

Supporting Information

Keto-enol tautomerization of ethyl acetoacetate in choline ionic liquids:

Role of cation and anion in switching the tautomeric equilibrium

Madhu Deepan Kumar and Madhavan Jaccob*

Department of Chemistry & Computational Chemistry Laboratory, Loyola Institute of Frontier
Energy (LIFE), Loyola College, University of Madras, Chennai 600 034, Tamil Nadu, India

Table of Contents

Figure S1	Free energy profile for enol to keto tautomerization reaction of EAA.	S2
Figure S2a	Computed free energy profile for keto-enol tautomeric equilibrium of EAA in the presence of organic solvents. (Energies are in Kcal/mol).	S2
Figure S2b	Optimized geometries of keto form, transition state and enol form involved in the tautomerization of EAA with the assistance of H ₂ O, CH ₃ OH and CH ₃ COOH solvents.	S3
Figure S2c	Optimized geometries of keto form, transition state and enol form involved in the tautomerization of EAA with the assistance of DCM, CH ₃ CN, CHCl ₃ and Toluene solvents.	S4
Figure S3a	Optimized geometries of keto form, transition state and enol form involved in the cation assisted tautomerization of EAA (CAT) by CS, NS _{Ca} and NS _{Cb} .	S5
Figure S3b	Optimized geometries of keto form, transition state and enol form involved in the cation assisted tautomerization of EAA (CAT) by CP, NP _{Ca} and NP _{Cb} .	S6
Figure S3c	Molecular graphs of keto and enol forms of EAA involved in the cation assisted tautomerization of EAA (CAT).	S7
Figure S4a	Optimized geometries of keto form, transition state and enol form involved in the anion-assisted tautomerization of EAA (AAT) by CS, NS _{Aa} and NS _{Ab} .	S8
Figure S4b	Optimized geometries of keto form, transition state and enol form involved in the anion-assisted tautomerization of EAA (AAT) by CP, NP _{Aa} and NP _{Ab} .	S9
Figure S4c	Molecular graphs of keto and enol forms of EAA involved in the anion-assisted tautomerization of EAA (AAT).	S10
Table S1	Topological properties of Keto forms of EAA in both CAT and AAT.	S11
Cartesian Coordinates and corresponding free energies in Hartrees		S12- S62

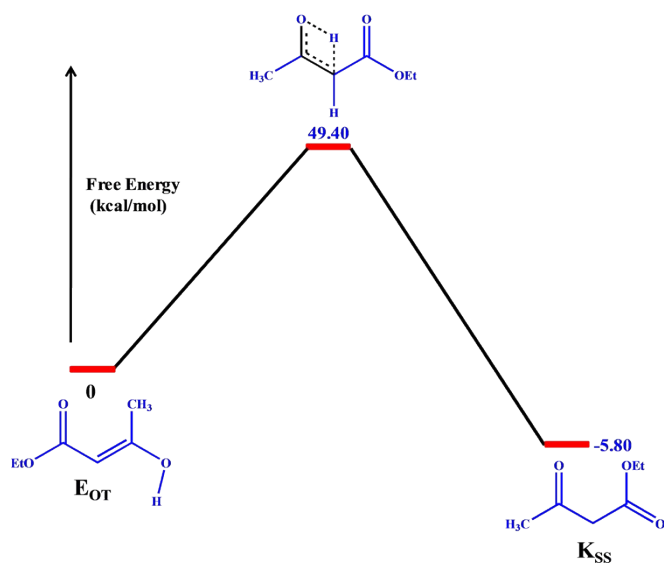


Figure S1. Free energy profile for enol to keto tautomerization reaction of EAA.

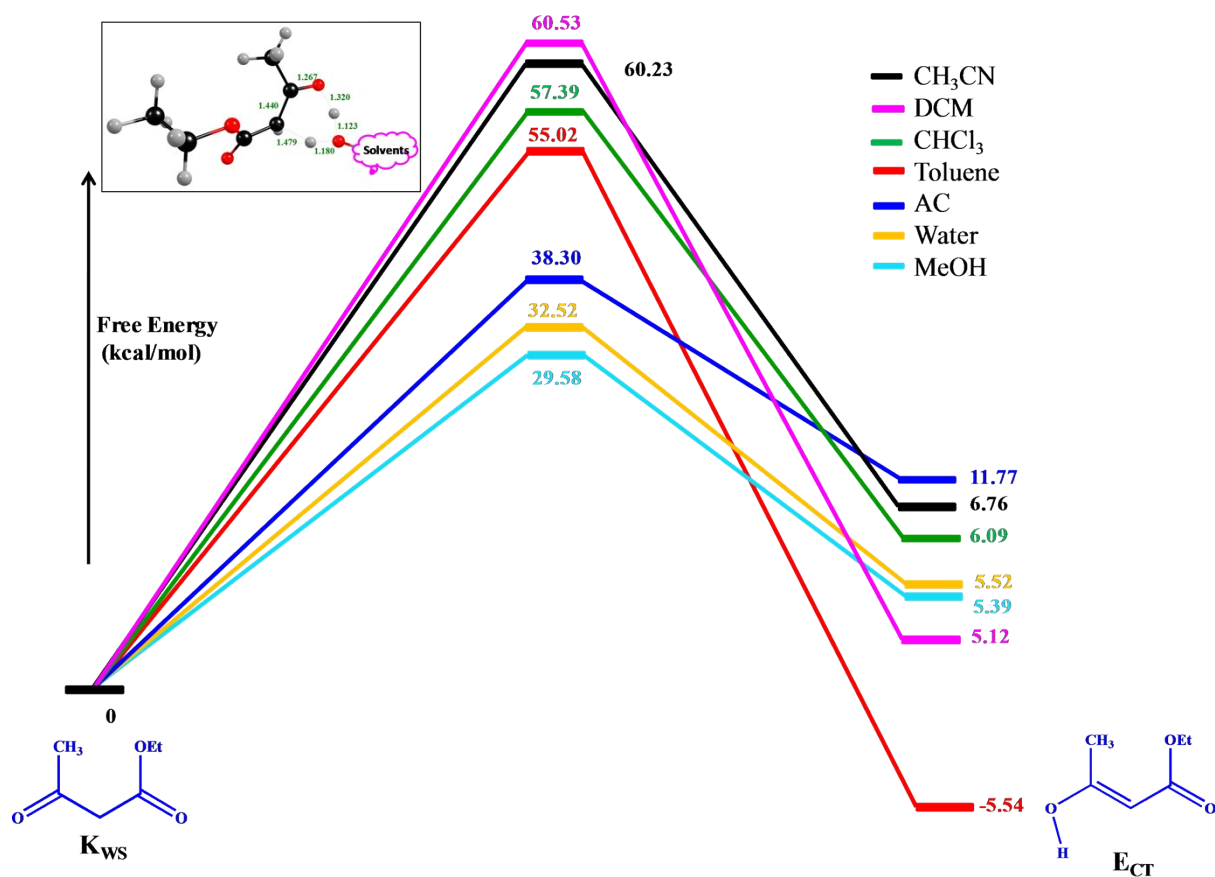


Figure S2a. Computed free energy profile for keto-enol tautomeric equilibrium of EAA in the presence of organic solvents. (Energies are in Kcal/mol).

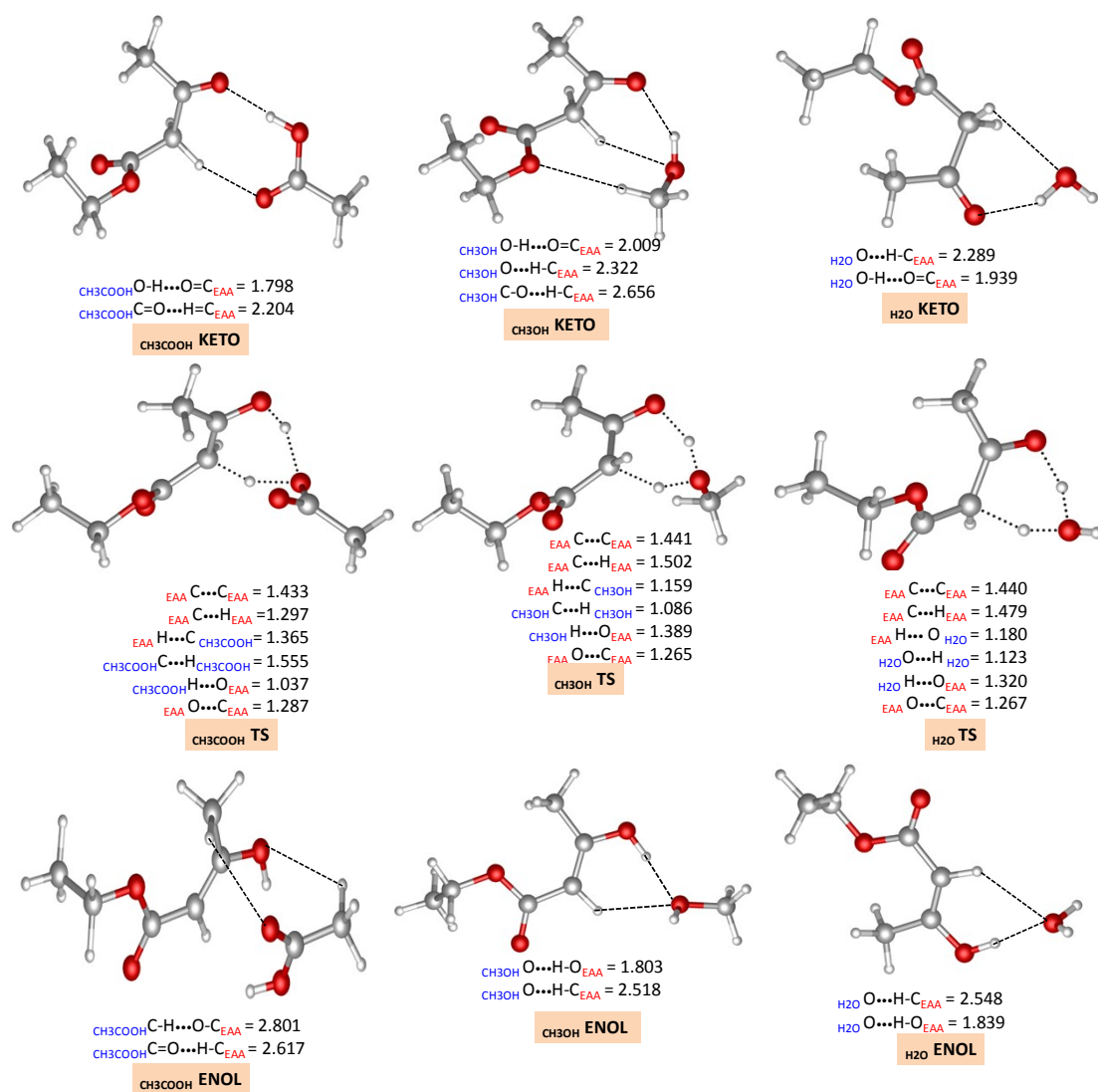


Figure S2b. Optimized geometries of keto form, transition state and enol form involved in the tautomerization of EAA with the assistance H₂O, CH₃OH and CH₃COOH solvents.

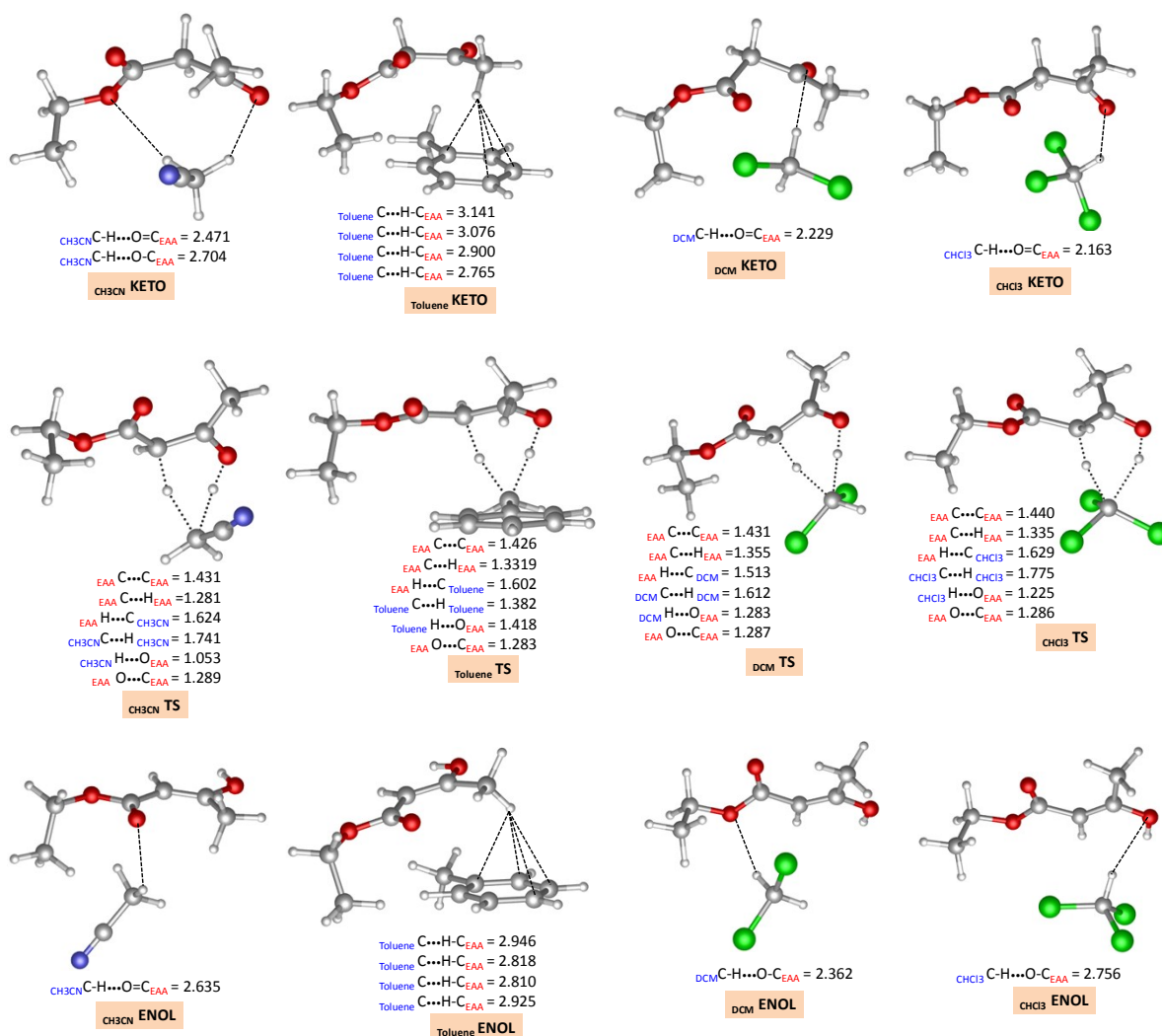


Figure S2c. Optimized geometries of keto form, transition state and enol form involved in the the tautomerization of EAA with the assistance of DCM, CH₃CN, CHCl₃ and Toluene solvents.

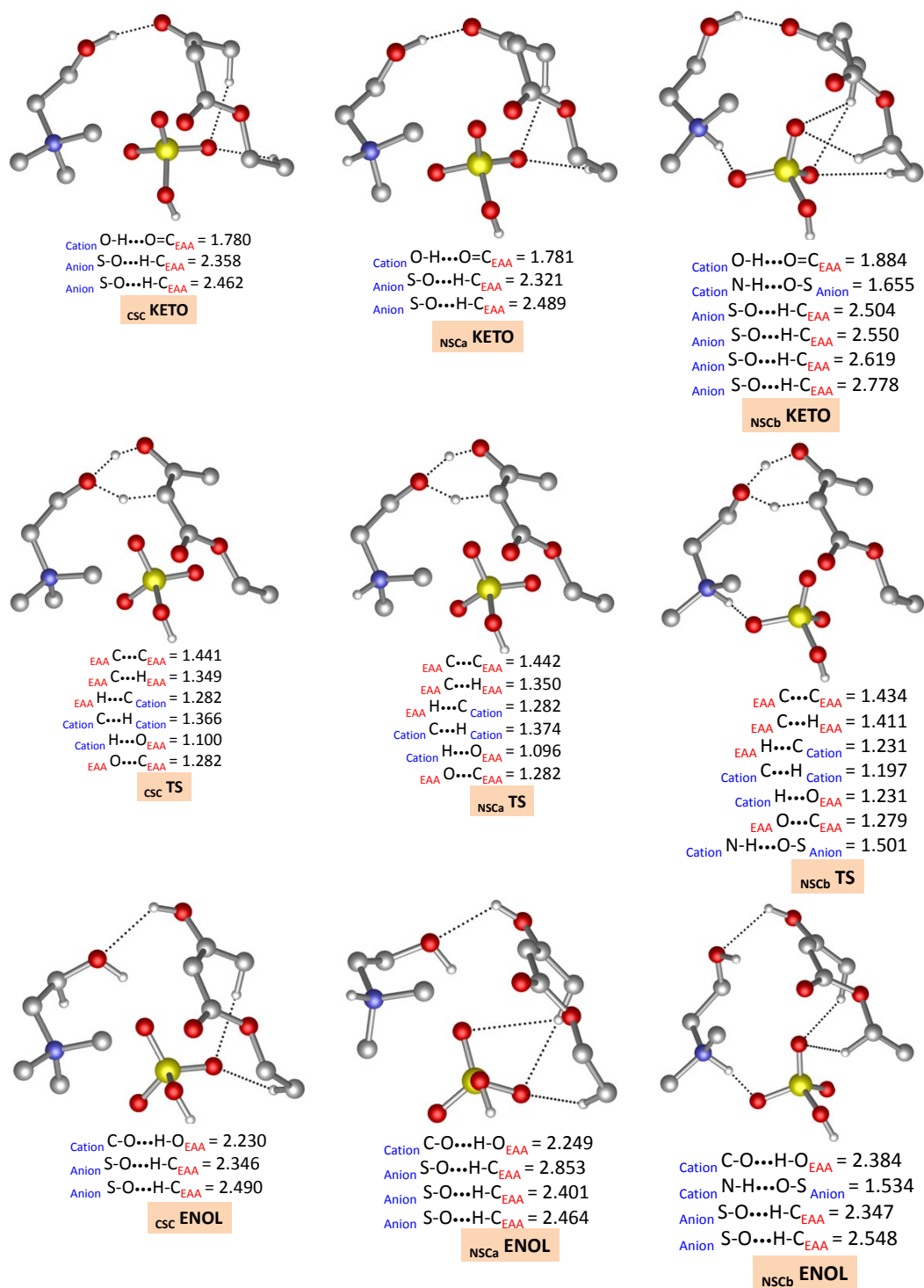


Figure S3a. Optimized geometries of keto form, transition state and enol form involved in the cation assisted tautomerization of EAA (CAT) by CS, NS_{Ca} and NS_{Cb}.

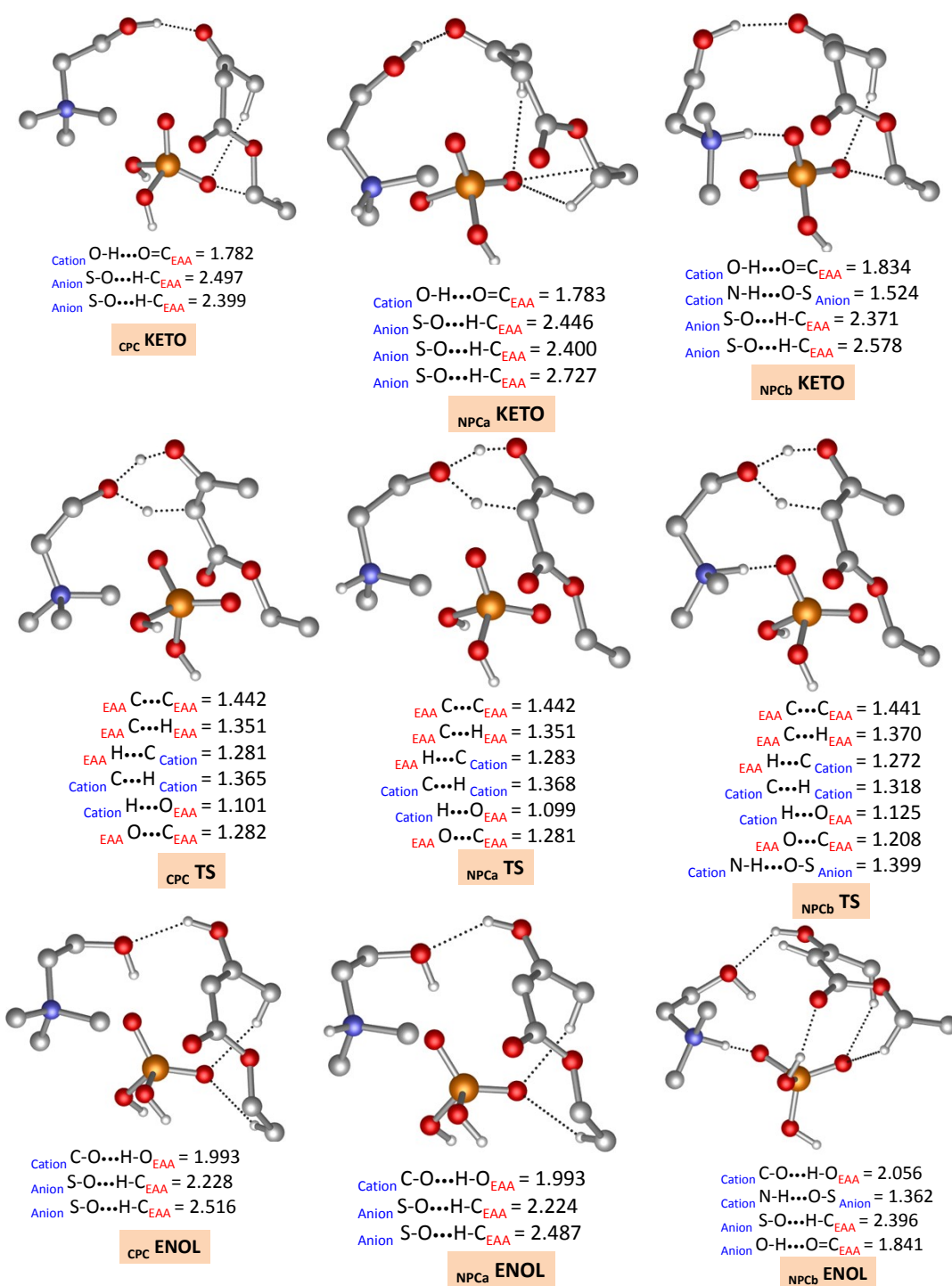


Figure S3b. Optimized geometries of keto form, transition state and enol form involved in the cation assisted tautomerization of EAA (CAT) by CP, NP_{Ca} and NP_{Cb}.

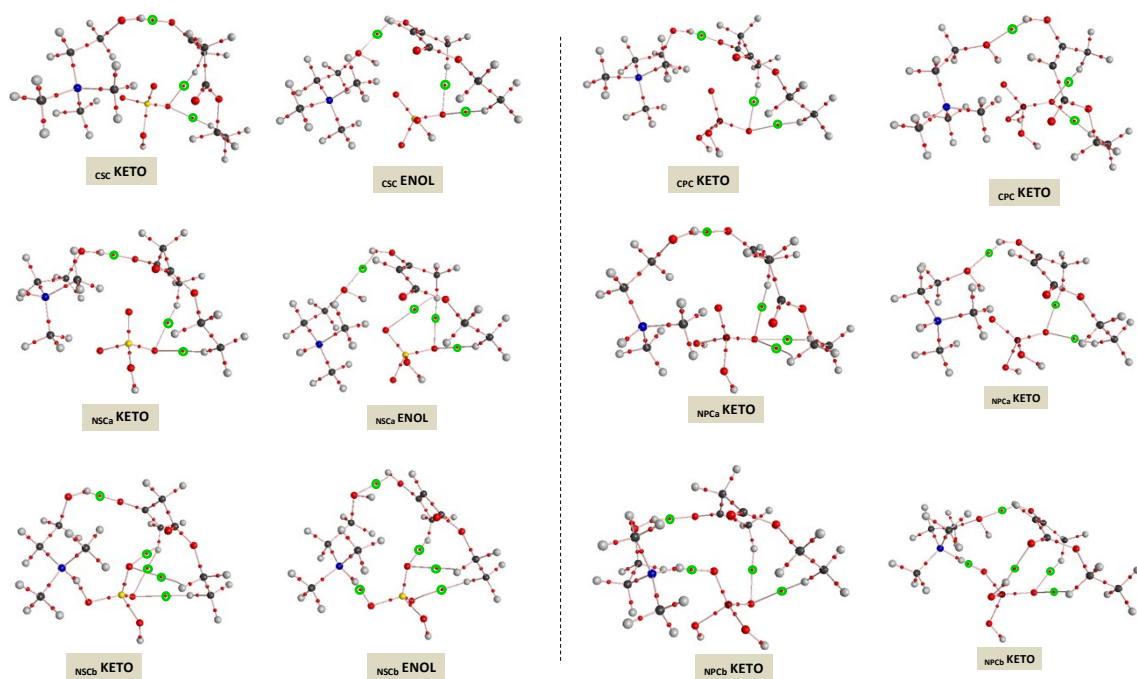


Figure S3c. Molecular graphs of keto and enol forms of EAA involved in the cation assisted tautomerization of EAA (CAT).

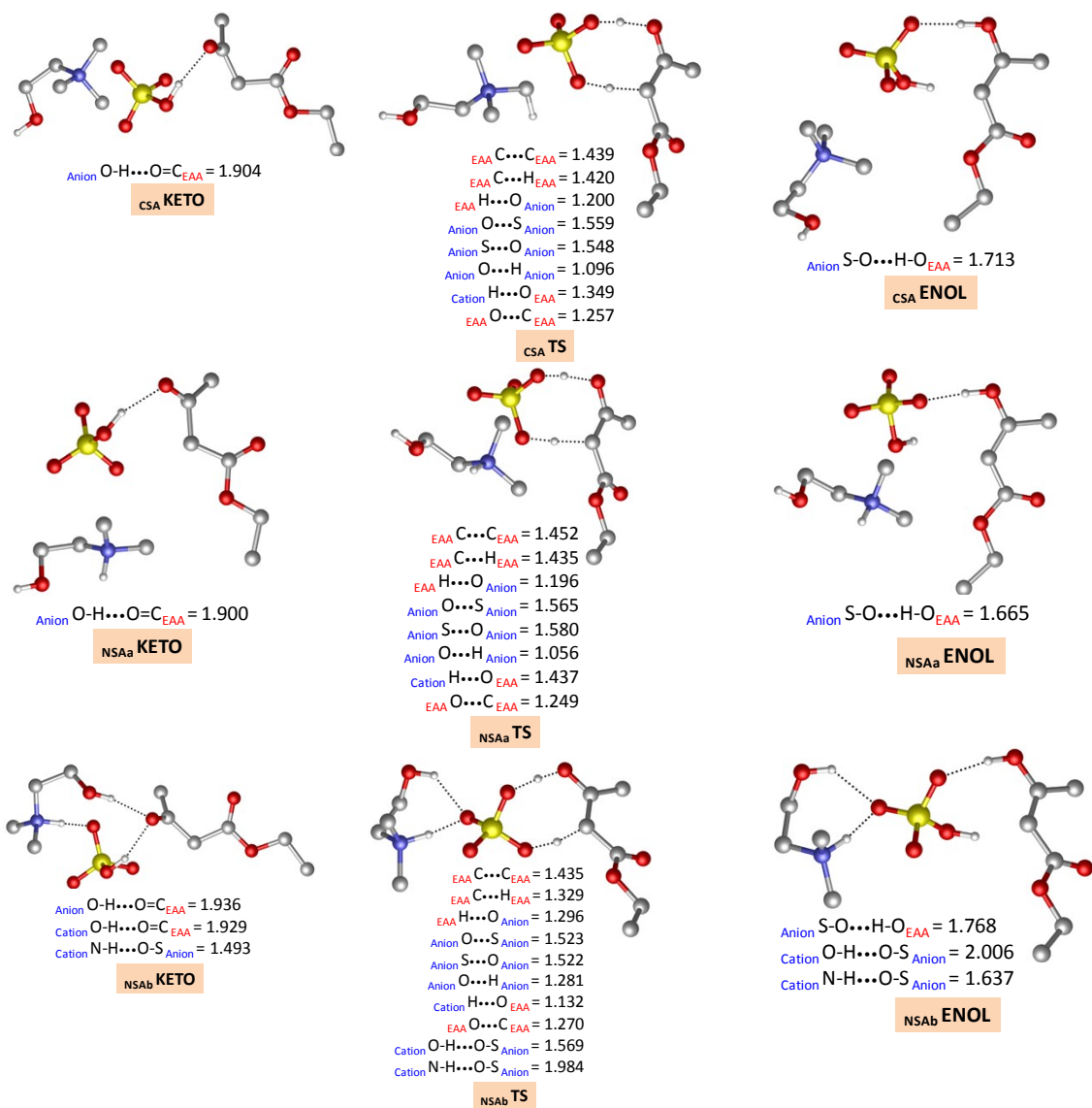


Figure S4a. Optimized geometries of keto form, transition state and enol form involved in the keto-enol interconversion (AAT) with the assistance of CS, NS_{Aa} and NS_{Ab}.

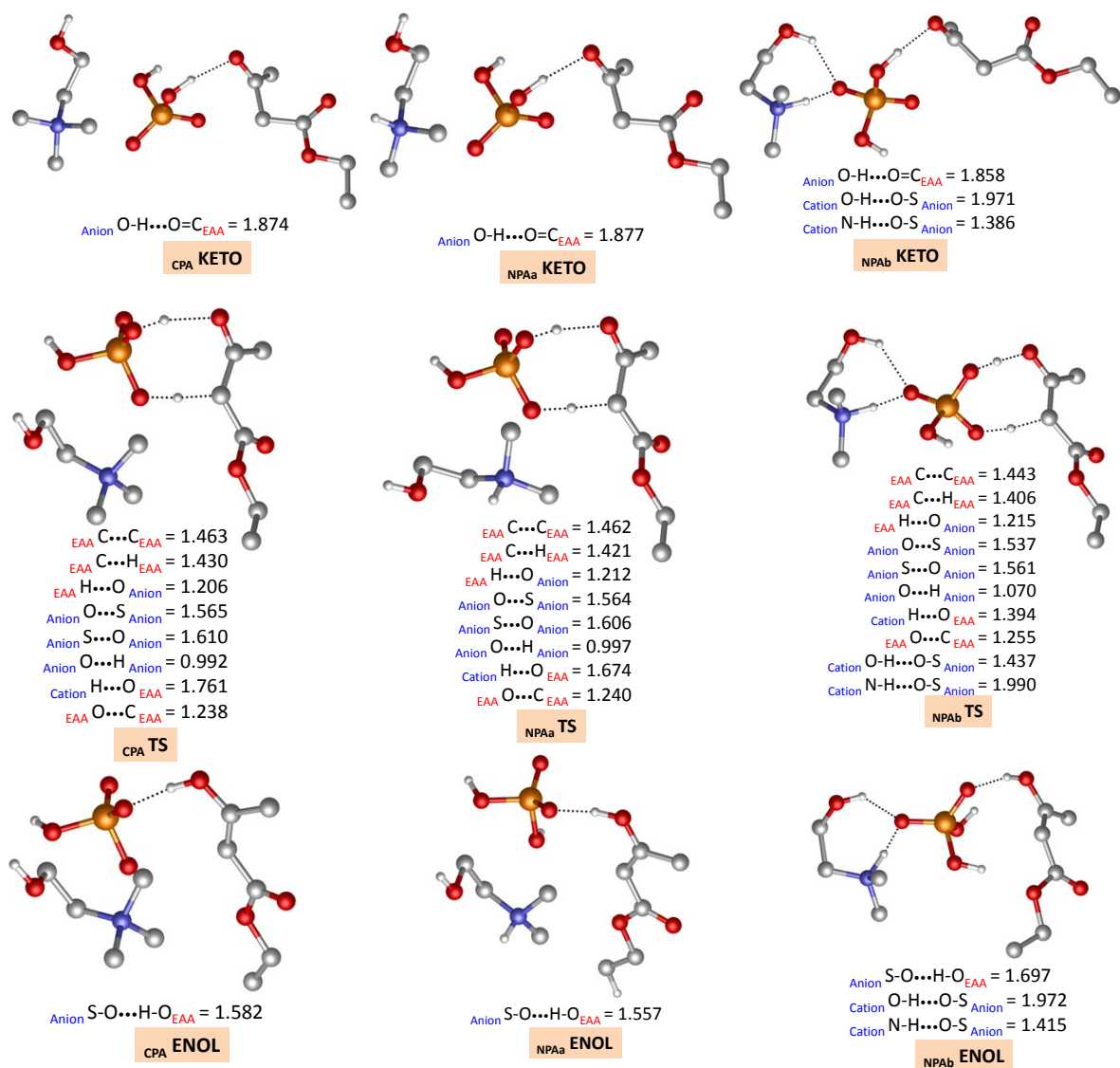


Figure S4b. Optimized geometries of keto form, transition state and enol form involved in the anion-assisted tautomerization of EAA (AAT) by CP, NP_{Aa} and NP_{Ab}.

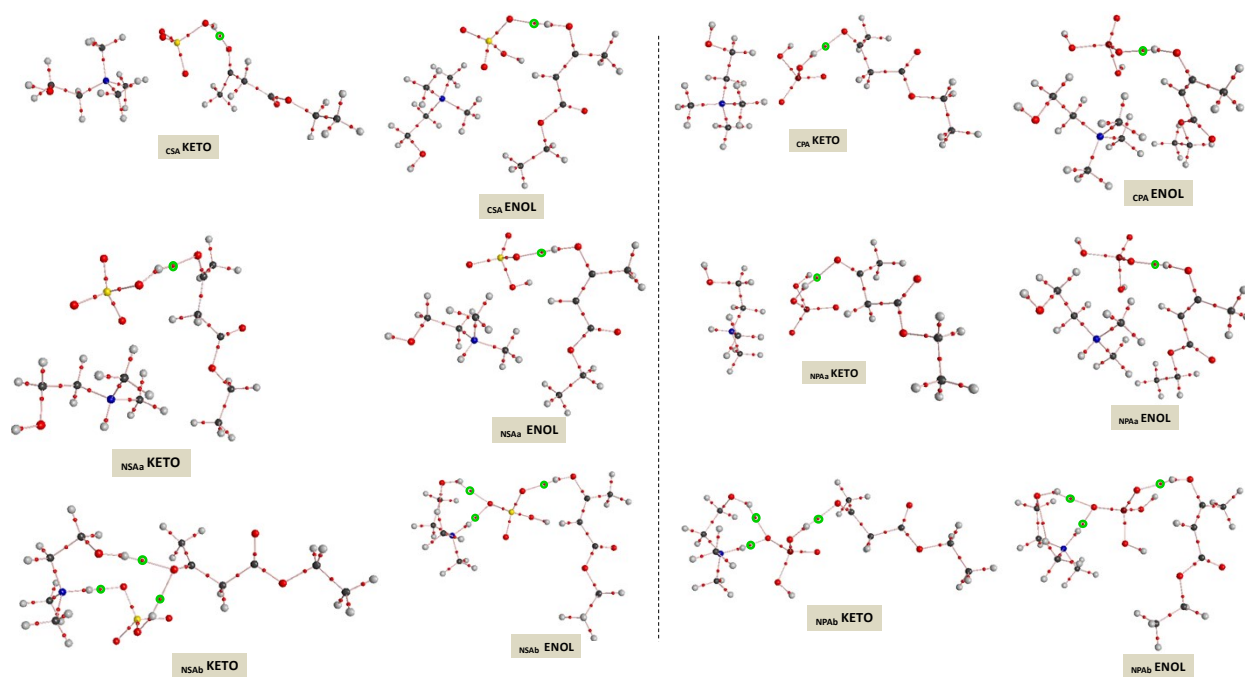


Figure S4c. Molecular graphs of keto and enol forms of EAA involved in the anion-assisted tautomerization of EAA (AAT).

Table S1. Topological properties at the BCPs of pertinent hydrogen bonding interactions in Keto forms of EAA in **CAT** and **AAT**.

Compound	Interactions	Length	$\rho_{H\cdots O}$	$\nabla^2\rho_{H\cdots O}$
CAT				
CS _C _KETO	Cation O-H1 $\cdots$ O1 _{EAA}	1.780	0.035	-0.028
	Anion S-O1 $\cdots$ H1-C _{EAA}	2.358	0.012	-0.009
	Anion S-O1 $\cdots$ H2-C _{EAA}	2.462	0.009	-0.008
NS _{Ca} _KETO	Cation O-H1 $\cdots$ O1 _{EAA}	1.781	0.034	-0.028
	Anion S-O1 $\cdots$ H1-C _{EAA}	2.321	0.012	-0.010
	Anion S-O1 $\cdots$ H2-C _{EAA}	2.489	0.009	-0.007
NS _{Cb} _KETO	Cation O-H1 $\cdots$ O1 _{EAA}	1.884	0.027	-0.023
	Cation N-H4 $\cdots$ O3-S _{Anion}	1.655	0.052	-0.036
	Anion S-O1 $\cdots$ H1-C _{EAA}	2.504	0.010	-0.009
	Anion S-O1 $\cdots$ H2-C _{EAA}	2.55	0.008	-0.008
	Anion S-O1 $\cdots$ H3-C _{EAA}	2.619	0.008	-0.007
	Anion S-O1 $\cdots$ H1-C _{EAA}	2.778	0.005	-0.005
CP _C _KETO	Cation O-H1 $\cdots$ O1 _{EAA}	1.780	0.035	-0.028
	Anion P-O1 $\cdots$ H1-C _{EAA}	2.497	0.009	-0.007
	Anion P-O1 $\cdots$ H2-C _{EAA}	2.399	0.011	-0.009
NP _{Ca} _KETO	Cation O-H1 $\cdots$ O1 _{EAA}	1.783	0.035	-0.028
	Anion P-O1 $\cdots$ H1-C _{EAA}	2.446	0.010	-0.008
	Anion P-O1 $\cdots$ H2-C _{EAA}	2.727	0.011	-0.009
	Anion P-O1 $\cdots$ H3-C _{EAA}	2.400	0.008	-0.007
NP _{Cb} _KETO	Cation O-H1 $\cdots$ O1 _{EAA}	1.834	0.03	-0.025
	Cation N-H4 $\cdots$ O3-P _{Anion}	1.524	0.071	-0.041
	Anion P-O1 $\cdots$ H1-C _{EAA}	2.371	0.012	-0.009
	Anion P-O1 $\cdots$ H2-C _{EAA}	2.578	0.008	-0.006
AAT				
CS _A _KETO	Anion O1-H1 $\cdots$ O _{EAA}	1.904	0.025	-0.021
NS _{Aa} _KETO	Anion O1-H1 $\cdots$ O _{EAA}	1.900	0.026	-0.020
NS _{Ab} _KETO	Cation O-H1 $\cdots$ O1 _{EAA}	1.929	0.024	-0.019
	Cation N-H4 $\cdots$ O3-S _{Anion}	1.493	0.080	-0.038
	Anion S-O1 $\cdots$ H2-C _{EAA}	1.936	0.023	-0.020
CP _A _KETO	Anion O-H1 $\cdots$ O1-C _{EAA}	1.874	0.027	-0.022
NP _{Aa} _KETO	Anion O-H1 $\cdots$ O1-C _{EAA}	1.877	0.027	-0.022
NP _{Ab} _KETO	Anion O-H1 $\cdots$ O1-C _{EAA}	1.858	0.026	-0.023
	Cation O-H1 $\cdots$ O2-P _{Anion}	1.971	0.024	-0.019
	Cation N-H4 $\cdots$ O3-P _{Anion}	1.386	0.104	-0.024

Cartesian Coordinates

Keto-enol tautomerization of EAA:

Keto SS

Reactant

FE=-460.047359

6	0.312677000	-0.192767000	-0.099616000
6	-0.908553000	-0.708187000	0.633182000
6	-2.211449000	-0.127978000	0.093082000
1	-0.787068000	-0.453560000	1.693057000
6	-2.458386000	1.344150000	0.303884000
1	-1.700062000	1.913839000	-0.240778000
1	-3.454675000	1.601922000	-0.054533000
1	-2.365057000	1.594477000	1.365819000
8	-3.007414000	-0.850803000	-0.462883000
8	0.315522000	0.695901000	-0.918762000
8	1.407572000	-0.862665000	0.280956000
6	2.649416000	-0.466884000	-0.335018000
6	3.222088000	0.766496000	0.337260000
1	3.299210000	-1.333632000	-0.207223000
1	2.472120000	-0.295688000	-1.399246000
1	3.359063000	0.590811000	1.407289000
1	4.195152000	1.006449000	-0.100150000
1	2.560852000	1.623807000	0.194496000
1	-0.939728000	-1.796869000	0.550146000

Keto SS

TS

i = -2022 cm⁻¹

FE=-459.958458

6	0.331522000	-0.185676000	-0.207500000
6	-0.915408000	-0.771383000	0.279184000
6	-2.158554000	-0.038762000	0.158128000
1	-0.849926000	-1.353987000	1.198621000
6	-2.428078000	1.415028000	0.247378000
1	-1.770916000	1.906058000	-0.478295000
1	-3.474626000	1.634456000	0.039775000
1	-2.136340000	1.782815000	1.235264000
8	-3.071674000	-0.882674000	-0.105971000
8	0.409325000	0.818739000	-0.894670000
8	1.408644000	-0.907598000	0.159296000
6	2.680211000	-0.441467000	-0.317073000
6	3.214587000	0.680595000	0.554576000
1	3.325059000	-1.321117000	-0.275101000
1	2.572580000	-0.117305000	-1.354984000
1	3.284717000	0.355293000	1.595901000
1	4.212906000	0.971962000	0.215543000
1	2.560754000	1.553175000	0.493973000
1	-2.040239000	-1.589091000	-0.228101000

Enol OPT**Product****FE=-460.037199**

6	0.352267000	-0.027232000	-0.229777000
6	-0.894519000	-0.762566000	-0.028495000
6	-2.088350000	-0.141046000	0.079417000
1	-0.822715000	-1.843899000	0.032646000
6	-2.338464000	1.333080000	0.016042000
1	-2.015488000	1.731308000	-0.948153000
1	-3.401978000	1.521008000	0.164692000
1	-1.750025000	1.852139000	0.774915000
8	-3.233620000	-0.834601000	0.263790000
8	0.472702000	1.178803000	-0.332222000
8	1.402273000	-0.875549000	-0.297094000
6	2.692871000	-0.274569000	-0.476791000
6	3.246193000	0.240495000	0.839778000
1	3.311710000	-1.076645000	-0.883265000
1	2.610255000	0.530118000	-1.211478000
1	3.291419000	-0.565817000	1.576501000
1	4.257252000	0.630465000	0.690894000
1	2.618800000	1.045799000	1.227456000
1	-3.050050000	-1.782677000	0.298961000

Solvent-assisted keto-enol tautomerization of EAA:

Methanol**Reactant****FE=-575.683265**

6	0.902248000	0.075146000	0.965179000
6	-0.475558000	0.686067000	1.067101000
6	-0.851365000	1.443982000	-0.202843000
6	0.214826000	2.306017000	-0.828681000
1	0.998969000	1.661150000	-1.241990000
1	-0.217390000	2.910788000	-1.625168000
1	0.685406000	2.941557000	-0.071888000
8	-1.970803000	1.369089000	-0.666304000
8	1.853797000	0.377617000	1.643517000
8	0.938603000	-0.846758000	-0.011680000
6	2.210683000	-1.479189000	-0.252919000
6	3.100343000	-0.593259000	-1.104573000
1	2.676018000	-1.705163000	0.709281000
1	1.957448000	-2.408390000	-0.765324000
1	4.036057000	-1.113068000	-1.328128000
1	2.608548000	-0.352949000	-2.051436000
1	3.341948000	0.331533000	-0.574589000
8	-3.205758000	-0.983415000	0.422193000
1	-3.148650000	-0.086459000	0.061707000
1	-1.232100000	-0.083580000	1.251301000

1	-0.461183000	1.394121000	1.901290000
6	-2.585505000	-1.855816000	-0.501698000
1	-1.523910000	-1.610695000	-0.650127000
1	-2.653575000	-2.864702000	-0.089462000
1	-3.088328000	-1.844098000	-1.476676000

Methanol

TS

i = -1270 cm⁻¹

FE=-575.636115

6	-0.876438000	-0.608061000	-0.557430000
6	0.483343000	-0.136763000	-0.823950000
6	1.006154000	1.128954000	-0.376474000
6	0.187626000	2.196672000	0.296358000
1	0.017397000	1.913736000	1.339259000
1	0.747847000	3.131510000	0.261910000
1	-0.793229000	2.305009000	-0.169172000
8	2.244465000	1.353892000	-0.503176000
8	-1.488605000	-1.391687000	-1.254461000
8	-1.383331000	-0.130172000	0.609562000
6	-2.722581000	-0.534055000	0.929433000
6	-3.740712000	0.294177000	0.166186000
1	-2.835291000	-1.598177000	0.708093000
1	-2.806589000	-0.375491000	2.006712000
1	-4.754086000	0.013292000	0.467389000
1	-3.602337000	1.358958000	0.374991000
1	-3.639454000	0.122419000	-0.907653000
8	2.814137000	-0.965506000	-0.204980000
1	2.827802000	0.094889000	-0.439669000
1	1.662762000	-0.927019000	-0.334539000
1	0.821183000	-0.417079000	-1.823196000
6	3.172852000	-1.160261000	1.168253000
1	2.446748000	-0.669627000	1.825702000
1	3.188310000	-2.231692000	1.366148000
1	4.164150000	-0.736936000	1.334206000

Methanol

Product

FE=-575.674664

6	1.094407000	-0.687000000	-0.155525000
6	-0.257658000	-0.167620000	0.024848000
6	-0.643172000	1.131106000	0.048063000
6	0.226948000	2.348593000	-0.068109000
1	0.707710000	2.383002000	-1.048382000
1	-0.394194000	3.234469000	0.067718000
1	1.024004000	2.330593000	0.676508000
8	-1.936836000	1.467071000	0.189245000
8	1.363524000	-1.873074000	-0.149269000
8	2.037897000	0.266348000	-0.347490000

6	3.384174000	-0.201056000	-0.512737000
6	4.025939000	-0.512812000	0.827053000
1	3.378326000	-1.081371000	-1.159904000
1	3.897035000	0.619524000	-1.018992000
1	5.069059000	-0.808549000	0.680454000
1	4.004383000	0.366850000	1.476232000
1	3.498815000	-1.333675000	1.317775000
8	-3.501079000	-0.804323000	-0.117187000
1	-2.505507000	0.670437000	0.173827000
1	-3.316349000	-1.252147000	-0.950386000
1	-1.002857000	-0.942633000	0.168897000
6	-4.887646000	-0.895365000	0.192463000
1	-5.499830000	-0.389332000	-0.560663000
1	-5.200967000	-1.939584000	0.284167000
1	-5.025636000	-0.400826000	1.154020000

Water

Reactant

FE=-536.433115

6	0.623612000	-0.547936000	0.684845000
6	-0.871763000	-0.343969000	0.677637000
6	-1.278893000	0.978328000	0.034637000
6	-0.322843000	2.136309000	0.154658000
1	0.565816000	1.929406000	-0.452297000
1	-0.801653000	3.050402000	-0.194659000
1	0.013057000	2.245152000	1.191024000
8	-2.355053000	1.092951000	-0.517076000
8	1.328272000	-0.506875000	1.665213000
8	1.082995000	-0.758624000	-0.559362000
6	2.506512000	-0.927191000	-0.697270000
6	3.213161000	0.415387000	-0.699286000
1	2.863560000	-1.563912000	0.115616000
1	2.626243000	-1.446402000	-1.649200000
1	3.074074000	0.923600000	0.258136000
1	4.285488000	0.269763000	-0.856620000
1	2.832967000	1.048547000	-1.506038000
1	-4.406830000	-1.705916000	-0.812740000
8	-3.586374000	-1.454659000	-0.380361000
1	-3.437325000	-0.514996000	-0.570826000
1	-1.381435000	-1.161416000	0.160759000
1	-1.211397000	-0.322138000	1.718208000

Water

TS

i = -1525 cm⁻¹

FE=-536.381279

6	-0.585003000	-0.766249000	-0.283279000
6	0.845761000	-0.499169000	-0.454419000
6	1.446502000	0.798721000	-0.283034000

6	0.681049000	2.072490000	-0.065231000
1	0.354367000	2.113941000	0.978129000
1	1.343725000	2.913794000	-0.270120000
1	-0.216378000	2.112916000	-0.684120000
8	2.710451000	0.884529000	-0.257483000
8	-1.194804000	-1.653890000	-0.843161000
8	-1.167281000	0.048608000	0.633282000
6	-2.573507000	-0.142454000	0.848529000
6	-3.389058000	0.536467000	-0.236973000
1	-2.783857000	-1.213883000	0.888229000
1	-2.762469000	0.302367000	1.827671000
1	-3.187061000	0.076131000	-1.206675000
1	-4.456714000	0.434901000	-0.021829000
1	-3.148212000	1.602324000	-0.286859000
1	3.238456000	-1.374620000	1.512179000
8	3.004178000	-1.329931000	0.576379000
1	3.131146000	-0.295968000	0.158050000
1	1.848777000	-1.205424000	0.372311000
1	1.263395000	-1.059846000	-1.292657000

Water

Product

FE=-536.424304

6	0.680696000	-0.679808000	-0.229972000
6	-0.726243000	-0.327970000	-0.065788000
6	-1.256374000	0.915692000	0.012547000
6	-0.532066000	2.229096000	-0.041796000
1	-0.004405000	2.337039000	-0.991552000
1	-1.259195000	3.033359000	0.072669000
1	0.219594000	2.289252000	0.747197000
8	-2.582100000	1.096199000	0.156177000
8	1.082886000	-1.825682000	-0.295963000
8	1.516538000	0.383872000	-0.311107000
6	2.910880000	0.080946000	-0.460253000
6	3.543250000	-0.279879000	0.871657000
1	3.022458000	-0.732204000	-1.181730000
1	3.344463000	0.994953000	-0.871998000
1	3.102657000	-1.198585000	1.264324000
1	4.618058000	-0.438287000	0.742178000
1	3.397870000	0.526163000	1.596059000
1	-4.251970000	-1.866351000	0.918196000
8	-3.921428000	-1.379211000	0.156813000
1	-3.050074000	0.240666000	0.177497000
1	-4.241023000	-1.829384000	-0.631653000
1	-1.386458000	-1.186509000	-0.006913000

Acetic acid

Reactant

FE=-689.009829

6	1.655104000	-0.390083000	0.837363000
6	0.347308000	0.339335000	1.035400000
6	0.213288000	1.535283000	0.106758000
6	1.444621000	2.365894000	-0.140685000
1	2.147996000	1.782231000	-0.745278000
1	1.178281000	3.280136000	-0.669809000
1	1.944935000	2.595227000	0.805459000
8	-0.857328000	1.828868000	-0.390411000
8	2.523281000	-0.507372000	1.668474000
8	1.735682000	-0.885382000	-0.408051000
6	2.949334000	-1.583893000	-0.745016000
6	4.049907000	-0.607199000	-1.114307000
1	3.239292000	-2.209270000	0.102262000
1	2.671499000	-2.216216000	-1.589221000
1	4.947097000	-1.155710000	-1.414344000
1	3.739375000	0.023085000	-1.952499000
1	4.305843000	0.024013000	-0.259633000
8	-3.377585000	0.681005000	-0.609100000
1	-2.468120000	1.033269000	-0.480972000
1	-0.503679000	-0.329603000	0.872257000
1	0.327882000	0.706853000	2.066428000
6	-3.467723000	-0.531909000	-0.065461000
6	-4.836412000	-1.132299000	-0.237730000
1	-5.587395000	-0.458382000	0.180800000
1	-5.050320000	-1.242634000	-1.303789000
1	-4.876349000	-2.101264000	0.255966000
8	-2.542663000	-1.079932000	0.498393000

Acetic acid

TS

i = -1332 cm⁻¹

FE=-688.948781

6	1.357676000	-0.324241000	0.813582000
6	0.105864000	0.436591000	1.043142000
6	-0.309997000	1.530323000	0.215371000
6	0.415461000	2.128103000	-0.928670000
1	0.200977000	1.468799000	-1.780868000
1	0.007429000	3.117550000	-1.137108000
1	1.493078000	2.145442000	-0.775076000
8	-1.492446000	1.993280000	0.422304000
8	1.961215000	-0.895384000	1.692990000
8	1.715885000	-0.358751000	-0.481634000
6	2.892753000	-1.126137000	-0.797576000
6	4.153609000	-0.329802000	-0.517946000
1	2.870838000	-2.051863000	-0.218195000
1	2.786164000	-1.356153000	-1.858813000
1	5.031477000	-0.906330000	-0.822703000
1	4.148179000	0.608383000	-1.080011000

1	4.238810000	-0.111263000	0.548725000
8	-2.371917000	-0.300161000	0.910696000
1	-2.053829000	1.219615000	0.823888000
1	-1.010070000	-0.214441000	0.931232000
1	-0.056479000	0.632849000	2.105830000
6	-2.670798000	-0.690831000	-0.321941000
6	-3.873586000	-1.596154000	-0.418934000
1	-3.674249000	-2.515153000	0.138524000
1	-4.734190000	-1.112210000	0.049201000
1	-4.086287000	-1.827390000	-1.461793000
8	-2.011205000	-0.347104000	-1.292480000

Acetic acid

Product

FE=-688.991063

6	-1.601770000	-0.655558000	-0.415971000
6	-0.326698000	-0.318677000	-1.054145000
6	0.417460000	0.794202000	-0.862350000
6	0.129092000	1.966011000	0.022628000
1	0.146598000	1.647664000	1.067372000
1	0.898553000	2.722353000	-0.135668000
1	-0.857382000	2.379281000	-0.189051000
8	1.602043000	0.941939000	-1.502698000
8	-2.184440000	-1.702324000	-0.618576000
8	-2.064803000	0.289561000	0.426581000
6	-3.309684000	-0.000799000	1.083761000
6	-4.489427000	0.296498000	0.176833000
1	-3.306851000	-1.046789000	1.398896000
1	-3.307051000	0.644949000	1.963877000
1	-5.425196000	0.128034000	0.717651000
1	-4.465406000	1.338040000	-0.154837000
1	-4.472290000	-0.358718000	-0.696579000
8	2.494585000	-1.475182000	-0.068299000
1	1.805825000	0.142016000	-2.008406000
1	1.574158000	-1.685050000	0.166538000
1	0.013039000	-1.077036000	-1.755194000
6	2.874608000	-0.443840000	0.717749000
6	4.259948000	0.035487000	0.395602000
1	4.925975000	-0.806655000	0.202515000
1	4.204725000	0.648890000	-0.508648000
1	4.629384000	0.645028000	1.218364000
8	2.141958000	0.025762000	1.554058000

Toluene

Reactant

FE=-731.378508

6	1.872623000	0.619386000	-0.405060000
6	0.983885000	1.679430000	0.073172000

6	-0.199675000	2.003373000	-0.492090000
6	-0.822432000	1.430597000	-1.718185000
1	-1.752384000	0.926135000	-1.432204000
1	-1.078532000	2.250049000	-2.396654000
1	-0.156003000	0.724008000	-2.205162000
8	-1.000260000	2.942871000	0.062479000
8	1.782871000	-0.031828000	-1.427232000
8	2.867808000	0.418880000	0.492384000
6	3.807096000	-0.618230000	0.176547000
6	3.251183000	-1.985984000	0.530649000
1	4.059692000	-0.558536000	-0.885043000
1	4.688207000	-0.378591000	0.774770000
1	4.011623000	-2.754206000	0.363237000
1	2.955115000	-2.017055000	1.583052000
1	2.384475000	-2.217733000	-0.093183000
1	-0.599583000	3.290461000	0.870096000
1	-0.383276000	0.556014000	2.455481000
1	1.297870000	2.174495000	0.988069000
6	-1.448352000	0.308521000	2.416590000
1	-2.024831000	1.237368000	2.461740000
1	-1.689047000	-0.274543000	3.312085000
6	-1.772322000	-0.465657000	1.164002000
6	-0.787993000	-1.212047000	0.509483000
6	-3.065363000	-0.459626000	0.631791000
6	-1.080274000	-1.928285000	-0.649073000
1	0.226446000	-1.215676000	0.903861000
6	-3.368218000	-1.184513000	-0.520346000
1	-3.840887000	0.124493000	1.121702000
6	-2.374791000	-1.919198000	-1.166827000
1	-0.290465000	-2.474461000	-1.156080000
1	-4.378295000	-1.166124000	-0.918796000
1	-2.605688000	-2.472095000	-2.071925000

Toluene

TS

i = -1849 cm⁻¹

FE=-731.290818

6	-1.787804000	-0.618626000	-0.375550000
6	-0.806035000	-1.578184000	0.172019000
6	0.373645000	-1.924213000	-0.550878000
6	0.758616000	-1.441591000	-1.910074000
1	0.966578000	-0.364228000	-1.858885000
1	1.658705000	-1.969535000	-2.226972000
1	-0.058819000	-1.568419000	-2.621212000
8	1.246833000	-2.541777000	0.157301000
8	-1.675851000	0.012968000	-1.404584000
8	-2.844993000	-0.498178000	0.452537000
6	-3.840419000	0.466557000	0.074107000

6	-3.397865000	1.873528000	0.433293000
1	-4.034072000	0.373740000	-0.997440000
1	-4.730159000	0.171366000	0.632746000
1	-4.196890000	2.585111000	0.206563000
1	-3.168899000	1.940718000	1.500520000
1	-2.513158000	2.152671000	-0.144014000
1	1.171761000	-1.960963000	1.174172000
1	-0.039684000	-1.138248000	1.206233000
1	-1.229251000	-2.364226000	0.796741000
6	1.146217000	-0.753724000	2.048121000
1	1.948838000	-1.260161000	2.597764000
1	0.432554000	-0.390003000	2.792760000
6	1.654231000	0.315276000	1.141907000
6	0.797696000	1.331988000	0.696173000
6	2.931189000	0.231595000	0.569405000
6	1.195923000	2.227754000	-0.292639000
1	-0.201845000	1.409564000	1.122059000
6	3.336339000	1.128251000	-0.414381000
1	3.601649000	-0.564110000	0.885758000
6	2.466602000	2.125908000	-0.857671000
1	0.508083000	2.996548000	-0.631843000
1	4.329223000	1.041527000	-0.845590000
1	2.777478000	2.817422000	-1.634381000

Toluene

Product

FE=-731.387341

6	1.758474000	0.920499000	-0.219461000
6	0.713587000	1.886141000	0.281668000
6	-0.604485000	2.006215000	-0.489831000
6	-0.772958000	1.336191000	-1.823149000
1	-0.603439000	0.258723000	-1.722698000
1	-1.782412000	1.528800000	-2.186175000
1	-0.022638000	1.706185000	-2.527338000
8	-1.479853000	2.677389000	0.015953000
8	2.052896000	0.746203000	-1.378837000
8	2.390340000	0.321614000	0.803980000
6	3.501070000	-0.527434000	0.459348000
6	3.031780000	-1.897169000	0.007297000
1	4.086464000	-0.035276000	-0.321398000
1	4.089919000	-0.584982000	1.376181000
1	3.897220000	-2.532337000	-0.202352000
1	2.434517000	-2.378241000	0.787329000
1	2.436208000	-1.811170000	-0.904251000
1	-1.836232000	1.396486000	2.092727000
1	0.477291000	1.686606000	1.328837000
1	1.171865000	2.883723000	0.250299000
6	-1.672264000	0.345513000	2.355598000
1	-2.470668000	0.046478000	3.042103000

1	-0.722669000	0.259659000	2.891445000
6	-1.681922000	-0.521075000	1.122005000
6	-0.596013000	-1.338018000	0.793590000
6	-2.800801000	-0.532511000	0.278847000
6	-0.635631000	-2.167977000	-0.329352000
1	0.286844000	-1.328662000	1.429119000
6	-2.844889000	-1.357084000	-0.841193000
1	-3.641993000	0.117592000	0.507243000
6	-1.762781000	-2.184647000	-1.147016000
1	0.213237000	-2.803971000	-0.561592000
1	-3.723416000	-1.352933000	-1.479390000
1	-1.796171000	-2.830200000	-2.018968000

Chloroform

Reactant

FE=-1879.215569

6	-2.184293000	0.092667000	-0.183172000
6	-1.445587000	1.190699000	-0.923592000
6	-0.944972000	2.282613000	0.010773000
6	-1.966945000	3.195418000	0.631129000
1	-2.659173000	2.596540000	1.230144000
1	-1.468288000	3.939923000	1.251149000
1	-2.547908000	3.690168000	-0.154499000
8	0.244747000	2.404089000	0.220038000
8	-2.635773000	0.187572000	0.934636000
8	-2.298332000	-0.995017000	-0.949771000
6	-2.998776000	-2.117614000	-0.376231000
6	-2.103595000	-2.898660000	0.566209000
1	-3.891798000	-1.748184000	0.134175000
1	-3.292071000	-2.715430000	-1.240226000
1	-2.628109000	-3.794005000	0.911854000
1	-1.188303000	-3.208002000	0.055203000
1	-1.843524000	-2.295464000	1.439205000
1	1.978820000	1.113433000	0.309339000
1	-0.604761000	0.755435000	-1.468526000
1	-2.146638000	1.612492000	-1.654750000
6	2.168809000	0.067253000	0.090514000
17	2.167247000	-0.118131000	-1.674538000
17	3.730901000	-0.402577000	0.776295000
17	0.846485000	-0.867194000	0.819062000

Chloroform

TS

i = -881 cm⁻¹

FE=-1879.124098

6	1.023954000	-0.584441000	-0.158708000
6	-0.283858000	-0.504599000	-0.861875000
6	-1.436748000	-1.139045000	-0.294167000

6	-1.503847000	-1.989630000	0.920299000
1	-1.336053000	-1.348246000	1.792678000
1	-2.492788000	-2.443669000	0.984140000
1	-0.707633000	-2.735131000	0.918555000
8	-2.549332000	-0.817643000	-0.860880000
8	1.194871000	-1.011566000	0.960792000
8	2.003729000	-0.094934000	-0.933002000
6	3.317613000	-0.046950000	-0.342802000
6	3.459826000	1.160949000	0.563678000
1	3.490602000	-0.977967000	0.202377000
1	3.993399000	0.006814000	-1.197613000
1	4.480446000	1.211913000	0.953104000
1	3.254968000	2.081013000	0.010397000
1	2.771420000	1.090375000	1.408513000
1	-2.416105000	0.163962000	-1.218301000
1	-0.834917000	0.649142000	-0.936229000
1	-0.208287000	-0.603586000	-1.946483000
6	-1.963339000	1.816092000	-0.907252000
1	-2.930130000	2.030270000	-1.372252000
1	-1.235007000	2.549883000	-1.255540000
6	-2.055079000	1.776500000	0.525780000
7	-2.053598000	1.540733000	1.664522000

Chloroform

Product

FE=-1879.205854

6	-2.091442000	0.577964000	-0.043620000
6	-0.939806000	1.296070000	-0.606315000
6	-0.264187000	2.280814000	0.022370000
6	-0.555089000	2.894157000	1.351906000
1	0.285006000	2.702347000	2.028015000
1	-0.627489000	3.978389000	1.225610000
1	-1.471297000	2.495431000	1.779222000
8	0.840872000	2.836879000	-0.529827000
8	-2.590377000	0.725274000	1.054594000
8	-2.545435000	-0.325679000	-0.935697000
6	-3.627837000	-1.162110000	-0.499085000
6	-3.116358000	-2.312546000	0.348901000
1	-4.346907000	-0.552575000	0.053550000
1	-4.085372000	-1.518877000	-1.423572000
1	-3.948521000	-2.962177000	0.635157000
1	-2.391470000	-2.908235000	-0.213061000
1	-2.644465000	-1.934254000	1.258810000
1	1.054552000	2.409960000	-1.371797000
1	1.450590000	0.411827000	0.631371000
1	-0.618142000	0.963182000	-1.589154000
6	1.844609000	-0.487541000	0.165284000
17	0.570158000	-1.712082000	0.178816000
17	2.298122000	-0.064055000	-1.503993000

17	3.261349000	-1.017843000	1.080274000
----	-------------	--------------	-------------

Dichloromethane

Reactant

FE=-1419.646309

6	-1.776365000	0.879614000	0.063230000
6	-0.883300000	1.769000000	-0.774347000
6	0.566542000	1.853005000	-0.302266000
6	0.852238000	2.034662000	1.163283000
1	0.677053000	1.083149000	1.676507000
1	1.893380000	2.332717000	1.287441000
1	0.169045000	2.759438000	1.612593000
8	1.454039000	1.800652000	-1.129836000
8	-1.861991000	0.924763000	1.268484000
8	-2.496720000	0.054411000	-0.706218000
6	-3.412735000	-0.821503000	-0.020646000
6	-2.693991000	-2.034895000	0.537869000
1	-3.912143000	-0.256149000	0.769902000
1	-4.138755000	-1.100921000	-0.785841000
1	-3.417571000	-2.707322000	1.007581000
1	-2.184602000	-2.581783000	-0.260417000
1	-1.962513000	-1.735258000	1.292278000
1	2.371466000	-0.212697000	-1.406425000
1	-0.891378000	1.455703000	-1.817902000
1	-1.301385000	2.782600000	-0.704718000
6	2.288412000	-1.101904000	-0.786584000
17	0.554726000	-1.392378000	-0.489838000
17	3.186220000	-0.815596000	0.716252000
1	2.693895000	-1.990392000	-1.262710000

Dichloromethane

TS

i = -1473 cm⁻¹

FE=-1419.549834

6	-1.436283000	0.709685000	-0.234288000
6	-0.108389000	0.828241000	-0.889546000
6	0.768353000	1.903927000	-0.542260000
6	0.477048000	3.055928000	0.349091000
1	0.459882000	2.688968000	1.381692000
1	1.264728000	3.801633000	0.238898000
1	-0.511550000	3.469540000	0.148585000
8	1.982570000	1.745854000	-0.939871000
8	-1.773447000	1.308570000	0.764052000
8	-2.206685000	-0.173119000	-0.879625000
6	-3.469844000	-0.491431000	-0.264523000

6	-3.277465000	-1.485998000	0.864926000
1	-3.932954000	0.433257000	0.088213000
1	-4.064331000	-0.912041000	-1.076903000
1	-4.249974000	-1.773046000	1.274661000
1	-2.773909000	-2.384484000	0.499577000
1	-2.681235000	-1.044813000	1.666842000
1	2.128189000	0.678389000	-0.925201000
1	0.772359000	-0.043824000	-0.567151000
1	-0.089599000	0.531705000	-1.940426000
6	2.081086000	-0.809835000	-0.220432000
17	1.383145000	-2.373797000	-0.743552000
17	1.928650000	-0.559319000	1.549205000
1	3.151340000	-0.895841000	-0.419158000

Dichloromethane

Product

FE=-1419.638145

6	1.043945000	1.299126000	-0.188744000
6	1.733617000	0.225287000	-0.912816000
6	2.556247000	-0.674731000	-0.332657000
6	2.917390000	-0.786320000	1.109379000
1	2.704573000	-1.806788000	1.441438000
1	3.992962000	-0.616987000	1.220637000
1	2.370500000	-0.064971000	1.710661000
8	3.155527000	-1.647861000	-1.056586000
8	1.286044000	1.722363000	0.921255000
8	0.039551000	1.793720000	-0.955022000
6	-0.747620000	2.847794000	-0.373439000
6	-1.817306000	2.281151000	0.541901000
1	-0.082586000	3.525952000	0.166534000
1	-1.182455000	3.366223000	-1.230029000
1	-2.434123000	3.091980000	0.940020000
1	-2.472561000	1.593769000	-0.002965000
1	-1.360320000	1.750090000	1.380233000
1	2.943402000	-1.552430000	-1.994176000
1	-1.083084000	-0.282618000	-0.866401000
1	1.517995000	0.156569000	-1.975893000
6	-1.346676000	-1.240491000	-0.422090000
17	-3.109497000	-1.438444000	-0.531596000
17	-0.768284000	-1.252534000	1.257950000
1	-0.878568000	-2.070841000	-0.944457000

Acetonitrile

Reactant

FE=-592.717055

6	0.459604000	-1.085519000	-0.451189000
6	-0.888935000	-0.889964000	-1.109969000
6	-2.032518000	-0.528472000	-0.157827000

6	-2.183052000	-1.315472000	1.112954000
1	-1.400357000	-0.998153000	1.810141000
1	-3.164039000	-1.115533000	1.543664000
1	-2.035492000	-2.383564000	0.934951000
8	-2.794141000	0.360260000	-0.476535000
8	0.690952000	-1.903355000	0.405813000
8	1.381431000	-0.263352000	-0.976940000
6	2.728500000	-0.413700000	-0.479047000
6	2.927894000	0.343433000	0.818641000
1	2.930769000	-1.479976000	-0.352207000
1	3.354417000	-0.016906000	-1.280543000
1	3.967186000	0.237829000	1.143344000
1	2.711789000	1.406578000	0.684891000
1	2.271568000	-0.045930000	1.599229000
1	0.294844000	2.176399000	-1.400666000
1	-0.837807000	-0.135158000	-1.895062000
1	-1.151078000	-1.854025000	-1.564888000
6	-0.451436000	2.561975000	-0.701310000
1	-1.454742000	2.347505000	-1.078577000
1	-0.321752000	3.638780000	-0.580339000
6	-0.282650000	1.888887000	0.584452000
7	-0.150811000	1.329532000	1.588162000

Acetonitrile

TS

i = -1335 cm⁻¹

FE=-592.62106

6	1.023954000	-0.584441000	-0.158708000
6	-0.283858000	-0.504599000	-0.861875000
6	-1.436748000	-1.139045000	-0.294167000
6	-1.503847000	-1.989630000	0.920299000
1	-1.336053000	-1.348246000	1.792678000
1	-2.492788000	-2.443669000	0.984140000
1	-0.707633000	-2.735131000	0.918555000
8	-2.549332000	-0.817643000	-0.860880000
8	1.194871000	-1.011566000	0.960792000
8	2.003729000	-0.094934000	-0.933002000
6	3.317613000	-0.046950000	-0.342802000
6	3.459826000	1.160949000	0.563678000
1	3.490602000	-0.977967000	0.202377000
1	3.993399000	0.006814000	-1.197613000
1	4.480446000	1.211913000	0.953104000
1	3.254968000	2.081013000	0.010397000
1	2.771420000	1.090375000	1.408513000
1	-2.416105000	0.163962000	-1.218301000
1	-0.834917000	0.649142000	-0.936229000
1	-0.208287000	-0.603586000	-1.946483000
6	-1.963339000	1.816092000	-0.907252000
1	-2.930130000	2.030270000	-1.372252000

1	-1.235007000	2.549883000	-1.255540000
6	-2.055079000	1.776500000	0.525780000
7	-2.053598000	1.540733000	1.664522000

Acetonitrile

Product

FE=-592.706274

6	-0.519390000	-1.010256000	0.036188000
6	-1.588609000	-0.360374000	-0.719429000
6	-2.540407000	0.391381000	-0.122637000
6	-2.666345000	0.678182000	1.340799000
1	-1.757249000	1.149565000	1.720353000
1	-3.525069000	1.329565000	1.504220000
1	-2.783520000	-0.252191000	1.900385000
8	-3.522951000	0.983628000	-0.833519000
8	-0.371081000	-0.985083000	1.244197000
8	0.331161000	-1.650305000	-0.792840000
6	1.425903000	-2.350532000	-0.174728000
6	2.560810000	-1.409258000	0.182977000
1	1.052643000	-2.873145000	0.709571000
1	1.734635000	-3.079700000	-0.925855000
1	3.413205000	-1.983263000	0.557281000
1	2.892380000	-0.845939000	-0.694196000
1	2.253715000	-0.711577000	0.965503000
1	-3.435597000	0.773412000	-1.772854000
1	0.761256000	1.335663000	0.714933000
1	-1.590106000	-0.508097000	-1.795095000
6	1.138344000	1.755195000	-0.221394000
1	0.562317000	2.645970000	-0.479094000
1	1.018501000	1.008753000	-1.010851000
6	2.553550000	2.095739000	-0.079047000
7	3.674674000	2.354943000	0.029517000

Ionic-liquid assisted tautomerization of EAA:

Cation-assisted keto-enol tautomerization:

CS_C

Reactant

FE=-1488.14258

6	1.479797000	1.046921000	1.527232000
6	1.253488000	2.334481000	0.763107000
6	1.406049000	2.277031000	-0.754078000
1	0.252232000	2.693301000	1.006194000
8	0.501641000	2.707524000	-1.450739000
8	0.719108000	0.638203000	2.376784000
8	2.626168000	0.458525000	1.201935000

6	2.843747000	-0.856692000	1.749502000
6	4.059773000	-1.426840000	1.054114000
1	2.980489000	-0.761765000	2.831721000
1	1.946099000	-1.451575000	1.557246000
1	4.938473000	-0.799185000	1.227505000
1	4.268940000	-2.427655000	1.442952000
1	3.868919000	-1.499863000	-0.019516000
7	-3.183143000	-0.428957000	0.677210000
6	-2.045317000	0.123894000	1.495128000
6	-3.627775000	0.546125000	-0.394561000
1	-4.189876000	1.335873000	0.112840000
1	-4.301559000	-0.019918000	-1.044056000
6	-2.508483000	1.194225000	-1.192551000
1	-2.318211000	1.118427000	1.846557000
1	-1.156902000	0.171152000	0.869084000
1	-1.869984000	-0.560010000	2.327051000
8	-0.397768000	-1.801368000	-2.218310000
8	0.296029000	-0.184513000	-0.508171000
8	2.009352000	-1.575183000	-1.631483000
8	0.415444000	-2.548485000	0.003535000
1	0.774371000	-3.388288000	-0.320004000
1	1.988604000	3.064647000	1.129076000
6	-4.340929000	-0.696892000	1.574560000
1	-4.062509000	-1.483607000	2.277117000
1	-4.585201000	0.217528000	2.116780000
1	-5.194123000	-1.017515000	0.973957000
1	-1.153130000	2.548664000	-0.813372000
1	-2.959210000	1.536395000	-2.135105000
1	-1.713501000	0.478419000	-1.439094000
8	-2.017436000	2.278164000	-0.441954000
6	-2.751489000	-1.715545000	0.039697000
1	-2.281553000	-2.338636000	0.801436000
1	-3.635434000	-2.206134000	-0.373134000
1	-2.028456000	-1.516748000	-0.752386000
6	2.684185000	1.778344000	-1.359173000
1	3.550248000	2.056820000	-0.754693000
1	2.643187000	0.682674000	-1.390186000
1	2.767333000	2.165608000	-2.375205000
16	0.613386000	-1.438072000	-1.219618000

CS_c
TS

i = -1521 cm⁻¹

FE=-1488.084545

6	1.239836000	1.204748000	1.479129000
6	0.626347000	2.110659000	0.490504000
6	1.093268000	2.288569000	-0.861470000
1	-0.650687000	1.837501000	0.153594000
8	0.276254000	2.853643000	-1.671802000

8	0.773456000	1.043803000	2.594571000
8	2.314658000	0.546381000	1.037634000
6	2.895850000	-0.413238000	1.935972000
6	3.994894000	-1.117160000	1.170846000
1	3.269034000	0.119365000	2.816937000
1	2.109008000	-1.100140000	2.255897000
1	4.774142000	-0.408879000	0.874933000
1	4.451761000	-1.886882000	1.799763000
1	3.586396000	-1.576086000	0.266353000
7	-2.977725000	-0.539078000	0.693005000
6	-1.722415000	-0.147222000	1.422720000
6	-3.512249000	0.603300000	-0.149967000
1	-3.877188000	1.360099000	0.550961000
1	-4.359421000	0.180735000	-0.699852000
6	-2.527837000	1.260898000	-1.113368000
1	-1.880066000	0.812815000	1.915793000
1	-0.914841000	-0.092964000	0.695106000
1	-1.493767000	-0.924833000	2.152693000
8	-0.119418000	-2.680498000	-1.829170000
8	0.052781000	-0.307529000	-1.180359000
8	2.111701000	-1.609813000	-1.601334000
8	0.688635000	-2.006531000	0.411125000
1	1.064185000	-2.895406000	0.499040000
1	0.271270000	3.036837000	0.948314000
6	-4.022405000	-0.899426000	1.692470000
1	-3.690014000	-1.780569000	2.242857000
1	-4.157800000	-0.062100000	2.378618000
1	-4.957395000	-1.115064000	1.172415000
1	-0.733169000	2.731756000	-1.251405000
1	-3.155500000	1.780591000	-1.851545000
1	-1.932004000	0.511644000	-1.648742000
8	-1.714479000	2.199540000	-0.463574000
6	-2.692409000	-1.732281000	-0.169948000
1	-2.215529000	-2.495826000	0.446190000
1	-3.636751000	-2.097443000	-0.577988000
1	-2.002636000	-1.455064000	-0.965194000
6	2.388406000	1.842186000	-1.432794000
1	3.215700000	2.084984000	-0.764468000
1	2.356390000	0.747676000	-1.521539000
1	2.516168000	2.287002000	-2.419843000
16	0.703148000	-1.634023000	-1.217575000

CS_C

Product

FE=-1488.126242

6	1.443869000	0.945274000	1.575826000
6	0.983357000	2.023838000	0.708494000
6	1.469839000	2.345114000	-0.515371000
1	-0.925624000	1.385690000	-1.026379000

8	0.840817000	3.265465000	-1.277151000
8	0.845448000	0.599608000	2.585011000
8	2.568843000	0.348592000	1.159324000
6	3.007770000	-0.803955000	1.884574000
6	3.951492000	-1.558075000	0.970768000
1	3.495971000	-0.472025000	2.807774000
1	2.131975000	-1.395407000	2.162897000
1	4.823958000	-0.945458000	0.727479000
1	4.299768000	-2.473142000	1.458938000
1	3.445553000	-1.811258000	0.033435000
7	-3.005159000	-0.376904000	0.832247000
6	-1.681983000	0.016917000	1.440059000
6	-3.616752000	0.760856000	0.043657000
1	-3.746185000	1.583452000	0.753388000
1	-4.602888000	0.406519000	-0.275100000
6	-2.845679000	1.263355000	-1.174207000
1	-1.811956000	0.950891000	1.987225000
1	-0.947608000	0.128177000	0.648942000
1	-1.360555000	-0.779880000	2.110452000
8	-0.375798000	-2.616809000	-1.922975000
8	-0.238935000	-0.208065000	-1.468109000
8	1.844098000	-1.498451000	-1.847296000
8	0.500210000	-1.754577000	0.228709000
1	0.974957000	-2.585825000	0.379362000
1	0.099957000	2.536887000	1.076741000
6	-3.944913000	-0.715159000	1.939789000
1	-3.529771000	-1.551264000	2.503475000
1	-4.049877000	0.153851000	2.590986000
1	-4.913021000	-0.991564000	1.518878000
1	-0.034778000	3.468129000	-0.912548000
1	-3.535631000	1.946319000	-1.685464000
1	-2.611386000	0.448224000	-1.867405000
8	-1.684446000	1.969931000	-0.828520000
6	-2.818665000	-1.586436000	-0.033744000
1	-2.363196000	-2.371818000	0.570407000
1	-3.796297000	-1.901420000	-0.404673000
1	-2.145310000	-1.351603000	-0.855443000
6	2.663653000	1.778472000	-1.214677000
1	3.541667000	1.791281000	-0.568925000
1	2.466828000	0.734604000	-1.486081000
1	2.846433000	2.359485000	-2.119339000
16	0.450582000	-1.518204000	-1.421106000

CP_C

Reactant

FE=-1432.054546

6	1.475152000	0.985494000	1.409140000
6	0.987665000	2.247547000	0.734868000
6	1.047243000	2.333288000	-0.787284000

1	-0.039878000	2.422471000	1.057244000
8	0.105919000	2.849939000	-1.369446000
8	0.851404000	0.407463000	2.271927000
8	2.695859000	0.637344000	1.010361000
6	3.239006000	-0.573138000	1.572014000
6	4.518478000	-0.870206000	0.824617000
1	3.397296000	-0.410664000	2.643552000
1	2.498984000	-1.366305000	1.443093000
1	5.227747000	-0.043459000	0.923550000
1	4.980964000	-1.773288000	1.233624000
1	4.285358000	-1.040036000	-0.228840000
7	-3.117113000	-0.594302000	0.641610000
6	-1.938645000	-0.089341000	1.434525000
6	-3.740496000	0.507781000	-0.187346000
1	-4.273285000	1.165592000	0.506129000
1	-4.463430000	0.009238000	-0.839756000
6	-2.760429000	1.351265000	-0.989010000
1	-2.252511000	0.790552000	1.996466000
1	-1.134015000	0.147639000	0.739445000
1	-1.606238000	-0.892953000	2.093098000
8	0.089938000	-0.141676000	-0.810904000
8	2.210580000	-1.646933000	-1.268919000
8	-0.098258000	-2.255067000	-2.190163000
8	0.313958000	-2.365326000	0.313010000
1	0.901356000	-3.126237000	0.401971000
1	1.611308000	3.072502000	1.109223000
1	-1.477505000	2.740242000	-0.558514000
1	-3.318236000	1.749959000	-1.848585000
1	-1.919882000	0.754146000	-1.369386000
8	-2.302530000	2.393303000	-0.160499000
6	-2.671873000	-1.706169000	-0.261157000
1	-2.099131000	-2.424527000	0.325904000
1	-3.559395000	-2.165182000	-0.701454000
1	-2.019240000	-1.299500000	-1.032282000
6	2.290494000	1.923329000	-1.517772000
1	3.172436000	2.363502000	-1.042116000
1	2.403719000	0.835678000	-1.460541000
1	2.207852000	2.244646000	-2.556159000
15	0.747789000	-1.479592000	-1.010793000
1	0.520889000	-2.659583000	-2.809855000
6	-4.147800000	-1.117462000	1.579342000
1	-5.032815000	-1.412407000	1.012314000
1	-3.734864000	-1.980495000	2.103223000
1	-4.402263000	-0.334258000	2.294727000

CP_C
TS

i = -1535 cm⁻¹

FE=-1431.997938

6	1.215173000	1.340863000	1.413112000
6	0.604123000	2.180520000	0.368653000
6	1.062300000	2.247361000	-0.996931000
1	-0.675120000	1.876704000	0.057057000
8	0.242291000	2.752770000	-1.842575000
8	0.757435000	1.253749000	2.540525000
8	2.281537000	0.643006000	1.008329000
6	2.838688000	-0.287119000	1.951777000
6	4.027208000	-0.938920000	1.277229000
1	3.113094000	0.258998000	2.859611000
1	2.060000000	-1.011316000	2.209293000
1	4.794437000	-0.192698000	1.050782000
1	4.465304000	-1.687044000	1.944948000
1	3.715351000	-1.416071000	0.342834000
7	-2.952656000	-0.516014000	0.727637000
6	-1.702992000	-0.068814000	1.437065000
6	-3.507508000	0.578872000	-0.163126000
1	-3.875342000	1.363605000	0.504935000
1	-4.354915000	0.120726000	-0.683612000
6	-2.540894000	1.200911000	-1.168068000
1	-1.883417000	0.905794000	1.892551000
1	-0.901989000	-0.027689000	0.698778000
1	-1.456336000	-0.813488000	2.195129000
8	0.023335000	-0.340624000	-1.102088000
8	2.229734000	-1.761231000	-1.398529000
8	-0.074110000	-2.750068000	-1.894052000
8	0.525879000	-2.183098000	0.498737000
1	1.134095000	-2.907520000	0.693143000
1	0.254996000	3.139527000	0.757289000
1	-0.764612000	2.660539000	-1.406270000
1	-3.184071000	1.667007000	-1.928883000
1	-1.927938000	0.436377000	-1.660979000
8	-1.742249000	2.190641000	-0.577959000
6	-2.647718000	-1.739744000	-0.084402000
1	-2.152196000	-2.465868000	0.561627000
1	-3.586849000	-2.135935000	-0.475509000
1	-1.963562000	-1.471221000	-0.888226000
6	2.357289000	1.761871000	-1.538257000
1	3.186487000	2.072685000	-0.900426000
1	2.341058000	0.663442000	-1.528944000
1	2.473752000	2.121331000	-2.560869000
15	0.785580000	-1.634941000	-1.039482000
1	0.522412000	-3.213224000	-2.494426000
6	-3.989174000	-0.851515000	1.743135000
1	-4.920051000	-1.110122000	1.235111000
1	-3.638088000	-1.698932000	2.333488000
1	-4.141397000	0.013737000	2.390130000

CP_C
Product

FE=-1432.044359

6	1.429926000	1.017206000	1.504927000
6	0.909697000	1.932787000	0.502918000
6	1.464355000	2.242305000	-0.698140000
1	-1.071317000	0.916830000	-1.299071000
8	0.766099000	2.962157000	-1.595414000
8	0.808689000	0.692940000	2.508763000
8	2.642372000	0.514712000	1.215790000
6	3.120419000	-0.561526000	2.024077000
6	4.129230000	-1.316728000	1.181757000
1	3.560347000	-0.152712000	2.940616000
1	2.269831000	-1.183101000	2.322230000
1	4.985441000	-0.679024000	0.945730000
1	4.492300000	-2.197147000	1.720235000
1	3.666982000	-1.620670000	0.236353000
7	-3.101026000	-0.277721000	0.907727000
6	-1.739577000	0.056500000	1.465759000
6	-3.663701000	0.872186000	0.096361000
1	-3.618653000	1.747907000	0.750538000
1	-4.713590000	0.620505000	-0.090512000
6	-2.983903000	1.189425000	-1.235611000
1	-1.812306000	0.984660000	2.033031000
1	-1.036523000	0.154330000	0.645517000
1	-1.419772000	-0.762118000	2.110065000
8	-0.575110000	-0.509186000	-1.564841000
8	1.975817000	-1.249427000	-1.589580000
8	0.070424000	-2.894687000	-1.998283000
8	0.348050000	-1.851963000	0.306099000
1	1.155986000	-2.253646000	0.650260000
1	-0.077974000	2.319222000	0.728395000
1	-0.180145000	2.962860000	-1.366095000
1	-3.623866000	1.950691000	-1.701310000
1	-2.990878000	0.310782000	-1.893092000
8	-1.689568000	1.690354000	-1.095410000
6	-3.006426000	-1.526048000	0.083298000
1	-2.677165000	-2.335248000	0.736505000
1	-3.994521000	-1.742842000	-0.329417000
1	-2.263496000	-1.374062000	-0.702337000
6	2.819054000	1.874927000	-1.211877000
1	3.584616000	2.022248000	-0.450580000
1	2.813175000	0.812328000	-1.486204000
1	3.031414000	2.480844000	-2.093975000
15	0.537038000	-1.497443000	-1.289604000
1	0.820632000	-3.270614000	-2.474430000
6	-4.027538000	-0.517725000	2.051030000
1	-5.007286000	-0.805457000	1.665881000
1	-3.618001000	-1.317860000	2.668495000
1	-4.107013000	0.397926000	2.639135000

NS_{Ca}

Reactant

FE=-1448.875293

6	-1.400597000	-1.304512000	1.351704000
6	-1.084553000	-2.473398000	0.441529000
6	-1.064821000	-2.182441000	-1.056708000
1	-0.116202000	-2.876623000	0.740977000
8	-0.062969000	-2.453166000	-1.697490000
8	-0.733955000	-1.021620000	2.322982000
8	-2.508528000	-0.665953000	0.991613000
6	-2.767713000	0.583262000	1.662618000
6	-3.823367000	1.307260000	0.856733000
1	-3.090803000	0.365300000	2.685863000
1	-1.831591000	1.146989000	1.695727000
1	-4.744142000	0.720003000	0.799199000
1	-4.053406000	2.264606000	1.333451000
1	-3.453263000	1.499072000	-0.154595000
7	3.214243000	0.459767000	1.210318000
6	2.057774000	-0.261922000	1.846395000
6	3.851724000	-0.297732000	0.067653000
1	4.401791000	-1.133010000	0.510345000
1	4.552014000	0.398487000	-0.400412000
6	2.859930000	-0.850540000	-0.942241000
1	2.341771000	-1.296857000	2.028497000
1	1.214582000	-0.216093000	1.159764000
1	1.808600000	0.257727000	2.772092000
8	0.877283000	2.025197000	-1.762761000
8	-0.097397000	0.287301000	-0.332183000
8	-1.578474000	1.645079000	-1.784861000
8	-0.489550000	2.608047000	0.225262000
1	-0.812389000	3.445433000	-0.139723000
1	-1.855148000	-3.237808000	0.610427000
1	1.517253000	-2.276449000	-0.896232000
1	3.426797000	-1.040196000	-1.864950000
1	2.074572000	-0.119764000	-1.174893000
8	2.334630000	-2.042379000	-0.411660000
6	2.821915000	1.845138000	0.801187000
1	2.258101000	2.302292000	1.614255000
1	3.729606000	2.412950000	0.590432000
1	2.195689000	1.793629000	-0.092210000
6	-2.295380000	-1.646308000	-1.724524000
1	-3.206520000	-2.030700000	-1.260991000
1	-2.295633000	-0.555729000	-1.608165000
1	-2.255140000	-1.888851000	-2.786997000
16	-0.318939000	1.557740000	-1.049492000
1	3.938981000	0.550487000	1.924487000

NS_{Ca}

TS

i = -1522 cm⁻¹
FE=-1448.817687

6	-1.126837000	-1.457120000	1.256178000
6	-0.306354000	-2.173034000	0.263515000
6	-0.572982000	-2.195229000	-1.153064000
1	0.966034000	-1.737778000	0.149174000
8	0.396894000	-2.566135000	-1.905077000
8	-0.844704000	-1.429904000	2.442743000
8	-2.166963000	-0.795702000	0.741711000
6	-2.928039000	0.013845000	1.654287000
6	-4.002045000	0.699383000	0.838032000
1	-3.339330000	-0.634449000	2.434443000
1	-2.246053000	0.729435000	2.120261000
1	-4.682318000	-0.036557000	0.399736000
1	-4.586434000	1.366070000	1.478929000
1	-3.548024000	1.276117000	0.027248000
7	2.916221000	0.722773000	1.285776000
6	1.639153000	0.146273000	1.828196000
6	3.699999000	-0.236021000	0.417344000
1	4.034362000	-1.047118000	1.070357000
1	4.566108000	0.331809000	0.064724000
6	2.928576000	-0.833326000	-0.756390000
1	1.823741000	-0.863598000	2.194155000
1	0.914550000	0.147424000	1.015533000
1	1.285283000	0.794212000	2.630447000
8	0.342157000	2.855341000	-1.467342000
8	0.220478000	0.453209000	-0.935951000
8	-1.834567000	1.662755000	-1.595755000
8	-0.731929000	2.039677000	0.610661000
1	-1.206660000	2.881570000	0.678968000
1	0.075990000	-3.121513000	0.647090000
1	1.321538000	-2.418332000	-1.335477000
1	3.695956000	-1.193004000	-1.456478000
1	2.336082000	-0.066083000	-1.270570000
8	2.134486000	-1.913596000	-0.349182000
6	2.666998000	2.031764000	0.601808000
1	2.055000000	2.652661000	1.256131000
1	3.628085000	2.506143000	0.398891000
1	2.114850000	1.858709000	-0.321584000
6	-1.823072000	-1.787137000	-1.841983000
1	-2.700307000	-2.183771000	-1.328898000
1	-1.890245000	-0.691356000	-1.794830000
1	-1.778620000	-2.107870000	-2.883023000
16	-0.496891000	1.742545000	-1.015415000
1	3.517916000	0.915605000	2.088954000

NS_{Ca}
Product
FE=-1448.858818

6	-1.425038000	-1.145404000	1.360531000
6	-0.779115000	-2.119608000	0.487721000
6	-1.055435000	-2.345553000	-0.819584000
1	1.306848000	-1.210832000	-0.858530000
8	-0.269202000	-3.166293000	-1.549082000
8	-1.018601000	-0.883915000	2.484068000
8	-2.488834000	-0.539865000	0.816466000
6	-3.109043000	0.499755000	1.581055000
6	-3.984316000	1.277902000	0.621046000
1	-3.681896000	0.041477000	2.394862000
1	-2.326243000	1.117828000	2.027279000
1	-4.765243000	0.634925000	0.205660000
1	-4.465823000	2.112118000	1.139693000
1	-3.381257000	1.659451000	-0.208852000
7	2.968955000	0.451069000	1.378778000
6	1.614431000	-0.053663000	1.804845000
6	3.784030000	-0.556352000	0.605241000
1	3.864717000	-1.440210000	1.244007000
1	4.775497000	-0.110379000	0.477268000
6	3.218432000	-0.964132000	-0.751575000
1	1.726686000	-1.046658000	2.238147000
1	0.969608000	-0.078466000	0.932119000
1	1.201203000	0.644134000	2.532262000
8	0.693573000	2.831818000	-1.494359000
8	0.577202000	0.401291000	-1.179527000
8	-1.479484000	1.653453000	-1.774886000
8	-0.431222000	1.833549000	0.474009000
1	-0.963058000	2.633681000	0.600289000
1	0.059713000	-2.633405000	0.947848000
1	0.552510000	-3.362596000	-1.073097000
1	4.010629000	-1.544605000	-1.239573000
1	3.010249000	-0.089497000	-1.377359000
8	2.075426000	-1.768433000	-0.627531000
6	2.868043000	1.772523000	0.681145000
1	2.279592000	2.444722000	1.305222000
1	3.875238000	2.162957000	0.527033000
1	2.349209000	1.643253000	-0.267224000
6	-2.158627000	-1.766227000	-1.646196000
1	-3.122976000	-1.879425000	-1.150544000
1	-1.985573000	-0.693191000	-1.789498000
1	-2.167127000	-2.266371000	-2.615276000
16	-0.156977000	1.687632000	-1.163856000
1	3.495417000	0.613224000	2.239875000

NS_{Cb}

Reactant

FE=-1448.899304

6	1.684753000	1.259193000	1.357862000
---	-------------	-------------	-------------

6	1.374338000	2.502733000	0.547750000
6	1.053422000	2.256951000	-0.923701000
1	0.532998000	3.014267000	1.016132000
8	-0.020544000	2.628676000	-1.364546000
8	1.076336000	0.941019000	2.352366000
8	2.721819000	0.593589000	0.855165000
6	2.961897000	-0.722232000	1.390322000
6	3.761982000	-1.477847000	0.352694000
1	3.497083000	-0.615519000	2.339566000
1	1.995848000	-1.196478000	1.574361000
1	4.719325000	-0.986559000	0.158131000
1	3.956890000	-2.493992000	0.707132000
1	3.197685000	-1.540785000	-0.582605000
7	-2.675666000	-0.592746000	0.727614000
6	-1.903237000	0.161372000	1.755007000
6	-3.552511000	0.266112000	-0.127708000
1	-4.276899000	0.766933000	0.523701000
1	-4.076354000	-0.418590000	-0.800147000
6	-2.774622000	1.288636000	-0.938580000
1	-2.610663000	0.592688000	2.467566000
1	-1.330116000	0.944883000	1.271478000
1	-1.214017000	-0.527248000	2.244256000
8	-1.317976000	-2.001405000	-1.118605000
8	0.237404000	-0.382379000	-0.186943000
8	0.921972000	-1.741872000	-2.162287000
8	0.716033000	-2.740138000	0.091366000
1	0.899620000	-3.548850000	-0.410062000
1	2.258962000	3.151573000	0.584585000
1	-1.672663000	2.807023000	-0.477098000
1	-3.398135000	1.568948000	-1.798276000
1	-1.852767000	0.833714000	-1.326078000
8	-2.494749000	2.414329000	-0.137474000
6	2.084840000	1.625819000	-1.813842000
1	3.099704000	1.886048000	-1.506589000
1	1.980022000	0.538340000	-1.732157000
1	1.890750000	1.921630000	-2.845454000
16	0.114101000	-1.628055000	-0.956747000
6	-3.446008000	-1.699573000	1.342417000
1	-3.911169000	-2.288577000	0.551173000
1	-2.756923000	-2.328167000	1.907377000
1	-4.206511000	-1.283121000	2.006689000
1	-2.010110000	-1.061594000	0.055320000

NS_{cb}

TS

i = -1792 cm⁻¹

FE=-1448.842096

6	1.655617000	0.989027000	1.393106000
6	1.139422000	2.125071000	0.607875000

6	1.444456000	2.406778000	-0.764479000
1	-0.249683000	2.089647000	0.361386000
8	0.691555000	3.249605000	-1.362572000
8	1.220709000	0.709037000	2.495999000
8	2.594730000	0.268427000	0.773994000
6	2.839611000	-1.047196000	1.297474000
6	3.494086000	-1.844870000	0.190478000
1	3.475950000	-0.959717000	2.184135000
1	1.882571000	-1.484966000	1.591202000
1	4.429709000	-1.377713000	-0.130435000
1	3.715383000	-2.856487000	0.542567000
1	2.821023000	-1.916108000	-0.669059000
7	-2.804124000	-0.088784000	0.583920000
6	-1.881248000	0.266349000	1.697509000
6	-3.122599000	1.050220000	-0.326859000
1	-3.651020000	1.813266000	0.255846000
1	-3.798521000	0.646190000	-1.085950000
6	-1.914910000	1.664454000	-1.015870000
1	-2.261529000	1.147508000	2.219514000
1	-0.886864000	0.448144000	1.299304000
1	-1.819298000	-0.585699000	2.375680000
8	-1.763505000	-1.992302000	-0.825744000
8	0.249758000	-0.655721000	-0.484965000
8	0.288835000	-2.594111000	-2.064534000
8	0.193745000	-2.922838000	0.379770000
1	0.241557000	-3.833442000	0.051730000
1	0.929742000	3.005393000	1.217682000
1	-0.401528000	3.139566000	-0.806711000
1	-2.278153000	2.206084000	-1.896387000
1	-1.225641000	0.878329000	-1.351781000
8	-1.245883000	2.584818000	-0.164935000
6	2.458889000	1.695688000	-1.598009000
1	3.427956000	1.652989000	-1.099950000
1	2.116325000	0.659533000	-1.713140000
1	2.522343000	2.182609000	-2.571122000
16	-0.264068000	-1.973842000	-0.872660000
6	-4.049707000	-0.704517000	1.097833000
1	-4.679272000	-0.992146000	0.255008000
1	-3.786246000	-1.593637000	1.671044000
1	-4.574298000	0.011734000	1.735358000
1	-2.317805000	-0.859445000	-0.011246000

NS_{Cb}

Product

FE=-1448.876971

6	1.726569000	1.110504000	1.331910000
6	1.371479000	2.275866000	0.516357000
6	1.458441000	2.351674000	-0.832603000
1	-0.947734000	2.446286000	0.724668000

8	0.870924000	3.367284000	-1.504561000
8	1.197602000	0.887110000	2.408811000
8	2.644356000	0.316740000	0.779958000
6	2.800850000	-0.987522000	1.363287000
6	3.482546000	-1.850214000	0.323952000
1	3.391979000	-0.890700000	2.279990000
1	1.811466000	-1.373858000	1.617266000
1	4.460740000	-1.441574000	0.054826000
1	3.622978000	-2.861273000	0.716534000
1	2.865131000	-1.910094000	-0.577463000
7	-2.798062000	-0.191709000	0.529184000
6	-2.011637000	0.218116000	1.723949000
6	-3.093856000	0.916394000	-0.430005000
1	-3.846062000	1.566611000	0.030739000
1	-3.525369000	0.434264000	-1.312266000
6	-1.887146000	1.753822000	-0.837566000
1	-2.513669000	1.054661000	2.215995000
1	-0.993695000	0.469780000	1.426549000
1	-1.950451000	-0.637462000	2.398185000
8	-1.693512000	-2.137572000	-0.800271000
8	0.178828000	-0.701494000	-0.219386000
8	0.414370000	-2.345136000	-2.085380000
8	0.342560000	-3.072701000	0.271540000
1	0.494688000	-3.907145000	-0.196949000
1	0.908301000	3.086326000	1.073913000
1	0.264263000	3.845829000	-0.918879000
1	-2.138509000	2.249692000	-1.779427000
1	-1.010735000	1.115328000	-1.008644000
8	-1.607987000	2.778894000	0.101859000
6	2.132977000	1.387881000	-1.758419000
1	3.192404000	1.297179000	-1.513140000
1	1.687536000	0.395345000	-1.644125000
1	2.011815000	1.739300000	-2.783465000
16	-0.203945000	-1.985717000	-0.819244000
6	-4.051288000	-0.879238000	0.922970000
1	-4.584278000	-1.185284000	0.021923000
1	-3.792709000	-1.763863000	1.505328000
1	-4.668030000	-0.200802000	1.517142000
1	-2.241246000	-0.943815000	-0.008652000

NP_{Ca}

Reactant

FE=-1392.788283

6	-1.322946000	-1.199444000	1.247046000
6	-0.657491000	-2.338191000	0.507692000
6	-0.537928000	-2.253553000	-1.010851000
1	0.338015000	-2.473767000	0.932981000
8	0.509668000	-2.615443000	-1.524344000
8	-0.843427000	-0.671788000	2.226261000

8	-2.521454000	-0.905273000	0.750884000
6	-3.223324000	0.192933000	1.365507000
6	-4.453817000	0.452932000	0.527875000
1	-3.459912000	-0.087899000	2.397306000
1	-2.551850000	1.054479000	1.381638000
1	-5.090723000	-0.435348000	0.487193000
1	-5.030742000	1.271851000	0.967485000
1	-4.145455000	0.739333000	-0.479931000
7	3.122995000	0.854536000	1.084139000
6	1.963433000	0.175464000	1.763897000
6	3.963224000	-0.077550000	0.245910000
1	4.501736000	-0.735216000	0.934231000
1	4.676036000	0.558745000	-0.285181000
6	3.158780000	-0.936724000	-0.717260000
1	2.329238000	-0.720707000	2.263750000
1	1.227130000	-0.068650000	0.999164000
1	1.521958000	0.884857000	2.464178000
8	0.186800000	0.288430000	-0.672201000
8	-2.035064000	1.591280000	-1.241263000
8	0.264806000	2.555983000	-1.807652000
8	-0.417453000	2.338520000	0.621833000
1	-1.059500000	3.056231000	0.692089000
1	-1.246817000	-3.243096000	0.715668000
1	1.978371000	-2.461115000	-0.525809000
1	3.833603000	-1.209578000	-1.541238000
1	2.305409000	-0.383789000	-1.135040000
8	2.725376000	-2.079662000	-0.019776000
6	2.675222000	2.043089000	0.289851000
1	1.964785000	2.618247000	0.883315000
1	3.554979000	2.633038000	0.028244000
1	2.163447000	1.689839000	-0.604670000
6	-1.726986000	-1.873427000	-1.841220000
1	-2.612163000	-2.427822000	-1.514505000
1	-1.944823000	-0.808834000	-1.702139000
1	-1.502772000	-2.081742000	-2.887581000
15	-0.601079000	1.561213000	-0.821590000
1	-0.315469000	2.897854000	-2.498561000
1	3.737704000	1.203610000	1.821669000

NP_{Ca}
TS

i = -1537 cm⁻¹

FE=-1392.730918

6	-1.106334000	-1.567143000	1.171771000
6	-0.258074000	-2.202187000	0.149047000
6	-0.498760000	-2.131531000	-1.271314000
1	1.014489000	-1.752581000	0.084913000
8	0.484967000	-2.453713000	-2.026602000
8	-0.845581000	-1.607778000	2.362603000

8	-2.155418000	-0.896415000	0.682994000
6	-2.941026000	-0.155366000	1.631031000
6	-4.058087000	0.505492000	0.852052000
1	-3.308304000	-0.845979000	2.396498000
1	-2.284252000	0.573537000	2.115755000
1	-4.715395000	-0.249425000	0.410789000
1	-4.657279000	1.130323000	1.521242000
1	-3.642078000	1.118159000	0.046204000
7	2.870646000	0.711096000	1.326418000
6	1.593724000	0.096180000	1.827990000
6	3.699414000	-0.220545000	0.471873000
1	4.017588000	-1.041048000	1.121404000
1	4.572532000	0.363964000	0.166380000
6	2.986369000	-0.801146000	-0.746680000
1	1.799604000	-0.907470000	2.200407000
1	0.899627000	0.080130000	0.988205000
1	1.195106000	0.735041000	2.616180000
8	0.323167000	0.530317000	-0.936362000
8	-1.971526000	1.747828000	-1.422565000
8	0.246265000	3.016725000	-1.431213000
8	-0.627485000	2.089553000	0.758233000
1	-1.348185000	2.707068000	0.936597000
1	0.126424000	-3.171031000	0.475217000
1	1.399084000	-2.339089000	-1.427577000
1	3.789755000	-1.134788000	-1.419521000
1	2.399894000	-0.033035000	-1.266226000
8	2.191749000	-1.902760000	-0.401869000
6	2.611739000	2.019857000	0.644302000
1	1.946750000	2.613482000	1.271882000
1	3.567271000	2.522615000	0.488014000
1	2.107301000	1.820982000	-0.300695000
6	-1.742713000	-1.694072000	-1.953830000
1	-2.620166000	-2.149837000	-1.491876000
1	-1.841774000	-0.607355000	-1.824560000
1	-1.670567000	-1.933622000	-3.014969000
15	-0.590767000	1.721581000	-0.854263000
1	-0.312016000	3.500352000	-2.051915000
1	3.444961000	0.910942000	2.147478000

NP_{Ca}

Product

FE=-1392.775362

6	-1.417791000	-1.195889000	1.300246000
6	-0.716510000	-1.990008000	0.303923000
6	-1.071603000	-2.181354000	-0.993397000
1	1.460778000	-0.721386000	-1.068703000
8	-0.219898000	-2.785359000	-1.842521000
8	-0.968919000	-0.964042000	2.415351000
8	-2.590296000	-0.695385000	0.878167000

6	-3.223682000	0.285642000	1.701279000
6	-4.138973000	1.080925000	0.791751000
1	-3.766257000	-0.220112000	2.507661000
1	-2.451360000	0.906171000	2.167463000
1	-4.916668000	0.435576000	0.374170000
1	-4.623178000	1.888576000	1.348712000
1	-3.560146000	1.494522000	-0.041126000
7	3.077997000	0.262667000	1.453776000
6	1.680984000	-0.159055000	1.830335000
6	3.832774000	-0.769556000	0.649143000
1	3.733941000	-1.710948000	1.196297000
1	4.881670000	-0.454700000	0.657130000
6	3.360754000	-0.958613000	-0.791151000
1	1.719851000	-1.156866000	2.265616000
1	1.066063000	-0.144707000	0.936998000
1	1.285662000	0.559915000	2.546799000
8	0.951648000	0.720387000	-1.238820000
8	-1.599986000	1.379317000	-1.567235000
8	0.265283000	3.119254000	-1.536481000
8	-0.278292000	1.842718000	0.593815000
1	-1.115836000	2.245393000	0.855572000
1	0.238099000	-2.378508000	0.640374000
1	0.681104000	-2.786371000	-1.473916000
1	4.081768000	-1.650471000	-1.245279000
1	3.419371000	-0.012024000	-1.343767000
8	2.076175000	-1.497664000	-0.870666000
6	3.082900000	1.619797000	0.820652000
1	2.632722000	2.320883000	1.523620000
1	4.115394000	1.897821000	0.601242000
1	2.473499000	1.575782000	-0.084675000
6	-2.346453000	-1.789697000	-1.668352000
1	-3.212825000	-2.053561000	-1.062159000
1	-2.347991000	-0.701168000	-1.805952000
1	-2.391154000	-2.284536000	-2.639573000
15	-0.231206000	1.643442000	-1.039277000
1	-0.417783000	3.510016000	-2.094735000
1	3.595258000	0.343445000	2.331497000

NP_{Cb}

Reactant

FE=-1392.819653

6	-1.087586000	-1.469364000	1.260968000
6	-0.497029000	-2.522536000	0.347429000
6	-0.491511000	-2.220701000	-1.149329000
1	0.527890000	-2.712857000	0.670496000
8	0.552082000	-2.344699000	-1.767915000
8	-0.531091000	-1.067207000	2.260095000
8	-2.298527000	-1.084763000	0.874339000
6	-2.857465000	0.056888000	1.552943000

6	-3.941141000	0.611779000	0.653978000
1	-3.241919000	-0.273325000	2.523364000
1	-2.056011000	0.782025000	1.716340000
1	-4.725605000	-0.130569000	0.483029000
1	-4.394593000	1.489951000	1.123255000
1	-3.516725000	0.905923000	-0.311671000
7	2.153636000	0.513863000	1.084628000
6	2.542104000	-0.540807000	2.058930000
6	3.172880000	0.698289000	0.002208000
1	4.161681000	0.568440000	0.455139000
1	3.072666000	1.718787000	-0.375762000
6	2.951045000	-0.268214000	-1.153734000
1	3.403893000	-0.178559000	2.627343000
1	2.809143000	-1.437621000	1.503776000
1	1.692256000	-0.730268000	2.713774000
8	-0.042511000	0.330464000	-0.258650000
8	-1.639257000	1.554996000	-1.954986000
8	0.775619000	2.334213000	-1.498666000
8	-1.008102000	2.568234000	0.314328000
1	-1.697228000	3.177825000	0.020883000
1	-1.082767000	-3.442327000	0.484251000
1	2.236073000	-2.073798000	-1.094346000
1	3.743671000	-0.083073000	-1.891594000
1	1.984888000	-0.047472000	-1.619174000
8	2.994552000	-1.604375000	-0.702581000
6	-1.772639000	-1.878294000	-1.851891000
1	-2.632716000	-2.360739000	-1.383785000
1	-1.922556000	-0.792988000	-1.791684000
1	-1.679995000	-2.159884000	-2.901684000
15	-0.568206000	1.587973000	-0.922034000
1	0.567879000	2.814113000	-2.310464000
6	1.852766000	1.786864000	1.784579000
1	1.486100000	2.511574000	1.056130000
1	1.073219000	1.593273000	2.523536000
1	2.761123000	2.153711000	2.270095000
1	1.226626000	0.272880000	0.582661000

NP_{cb}

TS

i = -1621 cm⁻¹

FE=-1392.7617

6	0.998528000	1.509324000	1.246172000
6	0.074264000	2.169681000	0.310045000
6	0.285789000	2.278397000	-1.111640000
1	-1.192717000	1.662923000	0.193805000
8	-0.719099000	2.654965000	-1.809299000
8	0.840469000	1.523593000	2.453947000
8	2.012144000	0.859506000	0.657254000
6	2.932705000	0.189827000	1.532899000

6	4.036808000	-0.371855000	0.662484000
1	3.303332000	0.910293000	2.268349000
1	2.386814000	-0.591309000	2.069615000
1	4.591119000	0.437223000	0.178238000
1	4.736480000	-0.947953000	1.275261000
1	3.617659000	-1.008452000	-0.122302000
7	-2.222709000	-0.839206000	0.868468000
6	-1.821488000	-0.222615000	2.157207000
6	-3.464264000	-0.232760000	0.293132000
1	-4.029900000	0.230401000	1.107947000
1	-4.066967000	-1.035040000	-0.141842000
6	-3.125435000	0.786433000	-0.785731000
1	-2.519701000	-0.539271000	2.938217000
1	-1.838208000	0.862878000	2.061720000
1	-0.805815000	-0.542611000	2.397458000
8	-0.407243000	-0.550320000	-0.859906000
8	1.915564000	-1.438408000	-1.692754000
8	-0.097039000	-2.998516000	-1.486983000
8	0.886551000	-2.042137000	0.625951000
1	1.604502000	-2.681650000	0.720971000
1	-0.363243000	3.069788000	0.747897000
1	-1.636722000	2.437053000	-1.195115000
1	-4.070708000	1.179636000	-1.181932000
1	-2.588944000	0.280443000	-1.600445000
8	-2.363942000	1.849652000	-0.265391000
6	1.525428000	1.944993000	-1.860628000
1	2.405336000	2.357695000	-1.364328000
1	1.649493000	0.852700000	-1.863169000
1	1.429983000	2.308481000	-2.883961000
15	0.647160000	-1.645296000	-0.945846000
1	0.359309000	-3.321698000	-2.273865000
6	-2.320177000	-2.312380000	0.992718000
1	-2.442958000	-2.740011000	-0.004363000
1	-1.387387000	-2.683479000	1.419555000
1	-3.169040000	-2.572209000	1.631713000
1	-1.392351000	-0.672900000	0.126485000

NP_{cb}

Product

FE=-1392.810418

6	-1.663421000	-0.417435000	1.241959000
6	-1.034357000	-1.651254000	0.794483000
6	-1.388622000	-2.344072000	-0.316056000
1	1.222030000	-1.396916000	-0.525977000
8	-0.647649000	-3.380685000	-0.751721000
8	-1.076501000	0.417179000	1.932795000
8	-2.925821000	-0.259371000	0.855488000
6	-3.496611000	1.047316000	1.026243000
6	-4.785641000	1.063850000	0.234667000

1	-3.657259000	1.224220000	2.094480000
1	-2.784543000	1.780110000	0.639684000
1	-5.473808000	0.292254000	0.590579000
1	-5.272515000	2.037574000	0.335790000
1	-4.570852000	0.887986000	-0.822451000
7	2.962830000	0.361808000	0.660440000
6	2.310255000	0.239900000	1.986254000
6	3.815351000	-0.830005000	0.353317000
1	4.028175000	-1.345409000	1.294732000
1	4.762278000	-0.486320000	-0.073288000
6	3.114857000	-1.771397000	-0.628810000
1	3.078350000	0.217580000	2.765994000
1	1.725630000	-0.679712000	2.002442000
1	1.643234000	1.088783000	2.128469000
8	1.182720000	0.349013000	-1.104020000
8	-1.333112000	1.057584000	-1.238079000
8	0.597536000	2.555284000	-2.098364000
8	0.321892000	2.213684000	0.365902000
1	-0.252858000	1.803724000	1.044987000
1	-0.138520000	-1.930254000	1.338854000
1	0.219469000	-3.391516000	-0.311525000
1	3.700385000	-2.692469000	-0.703940000
1	3.065904000	-1.306321000	-1.619995000
8	1.815072000	-2.101571000	-0.186480000
6	-2.547515000	-2.061203000	-1.220702000
1	-3.495594000	-2.182663000	-0.693739000
1	-2.480719000	-1.020939000	-1.557032000
1	-2.502164000	-2.740440000	-2.072315000
15	0.093397000	1.436764000	-1.046699000
1	-0.134700000	3.124021000	-2.367308000
6	3.681746000	1.647479000	0.533182000
1	4.075991000	1.730529000	-0.481085000
1	2.964576000	2.452450000	0.705049000
1	4.497450000	1.697199000	1.260969000
1	2.129934000	0.404409000	-0.127358000

Anion-assisted keto-eneol tautomerization of EAA:

CS_A

Reactant

FE=-1488.130612

6	4.331032000	0.201985000	0.540677000
6	2.931167000	-0.136106000	0.085969000
6	2.428629000	-1.437767000	0.688984000
1	2.256665000	0.676771000	0.377353000
6	2.109039000	-1.444128000	2.156093000
1	1.810055000	-2.446605000	2.461937000
1	2.976623000	-1.105263000	2.728307000

1	1.281933000	-0.743741000	2.312220000
8	2.281346000	-2.423210000	-0.010655000
8	4.932487000	-0.335159000	1.443168000
8	4.843220000	1.204886000	-0.186485000
6	6.172474000	1.620719000	0.168042000
6	6.558784000	2.738346000	-0.775479000
1	6.171118000	1.943881000	1.213492000
1	6.842030000	0.759463000	0.085486000
1	5.866188000	3.578386000	-0.682337000
1	7.566976000	3.090015000	-0.540849000
1	6.543754000	2.390539000	-1.811124000
7	-3.843467000	0.265474000	0.576599000
6	-4.151207000	-0.516440000	-0.666579000
6	-3.084865000	1.515254000	0.206681000
6	-5.103659000	0.599712000	1.333528000
1	-5.385584000	-0.302140000	1.885315000
6	-6.297433000	1.033967000	0.503744000
1	-6.606463000	0.231664000	-0.177305000
1	-7.115493000	1.201569000	1.217243000
8	-5.977606000	2.213706000	-0.201619000
1	-4.647819000	0.150032000	-1.372268000
1	-2.760111000	1.991107000	1.133652000
1	-3.753716000	2.169346000	-0.347775000
1	-4.796843000	-1.353632000	-0.391832000
1	-3.216149000	-0.888715000	-1.086050000
1	-2.225789000	1.223058000	-0.400975000
16	-0.559450000	-0.837562000	-1.158125000
8	-1.346533000	-2.046223000	-0.848409000
8	-1.264212000	0.118922000	-2.022643000
8	0.707386000	-1.300120000	-2.044367000
8	-0.012268000	-0.211571000	0.073191000
1	-6.744594000	2.522416000	-0.696424000
1	1.237353000	-1.942702000	-1.529193000
1	2.901082000	-0.197892000	-1.004454000
6	-2.975202000	-0.559958000	1.484910000
1	-1.983570000	-0.663052000	1.042465000
1	-2.913454000	-0.044189000	2.445513000
1	-3.435181000	-1.541995000	1.603847000
1	-4.836655000	1.381011000	2.050706000

CS_A
TS

i = -1123 cm⁻¹

FE=-1488.106917

6	3.503454000	0.746207000	0.484882000
6	2.906249000	-0.466334000	-0.076865000
6	2.999016000	-1.728901000	0.608111000
1	1.492985000	-0.331583000	-0.059653000
6	3.561904000	-1.857737000	1.995346000

1	3.574455000	-2.912310000	2.269986000
1	4.559076000	-1.415948000	2.052568000
1	2.942598000	-1.286884000	2.692605000
8	2.534302000	-2.771100000	0.079358000
8	3.767043000	0.967141000	1.653731000
8	3.700787000	1.681145000	-0.476029000
6	4.219497000	2.935425000	-0.026129000
6	4.326677000	3.836829000	-1.237921000
1	3.547449000	3.347943000	0.733401000
1	5.192044000	2.771220000	0.448869000
1	3.346518000	3.976101000	-1.701033000
1	4.716510000	4.815210000	-0.943295000
1	5.000160000	3.403658000	-1.981613000
7	-3.353247000	0.363175000	0.638308000
6	-3.823606000	-0.787709000	-0.201146000
6	-2.599830000	1.339710000	-0.229628000
6	-4.507764000	1.039646000	1.334341000
1	-4.756729000	0.422354000	2.202670000
6	-5.771322000	1.228954000	0.516646000
1	-6.183614000	0.258429000	0.214638000
1	-6.497210000	1.706270000	1.188533000
8	-5.491491000	2.040273000	-0.603153000
1	-4.375166000	-0.386147000	-1.051503000
1	-2.163142000	2.095674000	0.425077000
1	-3.303105000	1.791023000	-0.925254000
1	-4.458995000	-1.425726000	0.417068000
1	-2.952211000	-1.346412000	-0.543388000
1	-1.817158000	0.794304000	-0.758202000
16	-0.304300000	-1.508146000	-1.009045000
8	-1.025230000	-2.410471000	-0.104059000
8	-1.128362000	-0.922891000	-2.065416000
8	0.913061000	-2.212919000	-1.655518000
8	0.295958000	-0.356271000	-0.146890000
1	-6.297503000	2.201424000	-1.105936000
1	1.660382000	-2.532372000	-0.920804000
1	2.960176000	-0.536269000	-1.162649000
6	-2.418407000	-0.145846000	1.699523000
1	-1.503410000	-0.505875000	1.229293000
1	-2.200204000	0.679684000	2.379934000
1	-2.911789000	-0.961599000	2.229932000
1	-4.134340000	2.005213000	1.686161000

CS_A

Product

FE=-1488.124403

6	2.662267000	1.750420000	0.054810000
6	2.796895000	0.354099000	-0.329678000
6	3.949307000	-0.346156000	-0.109422000
1	1.374226000	-0.837811000	1.027986000

6	5.194001000	0.212795000	0.512396000
1	5.948560000	-0.572657000	0.555324000
1	5.557646000	1.067135000	-0.062147000
1	4.982991000	0.590806000	1.515376000
8	4.079591000	-1.624734000	-0.437520000
8	3.503908000	2.468085000	0.564531000
8	1.410859000	2.218176000	-0.220616000
6	1.219323000	3.610752000	0.038775000
6	-0.214704000	3.948887000	-0.311183000
1	1.443330000	3.818619000	1.089653000
1	1.927364000	4.186001000	-0.566726000
1	-0.911002000	3.412749000	0.339881000
1	-0.387664000	5.021065000	-0.183403000
1	-0.431907000	3.681580000	-1.348779000
7	-3.054059000	-0.361241000	0.503380000
6	-3.158025000	-1.204747000	-0.732540000
6	-2.003404000	0.702495000	0.296477000
6	-4.382927000	0.255534000	0.861157000
1	-4.965438000	-0.521936000	1.364363000
6	-5.210242000	0.787823000	-0.293841000
1	-5.479957000	-0.024820000	-0.979475000
1	-6.138003000	1.173422000	0.149554000
8	-4.493124000	1.805161000	-0.958212000
1	-3.322076000	-0.543833000	-1.584126000
1	-1.840512000	1.195575000	1.256701000
1	-2.374066000	1.409742000	-0.441787000
1	-3.989935000	-1.901069000	-0.604859000
1	-2.221336000	-1.748881000	-0.854566000
1	-1.090202000	0.216296000	-0.052253000
16	0.400188000	-2.260066000	-0.285816000
8	-0.664996000	-3.195284000	0.075811000
8	-0.025894000	-1.212345000	-1.233736000
8	1.704671000	-2.851494000	-0.616831000
8	0.628885000	-1.457811000	1.139181000
1	-5.025363000	2.175197000	-1.671006000
1	3.214938000	-2.043423000	-0.673618000
1	1.981271000	-0.081515000	-0.900500000
6	-2.628720000	-1.228890000	1.652933000
1	-1.614354000	-1.584592000	1.476417000
1	-2.675597000	-0.629959000	2.564472000
1	-3.310578000	-2.078479000	1.715476000
1	-4.170765000	1.054442000	1.577258000

CP_A

Reactant

FE=-1432.052524

6	-4.357166000	0.038267000	0.300941000
6	-2.916028000	-0.229276000	-0.060092000
6	-2.475908000	-1.625412000	0.342203000

1	-2.276309000	0.515089000	0.421407000
6	-3.017200000	-2.772099000	-0.458563000
1	-2.739489000	-3.716238000	0.010491000
1	-4.103407000	-2.693847000	-0.550714000
1	-2.564999000	-2.699500000	-1.453792000
8	-1.699834000	-1.786910000	1.269224000
8	-5.143786000	-0.775631000	0.728558000
8	-4.678329000	1.321935000	0.079400000
6	-6.038340000	1.685138000	0.367277000
6	-6.187585000	3.156256000	0.047417000
1	-6.702399000	1.061720000	-0.238884000
1	-6.244211000	1.467940000	1.419596000
1	-5.963331000	3.346950000	-1.004823000
1	-7.213382000	3.476591000	0.248528000
1	-5.509950000	3.755386000	0.660520000
7	4.287442000	1.266042000	-0.079672000
6	3.127048000	1.798040000	0.711078000
6	4.227499000	1.838125000	-1.464860000
6	4.243510000	-0.252374000	-0.206517000
1	5.261583000	-0.552752000	-0.472114000
1	3.548626000	-0.475699000	-1.018781000
6	3.768057000	-0.977736000	1.030873000
1	2.724266000	-0.724740000	1.245223000
1	3.799995000	-2.045059000	0.786333000
8	4.627937000	-0.661499000	2.123802000
1	3.189747000	2.887646000	0.682749000
1	3.256684000	1.572229000	-1.889803000
1	5.042970000	1.402961000	-2.046203000
1	3.220708000	1.443124000	1.737395000
1	-2.782832000	-0.113476000	-1.141041000
1	2.203552000	1.448246000	0.246180000
1	4.356657000	2.919732000	-1.392753000
8	-0.597500000	-1.085837000	-1.558636000
8	1.660647000	-2.000147000	-0.812542000
8	0.518926000	-0.195191000	0.585784000
8	1.606785000	0.400589000	-1.569101000
1	-0.195089000	-0.696790000	1.022964000
1	4.329103000	-1.138530000	2.905332000
15	0.711849000	-0.651818000	-0.978819000
1	1.112970000	-2.783078000	-0.947104000
6	5.562430000	1.695632000	0.571491000
1	5.632579000	1.224580000	1.550332000
1	6.396712000	1.383054000	-0.058648000
1	5.552752000	2.783605000	0.658206000

CP_A
TS

i = -1006 cm⁻¹

FE=-1432.028953

6	-2.590554000	0.788923000	-0.073121000
6	-1.910130000	-0.329869000	0.563280000
6	-2.559020000	-1.626944000	0.752339000
1	-1.333307000	-0.041429000	1.440945000
6	-3.777357000	-2.008576000	-0.045575000
1	-3.549116000	-1.941148000	-1.113370000
1	-4.062057000	-3.026623000	0.218569000
1	-4.594594000	-1.306447000	0.137669000
8	-2.048551000	-2.452521000	1.520885000
8	-3.510010000	0.774731000	-0.866305000
8	-2.007237000	1.986344000	0.292421000
6	-2.592727000	3.151611000	-0.291369000
6	-1.938075000	4.357249000	0.352738000
1	-2.439612000	3.131211000	-1.377403000
1	-3.672379000	3.139970000	-0.118089000
1	-0.857642000	4.369771000	0.169149000
1	-2.358111000	5.280082000	-0.055723000
1	-2.099557000	4.349268000	1.433674000
7	1.816988000	1.684705000	-0.271817000
6	1.124911000	1.254209000	0.987911000
6	0.802369000	1.863163000	-1.362707000
6	2.811782000	0.634536000	-0.734658000
1	3.486015000	1.144881000	-1.428864000
1	2.236390000	-0.131209000	-1.259221000
6	3.589056000	-0.041883000	0.374411000
1	2.920454000	-0.625124000	1.017150000
1	4.261236000	-0.753424000	-0.118117000
8	4.308045000	0.940278000	1.109358000
1	0.262577000	1.906799000	1.138244000
1	0.275011000	0.918497000	-1.496830000
1	1.333974000	2.140467000	-2.275157000
1	1.837243000	1.335525000	1.809372000
1	-0.868976000	-0.748966000	-0.323586000
1	0.790373000	0.224664000	0.861918000
1	0.111709000	2.651722000	-1.062311000
8	0.085890000	-3.769820000	-0.942684000
8	2.236889000	-2.380473000	-0.716456000
8	0.632920000	-2.352290000	1.190640000
8	0.089040000	-1.139393000	-0.943755000
1	-0.287356000	-2.469838000	1.541292000
1	4.840116000	0.506814000	1.785366000
15	0.635328000	-2.506328000	-0.412441000
1	2.559298000	-3.249774000	-0.988488000
6	2.493891000	2.996718000	-0.032211000
1	3.280397000	2.855822000	0.706160000
1	2.916295000	3.347138000	-0.975355000
1	1.742018000	3.703656000	0.323257000

CP_A
Product

FE=-1432.049742

6	-2.843710000	-0.092933000	0.415427000
6	-1.702706000	-0.846309000	0.900690000
6	-1.373583000	-0.967340000	2.217763000
1	-1.061733000	-1.294210000	0.149452000
6	-2.197906000	-0.501085000	3.378080000
1	-2.106323000	-1.239216000	4.178378000
1	-1.789181000	0.444064000	3.754644000
1	-3.237615000	-0.339324000	3.104558000
8	-0.233262000	-1.520345000	2.608273000
8	-3.612567000	0.616862000	1.044309000
8	-2.946577000	-0.206786000	-0.939477000
6	-4.026474000	0.508123000	-1.543604000
6	-3.931906000	0.281476000	-3.037708000
1	-4.973243000	0.142892000	-1.133571000
1	-3.947981000	1.570163000	-1.283811000
1	-4.007654000	-0.783597000	-3.269787000
1	-4.741071000	0.808338000	-3.550466000
1	-2.977370000	0.649645000	-3.424983000
7	0.842830000	2.065070000	-0.169189000
6	0.697776000	1.565650000	1.239389000
6	-0.341460000	1.618624000	-0.972404000
6	2.087512000	1.502693000	-0.842357000
1	2.329890000	2.200072000	-1.649744000
1	1.811520000	0.538652000	-1.270599000
6	3.272677000	1.301107000	0.073412000
1	3.041840000	0.537884000	0.825206000
1	4.078898000	0.908871000	-0.555777000
8	3.618368000	2.553322000	0.658506000
1	-0.291555000	1.860426000	1.594824000
1	-0.379922000	0.528628000	-0.967427000
1	-0.215392000	1.983453000	-1.994312000
1	1.480935000	2.027023000	1.841440000
1	0.361684000	-2.118384000	-2.276583000
1	0.796694000	0.479797000	1.227298000
1	-1.245713000	2.038746000	-0.525980000
8	1.767107000	-3.590229000	-0.764209000
8	3.135512000	-1.456610000	-1.160982000
8	1.487111000	-1.387531000	0.710144000
8	0.629998000	-1.456885000	-1.626162000
1	0.412243000	-1.642811000	1.842714000
1	4.399647000	2.439809000	1.210131000
15	1.739024000	-2.116981000	-0.591804000
1	3.631478000	-2.138753000	-1.631052000
6	0.890576000	3.558713000	-0.150259000
1	1.795433000	3.868234000	0.370490000
1	0.901244000	3.920795000	-1.179618000
1	-0.002210000	3.921345000	0.362169000

NS_{Aa}

Reactant

FE=-1448.872739

6	-3.121451000	0.632116000	0.078153000
6	-2.125548000	-0.484935000	0.233112000
6	-2.667992000	-1.900507000	0.308345000
1	-1.503730000	-0.296216000	1.114419000
6	-3.830775000	-2.298385000	-0.556748000
1	-3.885871000	-3.385811000	-0.597135000
1	-4.750761000	-1.880281000	-0.139608000
1	-3.719938000	-1.879726000	-1.561308000
8	-2.102360000	-2.708292000	1.022035000
8	-4.324458000	0.537786000	0.039881000
8	-2.482524000	1.818268000	-0.006790000
6	-3.332689000	2.967634000	-0.159590000
6	-2.437895000	4.186487000	-0.215683000
1	-3.921175000	2.848645000	-1.073990000
1	-4.027912000	3.006233000	0.683885000
1	-1.740920000	4.116576000	-1.055605000
1	-3.043383000	5.086867000	-0.347395000
1	-1.867324000	4.291617000	0.711368000
7	2.216385000	1.746301000	0.250910000
6	2.034052000	0.901660000	1.472915000
6	0.892459000	2.211189000	-0.257422000
6	3.006296000	1.095176000	-0.857431000
1	3.082327000	1.858749000	-1.637591000
1	2.438111000	0.232624000	-1.207667000
6	4.378973000	0.709074000	-0.358510000
1	4.316374000	-0.172772000	0.285380000
1	4.997527000	0.458030000	-1.227114000
8	4.880890000	1.854032000	0.331755000
1	1.594549000	1.538102000	2.242829000
1	0.351396000	1.326276000	-0.597977000
1	1.056177000	2.908180000	-1.080450000
1	3.001295000	0.529367000	1.801928000
1	-1.420056000	-0.464622000	-0.612367000
1	1.373622000	0.069663000	1.236449000
1	0.351847000	2.700370000	0.553574000
8	0.865542000	-3.312930000	-0.914939000
8	2.693533000	-1.817756000	-0.077702000
8	0.657689000	-2.045501000	1.210776000
8	0.631380000	-0.851551000	-0.952285000
1	-0.227630000	-2.464416000	1.214011000
1	5.746141000	1.661372000	0.707210000
1	2.783711000	2.551292000	0.535498000
16	1.260676000	-2.048358000	-0.315588000

NS_{Aa}

TS

i = -1072 cm⁻¹

FE=-1448.850813

6	-2.759249000	0.771337000	-0.143360000
6	-2.012745000	-0.338439000	0.444981000
6	-2.598284000	-1.661589000	0.562881000
1	-1.418968000	-0.056104000	1.315939000
6	-3.884882000	-2.028697000	-0.119965000
1	-4.116595000	-3.067563000	0.112702000
1	-4.691056000	-1.359096000	0.188311000
1	-3.776181000	-1.893062000	-1.199556000
8	-1.997266000	-2.553716000	1.198412000
8	-3.749692000	0.725628000	-0.844305000
8	-2.164504000	1.971940000	0.150084000
6	-2.835843000	3.120642000	-0.379098000
6	-2.024489000	4.340980000	0.002640000
1	-2.930503000	3.015472000	-1.463883000
1	-3.847365000	3.163700000	0.036591000
1	-1.032291000	4.309800000	-0.457660000
1	-2.526871000	5.248014000	-0.343748000
1	-1.907138000	4.405576000	1.088093000
7	2.279634000	1.582985000	0.462618000
6	2.161992000	0.586107000	1.571833000
6	0.970525000	2.256000000	0.220202000
6	2.826880000	1.023451000	-0.824885000
1	2.867631000	1.873202000	-1.512420000
1	2.130030000	0.267425000	-1.186635000
6	4.211292000	0.458542000	-0.598325000
1	4.155212000	-0.494450000	-0.064777000
1	4.671069000	0.280846000	-1.576563000
8	4.916990000	1.451917000	0.143402000
1	1.879008000	1.132127000	2.472805000
1	0.270156000	1.508625000	-0.153147000
1	1.114410000	3.045626000	-0.518127000
1	3.122380000	0.095719000	1.715615000
1	-0.867781000	-0.602069000	-0.378061000
1	1.401731000	-0.149605000	1.315856000
1	0.598787000	2.673000000	1.156764000
8	0.307955000	-3.247318000	-1.109335000
8	2.315942000	-1.926612000	-0.396665000
8	0.462959000	-2.210119000	1.143254000
8	0.219992000	-0.783505000	-0.841899000
1	-0.570193000	-2.398799000	1.253564000
1	5.808582000	1.148939000	0.343856000
1	2.975848000	2.273690000	0.763438000
16	0.868905000	-2.131102000	-0.382019000

NS_{Aa}

Product

FE=-1448.871796

6	-3.042314000	0.701795000	0.041649000
6	-2.231086000	-0.453528000	0.366055000
6	-2.782362000	-1.656395000	0.702145000
1	-1.152478000	-0.357091000	0.334421000
6	-4.251815000	-1.933804000	0.809346000
1	-4.390374000	-2.953894000	1.167922000
1	-4.732479000	-1.219645000	1.480346000
1	-4.732474000	-1.808943000	-0.164084000
8	-2.044415000	-2.724583000	0.970601000
8	-4.256165000	0.775438000	-0.004100000
8	-2.264881000	1.796773000	-0.240528000
6	-2.995170000	2.966664000	-0.623695000
6	-1.989110000	4.058347000	-0.922140000
1	-3.609501000	2.733097000	-1.498416000
1	-3.672807000	3.249797000	0.187510000
1	-1.311937000	3.750716000	-1.724683000
1	-2.507018000	4.966387000	-1.242052000
1	-1.399711000	4.301238000	-0.032564000
7	2.042700000	1.622447000	0.671097000
6	1.929884000	0.569934000	1.730156000
6	0.691161000	2.007617000	0.166089000
6	2.935954000	1.259187000	-0.486500000
1	2.991766000	2.161922000	-1.101742000
1	2.464445000	0.445909000	-1.037923000
6	4.306681000	0.862440000	0.009017000
1	4.267559000	-0.126277000	0.476992000
1	4.980093000	0.810720000	-0.853481000
8	4.698180000	1.881517000	0.925474000
1	1.291262000	0.971719000	2.517894000
1	0.283622000	1.155710000	-0.379808000
1	0.793791000	2.864954000	-0.500638000
1	2.921827000	0.362445000	2.126605000
1	-0.122547000	-1.201780000	-1.962169000
1	1.485206000	-0.332051000	1.307227000
1	0.041776000	2.253412000	1.005846000
8	1.071095000	-3.340833000	-1.446741000
8	2.678581000	-1.710753000	-0.428302000
8	0.519324000	-2.117496000	0.636451000
8	0.672121000	-0.887844000	-1.503717000
1	-1.074826000	-2.552321000	0.844210000
1	5.570722000	1.690069000	1.284675000
1	2.492061000	2.430626000	1.113072000
16	1.300092000	-2.164072000	-0.629542000

NS_{Ab}

Reactant

FE=-1448.900068

6	3.771393000	0.461908000	-0.165995000
---	-------------	-------------	--------------

6	2.460291000	-0.288242000	-0.083639000
6	1.283792000	0.645255000	-0.280205000
1	2.443191000	-1.063449000	-0.857713000
6	0.997017000	1.126243000	-1.666831000
1	0.291865000	1.957374000	-1.639786000
1	1.921297000	1.415374000	-2.171803000
1	0.536352000	0.283674000	-2.196415000
8	0.587957000	0.954864000	0.677848000
8	3.901246000	1.597857000	-0.560764000
8	4.787891000	-0.300155000	0.249488000
6	6.091103000	0.309894000	0.202193000
6	7.080804000	-0.707399000	0.724984000
1	6.302016000	0.599556000	-0.831500000
1	6.070791000	1.219412000	0.809311000
1	7.070092000	-1.609271000	0.108378000
1	8.088835000	-0.284979000	0.705878000
1	6.840399000	-0.986453000	1.753621000
7	-4.006486000	0.225235000	0.095204000
6	-4.059298000	-0.287196000	1.491517000
6	-4.186580000	1.709869000	0.021196000
1	-4.791454000	1.946054000	-0.858379000
6	-2.828622000	2.398049000	-0.073842000
1	-2.337087000	2.096820000	-1.007016000
1	-2.997363000	3.482749000	-0.106309000
8	-2.052864000	2.047019000	1.044402000
1	-5.073711000	-0.146779000	1.875622000
1	-3.334223000	0.270230000	2.082222000
1	-3.789354000	-1.344244000	1.475594000
16	-1.217103000	-1.571608000	-0.249035000
8	-1.663321000	-0.271158000	-0.869105000
8	-2.282812000	-2.566194000	-0.257503000
8	-1.075039000	-1.221827000	1.335095000
8	0.110935000	-1.943963000	-0.726228000
1	-1.170751000	1.743657000	0.765581000
1	-0.400669000	-0.523674000	1.442736000
1	2.381184000	-0.789660000	0.883222000
6	-4.926958000	-0.531576000	-0.785178000
1	-4.803951000	-0.176223000	-1.809285000
1	-4.647276000	-1.585574000	-0.733240000
1	-5.957759000	-0.381839000	-0.453164000
1	-4.726269000	2.033623000	0.916161000
1	-3.006701000	0.020337000	-0.286646000

NS_{Ab}

TS

i = -1256 cm⁻¹

FE=-1448.872073

6	3.835725000	-0.146333000	0.257224000
6	2.588020000	-0.684835000	-0.322795000

6	2.323848000	-2.095090000	-0.285371000
1	1.531108000	-0.270943000	0.368241000
6	3.159886000	-3.083280000	0.457159000
1	2.753664000	-4.082090000	0.302771000
1	4.203037000	-3.016192000	0.140970000
1	3.155801000	-2.822716000	1.519237000
8	1.278212000	-2.555644000	-0.840120000
8	4.548756000	-0.691059000	1.075589000
8	4.081330000	1.089233000	-0.212932000
6	5.226987000	1.752854000	0.340551000
6	5.285776000	3.132619000	-0.277717000
1	5.118383000	1.792480000	1.428521000
1	6.119978000	1.161985000	0.114711000
1	4.379235000	3.696549000	-0.045261000
1	6.147443000	3.679062000	0.115103000
1	5.382792000	3.064595000	-1.364094000
7	-3.935879000	1.119836000	0.146695000
6	-4.109205000	1.287250000	-1.323133000
6	-5.104802000	0.422926000	0.777696000
1	-5.287179000	0.872812000	1.757479000
6	-4.821246000	-1.071778000	0.932756000
1	-4.035119000	-1.218229000	1.682592000
1	-5.736054000	-1.552319000	1.295355000
8	-4.460155000	-1.660903000	-0.292784000
1	-4.911439000	2.008923000	-1.498341000
1	-4.369697000	0.316851000	-1.744898000
1	-3.161565000	1.641679000	-1.729547000
16	-0.748906000	0.030052000	-0.211617000
8	-1.971131000	-0.621643000	0.383858000
8	-1.075233000	1.398264000	-0.633737000
8	-0.266945000	-0.792463000	-1.397514000
8	0.352943000	-0.007183000	0.838538000
1	-3.488972000	-1.678861000	-0.335827000
1	0.543754000	-1.754657000	-1.155839000
1	2.278867000	-0.197749000	-1.248790000
6	-3.609605000	2.412927000	0.796249000
1	-3.372402000	2.225420000	1.844526000
1	-2.734761000	2.828781000	0.296297000
1	-4.471615000	3.080334000	0.717139000
1	-5.978598000	0.596282000	0.143072000
1	-3.087531000	0.475942000	0.272698000

NS_{Ab}

Product

FE=-1448.888925

6	-3.767665000	0.233488000	-0.098679000
6	-2.770893000	-0.715597000	0.390576000
6	-2.905937000	-2.061998000	0.218593000
1	-1.042493000	-0.747432000	-1.028648000

6	-4.044334000	-2.741960000	-0.479550000
1	-3.944076000	-3.819036000	-0.343896000
1	-5.001744000	-2.386274000	-0.096918000
1	-4.031544000	-2.500170000	-1.545562000
8	-2.000155000	-2.930018000	0.665013000
8	-4.750165000	-0.015296000	-0.773395000
8	-3.463835000	1.492710000	0.290153000
6	-4.376253000	2.510069000	-0.134455000
6	-3.841426000	3.831150000	0.376206000
1	-4.449413000	2.490227000	-1.226404000
1	-5.369993000	2.287448000	0.267365000
1	-2.845261000	4.023611000	-0.030228000
1	-4.505709000	4.645440000	0.074200000
1	-3.773192000	3.822900000	1.466898000
7	3.648784000	1.201291000	-0.081692000
6	3.599575000	1.409703000	1.394436000
6	5.013700000	0.782149000	-0.548186000
1	5.202166000	1.245793000	-1.520209000
6	5.097819000	-0.739521000	-0.666761000
1	4.454743000	-1.078716000	-1.487230000
1	6.132536000	-1.000480000	-0.912330000
8	4.745817000	-1.369353000	0.541136000
1	4.201783000	2.288099000	1.638941000
1	4.007558000	0.520759000	1.874272000
1	2.556022000	1.556370000	1.674446000
16	0.800199000	-0.645620000	0.042793000
8	2.162554000	-1.006572000	-0.449554000
8	0.719088000	0.785617000	0.363006000
8	0.303847000	-1.537397000	1.097695000
8	-0.103657000	-0.904093000	-1.262674000
1	3.822240000	-1.660966000	0.468734000
1	-1.189639000	-2.477455000	0.987940000
1	-1.967788000	-0.316758000	1.003765000
6	3.123033000	2.387216000	-0.803785000
1	3.072207000	2.153989000	-1.868095000
1	2.120998000	2.591869000	-0.426695000
1	3.794299000	3.232075000	-0.632821000
1	5.741207000	1.164546000	0.172831000
1	2.996746000	0.392064000	-0.284605000

NP_{Aa}

Reactant

FE=-1392.789359

6	-4.091470000	-0.073389000	0.250464000
6	-2.639217000	-0.265501000	-0.114926000
6	-2.120322000	-1.626417000	0.314144000
1	-2.039865000	0.523022000	0.347148000
6	-2.580813000	-2.816097000	-0.474007000
1	-2.251532000	-3.734515000	0.012490000

1	-3.668648000	-2.805158000	-0.578089000
1	-2.123468000	-2.730873000	-1.465783000
8	-1.351108000	-1.725159000	1.255754000
8	-4.840143000	-0.933304000	0.655124000
8	-4.470971000	1.199287000	0.060769000
6	-5.846060000	1.492905000	0.357115000
6	-6.059550000	2.965479000	0.083619000
1	-6.481910000	0.860325000	-0.269391000
1	-6.042368000	1.233813000	1.401775000
1	-5.844184000	3.198752000	-0.961917000
1	-7.098148000	3.234494000	0.293912000
1	-5.408107000	3.573717000	0.715823000
7	4.391560000	1.453906000	0.051366000
6	3.171663000	2.006232000	0.727314000
6	4.562850000	2.078564000	-1.293302000
6	4.431136000	-0.050988000	-0.086788000
1	5.462913000	-0.283820000	-0.368311000
1	3.737951000	-0.323299000	-0.882647000
6	4.075379000	-0.720343000	1.216720000
1	3.012300000	-0.579613000	1.442720000
1	4.261224000	-1.793764000	1.106324000
8	4.920730000	-0.128062000	2.203482000
1	3.297463000	3.089274000	0.775304000
1	3.677882000	1.808196000	-1.875141000
1	5.468933000	1.679922000	-1.751562000
1	3.111148000	1.592313000	1.731411000
1	-2.520125000	-0.164657000	-1.199034000
1	2.303022000	1.728107000	0.130642000
1	4.644239000	3.159348000	-1.172285000
8	-0.258222000	-1.017258000	-1.565616000
8	2.000645000	-1.841892000	-0.720002000
8	0.781433000	-0.018450000	0.571180000
8	1.905436000	0.526825000	-1.584256000
1	0.085656000	-0.541549000	1.012706000
1	4.728267000	-0.503209000	3.069078000
15	1.023839000	-0.525613000	-0.971876000
1	1.478046000	-2.643961000	-0.840492000
1	5.186829000	1.691428000	0.650287000

NP_{Aa}
TS

i = -1018 cm⁻¹

FE=-1392.76720

6	-2.781195000	0.452059000	-0.178353000
6	-1.885414000	-0.484525000	0.497312000
6	-2.266950000	-1.882525000	0.692269000
1	-1.400816000	-0.063654000	1.380338000
6	-3.389360000	-2.504313000	-0.095552000
1	-3.461761000	-3.556300000	0.179182000

1	-4.329778000	-1.979153000	0.088231000
1	-3.187535000	-2.400989000	-1.165408000
8	-1.609257000	-2.597658000	1.463114000
8	-3.677561000	0.209079000	-0.960674000
8	-2.466507000	1.752606000	0.135947000
6	-3.292963000	2.740662000	-0.486838000
6	-2.828127000	4.097103000	0.001511000
1	-3.211096000	2.646807000	-1.574454000
1	-4.337301000	2.552559000	-0.220277000
1	-1.793289000	4.289863000	-0.298091000
1	-3.454595000	4.884547000	-0.425936000
1	-2.892339000	4.158371000	1.091376000
7	1.884753000	1.881272000	0.443150000
6	1.908279000	0.893410000	1.565975000
6	0.484766000	2.284212000	0.115584000
6	2.585879000	1.397923000	-0.797360000
1	2.507637000	2.217850000	-1.516897000
1	2.047433000	0.519064000	-1.158531000
6	4.037089000	1.102336000	-0.490759000
1	4.127019000	0.178085000	0.088255000
1	4.566456000	0.968384000	-1.440802000
8	4.519344000	2.233093000	0.228949000
1	1.380001000	1.337259000	2.410605000
1	-0.022778000	1.411964000	-0.292937000
1	0.515373000	3.088788000	-0.620583000
1	2.943120000	0.695125000	1.839679000
1	-0.727887000	-0.677139000	-0.303685000
1	1.413523000	-0.024118000	1.247783000
1	-0.022428000	2.613346000	1.022564000
8	0.840584000	-3.391688000	-1.162858000
8	2.674592000	-1.687125000	-0.556866000
8	0.991182000	-2.236291000	1.181071000
8	0.358948000	-0.828073000	-0.817415000
1	0.057470000	-2.438089000	1.465305000
1	5.445820000	2.115439000	0.463118000
15	1.104437000	-2.144358000	-0.418515000
1	3.176893000	-2.450681000	-0.870850000
1	2.418406000	2.699543000	0.754814000

NP_{Aa}

Product

FE=-1392.786247

6	-2.876259000	-0.265886000	0.243274000
6	-1.626952000	-0.967182000	0.454340000
6	-1.390044000	-1.723728000	1.566206000
1	-0.868693000	-0.883614000	-0.316444000
6	-2.385830000	-1.973446000	2.661271000
1	-1.954590000	-2.676270000	3.374541000
1	-2.643830000	-1.037457000	3.164933000
1	-3.320299000	-2.362183000	2.253224000

8	-0.222584000	-2.303513000	1.792938000
8	-3.862816000	-0.243887000	0.959786000
8	-2.833889000	0.458659000	-0.916505000
6	-4.036640000	1.155479000	-1.250707000
6	-3.779211000	1.904028000	-2.541586000
1	-4.851004000	0.431600000	-1.355337000
1	-4.304079000	1.830643000	-0.430746000
1	-3.503377000	1.211095000	-3.340268000
1	-4.677686000	2.447263000	-2.846537000
1	-2.966900000	2.626598000	-2.417268000
7	0.892038000	2.118032000	0.818924000
6	0.732557000	1.055416000	1.865129000
6	-0.344498000	2.263732000	-0.005558000
6	2.074171000	1.895766000	-0.092633000
1	2.218389000	2.840950000	-0.624497000
1	1.800687000	1.116259000	-0.801815000
6	3.308968000	1.531840000	0.694554000
1	3.207868000	0.524687000	1.115280000
1	4.160228000	1.529198000	0.007255000
8	3.431728000	2.534716000	1.701557000
1	-0.245756000	1.182729000	2.329136000
1	-0.507244000	1.328485000	-0.544118000
1	-0.199101000	3.084265000	-0.710047000
1	1.527987000	1.184555000	2.597460000
1	0.575049000	-0.871916000	-2.797104000
1	0.810457000	0.084992000	1.374036000
1	-1.192312000	2.465022000	0.650355000
8	2.019096000	-2.792496000	-1.989177000
8	3.306669000	-0.650977000	-1.404038000
8	1.611679000	-1.411809000	0.256166000
8	0.816371000	-0.524310000	-1.929049000
1	0.478977000	-2.065511000	1.102325000
1	4.223265000	2.379705000	2.227485000
15	1.925235000	-1.527873000	-1.220182000
1	3.842386000	-1.060717000	-2.094875000
1	1.079166000	2.994312000	1.314121000

NP_{Ab}

Reactant

FE=-1392.816316

6	-4.374964000	-0.431722000	-0.017821000
6	-2.913649000	-0.054790000	-0.092307000
6	-2.002875000	-1.240822000	0.168911000
1	-2.699972000	0.347429000	-1.088688000
6	-1.880584000	-2.271421000	-0.913093000
1	-1.325482000	-3.133911000	-0.544130000
1	-2.869633000	-2.570290000	-1.268779000
1	-1.330364000	-1.799237000	-1.734842000
8	-1.386383000	-1.319705000	1.217659000

8	-4.814750000	-1.558074000	-0.015960000
8	-5.150085000	0.661130000	0.036357000
6	-6.567050000	0.421441000	0.087384000
6	-7.248423000	1.771174000	0.131456000
1	-6.855179000	-0.158586000	-0.794308000
1	-6.787531000	-0.182557000	0.972422000
1	-6.998449000	2.358267000	-0.755602000
1	-8.332837000	1.637666000	0.166119000
1	-6.939074000	2.331377000	1.017184000
7	4.485622000	0.692728000	0.043923000
6	4.210811000	0.945388000	1.481385000
6	5.500828000	-0.389099000	-0.150620000
1	6.137012000	-0.118927000	-0.998540000
6	4.820656000	-1.731174000	-0.420767000
1	4.308152000	-1.689400000	-1.390009000
1	5.597879000	-2.500651000	-0.476545000
8	3.922566000	-2.079896000	0.603455000
1	5.098359000	1.385172000	1.946571000
1	3.962921000	-0.005430000	1.953437000
1	3.360203000	1.625315000	1.554561000
8	2.277201000	-0.252980000	-0.703523000
8	1.639917000	2.099998000	-0.346259000
8	0.819581000	0.395720000	1.282741000
8	-0.225420000	0.437865000	-1.067219000
1	3.050860000	-1.728037000	0.351140000
1	0.040254000	-0.158696000	1.480343000
1	-2.702381000	0.734245000	0.632358000
6	4.831818000	1.942958000	-0.663546000
1	4.921149000	1.730653000	-1.730165000
1	4.023732000	2.658320000	-0.508173000
1	5.778201000	2.335468000	-0.279224000
1	6.121729000	-0.439338000	0.749478000
1	3.494991000	0.315612000	-0.364848000
1	0.924168000	2.746729000	-0.304523000
15	1.046767000	0.572377000	-0.307774000

NP_{Ab}

TS

i = -1113 cm⁻¹

FE=-1392.796752

6	-3.866537000	-0.141853000	-0.300513000
6	-2.677012000	-0.715618000	0.335161000
6	-2.402972000	-2.131918000	0.291429000
1	-1.528606000	-0.275670000	-0.345695000
6	-3.179067000	-3.072492000	-0.584781000
1	-2.773404000	-4.076993000	-0.467336000
1	-4.241722000	-3.040122000	-0.332108000
1	-3.111358000	-2.743826000	-1.625142000

8	-1.437426000	-2.601350000	0.940748000
8	-4.558968000	-0.639357000	-1.167534000
8	-4.107593000	1.106437000	0.175336000
6	-5.216822000	1.790308000	-0.416347000
6	-5.285003000	3.164952000	0.214441000
1	-5.067324000	1.843078000	-1.499231000
1	-6.129363000	1.213203000	-0.235811000
1	-4.363837000	3.721631000	0.023190000
1	-6.123852000	3.727516000	-0.204510000
1	-5.424637000	3.086481000	1.295725000
7	4.017675000	1.107893000	-0.188451000
6	4.276391000	1.249221000	1.267811000
6	5.146919000	0.421487000	-0.895336000
1	5.281618000	0.890586000	-1.873956000
6	4.848946000	-1.068930000	-1.066242000
1	4.027337000	-1.197210000	-1.780537000
1	5.742832000	-1.547698000	-1.479548000
8	4.540952000	-1.677892000	0.164185000
1	5.083894000	1.971266000	1.419051000
1	4.560569000	0.272137000	1.657999000
1	3.355823000	1.592751000	1.741550000
8	2.061768000	-0.510947000	-0.304499000
8	1.049949000	1.389386000	0.889141000
8	0.267276000	-0.924904000	1.517743000
8	-0.422227000	0.035269000	-0.738757000
1	3.572769000	-1.680763000	0.252792000
1	-0.477629000	-1.671936000	1.340217000
1	-2.421685000	-0.249970000	1.287255000
6	3.655188000	2.405893000	-0.799357000
1	3.358394000	2.235092000	-1.835392000
1	2.810894000	2.819326000	-0.246391000
1	4.512805000	3.083103000	-0.760141000
1	6.055748000	0.576207000	-0.305699000
1	3.130255000	0.449671000	-0.268422000
1	0.269040000	1.797026000	1.286607000
15	0.721846000	-0.091305000	0.279080000

NP_{Ab}

Product

FE=-1392.814828

6	3.409983000	0.741431000	-0.148134000
6	2.899987000	-0.534703000	-0.629999000
6	3.214743000	-1.742824000	-0.102902000
1	0.881375000	-2.325068000	1.170051000
6	4.285581000	-2.031175000	0.896871000
1	3.834430000	-2.472740000	1.791224000
1	4.963154000	-2.778194000	0.472109000
1	4.842093000	-1.133696000	1.157109000

8	2.515832000	-2.837638000	-0.431621000
8	4.422804000	1.000982000	0.464044000
8	2.494066000	1.715192000	-0.457487000
6	2.821868000	3.044739000	-0.033684000
6	1.666321000	3.937395000	-0.433650000
1	2.986036000	3.041116000	1.047970000
1	3.758463000	3.344855000	-0.513267000
1	0.741127000	3.607501000	0.048469000
1	1.866347000	4.967887000	-0.128650000
1	1.519446000	3.916955000	-1.516445000
7	-3.253964000	0.953840000	0.342385000
6	-3.067913000	1.615278000	-0.973972000
6	-4.680079000	0.557258000	0.572218000
1	-4.926914000	0.738227000	1.622271000
6	-4.893428000	-0.917937000	0.231373000
1	-4.360055000	-1.541389000	0.958695000
1	-5.964016000	-1.133516000	0.311981000
8	-4.474382000	-1.211551000	-1.079253000
1	-3.568476000	2.588085000	-0.960884000
1	-3.504833000	0.973610000	-1.739209000
1	-1.996747000	1.731546000	-1.144326000
8	-1.975469000	-1.218276000	0.111215000
8	-0.198307000	0.451652000	-0.072118000
8	0.183603000	-1.866495000	-1.211138000
8	0.224550000	-1.630528000	1.326801000
1	-3.556364000	-1.529004000	-1.025098000
1	1.698623000	-2.583059000	-0.942283000
1	2.107835000	-0.485781000	-1.368315000
6	-2.698936000	1.774377000	1.440639000
1	-2.756167000	1.203482000	2.368972000
1	-1.653340000	1.983557000	1.212778000
1	-3.270975000	2.702092000	1.533489000
1	-5.313080000	1.197360000	-0.049870000
1	-2.648676000	0.013721000	0.290246000
1	0.725127000	0.730874000	-0.207582000
15	-0.461134000	-1.155002000	-0.060148000