

Mechanism and Diastereoselectivity of Arsenic Ylide Mediated cyclopropanation – A Theoretical Study

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Supporting Information

Optimized Cartesian coordinates and energies of TSs, intermediates, products and reactants obtained at the B3LYP/6-31G(d) level (Energy in a. u.). Single point energies (at the PCM(CH₃CN)/B3LYP/6-311+G(d,p) //B3LYP/6-31G(d) level) imaginary frequencies, if any (in cm⁻¹) are also given before the respective coordinates.

Semistabilized Ylide (Ph)

TS1C_{rr} (-2894.36727)
E(CH₃CN) = -2896.66495
NIMAG = 1 (-185.7)

Cisoid Betaine_{rr} (-2894.40846)
E(CH₃CN) = -2896.69861
NIMAG = 0

6	-0.870506000	-2.891443000	-0.307716000
1	-1.736273000	-2.742843000	0.337655000
1	-1.191012000	-2.873620000	-1.351173000
6	1.003145000	-1.726577000	1.779848000
1	0.176617000	-1.520740000	2.463136000
1	1.849874000	-1.064880000	1.960625000
6	-0.276134000	0.246685000	-0.479580000
1	0.138266000	0.534730000	-1.443382000
6	0.830198000	1.872934000	0.755195000
6	1.976330000	2.225515000	0.053611000
1	1.307354000	-2.772284000	1.876091000
1	-0.383538000	-3.843213000	-0.080122000
33	0.428824000	-1.445535000	-0.050050000
6	1.889832000	-2.012122000	-1.188309000
1	2.749012000	-1.373872000	-0.984404000
1	2.108091000	-3.053377000	-0.938755000
1	1.563779000	-1.942563000	-2.228050000
6	-0.274499000	2.868324000	0.980778000
1	0.005584000	3.536051000	1.808614000
1	-0.440906000	3.493878000	0.096812000
1	-1.220880000	2.392115000	1.247091000
1	0.947335000	1.120990000	1.527646000
6	3.087650000	1.342301000	-0.023639000
8	3.071985000	0.177934000	0.454485000
1	1.991092000	3.147459000	-0.523713000
6	4.348824000	1.802952000	-0.744743000
1	5.212290000	1.675204000	-0.081823000
1	4.528595000	1.171346000	-1.624248000
1	4.299231000	2.847523000	-1.067492000
6	-1.724521000	0.377071000	-0.354691000
6	-2.477456000	1.063444000	-1.336109000
6	-2.429575000	-0.061843000	0.793035000
6	-3.844281000	1.278788000	-1.186615000
1	-1.970194000	1.425943000	-2.227622000
6	-3.799069000	0.146641000	0.935150000
1	-1.884746000	-0.555967000	1.595679000
6	-4.522516000	0.816628000	-0.054506000
1	-4.388232000	1.807100000	-1.966430000
1	-4.302883000	-0.208136000	1.831517000
1	-5.590061000	0.982571000	0.057882000

6	-0.500095000	-2.310596000	-1.145844000
1	-1.498803000	-2.344195000	-0.707448000
1	-0.570859000	-1.993697000	-2.190769000
6	0.596715000	-2.046077000	1.549596000
1	-0.407239000	-2.457109000	1.659250000
1	0.869818000	-1.375250000	2.359945000
6	-0.256979000	0.606178000	-0.553262000
1	-0.151970000	0.625272000	-1.645398000
6	0.354965000	1.906307000	0.041669000
6	1.848289000	2.021763000	-0.143635000
1	1.325226000	-2.858446000	1.483634000
1	-0.051985000	-3.309289000	-1.109448000
33	0.732057000	-1.081736000	-0.142065000
6	2.289591000	-1.473069000	-1.261516000
1	2.650921000	-0.526288000	-1.663375000
1	3.045614000	-1.896550000	-0.601434000
1	2.027590000	-2.163260000	-2.064783000
6	-0.370488000	3.134244000	-0.531611000
1	0.035660000	4.047560000	-0.082388000
1	-0.219606000	3.204788000	-1.616925000
1	-1.447395000	3.109463000	-0.338625000
1	0.149558000	1.864936000	1.123173000
6	2.665242000	1.098233000	0.414584000
8	2.171762000	0.010070000	0.998870000
1	2.251106000	2.905546000	-0.630319000
6	4.171368000	1.225234000	0.431789000
1	4.512015000	2.154182000	-0.036937000
1	4.531217000	1.206019000	1.468395000
1	4.644993000	0.377313000	-0.080471000
6	-1.707438000	0.403916000	-0.175922000
6	-2.723686000	0.457600000	-1.139386000
6	-2.070167000	0.193497000	1.164336000
6	-4.063405000	0.306143000	-0.778233000
1	-2.461596000	0.623999000	-2.181687000
6	-3.408288000	0.048787000	1.528729000
1	-1.296842000	0.156327000	1.927187000
6	-4.410986000	0.100546000	0.557765000
1	-4.835376000	0.351429000	-1.542078000
1	-3.668193000	-0.106980000	2.572570000
1	-5.453639000	-0.015277000	0.840779000

Cisoid Betaine _{tr} (-2894.39556) E(CH ₃ CN) = -2896.69107 NIMAG = 0				TS1T _{tr} (-2894.35986) E(CH ₃ CN) = -2896.66884 NIMAG = 1 (-248.2)			
6	-0.450034000	2.759595000	-0.069471000	6	1.274691000	2.841194000	-1.081499000
1	-1.454375000	2.487150000	-0.399733000	1	2.260118000	2.681798000	-0.641792000
1	-0.502410000	3.195475000	0.932751000	1	1.288853000	2.537188000	-2.129684000
6	0.812435000	0.853617000	-1.955940000	6	0.013704000	2.410139000	1.669625000
1	-0.143550000	1.161345000	-2.382168000	1	0.964227000	2.160487000	2.143645000
1	1.026223000	-0.190429000	-2.188093000	1	-0.809896000	1.972733000	2.236007000
6	-0.464920000	-0.054086000	1.060343000	6	0.121513000	-0.127994000	-0.284629000
1	-0.586341000	0.511807000	1.993688000	1	-0.509128000	-0.407159000	-1.125518000
6	0.469752000	-1.282767000	1.245396000	6	-1.182728000	-0.963476000	1.168781000
6	1.838186000	-0.916893000	0.690992000	6	-2.016056000	-1.899958000	0.539579000
1	1.609202000	1.506578000	-2.321571000	1	-0.104670000	3.496291000	1.633900000
1	-0.019591000	3.493839000	-0.756455000	1	0.979587000	3.889932000	-0.997569000
33	0.731440000	1.142979000	-0.034713000	33	-0.046552000	1.738906000	-0.152450000
6	2.337280000	2.113880000	0.561907000	6	-1.779926000	2.248063000	-0.821899000
1	3.206921000	1.585806000	0.172375000	1	-2.051734000	3.221204000	-0.407111000
1	2.299067000	3.147925000	0.209520000	1	-1.724626000	2.308850000	-1.911170000
1	2.352346000	2.092366000	1.653467000	1	-2.484121000	1.453360000	-0.533351000
6	0.496795000	-1.746583000	2.709196000	6	-0.216174000	-1.402152000	2.242233000
1	1.105298000	-2.650625000	2.818055000	1	-0.773273000	-1.668552000	3.150543000
1	0.927967000	-0.975391000	3.362263000	1	0.352543000	-2.284298000	1.930179000
1	-0.511019000	-1.972122000	3.079916000	1	0.504966000	-0.621429000	2.505820000
1	0.078022000	-2.096086000	0.626762000	1	-1.682716000	-0.015507000	1.364432000
6	2.278049000	-1.557124000	-0.508079000	6	-3.175442000	-1.474755000	-0.166787000
8	1.513437000	-2.151191000	-1.302971000	8	-3.498249000	-0.271769000	-0.337843000
1	2.612421000	-0.664603000	1.418368000	1	-1.746074000	-2.953335000	0.544824000
6	3.752342000	-1.429051000	-0.897563000	6	-4.100661000	-2.541139000	-0.749641000
1	4.191127000	-2.432610000	-0.951690000	1	-3.752504000	-3.562411000	-0.563949000
1	3.838471000	-0.994060000	-1.900240000	1	-5.102563000	-2.424945000	-0.319318000
1	4.340081000	-0.831829000	-0.191751000	1	-4.201990000	-2.389705000	-1.831260000
6	-1.798147000	-0.263606000	0.399772000	6	1.467863000	-0.707971000	-0.315777000
6	-2.972498000	0.276127000	0.944646000	6	1.687152000	-1.901478000	-1.039347000
6	-1.886297000	-1.005324000	-0.793149000	6	2.557871000	-0.197849000	0.424208000
6	-4.206514000	0.082175000	0.321612000	6	2.923691000	-2.541218000	-1.024064000
1	-2.919341000	0.844448000	1.870892000	1	0.866551000	-2.323825000	-1.613874000
6	-3.120371000	-1.203253000	-1.409544000	6	3.796864000	-0.833330000	0.429428000
1	-0.986493000	-1.446712000	-1.217019000	1	2.433144000	0.713249000	1.006858000
6	-4.283595000	-0.657503000	-0.858973000	6	3.992039000	-2.011602000	-0.295133000
1	-5.106146000	0.504073000	0.762260000	1	3.056347000	-3.458071000	-1.593538000
1	-3.174286000	-1.786775000	-2.324915000	1	4.614417000	-0.406700000	1.005873000
1	-5.243372000	-0.813576000	-1.344262000	1	4.958339000	-2.507740000	-0.290832000

Transoid Betaine _π (-2894.37448) E(CH ₃ CN) = -2896.68837 NIMAG = 0				TS1R _π (-2894.34468) E(CH ₃ CN) = -2896.67401 NIMAG = 1 (-46)			
6	-0.357340000	-2.402291000	-1.771767000	6	-2.376853000	1.881904000	-0.563294000
1	-1.441093000	-2.323790000	-1.677490000	1	-1.623137000	2.542284000	-0.134867000
1	-0.008959000	-1.788676000	-2.605251000	1	-2.343842000	1.941748000	-1.652547000
6	0.030691000	-2.949281000	1.264664000	6	-2.242011000	0.107641000	1.894059000
1	-1.048716000	-3.090486000	1.333337000	1	-1.555902000	0.840167000	2.320201000
1	0.420283000	-2.543157000	2.199811000	1	-2.065310000	-0.876002000	2.328184000
6	0.075283000	0.162471000	0.049038000	6	-0.180717000	-0.467855000	-0.684160000
1	0.686434000	0.506989000	-0.803185000	1	-0.380777000	-0.430365000	-1.762059000
6	0.854559000	0.739718000	1.299628000	6	0.351400000	-1.959811000	-0.306277000
6	1.462789000	2.051502000	0.902301000	6	1.610532000	-1.963224000	0.474857000
1	0.515100000	-3.904792000	1.047714000	1	-3.275420000	0.417497000	2.070353000
1	-0.057425000	-3.441555000	-1.923039000	1	-3.375625000	2.141836000	-0.203095000
33	0.487484000	-1.719081000	-0.169290000	33	-1.973491000	0.057661000	-0.024943000
6	2.398716000	-1.871962000	-0.428391000	6	-3.485650000	-0.963159000	-0.710919000
1	2.853441000	-2.153680000	0.523038000	1	-3.580068000	-1.894279000	-0.153279000
1	2.594352000	-2.639781000	-1.181074000	1	-4.387511000	-0.357926000	-0.592290000
1	2.733654000	-0.866621000	-0.733616000	1	-3.318464000	-1.174193000	-1.768638000
6	-0.012186000	0.822719000	2.558595000	6	-0.732680000	-2.872793000	0.277118000
1	0.598956000	1.163987000	3.401373000	1	-0.310118000	-3.873055000	0.412170000
1	-0.829756000	1.539173000	2.426821000	1	-1.071262000	-2.541594000	1.268480000
1	-0.457681000	-0.143662000	2.831942000	1	-1.609196000	-2.977284000	-0.375996000
1	1.658415000	0.003854000	1.510164000	1	0.593204000	-2.318365000	-1.316081000
6	2.296716000	2.118164000	-0.198616000	6	2.743066000	-1.530518000	-0.215254000
8	2.565046000	1.118769000	-0.972298000	8	2.679678000	-1.062519000	-1.393458000
1	1.263607000	2.924734000	1.516474000	1	1.636963000	-2.360190000	1.486455000
6	2.937172000	3.451741000	-0.571931000	6	4.111958000	-1.595935000	0.462168000
1	2.650732000	4.269232000	0.099526000	1	4.077917000	-2.046066000	1.461804000
1	4.030369000	3.352507000	-0.557773000	1	4.803870000	-2.175022000	-0.162168000
1	2.661925000	3.723124000	-1.599479000	1	4.531727000	-0.585128000	0.545702000
6	-1.372195000	0.531560000	-0.120033000	6	0.656344000	0.722913000	-0.288740000
6	-1.666664000	1.766737000	-0.722764000	6	1.058081000	1.663715000	-1.246094000
6	-2.441526000	-0.255340000	0.334333000	6	0.998932000	0.932760000	1.056850000
6	-2.986539000	2.197538000	-0.857409000	6	1.766535000	2.803112000	-0.871484000
1	-0.844688000	2.390898000	-1.058969000	1	0.836849000	1.481969000	-2.294712000
6	-3.763092000	0.168188000	0.187707000	6	1.723717000	2.071113000	1.430666000
1	-2.247215000	-1.206648000	0.824179000	1	0.746338000	0.178237000	1.793093000
6	-4.040555000	1.398266000	-0.410410000	6	2.100600000	3.009517000	0.472262000
1	-3.191403000	3.159202000	-1.320627000	1	2.078812000	3.518002000	-1.627876000
1	-4.574023000	-0.460869000	0.545953000	1	1.998138000	2.215049000	2.472624000
1	-5.068627000	1.731157000	-0.524539000	1	2.661069000	3.893754000	0.764780000

TS1E _{tr} (-2894.36841) E(CH ₃ CN) = -2896.67962 NIMAG = -174.9				TS1C _{rs} Conformer (-2894.36697) E(CH ₃ CN) = -2896.66574 NIMAG = 1 (-100.1)			
6	1.098491000	1.833823000	-1.975160000	6	-2.225161000	-2.750662000	-0.043977000
1	2.036625000	1.277794000	-2.023425000	1	-1.467676000	-3.369282000	-0.529732000
1	0.352544000	1.354751000	-2.613127000	1	-2.329380000	-3.059630000	0.998733000
6	1.688386000	3.020900000	0.778822000	6	-1.676320000	-0.485406000	-1.973965000
1	2.690315000	2.590546000	0.730531000	1	-0.922256000	-1.077270000	-2.495222000
1	1.376030000	3.123476000	1.819556000	1	-1.520946000	0.584066000	-2.111349000
6	-0.284968000	-0.250604000	0.161506000	6	-0.010867000	-0.695012000	0.865847000
1	-0.885560000	-0.120870000	-0.740184000	1	-0.157072000	-1.234106000	1.804268000
6	-1.227262000	-0.325337000	1.352000000	6	0.161757000	1.643601000	1.738547000
6	-2.129756000	-1.395446000	0.815424000	6	0.937062000	1.315581000	2.983033000
1	1.667238000	3.994488000	0.281699000	1	1.974561000	1.054915000	2.747163000
1	1.256301000	2.864662000	-2.301989000	1	0.958869000	2.182211000	3.660280000
33	0.431615000	1.813513000	-0.143001000	1	0.491390000	0.481675000	3.533437000
6	-1.211554000	2.847332000	-0.292270000	1	-0.914649000	1.537811000	1.785409000
1	-1.991184000	2.153747000	-0.627799000	6	0.675795000	2.417083000	0.729347000
1	-1.472557000	3.237299000	0.693663000	1	1.721450000	2.714510000	0.743766000
1	-1.068577000	3.674191000	-0.993067000	6	-0.108190000	2.714014000	-0.436779000
6	-0.589028000	-0.610886000	2.708201000	6	0.470412000	3.644107000	-1.495303000
1	-1.369677000	-0.678581000	3.473399000	1	1.424394000	4.088246000	-1.196480000
1	-0.037306000	-1.557204000	2.708468000	1	0.617017000	3.094801000	-2.433629000
1	0.106668000	0.186027000	3.005009000	1	-0.248473000	4.444441000	-1.704207000
1	-1.780290000	0.624112000	1.407226000	8	-1.234142000	2.206862000	-0.639378000
6	-3.039379000	-1.047173000	-0.197783000	1	-2.674215000	-0.779239000	-2.310989000
8	-3.094599000	0.106386000	-0.725236000	1	-3.184595000	-2.845128000	-0.559989000
1	-2.055856000	-2.407429000	1.200997000	33	-1.598652000	-0.884187000	-0.083961000
6	-4.019786000	-2.104129000	-0.702069000	6	-3.087052000	0.051436000	0.728715000
1	-3.884350000	-3.080214000	-0.223407000	1	-2.936404000	1.117557000	0.561419000
1	-5.046855000	-1.763946000	-0.521280000	1	-4.011711000	-0.295227000	0.260571000
1	-3.913847000	-2.221427000	-1.787874000	1	-3.106637000	-0.183325000	1.795452000
6	0.884360000	-1.171548000	-0.015070000	6	1.268768000	-0.919588000	0.218376000
6	0.838134000	-2.165674000	-1.005035000	6	2.286110000	-1.655575000	0.875631000
6	2.043067000	-1.069541000	0.772628000	6	1.618015000	-0.320733000	-1.017422000
6	1.908571000	-3.040581000	-1.191689000	6	3.554150000	-1.802605000	0.323961000
1	-0.058000000	-2.260677000	-1.610932000	1	2.060803000	-2.121110000	1.833304000
6	3.115303000	-1.942394000	0.586511000	6	2.885344000	-0.486688000	-1.573373000
1	2.103238000	-0.298594000	1.536354000	1	0.888792000	0.292590000	-1.535848000
6	3.051014000	-2.931834000	-0.396520000	6	3.866050000	-1.228774000	-0.913296000
1	1.848124000	-3.809304000	-1.957530000	1	4.304225000	-2.380975000	0.859256000
1	4.001011000	-1.849216000	1.209624000	1	3.111526000	-0.017172000	-2.528522000
1	3.885896000	-3.612103000	-0.541954000	1	4.854401000	-1.351755000	-1.347393000

TS1C _{rs} Conformer (-2894.35748) E(CH3CN) = -2896.66525 NIMAG = 1 (-246.1)				TS1C _{rs} Conformer 2 (-2894.364705) E(CH3CN) = -2896.66479 NIMAG = 1 (-157.7)			
6	0.660644000	2.911312000	-0.682613000	6	0.441299000	3.131870000	0.197815000
1	1.641401000	2.874610000	-0.206939000	1	1.273634000	2.904285000	0.866634000
1	0.778365000	2.826701000	-1.764468000	1	0.827667000	3.503683000	-0.753245000
6	-0.756149000	1.800417000	1.783511000	6	-1.315464000	1.112952000	1.613733000
1	-1.234050000	2.782356000	1.831648000	1	-0.714771000	1.625852000	2.368097000
1	0.175969000	1.815934000	2.350423000	1	-1.317440000	0.038795000	1.784314000
6	0.333328000	-0.277373000	-0.428937000	6	0.525985000	0.140481000	-0.879537000
1	-0.143856000	-0.645710000	-1.334947000	1	0.596011000	0.361834000	-1.945916000
6	-0.818676000	-1.706545000	0.786407000	6	-0.809409000	-1.791324000	-1.124006000
6	-0.023386000	-1.826661000	2.060699000	6	0.297841000	-2.635786000	-1.693315000
1	-0.333941000	-1.088635000	2.809794000	1	0.988938000	-2.971138000	-0.913174000
1	-0.191156000	-2.819596000	2.501160000	1	-0.130202000	-3.531425000	-2.166513000
1	1.051938000	-1.721046000	1.892916000	1	0.879336000	-2.105898000	-2.452697000
1	-0.528169000	-2.393543000	-0.003497000	1	-1.362979000	-1.179231000	-1.829505000
6	-2.179789000	-1.376487000	0.827419000	6	-1.502876000	-2.188479000	0.006511000
1	-2.625184000	-1.049657000	1.766349000	1	-1.117549000	-2.999366000	0.620737000
6	-2.995008000	-1.474012000	-0.341681000	6	-2.742358000	-1.568927000	0.365906000
6	-4.510951000	-1.341814000	-0.182812000	6	-3.589383000	-2.212955000	1.459444000
1	-4.818515000	-1.056753000	0.829304000	1	-3.114895000	-3.088373000	1.913563000
1	-4.900525000	-0.610437000	-0.900816000	1	-3.809069000	-1.475774000	2.241229000
1	-4.980672000	-2.302514000	-0.426886000	1	-4.553093000	-2.517571000	1.033920000
8	-2.530509000	-1.650266000	-1.489615000	8	-3.163395000	-0.515167000	-0.162594000
1	-1.427617000	1.038316000	2.178827000	1	-2.340699000	1.484694000	1.618569000
1	0.143604000	3.840246000	-0.429723000	1	-0.224253000	3.871227000	0.651287000
6	-2.128091000	1.595282000	-0.960207000	33	-0.547687000	1.470272000	-0.133226000
1	-2.212213000	2.605971000	-1.365060000	6	-1.938165000	2.000046000	-1.362923000
1	-2.207119000	0.841742000	-1.744978000	1	-1.474144000	2.300355000	-2.305138000
1	-2.905264000	1.409875000	-0.217682000	1	-2.611055000	1.151921000	-1.484173000
33	-0.413629000	1.394807000	-0.083422000	1	-2.463936000	2.850813000	-0.923252000
6	1.780127000	-0.437025000	-0.354200000	6	1.805210000	-0.136420000	-0.234720000
6	2.426977000	-1.356222000	-1.213900000	6	2.956632000	-0.391103000	-1.018348000
6	2.588453000	0.205423000	0.614555000	6	1.958915000	-0.248512000	1.168889000
6	3.792109000	-1.606064000	-1.115430000	6	4.175484000	-0.730581000	-0.440377000
1	1.837002000	-1.872903000	-1.967376000	1	2.881833000	-0.312380000	-2.101051000
6	3.957219000	-0.036882000	0.701122000	6	3.183325000	-0.582329000	1.743747000
1	2.132777000	0.900696000	1.317412000	1	1.101256000	-0.099250000	1.819196000
6	4.573677000	-0.944635000	-0.162906000	6	4.305310000	-0.824221000	0.948592000
1	4.253235000	-2.318541000	-1.795493000	1	5.035474000	-0.914775000	-1.080433000
1	4.544602000	0.481374000	1.455686000	1	3.258468000	-0.659000000	2.826266000
1	5.640305000	-1.137266000	-0.091970000	1	5.258223000	-1.085191000	1.400051000

Cisoid betaine _{rs} (-2894.40981) E(CH ₃ CN) = -2896.69107 NIMAG = 0				Cisoid Betaine _{rs} Conformer (-2894.41039) E(CH ₃ CN) = -2896.69716 NIMAG = 0			
6	-0.153800000	-2.867561000	0.243932000	6	-0.946032000	-2.835668000	0.712101000
1	0.858675000	-2.835627000	-0.165822000	1	0.097730000	-3.135824000	0.579680000
1	-0.108938000	-3.122366000	1.307312000	1	-1.185974000	-2.817521000	1.779824000
6	-1.066594000	-1.201014000	-1.988263000	6	-1.002890000	-1.576617000	-1.918995000
1	-0.474794000	-2.052855000	-2.327407000	1	0.023169000	-1.926801000	-2.042790000
1	-0.687755000	-0.267253000	-2.396936000	1	-1.222989000	-0.742853000	-2.579204000
6	0.261856000	-0.048565000	1.018402000	6	0.223406000	-0.169865000	1.028318000
1	0.391377000	-0.732940000	1.866370000	1	0.321282000	-0.896020000	1.841848000
6	-0.319049000	1.284818000	1.572303000	6	-0.240329000	1.166263000	1.684721000
6	0.664962000	1.913104000	2.569996000	6	0.822067000	1.642160000	2.691936000
1	1.588818000	2.226940000	2.071645000	1	1.750594000	1.920601000	2.182953000
1	0.214025000	2.799084000	3.031126000	1	0.455171000	2.523447000	3.230251000
1	0.933432000	1.214166000	3.371995000	1	1.054588000	0.868008000	3.434038000
1	-1.212175000	0.971537000	2.141031000	1	-1.125047000	0.881198000	2.285682000
6	-0.755886000	2.263532000	0.512474000	6	-0.614752000	2.268690000	0.729318000
1	-0.351070000	3.270947000	0.528191000	1	-0.421588000	3.285128000	1.060305000
6	-1.674278000	1.901355000	-0.416007000	6	-1.205586000	2.083057000	-0.474314000
6	-2.213260000	2.867772000	-1.447618000	6	-1.566696000	3.251822000	-1.365336000
1	-1.783058000	3.868629000	-1.339693000	1	-1.321903000	4.213851000	-0.904891000
1	-2.012634000	2.504559000	-2.464472000	1	-1.037912000	3.175915000	-2.324583000
1	-3.303858000	2.944503000	-1.352581000	1	-2.639601000	3.234045000	-1.596010000
8	-2.188826000	0.681266000	-0.474762000	8	-1.488033000	0.903264000	-1.018761000
1	-2.114064000	-1.309596000	-2.272650000	1	-1.694185000	-2.409088000	-2.072506000
1	-0.729865000	-3.637251000	-0.279594000	1	-1.595115000	-3.563595000	0.216046000
33	-1.061792000	-1.097412000	-0.038262000	33	-1.210537000	-1.001043000	-0.071677000
6	-2.716847000	-1.626321000	0.845584000	6	-3.073355000	-0.815795000	0.460515000
1	-2.475909000	-1.854435000	1.886590000	1	-3.097366000	-0.542035000	1.517895000
1	-3.439746000	-0.819737000	0.767198000	1	-3.524619000	-0.039829000	-0.152060000
1	-3.069391000	-2.535490000	0.352665000	1	-3.566368000	-1.781270000	0.324710000
6	1.575143000	0.016364000	0.271540000	6	1.529105000	-0.166930000	0.262427000
6	2.694192000	-0.667560000	0.774288000	6	2.653953000	-0.784129000	0.832777000
6	1.731710000	0.759497000	-0.911448000	6	1.674786000	0.454558000	-0.990031000
6	3.927691000	-0.614259000	0.124999000	6	3.890020000	-0.774655000	0.185770000
1	2.597365000	-1.242385000	1.692763000	1	2.561190000	-1.270685000	1.801389000
6	2.968442000	0.822496000	-1.554423000	6	2.911731000	0.464385000	-1.635434000
1	0.891710000	1.326092000	-1.296578000	1	0.809868000	0.904788000	-1.461542000
6	4.069511000	0.131685000	-1.045873000	6	4.023957000	-0.145872000	-1.052529000
1	4.777107000	-1.152834000	0.537226000	1	4.745468000	-1.258465000	0.650203000
1	3.068915000	1.411681000	-2.462467000	1	3.004448000	0.951271000	-2.603008000
1	5.028822000	0.177046000	-1.554469000	1	4.984844000	-0.134378000	-1.560249000

TS1R _{rs} (-2894.37118) E(CH ₃ CN) = -2896.67401 NIMAG = -51.3				Transoid Betaine _{rs} (-2894.37311) E(CH ₃ CN) = -2896.69069 NIMAG = 0			
6	-1.745178000	-2.012724000	-1.210496000	6	2.364897000	2.018709000	-0.581160000
1	-0.905367000	-2.018171000	-1.906458000	1	1.519175000	2.591771000	-0.964491000
1	-1.609842000	-2.796509000	-0.463495000	1	2.689930000	2.429968000	0.376392000
6	-2.010498000	1.083123000	-1.642339000	6	1.379976000	-0.574720000	-2.045544000
1	-2.223782000	0.596668000	-2.596949000	1	0.965621000	0.211669000	-2.678728000
1	-1.052909000	1.647163000	-1.651540000	1	0.618574000	-1.362782000	-1.854611000
6	-0.290265000	-0.157357000	0.949337000	6	0.329550000	0.116260000	0.967827000
1	-0.746114000	-0.665481000	1.809544000	1	0.824222000	0.533746000	1.855065000
6	-0.051092000	1.382539000	1.344769000	6	-0.048711000	-1.430390000	1.244091000
6	-0.172495000	1.488897000	2.875355000	6	0.272680000	-1.721690000	2.719941000
1	0.635787000	0.931519000	3.365223000	1	-0.404394000	-1.164425000	3.380067000
1	-0.086594000	2.535412000	3.184302000	1	0.135298000	-2.787167000	2.928408000
1	-1.127693000	1.097670000	3.253073000	1	1.302718000	-1.449737000	2.994138000
1	-0.900761000	1.935404000	0.905388000	1	0.631318000	-2.027298000	0.615468000
6	1.224449000	2.003997000	0.869756000	6	-1.429004000	-1.854667000	0.875586000
1	1.986751000	2.189608000	1.622121000	1	-2.187235000	-1.866999000	1.654176000
6	1.432985000	2.401025000	-0.431116000	6	-1.709493000	-2.309534000	-0.396287000
6	2.731771000	3.122114000	-0.782347000	6	-3.097778000	-2.868232000	-0.695347000
1	3.376401000	3.299322000	0.085730000	1	-3.585434000	-2.264832000	-1.472703000
1	3.293578000	2.539330000	-1.524495000	1	-3.002856000	-3.883280000	-1.101446000
1	2.499054000	4.085949000	-1.252830000	1	-3.749053000	-2.899484000	0.185473000
8	0.630336000	2.181908000	-1.418386000	8	-0.888128000	-2.280144000	-1.389438000
1	-2.853326000	1.706900000	-1.338090000	1	2.310012000	-0.956072000	-2.474488000
1	-2.687702000	-2.149662000	-1.745628000	1	3.189147000	2.031202000	-1.297764000
33	-1.784389000	-0.297036000	-0.315980000	6	3.317592000	-0.765789000	0.371995000
6	-3.407769000	-0.315361000	0.749938000	1	4.162344000	-0.613123000	-0.303594000
1	-3.390429000	-1.168523000	1.431336000	1	3.560594000	-0.378986000	1.363375000
1	-3.453488000	0.616877000	1.317155000	1	3.072670000	-1.827411000	0.429524000
1	-4.269676000	-0.386849000	0.082777000	33	1.782449000	0.187786000	-0.330127000
6	0.866090000	-0.999279000	0.470472000	6	-0.739117000	1.083109000	0.518333000
6	1.286897000	-2.092242000	1.238949000	6	-0.991727000	2.237521000	1.271377000
6	1.524476000	-0.717504000	-0.738441000	6	-1.478309000	0.858526000	-0.656737000
6	2.345306000	-2.899396000	0.814811000	6	-1.957754000	3.160815000	0.865704000
1	0.791798000	-2.309045000	2.183935000	1	-0.436330000	2.410182000	2.191543000
6	2.575673000	-1.531432000	-1.161294000	6	-2.437615000	1.788152000	-1.061344000
1	1.213639000	0.146679000	-1.327703000	1	-1.314514000	-0.047480000	-1.236070000
6	2.989115000	-2.622039000	-0.390982000	6	-2.680674000	2.938430000	-0.306765000
1	2.661426000	-3.741481000	1.425103000	1	-2.142945000	4.048317000	1.465236000
1	3.082957000	-1.303704000	-2.095391000	1	-3.008319000	1.603466000	-1.967746000
1	3.811658000	-3.248322000	-0.726932000	1	-3.433411000	3.653968000	-0.627553000

TS1E _{rs} (-2894.36351) E(CH ₃ CN) = -2896.68039 NIMAG = -141.4				Product Complex _{rr} (-2894.43152) E(CH ₃ CN) = -2896.73046 NIMAG = 0			
6	2.860473000	0.298576000	1.752481000	6	2.353282000	-1.134849000	-1.713104000
1	2.258866000	1.132041000	2.115959000	1	2.229548000	-2.221563000	-1.725565000
1	2.761624000	-0.562289000	2.416924000	1	1.475570000	-0.679195000	-2.179407000
6	2.335764000	1.345012000	-1.261493000	6	4.330956000	-1.246762000	0.474332000
1	1.928735000	1.060288000	-2.232728000	1	4.263977000	-2.336187000	0.540129000
1	3.390608000	1.615900000	-1.349538000	1	4.707139000	-0.867517000	1.428299000
6	-0.246845000	-0.610273000	0.490887000	6	-1.069266000	0.457461000	-0.020001000
1	0.031376000	-0.818994000	1.523734000	1	-0.253476000	0.523920000	-0.737757000
6	-0.791271000	-1.817498000	-0.220579000	6	-0.745656000	1.109181000	1.290912000
6	0.016228000	-3.101449000	-0.023055000	6	-1.671205000	1.823062000	0.302550000
1	0.213090000	-3.284163000	1.042106000	1	5.013197000	-0.962497000	-0.332104000
1	-0.552659000	-3.955627000	-0.403892000	1	3.246284000	-0.868191000	-2.287083000
1	0.978974000	-3.077428000	-0.545197000	33	2.513944000	-0.522022000	0.161449000
1	-0.960553000	-1.623888000	-1.283858000	6	3.039896000	1.336020000	-0.250147000
6	-2.101813000	-1.774291000	0.506871000	1	2.167138000	1.879875000	-0.619685000
1	-2.152269000	-2.213711000	1.499205000	1	3.388245000	1.819035000	0.667605000
6	-3.253718000	-1.197064000	-0.093052000	1	3.842722000	1.354775000	-0.993739000
6	-4.549957000	-1.177385000	0.716058000	6	-1.285809000	0.596457000	2.606210000
1	-4.825349000	-0.137099000	0.929598000	1	-1.324981000	1.397103000	3.354211000
1	-5.360105000	-1.606332000	0.116144000	1	-2.292278000	0.180000000	2.497539000
1	-4.478732000	-1.721050000	1.664142000	1	-0.637983000	-0.198004000	2.995396000
8	-3.261874000	-0.710103000	-1.245520000	1	0.255031000	1.532958000	1.335602000
1	1.753262000	2.161911000	-0.835982000	6	-1.144612000	3.006058000	-0.435700000
1	3.908844000	0.592786000	1.666781000	8	0.014893000	3.064262000	-0.820714000
6	3.455997000	-1.646442000	-0.760809000	1	-2.723076000	1.855286000	0.574606000
1	4.460162000	-1.220444000	-0.823873000	6	-2.116798000	4.143980000	-0.687199000
1	3.436248000	-2.495623000	-0.076155000	1	-2.972551000	3.789497000	-1.276047000
1	3.099958000	-1.946733000	-1.747549000	1	-2.517890000	4.520401000	0.262490000
33	2.097757000	-0.270312000	-0.049635000	1	-1.614679000	4.952996000	-1.221156000
6	-0.663939000	0.782867000	0.252584000	6	-1.901209000	-0.784621000	-0.134367000
6	-0.467858000	1.735562000	1.274979000	6	-3.271017000	-0.759218000	-0.422927000
6	-1.150405000	1.231330000	-0.991548000	6	-1.276734000	-2.032026000	0.033343000
6	-0.740186000	3.084269000	1.066685000	6	-4.003230000	-1.943902000	-0.532594000
1	-0.123350000	1.401045000	2.251293000	1	-3.770116000	0.193667000	-0.575564000
6	-1.430240000	2.582906000	-1.191036000	6	-2.005098000	-3.214918000	-0.079375000
1	-1.353340000	0.517891000	-1.779006000	1	-0.210664000	-2.064288000	0.244692000
6	-1.221164000	3.515812000	-0.173671000	6	-3.373458000	-3.175917000	-0.359420000
1	-0.591539000	3.796983000	1.873908000	1	-5.065591000	-1.900867000	-0.758962000
1	-1.821587000	2.906833000	-2.151714000	1	-1.503629000	-4.170142000	0.054324000
1	-1.439667000	4.567236000	-0.340002000	1	-3.941499000	-4.098472000	-0.445025000

Product Complex_{rs} (-2894.42842)
E(CH₃CN) = -2896.7294
NIMAG = 0

6	2.331112000	0.163968000	1.567919000
1	1.499418000	0.865802000	1.663667000
1	2.147449000	-0.693230000	2.222200000
6	3.148951000	1.244791000	-1.044290000
1	3.415286000	1.100659000	-2.094947000
1	4.028437000	1.577310000	-0.484887000
6	-1.378218000	-0.586897000	0.965669000
1	-1.256618000	-0.708360000	2.041880000
6	-1.015874000	-1.796180000	0.168564000
6	-0.288102000	-2.957673000	0.809567000
1	-0.589252000	-3.097185000	1.854914000
1	-0.482265000	-3.894116000	0.273473000
1	0.791654000	-2.770154000	0.785431000
1	-0.743793000	-1.606855000	-0.866737000
6	-2.485661000	-1.550170000	0.432221000
1	-2.971007000	-2.138206000	1.208675000
6	-3.366467000	-1.121070000	-0.693175000
6	-4.862739000	-1.243733000	-0.459075000
1	-5.160197000	-0.652419000	0.416421000
1	-5.405449000	-0.894038000	-1.339425000
1	-5.135748000	-2.285829000	-0.248858000
8	-2.918372000	-0.685097000	-1.742335000
1	2.360138000	1.998674000	-0.983546000
1	3.261706000	0.653791000	1.871125000
6	4.180413000	-1.385769000	-0.122948000
1	4.925632000	-0.743339000	0.355836000
1	4.029785000	-2.288699000	0.475576000
1	4.535996000	-1.684741000	-1.112748000
33	2.441250000	-0.448888000	-0.304731000
6	-1.224111000	0.837571000	0.540525000
6	-1.566835000	1.842795000	1.460488000
6	-0.728216000	1.227148000	-0.712895000
6	-1.427708000	3.193129000	1.142906000
1	-1.945895000	1.558104000	2.440042000
6	-0.594275000	2.579507000	-1.033364000
1	-0.451059000	0.477460000	-1.443479000
6	-0.942009000	3.567711000	-0.111115000
1	-1.698005000	3.950481000	1.874291000
1	-0.218360000	2.859637000	-2.014084000
1	-0.833697000	4.618566000	-0.366016000

Stabilized Ylides (COMe)

TS2C _{tr} (-2815.974812) E(CH3CN) = -2818.25821 NIMAG = 1 (-297.3)				TS2C _{tr} Conformer (-2815.95957) E(CH3CN) = -2818.25409 NIMAG = 1 (-323.2)			
6	-2.540730000	-1.693122000	-0.335348000	6	3.185399000	0.387439000	-0.630861000
1	-2.767055000	-1.565691000	-1.396266000	1	3.710154000	0.650792000	0.289663000
1	-2.617748000	-2.749593000	-0.065795000	1	3.757323000	-0.358654000	-1.188176000
6	-0.467111000	-1.448357000	1.860767000	6	0.670464000	-0.948936000	-1.832660000
1	-1.132800000	-0.759888000	2.382679000	1	0.468183000	-0.067402000	-2.437549000
1	0.580375000	-1.291902000	2.110592000	1	-0.254611000	-1.477594000	-1.604729000
6	-0.532216000	0.709310000	-0.588081000	6	0.368889000	0.772851000	0.905521000
1	-0.134052000	0.791149000	-1.595925000	1	0.791811000	0.931662000	1.896241000
6	0.991531000	1.604341000	0.528403000	6	-1.332632000	-0.222474000	1.470290000
6	2.236548000	1.347142000	-0.078711000	6	-1.895503000	-1.040236000	0.470071000
1	-0.761698000	-2.484194000	2.047913000	1	1.391676000	-1.612781000	-2.317195000
1	-3.210290000	-1.084215000	0.269839000	1	3.004485000	1.276814000	-1.232869000
33	-0.703899000	-1.104998000	-0.020978000	33	1.449205000	-0.353560000	-0.173606000
6	0.281352000	-2.386022000	-1.087302000	6	1.866647000	-1.997350000	0.768718000
1	-0.094319000	-3.377156000	-0.820788000	1	2.588653000	-2.563897000	0.175759000
1	0.068824000	-2.186575000	-2.140091000	1	2.293291000	-1.769387000	1.747282000
1	1.340476000	-2.286077000	-0.856487000	1	0.948292000	-2.573700000	0.887640000
6	0.567047000	3.047667000	0.697608000	6	-0.927864000	-0.854157000	2.789744000
1	1.235320000	3.520477000	1.429332000	1	-1.835778000	-1.121093000	3.345275000
1	0.660443000	3.613307000	-0.236212000	1	-0.355751000	-1.778980000	2.654253000
1	-0.453877000	3.147855000	1.074333000	1	-0.341657000	-0.179470000	3.423545000
1	0.753905000	0.984515000	1.388850000	1	-1.847181000	0.729136000	1.586170000
6	2.812541000	0.062173000	-0.016593000	6	-2.670398000	-0.439967000	-0.566223000
8	2.223113000	-0.929465000	0.503187000	8	-2.802636000	0.795797000	-0.693095000
1	2.716240000	2.126721000	-0.666028000	1	-1.752001000	-2.119622000	0.497507000
6	4.197483000	-0.166071000	-0.608465000	6	-3.381689000	-1.352292000	-1.567748000
1	4.656131000	0.751854000	-0.989348000	1	-3.187217000	-2.417703000	-1.400061000
1	4.851777000	-0.598691000	0.157336000	1	-4.462780000	-1.180806000	-1.506309000
1	4.140467000	-0.897080000	-1.425243000	1	-3.078327000	-1.088126000	-2.587994000
6	-1.741869000	1.429620000	-0.246027000	6	0.108687000	1.959215000	0.090840000
8	-2.385460000	1.155518000	0.783702000	8	0.536467000	2.012489000	-1.077191000
6	-2.192633000	2.570742000	-1.148243000	6	-0.753677000	3.062091000	0.656684000
1	-2.739167000	3.311708000	-0.558766000	1	-0.535414000	4.004695000	0.148645000
1	-1.359266000	3.050019000	-1.670507000	1	-1.794598000	2.780492000	0.448751000
1	-2.877897000	2.175432000	-1.910304000	1	-0.632889000	3.179718000	1.739165000

Cisoid Betaine _π Conformer (-2815.98799) E(CH ₃ CN) = - 2818.27429 NIMAG = 0				Cisoid Betaine _π (-2815.99809) E(CH ₃ CN) = -2818.27847 NIMAG = 0			
6	2.901555000	0.640063000	-0.178725000	6	-1.458977000	-2.196875000	-0.745888000
1	2.748719000	1.585550000	-0.697623000	1	-2.360538000	-2.091092000	-0.138981000
1	3.253421000	0.811345000	0.842003000	1	-1.666990000	-1.905996000	-1.780618000
6	0.797265000	-0.691532000	-1.974992000	6	0.024624000	-1.869855000	1.752470000
1	-0.198142000	-0.296795000	-2.193707000	1	-0.967794000	-1.668665000	2.156605000
1	0.824085000	-1.776125000	-2.094805000	1	0.807829000	-1.418023000	2.354097000
6	-0.010748000	0.948939000	0.828625000	6	-0.754808000	0.680866000	-0.396463000
1	0.647924000	1.485455000	1.531636000	1	-0.720007000	0.765379000	-1.488628000
6	-1.094492000	0.131503000	1.569078000	6	0.009136000	1.876875000	0.258098000
6	-1.438316000	-1.106616000	0.773415000	6	1.441479000	1.949319000	-0.197696000
1	1.560120000	-0.208016000	-2.586285000	1	0.178518000	-2.946197000	1.641047000
1	3.628670000	0.019847000	-0.709173000	1	-1.145377000	-3.245755000	-0.737874000
33	1.188204000	-0.300270000	-0.123939000	33	0.070844000	-1.099222000	-0.030883000
6	1.741992000	-1.953445000	0.742293000	6	1.356778000	-1.766221000	-1.346822000
1	2.631707000	-2.309815000	0.214359000	1	2.148961000	-2.250776000	-0.777710000
1	1.994904000	-1.754281000	1.784633000	1	0.882876000	-2.458479000	-2.044775000
1	0.925733000	-2.669017000	0.677065000	1	1.771846000	-0.905826000	-1.872564000
6	-0.641086000	-0.202647000	2.997253000	6	-0.724223000	3.205252000	0.015785000
1	-1.434154000	-0.733000000	3.535393000	1	-0.157804000	4.023305000	0.474096000
1	0.243694000	-0.850910000	3.004288000	1	-0.808347000	3.424771000	-1.056845000
1	-0.396364000	0.704282000	3.564852000	1	-1.730068000	3.215748000	0.450344000
1	-1.972531000	0.792438000	1.650826000	1	-0.008641000	1.662740000	1.336823000
6	-1.969347000	-0.963660000	-0.503562000	6	2.276864000	0.931068000	0.114096000
8	-2.003832000	0.152720000	-1.125324000	8	1.822006000	-0.153281000	0.732017000
1	-1.556182000	-2.043565000	1.313808000	1	1.790879000	2.832825000	-0.724039000
6	-2.506700000	-2.189663000	-1.238057000	6	3.757847000	0.945435000	-0.184145000
1	-2.402580000	-3.116564000	-0.662972000	1	4.071835000	1.878984000	-0.662092000
1	-3.569486000	-2.034637000	-1.460625000	1	4.324692000	0.822883000	0.747339000
1	-2.001356000	-2.310453000	-2.204487000	1	4.036568000	0.105244000	-0.833896000
6	-0.401847000	1.982640000	-0.234730000	6	-2.185242000	0.614971000	0.115215000
8	0.362473000	2.173274000	-1.175117000	8	-2.411724000	0.324000000	1.279897000
6	-1.598920000	2.868133000	0.016144000	6	-3.301958000	0.955376000	-0.852588000
1	-2.498766000	2.281682000	-0.187516000	1	-3.136936000	1.941757000	-1.301697000
1	-1.633313000	3.218944000	1.054657000	1	-3.318006000	0.229532000	-1.675610000
1	-1.552100000	3.722300000	-0.663291000	1	-4.262735000	0.938964000	-0.333571000

TS2R _{tr} (-2815.96936) E(CH ₃ CN) = - 2818.26495 NIMAG = -63.7				Transoid Betaine _{tr} (-2815.97708) E(CH ₃ CN) = -2818.27466 NIMAG = 0			
6	-2.786292000	-0.671767000	-0.967821000	6	-2.325621000	-0.711387000	-1.714990000
1	-3.294648000	0.239217000	-0.658004000	1	-2.615925000	0.286140000	-2.042974000
1	-2.545361000	-0.630573000	-2.032621000	1	-1.600348000	-1.151584000	-2.402683000
6	-1.678014000	-0.865162000	1.872463000	6	-2.787189000	0.113718000	1.250783000
1	-2.034335000	0.138173000	2.107066000	1	-3.067398000	1.114457000	0.923157000
1	-0.838278000	-1.144488000	2.509216000	1	-2.349965000	0.142887000	2.250415000
6	0.040537000	0.671394000	-0.347109000	6	0.165463000	0.455075000	-0.157648000
1	0.604040000	0.376945000	-1.230529000	1	0.712097000	-0.219506000	-0.855831000
6	1.132727000	0.912892000	0.858127000	6	1.069343000	0.369595000	1.152828000
6	2.503935000	0.666143000	0.347376000	6	2.494253000	0.174349000	0.746951000
1	-2.483654000	-1.595590000	1.981155000	1	-3.648234000	-0.558828000	1.244288000
1	-3.401218000	-1.553261000	-0.770563000	1	-3.197149000	-1.363973000	-1.627070000
33	-1.121494000	-0.854391000	0.025694000	33	-1.468116000	-0.559297000	0.008795000
6	-0.565437000	-2.648882000	-0.412066000	6	-0.991642000	-2.360344000	0.528832000
1	0.231935000	-2.927417000	0.271284000	1	0.014278000	-2.529745000	0.124316000
1	-1.451737000	-3.286719000	-0.342152000	1	-0.975104000	-2.425803000	1.617952000
1	-0.155877000	-2.638447000	-1.420666000	1	-1.727805000	-3.059267000	0.124399000
6	0.979927000	2.269218000	1.560965000	6	0.834929000	1.538410000	2.117004000
1	1.672163000	2.291573000	2.409388000	1	1.389234000	1.364436000	3.045833000
1	1.250933000	3.106377000	0.906810000	1	1.188678000	2.489307000	1.702878000
1	-0.030928000	2.447049000	1.941392000	1	-0.225970000	1.660549000	2.371426000
1	0.878720000	0.136025000	1.594294000	1	0.707682000	-0.541155000	1.664876000
6	2.764402000	-0.601547000	-0.130654000	6	2.800723000	-0.846057000	-0.136174000
8	1.850148000	-1.505912000	-0.192155000	8	1.910404000	-1.622972000	-0.660596000
1	3.250794000	1.453119000	0.387831000	1	3.259420000	0.822419000	1.164065000
6	4.154731000	-0.976972000	-0.625509000	6	4.244415000	-1.070485000	-0.566706000
1	4.869261000	-0.149287000	-0.553683000	1	4.943553000	-0.368977000	-0.097771000
1	4.539476000	-1.823938000	-0.043002000	1	4.551161000	-2.093551000	-0.314605000
1	4.105482000	-1.311552000	-1.670111000	1	4.327055000	-0.978184000	-1.657330000
6	-0.823906000	1.882386000	-0.564393000	6	-0.152836000	1.808459000	-0.702388000
8	-1.873439000	2.047404000	0.055723000	8	-1.321355000	2.193438000	-0.804655000
6	-0.299264000	2.909384000	-1.545541000	6	1.008430000	2.655171000	-1.164875000
1	0.787054000	3.022087000	-1.454402000	1	1.915478000	2.434639000	-0.591600000
1	-0.495615000	2.564032000	-2.570028000	1	1.231432000	2.394895000	-2.208648000
1	-0.802649000	3.867104000	-1.394135000	1	0.741649000	3.714882000	-1.125035000

TS2T _π (-2815.96799) E(CH ₃ CN) = -2818.26521 NIMAG = -314.17				TS2E _π (-2815.9606) E(CH ₃ CN) = -2818.25622 NIMAG = -211.7			
6	-2.965378000	-0.574789000	-1.210224000	6	-2.306422000	-0.875241000	-1.828576000
1	-3.412451000	0.409379000	-1.072797000	1	-2.199537000	-0.008138000	-2.480682000
1	-2.623293000	-0.694579000	-2.239879000	1	-1.660084000	-1.683630000	-2.178324000
6	-2.143260000	-0.432135000	1.734620000	6	-3.137323000	0.915051000	0.482754000
1	-2.514811000	0.591243000	1.781858000	1	-3.058754000	1.791800000	-0.161189000
1	-1.366630000	-0.599657000	2.481966000	1	-2.992903000	1.205128000	1.525654000
6	-0.020605000	0.512970000	-0.454268000	6	0.516048000	0.276010000	-0.051521000
1	0.641172000	0.057490000	-1.185020000	1	0.706467000	-0.486104000	-0.811267000
6	1.264523000	0.499569000	1.051359000	6	1.220211000	-0.130323000	1.220806000
6	2.582817000	0.452301000	0.528313000	6	2.589445000	0.027899000	0.651469000
1	-2.957670000	-1.145599000	1.883673000	1	-4.113353000	0.436991000	0.362897000
1	-3.665499000	-1.373246000	-0.953401000	1	-3.344299000	-1.217700000	-1.798089000
33	-1.422729000	-0.690050000	-0.037976000	33	-1.729259000	-0.340082000	-0.041614000
6	-0.739996000	-2.494560000	-0.144765000	6	-2.190096000	-1.942900000	0.996654000
1	-1.287410000	-3.131681000	0.553018000	1	-1.511743000	-2.747077000	0.703313000
1	-0.883275000	-2.853886000	-1.166410000	1	-2.066928000	-1.736353000	2.061870000
1	0.335302000	-2.450079000	0.066235000	1	-3.224425000	-2.232714000	0.790380000
6	0.889208000	1.644696000	1.972252000	6	0.855650000	0.639500000	2.486722000
1	1.356465000	1.488436000	2.952784000	1	1.358274000	0.203783000	3.356520000
1	1.255240000	2.602631000	1.586734000	1	1.139530000	1.696273000	2.440940000
1	-0.190494000	1.738975000	2.120076000	1	-0.228237000	0.597203000	2.659417000
1	0.927336000	-0.472755000	1.416426000	1	1.005185000	-1.197330000	1.368344000
6	3.023062000	-0.720363000	-0.128123000	6	3.055212000	-0.958724000	-0.255377000
8	2.279987000	-1.720419000	-0.328277000	8	2.333353000	-1.909635000	-0.649393000
1	3.204962000	1.343750000	0.545363000	1	3.203538000	0.878336000	0.927961000
6	4.458090000	-0.787128000	-0.642751000	6	4.484639000	-0.856185000	-0.781195000
1	5.026264000	0.129098000	-0.450609000	1	5.022811000	0.018818000	-0.401133000
1	4.975790000	-1.629137000	-0.167621000	1	5.039357000	-1.759082000	-0.499939000
1	4.455712000	-0.985874000	-1.721430000	1	4.472367000	-0.820202000	-1.877120000
6	-0.545100000	1.851345000	-0.668632000	6	0.363379000	1.663426000	-0.601879000
8	-1.664234000	2.184673000	-0.237109000	8	-0.579165000	1.891749000	-1.362962000
6	0.361045000	2.845030000	-1.368361000	6	1.337190000	2.781911000	-0.288787000
1	1.401723000	2.719865000	-1.044181000	1	1.734590000	2.733147000	0.726082000
1	0.342544000	2.667661000	-2.451737000	1	2.191396000	2.713511000	-0.971218000
1	0.016605000	3.863982000	-1.175260000	1	0.831196000	3.736574000	-0.458720000

Product Complex (-2816.01821) E(CH3CN) = -2818.308474 NIMAG = 0				TS2C _{rs} (-2815.97102) E(CH3CN) = -2818.25777 NIMAG = -294.7			
6	-2.576743000	-0.516038000	-1.863063000	6	-2.439402000	-1.799675000	-0.484363000
1	-1.938928000	0.231868000	-2.337401000	1	-2.452800000	-2.853737000	-0.195518000
1	-2.304098000	-1.507535000	-2.235891000	1	-3.189379000	-1.233466000	0.066001000
6	-3.110425000	1.296319000	0.431755000	6	-0.497962000	-1.421256000	1.814967000
1	-2.477788000	2.087533000	0.024462000	1	-1.229545000	-0.808449000	2.340578000
1	-3.206397000	1.434058000	1.513197000	1	0.525454000	-1.199770000	2.108547000
6	1.427922000	0.293589000	-0.352357000	6	-0.654249000	0.749709000	-0.689171000
1	1.165000000	-0.378897000	-1.164521000	1	-0.340433000	0.812617000	-1.727161000
6	1.470847000	-0.386413000	0.994293000	6	0.922528000	1.887496000	0.113309000
6	2.773909000	-0.000449000	0.317106000	6	2.143400000	1.456004000	-0.449266000
1	-4.104068000	1.343086000	-0.024811000	1	-0.717421000	-2.484168000	1.948431000
1	-3.628666000	-0.318338000	-2.090610000	1	-2.605816000	-1.706651000	-1.559645000
33	-2.251144000	-0.447557000	0.082896000	33	-0.685389000	-1.050533000	-0.066481000
6	-3.794670000	-1.568545000	0.631848000	6	0.494823000	-2.231784000	-1.046399000
1	-3.597089000	-2.609752000	0.361860000	1	0.145493000	-3.252418000	-0.871785000
1	-3.898575000	-1.509829000	1.719160000	1	0.420231000	-1.995718000	-2.109995000
1	-4.719867000	-1.233380000	0.153039000	1	1.508116000	-2.090750000	-0.672871000
6	0.991817000	0.259522000	2.275570000	6	2.802535000	0.264145000	-0.069865000
1	1.343250000	-0.306170000	3.145895000	8	2.300595000	-0.608595000	0.693745000
1	1.340165000	1.290954000	2.389775000	1	2.528978000	1.998115000	-1.309872000
1	-0.103846000	0.264268000	2.286016000	6	4.185262000	-0.019797000	-0.649700000
1	1.245438000	-1.447674000	0.916599000	1	4.560904000	0.789813000	-1.283157000
6	3.609208000	-1.088821000	-0.282759000	1	4.891610000	-0.180533000	0.173142000
8	3.097368000	-2.069641000	-0.797152000	1	4.165860000	-0.948629000	-1.234230000
1	3.312686000	0.844625000	0.738518000	6	-1.862492000	1.424868000	-0.278065000
6	5.114459000	-0.911515000	-0.213354000	8	-2.499098000	1.066624000	0.732573000
1	5.414587000	0.007874000	-0.732563000	6	-2.284141000	2.683859000	-1.024006000
1	5.439692000	-0.808957000	0.829880000	1	-1.828632000	2.770972000	-2.014932000
1	5.611526000	-1.769057000	-0.670674000	1	-3.374327000	2.697258000	-1.117184000
6	0.874324000	1.674405000	-0.551092000	1	-1.999583000	3.565273000	-0.435037000
8	-0.202924000	1.805512000	-1.112370000	6	0.659068000	1.814184000	1.603962000
6	1.660413000	2.893574000	-0.102296000	1	1.082091000	2.719510000	2.060687000
1	1.928796000	2.846162000	0.958532000	1	-0.406164000	1.791226000	1.850898000
1	2.599412000	2.958399000	-0.666659000	1	1.161463000	0.955247000	2.045436000
1	1.064597000	3.789410000	-0.287097000	1	0.543550000	2.811091000	-0.327435000

TS2C _{rs} conformer 1 (-2815.95489) E(CH3CN) = -2818.25409 NIMAG = -326.3				Cisoid Betaine _{rs} (-2815.99705) E(CH3CN) = -2818.27078 NIMAG = 0			
6	3.238650000	0.530073000	-0.681344000	6	-1.641865000	-1.668213000	1.186731000
1	2.941844000	1.117940000	-1.549061000	6	-0.130965000	-2.341369000	-1.283591000
1	3.676056000	1.172027000	0.085639000	6	-0.628954000	0.779421000	-0.449448000
6	1.065693000	-1.582373000	-1.294937000	6	0.087326000	1.862976000	0.382062000
1	1.090013000	-1.085050000	-2.262692000	6	-0.256107000	1.776038000	1.886567000
1	0.045694000	-1.881423000	-1.053773000	6	1.578539000	1.829516000	0.109147000
6	0.323818000	0.923505000	0.659436000	6	2.257619000	0.810196000	-0.487401000
1	0.647259000	1.461689000	1.549675000	8	1.750977000	-0.363006000	-0.844670000
6	-1.148583000	-0.187879000	1.505515000	6	3.730856000	0.953411000	-0.812790000
6	-1.753582000	-1.138456000	0.645181000	1	-1.789470000	-1.023250000	2.058087000
1	1.747164000	-2.436442000	-1.263863000	1	-1.405955000	-2.679918000	1.532044000
1	3.944368000	-0.255719000	-0.961479000	1	-2.546956000	-1.692338000	0.581269000
33	1.633823000	-0.298852000	0.027020000	1	-0.074456000	-3.329344000	-0.820656000
6	2.265972000	-1.368538000	1.520439000	1	-1.090900000	-2.214372000	-1.784978000
1	3.119024000	-1.966533000	1.191312000	1	0.707911000	-2.171912000	-1.954810000
1	2.572853000	-0.712353000	2.337652000	1	-0.184207000	0.760207000	-1.450918000
1	1.460694000	-2.024837000	1.855422000	1	-0.294521000	2.835604000	0.030479000
6	-2.724258000	-0.805612000	-0.345171000	1	-1.334148000	1.860450000	2.077980000
8	-3.076229000	0.358609000	-0.634761000	1	0.242066000	2.580277000	2.437792000
1	-1.413841000	-2.171337000	0.705292000	1	0.085942000	0.828717000	2.313640000
6	-3.371488000	-1.957013000	-1.122118000	1	2.128276000	2.727872000	0.377452000
1	-2.997622000	-2.946138000	-0.835082000	1	3.885003000	0.815833000	-1.890437000
1	-4.455433000	-1.932722000	-0.959122000	1	4.309463000	0.167936000	-0.310208000
1	-3.210143000	-1.809406000	-2.196510000	1	4.132048000	1.929752000	-0.523737000
6	-0.051839000	1.697774000	-0.519345000	6	-2.128055000	0.864837000	-0.712719000
8	0.355064000	1.312533000	-1.633779000	8	-2.704346000	-0.091813000	-1.209385000
6	-0.958805000	2.899758000	-0.405920000	33	-0.062991000	-1.030834000	0.138647000
1	-0.890848000	3.390159000	0.570028000	6	1.258324000	-1.462995000	1.524204000
1	-0.722328000	3.610114000	-1.202916000	1	1.868871000	-2.254527000	1.086725000
1	-1.984973000	2.540937000	-0.544872000	1	0.760224000	-1.810258000	2.431307000
6	-1.985705000	0.914447000	2.139330000	1	1.885055000	-0.595153000	1.719084000
1	-2.608544000	0.455646000	2.918883000	6	-2.866526000	2.167874000	-0.475344000
1	-1.374731000	1.689624000	2.617136000	1	-2.835769000	2.459540000	0.579886000
1	-2.650151000	1.365169000	1.404005000	1	-3.903848000	2.048524000	-0.794099000
1	-0.482422000	-0.642465000	2.244606000	1	-2.400114000	2.982272000	-1.043319000

Cisoid Betaine _{rs} conformer 1 (-2815.97604) E(CH ₃ CN) = -2818.26165 NIMAG = 0				Cisoid Betaine _{rs} conformer 2 (-2815.97029) E(CH ₃ CN) = -2818.25603 NIMAG = 0			
6	1.490551000	2.427633000	0.195013000	6	1.666482000	2.141449000	0.519104000
1	2.314814000	2.037198000	0.791765000	1	2.387935000	1.608614000	1.142148000
1	1.849501000	2.713140000	-0.798955000	1	2.152296000	2.419679000	-0.417813000
6	-0.455666000	0.882073000	1.854921000	6	-0.520860000	0.778672000	1.970096000
1	-1.192493000	0.086752000	1.985759000	1	-1.349010000	0.072302000	2.038661000
1	-0.870908000	1.850878000	2.145233000	1	-0.829086000	1.778432000	2.288141000
6	1.122161000	-0.452611000	-0.769056000	6	1.089486000	-0.586287000	-0.818083000
1	1.263214000	-0.185682000	-1.824288000	1	1.053802000	-0.144990000	-1.822089000
6	0.042855000	-1.588572000	-0.655891000	6	-0.065986000	-1.601602000	-0.668897000
6	-1.266845000	-0.820760000	-0.815364000	6	-1.271896000	-0.663507000	-0.813343000
1	0.460580000	0.680636000	2.410523000	1	0.324686000	0.452742000	2.578817000
1	1.061553000	3.307770000	0.682555000	1	1.313700000	3.033960000	1.043847000
33	0.052540000	1.052195000	-0.003729000	33	0.091368000	0.974865000	0.129265000
6	-1.175010000	2.249200000	-0.975246000	6	-0.980173000	2.405543000	-0.703911000
1	-0.996178000	3.286476000	-0.680430000	1	-0.739056000	3.367959000	-0.246111000
1	-0.983956000	2.129669000	-2.043651000	1	-0.738414000	2.437757000	-1.768780000
1	-2.192359000	1.934241000	-0.747204000	1	-2.032887000	2.155354000	-0.571439000
6	-2.454157000	-1.009121000	-0.028756000	6	-2.561726000	-0.822465000	-0.163026000
8	-2.494763000	-1.476460000	1.125587000	8	-2.739159000	-1.359693000	0.940531000
1	-1.462022000	-0.553746000	-1.857289000	1	-1.361888000	-0.298622000	-1.841268000
6	-3.777260000	-0.516284000	-0.633853000	6	-3.780174000	-0.225286000	-0.875501000
1	-4.412687000	-1.387705000	-0.835285000	1	-4.299929000	-1.030935000	-1.410859000
1	-4.310053000	0.099762000	0.099145000	1	-4.478379000	0.178088000	-0.136088000
1	-3.661405000	0.042550000	-1.568713000	1	-3.526209000	0.545946000	-1.610257000
6	2.450877000	-0.719440000	-0.088495000	6	2.557580000	-0.748985000	-0.513933000
8	2.642343000	-0.397488000	1.073291000	8	3.346717000	0.030326000	-1.034077000
6	3.505685000	-1.452418000	-0.895662000	6	3.064939000	-1.806658000	0.449267000
1	3.091911000	-2.373352000	-1.324821000	1	2.544605000	-1.758359000	1.411300000
1	3.833957000	-0.829062000	-1.737636000	1	2.896912000	-2.811803000	0.045510000
1	4.363132000	-1.690750000	-0.262576000	1	4.136053000	-1.654158000	0.597290000
6	0.193227000	-2.437951000	0.614020000	6	-0.051906000	-2.461297000	0.602736000
1	-0.638253000	-3.139279000	0.694488000	1	-1.004040000	-2.980397000	0.712437000
1	1.130957000	-3.007730000	0.581727000	1	0.747678000	-3.206320000	0.558501000
1	0.194565000	-1.839117000	1.525811000	1	0.085564000	-1.866562000	1.510731000
1	0.183167000	-2.263990000	-1.513913000	1	-0.034524000	-2.291765000	-1.527114000

TS2R _{TS} (-2815.95326) E(CH ₃ CN) = -2818.26669 NIMAG = -46.1				TS2T _{TS} (-2815.95311) E(CH ₃ CN) = -2818.25815 NIMAG = -335.0			
6	-2.780464000	-0.329844000	1.444798000	6	-2.205712000	-0.356525000	1.817453000
6	-2.814136000	0.861375000	-1.409963000	6	-3.157035000	1.264396000	-0.605838000
6	0.101940000	0.267945000	-0.196204000	6	-0.048096000	0.140422000	-0.545075000
6	1.183264000	-0.532740000	0.737941000	6	1.238426000	-1.014109000	0.290256000
6	0.515305000	-1.574260000	1.647140000	6	0.553979000	-2.374333000	0.301224000
6	2.312602000	-1.052402000	-0.065766000	6	2.496413000	-0.969426000	-0.374365000
6	3.494460000	-0.319018000	-0.165680000	6	3.574159000	-0.192846000	0.128226000
8	3.690319000	0.844041000	0.312842000	8	3.485488000	0.617349000	1.081220000
6	4.673986000	-0.959357000	-0.903155000	6	4.945819000	-0.374250000	-0.529605000
1	-2.534995000	-1.238642000	1.993569000	1	-1.551814000	-1.126049000	2.228038000
1	-3.842992000	-0.325040000	1.188937000	1	-3.251844000	-0.637258000	1.962166000
1	-2.519110000	0.560880000	2.013610000	1	-1.990850000	0.604320000	2.283676000
1	-3.791995000	0.403702000	-1.578221000	1	-4.167405000	0.920853000	-0.369822000
1	-2.914789000	1.840835000	-0.944296000	1	-2.907619000	2.172141000	-0.059994000
1	-2.275563000	0.942960000	-2.356259000	1	-3.060242000	1.427406000	-1.680959000
1	0.413166000	0.107434000	-1.232432000	1	0.106294000	-0.108090000	-1.594747000
1	1.596133000	0.252320000	1.383272000	1	1.274377000	-0.539845000	1.272799000
1	-0.283934000	-1.154703000	2.273083000	1	-0.437315000	-2.367524000	0.769402000
1	1.276994000	-1.981414000	2.317855000	1	1.175733000	-3.075431000	0.869297000
1	0.114354000	-2.425159000	1.080080000	1	0.454267000	-2.780652000	-0.713168000
1	2.221414000	-2.037638000	-0.520938000	1	2.659507000	-1.621859000	-1.230680000
1	5.531652000	-1.028290000	-0.222515000	1	5.669498000	-0.691474000	0.230526000
1	4.984744000	-0.313055000	-1.734059000	1	5.296461000	0.591113000	-0.914978000
1	4.453800000	-1.959551000	-1.294578000	1	4.946645000	-1.104272000	-1.346388000
6	0.048102000	1.744259000	0.165035000	6	0.202147000	1.541720000	-0.135596000
8	-0.960218000	2.177680000	0.727938000	8	-0.559201000	2.056487000	0.700006000
33	-1.785927000	-0.271471000	-0.214533000	33	-1.894273000	-0.125599000	-0.076119000
6	-1.974911000	-2.034370000	-1.002378000	6	-2.637742000	-1.688535000	-0.966471000
1	-1.488266000	-2.035567000	-1.979740000	1	-2.573728000	-1.528418000	-2.045374000
1	-3.040950000	-2.243669000	-1.119443000	1	-3.688013000	-1.772859000	-0.677002000
1	-1.513617000	-2.785497000	-0.361330000	1	-2.100480000	-2.597247000	-0.699554000
6	1.248661000	2.576848000	-0.148725000	6	1.395450000	2.289152000	-0.664177000
1	2.185192000	2.058857000	0.156075000	1	2.268694000	1.966982000	-0.080342000
1	1.148363000	3.562220000	0.312173000	1	1.241634000	3.361418000	-0.519632000
1	1.322326000	2.693180000	-1.239769000	1	1.590068000	2.066806000	-1.717347000

Transoid Betaine _{rs} (-2815.95896) E(CH ₃ CN) = -2818.26913 NIMAG = 0				TS2E _{rs} (-2815.95625) E(CH ₃ CN) = -2818.25874 NIMAG = -186.3			
6	3.084449000	1.191638000	-0.859218000	6	-2.994937000	-1.555897000	-0.418104000
1	2.852235000	1.280744000	-1.922531000	1	-2.978434000	-1.796465000	-1.483071000
1	2.932133000	2.145793000	-0.359204000	1	-2.564386000	-2.375990000	0.155841000
6	2.593486000	-1.768780000	-0.832313000	6	-3.031082000	1.435581000	-0.890643000
1	2.422896000	-1.750212000	-1.911341000	1	-3.078000000	1.279634000	-1.970721000
1	2.117286000	-2.647527000	-0.401214000	1	-2.619182000	2.424562000	-0.685795000
6	-0.081599000	0.084616000	-0.483661000	6	0.306757000	0.045193000	-0.570653000
6	-1.078270000	-0.884365000	0.271352000	6	1.010227000	1.145148000	0.203744000
6	-2.383497000	-0.885575000	-0.453962000	6	2.369218000	1.022814000	-0.412575000
1	3.668702000	-1.787480000	-0.636993000	1	-4.035142000	1.351938000	-0.465676000
1	4.109705000	0.834093000	-0.735076000	1	-4.020929000	-1.349970000	-0.101325000
33	1.876760000	-0.120435000	-0.074410000	33	-1.899876000	0.038222000	-0.091582000
6	2.302389000	-0.174448000	1.810379000	6	-2.173253000	0.312605000	1.813609000
1	3.351975000	-0.458910000	1.916251000	1	-3.245505000	0.290108000	2.026755000
1	2.128323000	0.824182000	2.209208000	1	-1.660510000	-0.499264000	2.328986000
1	1.665072000	-0.899155000	2.318360000	1	-1.757411000	1.272571000	2.124725000
6	-0.513484000	-2.304254000	0.443318000	6	0.382365000	2.533480000	0.050624000
1	-1.258519000	-2.907741000	0.969383000	1	1.017088000	3.274673000	0.546476000
1	-0.332758000	-2.783733000	-0.528092000	1	0.304610000	2.818773000	-1.006868000
1	0.418526000	-2.349203000	1.026978000	1	-0.619786000	2.601793000	0.493544000
1	-1.257266000	-0.446890000	1.262230000	1	1.070161000	0.857032000	1.259495000
6	-3.503321000	-0.252077000	0.081279000	6	3.387450000	0.277367000	0.210034000
8	-3.488040000	0.530297000	1.085915000	8	3.206682000	-0.462671000	1.213399000
1	-2.472289000	-1.540499000	-1.319821000	1	2.566654000	1.600336000	-1.312623000
6	-4.855261000	-0.483271000	-0.598497000	6	4.797490000	0.355607000	-0.380702000
1	-4.802489000	-1.162327000	-1.457502000	1	4.873823000	1.027645000	-1.242517000
1	-5.561150000	-0.894802000	0.133558000	1	5.491904000	0.696587000	0.396069000
1	-5.271882000	0.476934000	-0.929001000	1	5.129669000	-0.645934000	-0.682253000
6	-0.293071000	1.556125000	-0.110227000	6	0.589793000	-1.404689000	-0.154995000
8	0.616904000	2.105545000	0.515425000	8	-0.104010000	-1.902166000	0.724822000
6	-1.570763000	2.238751000	-0.430215000	6	1.665998000	-2.202230000	-0.836120000
1	-1.921109000	1.992157000	-1.436160000	1	1.883055000	-1.845281000	-1.845183000
1	-2.342831000	1.832292000	0.266891000	1	2.566209000	-2.073291000	-0.219440000
1	-1.459162000	3.316530000	-0.288505000	1	1.388883000	-3.260489000	-0.837179000
1	-0.157732000	-0.096763000	-1.562014000	1	0.301603000	0.218541000	-1.648123000

Product Complex_{rs} (-2816.01943)
E(CH₃CN) = -2818.30792
NIMAG = 0

6	3.051156000	1.700782000	0.129374000
1	3.387595000	2.126518000	-0.820257000
1	2.235208000	2.310608000	0.522773000
6	4.114821000	-1.022988000	-0.401451000
1	4.542090000	-0.757991000	-1.372688000
1	3.952578000	-2.104737000	-0.382064000
6	-1.353078000	0.019307000	-0.875524000
6	-1.283363000	-1.206173000	-0.045493000
6	-2.646401000	-0.749883000	-0.596064000
1	4.809528000	-0.737971000	0.394415000
1	3.886026000	1.681976000	0.836463000
33	2.357037000	-0.126313000	-0.173660000
6	2.138571000	-0.598215000	1.727951000
1	3.034022000	-0.331673000	2.298349000
1	1.274832000	-0.057341000	2.118945000
1	1.965237000	-1.674830000	1.821506000
6	-0.642935000	-2.479030000	-0.551386000
1	-0.984893000	-3.353868000	0.013476000
1	-0.872658000	-2.647305000	-1.610265000
1	0.445969000	-2.403713000	-0.457855000
1	-1.160167000	-1.004760000	1.017019000
6	-3.660556000	-0.219768000	0.359970000
8	-3.383419000	0.636582000	1.186447000
1	-3.040548000	-1.341323000	-1.420032000
6	-5.054502000	-0.813882000	0.265277000
1	-5.489555000	-0.606432000	-0.720931000
1	-5.015673000	-1.905071000	0.373054000
1	-5.692406000	-0.388546000	1.042294000
6	-1.065183000	1.387835000	-0.284935000
8	-0.261296000	1.534417000	0.616998000
6	-1.767376000	2.565116000	-0.928792000
1	-1.795185000	2.470920000	-2.020689000
1	-2.803191000	2.588770000	-0.570180000
1	-1.272921000	3.496149000	-0.643259000
1	-1.017328000	-0.057629000	-1.910409000