

Theoretical Study Of The Rate Constants For The Hydrogen Atom Abstraction Reactions Of Esters With $\dot{\text{O}}\text{H}$ Radicals.

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Table S1: Energies of the reactions of methyl ethanoate with the $\dot{\text{O}}\text{H}$ radical computed at CCSD(T)/cc-pVXZ (X=D, T, Q) and CCSD(T)/CBS, based on MP2/6-311G(d,p) geometries.

	CCSD(T)/cc-pVDZ		CCSD(T)/cc-pVTZ		CCSD(T)/cc-pVQZ		CCSD(T)/CBS	
		ΔE Kcal mol ⁻¹		ΔE Kcal mol ⁻¹		ΔE Kcal mol ⁻¹	AU	ΔE Kcal mol ⁻¹
ME	-267.608510		-267.885609		-267.968301		-268.136812	
$\dot{\text{O}}\text{H}$	-75.550421		-75.628926		-75.652846		-75.700792	
RC α'	-343.169862	-6.86	-343.523427	-5.58	-343.629363	-5.16	-343.845440	-4.92
RC α	-343.168467	-5.98	-343.522452	-4.97	-343.628770	-4.78	-343.845090	-4.70
TS α'	-343.150673	5.18	-343.508741	3.64	-343.615625	3.46	-343.832178	3.40
TS α	-343.155161	2.37	-343.512920	1.01	-343.619859	0.81	-343.836462	0.72
PC α'	-343.190648	-19.90	-343.550733	-22.71	-343.658687	-23.56	-343.875916	-24.04
PC α	-343.187068	-17.66	-343.546955	-20.34	-343.654566	-20.97	-343.871566	-21.31
P α'	-266.960006		-267.231473		-267.312907		-267.480459	
H ₂ O	-76.219330	-12.80	-76.310338	-17.12	-76.337891	-18.61	-76.388179	-19.47
P α	-266.959973		-267.230948		-267.312287		-267.479790	
H ₂ O	-76.219330	-12.78	-76.310338	-16.79	-76.337891	-18.22	-76.388179	-19.05

Table S2: Geometry co-ordinates and frequencies of Reactants and Transition States computed at MP2/6-311G(d,p) level. Frequencies corresponding to the torsional modes are shown in bold.

Species	Geometry co-ordinates				Frequencies (cm ⁻¹)		
ME	6	0.000000000	0.489773000	0.000000000	39.5188 ,	161.5672 ,	183.8715 ,
	8	1.180762000	0.749872000	0.000000000	295.2705,	429.1168,	603.8964,
	6	-1.129229000	1.488362000	0.000000000	654.4588,	876.2044,	1002.4336,
	1	-1.754178000	1.334132000	0.882285000	1074.0336,	1104.0245,	1202.0337,
	1	-0.718963000	2.496807000	0.000000000	1227.7500,	1294.7329,	1414.7208,
	1	-1.754178000	1.334132000	-0.882285000	1493.6312,	1498.4476,	1500.6687,
	8	-0.487478000	-0.772597000	0.000000000	1509.6116,	1527.5905,	1828.4679,
	6	0.526200000	-1.786306000	0.000000000	3098.1493,	3101.3958,	3187.6806,
	1	1.155266000	-1.700963000	0.887888000	3188.0931,	3223.4610,	3224.9263
	1	-0.011315000	-2.732311000	0.000000000			
	1	1.155266000	-1.700963000	-0.887888000			
OH	8	0.000000000	0.000000000	0.107391000	3853.7250		
	1	0.000000000	0.000000000	-0.859130000			
TSα'	6	0.143618000	0.089259000	0.192193000	2118.5969 <i>i</i> ,	37.5163 ,	130.1354,
	8	0.006655000	-1.088404000	0.451625000	162.6722 ,	197.0028 ,	287.5405,
	6	-0.959696000	1.103069000	0.254716000	320.1509,	395.3238 ,	400.6668,
	1	-0.773609000	1.996042000	-0.338287000	613.3855,	651.1465,	765.2532,
	1	-1.937372000	0.545024000	-0.205629000	889.3391,	957.5215,	1036.6232,
	1	-1.230149000	1.330129000	1.285763000	1063.5399,	1118.1441,	1200.5617,
	8	1.309708000	0.644549000	-0.175199000	1228.2530,	1248.7701,	1331.0308,
	6	2.406552000	-0.283259000	-0.237033000	1468.7164,	1501.6084,	1509.9396,
	1	2.193255000	-1.074977000	-0.956668000	1524.8223,	1565.0831,	1804.1717,
	1	3.263180000	0.307272000	-0.553530000	3103.1765,	3151.6744,	3196.0757,
	1	2.583253000	-0.728865000	0.743040000	3232.8756,	3245.3407,	3799.3383
	8	-2.748184000	-0.398123000	-0.424759000			
	1	-2.186834000	-1.093204000	-0.047283000			
TSα	6	-0.853974000	-0.147769000	0.133460000	2022.2413 <i>i</i> ,	34.9923 ,	77.6274 ,
	8	-0.315125000	-1.035342000	0.756086000	142.5363 ,	202.3090,	284.8099,
	6	-2.256219000	-0.171544000	-0.409705000	371.2811,	409.9989 ,	436.7164,
	1	-2.220617000	-0.111329000	-1.499920000	605.3651,	652.7098,	763.1584,
	1	-2.746432000	-1.093198000	-0.101308000	885.6256,	945.4105,	1018.3958,
	1	-2.808650000	0.696200000	-0.044110000	1075.6176,	1128.1414,	1137.0662,
	8	-0.246120000	1.024751000	-0.168453000	1245.0025,	1296.5683,	1374.7624,
	6	1.076771000	1.147863000	0.315571000	1418.4488,	1492.3241,	1495.5854,
	1	1.777009000	0.318268000	-0.199585000	1496.9067,	1532.1171,	1822.1766,
	1	1.446689000	2.118281000	-0.006479000	3102.7315,	3140.6542,	3189.9856,
	1	1.141491000	0.988146000	1.391967000	3226.5195,	3248.3891,	3813.5517
	8	2.299427000	-0.806476000	-0.557320000			
	1	1.705586000	-1.351142000	-0.019031000			

MP	6	0.053267000	0.081963000	-0.000013000	21.8821,	146.3072,	172.1088,
	8	0.109478000	1.290801000	-0.000025000	214.0209,	236.0232,	342.0649,
	6	-1.212651000	-0.744980000	-0.000038000	453.5201,	581.4592,	669.2477,
	1	-1.175992000	-1.402106000	0.875155000	821.3703,	876.0333,	1012.8060,
	1	-1.176026000	-1.401987000	-0.875324000	1052.3909,	1121.8854,	1133.0078,
	8	1.143748000	-0.717443000	0.000016000	1201.3732,	1221.3385,	1244.8161,
	6	2.388087000	-0.004761000	0.000016000	1295.7379,	1403.2948,	1438.4932,
	1	2.470510000	0.624600000	0.888037000	1481.2616,	1499.2588,	1509.5284,
	1	3.160197000	-0.771414000	0.000041000	1517.0436,	1521.6218,	1527.3639,
	1	2.470531000	0.624564000	-0.888028000	1819.2595,	3091.6364,	3096.6481,
	6	-2.467273000	0.120152000	0.000038000	3098.2429,	3142.8853,	3182.1140,
	1	-2.489896000	0.765080000	-0.880813000	3187.1796,	3187.8943,	3224.6351
	1	-3.363835000	-0.504807000	0.000007000			
	1	-2.489875000	0.764957000	0.880980000			
	6	0.474672000	0.114106000	0.024136000	1929.5558 <i>j</i> ,	34.7936,	106.5571,
TSβ'	8	0.236204000	-1.002805000	0.437559000	149.9586,	161.2485,	179.5492,
	6	-0.553735000	1.173442000	-0.300474000	229.2704,	339.7191,	380.4279,
	1	-0.730168000	1.124169000	-1.381133000	444.2576,	475.8928,	589.5923,
	1	-0.109056000	2.151863000	-0.094612000	658.2507,	743.0588,	857.5150,
	8	1.718266000	0.557547000	-0.223438000	913.6489,	989.9137,	1014.8679,
	6	2.748432000	-0.419185000	0.001431000	1067.2542,	1109.6914,	1154.3971,
	1	2.596484000	-1.287863000	-0.641126000	1201.0556,	1222.8170,	1251.2323,
	1	3.679901000	0.085191000	-0.245305000	1273.2947,	1327.7814,	1415.5719,
	1	2.746235000	-0.741318000	1.043738000	1470.4072,	1482.8587,	1501.6838,
	6	-1.857290000	0.976654000	0.448480000	1510.2339,	1510.5372,	1524.8190,
	1	-1.727115000	0.866220000	1.525684000	1803.7497,	3093.5355,	3102.7333,
	1	-2.595297000	1.745603000	0.214547000	3129.9954,	3148.5552,	3195.1791,
	1	-2.365659000	-0.043658000	0.067238000	3215.9487,	3231.7039,	3789.0651
	8	-2.539179000	-1.231400000	-0.397944000			
	1	-1.690122000	-1.557049000	-0.059885000			
TSα'	6	0.247362000	-0.501323000	0.048799000	1727.9093 <i>j</i> ,	45.3461,	100.8630,
	8	0.506580000	-1.511144000	-0.561786000	135.8553,	151.2961,	173.3901,
	6	-1.120422000	-0.069416000	0.497954000	212.6342,	229.0929,	320.3944,
	1	-1.275184000	1.011681000	0.017595000	336.6572,	440.8223,	583.7451,
	1	-1.118049000	0.125277000	1.573390000	609.0534,	673.0684,	847.4572,
	8	1.181303000	0.414694000	0.414693000	874.0805,	944.5065,	1024.1650,
	6	2.518779000	0.073842000	0.016186000	1081.2877,	1104.4494,	1154.2224,
	1	2.585982000	-0.001761000	-1.070360000	1201.4181,	1220.4214,	1235.7298,
	1	3.145564000	0.882499000	0.386196000	1302.1798,	1372.9892,	1431.2094,
	1	2.816698000	-0.877706000	0.459089000	1492.1685,	1501.3416,	1509.1018,
	8	-1.051721000	2.232296000	-0.422655000	1510.8008,	1524.0087,	1529.1422,
	1	-0.132150000	2.254432000	-0.120139000	1827.3409,	3087.0407,	3101.2069,
	6	-2.239490000	-0.977635000	0.031942000	3148.8694,	3174.2182,	3193.4789,
	1	-2.110221000	-1.980186000	0.450342000	3193.7101,	3227.7823,	3828.4039
	1	-3.208614000	-0.586207000	0.348446000			
	1	-2.230699000	-1.067604000	-1.055855000			
TSα	6	-0.387271000	0.192892000	0.145048000	2019.7229 <i>j</i> ,	21.7185,	62.4309,
	8	-0.082695000	-0.793023000	0.780253000	135.4263,	182.1973,	213.2710,
	6	-1.767274000	0.521441000	-0.368475000	240.2141,	336.2634,	370.0999,
	1	-1.679505000	0.714774000	-1.442416000	415.9469,	457.0169,	583.1444,

1	-2.067802000	1.470283000	0.088888000	665.9829, 764.7939, 821.4349,
8	0.493941000	1.164710000	-0.189760000	881.8368, 950.8363, 1020.5206,
6	1.811164000	0.960978000	0.283249000	1074.2310, 1123.7310, 1135.9575,
1	2.273286000	-0.029828000	-0.215177000	1140.3840, 1228.3547, 1258.4385,
1	2.409877000	1.799131000	-0.065176000	1296.7299, 1371.7674, 1407.7657,
1	1.846678000	0.814792000	1.363016000	1440.0089, 1479.0713, 1495.0924,
8	2.489771000	-1.258504000	-0.547628000	1517.6131, 1522.0796, 1532.9964,
1	1.779563000	-1.620790000	0.003299000	1812.8075, 3093.3458, 3097.9522,
6	-2.772926000	-0.584995000	-0.073335000	3139.8478, 3144.6082, 3184.6885,
1	-3.761418000	-0.311121000	-0.449699000	3189.4803, 3247.7433, 3812.4581
1	-2.466667000	-1.520586000	-0.545873000	
1	-2.844300000	-0.764014000	1.001290000	

MB	6	-0.629935000	0.141094000	-0.000002000	3.7114,	81.3271,	149.9505,
	8	-0.813014000	1.337455000	-0.000012000	156.3214,	180.0917,	247.6378,
	6	0.715283000	-0.548220000	0.000003000	316.2951,	343.4599,	440.8717,
	1	0.754052000	-1.206475000	-0.875972000	584.2127,	714.2431,	758.9692,
	1	0.754031000	-1.206505000	0.875955000	896.3014,	909.2861,	934.9215,
	8	-1.630554000	-0.768635000	0.000006000	1050.9757,	1084.0181,	1134.5465,
	6	-2.943595000	-0.191740000	-0.000002000	1155.6298,	1200.8931,	1214.9362,
	1	-3.092231000	0.425152000	-0.888188000	1235.5968,	1266.9757,	1340.5445,
	1	-3.629837000	-1.036146000	0.000004000	1343.6067,	1424.4439,	1434.1067,
	1	-3.092235000	0.425168000	0.888171000	1478.1819,	1498.9514,	1508.9300,
	6	1.882222000	0.432991000	0.000028000	1509.4072,	1521.3554,	1527.429,
	1	1.799421000	1.084411000	0.875571000	1528.3370,	1817.0627,	3070.9026,
	1	1.799402000	1.084477000	-0.875464000	3082.1186,	3097.4341,	3098.5865,
	6	3.230916000	-0.285300000	-0.000016000	3125.3318,	3143.9030,	3164.2060
	1	3.334006000	-0.921461000	-0.884909000			
	1	4.058516000	0.429315000	-0.000057000			
	1	3.334078000	-0.921444000	0.884880000			
TSy'	6	-1.284425000	0.104951000	0.079433000	1659.8932 <i>i</i> ,	20.7250,	66.4827,
	8	-1.270782000	1.304021000	0.243470000	80.5994,	84.7077,	132.2010,
	6	-0.074047000	-0.801108000	0.120817000	151.5903,	166.1011,	191.1734,
	1	-0.175779000	-1.555352000	-0.665489000	295.8422,	331.6473,	370.4492,
	1	-0.103201000	-1.340474000	1.076002000	438.8120,	593.1064,	701.6894,
	8	-2.407571000	-0.608379000	-0.149383000	745.8544,	770.7978,	886.9662,
	6	-3.607424000	0.179505000	-0.159981000	919.1018,	944.9255,	1012.1984,
	1	-3.562519000	0.934121000	-0.947102000	1063.6165,	1092.4459,	1130.9893,
	1	-4.413634000	-0.526113000	-0.348965000	1171.5694,	1200.9414,	1217.7840,
	1	-3.747699000	0.677151000	0.801262000	1238.4754,	1262.7178,	1322.1935,
	6	1.233348000	-0.022900000	-0.014919000	1337.2718,	1353.4273,	1422.9808,
	1	1.250163000	0.764591000	0.744573000	1471.0161,	1480.2957,	1494.3209,
	1	1.255153000	0.481328000	-0.986079000	1499.0860,	1509.7834,	1513.6263,
	6	2.449917000	-0.920506000	0.122502000	1526.9279,	1816.9326,	3082.5404,
	1	2.491756000	-1.706709000	-0.635653000	3098.0822,	3099.1827,	3112.6202,
	1	3.426851000	-0.276892000	-0.083366000	3136.5061,	3155.9736,	3189.6306,
	1	2.568002000	-1.343884000	1.122945000	3194.3246,	3227.0045,	3846.3602
	8	4.284071000	0.720277000	-0.260255000			
	1	3.860953000	1.325228000	0.364100000			
TSβ'	6	-0.863190000	-0.033019000	-0.032271000	1674.0439 <i>i</i> ,	27.7419,	82.9991,
	8	-0.906660000	1.123318000	0.338437000	123.5548,	146.1340,	156.2934,
	6	0.391584000	-0.794093000	-0.390572000	171.8381,	211.1200,	232.0827,
	1	0.587577000	-0.609819000	-1.454271000	315.9629,	343.4949,	427.4646,
	1	0.194343000	-1.865040000	-0.277094000	482.2634,	607.0187,	652.5168,
	8	-1.958321000	-0.794896000	-0.191260000	743.9290,	759.1383,	905.9569,
	6	-3.195220000	-0.113784000	0.078528000	931.0925,	948.5802,	1026.2749,
	1	-3.312530000	0.741147000	-0.589216000	1055.4851,	1105.9092,	1133.7014,
	1	-3.973273000	-0.852654000	-0.099471000	1159.0739,	1200.5590,	1222.2063,
	1	-3.219935000	0.234213000	1.112221000	1250.3471,	1268.3556,	1337.7423,
	6	1.601696000	-0.366964000	0.424185000	1363.4603,	1408.0339,	1424.8286,
	1	1.381793000	-0.359446000	1.496021000	1466.2716,	1474.3168,	1500.8662,
	1	1.829472000	0.766108000	0.147790000	1510.1849,	1514.3876,	1517.6988,
	8	1.781251000	1.997757000	-0.314701000	1525.0423,	1800.9068,	3066.3977,

TS α'	1	0.849575000	2.103361000	-0.063975000	3082.0817, 3102.5701, 3126.9199,
	6	2.862605000	-1.146641000	0.094185000	3142.5417, 3151.9145, 3175.0900,
	1	3.103366000	-1.052112000	-0.968837000	3195.2091, 3231.5084, 3781.9087
	1	3.713763000	-0.777053000	0.671299000	
	1	2.730838000	-2.211124000	0.321406000	
	6	0.691869000	-0.504127000	0.023961000	1672.3264 <i>i</i> , 41.0695 , 73.2539 ,
	8	0.931195000	-1.529849000	-0.568243000	96.0352 , 118.0612, 143.6927,
	6	-0.673199000	0.000463000	0.397593000	159.4561 , 185.7501, 249.2761 ,
	1	-0.744422000	1.095177000	-0.068128000	308.4359 , 319.2693, 342.0713,
	1	-0.732544000	0.174709000	1.476475000	428.8194, 588.7848, 620.8207,
TS α	8	1.651043000	0.364837000	0.437221000	710.4259, 772.8840, 890.9900,
	6	2.989226000	-0.047568000	0.115711000	903.6490, 951.6493, 962.9892,
	1	3.113120000	-0.133037000	-0.965130000	1054.714, 1095.3218, 1127.0463,
	1	3.635556000	0.729789000	0.517856000	1171.8432, 1200.9756, 1216.0740,
	1	3.211747000	-1.010568000	0.577841000	1231.8812, 1283.7923, 1316.0198,
	8	-0.449121000	2.315060000	-0.479580000	1332.4616, 1405.3640, 1432.8645,
	1	0.454128000	2.290601000	-0.131251000	1489.8875, 1497.9342, 1507.5856,
	6	-1.825053000	-0.818376000	-0.150863000	1508.975, 1522.0262, 1527.1503,
	1	-1.746093000	-1.838774000	0.242827000	1527.8111, 1824.9779, 3074.3894,
	1	-1.715693000	-0.896772000	-1.236786000	3084.8774, 3100.8780, 3129.0417,
	6	-3.178706000	-0.207084000	0.208314000	3142.2700, 3165.1759, 3170.6709,
	1	-3.998215000	-0.805136000	-0.199019000	3193.3811, 3227.4644, 3827.2561
	1	-3.305091000	-0.153567000	1.294297000	
	1	-3.262256000	0.807347000	-0.192453000	
	6	-0.167930000	-0.224122000	0.226027000	2020.6116 <i>i</i> , 16.2602 , 49.1881 ,
	8	-0.496387000	0.751718000	0.865234000	98.2938 , 123.7619 , 161.7866,
	6	1.240082000	-0.580753000	-0.179465000	200.4356, 249.1354 , 308.0403,
	1	1.230127000	-0.831627000	-1.245880000	344.8148, 370.2683, 415.6435 ,
	1	1.510607000	-1.503366000	0.349056000	445.0340, 588.1707, 702.6694,
	8	-1.045404000	-1.159589000	-0.208195000	760.8393, 776.0720, 896.5768,
	6	-2.389610000	-0.935970000	0.171405000	910.0294, 938.7621, 953.0358,
	1	-2.788539000	0.082057000	-0.326965000	1079.2968, 1084.7442, 1134.9641,
	1	-2.979946000	-1.746644000	-0.248954000	1138.1654, 1159.0914, 1219.2336,
	1	-2.503242000	-0.823233000	1.249811000	1253.6443, 1268.6909, 1338.6461,
	8	-2.950348000	1.326121000	-0.631403000	1346.5069, 1375.3195, 1426.8314,
	1	-2.271666000	1.650441000	-0.020303000	1435.7381, 1476.3827, 1495.0731,
	6	2.241582000	0.529207000	0.121652000	1509.9130, 1521.7294, 1528.3694,
	1	1.939643000	1.436095000	-0.412077000	1533.4385, 1810.5089, 3071.5026,
	1	2.196372000	0.769219000	1.188092000	3081.9638, 3098.5201, 3128.4141,
	6	3.663198000	0.133299000	-0.274496000	3139.6180, 3145.4910, 3164.9825,
	1	3.722615000	-0.089816000	-1.344506000	3166.6691, 3247.5935, 3811.8161
	1	4.370553000	0.938309000	-0.057788000	
	1	3.986662000	-0.757402000	0.273682000	

MiB	6	0.298657000	-0.268530000	0.019969000	21.5761,	132.0848,	172.2190,
	8	0.508355000	-1.201583000	0.763146000	211.5648,	221.5761,	259.4064,
	6	-1.065869000	0.227563000	-0.408259000	294.0664,	327.1352,	359.8031,
	1	-0.964331000	0.624027000	-1.423782000	485.3731,	659.0149,	768.7606,
	8	1.278088000	0.504697000	-0.502319000	850.7076,	932.0677,	947.5670,
	6	2.598014000	0.139531000	-0.074850000	993.8920,	1048.4398,	1128.9688,
	1	2.827721000	-0.884823000	-0.373484000	1162.9971,	1201.6621,	1205.2811,
	1	3.266294000	0.842807000	-0.567622000	1224.9419,	1241.5208,	1353.1938,
	1	2.685685000	0.219586000	1.010302000	1399.1305,	1418.8244,	1435.0575,
	6	-2.081869000	-0.910582000	-0.379782000	1498.0931,	1507.4937,	1508.7196,
	1	-2.147637000	-1.328693000	0.627630000	1509.4743,	1521.9321,	1525.9855,
	1	-3.068719000	-0.543011000	-0.676162000	1532.9334,	1813.2746,	3071.2518,
	1	-1.792388000	-1.717058000	-1.059030000	3079.5188,	3097.6250,	3112.3096,
	6	-1.474769000	1.376537000	0.525842000	3162.2128,	3168.9350,	3171.9525,
	1	-0.743598000	2.188619000	0.492115000	3179.5326,	3187.6448,	3224.6362
	1	-2.450350000	1.773388000	0.229935000			
	1	-1.549201000	1.013124000	1.555962000			
TSβ'	6	0.460676000	-0.133144000	0.098600000	1857.6160 <i>i</i> ,	33.3407,	77.1857,
	8	0.278173000	-1.100325000	0.810376000	127.0187,	154.2039,	175.0958,
	6	-0.592312000	0.874988000	-0.320629000	211.0310,	238.6999,	297.2073,
	1	-0.647838000	0.821091000	-1.414793000	336.5253,	357.5227,	399.3545,
	8	1.662463000	0.180473000	-0.418594000	432.8326,	480.7741,	619.6601,
	6	2.710535000	-0.740573000	-0.076132000	759.1817,	788.5434,	853.9943,
	1	2.472569000	-1.740804000	-0.441636000	927.4875,	955.4073,	987.2330,
	1	3.602632000	-0.353980000	-0.563893000	1019.0457,	1045.4678,	1135.3292,
	1	2.845990000	-0.778774000	1.005825000	1165.9553,	1198.9152,	1201.4919,
	6	-1.944147000	0.521226000	0.267688000	1227.0327,	1261.3334,	1302.8886,
	1	-1.927887000	0.447036000	1.356392000	1336.1901,	1403.2488,	1423.7940,
	1	-2.734543000	1.193507000	-0.073423000	1477.7618,	1499.4526,	1509.0386,
	1	-2.272287000	-0.559185000	-0.134416000	1510.3278,	1519.2087,	1523.3651,
	8	-2.257826000	-1.810691000	-0.473592000	1525.9283,	1797.5593,	3077.0267,
	1	-1.519545000	-2.030356000	0.114538000	3096.1877,	3101.6410,	3122.7739,
	6	-0.155182000	2.295013000	0.075765000	3164.3974,	3189.0696,	3193.9179,
	1	-0.039154000	2.366079000	1.162117000	3208.1296,	3230.0633,	3810.3528
	1	0.794702000	2.556485000	-0.393719000			
	1	-0.914536000	3.018204000	-0.234255000			
TSα'	6	0.445684000	-0.523838000	-0.107679000	1464.7497 <i>i</i> ,	41.6875,	92.1663,
	8	0.841080000	-1.599414000	-0.493225000	109.8562,	142.6224,	171.2271,
	6	-0.997895000	-0.126334000	0.074082000	201.0031,	209.7757,	239.1371,
	1	-1.099762000	0.925835000	-0.454803000	304.5281,	327.3106,	339.4331,
	8	1.277393000	0.493720000	0.241692000	351.0441,	449.0245,	595.6151,
	6	2.673173000	0.172139000	0.127068000	666.2542,	767.3540,	845.6532,
	1	2.923576000	-0.076873000	-0.905394000	937.9430,	943.0896,	971.6124,
	1	3.203260000	1.066458000	0.448059000	1012.6122,	1047.6924,	1133.7698,
	1	2.921662000	-0.674579000	0.768702000	1172.4793,	1200.8533,	1202.0956,
	8	-0.896848000	2.197175000	-0.839590000	1229.6220,	1263.0845,	1312.5839,
	1	0.009927000	2.216253000	-0.500274000	1412.9644,	1432.4497,	1485.1707,
	6	-1.943413000	-1.083194000	-0.629076000	1498.3602,	1499.6484,	1504.0947,
	1	-1.873024000	-2.077061000	-0.175166000	1508.8262,	1516.8558,	1525.8499,
	1	-2.972857000	-0.726322000	-0.539775000	1534.2102,	1817.5656,	3069.3601,

TS α

1	-1.691653000	-1.178833000	-1.687487000	3078.0711, 3101.2566, 3157.9255,
6	-1.332500000	0.110895000	1.543689000	3166.7098, 3184.1895, 3187.6959,
1	-0.667330000	0.857231000	1.982057000	3194.1653, 3227.5309, 3826.7041
1	-2.363396000	0.462421000	1.637186000	
1	-1.233704000	-0.824376000	2.107378000	
6	-0.105873000	0.028728000	0.086421000	2025.6832 <i>i</i> , 19.2564 , 54.3335 ,
8	0.329450000	-0.692823000	0.958782000	137.5893 , 161.0358, 213.0195,
6	-1.520812000	0.012846000	-0.440649000	222.3377 , 265.1619 , 294.1559,
1	-1.481408000	0.337212000	-1.485305000	322.8847, 357.1733, 372.0002,
8	0.624458000	1.003812000	-0.505317000	424.9518 , 487.9840, 659.0238,
6	1.936892000	1.153134000	0.002091000	755.9265, 774.7690, 859.3110,
1	2.570259000	0.154277000	-0.212622000	933.8697, 948.6963, 952.2783,
1	2.408779000	1.954803000	-0.561010000	994.6351, 1078.2658, 1131.4244,
1	1.949339000	1.306559000	1.081381000	1136.0215, 1162.0739, 1208.4856,
8	2.987130000	-1.066276000	-0.205466000	1228.8904, 1256.4909, 1351.5951,
1	2.315270000	-1.379959000	0.418752000	1369.5901, 1402.9145, 1421.3993,
6	-2.112953000	-1.390285000	-0.339044000	1435.8294, 1494.5869, 1507.6535,
1	-3.141287000	-1.391282000	-0.711534000	1509.2547, 1522.5330, 1530.6797,
1	-1.531155000	-2.108624000	-0.922918000	1535.7903, 1806.1899, 3072.7944,
1	-2.113862000	-1.722832000	0.701807000	3080.9786, 3117.1027, 3139.4735,
6	-2.340547000	1.035441000	0.361662000	3165.7585, 3171.1887, 3172.3018,
1	-1.911201000	2.037511000	0.277482000	3180.9252, 3247.7760, 3809.9554
1	-3.368322000	1.065375000	-0.011083000	
1	-2.364965000	0.750065000	1.418180000	

EE	6	-1.032077000	0.148055000	0.000000000	40.3564,	76.6762,	153.4885,
	8	-1.182348000	1.347940000	-0.000001000	199.7845,	274.1527,	376.6802,
	6	-2.132832000	-0.882592000	-0.000001000	432.7745,	602.6397,	648.5761,
	1	-2.037777000	-1.519382000	0.882263000	826.1009,	880.6848,	965.8034,
	1	-3.098450000	-0.379546000	-0.000013000	1024.9469,	1073.4548,	1109.9061,
	1	-2.037762000	-1.519397000	-0.882252000	1159.1298,	1203.4304,	1287.9148,
	8	0.179126000	-0.456370000	0.000003000	1321.9846,	1404.8617,	1418.8156,
	6	1.297967000	0.450427000	0.000002000	1453.2780,	1493.8666,	1498.7176,
	1	1.237960000	1.092150000	0.883373000	1505.2174,	1521.2253,	1545.1189,
	1	1.237956000	1.092148000	-0.883369000	1824.5184,	3088.2875,	3100.3926,
	6	2.553192000	-0.396308000	-0.000002000	3102.2332,	3153.4221,	3180.7359,
	1	3.436041000	0.248859000	0.000051000	3187.2691,	3190.1419,	3222.5951
	1	2.585130000	-1.032483000	0.887181000			
	1	2.585183000	-1.032405000	-0.887241000			
	6	0.410065000	0.011668000	-0.265577000	2114.3876 <i>i,</i>	29.9113,	77.6663,
TS α'	8	0.656208000	-1.166187000	-0.425900000	119.6033,	167.4747,	201.4116,
	6	1.437757000	1.103342000	-0.320038000	276.9646,	318.4023,	365.1801,
	1	1.139070000	2.017570000	0.188688000	397.7365,	415.2873,	612.2166,
	1	2.413224000	0.657163000	0.252764000	641.1419,	771.6164,	826.4906,
	1	1.773210000	1.279666000	-1.341960000	892.2415,	936.8494,	985.7504,
	8	-0.819421000	0.497376000	-0.029250000	1055.4073,	1076.3510,	1115.2880,
	6	-1.861890000	-0.502520000	0.021923000	1158.5893,	1202.279,	1248.2955,
	1	-1.614780000	-1.228259000	0.800956000	1322.1144,	1324.5513,	1412.8564,
	1	-1.890696000	-1.030688000	-0.934673000	1449.4317,	1474.6948,	1505.6786,
	8	3.270382000	-0.203104000	0.601527000	1521.0166,	1542.7704,	1565.6398,
	1	2.791530000	-0.963457000	0.236267000	1799.7948,	3089.4628,	3107.5581,
	6	-3.156446000	0.225959000	0.310335000	3150.8158,	3160.5981,	3182.3272,
	1	-3.980366000	-0.491283000	0.357653000	3192.5766,	3244.4667,	3798.1922
	1	-3.095144000	0.751287000	1.265790000			
	1	-3.370324000	0.952626000	-0.476357000			
TS α	6	-1.211072000	-0.012283000	-0.132943000	1758.6003 <i>i,</i>	34.3802,	75.2791,
	8	-1.136844000	1.042281000	-0.724090000	120.6992,	153.8079,	179.7375,
	6	-2.468699000	-0.627704000	0.418521000	204.4416,	274.5480,	370.2580,
	1	-2.392637000	-0.684849000	1.506975000	408.1999,	440.6071,	597.0994,
	1	-3.323688000	-0.016348000	0.135100000	605.7617,	651.8566,	859.7961,
	1	-2.581180000	-1.644323000	0.036936000	896.1653,	962.6625,	977.9630,
	8	-0.142670000	-0.803520000	0.122605000	1042.0117,	1075.2115,	1146.6871,
	6	1.102747000	-0.322880000	-0.370319000	1175.2769,	1176.6678,	1293.5259,
	1	1.334854000	0.722457000	0.145182000	1329.8677,	1402.8671,	1419.3009,
	1	1.037912000	-0.116316000	-1.441483000	1441.7454,	1492.8256,	1497.1099,
	8	1.326415000	1.974519000	0.556204000	1497.2761,	1506.1062,	1520.8552,
	1	0.534704000	2.206685000	0.047665000	1818.1391,	3084.9928,	3101.8249,
	6	2.184686000	-1.296981000	0.017142000	3141.7153,	3176.4368,	3189.1340,
	1	3.153428000	-0.923904000	-0.323505000	3193.1545,	3225.4432,	3811.8253
	1	2.214697000	-1.417223000	1.101829000			
	1	2.000728000	-2.273330000	-0.440860000			
TS β	6	1.439760000	-0.074863000	-0.039216000	1864.7721 <i>i,</i>	49.1766,	67.7896,
	8	1.874441000	-1.046391000	-0.608502000	80.8358,	141.5612,	192.6753,
	6	2.220241000	1.153941000	0.350144000	205.7262,	334.1912,	373.6916,
	1	1.941631000	1.979374000	-0.310515000	396.9359,	434.0129,	600.5537,

1	1.981053000	1.444475000	1.374289000	646.9395,	697.8430,	855.3963,
1	3.284807000	0.950329000	0.245798000	942.5804,	957.5787,	972.0097,
8	0.135542000	0.054063000	0.327593000	1029.4348,	1074.301,	1108.3599,
6	-0.701674000	-1.059330000	-0.047174000	1177.7216,	1192.8629,	1273.6815,
1	-0.279762000	-1.979256000	0.368389000	1296.0788,	1329.234,	1410.5621,
1	-0.710089000	-1.147256000	-1.136426000	1433.4763,	1475.8957,	1493.8471,
6	-2.077226000	-0.771704000	0.493000000	1500.6067,	1528.1248,	1544.4194,
1	-2.811974000	-1.512203000	0.172057000	1831.5143,	3099.4298,	3102.4108,
1	-2.091270000	-0.627979000	1.573716000	3133.3324,	3161.9309,	3187.5930,
1	-2.441338000	0.263046000	0.006442000	3221.5660,	3223.4337,	3827.2997
8	-2.350045000	1.436096000	-0.541784000			
1	-1.439166000	1.591066000	-0.252726000			

PE	6	-1.591073000	0.179597000	-0.000001000	42.1892,	66.4901,	84.9284,
	8	-1.650183000	1.387382000	-0.000004000	137.3961,	193.8494,	239.3637,
	6	-2.766007000	-0.765708000	0.000000000	314.4645,	346.5921,	484.6211,
	1	-2.718591000	-1.407868000	0.882229000	602.2574,	651.7175,	779.3165,
	1	-3.691324000	-0.191873000	0.000000000	907.8944,	917.2716,	938.0089,
	1	-2.718593000	-1.407869000	-0.882229000	1006.1671,	1073.7477,	1077.6736,
	8	-0.428671000	-0.514618000	0.000001000	1103.6237,	1172.8556,	1208.2964,
	6	0.754253000	0.304175000	0.000000000	1286.4409,	1294.5035,	1334.0530,
	1	0.747749000	0.949677000	0.884412000	1345.4548,	1411.6016,	1431.7345,
	1	0.747750000	0.949673000	-0.884415000	1451.4760,	1494.0921,	1499.0521,
	6	1.952896000	-0.623483000	0.000002000	1513.8944,	1521.3593,	1527.1925,
	1	1.898472000	-1.270097000	0.881687000	1541.1788,	1824.0568,	3076.0268,
	1	1.898473000	-1.270101000	-0.881679000	3086.0962,	3094.6019,	3100.4173,
	6	3.262509000	0.165662000	0.000001000	3132.4863,	3150.1124,	3168.2719,
	1	4.124631000	-0.505846000	0.000003000	3171.5992,	3187.1892,	3222.5269
	1	3.333401000	0.805366000	-0.884970000			
	1	3.333400000	0.805370000	0.884971000			
TSα'	6	-0.978496000	0.063973000	0.276519000	2114.6025 <i>i</i> ,	27.0238,	71.9818,
	8	-1.136530000	-1.118363000	0.501592000	77.2456,	107.6439,	161.0422,
	6	-2.089416000	1.071598000	0.235188000	205.7179,	240.6100,	294.5000,
	1	-1.847131000	1.973660000	-0.322884000	319.1134,	345.5862,	398.6759,
	1	-3.009417000	0.514838000	-0.332625000	466.7054,	611.6957,	647.8973,
	1	-2.468124000	1.283326000	1.235069000	772.6109,	779.8770,	907.8845,
	8	0.216448000	0.632193000	0.045773000	912.4508,	936.3848,	973.0939,
	6	1.334346000	-0.280898000	0.085737000	1035.1049,	1061.8543,	1086.8726,
	1	1.175704000	-1.070493000	-0.655265000	1112.5427,	1173.7377,	1207.2898,
	1	1.377453000	-0.749057000	1.074124000	1248.5296,	1294.497,	1320.6371,
	8	-3.785878000	-0.430677000	-0.647918000	1335.2752,	1349.3431,	1432.6403,
	1	-3.259359000	-1.126946000	-0.225005000	1445.8475,	1474.2456,	1514.1163,
	6	2.586681000	0.519249000	-0.208745000	1521.7296,	1526.7917,	1539.3911,
	1	2.479035000	0.995043000	-1.188609000	1565.7609,	1799.3147,	3076.3907,
	1	2.678167000	1.318068000	0.534007000	3090.6509,	3097.4925,	3137.0428,
	6	3.827914000	-0.373556000	-0.184979000	3150.5948,	3154.4150,	3170.1710,
	1	3.752636000	-1.167998000	-0.933728000	3172.9661,	3244.2440,	3797.9886
	1	4.729484000	0.205808000	-0.398218000			
	1	3.953056000	-0.843666000	0.795235000			
TSα	6	1.667274000	-0.107919000	0.159881000	1687.3775 <i>i</i> ,	35.8286,	68.9937,
	8	1.667005000	0.939937000	0.767340000	82.0393,	114.2778,	124.3650,
	6	2.884700000	-0.843250000	-0.331957000	156.0776,	223.9499,	244.9635,
	1	2.863717000	-0.882132000	-1.423648000	313.3629,	343.5615,	411.9170,
	1	3.780429000	-0.325682000	0.007044000	488.4308,	598.7995,	605.1573,
	1	2.871406000	-1.869649000	0.039787000	654.3683,	793.6090,	914.0301,
	8	0.539410000	-0.779989000	-0.172475000	923.0471,	953.2958,	983.4368,
	6	-0.673690000	-0.178000000	0.260446000	1021.0792,	1075.4077,	1085.6073,
	1	-0.764955000	0.894218000	-0.239447000	1131.0987,	1182.0825,	1192.0876,
	1	-0.656957000	-0.003305000	1.340534000	1288.1663,	1293.6499,	1329.6303,
	8	-0.630535000	2.160271000	-0.604683000	1359.6736,	1413.0275,	1433.346,
	1	0.146861000	2.302994000	-0.043563000	1437.1700,	1493.0751,	1497.5463,
	6	-1.844741000	-1.004325000	-0.210950000	1499.0794,	1509.0763,	1520.9555,
	1	-1.791728000	-1.094147000	-1.300307000	1530.1599,	1817.7416,	3079.5946,

TS β	1	-1.754695000	-2.014299000	0.206593000	3083.2369,	3101.7024,	3125.2898,
	6	-3.166798000	-0.362181000	0.211275000	3143.1483,	3169.5709,	3178.6009,
	1	-4.016211000	-0.940669000	-0.159684000	3189.0236,	3225.2640,	3810.6084
	1	-3.243091000	-0.309935000	1.301650000			
	1	-3.242290000	0.654900000	-0.182577000			
	6	1.824232000	-0.277805000	-0.037893000	1573.2229 <i>j</i> ,	47.4386,	61.5864,
	8	2.015891000	-1.320277000	-0.615458000	76.7421,	116.4721,	130.9138,
	6	2.874807000	0.724842000	0.364914000	160.1535,	197.2730,	226.8041,
	1	2.807153000	1.597152000	-0.290827000	311.6419,	342.7109,	352.3562,
	1	2.705306000	1.057926000	1.389989000	479.9371,	600.3713,	628.5839,
TS γ	1	3.860063000	0.272190000	0.264301000	650.9406,	772.5875,	914.4069,
	8	0.587586000	0.157534000	0.327155000	925.2468,	967.5765,	999.2001,
	6	-0.490574000	-0.718906000	-0.056958000	1012.722,	1074.3231,	1089.4455,
	1	-0.301129000	-1.720633000	0.343018000	1121.9361,	1175.6131,	1194.2507,
	1	-0.526840000	-0.785978000	-1.148417000	1273.3691,	1297.8008,	1334.8486,
	6	-1.767942000	-0.132292000	0.490847000	1359.5995,	1411.8838,	1427.8734,
	1	-1.708136000	-0.004603000	1.575284000	1437.5095,	1494.018,	1500.9029,
	1	-1.841724000	0.965218000	0.049130000	1507.5536,	1514.4902,	1525.0738,
	8	-1.481506000	2.106860000	-0.535955000	1543.2292,	1830.7436,	3070.5638,
	1	-0.556396000	2.031868000	-0.260406000	3090.5255,	3099.3129,	3134.5380,
	6	-3.012052000	-0.884316000	0.049335000	3151.4211,	3157.8549,	3180.6671,
	1	-3.914286000	-0.412149000	0.444199000	3187.4638,	3223.0950,	3826.8002
	1	-3.085278000	-0.903272000	-1.041628000			
	1	-2.985323000	-1.919797000	0.407948000			
	6	-2.308703000	0.036856000	0.004895000	1667.2792 <i>j</i> ,	33.4989,	45.6947,
	8	-2.567986000	1.217350000	0.024395000	61.0348,	76.6986,	100.7788,
	6	-3.306694000	-1.092896000	-0.010956000	117.1207,	143.2997,	194.7852,
	1	-3.139729000	-1.741411000	0.851772000	290.9086,	352.8851,	377.7183,
	1	-4.315376000	-0.683759000	0.012945000	471.9565,	601.7877,	649.6799,
	1	-3.163474000	-1.693471000	-0.911975000	753.2639,	788.0090,	894.4444,
	8	-1.044102000	-0.451490000	-0.007255000	920.9238,	950.4917,	995.4480,
	6	-0.019702000	0.556771000	0.000542000	1028.0337,	1074.0240,	1085.5373,
	1	-0.127259000	1.177969000	0.895550000	1103.0279,	1171.3277,	1209.4132,
	1	-0.139817000	1.204536000	-0.873611000	1282.7081,	1290.2334,	1317.4916,
	6	1.318055000	-0.160709000	-0.022298000	1334.2489,	1352.3595,	1411.4209,
	1	1.371241000	-0.830240000	0.842386000	1448.6447,	1466.4026,	1493.9426,
	1	1.376343000	-0.782289000	-0.920461000	1495.4273,	1498.9643,	1514.7827,
	6	2.474563000	0.823878000	-0.000074000	1539.4116,	1825.6323,	3088.5228,
	1	3.488950000	0.214480000	-0.106586000	3096.9796,	3100.8093,	3115.7593,
	1	2.485878000	1.494982000	-0.862502000	3138.8456,	3160.5053,	3187.6970,
	1	2.548981000	1.392744000	0.929479000	3197.4304,	3223.2374,	3845.8779
	8	4.425218000	-0.720736000	-0.075319000			
	1	4.164105000	-1.097937000	0.775782000			

iPE	6	1.252307000	0.077075000	-0.136594000	41.1982,	89.8387,	115.5851,
	8	1.293484000	1.097048000	-0.786213000	200.1968,	221.9548,	276.1897,
	6	2.445776000	-0.659287000	0.419128000	318.3728,	408.7779,	433.7438,
	1	2.409956000	-1.706896000	0.114117000	481.9104,	607.5225,	646.3293,
	1	3.359791000	-0.187504000	0.061705000	847.4532,	915.6352,	948.0165,
	1	2.411372000	-0.627931000	1.510914000	968.2521,	992.6694,	1052.5751,
	8	0.109272000	-0.564470000	0.202245000	1072.9432,	1165.6177,	1195.3715,
	6	-1.119337000	0.050912000	-0.257645000	1225.2918,	1286.0707,	1378.3172,
	1	-0.938956000	0.453846000	-1.258187000	1400.6478,	1418.9004,	1426.0724,
	6	-2.144625000	-1.066460000	-0.306460000	1436.3885,	1493.4852,	1499.0653,
	1	-3.102660000	-0.677905000	-0.663616000	1501.6904,	1505.9371,	1517.8746,
	1	-1.814293000	-1.860922000	-0.979879000	1531.7971,	1818.7400,	3077.8215,
	1	-2.287855000	-1.490349000	0.691526000	3080.7941,	3099.6564,	3124.9997,
	6	-1.506949000	1.176978000	0.687306000	3167.2380,	3176.3457,	3180.0780,
	1	-1.623324000	0.784603000	1.701993000	3187.0367,	3188.6111,	3221.7264
	1	-0.742882000	1.956587000	0.686926000			
	1	-2.456225000	1.620532000	0.371837000			
TS α'	6	0.681284000	0.072389000	0.195243000	2107.3044 <i>i</i> ,	29.7037,	77.2400,
	8	0.844505000	1.084078000	-0.457193000	117.6797,	133.6637,	206.0188,
	6	1.777050000	-0.621621000	0.950098000	221.1223,	275.8159,	308.1698,
	1	1.565319000	-1.663885000	1.179462000	320.5396,	400.6250,	405.1543,
	1	2.745311000	-0.587201000	0.215655000	423.5362,	479.2978,	616.8733,
	1	2.075597000	-0.047773000	1.827405000	637.5671,	773.0262,	856.5652,
	8	-0.494208000	-0.560207000	0.340606000	913.7105,	949.6632,	954.0065,
	6	-1.628951000	0.040968000	-0.343269000	969.3116,	1005.7538,	1058.6207,
	1	-1.271634000	0.423412000	-1.303170000	1104.1742,	1160.2599,	1196.2169,
	8	3.557340000	-0.101327000	-0.623117000	1225.8379,	1247.9700,	1323.4995,
	1	3.009400000	0.667909000	-0.844502000	1380.3655,	1406.4029,	1426.8030,
	6	-2.623772000	-1.085380000	-0.547308000	1436.3745,	1472.3178,	1501.7358,
	1	-3.503743000	-0.710498000	-1.077551000	1505.9688,	1518.0148,	1531.5997,
	1	-2.176728000	-1.891206000	-1.134032000	1566.5916,	1792.9533,	3079.6096,
	1	-2.941116000	-1.488167000	0.418569000	3082.4504,	3129.5078,	3150.2596,
	6	-2.175041000	1.181851000	0.498791000	3169.7851,	3178.5905,	3182.4747,
	1	-2.465166000	0.808381000	1.485229000	3189.3884,	3244.5117,	3796.9090
	1	-1.425504000	1.966878000	0.615150000			
	1	-3.056262000	1.612552000	0.014093000			
TS α	6	1.381118000	0.043327000	0.024160000	1648.0623 <i>i</i> ,	37.0465,	66.5423,
	8	1.253454000	1.161238000	0.474612000	110.2591,	125.4866,	162.2970,
	6	2.694959000	-0.624758000	-0.286018000	198.1991,	207.3279,	258.1356,
	1	2.682951000	-1.004078000	-1.309483000	324.8415,	393.9234,	408.8761,
	1	3.504258000	0.090950000	-0.151395000	436.8796,	449.3990,	607.8736,
	1	2.832533000	-1.476056000	0.385187000	640.8950,	668.5138,	853.4602,
	8	0.354921000	-0.788433000	-0.262785000	877.8342,	923.9290,	962.4886,
	6	-0.977694000	-0.340673000	0.028023000	995.4460,	1003.4895,	1061.5882,
	1	-1.111210000	0.762742000	-0.380895000	1074.9679,	1180.3270,	1194.4182,
	8	-1.196541000	2.044635000	-0.704032000	1256.0740,	1297.3558,	1305.5630,
	1	-0.370271000	2.258076000	-0.244313000	1414.0203,	1416.4897,	1425.4110,
	6	-1.912086000	-1.202475000	-0.789072000	1453.6960,	1492.0917,	1494.5165,
	1	-2.941344000	-0.863193000	-0.649037000	1498.4147,	1501.3708,	1511.3814,
	1	-1.659121000	-1.135979000	-1.849258000	1526.4497,	1813.2586,	3075.9938,

TSβ

1	-1.834955000	-2.247513000	-0.470372000	3078.4506, 3101.0027, 3167.9513,
6	-1.254087000	-0.330410000	1.516409000	3171.7388, 3188.7115, 3190.5667,
1	-1.134635000	-1.342662000	1.918208000	3198.2472, 3224.5916, 3808.6620
1	-0.575516000	0.347065000	2.036026000	
1	-2.280629000	0.001058000	1.691958000	
6	1.589113000	0.021796000	0.084978000	1842.4621 <i>i</i> , 60.7517 , 81.3591 ,
8	2.026679000	-1.103097000	0.128187000	84.9174 , 115.5062, 139.5564 ,
6	2.397458000	1.280096000	-0.103407000	210.1684, 263.4092 , 316.7465,
1	2.176308000	1.704477000	-1.086246000	352.3815 , 400.9385, 408.9106,
1	2.123159000	2.018258000	0.652391000	442.1550, 483.0201, 603.8085,
1	3.457399000	1.039572000	-0.037635000	645.1237, 742.6096, 864.2544,
8	0.267090000	0.324066000	0.192653000	909.7425, 951.0479, 971.3371,
6	-0.631444000	-0.807289000	0.338444000	991.6437, 1007.3166, 1053.3060,
1	-0.133154000	-1.549434000	0.970079000	1073.0783, 1166.7635, 1205.8778,
6	-1.857046000	-0.259177000	1.030088000	1211.4450, 1273.6650, 1322.5741,
1	-2.665488000	-0.990496000	1.089334000	1369.0329, 1395.5273, 1417.1613,
1	-1.637508000	0.182944000	2.002777000	1431.4798, 1472.5053, 1493.7531,
1	-2.284871000	0.632276000	0.349772000	1500.3835, 1516.8637, 1519.9110,
8	-2.301616000	1.633642000	-0.486605000	1532.6375, 1826.1036, 3085.2694,
1	-1.342128000	1.765944000	-0.469028000	3099.0307, 3115.5131, 3130.8404,
6	-0.931159000	-1.401012000	-1.028223000	3177.5649, 3186.8833, 3197.1783,
1	-0.011712000	-1.750570000	-1.501420000	3216.9063, 3222.6346, 3819.8702
1	-1.610714000	-2.251910000	-0.921360000	
1	-1.410048000	-0.644434000	-1.653817000	