

# Electronic Supplementary Information

## Can Carbene Decorated [FeFe]-Hydrogenase Model Complexes Catalytically Produce Dihydrogen? An Insight from Theory

Bitupon Borthakur and Ashwini K. Phukan \*

*Department of Chemical Sciences, Tezpur University, Napaam 784028, Assam, India*  
E-mail: [ashwini@tezu.ernet.in](mailto:ashwini@tezu.ernet.in)

### Contents

1. Total charge, multiplicity and $\langle S^2 \rangle$ values for all the complexes considered in the present study.	S1
2. Cartesian coordinates of all the complexes	S2-S34

**Table S1:** Total charge, multiplicity and  $\langle S^2 \rangle$  values for all the complexes considered in the present study.

Complex	Charge	Multiplicity	$\langle S^2 \rangle$
[1] <sup>0</sup>	0	Singlet	-
[1- <i>adtH</i> ] <sup>+</sup>	1	Singlet	-
[1- <i>tH</i> ] <sup>+</sup>	1	Singlet	-
[1- <i>tH</i> ] <sup>0</sup>	0	Doublet	0.7678
[1- <i>tH-adtH</i> ] <sup>+</sup>	1	Doublet	0.7676
[1- <b>H<sub>2</sub></b> ] <sup>+</sup>	1	Doublet	0.7570
[2] <sup>0</sup>	0	Singlet	-
[2- <i>adtH(a)</i> ] <sup>+</sup>	1	Singlet	-
[2- <i>adtH(b)</i> ] <sup>+</sup>	1	Singlet	-
[2- <i>tH</i> ] <sup>+</sup>	1	Singlet	-
[2- <i>tH</i> ] <sup>0</sup>	0	Doublet	0.7641
[2- <i>tH-adtH(a)</i> ] <sup>+</sup>	1	Doublet	0.7639
[2- <i>tH-adtH(b)</i> ] <sup>+</sup>	1	Doublet	0.7642
[2- <b>H<sub>2</sub></b> ] <sup>+</sup>	1	Doublet	0.7547

Cartesian coordinates of all the complexes along with their total energies (T. E. in hartrees) including zero point vibrational correction.

[1]<sup>0</sup>, T. E. = -5069.115539

Fe	-0.008053000	-2.244981000	-0.132817000
Fe	0.011153000	0.187703000	0.833476000
C	0.002236000	-0.850078000	-1.224539000
O	0.005593000	-0.407813000	-2.302458000
C	-1.161454000	-2.286280000	3.145916000
C	1.257164000	-2.299835000	3.097563000
S	-1.609963000	-1.488451000	1.546372000
S	1.649465000	-1.494618000	1.486401000
C	-1.515455000	1.509643000	0.174540000
C	-2.507360000	3.662560000	-0.426588000
C	1.495317000	1.532460000	0.124002000
C	2.387593000	3.693531000	-0.586944000
C	0.051339000	0.695589000	2.636795000
O	0.082852000	0.783901000	3.763816000
C	-0.048439000	3.520512000	-0.189505000
C	3.416135000	2.606446000	-0.877602000
C	-3.509595000	2.550084000	-0.708208000
N	0.045165000	-3.065843000	3.199267000
H	0.026830000	-3.779501000	2.475922000
C	1.222437000	-3.324228000	-0.865539000
O	1.992588000	-4.038173000	-1.310609000
H	-2.006911000	-2.931678000	3.378767000
H	-1.106365000	-1.515297000	3.916495000
H	2.104167000	-2.956126000	3.290848000
H	1.244353000	-1.532225000	3.873370000
C	-1.284185000	-3.276744000	-0.868719000
O	-2.067622000	-3.976549000	-1.310089000
C	-1.373096000	3.018654000	0.397847000
C	1.317421000	3.042398000	0.312865000
N	-2.656543000	1.325334000	-0.434089000
N	2.632313000	1.364853000	-0.497399000
C	3.275391000	0.121059000	-0.842064000
C	4.226737000	-0.409582000	0.016158000
C	3.051469000	-0.451542000	-2.085833000
C	4.950736000	-1.528599000	-0.368502000
H	4.382816000	0.043548000	0.985243000
C	3.771717000	-1.575646000	-2.462145000
H	2.320669000	-0.016269000	-2.750906000
C	4.723870000	-2.113122000	-1.606512000
H	5.685232000	-1.947721000	0.306332000

H	3.586659000	-2.030389000	-3.426320000
H	5.283921000	-2.990585000	-1.902306000
C	-3.247914000	0.080395000	-0.858582000
C	-4.169321000	-0.554274000	-0.039425000
C	-3.020112000	-0.377854000	-2.148911000
C	-4.861024000	-1.660641000	-0.512566000
H	-4.331611000	-0.188737000	0.964415000
C	-3.710634000	-1.486098000	-2.615370000
H	-2.310796000	0.136918000	-2.780134000
C	-4.635967000	-2.124712000	-1.800433000
H	-5.573156000	-2.160196000	0.130800000
H	-3.525308000	-1.848291000	-3.617992000
H	-5.173319000	-2.989876000	-2.166210000
C	-1.581543000	3.383657000	1.874341000
H	-1.393421000	4.451322000	2.005384000
H	-2.611209000	3.187313000	2.172102000
H	-0.939904000	2.846225000	2.559514000
H	2.843543000	4.563010000	-0.114346000
H	1.939389000	4.024241000	-1.524578000
H	-2.970462000	4.497402000	0.098325000
H	-2.117774000	4.042103000	-1.372019000
C	-4.715077000	2.567990000	0.229336000
H	-5.232599000	3.520559000	0.111272000
H	-5.417409000	1.772040000	-0.016037000
H	-4.419746000	2.461167000	1.272505000
C	-3.987430000	2.582352000	-2.154386000
H	-4.713562000	1.797255000	-2.363078000
H	-4.466942000	3.546562000	-2.329579000
H	-3.149796000	2.486624000	-2.846163000
C	4.680236000	2.723249000	-0.028938000
H	5.396415000	1.940604000	-0.276886000
H	5.148348000	3.685597000	-0.238476000
H	4.462905000	2.670661000	1.037124000
C	3.794648000	2.578315000	-2.353568000
H	4.219858000	3.548964000	-2.612783000
H	4.537792000	1.811514000	-2.570162000
H	2.916392000	2.411072000	-2.978422000
H	-0.081544000	3.289453000	-1.259506000
H	-0.055245000	4.614733000	-0.116887000
C	1.610659000	3.427846000	1.771147000
H	2.661033000	3.257689000	2.005280000
H	1.405007000	4.491954000	1.904923000
H	1.026245000	2.880307000	2.499116000

[1-adtH]<sup>+</sup>, T. E. = -5069.548323

Fe	0.042365000	-2.209265000	-0.280897000
Fe	0.040416000	0.181191000	0.836260000
C	0.070806000	-0.789627000	-1.340703000
O	0.121936000	-0.245129000	-2.361181000
C	-0.977378000	-2.409288000	3.026217000
C	1.522831000	-2.379816000	2.812586000
S	-1.501551000	-1.571327000	1.521048000
S	1.765630000	-1.486846000	1.267280000
C	-1.600405000	1.427690000	0.341911000
C	-2.844341000	3.513231000	0.032797000
C	1.380444000	1.614714000	0.031074000
C	1.945530000	3.744599000	-1.009018000
C	0.215852000	0.685646000	2.646640000
O	0.365806000	0.756283000	3.761858000
C	-0.376288000	3.503546000	-0.175801000
C	3.049419000	2.731960000	-1.311904000
C	-3.763137000	2.328636000	-0.228532000
N	0.277207000	-3.206232000	2.857039000
H	0.206594000	-3.727538000	1.970813000
C	1.233963000	-3.328362000	-1.030960000
O	2.000260000	-4.023328000	-1.507089000
H	-1.755590000	-3.112666000	3.311628000
H	-0.800539000	-1.722982000	3.852919000
H	2.354630000	-3.068557000	2.936690000
H	1.484810000	-1.714232000	3.673905000
C	-1.277648000	-3.210835000	-1.048108000
O	-2.052149000	-3.909792000	-1.492078000
C	-1.547573000	2.928662000	0.635278000
C	1.075476000	3.112125000	0.094143000
N	-2.763485000	1.184122000	-0.195379000
N	2.509166000	1.499530000	-0.614202000
C	3.354624000	0.335029000	-0.676959000
C	4.326097000	0.193808000	0.305979000
C	3.276252000	-0.562500000	-1.729299000
C	5.216008000	-0.864510000	0.245249000
H	4.364473000	0.906128000	1.120640000
C	4.166880000	-1.628383000	-1.779065000
H	2.532034000	-0.429598000	-2.501086000
C	5.133719000	-1.780953000	-0.796273000
H	5.968258000	-0.978359000	1.014449000
H	4.101953000	-2.337773000	-2.592869000
H	5.826690000	-2.610689000	-0.843827000
C	-3.236844000	-0.035726000	-0.799486000
C	-4.118017000	-0.863815000	-0.119063000

C	-2.958947000	-0.252840000	-2.142365000
C	-4.724680000	-1.915333000	-0.792473000
H	-4.320917000	-0.690011000	0.927689000
C	-3.565584000	-1.306758000	-2.808496000
H	-2.286684000	0.417031000	-2.660392000
C	-4.458483000	-2.131162000	-2.137087000
H	-5.409507000	-2.563612000	-0.262145000
H	-3.347203000	-1.475285000	-3.854646000
H	-4.936059000	-2.950151000	-2.658454000
C	-1.510380000	3.262712000	2.129413000
H	-1.493464000	4.347959000	2.245800000
H	-2.406481000	2.887874000	2.625897000
H	-0.651216000	2.869438000	2.654359000
H	2.354215000	4.705939000	-0.698761000
H	1.349615000	3.912207000	-1.906376000
H	-3.310939000	4.238418000	0.697748000
H	-2.629891000	4.019186000	-0.909143000
C	-4.796763000	2.126555000	0.876781000
H	-5.414650000	3.022633000	0.941949000
H	-5.452645000	1.284506000	0.659571000
H	-4.320436000	1.961859000	1.843587000
C	-4.458154000	2.435134000	-1.578326000
H	-5.121200000	1.590565000	-1.765501000
H	-5.057966000	3.346261000	-1.575289000
H	-3.733537000	2.505976000	-2.390103000
C	4.418417000	3.137328000	-0.774435000
H	5.174039000	2.387735000	-1.006783000
H	4.709110000	4.069687000	-1.259295000
H	4.410586000	3.302286000	0.301944000
C	3.151766000	2.448997000	-2.807462000
H	3.383368000	3.383597000	-3.319773000
H	3.943128000	1.734004000	-3.031090000
H	2.204919000	2.067700000	-3.193189000
H	-0.583391000	3.256631000	-1.222349000
H	-0.436093000	4.595861000	-0.107257000
C	1.595326000	3.591798000	1.465454000
H	2.684014000	3.596842000	1.472960000
H	1.248951000	4.610304000	1.649924000
H	1.277487000	2.967997000	2.295098000
H	0.352206000	-3.886256000	3.617539000

**TS1<sub>[1]</sub><sup>0</sup>**, T. E. = -5069.540844

Fe	-0.032842000	-2.369634000	-0.117579000
Fe	0.025032000	0.269341000	0.823523000

C	-0.011725000	-1.220145000	-1.529205000
O	0.044979000	-0.737227000	-2.562353000
C	-1.070479000	-2.362073000	2.953908000
C	1.370405000	-2.393692000	2.788548000
S	-1.574695000	-1.400847000	1.470244000
S	1.690334000	-1.419733000	1.263008000
C	-1.554406000	1.549376000	0.265114000
C	-2.726989000	3.668633000	-0.084223000
C	1.418962000	1.658444000	0.060258000
C	2.147378000	3.835646000	-0.759934000
C	0.184480000	0.729595000	2.649746000
O	0.306849000	0.749431000	3.774374000
C	-0.240485000	3.620115000	-0.102169000
C	3.225701000	2.796901000	-1.078942000
C	-3.664286000	2.507705000	-0.410988000
N	0.127923000	-3.144119000	2.693764000
H	0.036313000	-3.347084000	1.302125000
C	1.251501000	-3.555102000	-0.643609000
O	2.076449000	-4.294147000	-0.903778000
H	-1.895349000	-3.045977000	3.183598000
H	-0.926405000	-1.684649000	3.808206000
H	2.201726000	-3.100689000	2.890207000
H	1.367212000	-1.725872000	3.662483000
C	-1.404783000	-3.512787000	-0.547186000
O	-2.248759000	-4.253803000	-0.722250000
C	-1.485130000	3.043267000	0.597019000
C	1.182590000	3.162853000	0.241097000
N	-2.699394000	1.338763000	-0.333157000
N	2.557876000	1.531985000	-0.575053000
C	3.281781000	0.308732000	-0.811538000
C	4.272070000	-0.069733000	0.095398000
C	3.054520000	-0.438078000	-1.964841000
C	5.017561000	-1.221128000	-0.139869000
H	4.430872000	0.523671000	0.996376000
C	3.788561000	-1.603968000	-2.183892000
H	2.312094000	-0.104623000	-2.687187000
C	4.767778000	-1.996888000	-1.272206000
H	5.783894000	-1.522955000	0.574905000
H	3.597267000	-2.200908000	-3.076604000
H	5.341406000	-2.907880000	-1.447784000
C	-3.156078000	0.119068000	-0.948150000
C	-4.046404000	-0.725944000	-0.283312000
C	-2.802241000	-0.127948000	-2.272621000
C	-4.555292000	-1.840714000	-0.945566000
H	-4.313941000	-0.524107000	0.752423000
C	-3.306795000	-1.250604000	-2.927497000

H	-2.127937000	0.559343000	-2.783749000
C	-4.185450000	-2.106098000	-2.264817000
H	-5.238404000	-2.511178000	-0.422892000
H	-3.016144000	-1.449056000	-3.959801000
H	-4.582356000	-2.984406000	-2.775491000
C	-1.561093000	3.328879000	2.103895000
H	-1.474270000	4.413304000	2.265276000
H	-2.531022000	3.005473000	2.506602000
H	-0.782573000	2.847331000	2.696603000
H	2.579281000	4.761095000	-0.355931000
H	1.609437000	4.096834000	-1.681935000
H	-3.217555000	4.414147000	0.555020000
H	-2.437057000	4.174083000	-1.016073000
C	-4.769992000	2.318548000	0.628700000
H	-5.384812000	3.228679000	0.659194000
H	-5.426835000	1.479011000	0.364601000
H	-4.355936000	2.142510000	1.631135000
C	-4.272174000	2.639874000	-1.803181000
H	-4.939583000	1.800560000	-2.041220000
H	-4.862223000	3.566912000	-1.831151000
H	-3.491261000	2.707329000	-2.573702000
C	4.552933000	3.048030000	-0.361860000
H	5.297506000	2.283641000	-0.620730000
H	4.942149000	4.021589000	-0.690088000
H	4.439778000	3.074741000	0.729676000
C	3.471086000	2.684866000	-2.582361000
H	3.822801000	3.659474000	-2.949294000
H	4.238321000	1.934370000	-2.816505000
H	2.543455000	2.430590000	-3.114955000
H	-0.381579000	3.434100000	-1.179983000
H	-0.270965000	4.717237000	0.019556000
C	1.618384000	3.541053000	1.671262000
H	2.703296000	3.422195000	1.786164000
H	1.369532000	4.596142000	1.856847000
H	1.146896000	2.940950000	2.453376000
H	0.153517000	-4.009549000	3.235457000

[1-*rH*]<sup>+</sup>, T. E. = -5069.560363

Fe	-0.000026000	-2.397525000	0.009907000
Fe	0.000015000	0.218637000	0.872585000
C	0.000037000	-0.941489000	-1.290741000
O	0.000090000	-0.470786000	-2.312696000
C	-1.213842000	-2.200821000	3.175256000
C	1.213766000	-2.200877000	3.175262000



S	-1.600401000	-1.456088000	1.517221000
S	1.600367000	-1.456152000	1.517233000
C	-1.496844000	1.545714000	0.145940000
C	-2.452113000	3.703817000	-0.475527000
C	1.496897000	1.545692000	0.145968000
C	2.452187000	3.703786000	-0.475497000
C	0.000043000	0.769334000	2.677700000
O	0.000092000	0.871278000	3.799208000
C	0.000035000	3.555619000	-0.146161000
C	3.451958000	2.599949000	-0.798113000
C	-3.451901000	2.599990000	-0.798120000
N	-0.000055000	-2.933758000	3.337944000
H	-0.000073000	-3.768667000	2.765497000
C	1.383336000	-3.354948000	-0.811283000
O	2.194641000	-4.039034000	-1.179671000
H	-2.054779000	-2.859918000	3.377318000
H	-1.242032000	-1.384357000	3.897310000
H	2.054672000	-2.860013000	3.377324000
H	1.241992000	-1.384417000	3.897319000
C	-1.383426000	-3.354894000	-0.811289000
O	-2.194779000	-4.038916000	-1.179690000
C	-1.348968000	3.051477000	0.385294000
C	1.349022000	3.051457000	0.385308000
N	-2.613502000	1.367529000	-0.503122000
N	2.613559000	1.367495000	-0.503084000
C	3.197051000	0.122181000	-0.938000000
C	4.109122000	-0.529056000	-0.120048000
C	2.972929000	-0.321301000	-2.235113000
C	4.784439000	-1.642733000	-0.598301000
H	4.279878000	-0.167664000	0.884023000
C	3.646163000	-1.439137000	-2.706185000
H	2.295829000	0.222500000	-2.878528000
C	4.555939000	-2.097326000	-1.889424000
H	5.490284000	-2.153810000	0.042516000
H	3.468176000	-1.784637000	-3.715775000
H	5.084034000	-2.966469000	-2.258594000
C	-3.197036000	0.122225000	-0.938010000
C	-4.109172000	-0.528934000	-0.120068000
C	-2.972903000	-0.321309000	-2.235104000
C	-4.784538000	-1.642587000	-0.598307000
H	-4.279948000	-0.167493000	0.883982000
C	-3.646183000	-1.439124000	-2.706161000
H	-2.295743000	0.222426000	-2.878511000
C	-4.556023000	-2.097234000	-1.889408000
H	-5.490437000	-2.153601000	0.042502000
H	-3.468182000	-1.784667000	-3.715733000

H	-5.084160000	-2.966357000	-2.258568000
C	-1.613849000	3.412554000	1.854394000
H	-1.459038000	4.485420000	1.982955000
H	-2.646113000	3.189990000	2.122101000
H	-0.978621000	2.902697000	2.565439000
H	2.928977000	4.537199000	0.038403000
H	2.029055000	4.087368000	-1.404365000
H	-2.928890000	4.537240000	0.038366000
H	-2.028976000	4.087386000	-1.404399000
C	-4.685576000	2.608413000	0.101241000
H	-5.202432000	3.559247000	-0.030180000
H	-5.376818000	1.811090000	-0.170317000
H	-4.423945000	2.499402000	1.152934000
C	-3.881633000	2.643597000	-2.258323000
H	-4.604129000	1.863778000	-2.496732000
H	-4.353307000	3.610388000	-2.438853000
H	-3.023161000	2.554714000	-2.924857000
C	4.685677000	2.608383000	0.101188000
H	5.376920000	1.811077000	-0.170414000
H	5.202509000	3.559227000	-0.030251000
H	4.424105000	2.499357000	1.152893000
C	3.881627000	2.643537000	-2.258335000
H	4.353298000	3.610323000	-2.438900000
H	4.604107000	1.863711000	-2.496766000
H	3.023123000	2.554650000	-2.924829000
H	0.000038000	3.355657000	-1.222629000
H	0.000041000	4.646787000	-0.043153000
C	1.613864000	3.412526000	1.854418000
H	2.646100000	3.189900000	2.122180000
H	1.459114000	4.485404000	1.982958000
H	0.978563000	2.902721000	2.565436000
H	-0.000056000	-3.720735000	0.748755000

[1- $\tau$ H]<sup>0</sup>, T. E. = -5069.691710

Fe	-0.000070000	-2.540751000	0.024699000
Fe	0.000055000	0.217158000	0.784278000
C	0.000000000	-0.715063000	-1.042871000
O	0.000055000	-0.439854000	-2.180556000
C	-1.216584000	-2.202300000	3.179485000
C	1.216976000	-2.202410000	3.179272000
S	-1.629452000	-1.512529000	1.512706000
S	1.629590000	-1.512611000	1.512442000
C	-1.497745000	1.562298000	0.140181000
C	-2.451690000	3.721303000	-0.495660000

C	1.497681000	1.562387000	0.139980000
C	2.451169000	3.721404000	-0.496460000
C	0.000268000	0.723400000	2.652855000
O	0.000440000	0.794554000	3.780402000
C	-0.000204000	3.568976000	-0.180279000
C	3.462561000	2.619228000	-0.789609000
C	-3.462943000	2.619014000	-0.788855000
N	0.000176000	-2.951190000	3.330719000
H	0.000083000	-3.719252000	2.666051000
C	1.347821000	-3.371260000	-0.934895000
O	2.147126000	-3.995809000	-1.433940000
H	-2.053860000	-2.853940000	3.424039000
H	-1.215710000	-1.380216000	3.896443000
H	2.054238000	-2.854137000	3.423643000
H	1.216318000	-1.380348000	3.896257000
C	-1.348147000	-3.371123000	-0.934768000
O	-2.147518000	-3.995644000	-1.433741000
C	-1.345378000	3.071103000	0.360765000
C	1.345161000	3.071210000	0.360358000
N	-2.634091000	1.387028000	-0.480860000
N	2.634018000	1.387168000	-0.481092000
C	3.235635000	0.142145000	-0.888300000
C	4.169509000	-0.466499000	-0.063152000
C	3.004273000	-0.344730000	-2.167882000
C	4.873132000	-1.571990000	-0.519719000
H	4.332619000	-0.080114000	0.932914000
C	3.707656000	-1.451724000	-2.618352000
H	2.284988000	0.149402000	-2.804441000
C	4.646688000	-2.062550000	-1.797679000
H	5.594744000	-2.050832000	0.128729000
H	3.521260000	-1.835009000	-3.612914000
H	5.193807000	-2.926711000	-2.151157000
C	-3.235509000	0.142020000	-0.888414000
C	-4.169292000	-0.467025000	-0.063462000
C	-3.004118000	-0.344381000	-2.168174000
C	-4.872784000	-1.572451000	-0.520406000
H	-4.332464000	-0.080984000	0.932724000
C	-3.707385000	-1.451286000	-2.619031000
H	-2.284894000	0.150058000	-2.804567000
C	-4.646331000	-2.062510000	-1.798553000
H	-5.594326000	-2.051607000	0.127888000
H	-3.520973000	-1.834191000	-3.613736000
H	-5.193356000	-2.926609000	-2.152326000
C	-1.596035000	3.434433000	1.831687000
H	-1.398080000	4.499091000	1.972607000
H	-2.636585000	3.250168000	2.097026000

H	-0.982587000	2.884994000	2.533237000
H	2.914399000	4.568466000	0.008554000
H	2.034438000	4.084853000	-1.436652000
H	-2.914965000	4.568164000	0.009648000
H	-2.035231000	4.085045000	-1.435861000
C	-4.693369000	2.665689000	0.114727000
H	-5.195413000	3.622623000	-0.031543000
H	-5.398565000	1.874697000	-0.138734000
H	-4.429337000	2.570785000	1.167231000
C	-3.902095000	2.639465000	-2.247700000
H	-4.633027000	1.861311000	-2.465631000
H	-4.363911000	3.607422000	-2.447882000
H	-3.047636000	2.523716000	-2.915464000
C	4.693235000	2.666436000	0.113607000
H	5.398530000	1.875519000	-0.139808000
H	5.195028000	3.623433000	-0.033114000
H	4.429534000	2.571819000	1.166219000
C	3.901294000	2.639318000	-2.248587000
H	4.362863000	3.607303000	-2.449205000
H	4.632316000	1.861240000	-2.466484000
H	3.046661000	2.523191000	-2.916064000
H	-0.000365000	3.349441000	-1.253208000
H	-0.000231000	4.662404000	-0.095637000
C	1.596251000	3.434697000	1.831174000
H	2.636872000	3.250438000	2.096238000
H	1.398355000	4.499375000	1.972026000
H	0.982987000	2.885347000	2.532955000
H	-0.000091000	-3.971063000	0.717856000

[1-*t*H-*adt*H]<sup>+</sup>, T. E. = -5070.131403

Fe	0.000371000	-2.544440000	0.015601000
Fe	-0.000174000	0.231972000	0.783110000
C	0.000258000	-0.709454000	-1.052566000
O	0.000328000	-0.450240000	-2.188408000
C	-1.259057000	-2.200661000	3.106630000
C	1.258208000	-2.199848000	3.107321000
S	-1.646425000	-1.501399000	1.485319000
S	1.646181000	-1.500799000	1.486063000
C	-1.500805000	1.579117000	0.143367000
C	-2.450966000	3.735855000	-0.494938000
C	1.500747000	1.579143000	0.143870000
C	2.451322000	3.735987000	-0.493588000
C	-0.001366000	0.750308000	2.664190000
O	-0.002368000	0.794677000	3.790719000

C	0.000116000	3.583114000	-0.179247000
C	3.464532000	2.635222000	-0.785558000
C	-3.464213000	2.635134000	-0.786920000
N	-0.000177000	-2.997845000	3.136541000
H	0.000231000	-3.597620000	2.271215000
C	1.360022000	-3.373168000	-0.983147000
O	2.148789000	-3.984251000	-1.503648000
H	-2.060997000	-2.883272000	3.376731000
H	-1.179224000	-1.434514000	3.876076000
H	2.060406000	-2.881861000	3.378157000
H	1.177366000	-1.433538000	3.876505000
C	-1.358532000	-3.373510000	-0.983885000
O	-2.146907000	-3.984672000	-1.504886000
C	-1.344965000	3.086740000	0.362848000
C	1.344922000	3.086720000	0.363575000
N	-2.636458000	1.401508000	-0.474419000
N	2.636496000	1.401592000	-0.473767000
C	3.238383000	0.155597000	-0.877393000
C	4.173829000	-0.448939000	-0.050466000
C	3.007486000	-0.333915000	-2.156623000
C	4.875100000	-1.557714000	-0.502895000
H	4.342256000	-0.055915000	0.942550000
C	3.711094000	-1.442118000	-2.603180000
H	2.293135000	0.161833000	-2.797680000
C	4.648334000	-2.051908000	-1.779358000
H	5.599129000	-2.032769000	0.145511000
H	3.527858000	-1.826062000	-3.597953000
H	5.196817000	-2.915795000	-2.131054000
C	-3.238453000	0.155413000	-0.877550000
C	-4.174161000	-0.448523000	-0.050483000
C	-3.007278000	-0.334900000	-2.156419000
C	-4.875410000	-1.557518000	-0.502390000
H	-4.342766000	-0.054889000	0.942266000
C	-3.710847000	-1.443345000	-2.602445000
H	-2.292732000	0.160392000	-2.797608000
C	-4.648328000	-2.052557000	-1.778472000
H	-5.599636000	-2.032114000	0.146133000
H	-3.527379000	-1.827936000	-3.596925000
H	-5.196782000	-2.916630000	-2.129759000
C	-1.596350000	3.452595000	1.833255000
H	-1.396701000	4.517033000	1.971392000
H	-2.637141000	3.270535000	2.098567000
H	-0.983435000	2.906856000	2.538497000
H	2.913122000	4.583605000	0.011244000
H	2.034762000	4.098416000	-1.434003000
H	-2.912861000	4.583687000	0.009448000

H	-2.033992000	4.097935000	-1.435306000
C	-4.695151000	2.683884000	0.115302000
H	-5.194852000	3.641416000	-0.033778000
H	-5.402008000	1.894518000	-0.138375000
H	-4.433034000	2.591424000	1.168520000
C	-3.899949000	2.649660000	-2.246477000
H	-4.631532000	1.871768000	-2.462931000
H	-4.360975000	3.617061000	-2.450173000
H	-3.044442000	2.532304000	-2.912491000
C	4.695146000	2.683444000	0.117141000
H	5.402067000	1.894194000	-0.136719000
H	5.194943000	3.641035000	-0.031226000
H	4.432650000	2.590387000	1.170212000
C	3.900834000	2.650239000	-2.244939000
H	4.362061000	3.617660000	-2.448091000
H	4.632404000	1.872337000	-2.461405000
H	3.045577000	2.533244000	-2.911335000
H	0.000420000	3.362968000	-1.251816000
H	0.000095000	4.676184000	-0.095339000
C	1.595684000	3.452236000	1.834190000
H	2.636778000	3.271723000	2.099338000
H	1.394329000	4.516267000	1.972996000
H	0.983793000	2.904999000	2.539176000
H	0.000427000	-3.971240000	0.764973000
H	-0.000220000	-3.601147000	3.960669000

**TS2<sub>[1]</sub><sup>0</sup>**, T. E. = -5070.130205

Fe	0.010019000	-2.548381000	0.132134000
Fe	0.000490000	0.214339000	0.796245000
C	0.007750000	-0.764387000	-1.044391000
O	0.012864000	-0.637830000	-2.191022000
C	-1.229467000	-2.193863000	3.168337000
C	1.241647000	-2.187053000	3.170148000
S	-1.650010000	-1.474429000	1.546443000
S	1.661138000	-1.464671000	1.549226000
C	-1.498855000	1.558563000	0.152450000
C	-2.484253000	3.717686000	-0.416713000
C	1.481636000	1.575034000	0.140653000
C	2.422006000	3.744581000	-0.463701000
C	-0.000152000	0.741220000	2.672971000
O	0.001171000	0.799222000	3.798004000
C	-0.026735000	3.585576000	-0.113505000
C	3.428279000	2.649712000	-0.798683000
C	-3.476037000	2.609059000	-0.748030000

N	0.008254000	-2.978913000	3.153257000
H	0.010883000	-3.595739000	1.980304000
C	1.388790000	-3.343393000	-0.895453000
O	2.186538000	-3.907611000	-1.450295000
H	-1.171086000	-1.412370000	3.927149000
H	-2.042138000	-2.867094000	3.430368000
H	1.177980000	-1.406104000	3.929127000
H	2.057606000	-2.855916000	3.433127000
C	-1.361584000	-3.348818000	-0.900592000
O	-2.154703000	-3.915844000	-1.459180000
C	-1.366289000	3.061051000	0.421174000
C	1.328226000	3.077517000	0.397097000
N	-2.619424000	1.381881000	-0.490253000
N	2.601382000	1.410075000	-0.506839000
C	3.191870000	0.172166000	-0.951423000
C	2.958613000	-0.268166000	-2.248224000
C	4.815427000	-1.565854000	-0.640717000
C	4.121878000	-0.469589000	-0.146658000
H	2.247650000	0.255597000	-2.871138000
C	3.654418000	-1.363358000	-2.736253000
H	5.536272000	-2.069241000	-0.010465000
C	4.588085000	-2.008701000	-1.935505000
H	3.469832000	-1.707847000	-3.745068000
H	5.131969000	-2.861747000	-2.319261000
H	4.296236000	-0.112136000	0.858397000
C	-3.182777000	0.142863000	-0.965756000
C	-4.111330000	-0.533431000	-0.187766000
C	-2.927721000	-0.261895000	-2.269893000
C	-4.781872000	-1.627500000	-0.717331000
H	-4.302704000	-0.204448000	0.823691000
C	-3.599790000	-1.355645000	-2.793126000
H	-2.218752000	0.289189000	-2.871246000
C	-4.533041000	-2.034327000	-2.020028000
H	-5.502071000	-2.157428000	-0.108458000
H	-3.398216000	-1.671715000	-3.807972000
H	-5.059319000	-2.885641000	-2.431158000
C	-1.618145000	3.393174000	1.898950000
H	-1.481361000	4.466485000	2.043782000
H	-2.642384000	3.147148000	2.177262000
H	-0.962624000	2.883414000	2.591430000
H	2.894511000	4.578762000	0.053242000
H	1.991239000	4.130363000	-1.388203000
H	-2.963804000	4.538123000	0.115391000
H	-2.074004000	4.120032000	-1.343550000
C	-4.697277000	2.586781000	0.168326000
H	-5.221525000	3.537700000	0.070385000

H	-5.387952000	1.793211000	-0.115318000
H	-4.420407000	2.450016000	1.212993000
C	-3.927415000	2.677980000	-2.200786000
H	-4.643184000	1.893651000	-2.445032000
H	-4.413140000	3.642408000	-2.355358000
H	-3.077433000	2.612088000	-2.880597000
C	4.669731000	2.665538000	0.090093000
H	5.367470000	1.878272000	-0.193909000
H	5.174770000	3.623230000	-0.037983000
H	4.419150000	2.544865000	1.143212000
C	3.846725000	2.705381000	-2.262063000
H	4.309351000	3.676844000	-2.441447000
H	4.572963000	1.932094000	-2.510336000
H	2.983453000	2.612343000	-2.921783000
H	-0.035553000	3.404155000	-1.193085000
H	-0.032022000	4.674864000	0.009123000
C	1.605689000	3.416472000	1.869427000
H	2.646337000	3.211760000	2.118112000
H	1.428934000	4.482739000	2.023127000
H	0.992822000	2.875243000	2.577462000
H	0.012790000	-4.006647000	1.056868000
H	0.009563000	-3.650876000	3.916873000

[1-H<sub>2</sub>]<sup>+</sup>, T. E. = -5070.161306

Fe	-0.468590000	-2.834725000	0.068450000
Fe	0.068806000	0.224035000	0.636695000
C	-0.014050000	-0.283178000	-1.232733000
O	0.057527000	-0.431729000	-2.344394000
C	-1.136788000	-1.890860000	3.199318000
C	1.260635000	-2.292718000	2.850300000
S	-1.677505000	-1.327528000	1.539606000
S	1.454247000	-1.782064000	1.101091000
C	-1.391784000	1.699359000	0.231734000
C	-2.362148000	3.906976000	-0.123966000
C	1.602767000	1.538779000	0.004726000
C	2.493391000	3.610715000	-0.889787000
C	0.411352000	0.688526000	2.466092000
O	0.685834000	0.845176000	3.545143000
C	0.101468000	3.624697000	-0.203102000
C	3.493585000	2.485570000	-1.152818000
C	-3.420833000	2.840246000	-0.378401000
N	-0.041236000	-2.832266000	3.171786000
C	0.601044000	-3.533872000	-1.291473000
O	1.240264000	-3.915558000	-2.142115000



H	-2.000878000	-2.400454000	3.621460000
H	-0.939479000	-1.012534000	3.822352000
H	1.993949000	-3.083876000	2.998596000
H	1.551225000	-1.451229000	3.487915000
C	-2.021805000	-3.503143000	-0.735521000
O	-2.926259000	-3.999991000	-1.193119000
C	-1.171204000	3.178671000	0.536775000
C	1.480853000	3.057878000	0.132479000
N	-2.566976000	1.584173000	-0.317213000
N	2.739283000	1.298827000	-0.584282000
C	3.394348000	0.020415000	-0.698168000
C	4.282182000	-0.344851000	0.303758000
C	3.207981000	-0.782619000	-1.810621000
C	4.980555000	-1.535479000	0.197266000
H	4.403875000	0.296137000	1.167717000
C	3.900372000	-1.984312000	-1.903272000
H	2.545394000	-0.469537000	-2.605019000
C	4.785464000	-2.360098000	-0.903731000
H	5.667812000	-1.825443000	0.980755000
H	3.751354000	-2.619181000	-2.766018000
H	5.326239000	-3.293724000	-0.983916000
C	-3.168007000	0.408663000	-0.895588000
C	-4.117101000	-0.316538000	-0.187340000
C	-2.924056000	0.131874000	-2.233899000
C	-4.816071000	-1.329550000	-0.827187000
H	-4.298318000	-0.093383000	0.853400000
C	-3.617701000	-0.890834000	-2.864704000
H	-2.217423000	0.737159000	-2.785636000
C	-4.572127000	-1.614373000	-2.163904000
H	-5.551928000	-1.899069000	-0.275363000
H	-3.423998000	-1.105286000	-3.907105000
H	-5.119644000	-2.407020000	-2.656103000
C	-1.188500000	3.482654000	2.040446000
H	-0.861385000	4.511642000	2.200641000
H	-2.201703000	3.391500000	2.429845000
H	-0.559076000	2.837123000	2.637983000
H	2.986491000	4.510179000	-0.522925000
H	1.983123000	3.866785000	-1.818984000
H	-2.744834000	4.712613000	0.500761000
H	-2.058192000	4.342659000	-1.076462000
C	-4.492405000	2.771950000	0.706835000
H	-4.994533000	3.738020000	0.762150000
H	-5.243518000	2.018783000	0.471093000
H	-4.064697000	2.544213000	1.682751000
C	-4.074324000	3.007898000	-1.742570000
H	-4.828889000	2.244475000	-1.931131000

H	-4.563056000	3.982830000	-1.761073000
H	-3.333205000	2.983503000	-2.542137000
C	4.839806000	2.678670000	-0.462124000
H	5.510064000	1.843956000	-0.663922000
H	5.298693000	3.582500000	-0.863302000
H	4.742951000	2.796910000	0.615636000
C	3.713977000	2.268883000	-2.646097000
H	4.113743000	3.191108000	-3.069299000
H	4.427994000	1.468626000	-2.838538000
H	2.773753000	2.039852000	-3.150376000
H	-0.077263000	3.424103000	-1.264593000
H	0.166386000	4.714635000	-0.110048000
C	1.956185000	3.445315000	1.545563000
H	2.995339000	3.156524000	1.695424000
H	1.886027000	4.529322000	1.649827000
H	1.377384000	2.998309000	2.343536000
H	-0.344268000	-4.875812000	0.917976000
H	0.003862000	-3.334341000	4.051644000
H	-0.305059000	-4.442246000	1.534844000

[2]<sup>0</sup>, T. E. = -5101.950177

C	2.312987000	-0.089744000	3.217150000
P	2.483675000	-1.112382000	1.721668000
C	4.276962000	-1.040910000	1.304723000
C	4.544469000	0.120731000	0.341801000
P	3.360761000	0.043291000	-1.062976000
Fe	1.291085000	-0.470544000	-0.161638000
C	1.287701000	-2.197122000	-0.847822000
O	1.282917000	-3.241197000	-1.276482000
C	4.109131000	-1.172672000	-2.197124000
C	3.583784000	1.610606000	-1.954466000
S	0.051244000	0.423179000	-2.020785000
Fe	-0.372227000	1.516177000	0.113940000
C	-1.051412000	2.202294000	1.643923000
O	-1.468483000	2.603749000	2.620769000
S	-0.817696000	-0.719212000	0.966330000
C	-1.920620000	-1.642612000	-0.203799000
C	-1.300155000	-0.796777000	-2.386176000
C	1.342285000	1.585351000	0.584619000
O	2.153164000	2.310868000	1.033934000
C	2.244095000	-2.798174000	2.364601000
H	4.367633000	1.076910000	0.839574000
H	-1.405945000	-2.565730000	-0.473439000

H	-2.804051000	-1.900592000	0.377020000
H	-0.819482000	-1.757856000	-2.575186000
H	-1.756619000	-0.451421000	-3.312832000
H	4.879685000	-0.960103000	2.210914000
H	4.172397000	-2.146914000	-1.711572000
H	3.474538000	-1.269639000	-3.079038000
H	5.106982000	-0.858091000	-2.503428000
H	3.276061000	2.437587000	-1.316463000
H	4.625042000	1.741263000	-2.250002000
H	2.952166000	1.596528000	-2.843074000
H	2.868981000	-0.528791000	4.045517000
H	2.680450000	0.914868000	3.015642000
H	1.255564000	-0.027250000	3.479352000
H	1.213519000	-2.894023000	2.707355000
H	2.417252000	-3.526590000	1.572534000
H	2.921887000	-2.999408000	3.194496000
C	-0.445785000	3.109047000	-0.732056000
O	-0.463781000	4.099893000	-1.286958000
N	-2.332630000	-0.987748000	-1.411241000
H	5.573274000	0.113079000	-0.022419000
H	4.527883000	-1.993874000	0.830768000
C	-3.244224000	0.139262000	-1.256395000
H	-2.765815000	0.996898000	-0.767703000
H	-3.521892000	0.460041000	-2.263995000
C	-4.481542000	-0.238678000	-0.483267000
C	-4.753571000	0.342702000	0.749655000
C	-5.364390000	-1.190408000	-0.990105000
C	-5.891235000	-0.013678000	1.466140000
H	-4.065035000	1.076883000	1.153347000
C	-6.499339000	-1.549615000	-0.279324000
H	-5.150504000	-1.652159000	-1.947192000
C	-6.765609000	-0.960486000	0.952905000
H	-6.089872000	0.446112000	2.425786000
H	-7.179768000	-2.287634000	-0.684768000
H	-7.651279000	-1.240615000	1.508532000

**[2-adtH(a)]<sup>+</sup>**, T. E. = -5102.371567

C	2.302604000	0.006158000	3.206146000
P	2.494566000	-1.054045000	1.740843000
C	4.284128000	-0.968576000	1.322160000
C	4.547023000	0.185506000	0.349839000
P	3.380684000	0.081050000	-1.064827000
Fe	1.292145000	-0.465580000	-0.174412000
C	1.399485000	-2.208774000	-0.832813000

O	1.455332000	-3.257889000	-1.238170000
C	4.141346000	-1.150735000	-2.171104000
C	3.590416000	1.632978000	-1.983996000
S	0.048864000	0.427710000	-2.021971000
Fe	-0.390130000	1.505130000	0.123493000
C	-1.061730000	2.155887000	1.697048000
O	-1.472391000	2.533241000	2.681604000
S	-0.828424000	-0.773095000	0.906223000
C	-1.851048000	-1.733746000	-0.222776000
C	-1.209863000	-0.781244000	-2.477279000
C	1.317205000	1.681422000	0.544614000
O	2.157289000	2.382015000	0.952501000
C	2.266945000	-2.726817000	2.416581000
H	4.365852000	1.146330000	0.836134000
H	-1.328999000	-2.631828000	-0.549596000
H	-2.755708000	-2.032453000	0.301026000
H	-0.748023000	-1.746324000	-2.680333000
H	-1.706834000	-0.437575000	-3.381676000
H	4.881027000	-0.871954000	2.230388000
H	4.220655000	-2.114218000	-1.666942000
H	3.513316000	-1.273123000	-3.054460000
H	5.135332000	-0.825814000	-2.478558000
H	3.278993000	2.472875000	-1.365757000
H	4.632341000	1.760956000	-2.277854000
H	2.965576000	1.597873000	-2.876762000
H	2.879185000	-0.396337000	4.038897000
H	2.641754000	1.015028000	2.978309000
H	1.247763000	0.045473000	3.481969000
H	1.238609000	-2.827043000	2.764285000
H	2.449316000	-3.470912000	1.641558000
H	2.947940000	-2.900938000	3.249822000
C	-0.680679000	3.094104000	-0.700416000
O	-0.823150000	4.080864000	-1.240090000
N	-2.316566000	-1.062112000	-1.491204000
H	5.577162000	0.179112000	-0.010031000
H	4.546720000	-1.924785000	0.861684000
C	-3.241274000	0.115736000	-1.289452000
H	-2.660539000	0.906542000	-0.824861000
H	-3.528385000	0.431607000	-2.291840000
C	-4.435913000	-0.254592000	-0.461188000
C	-4.473103000	0.060387000	0.894507000
C	-5.512812000	-0.920258000	-1.041014000
C	-5.573143000	-0.292160000	1.663233000
H	-3.635215000	0.578918000	1.346046000
C	-6.611160000	-1.276535000	-0.271708000
H	-5.498910000	-1.149884000	-2.100830000

C	-6.640978000	-0.962997000	1.081186000
H	-5.596988000	-0.041301000	2.715362000
H	-7.446330000	-1.789625000	-0.729540000
H	-7.499528000	-1.236104000	1.680462000
H	-2.889623000	-1.777228000	-1.951045000

[2-*adt*H(b)]<sup>+</sup>, T. E. = -5102.378507

C	-3.506098000	2.166662000	-0.998653000
P	-3.369229000	0.353437000	-1.057634000
C	-4.750375000	-0.250732000	-0.003234000
C	-4.298448000	-0.365581000	1.455832000
P	-2.718361000	-1.298474000	1.535185000
Fe	-1.363582000	-0.504954000	-0.221473000
C	-1.510630000	-2.116260000	-1.149756000
O	-1.553055000	-3.075273000	-1.736830000
C	-3.238335000	-3.037481000	1.356361000
C	-2.192605000	-1.235961000	3.273613000
S	0.642338000	-0.877730000	0.956326000
Fe	0.269730000	1.447985000	0.363116000
C	-0.064630000	3.139297000	-0.321816000
O	-0.272645000	4.158329000	-0.760466000
S	-0.091756000	0.572935000	-1.879825000
C	1.333779000	-0.443482000	-2.318648000
C	1.951958000	-1.484469000	-0.129353000
C	-1.123343000	1.545333000	1.431925000
O	-1.913852000	1.855994000	2.214625000
C	-3.883060000	-0.045945000	-2.754360000
H	-4.105855000	0.622539000	1.879330000
H	1.052081000	-1.460336000	-2.587730000
H	1.829019000	0.022121000	-3.166758000
H	1.670344000	-2.420781000	-0.608861000
H	2.836881000	-1.648240000	0.479723000
H	-5.614793000	0.407500000	-0.104033000
H	-3.719366000	-3.198432000	0.391363000
H	-2.357923000	-3.678741000	1.412919000
H	-3.932103000	-3.311425000	2.151180000
H	-1.963561000	-0.213349000	3.563981000
H	-2.979984000	-1.630516000	3.916096000
H	-1.295589000	-1.845222000	3.387049000
H	-4.477335000	2.488497000	-1.375150000
H	-3.378705000	2.515100000	0.025997000
H	-2.718823000	2.599761000	-1.617011000
H	-3.151303000	0.367349000	-3.448712000
H	-3.917919000	-1.127259000	-2.885478000

H	-4.864815000	0.376046000	-2.969558000
C	1.751727000	2.001534000	1.234202000
O	2.616655000	2.336093000	1.892844000
N	2.358710000	-0.547601000	-1.228053000
H	-5.057864000	-0.850900000	2.071290000
H	-5.041673000	-1.229859000	-0.391150000
C	3.715039000	-0.914240000	-1.788315000
H	3.641635000	-1.942622000	-2.139079000
C	4.801363000	-0.737072000	-0.767681000
C	5.423713000	-1.839663000	-0.191703000
C	5.186716000	0.546474000	-0.386854000
C	6.419053000	-1.661716000	0.759434000
H	5.129209000	-2.839393000	-0.489013000
C	6.173714000	0.724294000	0.570787000
H	4.722631000	1.412755000	-0.847047000
C	6.790956000	-0.380724000	1.143992000
H	6.901425000	-2.523522000	1.200956000
H	6.465972000	1.723887000	0.863417000
H	7.564731000	-0.242244000	1.887442000
H	3.872405000	-0.259939000	-2.644067000
H	2.425213000	0.391156000	-0.806745000

**TS1<sub>121</sub><sup>0</sup>**, T. E. = -5102.362919

C	-3.479516000	2.517369000	-0.551577000
P	-3.453733000	0.723896000	-0.855382000
C	-4.794494000	0.048704000	0.206429000
C	-4.245776000	-0.259275000	1.602543000
P	-2.730812000	-1.289458000	1.459572000
Fe	-1.477753000	-0.426748000	-0.330782000
C	-1.895992000	-1.835828000	-1.487334000
O	-2.087113000	-2.683430000	-2.199752000
C	-3.349584000	-2.985145000	1.230814000
C	-2.020615000	-1.331071000	3.130512000
S	0.503962000	-1.261791000	0.540675000
Fe	0.612149000	1.136602000	0.487779000
C	1.262640000	2.767419000	-0.037273000
O	1.698482000	3.738055000	-0.420336000
S	-0.245178000	0.926129000	-1.748818000
C	1.160590000	0.018640000	-2.498694000
C	1.719315000	-1.617347000	-0.783688000
C	1.855139000	0.986794000	1.829292000
O	2.642086000	0.846996000	2.627925000
C	-4.079006000	0.578278000	-2.554187000
H	-3.955491000	0.663241000	2.112718000

H	0.773057000	-0.825852000	-3.069633000
H	1.649710000	0.711119000	-3.179202000
H	1.299162000	-2.354545000	-1.469005000
H	2.590674000	-2.043825000	-0.293516000
H	-5.631555000	0.747232000	0.248885000
H	-3.935285000	-3.054247000	0.314261000
H	-2.498163000	-3.661905000	1.149576000
H	-3.968766000	-3.283761000	2.076455000
H	-1.709829000	-0.332413000	3.433111000
H	-2.753571000	-1.712354000	3.841814000
H	-1.147996000	-1.984354000	3.124882000
H	-4.412215000	2.943525000	-0.920912000
H	-3.391080000	2.718644000	0.514656000
H	-2.638404000	2.981669000	-1.068088000
H	-3.353331000	1.025674000	-3.233574000
H	-4.204976000	-0.472187000	-2.815200000
H	-5.034995000	1.091686000	-2.655649000
C	-0.842329000	1.609415000	1.463058000
O	-1.610133000	2.032419000	2.187603000
N	2.130018000	-0.413922000	-1.498889000
H	-4.989033000	-0.758732000	2.226056000
H	-5.155762000	-0.864769000	-0.274030000
H	1.893933000	0.581844000	-0.469058000
C	3.519913000	-0.474279000	-2.015205000
H	3.626435000	-1.329528000	-2.688780000
H	3.673207000	0.434881000	-2.596638000
C	4.529402000	-0.544091000	-0.900703000
C	4.764980000	0.576907000	-0.107480000
C	5.235674000	-1.714736000	-0.646662000
C	5.683991000	0.524276000	0.929309000
H	4.228944000	1.497552000	-0.310743000
C	6.159498000	-1.769768000	0.389658000
H	5.062254000	-2.588409000	-1.264407000
C	6.382240000	-0.651193000	1.180211000
H	5.858398000	1.400382000	1.540151000
H	6.703938000	-2.685799000	0.577823000
H	7.100957000	-0.692254000	1.988138000

[2-*t*H]<sup>+</sup>, T. E. = -5102.379396

C	3.142396000	-0.130398000	3.053981000
P	2.616074000	-1.227224000	1.705391000
C	4.176719000	-1.802717000	0.924557000
C	4.636902000	-0.801314000	-0.140698000
P	3.270427000	-0.458043000	-1.317465000

Fe	1.319133000	-0.342672000	-0.033421000
C	0.917085000	-2.131365000	-0.533251000
O	0.706035000	-3.192903000	-0.830939000
C	3.330181000	-1.806259000	-2.532592000
C	3.775428000	0.995349000	-2.276079000
S	-0.038881000	0.463686000	-1.845884000
Fe	-0.321368000	1.854520000	0.052756000
C	-0.516029000	2.821560000	1.639591000
O	-0.767019000	3.396479000	2.572877000
S	-0.687955000	-0.171018000	1.275614000
C	-1.953263000	-1.218163000	0.381444000
C	-1.501735000	-0.705702000	-1.946941000
C	2.029158000	1.363479000	0.505699000
O	2.729122000	2.182057000	0.841455000
C	1.925254000	-2.658540000	2.577427000
H	4.912682000	0.151141000	0.320218000
H	-1.522692000	-2.212781000	0.271704000
H	-2.790128000	-1.287443000	1.074181000
H	-1.083983000	-1.699722000	-2.107450000
H	-2.017883000	-0.404341000	-2.855174000
H	4.942570000	-1.950004000	1.687315000
H	3.252340000	-2.774182000	-2.038722000
H	2.496830000	-1.694993000	-3.227134000
H	4.269025000	-1.761341000	-3.083701000
H	3.885246000	1.865690000	-1.630879000
H	4.723039000	0.798532000	-2.777561000
H	3.006400000	1.200253000	-3.021499000
H	3.679950000	-0.709888000	3.803977000
H	3.794057000	0.656596000	2.677661000
H	2.263490000	0.325811000	3.510527000
H	1.026299000	-2.338256000	3.103876000
H	1.660673000	-3.447948000	1.875271000
H	2.651495000	-3.041837000	3.294012000
C	0.124768000	3.337033000	-0.990934000
O	0.270653000	4.227293000	-1.662376000
N	-2.426075000	-0.739919000	-0.871048000
H	5.513344000	-1.166487000	-0.677456000
H	3.976988000	-2.778754000	0.474355000
C	-3.463637000	0.278508000	-0.803592000
H	-3.179258000	1.102496000	-0.144143000
H	-3.576988000	0.700699000	-1.804474000
C	-4.785740000	-0.291865000	-0.338956000
C	-5.542797000	0.381749000	0.612733000
C	-5.275339000	-1.482867000	-0.870562000
C	-6.773967000	-0.117360000	1.023025000
H	-5.164386000	1.303801000	1.039226000



C	-6.501954000	-1.985108000	-0.462735000
H	-4.682115000	-2.017187000	-1.602967000
C	-7.256148000	-1.302010000	0.485701000
H	-7.351273000	0.416669000	1.766826000
H	-6.872699000	-2.910682000	-0.884479000
H	-8.212382000	-1.695357000	0.805486000
H	-1.662187000	2.469744000	-0.163977000

[2-*t*H]<sup>0</sup>, T. E. = -5102.518651

C	3.230625000	0.216983000	2.880063000
P	2.833988000	-1.038939000	1.622769000
C	4.451052000	-1.413957000	0.823111000
C	4.652437000	-0.504496000	-0.393599000
P	3.161368000	-0.568895000	-1.467665000
Fe	1.329619000	-0.481445000	-0.054283000
C	0.895383000	-2.324294000	-0.353422000
O	0.641456000	-3.404062000	-0.554625000
C	3.400844000	-2.076090000	-2.466349000
C	3.411667000	0.754917000	-2.688388000
S	-0.209582000	0.283721000	-1.764177000
Fe	-0.205247000	1.870607000	0.076956000
C	-0.277648000	2.947153000	1.577595000
O	-0.416081000	3.580488000	2.502789000
S	-0.474423000	-0.092846000	1.516818000
C	-1.892365000	-1.097890000	0.851082000
C	-1.733744000	-0.771284000	-1.565684000
C	1.833761000	1.489064000	0.207957000
O	2.796326000	2.144745000	0.342453000
C	2.484816000	-2.510252000	2.635886000
H	4.758725000	0.536288000	-0.077708000
H	-1.520795000	-2.118669000	0.737958000
H	-2.653562000	-1.105355000	1.630312000
H	-1.396810000	-1.803219000	-1.691198000
H	-2.377334000	-0.525855000	-2.408183000
H	5.267763000	-1.314568000	1.540185000
H	3.441834000	-2.952305000	-1.818743000
H	2.552189000	-2.188534000	-3.142358000
H	4.320326000	-2.016683000	-3.048877000
H	3.397201000	1.722184000	-2.188294000
H	4.361716000	0.626772000	-3.207644000
H	2.595165000	0.719652000	-3.410012000
H	3.897646000	-0.198311000	3.635515000
H	3.702929000	1.075544000	2.405932000
H	2.304180000	0.546226000	3.353061000

H	1.573134000	-2.329453000	3.205955000
H	2.327927000	-3.375477000	1.991886000
H	3.306584000	-2.715605000	3.322214000
C	-0.020455000	3.249592000	-1.139275000
O	0.002341000	4.071327000	-1.914242000
N	-2.488085000	-0.663546000	-0.365174000
H	5.546136000	-0.776991000	-0.957714000
H	4.415082000	-2.461939000	0.513017000
C	-3.548210000	0.311912000	-0.265003000
H	-3.370987000	0.982898000	0.579954000
H	-3.528820000	0.953351000	-1.148985000
C	-4.930904000	-0.302207000	-0.123770000
C	-6.010864000	0.528375000	0.174357000
C	-5.161207000	-1.661506000	-0.294179000
C	-7.292672000	0.013512000	0.291764000
H	-5.840266000	1.590274000	0.316292000
C	-6.445629000	-2.182806000	-0.173934000
H	-4.324299000	-2.310622000	-0.519454000
C	-7.514962000	-1.348743000	0.117402000
H	-8.119894000	0.672759000	0.522933000
H	-6.608561000	-3.244923000	-0.308183000
H	-8.514156000	-1.754022000	0.211624000
H	-1.700272000	2.308810000	-0.026256000

[2-*t*H-*adt*H(a)]<sup>+</sup>, T. E. = -5102.941146

C	2.341194000	-0.139717000	3.259636000
P	2.450932000	-1.163071000	1.758859000
C	4.241857000	-1.193924000	1.335367000
C	4.575943000	-0.057907000	0.363289000
P	3.399880000	-0.074952000	-1.047493000
Fe	1.292525000	-0.444358000	-0.134019000
C	1.269271000	-2.247530000	-0.829045000
O	1.295607000	-3.289810000	-1.252999000
C	4.069731000	-1.339383000	-2.174766000
C	3.713717000	1.471362000	-1.948047000
S	0.022749000	0.488096000	-1.998234000
Fe	-0.548135000	1.711333000	0.050260000
C	-0.989663000	2.470902000	1.697210000
O	-1.354156000	2.902556000	2.671138000
S	-0.888404000	-0.538168000	0.953759000
C	-1.859518000	-1.615120000	-0.119876000
C	-1.175329000	-0.792661000	-2.434525000
C	1.463283000	1.452718000	0.559158000
O	2.265514000	2.165656000	1.021950000

C	2.102952000	-2.833086000	2.390579000
H	4.462539000	0.911652000	0.853389000
H	-1.300912000	-2.527042000	-0.323894000
H	-2.776305000	-1.889150000	0.395385000
H	-0.655153000	-1.734591000	-2.600777000
H	-1.668873000	-0.507246000	-3.361058000
H	4.847768000	-1.137968000	2.241036000
H	4.084397000	-2.312231000	-1.683170000
H	3.428100000	-1.405929000	-3.054406000
H	5.081407000	-1.080035000	-2.486322000
H	3.439537000	2.323844000	-1.328794000
H	4.766392000	1.545529000	-2.221636000
H	3.104726000	1.479296000	-2.852276000
H	2.880501000	-0.615763000	4.078255000
H	2.762778000	0.845472000	3.069649000
H	1.291816000	-0.025143000	3.535908000
H	1.063058000	-2.874852000	2.715806000
H	2.254980000	-3.570554000	1.602675000
H	2.753205000	-3.069154000	3.232978000
C	-0.229785000	3.347645000	-0.794329000
O	-0.118239000	4.320522000	-1.349262000
N	-2.294982000	-1.111644000	-1.473454000
H	5.602152000	-0.130824000	-0.000724000
H	4.440242000	-2.163893000	0.872054000
C	-3.353969000	-0.030765000	-1.461920000
H	-2.856243000	0.885169000	-1.160274000
H	-3.678667000	0.054537000	-2.498159000
C	-4.498672000	-0.367361000	-0.554307000
C	-4.540405000	0.160394000	0.734189000
C	-5.518802000	-1.212376000	-0.983877000
C	-5.587732000	-0.160995000	1.585887000
H	-3.745930000	0.820751000	1.062859000
C	-6.564177000	-1.536593000	-0.130630000
H	-5.502646000	-1.610995000	-1.992375000
C	-6.597825000	-1.011899000	1.155158000
H	-5.616159000	0.253866000	2.584784000
H	-7.355293000	-2.191247000	-0.471417000
H	-7.414987000	-1.261303000	1.819285000
H	-2.021928000	2.153457000	-0.226978000
H	-2.753682000	-1.927605000	-1.890287000

[2-*t*H-*adt*H(b)]<sup>+</sup>, T. E. = -5102.959881

C	3.347950000	-0.486163000	2.637507000
P	2.354715000	-1.577333000	1.572364000

C	3.587189000	-2.600343000	0.667273000
C	3.973287000	-1.912071000	-0.645349000
P	2.456151000	-1.460183000	-1.574848000
Fe	0.977378000	-0.562400000	-0.018759000
C	-0.190853000	-2.099504000	-0.082787000
O	-0.896935000	-2.973072000	-0.130351000
C	1.956322000	-3.001813000	-2.405282000
C	3.036486000	-0.426625000	-2.951686000
S	-0.296928000	0.669432000	-1.651839000
Fe	0.494703000	2.239445000	0.036357000
C	1.065090000	3.338016000	1.459185000
O	1.333227000	3.993853000	2.331583000
S	-0.311517000	0.599759000	1.647963000
C	-2.065914000	0.433462000	1.241741000
C	-2.054011000	0.485690000	-1.264746000
C	2.233344000	1.093353000	-0.003792000
O	3.376407000	1.328037000	-0.037000000
C	1.595572000	-2.722239000	2.763415000
H	4.507130000	-0.979321000	-0.446613000
H	-2.357056000	-0.610057000	1.130135000
H	-2.637021000	0.868636000	2.058769000
H	-2.344664000	-0.561647000	-1.198025000
H	-2.618187000	0.954046000	-2.068113000
H	4.460065000	-2.789819000	1.294023000
H	1.729862000	-3.771201000	-1.667021000
H	1.056319000	-2.811420000	-2.991336000
H	2.746858000	-3.358659000	-3.065049000
H	3.465452000	0.496803000	-2.565397000
H	3.787157000	-0.958913000	-3.536110000
H	2.187922000	-0.182490000	-3.591223000
H	3.884542000	-1.072985000	3.382476000
H	4.058981000	0.074298000	2.033041000
H	2.685777000	0.219473000	3.141599000
H	0.896425000	-2.166280000	3.388472000
H	1.049204000	-3.502048000	2.233598000
H	2.357175000	-3.181349000	3.393904000
C	1.067997000	3.406454000	-1.330085000
O	1.339360000	4.103750000	-2.168604000
N	-2.483249000	1.157487000	0.001041000
H	4.620111000	-2.543796000	-1.256441000
H	3.113769000	-3.565358000	0.467454000
C	-3.962322000	1.461806000	0.001507000
H	-4.142912000	2.061680000	0.891745000
H	-4.140299000	2.080750000	-0.876095000
C	-4.820497000	0.227335000	-0.012797000
C	-5.237426000	-0.355202000	1.181825000

C	-5.217053000	-0.342084000	-1.220623000
C	-6.018564000	-1.501836000	1.169716000
H	-4.960500000	0.095353000	2.127675000
C	-5.997866000	-1.488898000	-1.234339000
H	-4.924662000	0.119039000	-2.156565000
C	-6.395286000	-2.072724000	-0.038742000
H	-6.338997000	-1.944068000	2.103620000
H	-6.302186000	-1.921002000	-2.178321000
H	-7.007662000	-2.964755000	-0.048845000
H	-0.828254000	3.152431000	0.053751000
H	-1.960730000	2.072522000	0.022664000

TS2<sub>12</sub><sup>0</sup>, T. E. = -5102.957615

C	3.375366000	-0.269985000	2.640637000
P	2.482636000	-1.452696000	1.583770000
C	3.808725000	-2.370701000	0.699634000
C	4.141911000	-1.664573000	-0.618095000
P	2.599580000	-1.346639000	-1.562085000
Fe	1.037461000	-0.556949000	-0.021712000
C	-0.034939000	-2.162147000	-0.103410000
O	-0.706260000	-3.060061000	-0.172272000
C	2.229155000	-2.930415000	-2.379811000
C	3.103700000	-0.277799000	-2.941263000
S	-0.311789000	0.550391000	-1.671864000
Fe	0.325173000	2.153538000	0.029449000
C	0.858613000	3.267940000	1.492596000
O	1.147553000	3.886115000	2.382085000
S	-0.340415000	0.477471000	1.644516000
C	-2.095231000	0.255960000	1.199359000
C	-2.072279000	0.304864000	-1.259598000
C	2.161040000	1.205089000	-0.003406000
O	3.263790000	1.574033000	-0.034771000
C	1.806186000	-2.641400000	2.780310000
H	4.597079000	-0.689434000	-0.425979000
H	-2.325317000	-0.807745000	1.106896000
H	-2.676024000	0.661230000	2.024907000
H	-2.298021000	-0.762451000	-1.209882000
H	-2.642152000	0.738134000	-2.078470000
H	4.689847000	-2.468269000	1.335798000
H	2.055972000	-3.706953000	-1.634600000
H	1.323160000	-2.816616000	-2.976188000
H	3.052359000	-3.231454000	-3.027652000
H	3.454271000	0.679508000	-2.557928000
H	3.899452000	-0.750325000	-3.517181000

H	2.242312000	-0.106728000	-3.587254000
H	3.957146000	-0.802055000	3.393079000
H	4.041477000	0.339651000	2.032284000
H	2.656512000	0.385232000	3.134811000
H	1.054232000	-2.136621000	3.387226000
H	1.334775000	-3.471757000	2.255589000
H	2.594422000	-3.026223000	3.427248000
C	0.881623000	3.352491000	-1.358859000
O	1.189580000	4.023350000	-2.202418000
N	-2.491260000	0.972985000	-0.020148000
H	4.842832000	-2.245194000	-1.219794000
H	3.432037000	-3.378885000	0.510632000
H	-1.210110000	2.930589000	0.037335000
H	-1.755937000	2.103963000	0.011079000
C	-3.928697000	1.351761000	-0.022737000
H	-4.086492000	1.971780000	0.860188000
H	-4.083468000	1.974414000	-0.904169000
C	-4.873605000	0.176628000	-0.023117000
C	-5.343506000	-0.352215000	1.176731000
C	-5.279034000	-0.406865000	-1.221481000
C	-6.187686000	-1.454194000	1.180865000
H	-5.058585000	0.108592000	2.115510000
C	-6.122467000	-1.509131000	-1.220530000
H	-4.944164000	0.010597000	-2.163875000
C	-6.574804000	-2.037328000	-0.018360000
H	-6.548578000	-1.852059000	2.120254000
H	-6.432598000	-1.950163000	-2.158752000
H	-7.235809000	-2.894093000	-0.016722000

[2-H<sub>2</sub>]<sup>+</sup>, T. E. = -5102.984517

C	-3.484843000	-1.156212000	-2.496858000
P	-2.093068000	-1.876655000	-1.576049000
C	-2.812149000	-3.285194000	-0.638972000
C	-3.383353000	-2.803355000	0.699240000
P	-2.130434000	-1.802409000	1.596921000
Fe	-1.010032000	-0.512782000	-0.005265000
C	0.412656000	-1.787723000	0.003028000
O	1.217005000	-2.571080000	0.007094000
C	-1.118725000	-3.009928000	2.503048000
C	-3.026983000	-0.936000000	2.914028000
S	0.136286000	0.870089000	1.600091000
Fe	-0.542989000	2.565511000	-0.017227000
C	-1.359756000	3.549120000	-1.391286000
O	-1.872790000	4.098460000	-2.232377000

S	0.139331000	0.857382000	-1.618720000
C	1.920347000	0.661977000	-1.232990000
C	1.917794000	0.672086000	1.218218000
C	-1.366044000	3.559413000	1.345870000
O	-1.884126000	4.114764000	2.179892000
C	-1.074677000	-2.621923000	-2.878549000
H	-4.254533000	-2.162967000	0.536670000
H	2.171393000	-0.405289000	-1.270369000
H	2.443058000	1.142992000	-2.058917000
H	2.168946000	-0.394768000	1.264893000
H	2.438847000	1.159775000	2.041295000
H	-3.572419000	-3.788185000	-1.238415000
H	-0.677086000	-3.733572000	1.818717000
H	-0.317127000	-2.481605000	3.020427000
H	-1.734038000	-3.537667000	3.231408000
H	-3.762007000	-0.253855000	2.489123000
H	-3.532368000	-1.651234000	3.562369000
H	-2.308140000	-0.360913000	3.498464000
H	-3.881132000	-1.886780000	-3.201508000
H	-4.279378000	-0.848986000	-1.817890000
H	-3.133608000	-0.280539000	-3.043980000
H	-0.681354000	-1.823056000	-3.507218000
H	-0.240001000	-3.169222000	-2.442618000
H	-1.674363000	-3.301705000	-3.483630000
C	-2.569752000	0.620157000	-0.010333000
O	-3.561113000	1.149794000	-0.005374000
N	2.354143000	1.301052000	-0.009497000
H	-3.710095000	-3.641399000	1.316890000
H	-2.003500000	-4.002371000	-0.474441000
H	0.994770000	4.073492000	-0.020111000
H	1.396714000	3.432783000	-0.018077000
C	3.798860000	1.579151000	-0.008358000
H	4.014063000	2.179699000	-0.893923000
H	4.009862000	2.193719000	0.868651000
C	4.676641000	0.346001000	0.004098000
C	5.068442000	-0.259864000	-1.187843000
C	5.071154000	-0.232361000	1.208636000
C	5.824746000	-1.424356000	-1.177992000
H	4.786108000	0.189813000	-2.133366000
C	5.827565000	-1.396693000	1.224123000
H	4.790371000	0.239004000	2.143978000
C	6.202779000	-1.997557000	0.029392000
H	6.124456000	-1.880660000	-2.112649000
H	6.129403000	-1.831210000	2.168422000
H	6.795345000	-2.903108000	0.039176000

**HBF<sub>4</sub>.Et<sub>2</sub>O**, T. E. = -658.587330

B	-1.943506000	-0.156048000	0.076220000
F	-2.262709000	1.181423000	0.171698000
F	-3.052968000	-0.954194000	-0.038115000
F	-1.141901000	-0.327177000	-1.140645000
O	1.246078000	-0.180837000	-0.769749000
C	1.587242000	1.244603000	-0.675399000
C	1.758041000	-1.092343000	0.261421000
C	1.227271000	1.839074000	0.661671000
C	3.262842000	-1.077634000	0.262151000
F	-1.119252000	-0.551133000	1.123557000
H	1.025210000	1.693173000	-1.490975000
H	2.648095000	1.305290000	-0.901706000
H	1.356934000	-2.059239000	-0.031612000
H	1.322336000	-0.796700000	1.212553000
H	0.226982000	-0.291148000	-0.913541000
H	0.173740000	1.680830000	0.891017000
H	1.410886000	2.912033000	0.609701000
H	3.606241000	-1.861472000	0.936255000
H	3.655272000	-1.281736000	-0.733237000
H	3.664300000	-0.131329000	0.622941000
H	1.838004000	1.434767000	1.467974000

**BF<sub>4</sub><sup>-</sup>.Et<sub>2</sub>O**, T. E. = -658.167031

B	1.874766000	-0.114335000	-0.002906000
F	1.115728000	-1.107307000	-0.634867000
F	3.225123000	-0.485610000	-0.009702000
F	1.721643000	1.096631000	-0.686042000
O	-2.614261000	0.259679000	0.042897000
C	-1.704409000	1.101241000	-0.651454000
C	-1.993576000	-0.861475000	0.655129000
C	-1.113145000	2.157435000	0.263209000
C	-1.950407000	-2.050359000	-0.286563000
F	1.441753000	0.032397000	1.322020000
H	-2.271163000	1.570163000	-1.458326000
H	-0.904050000	0.503880000	-1.100307000
H	-2.584706000	-1.100070000	1.541726000
H	-0.982056000	-0.601099000	0.981708000
H	-1.908797000	2.749655000	0.718027000
H	-0.457195000	2.820159000	-0.302075000
H	-1.476718000	-2.904122000	0.200717000
H	-2.960141000	-2.334150000	-0.586564000
H	-1.368748000	-1.810034000	-1.176541000
H	-0.515157000	1.693818000	1.048386000



[Cp\*<sub>2</sub>Cr], T. E. = -1824.147249

Cr	0.001354000	0.014621000	0.000816000
C	-1.881662000	-1.023302000	0.459420000
C	-1.865668000	0.173605000	1.230812000
C	-1.849104000	-0.656741000	-0.922677000
C	-1.822794000	1.276507000	0.337849000
C	-1.811478000	0.770896000	-0.993258000
C	1.881285000	0.329678000	1.108993000
C	1.764851000	-1.039813000	0.715697000
C	1.952606000	1.121145000	-0.072032000
C	1.763902000	-1.083548000	-0.714023000
C	1.880134000	0.252853000	-1.193174000
C	-1.956808000	-2.421238000	0.993841000
H	-2.990768000	-2.771615000	1.054850000
H	-1.412790000	-3.120106000	0.355985000
H	-1.527062000	-2.488114000	1.993875000
C	-1.919648000	-1.596673000	-2.087920000
H	-2.953781000	-1.787912000	-2.387716000
H	-1.396351000	-1.192553000	-2.956007000
H	-1.463691000	-2.558704000	-1.850262000
C	-1.863783000	0.245241000	2.727647000
H	-1.400462000	1.166157000	3.082232000
H	-2.880039000	0.211458000	3.128694000
H	-1.312798000	-0.589217000	3.164923000
C	-1.766802000	2.724056000	0.721635000
H	-1.192570000	3.304263000	-0.001844000
H	-2.767305000	3.161241000	0.772390000
H	-1.298872000	2.860327000	1.697157000
C	-1.798070000	1.585052000	-2.251595000
H	-2.811215000	1.774997000	-2.616246000
H	-1.318780000	2.552131000	-2.094641000
H	-1.254246000	1.075348000	-3.048376000
C	1.691385000	-2.324385000	-1.551107000
H	2.681827000	-2.760052000	-1.708412000
H	1.071035000	-3.087007000	-1.076834000
H	1.262741000	-2.118371000	-2.532399000
C	1.888650000	0.666015000	-2.633505000
H	1.491293000	1.673255000	-2.761218000
H	2.900961000	0.655131000	-3.045595000
H	1.280973000	-0.005552000	-3.242271000
C	2.051643000	2.615771000	-0.116523000
H	1.532881000	3.072975000	0.727092000
H	3.092696000	2.946788000	-0.079911000
H	1.611311000	3.017416000	-1.029800000
C	1.949303000	0.832075000	2.519454000

H	1.341764000	0.220874000	3.188627000
H	2.973851000	0.815469000	2.900949000
H	1.587759000	1.858326000	2.593583000
C	1.731389000	-2.222622000	1.635571000
H	2.738459000	-2.583926000	1.861832000
H	1.251662000	-1.974732000	2.583736000
H	1.176646000	-3.052486000	1.195831000

[Cp\*<sub>2</sub>Cr]<sup>+</sup>, T. E. = -1824.041132

Cr	-0.000557000	-0.009745000	-0.001435000
C	-1.886502000	-0.559503000	1.064842000
C	-1.881784000	0.848700000	0.844703000
C	-1.879211000	-1.204135000	-0.206629000
C	-1.869774000	1.075283000	-0.561980000
C	-1.868031000	-0.193262000	-1.211590000
C	1.861649000	1.088829000	0.555705000
C	1.866898000	-0.176747000	1.211118000
C	1.876681000	0.855986000	-0.849840000
C	1.885046000	-1.192169000	0.210803000
C	1.889601000	-0.553159000	-1.063603000
C	-1.909587000	-1.235635000	2.400170000
H	-2.939685000	-1.402660000	2.721727000
H	-1.411726000	-2.204115000	2.368050000
H	-1.419770000	-0.629930000	3.161934000
C	-1.886942000	-2.681091000	-0.450959000
H	-2.908185000	-3.032592000	-0.611601000
H	-1.304785000	-2.943205000	-1.334243000
H	-1.477678000	-3.227743000	0.397320000
C	-1.902337000	1.903053000	1.906612000
H	-1.434355000	2.825069000	1.564208000
H	-2.932084000	2.138059000	2.184328000
H	-1.385414000	1.574306000	2.807756000
C	-1.878866000	2.412195000	-1.235022000
H	-1.424178000	2.364675000	-2.223666000
H	-2.904817000	2.765322000	-1.358328000
H	-1.341376000	3.158192000	-0.649693000
C	-1.867733000	-0.423137000	-2.690571000
H	-2.888948000	-0.403025000	-3.076753000
H	-1.301385000	0.346027000	-3.215607000
H	-1.437516000	-1.391646000	-2.942233000
C	1.901249000	-2.668006000	0.461450000
H	2.925214000	-3.014148000	0.616323000
H	1.326537000	-2.928963000	1.349877000
H	1.488546000	-3.220379000	-0.381477000

C	1.917215000	-1.234780000	-2.396032000
H	1.417623000	-0.638514000	-3.158949000
H	2.948343000	-1.390350000	-2.720040000
H	1.431583000	-2.209201000	-2.358202000
C	1.893022000	1.905527000	-1.916511000
H	1.417673000	2.825857000	-1.579802000
H	2.921969000	2.146335000	-2.192220000
H	1.381080000	1.569112000	-2.817646000
C	1.861082000	2.428791000	1.222892000
H	1.400004000	2.383939000	2.208745000
H	2.884827000	2.786391000	1.351663000
H	1.324851000	3.170269000	0.630699000
C	1.868580000	-0.398561000	2.691360000
H	2.889176000	-0.361183000	3.077900000
H	1.290897000	0.365296000	3.211825000
H	1.452605000	-1.371805000	2.948399000