6	-2.744780000	2.154754000	0.392291000
1	-3.395548000	2.736282000	-1.292744000	1	-3.063617000	3.180457000	0.162503000
1	-3.399620000	2.194099000	0.390435000	1	-2.918119000	2.008928000	1.464593000
6	-0.886628000	3.166812000	-0.910023000	6	-0.780781000	3.130929000	-0.725355000
1	0.161020000	2.949272000	-1.104026000	1	0.135691000	2.801152000	-1.210346000
1	-1.316282000	3.580545000	-1.829753000	1	-1.492613000	3.373170000	-1.535672000
6	0.005990000	4.720421000	0.837587000	6	0.618255000	5.077017000	0.045455000
1	1.033156000	4.473499000	0.584736000	1	1.462333000	4.766861000	-0.564890000
6	-4.493348000	-0.135935000	-0.300485000	6	-4.535696000	0.368267000	0.146833000
1	-4.849956000	0.207054000	0.663774000	1	-4.776979000	0.416396000	1.203146000

1	-0.137940000	5.454132000	1.623486000	1	0.750634000	5.978773000	0.636375000
1	-5.074747000	-0.925122000	-0.759599000	1	-5.279896000	-0.107819000	-0.479940000
8	4.621811000	0.405068000	-0.339306000	8	4.706158000	-0.102988000	-0.695173000
6	5.240236000	-0.699485000	0.132924000	6	5.394937000	-0.837548000	0.177564000
9	4.890537000	-1.818843000	-0.532723000	9	4.985831000	-2.125819000	0.255993000
9	6.554949000	-0.520968000	-0.007055000	9	6.686583000	-0.851384000	-0.211415000
9	4.981638000	-0.924300000	1.438466000	9	5.365645000	-0.353229000	1.444715000
E=-2469.60707763 Hartrees				E=-2469.64840983 Hartrees			
2m				2m'			
24	-1.773874000	-0.548613000	0.075884000	24	-1.921417000	-0.453918000	0.021180000
6	-1.671367000	-1.469093000	-1.593942000	6	-1.769648000	-0.970361000	-1.796470000
8	-1.576378000	-2.049091000	-2.582211000	8	-1.651603000	-1.312531000	-2.894357000
6	-3.285834000	-1.566401000	0.575359000	6	-3.565428000	-1.286923000	0.220215000
8	-4.194459000	-2.198551000	0.892310000	8	-4.590038000	-1.825024000	0.345994000
6	-1.779191000	0.320642000	1.773281000	6	-1.818767000	0.046533000	1.850895000
8	-1.748091000	0.801380000	2.818483000	8	-1.725976000	0.278654000	2.978961000
6	-0.721642000	-1.902731000	0.823680000	6	-1.178856000	-2.074952000	0.555470000
8	-0.109994000	-2.757514000	1.291888000	8	-0.819041000	-3.111403000	0.921713000
6	-0.067054000	0.575363000	-0.373243000	6	0.063173000	0.522395000	-0.166876000
7	-0.180358000	1.845340000	-0.722512000	7	0.041035000	1.923174000	-0.135694000
6	1.315939000	0.039515000	-0.256154000	6	1.346649000	-0.104671000	-0.099207000
6	2.048808000	0.191993000	0.929491000	6	2.473776000	0.490381000	0.565661000
6	1.880601000	-0.694139000	-1.308948000	6	1.590091000	-1.395337000	-0.667382000
6	3.316798000	-0.360801000	1.057719000	6	3.703350000	-0.128817000	0.638033000
1	1.620805000	0.736726000	1.763910000	1	2.339850000	1.433965000	1.080931000
6	3.152698000	-1.240922000	-1.193465000	6	2.822781000	-2.007141000	-0.620237000
1	1.318798000	-0.847540000	-2.223930000	1	0.783499000	-1.895234000	-1.187652000
6	3.873591000	-1.072888000	-0.008219000	6	3.909802000	-1.383320000	0.030286000
1	3.878923000	-0.248693000	1.977486000	1	4.521280000	0.336389000	1.180367000
1	3.588563000	-1.804592000	-2.009976000	1	2.970968000	-2.976439000	-1.085388000
6	1.042625000	3.864026000	0.089187000	6	1.549580000	3.907956000	-0.017277000
1	0.164697000	4.480011000	0.273446000	1	0.799786000	4.514083000	0.490083000
6	-2.491928000	1.268395000	-1.198976000	6	-2.294014000	1.680247000	-0.788363000
1	-2.416732000	0.954828000	-2.235602000	1	-2.132953000	1.624136000	-1.861255000
6	-1.557837000	2.372577000	-0.800349000	6	-1.293052000	2.512107000	-0.035111000
1	-1.570879000	3.187650000	-1.532436000	1	-1.259975000	3.530273000	-0.446366000
1	-1.836860000	2.794886000	0.170578000	1	-1.599818000	2.609566000	1.013226000
6	0.918219000	2.811216000	-0.980275000	6	1.026331000	2.759391000	-0.841547000
1	1.846781000	2.254518000	-1.082314000	1	1.849795000	2.132649000	-1.176701000
1	0.703749000	3.281460000	-1.946938000	1	0.551221000	3.166522000	-1.751716000
6	2.158623000	4.092476000	0.775373000	6	2.835624000	4.227931000	0.112139000
1	3.058850000	3.504699000	0.620164000	1	3.619805000	3.643503000	-0.361596000
6	-3.594427000	0.898390000	-0.476383000	6	-3.503460000	1.282436000	-0.278900000
1	-3.860234000	1.396723000	0.448694000	1	-3.811369000	1.564204000	0.722092000
1	2.216046000	4.882033000	1.516939000	1	3.154934000	5.079247000	0.706189000
1	-4.381039000	0.312965000	-0.934733000	1	-4.297993000	0.943826000	-0.932571000
7	5.141584000	-1.617887000	0.112502000	7	5.146381000	-1.990920000	0.078532000
6	6.218759000	-2.074439000	0.212501000	6	6.203123000	-2.507189000	0.119282000
E=-2149.45022933 Hartrees				E=-2149.49872863 Hartrees			

2n				2n'			
24	-1.772839000	-0.564651000	0.074992000	24	-1.919124000	-0.472594000	0.026367000
6	-1.654825000	-1.486924000	-1.593570000	6	-1.778371000	-1.041004000	-1.777204000
8	-1.550993000	-2.067090000	-2.580562000	8	-1.671121000	-1.414010000	-2.865787000
6	-3.275397000	-1.599099000	0.570526000	6	-3.547762000	-1.327638000	0.260884000
8	-4.177778000	-2.240898000	0.885103000	8	-4.562288000	-1.878079000	0.409317000
6	-1.796309000	0.306969000	1.771118000	6	-1.824670000	0.080147000	1.841714000
8	-1.776886000	0.789685000	2.815561000	8	-1.739772000	0.345222000	2.962941000
6	-0.708987000	-1.906545000	0.828558000	6	-1.142495000	-2.065595000	0.601207000
8	-0.090303000	-2.754255000	1.300199000	8	-0.761342000	-3.083884000	0.993690000
6	-0.081477000	0.581087000	-0.372158000	6	0.048890000	0.528151000	-0.194035000
7	-0.207800000	1.848413000	-0.724858000	7	0.000761000	1.922513000	-0.198275000
6	1.305235000	0.058236000	-0.255261000	6	1.338415000	-0.082820000	-0.117071000
6	2.021563000	0.182776000	0.944257000	6	2.456860000	0.527062000	0.551588000
6	1.889964000	-0.634117000	-1.325792000	6	1.597106000	-1.375502000	-0.676488000
6	3.295067000	-0.355908000	1.066838000	6	3.690316000	-0.077321000	0.629553000
1	1.575492000	0.694967000	1.789703000	1	2.309464000	1.469010000	1.066354000
6	3.166683000	-1.167801000	-1.211287000	6	2.835818000	-1.969357000	-0.626371000
1	1.339182000	-0.764039000	-2.251084000	1	0.796197000	-1.887112000	-1.194592000
6	3.882344000	-1.030348000	-0.013395000	6	3.928884000	-1.336713000	0.023755000
1	3.839502000	-0.258672000	1.999218000	1	4.493929000	0.406602000	1.177529000
1	3.611521000	-1.697794000	-2.045748000	1	2.986308000	-2.938695000	-1.091403000
6	0.988822000	3.875143000	0.104168000	6	1.483177000	3.922980000	-0.002654000
1	0.104749000	4.483309000	0.284864000	1	0.710312000	4.512044000	0.489956000
6	-2.510555000	1.242729000	-1.207001000	6	-2.328557000	1.627282000	-0.840543000
1	-2.427899000	0.927126000	-2.242439000	1	-2.170226000	1.544488000	-1.912052000
6	-1.591293000	2.359204000	-0.807928000	6	-1.340436000	2.498635000	-0.116790000
1	-1.611727000	3.172424000	-1.541825000	1	-1.318747000	3.501361000	-0.565251000
1	-1.878084000	2.780104000	0.161334000	1	-1.648845000	2.630377000	0.927559000
6	0.881358000	2.827780000	-0.972495000	6	1.000174000	2.779149000	-0.857654000
1	1.816792000	2.282281000	-1.073021000	1	1.839910000	2.165945000	-1.176741000
1	0.666683000	3.300848000	-1.937621000	1	0.546368000	3.193681000	-1.774641000
6	2.097425000	4.107456000	0.800926000	6	2.760206000	4.259171000	0.167474000
1	3.003478000	3.527761000	0.649359000	1	3.566000000	3.692167000	-0.290769000
6	-3.610229000	0.860840000	-0.486739000	6	-3.530285000	1.225197000	-0.315259000
1	-3.884511000	1.357917000	0.436522000	1	-3.840239000	1.532110000	0.677641000
1	2.142777000	4.892643000	1.547922000	1	3.049804000	5.107198000	0.781018000
1	-4.387978000	0.263994000	-0.945467000	1	-4.321286000	0.856136000	-0.956573000
6	5.199234000	-1.574689000	0.106142000	6	5.205518000	-1.941076000	0.075952000
7	6.266961000	-2.007201000	0.199807000	7	6.259165000	-2.434158000	0.118210000
E= -2149.48533523 Hartrees				E= -2149.53842976 Hartrees			
3a				3a'			
24	1.298962000	-0.332318000	0.060526000	24	1.373521000	-0.341127000	-0.007641000
6	1.733392000	0.383782000	1.773267000	6	1.948325000	0.296568000	1.679352000
8	2.008047000	0.783549000	2.815335000	8	2.321577000	0.650686000	2.714714000
6	2.760702000	-1.507476000	0.202615000	6	2.911689000	-1.339639000	-0.257805000
8	3.657390000	-2.223162000	0.291679000	8	3.876847000	-1.968652000	-0.421523000
6	0.888528000	-1.098343000	-1.652366000	6	0.619033000	-0.865617000	-1.677764000
8	0.711512000	-1.574618000	-2.678941000	8	0.187508000	-1.159404000	-2.704598000
6	2.464385000	0.872453000	-0.845735000	6	2.268573000	1.073871000	-0.891369000

8	3.219952000	1.533531000	-1.406126000	8	2.906064000	1.861512000	-1.451017000
6	0.236227000	-1.665720000	0.937882000	6	0.628268000	-1.854895000	0.889872000
8	-0.339312000	-2.499045000	1.474804000	8	0.291334000	-2.801387000	1.452608000
6	-0.436839000	0.956662000	-0.118343000	6	-0.547905000	0.767863000	0.184510000
7	-0.487119000	2.288457000	-0.109653000	7	-0.695460000	2.197733000	0.244330000
6	-1.647334000	3.120275000	-0.487221000	6	-0.945179000	2.844553000	-1.040336000
1	-2.133194000	3.541849000	0.397019000	1	-1.271753000	3.879574000	-0.880712000
1	-1.285314000	3.947406000	-1.101393000	1	-0.047313000	2.868409000	-1.682553000
1	-2.370202000	2.543547000	-1.054438000	1	-1.732801000	2.315956000	-1.577664000
6	0.668670000	3.135772000	0.204406000	6	0.257590000	2.935940000	1.049118000
1	1.425716000	2.573537000	0.732605000	1	0.329375000	2.494880000	2.042763000
1	1.095724000	3.552523000	-0.711683000	1	1.270723000	2.974273000	0.616983000
1	0.335023000	3.961227000	0.837494000	1	-0.095675000	3.967738000	1.162727000
6	-1.751299000	0.315788000	-0.212503000	6	-1.813461000	0.160598000	0.099888000
6	-2.943592000	0.522702000	0.442054000	6	-3.123295000	0.641243000	0.268877000
6	-3.814666000	-0.564731000	0.121919000	6	-4.017413000	-0.450333000	0.099556000
1	-3.167348000	1.339592000	1.112433000	1	-3.372782000	1.657706000	0.533340000
6	-3.093488000	-1.350940000	-0.727530000	6	-3.232039000	-1.537719000	-0.168949000
1	-3.320462000	-2.262282000	-1.258062000	1	-3.456571000	-2.575382000	-0.363728000
8	-1.849336000	-0.851644000	-0.925450000	8	-1.911205000	-1.201882000	-0.178453000
6	-5.209712000	-0.792197000	0.617669000	6	-5.513012000	-0.431368000	0.203642000
1	-5.637125000	-1.702828000	0.192983000	1	-5.937739000	-1.424884000	0.031440000
1	-5.232815000	-0.893750000	1.706695000	1	-5.844697000	-0.098613000	1.193866000
1	-5.871102000	0.038569000	0.354203000	1	-5.961120000	0.249895000	-0.528771000
E=-2052.88168819 Hartrees				E=-2052.92758266 Hartrees			
3b				3b'			
24	1.511191000	-0.427342000	0.059242000	24	1.605081000	-0.421940000	-0.007165000
6	2.059842000	0.235159000	1.761336000	6	2.257255000	0.166361000	1.670054000
8	2.403595000	0.597420000	2.796465000	8	2.676965000	0.486356000	2.698570000
6	2.819993000	-1.771523000	0.195933000	6	3.037392000	-1.567909000	-0.256004000
8	3.623275000	-2.590878000	0.282371000	8	3.935861000	-2.289008000	-0.418739000
6	0.997369000	-1.156354000	-1.641916000	6	0.800965000	-0.892322000	-1.670810000
8	0.761154000	-1.622521000	-2.661232000	8	0.346054000	-1.158739000	-2.694858000
6	2.799587000	0.624613000	-0.871091000	6	2.622606000	0.894728000	-0.910270000
8	3.618871000	1.189955000	-1.446258000	8	3.323790000	1.615821000	-1.482819000
6	0.299315000	-1.610107000	0.959425000	6	0.715528000	-1.845149000	0.907472000
8	-0.373153000	-2.358871000	1.507990000	8	0.285406000	-2.747133000	1.479579000
6	-0.055084000	1.061761000	-0.111297000	6	-0.193884000	0.875370000	0.184475000
7	0.052651000	2.389434000	-0.098409000	7	-0.200651000	2.310543000	0.245672000
6	-1.003549000	3.355575000	-0.463206000	6	-0.417788000	2.985650000	-1.030792000
1	-1.434016000	3.821250000	0.427418000	1	-0.648343000	4.044193000	-0.859496000
1	-0.548736000	4.140842000	-1.070293000	1	0.466847000	2.934091000	-1.689455000
1	-1.791029000	2.874420000	-1.033444000	1	-1.259041000	2.532857000	-1.555416000
6	1.304329000	3.091215000	0.207533000	6	0.829836000	2.956181000	1.034527000
1	1.990447000	2.442621000	0.733610000	1	0.880612000	2.505667000	2.024997000
1	1.773354000	3.450319000	-0.712337000	1	1.833753000	2.906938000	0.582560000
1	1.076738000	3.952627000	0.839555000	1	0.572044000	4.014605000	1.158573000
6	-1.437527000	0.580471000	-0.206546000	6	-1.512483000	0.392160000	0.101559000
6	-2.593325000	0.932238000	0.449138000	6	-2.764903000	1.003624000	0.277578000
6	-3.575334000	-0.041193000	0.106755000	6	-3.742049000	-0.001888000	0.105570000

1	-2.736494000	1.758066000	1.128141000	1	-2.931010000	2.033238000	0.549641000
6	-2.969483000	-0.918416000	-0.752345000	6	-3.087216000	-1.176533000	-0.171156000
1	-3.294562000	-1.789714000	-1.293863000	1	-3.401892000	-2.187057000	-0.367453000
8	-1.668363000	-0.556600000	-0.930431000	8	-1.736245000	-0.951679000	-0.180191000
8	-4.836382000	-0.013499000	0.589674000	8	-5.087292000	0.227052000	0.219958000
6	-5.678165000	-1.086993000	0.180189000	6	-5.908613000	-0.907716000	0.035681000
1	-5.816216000	-1.081718000	-0.906438000	1	-5.780968000	-1.332099000	-0.968345000
1	-5.259818000	-2.049319000	0.493104000	1	-5.686678000	-1.683756000	0.779076000
1	-6.636568000	-0.927974000	0.669543000	1	-6.938900000	-0.572616000	0.158270000
E= -2128.10405832 Hartrees				E=-2128.15150285 Hartrees			
3c				3c'			
24	1.075068000	-0.221601000	0.036878000	24	1.109870000	-0.284138000	-0.017910000
6	1.521436000	0.634919000	1.681219000	6	1.671685000	0.404868000	1.653497000
8	1.810023000	1.120355000	2.682152000	8	2.038889000	0.791133000	2.679393000
6	2.697608000	-1.170396000	0.119623000	6	2.712875000	-1.167324000	-0.295110000
8	3.692161000	-1.746424000	0.172182000	8	3.719125000	-1.722950000	-0.475555000
6	0.668407000	-1.128223000	-1.606675000	6	0.360943000	-0.877334000	-1.667221000
8	0.496333000	-1.679554000	-2.595845000	8	-0.070068000	-1.212882000	-2.681380000
6	1.988682000	1.086935000	-1.005180000	6	1.878654000	1.185488000	-0.930932000
8	2.598584000	1.818469000	-1.648916000	8	2.443519000	2.012826000	-1.510787000
6	0.274554000	-1.641295000	1.046952000	6	0.497367000	-1.843165000	0.902249000
8	-0.141418000	-2.516603000	1.658979000	8	0.242546000	-2.809257000	1.474778000
6	-0.834611000	0.802880000	-0.064981000	6	-0.880003000	0.687531000	0.210251000
7	-1.073698000	2.113318000	-0.099687000	7	-1.128165000	2.103684000	0.262669000
6	-2.364096000	2.757453000	-0.418078000	6	-1.455143000	2.720243000	-1.019509000
1	-2.845268000	3.140728000	0.485867000	1	-1.854424000	3.729206000	-0.858216000
1	-2.166421000	3.602358000	-1.080800000	1	-0.576119000	2.806403000	-1.682064000
1	-3.032786000	2.062649000	-0.915029000	1	-2.212899000	2.130600000	-1.535742000
6	-0.031445000	3.126768000	0.099242000	6	-0.213379000	2.916765000	1.039156000
1	0.830145000	2.699974000	0.592685000	1	-0.077451000	2.485070000	2.030098000
1	0.271201000	3.554798000	-0.860069000	1	0.780323000	3.034955000	0.577196000
1	-0.436383000	3.926735000	0.723234000	1	-0.644012000	3.917571000	1.163193000
6	-2.049089000	-0.018175000	-0.044435000	6	-2.101064000	-0.008363000	0.158214000
6	-3.214851000	0.047710000	0.684235000	6	-3.438696000	0.381034000	0.350594000
6	-3.930609000	-1.161198000	0.449092000	6	-4.245473000	-0.775182000	0.204949000
1	-3.510064000	0.850242000	1.342560000	1	-3.754460000	1.378992000	0.610427000
6	-3.168506000	-1.880041000	-0.420377000	6	-3.398289000	-1.812229000	-0.071089000
1	-4.880137000	-1.455782000	0.869679000	1	-5.321229000	-0.843536000	0.299358000
1	-3.293886000	-2.833395000	-0.907698000	1	-3.545899000	-2.864763000	-0.254172000
8	-2.026563000	-1.217135000	-0.713743000	8	-2.107813000	-1.378242000	-0.107603000
E= -2013.55461300 Hartrees				E=-2013.60169949 Hartrees			
3d				3d'			
24	1.465795000	-0.424813000	0.066918000	24	1.573275000	-0.403833000	-0.005548000
6	1.960147000	0.211241000	1.795770000	6	2.216678000	0.215431000	1.664372000
8	2.269723000	0.558388000	2.846659000	8	2.632340000	0.554451000	2.688173000
6	2.782775000	-1.760393000	0.212861000	6	3.034180000	-1.515729000	-0.247906000
8	3.590585000	-2.574445000	0.305089000	8	3.949871000	-2.215155000	-0.406518000
6	1.001253000	-1.123068000	-1.660664000	6	0.779192000	-0.911535000	-1.662738000
8	0.791332000	-1.568538000	-2.694894000	8	0.327574000	-1.199962000	-2.682166000

6	2.772070000	0.653157000	-0.807866000	6	2.555475000	0.930652000	-0.922528000
8	3.603888000	1.233279000	-1.349168000	8	3.237089000	1.664655000	-1.501811000
6	0.244975000	-1.636739000	0.913722000	6	0.722951000	-1.839797000	0.925412000
8	-0.431611000	-2.403656000	1.431315000	8	0.314898000	-2.745635000	1.507309000
6	-0.108033000	1.056440000	-0.118303000	6	-0.255862000	0.847059000	0.179090000
7	-0.007080000	2.384914000	-0.081010000	7	-0.299536000	2.283596000	0.229912000
6	-1.058050000	3.351338000	-0.458103000	6	-0.523215000	2.940922000	-1.054739000
1	-1.515733000	3.799767000	0.427950000	1	-0.778282000	3.995697000	-0.895437000
1	-0.591775000	4.149588000	-1.038998000	1	0.366099000	2.902774000	-1.707743000
1	-1.826346000	2.875511000	-1.058521000	1	-1.350761000	2.464346000	-1.580333000
6	1.231680000	3.088106000	0.270620000	6	0.713700000	2.958766000	1.016847000
1	1.908294000	2.433660000	0.801603000	1	0.770733000	2.518156000	2.011469000
1	1.721981000	3.468230000	-0.629547000	1	1.720066000	2.927525000	0.568923000
1	0.982458000	3.935591000	0.913299000	1	0.432289000	4.012274000	1.130544000
6	-1.484563000	0.572721000	-0.255707000	6	-1.563155000	0.336175000	0.105501000
6	-2.665570000	0.902920000	0.364383000	6	-2.832011000	0.907933000	0.281384000
6	-3.643744000	-0.079012000	0.005452000	6	-3.808921000	-0.114938000	0.118299000
1	-2.819489000	1.727542000	1.044302000	1	-3.010665000	1.940012000	0.541441000
6	-2.986293000	-0.928270000	-0.846222000	6	-3.100715000	-1.265267000	-0.151239000
1	-3.300246000	-1.782303000	-1.424369000	1	-3.391299000	-2.288306000	-0.329027000
8	-1.694488000	-0.567096000	-0.994021000	8	-1.766407000	-1.020390000	-0.166640000
6	-5.033426000	-0.124541000	0.459004000	6	-5.251542000	0.064530000	0.235544000
1	-5.423431000	0.810373000	0.856625000	1	-5.557422000	1.061521000	0.551819000
6	-5.836035000	-1.191934000	0.433403000	6	-6.214611000	-0.836888000	0.000045000
1	-5.501473000	-2.163201000	0.082206000	1	-5.996075000	-1.849135000	-0.327575000
1	-6.862334000	-1.128875000	0.776538000	1	-7.262331000	-0.585639000	0.128870000
E=-2090.97032506 Hartrees				E= -2091.01991085 Hartrees			
3e				3e'			
24	1.528210000	-0.378710000	0.073496000	24	1.631814000	-0.360790000	0.000743000
6	1.965188000	0.301148000	1.801394000	6	2.250156000	0.285554000	1.670629000
8	2.240239000	0.676263000	2.852044000	8	2.658108000	0.638847000	2.692661000
6	2.909823000	-1.645012000	0.254335000	6	3.146647000	-1.401973000	-0.227775000
8	3.756119000	-2.415479000	0.368037000	8	4.095688000	-2.057357000	-0.376260000
6	1.127989000	-1.120923000	-1.652872000	6	0.888976000	-0.921123000	-1.664134000
8	0.958813000	-1.590208000	-2.683728000	8	0.474158000	-1.243051000	-2.688863000
6	2.789577000	0.757168000	-0.796487000	6	2.544282000	1.024501000	-0.914570000
8	3.595634000	1.375506000	-1.333589000	8	3.182574000	1.796680000	-1.492854000
6	0.355337000	-1.639565000	0.914300000	6	0.835672000	-1.826306000	0.933478000
8	-0.296290000	-2.429934000	1.429128000	8	0.455336000	-2.741369000	1.519447000
6	-0.112049000	1.016635000	-0.142962000	6	-0.255753000	0.801854000	0.166366000
7	-0.090268000	2.347269000	-0.111725000	7	-0.369075000	2.231422000	0.231778000
6	-1.198277000	3.248858000	-0.489581000	6	-0.644879000	2.896951000	-1.039163000
1	-1.675184000	3.675247000	0.396942000	1	-0.966962000	3.929531000	-0.858408000
1	-0.781787000	4.068371000	-1.078351000	1	0.241336000	2.929289000	-1.696560000
1	-1.941581000	2.725769000	-1.081649000	1	-1.442832000	2.378124000	-1.569837000
6	1.105070000	3.123667000	0.237497000	6	0.611322000	2.951761000	1.020010000
1	1.822082000	2.509835000	0.763995000	1	0.700837000	2.503091000	2.008379000
1	1.567163000	3.534005000	-0.664218000	1	1.613467000	2.982314000	0.563179000
1	0.807247000	3.953264000	0.882636000	1	0.272380000	3.986256000	1.149215000
6	-1.460719000	0.453462000	-0.285627000	6	-1.536865000	0.228831000	0.068478000

6	-2.648123000	0.695209000	0.359357000	6	-2.833796000	0.741547000	0.233424000
6	-3.560062000	-0.333142000	-0.035036000	6	-3.738030000	-0.338110000	0.054861000
1	-2.854833000	1.489064000	1.060359000	1	-3.074610000	1.759996000	0.491535000
6	-2.875120000	-1.116213000	-0.917594000	6	-2.986492000	-1.447731000	-0.220913000
1	-3.150700000	-1.980820000	-1.499438000	1	-3.242605000	-2.475698000	-0.419920000
8	-1.609662000	-0.669842000	-1.066035000	8	-1.666519000	-1.133244000	-0.226513000
16	-5.270041000	-0.515889000	0.412707000	16	-5.517867000	-0.306905000	0.085625000
1	-5.067551000	-1.080546000	1.627378000	1	-5.677346000	-0.101990000	1.417053000
E=-2411.76501728 Hartrees				E=-2411.81778480 Hartrees			
3f				3f			
24	2.014358000	-0.407225000	0.087163000	24	2.152123000	-0.375058000	0.007462000
6	2.420404000	0.230372000	1.839372000	6	2.760760000	0.263786000	1.684106000
8	2.676183000	0.579643000	2.903457000	8	3.161948000	0.611733000	2.710316000
6	3.346467000	-1.723338000	0.289690000	6	3.653835000	-1.439827000	-0.201617000
8	4.162377000	-2.523688000	0.416157000	8	4.594741000	-2.108868000	-0.338557000
6	1.643934000	-1.109379000	-1.662097000	6	1.422306000	-0.930029000	-1.665151000
8	1.490299000	-1.556826000	-2.705052000	8	1.016546000	-1.250013000	-2.693995000
6	3.342273000	0.696329000	-0.722446000	6	3.096985000	0.992545000	-0.900987000
8	4.187449000	1.293141000	-1.222521000	8	3.753185000	1.753019000	-1.474440000
6	0.774681000	-1.643078000	0.870680000	6	1.322348000	-1.828256000	0.931139000
8	0.084522000	-2.422131000	1.350268000	8	0.921698000	-2.738583000	1.510493000
6	0.434252000	1.047244000	-0.162809000	6	0.286290000	0.823676000	0.150998000
7	0.503154000	2.376089000	-0.117878000	7	0.197178000	2.254440000	0.218495000
6	-0.553760000	3.321767000	-0.532856000	6	-0.053668000	2.926874000	-1.054074000
1	-1.046776000	3.763879000	0.336984000	1	-0.356170000	3.965468000	-0.874813000
1	-0.083520000	4.126245000	-1.101618000	1	0.839054000	2.941368000	-1.702987000
1	-1.293879000	2.830835000	-1.155755000	1	-0.856908000	2.424955000	-1.592999000
6	1.712140000	3.104099000	0.285155000	6	1.181140000	2.956660000	1.019236000
1	2.378932000	2.462484000	0.843803000	1	1.252583000	2.504170000	2.007247000
1	2.231118000	3.494420000	-0.594151000	1	2.188453000	2.972421000	0.573361000
1	1.418682000	3.945670000	0.916529000	1	0.857356000	3.995971000	1.147663000
6	-0.928843000	0.535747000	-0.358032000	6	-1.000901000	0.270399000	0.038662000
6	-2.127876000	0.825690000	0.248258000	6	-2.290411000	0.810508000	0.199552000
6	-3.055869000	-0.157264000	-0.198370000	6	-3.193250000	-0.253965000	-0.002213000
1	-2.325754000	1.617547000	0.953122000	1	-2.515433000	1.825803000	0.479857000
6	-2.383112000	-0.973379000	-1.055313000	6	-2.478544000	-1.383801000	-0.277049000
1	-2.669786000	-1.825660000	-1.648234000	1	-2.752095000	-2.403479000	-0.488579000
8	-1.092608000	-0.575037000	-1.147216000	8	-1.149521000	-1.086694000	-0.259657000
35	-4.865418000	-0.301837000	0.296413000	35	-5.094804000	-0.162929000	0.102109000
E=-4587.09724435 Hartrees				E=-4587.14970941 Hartrees			
3g				3g			
24	1.978356000	-0.463740000	0.098744000	24	2.109096000	-0.439038000	0.010360000
6	2.466192000	0.227674000	1.809761000	6	2.780835000	0.194917000	1.664984000
8	2.772332000	0.605323000	2.850531000	8	3.217977000	0.536729000	2.678430000
6	3.237309000	-1.843248000	0.336553000	6	3.537979000	-1.599902000	-0.194274000
8	4.008917000	-2.683252000	0.483984000	8	4.432634000	-2.330132000	-0.329446000
6	1.530373000	-1.228890000	-1.604418000	6	1.323076000	-0.982747000	-1.639124000
8	1.330188000	-1.719486000	-2.619977000	8	0.881881000	-1.299942000	-2.654511000
6	3.344180000	0.522682000	-0.794912000	6	3.121553000	0.848996000	-0.942078000

8	4.206737000	1.046656000	-1.344412000	8	3.811792000	1.555913000	-1.543033000
6	0.687473000	-1.582177000	0.968658000	6	1.200961000	-1.814191000	0.975608000
8	-0.038493000	-2.292603000	1.499882000	8	0.745629000	-2.682895000	1.578755000
6	0.476537000	1.069349000	-0.188356000	6	0.322882000	0.878863000	0.148240000
7	0.623010000	2.392158000	-0.199480000	7	0.327003000	2.311327000	0.188621000
6	-0.388255000	3.382130000	-0.625475000	6	0.078597000	2.982579000	-1.084968000
1	-0.843618000	3.872559000	0.238731000	1	-0.166020000	4.037052000	-0.910889000
1	0.115489000	4.144328000	-1.222838000	1	0.954984000	2.943746000	-1.755004000
1	-1.163441000	2.915085000	-1.223681000	1	-0.762694000	2.517565000	-1.597821000
6	1.880557000	3.063329000	0.150438000	6	1.365931000	2.968291000	0.956872000
1	2.519140000	2.408121000	0.725888000	1	1.432088000	2.528995000	1.951080000
1	2.404121000	3.382765000	-0.754342000	1	2.362903000	2.918929000	0.490395000
1	1.649799000	3.947622000	0.748391000	1	1.105006000	4.026411000	1.073556000
6	-0.916844000	0.631662000	-0.341810000	6	-1.002026000	0.411458000	0.057618000
6	-2.091092000	1.014932000	0.251241000	6	-2.255093000	1.015490000	0.214226000
6	-3.086466000	0.063536000	-0.128508000	6	-3.242308000	0.002379000	0.042051000
1	-2.247118000	1.852265000	0.912661000	1	-2.428503000	2.047026000	0.470976000
6	-2.453897000	-0.832096000	-0.945693000	6	-2.564053000	-1.165186000	-0.214503000
1	-2.792821000	-1.699207000	-1.488082000	1	-2.891465000	-2.173967000	-0.404118000
8	-1.153931000	-0.517282000	-1.071358000	8	-1.236359000	-0.949822000	-0.214740000
6	-4.496780000	0.085559000	0.289894000	6	-4.688667000	0.171775000	0.131359000
8	-4.979624000	0.930172000	1.008407000	8	-5.273739000	1.210376000	0.358425000
8	-5.190395000	-0.949762000	-0.228164000	8	-5.361513000	-1.003105000	-0.075060000
6	-6.582815000	-1.017606000	0.128564000	6	-6.784747000	-0.919995000	-0.002236000
1	-6.694251000	-1.108436000	1.209191000	1	-7.106550000	-0.577034000	0.983241000
1	-7.107825000	-0.125809000	-0.214636000	1	-7.175713000	-0.234106000	-0.756668000
1	-6.965771000	-1.903766000	-0.371554000	1	-7.147318000	-1.930303000	-0.186940000

E=-2241.49995055 Hartrees

3h

24	1.524924000	-0.371127000	0.073832000
6	1.960611000	0.312374000	1.801582000
8	2.235669000	0.690736000	2.850797000
6	2.921383000	-1.623027000	0.247998000
8	3.776432000	-2.384149000	0.356950000
6	1.126193000	-1.114983000	-1.651716000
8	0.956165000	-1.583441000	-2.682869000
6	2.773284000	0.776919000	-0.797901000
8	3.573374000	1.401804000	-1.336436000
6	0.370617000	-1.649902000	0.916337000
8	-0.266203000	-2.452543000	1.429658000
6	-0.127866000	1.006765000	-0.139771000
7	-0.116896000	2.338097000	-0.118141000
6	-1.228646000	3.229383000	-0.509353000
1	-1.710966000	3.663180000	0.370671000
1	-0.814440000	4.044686000	-1.105507000
1	-1.966871000	2.696625000	-1.099125000
6	1.072000000	3.125518000	0.229006000
1	1.788510000	2.522386000	0.768509000
1	1.538318000	3.527071000	-0.674418000
1	0.764658000	3.961359000	0.861432000

E= -2241.55372594 Hartrees

3h'

24	1.624486000	-0.357994000	0.001074000
6	2.238115000	0.297250000	1.669440000
8	2.642941000	0.655854000	2.690616000
6	3.144895000	-1.392489000	-0.223258000
8	4.097686000	-2.042558000	-0.369778000
6	0.885800000	-0.930253000	-1.661724000
8	0.473680000	-1.259769000	-2.685066000
6	2.531345000	1.026463000	-0.920282000
8	3.166152000	1.798537000	-1.502418000
6	0.835450000	-1.825999000	0.936984000
8	0.460614000	-2.743193000	1.522821000
6	-0.264737000	0.801289000	0.163984000
7	-0.383191000	2.230480000	0.228495000
6	-0.657942000	2.892950000	-1.044335000
1	-0.977959000	3.926515000	-0.866188000
1	0.228196000	2.921312000	-1.701787000
1	-1.456853000	2.374072000	-1.573611000
6	0.594294000	2.954514000	1.017620000
1	0.683042000	2.507424000	2.006743000
1	1.597204000	2.987235000	0.562782000
1	0.252148000	3.988098000	1.144815000

6	-1.472607000	0.432190000	-0.276639000	6	-1.541307000	0.221459000	0.067842000
6	-2.663287000	0.683678000	0.362726000	6	-2.839734000	0.736062000	0.239363000
6	-3.558460000	-0.348422000	-0.033380000	6	-3.722880000	-0.346449000	0.051792000
1	-2.876081000	1.480345000	1.057729000	1	-3.084460000	1.747622000	0.517086000
6	-2.880543000	-1.154277000	-0.895964000	6	-2.988630000	-1.463303000	-0.225680000
1	-3.150404000	-2.031134000	-1.460137000	1	-3.245522000	-2.488993000	-0.429139000
8	-1.613044000	-0.701680000	-1.036935000	8	-1.665565000	-1.139177000	-0.223292000
17	-5.200461000	-0.538073000	0.480529000	17	-5.470189000	-0.292430000	0.165913000
E=-2473.17308352 Hartrees				E= -2473.22867914 Hartrees			
3i				3i'			
24	2.118205000	-0.469063000	0.114340000	24	2.359145000	-0.361217000	0.078018000
6	2.338741000	-0.022525000	1.957471000	6	2.743121000	0.253699000	1.829248000
8	2.481242000	0.209015000	3.073364000	8	3.008568000	0.586906000	2.903067000
6	3.323984000	-1.897577000	0.352159000	6	3.898562000	-1.392451000	0.039780000
8	4.062345000	-2.766249000	0.500051000	8	4.863354000	-2.040043000	0.009742000
6	1.938927000	-0.990737000	-1.725547000	6	1.859633000	-0.899501000	-1.681940000
8	1.897928000	-1.336628000	-2.816566000	8	1.594671000	-1.209509000	-2.758686000
6	3.607661000	0.597256000	-0.416144000	6	3.378092000	1.043763000	-0.681578000
8	4.545290000	1.171497000	-0.749780000	8	4.081689000	1.829490000	-1.155929000
6	0.705894000	-1.665608000	0.616330000	6	1.450805000	-1.848188000	0.863770000
8	-0.094358000	-2.423750000	0.928971000	8	0.997913000	-2.777244000	1.370043000
6	0.686711000	1.118659000	-0.189909000	6	0.467016000	0.798201000	0.007508000
7	0.834393000	2.428963000	-0.006531000	7	0.339415000	2.224731000	0.091307000
6	-0.091968000	3.487101000	-0.460607000	6	0.234651000	2.922313000	-1.188352000
1	-0.672506000	3.884594000	0.376090000	1	-0.113797000	3.949222000	-1.026629000
1	0.503670000	4.301447000	-0.877220000	1	1.201608000	2.972149000	-1.717933000
1	-0.766985000	3.114435000	-1.223626000	1	-0.480965000	2.416413000	-1.836045000
6	2.022407000	3.022544000	0.618956000	6	1.198946000	2.927834000	1.024048000
1	2.557488000	2.286920000	1.202728000	1	1.154712000	2.454905000	2.003963000
1	2.685658000	3.437889000	-0.144055000	1	2.253698000	2.973042000	0.709501000
1	1.701305000	3.832096000	1.277907000	1	0.838444000	3.957341000	1.130873000
6	-0.669361000	0.734965000	-0.608467000	6	-0.783819000	0.225552000	-0.280309000
6	-1.917297000	1.064417000	-0.138169000	6	-2.092956000	0.741781000	-0.283610000
6	-2.828657000	0.199350000	-0.803949000	6	-2.933934000	-0.338961000	-0.613382000
1	-2.160357000	1.801232000	0.610344000	1	-2.371366000	1.748708000	-0.023186000
6	-2.106709000	-0.584898000	-1.648334000	6	-2.171645000	-1.452132000	-0.810927000
1	-2.370784000	-1.344245000	-2.365170000	1	-2.399229000	-2.467940000	-1.086343000
8	-0.796705000	-0.278761000	-1.526345000	8	-0.865084000	-1.128428000	-0.619532000
8	-4.212013000	0.210378000	-0.714768000	8	-4.326866000	-0.315002000	-0.813810000
6	-4.776057000	-0.328349000	0.397532000	6	-5.116893000	-0.128920000	0.249531000
9	-6.095442000	-0.208960000	0.275527000	9	-6.394128000	-0.217118000	-0.165103000
9	-4.471038000	-1.626828000	0.552469000	9	-4.939451000	-1.045669000	1.225042000
9	-4.392481000	0.307875000	1.525028000	9	-4.966633000	1.085559000	0.830318000
E= -2425.93726075 Hartrees				E= -2425.99631560 Hartrees			
3j				3j'			
24	1.959618000	-0.408122000	0.082807000	24	2.102609000	-0.376646000	0.007409000
6	2.363098000	0.229731000	1.836755000	6	2.735942000	0.275297000	1.670723000
8	2.615919000	0.581541000	2.900247000	8	3.156086000	0.628751000	2.687135000
6	3.282563000	-1.735134000	0.291804000	6	3.601414000	-1.447327000	-0.200265000

8	4.091509000	-2.541135000	0.422297000	8	4.539533000	-2.119793000	-0.336165000
6	1.593129000	-1.106970000	-1.668382000	6	1.370149000	-0.956546000	-1.655353000
8	1.439467000	-1.551993000	-2.712274000	8	0.964645000	-1.294302000	-2.678551000
6	3.301087000	0.685497000	-0.720190000	6	3.035196000	0.984422000	-0.924580000
8	4.153518000	1.275001000	-1.215796000	8	3.679170000	1.743329000	-1.512923000
6	0.708718000	-1.636869000	0.858576000	6	1.268673000	-1.811467000	0.954366000
8	0.008661000	-2.411650000	1.330666000	8	0.857254000	-2.708261000	1.547021000
6	0.394398000	1.053232000	-0.170079000	6	0.241099000	0.825798000	0.147082000
7	0.462803000	2.380825000	-0.127747000	7	0.153222000	2.254556000	0.217203000
6	-0.598854000	3.326247000	-0.533301000	6	-0.130266000	2.934950000	-1.044772000
1	-1.078556000	3.772275000	0.341771000	1	-0.442600000	3.967878000	-0.851185000
1	-0.135277000	4.127255000	-1.112094000	1	0.751008000	2.966221000	-1.708299000
1	-1.348435000	2.834202000	-1.143690000	1	-0.936194000	2.427947000	-1.574414000
6	1.676039000	3.108408000	0.264696000	6	1.147321000	2.960036000	1.002614000
1	2.342375000	2.469089000	0.826741000	1	1.240257000	2.504370000	1.987126000
1	2.192710000	3.488498000	-0.620287000	1	2.145461000	2.984872000	0.537330000
1	1.387547000	3.956557000	0.889159000	1	0.818721000	3.996375000	1.141289000
6	-0.973700000	0.544215000	-0.358564000	6	-1.050820000	0.277377000	0.036275000
6	-2.157771000	0.806434000	0.279821000	6	-2.337833000	0.808564000	0.204717000
6	-3.096604000	-0.165318000	-0.182500000	6	-3.256261000	-0.256680000	0.003707000
1	-2.338493000	1.574956000	1.015194000	1	-2.559736000	1.823518000	0.490668000
6	-2.432798000	-0.943609000	-1.080813000	6	-2.522929000	-1.376013000	-0.278712000
1	-2.728326000	-1.776603000	-1.696854000	1	-2.792926000	-2.396254000	-0.494193000
8	-1.151931000	-0.539624000	-1.186331000	8	-1.204284000	-1.082038000	-0.268614000
6	-4.519770000	-0.296915000	0.225159000	6	-4.728750000	-0.193730000	0.089226000
9	-5.227977000	0.827727000	-0.049483000	9	-5.277826000	0.682281000	-0.801394000
9	-5.128555000	-1.319063000	-0.411876000	9	-5.316634000	-1.395903000	-0.150223000
9	-4.649951000	-0.511761000	1.554531000	9	-5.176208000	0.212857000	1.311621000
E= -2350.70395189 Hartrees				E= -2350.76411335 Hartrees			

3k				3k'			
24	1.416544000	-0.366529000	0.077335000	24	1.512631000	-0.351485000	0.003129000
6	1.846854000	0.321307000	1.806192000	6	2.149610000	0.327504000	1.654471000
8	2.117730000	0.703205000	2.854683000	8	2.573585000	0.697597000	2.663245000
6	2.822247000	-1.610790000	0.254448000	6	3.041208000	-1.376984000	-0.218150000
8	3.681280000	-2.366217000	0.365129000	8	3.997563000	-2.021166000	-0.362260000
6	1.027543000	-1.114672000	-1.648439000	6	0.779544000	-0.966607000	-1.646805000
8	0.861336000	-1.585427000	-2.679036000	8	0.373992000	-1.325377000	-2.662732000
6	2.660190000	0.789784000	-0.793002000	6	2.389358000	1.032552000	-0.949435000
8	3.456480000	1.419465000	-1.330621000	8	3.000047000	1.808193000	-1.551074000
6	0.269080000	-1.653140000	0.915566000	6	0.734405000	-1.804872000	0.969164000
8	-0.367693000	-2.459369000	1.423415000	8	0.357323000	-2.709640000	1.572348000
6	-0.239475000	0.998526000	-0.137497000	6	-0.381019000	0.795554000	0.160101000
7	-0.244444000	2.328846000	-0.118210000	7	-0.511770000	2.220990000	0.227405000
6	-1.369219000	3.207138000	-0.503448000	6	-0.834671000	2.888902000	-1.031951000
1	-1.847076000	3.639468000	0.379568000	1	-1.177346000	3.911651000	-0.835969000
1	-0.968762000	4.023788000	-1.106871000	1	0.035939000	2.946994000	-1.707488000
1	-2.107505000	2.665166000	-1.084530000	1	-1.630900000	2.355061000	-1.549709000
6	0.938075000	3.129703000	0.221779000	6	0.471786000	2.959543000	0.995859000
1	1.660791000	2.536382000	0.764075000	1	0.593314000	2.510589000	1.980283000
1	1.398737000	3.529162000	-0.685316000	1	1.461457000	3.013381000	0.515438000

1	0.623665000	3.966690000	0.848888000	1	0.113324000	3.985648000	1.136159000
6	-1.581915000	0.410188000	-0.267583000	6	-1.655448000	0.207100000	0.067766000
6	-2.759862000	0.628438000	0.399263000	6	-2.955777000	0.702168000	0.250529000
6	-3.655086000	-0.407932000	-0.008627000	6	-3.838368000	-0.393035000	0.065930000
1	-2.972506000	1.403072000	1.118867000	1	-3.216031000	1.707742000	0.535787000
6	-2.975135000	-1.180427000	-0.907529000	6	-3.078610000	-1.497957000	-0.222500000
1	-3.245591000	-2.046047000	-1.489007000	1	-3.326451000	-2.525899000	-0.428100000
8	-1.723171000	-0.705743000	-1.057236000	8	-1.769505000	-1.157511000	-0.229206000
7	-4.946113000	-0.586002000	0.413607000	7	-5.212341000	-0.373273000	0.165201000
6	-6.052060000	-0.712824000	0.788848000	6	-6.380639000	-0.330586000	0.252969000
E= -2105.78184114 Hartrees				E= -2105.84419601 Hartrees			
3l				3l'			
24	1.422232000	-0.373561000	0.079807000	24	1.522041000	-0.355285000	0.004543000
6	1.849310000	0.307385000	1.812787000	6	2.167912000	0.325844000	1.652020000
8	2.117677000	0.685642000	2.863032000	8	2.598767000	0.696181000	2.657617000
6	2.816954000	-1.630429000	0.261926000	6	3.046790000	-1.387616000	-0.214585000
8	3.668824000	-2.393160000	0.375606000	8	4.000405000	-2.035842000	-0.357191000
6	1.037241000	-1.114309000	-1.649813000	6	0.788834000	-0.976364000	-1.642925000
8	0.872282000	-1.581008000	-2.682445000	8	0.383686000	-1.339751000	-2.657363000
6	2.681059000	0.774356000	-0.780734000	6	2.399763000	1.023840000	-0.954844000
8	3.485698000	1.398196000	-1.312364000	8	3.008776000	1.797014000	-1.560937000
6	0.260023000	-1.653018000	0.908083000	6	0.736469000	-1.799901000	0.977107000
8	-0.387013000	-2.455525000	1.408808000	8	0.351296000	-2.698921000	1.583744000
6	-0.219611000	1.005294000	-0.139221000	6	-0.366399000	0.800330000	0.158017000
7	-0.216527000	2.335045000	-0.116832000	7	-0.491285000	2.225168000	0.226536000
6	-1.336058000	3.221573000	-0.499484000	6	-0.826171000	2.898059000	-1.027152000
1	-1.810402000	3.654265000	0.385150000	1	-1.170396000	3.918812000	-0.824016000
1	-0.930660000	4.037124000	-1.100973000	1	0.039466000	2.961790000	-1.708465000
1	-2.078249000	2.685947000	-1.081458000	1	-1.624501000	2.364450000	-1.541698000
6	0.971007000	3.127318000	0.226579000	6	0.497984000	2.961702000	0.989556000
1	1.688083000	2.528417000	0.770281000	1	0.626425000	2.510823000	1.972105000
1	1.436456000	3.523692000	-0.679370000	1	1.483973000	3.016524000	0.501867000
1	0.661015000	3.966168000	0.853258000	1	0.140747000	3.987520000	1.134533000
6	-1.566905000	0.426810000	-0.274806000	6	-1.644691000	0.218039000	0.064574000
6	-2.741040000	0.639384000	0.396400000	6	-2.942895000	0.711570000	0.250345000
6	-3.651858000	-0.386595000	-0.021880000	6	-3.840522000	-0.381353000	0.063841000
1	-2.942993000	1.406399000	1.127260000	1	-3.197059000	1.717713000	0.539084000
6	-2.968363000	-1.144201000	-0.934486000	6	-3.069563000	-1.481671000	-0.229264000
1	-3.241271000	-1.999763000	-1.530406000	1	-3.314510000	-2.509881000	-0.439458000
8	-1.717778000	-0.678065000	-1.082534000	8	-1.764982000	-1.147920000	-0.237406000
6	-4.989875000	-0.575289000	0.406851000	6	-5.253630000	-0.369032000	0.164983000
7	-6.081240000	-0.711486000	0.760668000	7	-6.408713000	-0.349121000	0.247646000
E= -2105.82010061 Hartrees				E= -2105.88416651 Hartrees			