

Theoretical and Kinetic Study of the Reactions of Ketones with HO₂ Radicals.

Part I: Abstraction Reaction Channels

Jorge Mendes, Chong-Wen Zhou, Henry J. Curran

Combustion Chemistry Centre, National University of Ireland, Galway, Ireland

Table S1: Energies of the reactions of DMK with the HO₂ 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			ΔE			ΔE			ΔE		
	AU	KJ mol ⁻¹	Kcal mol ⁻¹	AU	KJ mol ⁻¹	Kcal mol ⁻¹	AU	KJ mol ⁻¹	Kcal mol ⁻¹	AU	KJ mol ⁻¹	Kcal mol ⁻¹
DMK	-192.556954			-192.756214			-192.815041			-192.935810		
HO ₂	-150.543942			-150.698246			-150.745644			-150.841067		
RC1a	-343.117732	-44.2	-10.6	-343.469631	-39.8	-9.5	-343.575470	-38.8	-9.3	-343.791467	-38.3	-9.2
TS1a	-343.066022	91.6	21.9	-343.422203	84.7	20.2	-343.528384	84.8	20.3	-343.744441	85.2	20.4
TS2a	-343.066831	89.4	21.4	-343.421917	85.4	20.4	-343.527797	86.3	20.6	-343.743689	87.1	20.8
PC1a	-343.091517	24.6	5.9	-343.448863	14.7	3.5	-343.555698	13.1	3.1	-343.772170	12.4	3.0
DMK radical	-191.908907	63.0	15.0	-192.102830	49.3	11.8	-192.160515	46.4	11.1	-192.280400	45.0	10.8
H ₂ O ₂	-151.168010			-151.332861			-151.382489			-151.479345		

Table S2: Geometry co-ordinates and frequencies of Reactants, Complexes, Transition States and Products 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)		
DMK	6	-1.286590000	-0.617666000	-0.002327000	79.1917 ,	138.9562 ,	376.7058,
	6	0.000000000	0.186974000	0.000001000	481.3631,	534.4036,	803.4766,
	6	1.286591000	-0.617664000	0.002327000	889.08	, 906.072,	1091.3231,
	8	-0.000001000	1.403555000	0.000000000	1121.2464,	1253.8722,	1395.4248,
	1	-1.259606000	-1.384255000	-0.782534000	1405.8329,	1482.3337,	1486.2292,
	1	-2.136356000	0.047765000	-0.155590000	1491.5693,	1506.8482,	1787.6488,
	1	-1.394232000	-1.132663000	0.958265000	3075.2543,	3080.0048,	3158.2195,
	1	2.136356000	0.047768000	0.155586000	3163.1243,	3204.2565,	3205.3882
	1	1.259609000	-1.384252000	0.782535000			
	1	1.394230000	-1.132664000	-0.958264000			
HÖ₂	8	0.055115000	0.707840000	0.000000000	1246.4613,	1460.647,	3735.4228
	8	0.055115000	-0.601517000	0.000000000			
	1	-0.881845000	-0.850582000	0.000000000			
RC1a	6	0.766408000	1.384330000	0.080975000	36.2805,	57.4053,	102.0941,
	6	1.157772000	-0.072014000	0.010853000	127.2467,	141.091,	148.8504,
	6	2.634288000	-0.378586000	-0.072639000	224.3644,	392.1097,	483.7496,
	8	0.333267000	-0.977484000	0.028873000	554.6181,	687.7175,	816.4993,
	1	1.359955000	1.972715000	-0.623941000	899.9024,	929.7759,	1103.3252,
	1	0.996098000	1.752922000	1.087241000	1125.585,	1277.1609,	1325.3138,
	1	-0.299260000	1.506102000	-0.112824000	1404.249,	1416.9794,	1482.5405,
	1	2.803438000	-1.445151000	0.073547000	1486.0657,	1494.9022,	1513.9987,
	1	3.002377000	-0.081222000	-1.060414000	1591.7416,	1770.7228,	3076.4583,
	1	3.187199000	0.203566000	0.669980000	3082.2063,	3160.7912,	3165.8926,
	8	-2.570692000	0.578940000	-0.145956000	3210.0107,	3210.4856,	3470.9859
	8	-2.386445000	-0.689211000	0.088755000			
	1	-1.409650000	-0.809277000	0.077895000			
TS1a	6	-0.274933000	1.416841000	-0.076356000	1938.0639 <i>j</i> ,	56.4024 ,	101.9655 ,
	6	-0.954755000	0.114548000	0.258566000	122.7906 ,	138.2498,	250.0034,
	6	-1.751298000	-0.518990000	-0.857311000	371.4238,	412.3044,	514.0436 ,
	8	-0.814174000	-0.393562000	1.341967000	547.9607,	590.7968,	650.1484,
	1	-0.523309000	1.895129000	-1.022205000	817.3609,	924.1783,	967.4764,
	1	0.958052000	0.948293000	-0.220633000	1067.0618,	1099.2661,	1126.4104,
	1	-0.164337000	2.081622000	0.778075000	1186.0544,	1261.7035,	1396.2337,
	1	-2.163380000	-1.469992000	-0.521173000	1436.5733,	1470.3924,	1480.5346,
	1	-2.553361000	0.153893000	-1.176130000	1483.2702,	1495.1161,	2260.4026,
	1	-1.085464000	-0.675594000	-1.711843000	3080.8671,	3153.3367,	3168.3957,
	8	1.957523000	0.380307000	-0.161968000	3213.6437,	3264.3398,	3777.8511
	8	1.607070000	-0.962678000	-0.270469000			
	1	1.414363000	-1.200275000	0.648279000			
TS2a	6	-0.246252000	-1.042015000	0.713734000	1903.8791 <i>j</i> ,	40.833,	143.1062 ,
	6	-0.971905000	0.165062000	0.189891000	158.6767,	165.7043,	220.8932,
	6	-2.300955000	-0.088123000	-0.480962000	372.9178,	506.52,	525.1047,
	8	-0.486808000	1.274287000	0.274592000	567.348,	647.0685,	664.5862,

	1	0.280819000	-0.868827000	1.650679000	818.1209,	868.3044,	943.0886,
	1	0.805628000	-1.006577000	-0.097797000	1059.126,	1103.0194,	1122.5662,
	1	-0.727848000	-2.011834000	0.609032000	1240.8483,	1276.3425,	1400.0261,
	1	-2.706828000	0.847536000	-0.864323000	1469.3078,	1480.9833,	1493.2736,
	1	-2.160956000	-0.804383000	-1.297048000	1493.8973,	1530.7915,	2129.1141,
	1	-2.994801000	-0.539075000	0.235467000	3079.5628,	3153.6826,	3164.1702,
	1	1.553012000	1.123009000	0.047760000	3213.4136,	3264.8833,	3702.141
	8	2.215300000	0.412411000	0.097927000			
	8	1.654714000	-0.555372000	-0.724988000			
PC1a	6	0.694676000	1.323669000	-0.168014000	36.3409,	47.9193,	93.0086,
	6	1.207976000	-0.042079000	0.030532000	117.4962,	135.0837,	207.4635,
	6	2.712448000	-0.201912000	0.023032000	241.3309,	303.2903,	401.5331,
	8	0.470539000	-0.987965000	0.195305000	536.4242,	553.1179,	683.3909,
	1	1.372579000	2.147057000	-0.356028000	756.7151,	840.2478,	929.6929,
	1	-3.062610000	0.287176000	0.939320000	944.3818,	1043.5154,	1094.2803,
	1	-0.373583000	1.490832000	-0.105013000	1296.4658,	1348.4606,	1405.7445,
	1	2.968952000	-1.247860000	0.183338000	1479.8703,	1495.0857,	1495.8287,
	1	3.110678000	0.143577000	-0.935926000	1553.103,	2040.5736,	3084.5908,
	1	3.152476000	0.422079000	0.806731000	3169.5763,	3200.0226,	3221.4865,
	8	-2.446419000	0.569835000	0.256995000	3336.5597,	3631.9857,	3871.1221
	8	-2.219686000	-0.690238000	-0.414032000			
	1	-1.294573000	-0.853985000	-0.151867000			
P1a	6	1.165542000	-0.845979000	-0.000007000	102.328,	262.5055,	382.9542,
	6	0.073865000	0.158433000	-0.000001000	518.3789,	535.0272,	645.025,
	6	-1.334220000	-0.410124000	-0.000001000	818.8668,	897.9421,	1046.3537,
	8	0.303067000	1.331768000	0.000003000	1081.481,	1265.4255,	1398.4372,
	1	0.966826000	-1.910715000	0.000033000	1473.6525,	1486.4871,	1496.2492,
	1	2.185339000	-0.483358000	-0.000003000	2117.9842,	3083.3953,	3169.233,
	1	-2.054016000	0.407117000	-0.000021000	3204.1346,	3218.9637,	3338.0563
	1	-1.476899000	-1.040601000	-0.882929000			
	1	-1.476908000	-1.040571000	0.882946000			
EMK	6	-1.882934000	-0.503658000	0.043221000	68.6726,	108.639,	221.1884,
	6	-0.524574000	0.169166000	-0.024019000	252.3333,	400.7056,	469.5599,
	6	0.679719000	-0.759233000	-0.073896000	595.5589,	762.7693,	782.0814,
	6	2.007035000	-0.023251000	0.060161000	955.8814,	965.8901,	1019.1684,
	8	-0.404770000	1.380654000	-0.028129000	1124.8802,	1139.0134,	1205.1977,
	1	-2.024875000	-0.919613000	1.046687000	1296.6598,	1381.5141,	1406.8089,
	1	-1.944041000	-1.332285000	-0.668143000	1432.7377,	1471.8984,	1487.891,
	1	-2.667041000	0.227479000	-0.156114000	1499.1476,	1516.3058,	1520.6906,
	1	0.626148000	-1.305720000	-1.025220000	1781.4435,	3066.8428,	3077.9103,
	1	0.557589000	-1.517546000	0.709946000	3090.3996,	3112.4008,	3161.5771,
	1	2.845664000	-0.721629000	0.000042000	3179.2271,	3187.3289,	3202.2088
	1	2.058528000	0.503817000	1.015655000			
	1	2.110715000	0.722120000	-0.730623000			
RC1b	6	-0.033574000	1.695328000	0.119418000	30.4874,	52.413,	80.2443,
	6	0.669737000	0.364143000	0.004276000	93.5407,	128.9634,	142.5218,
	6	2.179034000	0.393077000	-0.111253000	212.3534,	225.7072,	289.5603,

	6	2.827457000	-0.980527000	0.004646000	413.1427,	471.3449,	607.8625,
	8	0.063417000	-0.700660000	0.021719000	689.5636,	760.8062,	796.5317,
	1	0.466783000	2.453843000	-0.487596000	964.724,	989.6384,	1022.889,
	1	0.024031000	2.017734000	1.165604000	1128.5927,	1141.5995,	1223.4413,
	1	-1.082655000	1.599129000	-0.161956000	1298.3751,	1324.6434,	1392.7668,
	1	2.558316000	1.088223000	0.648363000	1418.2157,	1435.3248,	1467.7227,
	1	2.409690000	0.860854000	-1.078141000	1487.7031,	1511.7048,	1517.1873,
	1	3.911732000	-0.902877000	-0.105308000	1521.6024,	1592.2493,	1764.0002,
	1	2.442747000	-1.651712000	-0.765383000	3068.8962,	3077.818,	3092.7917,
	1	2.606864000	-1.430122000	0.975490000	3114.8645,	3163.6875,	3182.3114,
	1	-1.672934000	-0.901080000	0.106569000	3189.5732,	3207.4779,	3466.8343
	8	-2.653323000	-0.985956000	0.132253000			
	8	-3.100157000	0.190851000	-0.203993000			
RC2b (identified as RC1b in PES)	6	-0.033052000	1.695606000	0.119454000	30.6726,	52.4138,	80.2719,
	6	0.669844000	0.364261000	0.003885000	93.4334,	128.9058,	142.5652,
	1	0.024090000	2.017265000	1.165902000	212.331,	225.7132,	289.5284,
	1	0.467899000	2.454368000	-0.486757000	413.1049,	471.3605,	607.8502,
	6	2.179189000	0.392845000	-0.111132000	689.5075,	760.7982,	796.5325,
	8	0.063236000	-0.700374000	0.020727000	964.718,	989.655,	1022.904,
	6	2.827253000	-0.980900000	0.005101000	1128.5881,	1141.5837,	1223.4306,
	1	2.558401000	1.087995000	0.648514000	1298.3757,	1324.5552,	1392.7596,
	1	2.410243000	0.860451000	-1.078011000	1418.2113,	1435.3236,	1467.7302,
	1	3.911579000	-0.903527000	-0.104543000	1487.6912,	1511.6628,	1517.1896,
	1	2.442599000	-1.652071000	-0.764967000	1521.6048,	1592.1618,	1764.0624,
	1	2.606269000	-1.430338000	0.975931000	3068.8806,	3077.8175,	3092.7889,
	1	-1.082021000	1.599955000	-0.162481000	3114.8585,	3163.6746,	3182.3021,
	8	-3.100385000	0.190821000	-0.203839000	3189.5797,	3207.5707,	3467.0138
	8	-2.653516000	-0.985878000	0.132793000			
	1	-1.673141000	-0.901522000	0.105129000			
RC3b	6	2.574932000	-0.739349000	-0.119169000	38.8728,	64.4396,	73.9679,
	6	1.102528000	-0.416837000	-0.090280000	110.2248,	144.3775,	169.9803,
	1	3.138776000	0.067636000	0.359678000	221.2811,	230.9406,	253.4064,
	1	2.908499000	-0.791567000	-1.161095000	397.8857,	540.3716,	597.7132,
	1	2.765980000	-1.688359000	0.381623000	732.2985,	789.0924,	823.4939,
	6	0.670384000	0.942773000	-0.595265000	962.9061,	996.9523,	1022.6307,
	8	0.289990000	-1.217332000	0.360670000	1117.6111,	1135.1163,	1246.2242,
	6	0.294825000	1.841136000	0.594665000	1309.3445,	1314.6706,	1367.3999,
	1	1.472088000	1.400434000	-1.181589000	1407.1805,	1427.0506,	1480.0789,
	1	-0.009909000	2.828986000	0.242108000	1495.6396,	1507.6325,	1522.0212,
	1	1.139731000	1.965992000	1.278870000	1527.0906,	1595.8886,	1761.2829,
	1	-0.539034000	1.402877000	1.146654000	3076.9973,	3083.2408,	3104.2421,
	1	-0.207720000	0.804412000	-1.231570000	3158.9929,	3163.7442,	3176.8779,
	8	-2.552556000	0.048217000	-0.648900000	3190.856,	3208.3626,	3426.9494
	8	-2.376305000	-0.687710000	0.414595000			
	1	-1.413463000	-0.902147000	0.414704000			
RC4b	6	-2.577003000	-0.732977000	0.114418000	39.3414,	64.7666,	74.2917,
	6	-1.102890000	-0.417506000	0.092908000	110.384,	143.9965,	169.3946,
	6	-0.667486000	0.941345000	0.596851000	221.1686,	230.987,	253.3798,

	6	-0.294978000	1.838801000	-0.594846000	398.0466,	540.6485,	597.6126,
	8	-0.291802000	-1.222861000	-0.351911000	730.783,	789.3382,	823.7396,
	1	-3.135182000	0.077279000	-0.365475000	962.7615,	996.9397,	1022.3873,
	1	-2.915255000	-0.785623000	1.154821000	1117.4881,	1135.0521,	1246.4134,
	1	-2.770181000	-1.680346000	-0.388662000	1309.3867,	1314.5763,	1367.0238,
	1	0.212315000	0.802493000	1.230568000	1407.1294,	1427.0239,	1480.1017,
	1	-1.467108000	1.400075000	1.185222000	1495.6474,	1507.8823,	1522.0459,
	1	0.011776000	2.826550000	-0.243754000	1527.2484,	1595.9232,	1761.3549,
	1	-1.141988000	1.964152000	-1.276361000	3077.0692,	3083.1602,	3104.3707,
	1	0.536701000	1.399340000	-1.149210000	3159.1065,	3163.8822,	3177.014,
	1	1.413129000	-0.912215000	-0.403097000	3190.7681,	3208.3395,	3427.6055
	8	2.373501000	-0.687469000	-0.416587000			
	8	2.557042000	0.051620000	0.643492000			
RC5b (identified as RC4b in PES)	6	-2.632285000	-0.986851000	-0.157049000	34.6275,	60.7288,	86.9427,
	6	-1.281818000	-0.323903000	-0.004400000	91.5611,	104.5017,	135.0831,
	6	0.095060000	1.810227000	0.224645000	210.8574,	251.3287,	272.1526,
	8	-0.280994000	-0.990938000	0.217152000	411.8113,	469.1765,	592.1858,
	1	-3.201982000	-0.530356000	-0.970605000	637.3573,	762.1361,	791.0936,
	1	-3.199967000	-0.838504000	0.768169000	961.0735,	977.588,	1025.8648,
	1	-2.504071000	-2.055487000	-0.329961000	1128.2197,	1142.6119,	1215.3669,
	1	0.869772000	1.466911000	-0.462219000	1298.7861,	1307.1668,	1388.9562,
	1	0.400635000	1.541543000	1.238961000	1415.1535,	1440.1181,	1466.5678,
	1	0.034617000	2.899254000	0.161925000	1485.5655,	1498.9888,	1523.4177,
	1	1.476617000	-0.768786000	0.377375000	1535.1674,	1573.0363,	1773.8691,
	8	2.454410000	-0.736225000	0.444843000	3068.9906,	3081.5625,	3092.85,
	8	2.846081000	-0.127348000	-0.641512000	3113.4608,	3166.499,	3179.033,
	6	-1.251969000	1.186242000	-0.117161000	3198.1883,	3208.1385,	3548.2406
	1	-2.054776000	1.576279000	0.521661000			
	1	-1.550748000	1.430952000	-1.145368000			
RC6b (identified as RC4b in PES)	6	-2.632124000	-0.986838000	0.157480000	34.697,	60.7892,	86.8477,
	6	-1.281733000	-0.323878000	0.004223000	91.4987,	104.5296,	135.1311,
	6	-1.251808000	1.186257000	0.117199000	210.8826,	251.3576,	272.0933,
	6	0.095173000	1.810203000	-0.224842000	411.8183,	469.1837,	592.2258,
	8	-0.281012000	-0.990875000	-0.217980000	637.4722,	762.1443,	791.085,
	1	-3.201024000	-0.530980000	0.971954000	961.0607,	977.5348,	1025.8644,
	1	-2.503851000	-2.055629000	0.329385000	1128.2289,	1142.6236,	1215.3757,
	1	-3.200655000	-0.837626000	-0.767076000	1298.7767,	1307.1632,	1388.9491,
	1	-1.550388000	1.430889000	1.145478000	1415.1496,	1440.1196,	1466.5688,
	1	-2.054705000	1.576406000	-0.521443000	1485.5679,	1498.9764,	1523.4192,
	1	0.869975000	1.466959000	0.461935000	1535.1763,	1573.0707,	1773.8004,
	1	0.034734000	2.899236000	-0.162211000	3069.0069,	3081.5657,	3092.873,
	1	0.400603000	1.541430000	-1.239180000	3113.4703,	3166.4938,	3179.0249,
	1	1.476640000	-0.768958000	-0.377705000	3198.2874,	3208.1457,	3547.9838
	8	2.454502000	-0.736540000	-0.444505000			
	8	2.845461000	-0.127109000	0.641799000			
TS1b	6	0.701961000	1.540258000	-0.301060000	1913.6096i,	41.1509,	75.2071,
	6	-0.392617000	0.674900000	0.261077000	99.7794,	138.8147,	217.1939,
	6	-1.449714000	0.221489000	-0.723607000	252.1839,	261.2107,	393.5768,

	6	-2.403087000	-0.810451000	-0.137887000	418.4284,	512.5253,	570.151,
	8	-0.383253000	0.338484000	1.420588000	606.6356,	645.1437,	786.4052,
	1	0.572807000	1.931677000	-1.308908000	814.1888,	976.987,	1006.6962,
	1	1.632431000	0.603406000	-0.395828000	1023.757,	1103.8106,	1123.0793,
	1	1.136069000	2.225763000	0.424292000	1133.2292,	1184.6705,	1210.3051,
	1	-0.921905000	-0.167421000	-1.603190000	1298.8994,	1395.7179,	1430.5708,
	1	-1.982469000	1.120878000	-1.061771000	1436.0929,	1460.6286,	1475.7423,
	1	-3.161159000	-1.096035000	-0.871229000	1485.6436,	1515.1191,	1520.2604,
	1	-2.899369000	-0.413647000	0.749668000	2208.6197,	3069.7863,	3093.0002,
	1	-1.852123000	-1.704672000	0.161187000	3120.12,	3151.37,	3183.5827,
	1	1.316200000	-1.380044000	0.858173000	3190.4628,	3262.2041,	3777.3781
	8	1.478372000	-1.391910000	-0.096450000			
	8	2.332413000	-0.306209000	-0.267080000			
TS2b	6	0.519456000	1.352865000	-0.457178000	1928.2658 <i>j</i> ,	32.6387,	83.5025,
	6	-0.479936000	0.236024000	-0.380006000	139.4192,	162.7841,	216.4199,
	1	1.136410000	1.336117000	-1.354492000	224.2999,	266.8927,	394.8191,
	1	0.207876000	2.336221000	-0.110818000	492.5343,	558.4974,	584.7545,
	6	-1.824999000	0.572448000	0.228518000	648.1244,	654.9521,	783.9636,
	8	-0.199382000	-0.886606000	-0.754741000	799.1168,	917.0002,	992.4344,
	6	-2.740759000	-0.635718000	0.369544000	1023.3998,	1104.5641,	1125.0818,
	1	-2.276891000	1.353052000	-0.398101000	1133.8205,	1208.3668,	1250.0936,
	1	-1.627928000	1.048840000	1.198104000	1296.6867,	1395.9415,	1433.7096,
	1	-3.700166000	-0.342215000	0.802450000	1462.089,	1470.9159,	1491.8647,
	1	-2.281583000	-1.390320000	1.011398000	1515.2745,	1520.3968,	1533.0913,
	1	-2.919162000	-1.095552000	-0.604393000	2049.205,	3067.9816,	3093.4518,
	1	1.414127000	0.873539000	0.395465000	3112.901,	3151.3656,	3184.8211,
	8	2.066517000	0.093673000	0.936088000	3189.5716,	3262.0085,	3702.7837
	8	2.560631000	-0.710083000	-0.081360000			
	1	1.782628000	-1.249265000	-0.304773000			
TS3b	6	-1.003519000	1.799373000	-0.662438000	1956.842 <i>j</i> ,	62.6703,	87.9905,
	6	-0.799108000	0.542827000	0.149494000	112.0943,	131.4659,	159.4226,
	1	-1.939866000	1.726171000	-1.225415000	177.8566,	241.873,	263.2746,
	1	-0.185068000	1.894337000	-1.382392000	397.916,	510.9689,	559.0579,
	1	-1.028510000	2.666057000	-0.001953000	606.0616,	656.2229,	782.6651,
	6	-0.601492000	-0.730382000	-0.635647000	811.8517,	971.6134,	1017.7339,
	8	-0.742386000	0.539174000	1.358948000	1056.4857,	1106.6392,	1137.4734,
	6	-0.985670000	-2.008063000	0.066555000	1175.484,	1214.6796,	1232.6728,
	1	-0.860366000	-0.661491000	-1.694551000	1382.3033,	1407.7871,	1423.4556,
	1	-0.588511000	-2.881129000	-0.456822000	1435.9062,	1478.6901,	1483.4205,
	1	-2.077098000	-2.103631000	0.113543000	1497.7897,	1505.2027,	1511.6961,
	1	-0.606240000	-1.993232000	1.089384000	2135.8463,	3070.9275,	3078.9755,
	1	0.684873000	-0.713084000	-0.618203000	3155.0876,	3159.3608,	3166.7278,
	8	1.841196000	-0.666056000	-0.322997000	3196.2926,	3209.5674,	3778.7118
	8	2.041537000	0.616381000	0.160398000			
	1	1.816752000	0.527473000	1.097830000			
TS4b	6	2.241610000	-0.669025000	-0.420699000	1995.1446 <i>i</i> ,	51.5073,	117.9126,
	6	1.030991000	-0.041317000	0.230082000	137.8229,	151.2272,	161.5617,
	6	0.215844000	0.887595000	-0.624431000	177.2237,	249.3785,	293.7991,

	6	-0.563880000	1.955245000	0.097854000	411.8174,	508.5891,	522.9345,
	8	0.681413000	-0.312652000	1.365061000	606.5248,	647.8226,	793.4301,
	1	2.973056000	0.108712000	-0.663054000	857.7557,	969.6585,	994.9333,
	1	1.940949000	-1.144879000	-1.359537000	1059.2963,	1091.8092,	1136.2078,
	1	2.685043000	-1.404585000	0.250462000	1178.6829,	1209.7858,	1235.7873,
	1	-0.659943000	-0.011139000	-0.948629000	1385.1385,	1409.5468,	1432.1765,
	1	0.682742000	1.175359000	-1.568555000	1466.9599,	1480.446,	1495.8926,
	1	-1.205683000	2.507109000	-0.592103000	1501.9404,	1506.5004,	1533.4828,
	1	0.121520000	2.662862000	0.580349000	1973.2239,	3068.6815,	3077.9094,
	1	-1.179605000	1.504629000	0.878317000	3156.5678,	3162.3111,	3163.3925,
	1	-1.351939000	-1.160974000	0.979750000	3195.5578,	3207.9641,	3730.7908
	8	-2.013684000	-0.843645000	0.343886000			
	8	-1.361920000	-0.972714000	-0.865677000			
TS5b	6	-2.180175000	-0.695214000	-0.536398000	2109.4286 <i>j</i> ,	53.9401,	89.4504,
	6	-1.135609000	0.101967000	0.211890000	108.1743,	149.7087,	158.2056,
	6	0.897391000	1.592162000	0.054572000	228.2636,	290.997,	401.4869,
	8	-0.912695000	-0.063681000	1.397916000	455.0076,	457.9463,	550.6899,
	1	-1.661253000	-1.413665000	-1.179835000	610.3658,	625.5154,	780.9377,
	1	-2.780057000	-0.045430000	-1.180276000	796.8997,	968.2998,	988.2173,
	1	-2.818898000	-1.228714000	0.168265000	1028.1394,	1117.3968,	1140.1459,
	1	1.653852000	0.555897000	0.037958000	1179.9529,	1198.268,	1208.3688,
	1	0.790912000	1.822182000	1.113786000	1273.9318,	1383.2975,	1410.0084,
	1	1.465949000	2.336272000	-0.503341000	1421.3043,	1448.9983,	1471.5722,
	1	0.991220000	-1.681884000	0.634574000	1488.0801,	1499.0357,	1519.2459,
	8	1.227893000	-1.432162000	-0.268668000	1785.7522,	3038.74,	3078.4031,
	8	2.228509000	-0.485203000	-0.060468000	3125.6941,	3141.7012,	3164.6249,
	6	-0.374054000	1.133926000	-0.609792000	3202.9267,	3239.6698,	3799.2809
	1	-1.059314000	1.984467000	-0.757384000			
	1	-0.177383000	0.722201000	-1.605624000			
TS6b	6	-2.665128000	-0.538831000	0.271714000	2214.2823 <i>j</i> ,	49.1564,	103.9364,
	6	-1.220041000	-0.241877000	-0.067425000	117.3504,	148.2763,	173.6401,
	6	-0.784503000	1.205240000	0.106372000	183.0158,	251.085,	405.9139,
	6	0.574059000	1.523458000	-0.464675000	454.8937,	560.6939,	573.5098,
	8	-0.469050000	-1.114384000	-0.469724000	612.8267,	641.6016,	776.8571,
	1	-2.964992000	-0.022770000	1.187849000	797.9394,	960.0694,	976.4547,
	1	-2.806708000	-1.614786000	0.375271000	1026.9644,	1088.6366,	1133.8748,
	1	-3.301210000	-0.168926000	-0.539948000	1153.3208,	1199.6624,	1242.5183,
	1	-0.815175000	1.421212000	1.183062000	1288.0694,	1385.8693,	1412.399,
	1	-1.563930000	1.840936000	-0.340412000	1449.6852,	1472.8074,	1478.1142,
	1	1.422224000	0.818044000	0.223565000	1485.5854,	1499.0326,	1521.3164,
	1	0.892976000	2.557325000	-0.334083000	1781.3933,	3048.5165,	3079.8045,
	1	0.754168000	1.137670000	-1.468336000	3098.0463,	3137.2799,	3164.5686,
	1	1.532678000	-1.383160000	-0.327127000	3206.6583,	3234.3004,	3763.0454
	8	2.372323000	-0.916613000	-0.200193000			
	8	2.024682000	-0.003190000	0.790447000			
PC1b	6	1.579873000	-1.668225000	-0.348283000	23.491,	66.4862,	90.7147,
	6	0.962073000	-0.461392000	0.222790000	115.2636,	162.8048,	218.9724,
	6	1.190098000	0.833292000	-0.534461000	225.6825,	255.8729,	261.9658,

	6	0.526426000	2.034418000	0.125478000	277.4876,	411.411,	501.0544,
	8	0.324144000	-0.512008000	1.254961000	589.2506,	616.9442,	646.6932,
	1	2.150985000	-1.632571000	-1.267528000	791.5478,	820.759,	933.0443,
	1	-2.092938000	0.344401000	-1.366140000	977.9333,	1029.774,	1093.2593,
	1	1.429005000	-2.609166000	0.164564000	1125.6834,	1229.2787,	1294.9511,
	1	0.820587000	0.675596000	-1.554291000	1323.0599,	1402.2893,	1433.4067,
	1	2.276019000	0.971633000	-0.621032000	1465.5968,	1482.8512,	1515.4545,
	1	0.714919000	2.943602000	-0.451039000	1527.5496,	1535.3325,	2007.5786,
	1	0.909910000	2.174764000	1.138081000	3074.9242,	3095.23,	3126.6699,
	1	-0.550994000	1.880773000	0.200575000	3184.0766,	3197.1641,	3207.71,
	1	-1.461160000	-0.240981000	0.919153000	3340.9512,	3687.5796,	3864.6389
	8	-2.288812000	-0.171838000	0.412061000			
	8	-1.753726000	-0.433230000	-0.911458000			
PC2b	6	0.059425000	1.605853000	-0.130601000	32.8056,	43.0856,	63.225,
	6	-0.702591000	0.353069000	-0.001624000	100.0319,	126.2857,	192.3043,
	1	1.138502000	1.569698000	-0.042943000	219.4561,	240.9141,	286.9357,
	1	-0.451393000	2.547303000	-0.291470000	305.5667,	422.3764,	511.1659,
	6	-2.214282000	0.477439000	-0.041037000	609.0636,	668.1134,	750.5848,
	8	-0.157987000	-0.721641000	0.134960000	800.1115,	822.8167,	944.5171,
	6	-2.928379000	-0.861713000	0.078555000	985.3841,	1031.5882,	1094.3451,
	1	-2.472558000	0.992580000	-0.975350000	1128.8459,	1234.4365,	1292.7619,
	1	-2.502964000	1.163619000	0.765832000	1348.574,	1404.0731,	1434.9388,
	1	-4.011852000	-0.722137000	0.049873000	1465.4896,	1491.3361,	1514.7547,
	1	-2.660371000	-1.355221000	1.014490000	1520.4851,	1552.2088,	2027.4267,
	1	-2.636444000	-1.524783000	-0.737949000	3071.6426,	3094.7012,	3117.5341,
	1	3.539399000	-0.159681000	0.970691000	3185.7141,	3192.8559,	3198.5519,
	8	2.999899000	0.256315000	0.291677000	3335.0125,	3634.3498,	3870.9556
	8	2.553531000	-0.915804000	-0.426814000			
	1	1.609103000	-0.910229000	-0.183511000			
PC3b	6	-0.091395000	-1.583693000	0.223428000	23.9658,	54.065,	57.8216,
	6	0.723252000	-0.311146000	0.139053000	94.3259,	118.7921,	126.7369,
	1	0.488475000	-2.481193000	0.005205000	148.1101,	202.4583,	215.1077,
	1	-0.931286000	-1.487960000	-0.468339000	298.2031,	433.7993,	543.8204,
	1	-0.508883000	-1.647798000	1.232164000	612.9625,	640.4328,	752.8549,
	6	2.161296000	-0.429994000	-0.130673000	799.1711,	936.3301,	985.0293,
	8	0.206850000	0.778994000	0.295533000	1015.7183,	1049.4585,	1055.2485,
	6	3.023233000	0.774766000	-0.225113000	1152.9597,	1229.9158,	1320.4461,
	1	2.588110000	-1.419174000	-0.261408000	1402.501,	1409.2216,	1450.2086,
	1	3.508341000	0.825223000	-1.207036000	1493.4121,	1499.7268,	1502.5291,
	1	3.823308000	0.735960000	0.523591000	1518.8224,	1582.9439,	1996.7563,
	1	2.424742000	1.672621000	-0.070077000	3061.9114,	3090.4454,	3128.107,
	1	-3.461869000	-0.554106000	-0.472759000	3183.0387,	3200.3298,	3205.3495,
	8	-2.822714000	0.099150000	-0.772197000	3240.7214,	3603.9385,	3876.6041
	8	-2.541403000	0.727761000	0.507755000			
	1	-1.571115000	0.809584000	0.429773000			
PC4b	6	1.909702000	-1.290444000	-0.414487000	18.3678,	53.7106,	81.1267,
	6	1.034593000	-0.246259000	0.238866000	89.5969,	105.1329,	139.4393,
	6	0.959546000	1.062833000	-0.421662000	168.8334,	226.1753,	253.582,

	6	0.059983000	2.125234000	0.097681000	268.4373,	420.1498,	504.467,
	8	0.400560000	-0.487446000	1.252698000	597.1831,	613.4506,	643.9656,
	1	2.830690000	-0.858816000	-0.813585000	808.1204,	934.5604,	972.0802,
	1	1.338823000	-1.713997000	-1.248282000	993.5931,	1045.6625,	1065.2618,
	1	2.130509000	-2.079938000	0.303315000	1152.6019,	1231.6456,	1329.3956,
	1	-2.082387000	0.226281000	-1.263414000	1390.8551,	1413.0802,	1459.7966,
	1	1.584176000	1.246848000	-1.289902000	1483.9563,	1495.6935,	1498.4788,
	1	-0.369377000	2.711488000	-0.719646000	1512.9417,	1534.9846,	1962.1421,
	1	0.615975000	2.821452000	0.740159000	3056.915,	3082.0283,	3136.0877,
	1	-0.735744000	1.684482000	0.699122000	3171.2294,	3198.0007,	3213.585,
	1	-1.374049000	-0.605291000	0.901308000	3238.2192,	3666.6606,	3865.6724
	8	-2.208862000	-0.605651000	0.399260000			
	8	-1.656893000	-0.574489000	-0.940890000			
PC5b	6	-1.840927000	-1.184362000	-0.522257000	40.7427,	66.4671,	83.3816,
	6	-1.136756000	-0.061368000	0.205246000	95.1701,	117.6269,	142.1486,
	6	0.290367000	2.010892000	0.005687000	151.6192,	221.0187,	271.557,
	8	-0.956416000	-0.071589000	1.408501000	288.5497,	403.476,	447.7461,
	1	-1.095958000	-1.731610000	-1.108544000	514.2802,	573.9439,	600.4264,
	1	-2.588006000	-0.788012000	-1.216455000	769.4931,	818.0233,	943.4764,
	1	-2.311357000	-1.855970000	0.196680000	965.8946,	1025.7231,	1041.161,
	1	1.954958000	0.526783000	-0.032437000	1135.1743,	1197.9888,	1212.1066,
	1	0.290694000	2.059499000	1.087260000	1369.6253,	1380.276,	1408.0135,
	1	0.767061000	2.804875000	-0.556397000	1444.8336,	1456.7548,	1475.1468,
	1	1.316747000	-1.559248000	0.704378000	1490.3863,	1500.214,	1795.1292,
	8	1.437669000	-1.266104000	-0.206405000	3010.2321,	3079.7468,	3106.2701,
	8	2.481449000	-0.286108000	-0.028763000	3166.9826,	3202.295,	3202.5733,
	6	-0.675457000	1.099861000	-0.670751000	3323.5407,	3742.995,	3839.9451
	1	-1.589126000	1.647727000	-0.962313000			
	1	-0.270001000	0.696225000	-1.606382000			
PC6b	6	-2.689780000	-0.516683000	0.078694000	35.6334,	55.564,	91.6802,
	6	-1.186486000	-0.389914000	0.115493000	114.1268,	126.3515,	157.1086,
	6	-0.615815000	0.950045000	0.581720000	166.7411,	195.322,	240.9657,
	6	-0.294044000	1.774364000	-0.627734000	248.7544,	378.8744,	491.9791,
	8	-0.452625000	-1.297706000	-0.243441000	535.0517,	598.7743,	689.1831,
	1	-3.076019000	-0.496447000	1.103369000	807.5312,	812.7805,	938.0334,
	1	-2.976922000	-1.449485000	-0.406756000	963.2575,	1033.6969,	1082.0343,
	1	-3.119507000	0.339270000	-0.450561000	1121.3012,	1225.4219,	1283.4405,
	1	0.295779000	0.731294000	1.147184000	1323.9281,	1331.2714,	1401.9131,
	1	-1.333807000	1.463664000	1.226247000	1480.397,	1485.5372,	1496.4287,
	1	2.834083000	0.825766000	0.482299000	1502.7077,	1547.7612,	1775.3299,
	1	-0.928959000	2.594490000	-0.934618000	3077.7842,	3091.9452,	3161.5853,
	1	0.502912000	1.446315000	-1.282396000	3164.8385,	3207.2457,	3210.6718,
	1	1.360254000	-0.902247000	-0.443372000	3335.0508,	3684.764,	3863.7908
	8	2.250035000	-0.553693000	-0.624784000			
	8	2.597457000	-0.081038000	0.701921000			
P1b	6	1.886264000	-0.558155000	0.000061000	68.3374,	212.4426,	252.6323,
	6	0.578876000	0.142176000	-0.000020000	261.2242,	405.3011,	497.6528,
	6	-0.646984000	-0.760823000	-0.000092000	599.2143,	623.247,	783.4262,

	6	-1.953318000	0.020657000	0.000078000	824.7064,	956.3379,	1026.3866,
	8	0.505084000	1.337161000	-0.000044000	1095.6582,	1124.8828,	1205.9576,
	1	1.955922000	-1.639141000	0.000037000	1292.4283,	1394.4196,	1433.4775,
	1	2.785104000	0.045090000	0.000162000	1467.8213,	1475.2742,	1514.3572,
	1	-0.568464000	-1.418517000	0.875304000	1519.9049,	2121.749,	3071.0359,
	1	-0.568544000	-1.418271000	-0.875682000	3093.4233,	3117.8017,	3184.0096,
	1	-2.810146000	-0.657913000	-0.000010000	3191.9019,	3202.7794,	3336.5119
	1	-2.011806000	0.664316000	-0.879613000			
	1	-2.011759000	0.664017000	0.879993000			
P2b	6	-1.844266000	-0.568235000	-0.000049000	64.7822,	77.4848,	129.9334,
	6	-0.516955000	0.169147000	-0.000021000	257.1602,	413.6162,	513.6643,
	6	0.689004000	-0.691409000	0.000069000	606.9907,	614.2599,	782.5736,
	6	2.047257000	-0.089590000	-0.000026000	959.2842,	981.374,	1048.8023,
	8	-0.442054000	1.367383000	0.000037000	1052.1473,	1158.1339,	1218.3427,
	1	-1.909514000	-1.210357000	0.883727000	1385.8906,	1405.5046,	1444.8214,
	1	-1.909052000	-1.211545000	-0.882986000	1484.2893,	1495.5419,	1501.9362,
	1	-2.659505000	0.154157000	-0.000712000	1505.955,	2090.5102,	3059.0281,
	1	0.566047000	-1.770564000	0.000158000	3081.9214,	3124.0025,	3167.7457,
	1	2.617012000	-0.409109000	0.880720000	3194.1274,	3215.9881,	3229.1881
	1	1.964426000	0.997875000	-0.000051000			
	1	2.616777000	-0.408999000	-0.880989000			
P3b	6	1.808312000	-0.533648000	-0.065940000	76.8851,	123.9642,	171.8955,
	6	0.471776000	0.176427000	0.026005000	269.3272,	372.9319,	409.1264,
	6	-0.751908000	-0.732310000	0.107612000	462.6362,	594.471,	766.7148,
	6	-2.043247000	-0.022725000	-0.106853000	810.8273,	963.522,	1024.958,
	8	0.382855000	1.388538000	0.035691000	1035.3921,	1137.2031,	1196.2224,
	1	1.929044000	-0.930163000	-1.079997000	1203.4894,	1380.3271,	1407.7375,
	1	1.850022000	-1.379653000	0.626106000	1451.2187,	1474.6614,	1486.9339,
	1	2.615372000	0.169343000	0.142234000	1499.3782,	1802.6917,	3011.1106,
	1	-0.711340000	-1.206150000	1.104207000	3076.7278,	3079.5277,	3161.841,
	1	-0.618074000	-1.563382000	-0.598755000	3203.4906,	3219.9317,	3343.3803
	1	-2.965847000	-0.580859000	-0.190607000			
	1	-2.071605000	1.056098000	-0.053664000			
nPMK	6	-2.337893000	-0.774567000	0.041573000	58.0089,	97.8831,	109.9588,
	6	-1.132859000	0.145238000	-0.024331000	175.4181,	250.2845,	343.299,
	6	0.226318000	-0.536351000	-0.068033000	393.2032,	470.8723,	601.0211,
	6	1.398949000	0.426636000	0.074469000	734.4541,	835.4243,	849.4764,
	6	2.746372000	-0.289897000	-0.004929000	928.1127,	976.2636,	985.8279,
	8	-1.246316000	1.357562000	-0.032851000	1085.2116,	1147.0698,	1147.8433,
	1	-3.248427000	-0.204617000	-0.146546000	1196.8769,	1266.5225,	1328.7553,
	1	-2.391184000	-1.221596000	1.040301000	1340.5587,	1396.8827,	1418.8343,
	1	-2.243557000	-1.591689000	-0.679590000	1431.2587,	1469.2001,	1487.6313,
	1	0.252234000	-1.307842000	0.713966000	1498.7293,	1507.5866,	1521.8338,
	1	0.289347000	-1.080916000	-1.021536000	1526.7494,	1779.1895,	3052.6007,
	1	1.307899000	0.957368000	1.027935000	3068.6472,	3076.8835,	3095.9238,
	1	1.325371000	1.189316000	-0.706381000	3098.2218,	3139.7517,	3160.7927,
	1	2.836957000	-1.041955000	0.785650000	3161.731,	3162.3226,	3201.4248
	1	2.860723000	-0.799528000	-0.967249000			

RC1c	1	3.575842000	0.414609000	0.103762000			
	6	2.820737000	-0.491393000	-0.073856000	40.7938,	50.0729,	66.3545,
	6	1.314560000	-0.551903000	-0.097952000	99.8848,	120.3626,	142.359,
	1	3.144683000	0.430071000	0.420488000	162.0014,	186.9886,	233.4389,
	1	3.228302000	-1.363367000	0.437702000	257.6352,	328.8166,	403.7983,
	6	0.568694000	0.657261000	-0.613303000	545.2316,	598.8474,	728.7272,
	8	0.714727000	-1.536691000	0.321775000	761.57,	833.6683,	897.194,
	6	-0.032188000	1.446375000	0.563981000	923.7465,	988.6739,	1021.8627,
	1	-0.247833000	0.310804000	-1.253555000	1081.9765,	1133.9818,	1140.4575,
	1	1.235310000	1.303118000	-1.194131000	1240.3266,	1282.7753,	1316.3101,
	1	0.773287000	1.792306000	1.223690000	1330.0747,	1349.5432,	1390.667,
	1	-0.663061000	0.769904000	1.148441000	1406.7098,	1429.2083,	1480.4206,
	1	3.192714000	-0.453615000	-1.103388000	1495.0098,	1505.5514,	1513.0918,
	8	-2.371903000	-0.867058000	-0.605059000	1520.1723,	1527.5414,	1597.0068,
	8	-2.004057000	-1.613846000	0.399605000	1757.5906,	3073.8787,	3076.1711,
	1	-1.017474000	-1.617469000	0.365904000	3077.0094,	3093.3402,	3136.5064,
	6	-0.861466000	2.634449000	0.080237000	3158.8737,	3161.3659,	3166.9402,
	1	-1.277259000	3.191339000	0.924542000	3172.2001,	3207.374,	3414.5168
	1	-1.690942000	2.287068000	-0.542161000			
	1	-0.249891000	3.321865000	-0.512736000			
RC2c	6	0.740151000	1.750954000	-0.106787000	28.3304,	45.1726,	67.6282,
	6	-0.068932000	0.479547000	-0.011708000	79.4782,	105.6889,	121.445,
	1	0.699433000	2.100922000	-1.144887000	142.1367,	193.1909,	232.8145,
	1	0.306361000	2.533369000	0.521141000	249.9439,	358.7977,	405.1241,
	6	-1.572441000	0.629186000	0.080230000	472.9193,	613.7546,	688.9748,
	8	0.450200000	-0.630679000	-0.024852000	734.1871,	840.0688,	860.0157,
	6	-2.342782000	-0.677125000	-0.071632000	933.9006,	988.3468,	1001.0229,
	1	-1.887051000	1.366903000	-0.670599000	1085.6789,	1149.2549,	1151.6389,
	1	-1.786309000	1.093929000	1.054058000	1212.903,	1268.5669,	1324.6703,
	1	-1.987103000	-1.387122000	0.680709000	1335.1936,	1344.176,	1407.6801,
	1	-2.106902000	-1.117982000	-1.045887000	1426.0265,	1433.1597,	1464.7599,
	1	1.779990000	1.564844000	0.163656000	1487.7372,	1508.4852,	1511.0183,
	8	3.677829000	-0.002325000	0.203835000	1522.3408,	1527.0577,	1592.3357,
	8	3.134190000	-1.143145000	-0.113140000	1762.0226,	3054.7247,	3071.023,
	1	2.164287000	-0.976160000	-0.091109000	3076.6561,	3096.5232,	3100.5246,
	6	-3.850895000	-0.469820000	0.062304000	3141.6692,	3162.5705,	3163.6598,
	1	-4.389621000	-1.414027000	-0.054611000	3166.0903,	3206.973,	3466.4388
	1	-4.219636000	0.225564000	-0.698551000			
	1	-4.101819000	-0.057495000	1.044897000			
RC3c (identified as RC1c in PES)	6	-2.820664000	0.491877000	-0.073844000	40.7557,	50.0527,	66.3165,
	6	-1.314476000	0.552069000	-0.097959000	99.8436,	120.364,	142.3468,
	1	-3.144816000	-0.429574000	0.420387000	161.9931,	186.9999,	233.3886,
	1	-3.192650000	0.454299000	-1.103382000	257.6334,	328.8144,	403.8029,
	1	-3.228031000	1.363887000	0.437807000	545.2318,	598.8435,	728.5958,
	6	-0.568870000	-0.657237000	-0.613330000	761.5601,	833.6714,	897.1921,
	8	-0.714433000	1.536708000	0.321821000	923.7393,	988.6744,	1021.8594,
	6	0.031888000	-1.446408000	0.563987000	1081.9776,	1133.9757,	1140.4589,
	1	-1.235648000	-1.302991000	-1.194087000	1240.3244,	1282.7605,	1316.341,

	1	-0.773650000	-1.792185000	1.223702000	1330.0704,	1349.5413,	1390.6572,
	1	0.662857000	-0.770001000	1.148414000	1406.7081,	1429.2046,	1480.4208,
	1	0.247718000	-0.310994000	-1.253609000	1495.0084,	1505.5425,	1513.0853,
	8	2.372110000	0.866212000	-0.604683000	1520.1722,	1527.5373,	1596.9812,
	8	2.004408000	1.614155000	0.399165000	1757.5884,	3073.8811,	3076.1698,
	1	1.017829000	1.617811000	0.365561000	3077.0071,	3093.3533,	3136.5194,
	6	0.860987000	-2.634625000	0.080298000	3158.8721,	3161.3872,	3166.9505,
	1	1.690539000	-2.287382000	-0.542073000	3172.2138,	3207.3855,	3414.6501
	1	0.249321000	-3.321957000	-0.512679000			
	1	1.276662000	-3.191564000	0.924630000			
RC4c (identified as RC1c in PES)	6	2.820615000	0.491469000	-0.074331000	40.9506,	50.0618,	66.3879,
	6	1.314405000	0.551740000	-0.097750000	99.9469,	120.5862,	142.4566,
	6	0.568526000	-0.657382000	-0.613177000	162.1203,	187.0364,	233.3848,
	6	-0.032280000	-1.446623000	0.564081000	257.7296,	328.8271,	403.8396,
	6	-0.861811000	-2.634505000	0.080304000	545.2249,	598.8615,	728.685,
	8	0.714603000	1.536272000	0.322634000	761.5715,	833.6547,	897.1997,
	1	3.228257000	1.363355000	0.437315000	923.7368,	988.6841,	1021.8648,
	1	3.192151000	0.454071000	-1.104043000	1081.9671,	1133.9803,	1140.4735,
	1	3.144937000	-0.430099000	0.419589000	1240.3121,	1282.7926,	1316.3088,
	1	-0.248046000	-0.310904000	-1.253362000	1330.0755,	1349.5536,	1390.6704,
	1	1.235153000	-1.303160000	-1.194088000	1406.7067,	1429.2136,	1480.4239,
	1	-0.662941000	-0.770144000	1.148783000	1495.0144,	1505.544,	1513.0843,
	1	0.773264000	-1.792775000	1.223605000	1520.176,	1527.5434,	1596.9434,
	1	-1.691357000	-2.286913000	-0.541895000	1757.5756,	3073.8217,	3076.1116,
	1	-0.250426000	-3.321917000	-0.512883000	3076.9468,	3093.3194,	3136.4118,
	1	-1.277527000	-3.191465000	0.924608000	3158.8163,	3161.3334,	3166.8909,
	1	-1.017559000	1.618103000	0.366841000	3172.1423,	3207.3639,	3414.4773
	8	-2.004199000	1.614830000	0.398986000			
	8	-2.370734000	0.866854000	-0.605275000			
RC5c	6	2.692225000	-1.335167000	0.129804000	32.9346,	60.2867,	72.5473,
	6	1.315842000	-0.720805000	0.007434000	81.8137,	98.3798,	114.8618,
	6	-0.142314000	1.374144000	-0.159066000	130.5232,	176.1696,	212.5316,
	8	0.335515000	-1.421786000	-0.202347000	250.8136,	345.831,	403.8945,
	1	3.247814000	-0.882976000	0.955622000	469.3891,	598.3815,	640.4485,
	1	3.248663000	-1.133198000	-0.792073000	741.6796,	844.6605,	856.1475,
	1	2.607318000	-2.413094000	0.268876000	935.9235,	983.9245,	991.3534,
	1	-0.870959000	0.955389000	0.539602000	1087.0613,	1148.8729,	1151.4506,
	1	-0.457188000	1.065426000	-1.161842000	1205.5581,	1273.1535,	1305.8486,
	1	-1.426311000	-1.239884000	-0.374096000	1339.5898,	1348.9412,	1402.5924,
	8	-2.403012000	-1.228468000	-0.463628000	1426.3571,	1433.9894,	1463.244,
	8	-2.834965000	-0.661581000	0.630337000	1485.5518,	1498.3229,	1517.0061,
	6	1.232368000	0.785881000	0.135257000	1522.3352,	1531.5863,	1571.3852,
	1	1.997942000	1.217327000	-0.524875000	1771.1326,	3054.9788,	3070.7691,
	1	1.550899000	1.040316000	1.156479000	3080.7245,	3094.3113,	3100.25,
	6	-0.141085000	2.899080000	-0.060371000	3146.215,	3165.7879,	3167.6123,
	1	0.561832000	3.338517000	-0.775618000	3169.2556,	3207.3655,	3544.7098
	1	-1.134522000	3.304777000	-0.268659000			
	1	0.151996000	3.223286000	0.943342000			

RC6c (identified as RC1c in PES)	6	-2.820666000	-0.491934000	0.074134000	40.6447,	50.0509,	66.2777,
	6	-1.314460000	-0.551953000	0.097846000	99.8138,	120.4116,	142.3568,
	6	-0.568882000	0.657330000	0.613301000	162.005,	187.0124,	233.3394,
	6	0.032020000	1.446397000	-0.564009000	257.6162,	328.8241,	403.8079,
	6	0.861178000	2.634593000	-0.080374000	545.2134,	598.8431,	728.4975,
	8	-0.714386000	-1.536367000	-0.322374000	761.5316,	833.6668,	897.1951,
	1	-3.192425000	-0.454452000	1.103756000	923.7262,	988.6671,	1021.8531,
	1	-3.228057000	-1.363956000	-0.437479000	1081.9878,	1133.9774,	1140.4657,
	1	-3.145035000	0.429503000	-0.419983000	1240.3097,	1282.7503,	1316.3752,
	1	-1.235658000	1.303123000	1.194019000	1330.0783,	1349.5469,	1390.6547,
	1	0.247645000	0.311042000	1.253641000	1406.7066,	1429.2014,	1480.4187,
	1	-0.773422000	1.792131000	-1.223863000	1495.0112,	1505.5327,	1513.0795,
	1	0.662995000	0.769852000	-1.148249000	1520.1705,	1527.5316,	1596.952,
	1	0.249516000	3.322072000	0.512436000	1757.6578,	3073.8878,	3076.1833,
	1	1.690621000	2.287351000	0.542143000	3077.0206,	3093.3404,	3136.5914,
	1	1.277010000	3.191372000	-0.924734000	3158.8762,	3161.3777,	3166.9549,
	1	1.017871000	-1.617594000	-0.366100000	3172.2186,	3207.3799,	3414.9234
	8	2.004457000	-1.614502000	-0.398899000			
	8	2.371654000	-0.866261000	0.604901000			
RC7c (identified as RC1c in PES)	6	2.820693000	-0.491924000	-0.073773000	40.7033,	50.0485,	66.2848,
	6	1.314496000	-0.551935000	-0.097949000	99.8787,	120.3641,	142.3724,
	6	0.569038000	0.657460000	-0.613330000	161.9907,	187.0291,	233.3805,
	6	-0.031948000	1.446459000	0.564002000	257.636,	328.8189,	403.8066,
	6	-0.861295000	2.634509000	0.080330000	545.2182,	598.8524,	728.6508,
	8	0.714315000	-1.536514000	0.321767000	761.5538,	833.6627,	897.1852,
	1	3.227931000	-1.364063000	0.437762000	923.7245,	988.6685,	1021.8546,
	1	3.144935000	0.429404000	0.420630000	1081.9638,	1133.9666,	1140.4568,
	1	3.192736000	-0.454218000	-1.103284000	1240.3125,	1282.7359,	1316.3897,
	1	1.235957000	1.303297000	-1.193832000	1330.0731,	1349.5397,	1390.6654,
	1	-0.247413000	0.311329000	-1.253832000	1406.7053,	1429.2071,	1480.4187,
	1	0.773501000	1.792399000	1.223742000	1495.0074,	1505.5341,	1513.0777,
	1	-0.662734000	0.769873000	1.148462000	1520.1712,	1527.5394,	1596.9785,
	1	-1.277133000	3.191323000	0.924665000	1757.6001,	3073.879,	3076.1573,
	1	-0.249743000	3.322000000	-0.512582000	3076.993,	3093.3741,	136.3895,
	1	-1.690736000	2.287127000	-0.542114000	3158.8767,	3161.4078,	3166.9413,
	1	-1.017781000	-1.617762000	0.365850000	3172.2027,	3207.3856,	3414.6897
	8	-2.004380000	-1.614819000	0.398776000			
	8	-2.371863000	-0.865932000	-0.604437000			
TS1c	6	-1.414453000	-1.342839000	-0.666131000	1914.4518 <i>i</i> ,	34.1797,	61.3661,
	6	-0.279525000	-0.881746000	0.207409000	95.0222,	102.888,	139.8342,
	1	-1.199285000	-1.538271000	-1.715546000	179.328,	250.287,	251.3822,
	1	-2.087699000	-2.045269000	-0.178261000	344.4008,	388.2408,	419.4716,
	6	0.984074000	-0.466913000	-0.515274000	514.8882,	572.0264,	611.2176,
	8	-0.408195000	-0.811365000	1.405894000	644.7276,	756.0037,	849.4684,
	6	2.012230000	0.198257000	0.389777000	881.1715,	935.5002,	986.6695,
	1	0.686461000	0.201081000	-1.334702000	1017.9743,	1086.4797,	1116.2361,
	1	1.399323000	-1.366823000	-0.992729000	1128.2827,	1150.2871,	1185.2996,
	1	2.248549000	-0.478566000	1.216099000	1201.9449,	1269.038,	1332.4483,

	1	1.556239000	1.086482000	0.838478000	1341.7003, 1419.1537, 1431.7751,
	1	-2.111725000	-0.218856000	-0.647122000	1434.879, 1457.7697, 1475.205,
	8	-2.626885000	0.784303000	-0.392531000	1485.5605, 1507.0851, 1521.9777,
	8	-1.613873000	1.582323000	0.131392000	1526.5753, 2209.5972, 3055.3044,
	1	-1.622479000	1.340244000	1.068993000	3069.9504, 3099.8503, 3105.8821,
	6	3.281595000	0.582643000	-0.368962000	3142.582, 3150.5946, 3163.4961,
	1	4.004089000	1.068642000	0.292555000	3164.8774, 3261.6559, 3777.2976
	1	3.053239000	1.274583000	-1.185929000	
	1	3.761382000	-0.301750000	-0.800779000	
TS2c	6	1.132669000	1.380727000	-0.394604000	1926.8475 <i>j</i> , 25.7387, 67.1983 ,
	6	0.107669000	0.288968000	-0.493631000	105.1641 , 121.6787, 158.5676,
	1	1.842813000	1.400643000	-1.220167000	197.7405, 226.0983, 250.7704 ,
	1	0.805620000	2.349591000	-0.022525000	346.9418, 390.0257, 493.4508,
	6	-1.284478000	0.622390000	-0.001682000	557.612, 581.7068, 650.9021,
	8	0.401900000	-0.814783000	-0.912134000	659.8313, 751.0081, 846.5353,
	6	-2.245992000	-0.558777000	-0.022737000	854.4671, 933.8055, 944.309,
	1	-1.661220000	1.450935000	-0.618845000	1000.8231, 1085.5402, 1120.7407,
	1	-1.182045000	1.033634000	1.012852000	1129.1552, 1150.5778, 1202.1263,
	1	-1.833418000	-1.360403000	0.597710000	1246.8545, 1267.3866, 1336.361,
	1	-2.296314000	-0.954993000	-1.041399000	1339.6933, 1419.5775, 1432.5991,
	1	1.917022000	0.826290000	0.518715000	1458.9525, 1470.2183, 1491.7081,
	8	2.485482000	-0.004691000	1.078630000	1507.9095, 1522.2612, 1527.0368,
	8	3.071274000	-0.761686000	0.074126000	1532.7144, 2047.9145, 3053.3696,
	1	2.310751000	-1.262826000	-0.267143000	3070.0728, 3097.9312, 3100.4837,
	6	-3.640115000	-0.170640000	0.468202000	3141.9112, 3150.7316, 3163.7089,
	1	-4.316623000	-1.029449000	0.450223000	3165.2161, 3261.5993, 3702.0548
	1	-4.072544000	0.612701000	-0.162761000	
	1	-3.601811000	0.207154000	1.495068000	
TS3c	6	2.022581000	-1.222593000	0.811921000	1929.1878 <i>j</i> , 58.5032 , 73.2666 ,
	6	0.910943000	-0.848674000	-0.139155000	87.0907 , 114.8878 , 128.6051,
	1	1.765889000	-2.148872000	1.336230000	133.0891, 188.5158, 240.9818,
	1	2.126556000	-0.431103000	1.560705000	270.9469 , 341.7681, 396.5492,
	1	2.955203000	-1.346098000	0.261351000	514.1799 , 563.099, 608.3808,
	6	-0.424932000	-0.539090000	0.488627000	652.2613, 765.7927, 837.9094,
	8	1.071777000	-0.746092000	-1.335203000	876.6334, 942.9615, 986.4013,
	6	-1.645800000	-0.766313000	-0.368838000	1038.889, 1088.5516, 1124.5751,
	1	-0.520831000	-0.824299000	1.540141000	1155.0603, 1177.8627, 1212.5863,
	1	-1.816791000	-1.849061000	-0.453205000	1233.0482, 1297.6202, 1334.4896,
	1	-1.423564000	-0.406307000	-1.377034000	1393.2748, 1420.8339, 1430.3525,
	1	-0.286852000	0.740105000	0.514420000	1436.3889, 1478.9642, 1482.1329,
	8	-0.098229000	1.891363000	0.250757000	1495.1564, 1498.8714, 1521.9799,
	8	1.245326000	1.976031000	-0.075614000	1526.4827, 2132.4074, 3057.5268,
	1	1.249173000	1.756519000	-1.018659000	3074.5956, 3078.1285, 3138.1529,
	6	-2.892234000	-0.080847000	0.192831000	3149.0148, 3165.6049, 3166.5585,
	1	-2.749876000	1.003225000	0.225884000	3169.9584, 3208.6988, 3776.4971
	1	-3.107088000	-0.428640000	1.208062000	
	1	-3.766158000	-0.290776000	-0.429724000	
TS4c	6	2.555320000	-0.739452000	-0.554369000	1965.2468 <i>j</i> , 41.2264, 66.1407 ,

	6	1.310089000	-0.337549000	0.200609000	123.7959,	136.5651,	148.8251,
	6	-0.004657000	-0.754045000	-0.398252000	159.5002,	189.9504,	237.0531,
	6	-1.128887000	-1.065106000	0.558340000	297.366,	339.9934,	426.8059,
	6	-2.483216000	-1.148786000	-0.145241000	522.1597,	530.3424,	607.8893,
	8	1.348651000	0.336511000	1.214495000	649.7924,	767.8719,	849.3674,
	1	3.436705000	-0.314085000	-0.074284000	903.5938,	947.0492,	987.2327,
	1	2.479184000	-0.387473000	-1.588345000	1022.759,	1092.8832,	1096.4214,
	1	2.629927000	-1.831386000	-0.583468000	1153.9611,	1182.1364,	1193.6815,
	1	-0.307548000	0.412554000	-0.871621000	1226.3746,	1305.0189,	1333.8307,
	1	0.067315000	-1.403743000	-1.274701000	1395.5303,	1427.8529,	1431.5237,
	1	-1.146125000	-0.293472000	1.332233000	1471.663,	1480.0735,	1488.6517,
	1	-0.901378000	-2.014557000	1.065187000	1495.252,	1518.6639,	1523.8288,
	1	-2.728092000	-0.187500000	-0.605258000	1530.6742,	1985.0294,	3051.4793,
	1	-2.471440000	-1.912979000	-0.928903000	3075.1063,	3076.7156,	3141.4581,
	1	-3.275857000	-1.401562000	0.564057000	3151.4984,	3161.6084,	3166.5684,
	1	-0.015554000	2.002220000	0.795990000	3173.8468,	3207.6219,	3724.3223
	8	-0.837689000	2.018465000	0.278696000			
	8	-0.418340000	1.595226000	-0.967869000			
TS5c	6	2.500188000	-0.552584000	-0.679492000	2052.8677i,	50.8699,	81.5501,
	6	1.285927000	-0.536110000	0.222412000	103.0692,	133.2646,	150.5405,
	6	-1.241389000	-0.636766000	0.372361000	158.448,	177.426,	213.6484,
	8	1.333502000	-0.141913000	1.374332000	277.8649,	354.3758,	395.9883,
	1	2.388138000	0.252309000	-1.413732000	457.2918,	523.3921,	601.167,
	1	2.565325000	-1.496462000	-1.228728000	629.9349,	776.0444,	834.0345,
	1	3.404573000	-0.389994000	-0.092080000	863.4678,	936.9134,	984.0279,
	1	-1.251551000	0.617951000	0.259428000	1003.4092,	1109.1485,	1138.8165,
	1	-1.126646000	-0.784737000	1.448351000	1164.2064,	1182.3972,	1196.8927,
	1	0.586385000	2.191872000	0.412004000	1230.5609,	1288.8291,	1318.9894,
	8	0.130611000	2.009974000	-0.420819000	1392.7,	1414.7319,	1420.883,
	8	-1.179656000	1.807942000	-0.003711000	1425.1149,	1453.1231,	1488.0129,
	6	-0.008917000	-1.041050000	-0.398521000	1498.8724,	1504.1745,	1511.8583,
	1	0.065059000	-2.140541000	-0.446971000	1520.8378,	1783.0466,	3029.5422,
	1	-0.065983000	-0.691443000	-1.436458000	3057.9691,	3077.7587,	3112.4661,
	6	-2.560405000	-1.109722000	-0.195552000	3140.3766,	3156.7721,	3164.1254,
	1	-2.630441000	-2.204035000	-0.144326000	3173.9367,	3201.8182,	3797.0924
	1	-3.403855000	-0.692419000	0.360735000			
	1	-2.659090000	-0.813137000	-1.243881000			
TS6c	6	-2.961354000	0.095887000	0.227482000	2196.1442i,	47.6271,	92.1293,
	6	-1.492097000	-0.116924000	-0.069571000	112.8221,	120.2646,	137.9844,
	6	-0.586579000	1.079222000	0.180015000	164.7696,	189.0913,	217.2003,
	6	0.816744000	0.937555000	-0.359803000	231.1302,	358.6188,	399.7512,
	6	1.734240000	2.113728000	-0.118178000	464.5901,	565.1425,	607.2227,
	8	-1.076447000	-1.181491000	-0.495507000	629.7388,	792.4528,	844.0116,
	1	-3.092945000	0.631189000	1.171964000	881.4851,	944.9401,	986.5836,
	1	-3.475816000	-0.864866000	0.257979000	993.9089,	1115.2862,	1125.6863,
	1	-3.396668000	0.713615000	-0.565696000	1149.9799,	1171.6967,	1199.6537,
	1	-1.080079000	1.970971000	-0.238365000	1219.8819,	1264.8069,	1331.651,
	1	-0.562368000	1.243865000	1.267254000	1398.7447,	1417.976,	1430.4801,

	1	0.843448000	0.545584000	-1.380415000	1452.6026, 1470.5392, 1485.5192,
	1	1.312262000	-0.054626000	0.272459000	1498.5956, 1508.6918, 1510.3468,
	1	1.380567000	3.001194000	-0.659762000	1529.7803, 1779.7632, 3036.016,
	1	1.772833000	2.365286000	0.946321000	3054.3576, 3078.9595, 3084.932,
	1	2.749980000	1.893766000	-0.455780000	3133.5878, 3143.5893, 3163.651,
	1	0.717633000	-2.151918000	-0.371008000	3173.4252, 3205.6648, 3763.9772
	8	1.663450000	-1.993828000	-0.232495000	
	8	1.633676000	-1.068539000	0.802423000	
TS7c	6	2.713191000	-1.138908000	-0.548334000	2075.8686i, 31.3984 , 38.9281 ,
	6	1.897964000	-0.015487000	0.061272000	65.0233 , 111.2737 , 118.9426 ,
	6	0.551898000	0.257096000	-0.589181000	150.604, 178.0864, 257.0044,
	6	-0.319347000	1.209450000	0.221422000	354.7666, 394.3885, 435.3087 ,
	6	-1.657764000	1.457725000	-0.430755000	469.5907, 539.2349, 603.4914,
	8	2.290078000	0.623703000	1.021166000	628.293, 739.2766, 838.603,
	1	3.729416000	-1.116696000	-0.153244000	886.0045, 928.1822, 979.6342,
	1	2.725498000	-1.061588000	-1.639510000	997.4002, 1104.8578, 1133.1104,
	1	2.243595000	-2.094858000	-0.292303000	1148.5452, 1179.8631, 1198.8977,
	1	0.746186000	0.668955000	-1.590305000	1235.774, 1256.1574, 1314.3418,
	1	0.033948000	-0.695743000	-0.748608000	1350.7362, 1397.8604, 1403.1073,
	1	0.212186000	2.159927000	0.360006000	1423.6218, 1471.7863, 1477.1394,
	1	-0.464261000	0.792078000	1.222502000	1485.9881, 1487.6837, 1498.2915,
	1	-2.350087000	2.074996000	0.145339000	1506.8284, 1779.1323, 3060.3595,
	1	-1.613819000	1.754236000	-1.481457000	3074.3456, 3077.2882, 3113.9629,
	1	-2.214013000	0.313556000	-0.474855000	3123.0896, 3140.9442, 3161.6365,
	1	-2.826609000	-1.174242000	1.388047000	3201.7123, 3205.6133, 3813.1675
	8	-2.098288000	-1.326999000	0.773513000	
	8	-2.609002000	-0.826688000	-0.422449000	
PC1c	6	2.938282000	-0.355328000	-0.201087000	26.9827, 59.2757, 71.2457,
	6	1.475877000	-0.419706000	-0.065171000	107.7178, 121.7004, 137.4319,
	1	3.432694000	0.498339000	-0.646099000	187.226, 209.4791, 221.6296,
	1	3.518137000	-1.195277000	0.160439000	259.2774, 285.0465, 337.7928,
	6	0.658441000	0.756654000	-0.557424000	417.5429, 554.1695, 612.6018,
	8	0.950409000	-1.386008000	0.443690000	733.9919, 748.7283, 764.7996,
	6	-0.128447000	1.386685000	0.602326000	874.5138, 893.0935, 931.8527,
	1	-0.054819000	0.358015000	-1.286572000	933.86, 992.5284, 1084.6749,
	1	1.289393000	1.505463000	-1.046365000	1120.3606, 1139.6312, 1240.1639,
	1	0.573360000	1.790326000	1.342274000	1275.8116, 1324.751, 1336.065,
	1	-0.701656000	0.598394000	1.095354000	1358.856, 1402.3755, 1426.9313,
	1	-2.829979000	-0.451600000	-0.429966000	1482.1629, 1498.8671, 1514.615,
	8	-2.122507000	-1.009261000	-0.767891000	1520.3975, 1527.6298, 1574.9915,
	8	-1.799757000	-1.725073000	0.454616000	2035.9089, 3072.1171, 3082.2199,
	1	-0.830236000	-1.606661000	0.456133000	3092.767, 3148.1518, 3157.5023,
	6	-1.063334000	2.491136000	0.113598000	3166.1587, 3174.5694, 3208.4478,
	1	-1.613469000	2.938707000	0.946161000	3342.246, 3609.744, 3871.3028
	1	-1.788138000	2.083819000	-0.597747000	
	1	-0.505356000	3.286573000	-0.390388000	
PC2c	6	0.764110000	1.668891000	-0.101075000	22.9764, 41.0084, 53.9543,
	6	-0.071175000	0.460985000	-0.208008000	90.6052, 97.3184, 120.7665,

	1	1.825538000	1.587992000	-0.296153000	173.4117,	230.6458,	239.451,
	1	0.327171000	2.619399000	0.178625000	249.8465,	297.1295,	361.2669,
	6	-1.548505000	0.640234000	0.084493000	412.0266,	512.3108,	614.9654,
	8	0.388948000	-0.618038000	-0.516410000	663.7998,	761.0823,	811.7098,
	6	-2.359170000	-0.643156000	-0.038892000	852.8213,	892.1519,	940.2437,
	1	-1.927670000	1.414610000	-0.597239000	943.827,	998.4761,	1085.7955,
	1	-1.633850000	1.066595000	1.093974000	1111.5227,	1150.8612,	1218.7828,
	1	-1.942591000	-1.390707000	0.642655000	1263.2397,	1338.2403,	1344.8704,
	1	-2.232108000	-1.045547000	-1.048230000	1350.4981,	1423.6063,	1433.0472,
	1	3.806774000	-1.117142000	1.087095000	1462.4869,	1488.3598,	1508.0987,
	8	3.293060000	-0.330753000	0.880282000	1522.1089,	1527.3671,	1540.3627,
	8	3.140803000	-0.509529000	-0.548798000	2025.7655,	3057.1885,	3069.8915,
	1	2.180547000	-0.683726000	-0.586568000	3102.9348,	3103.9046,	3143.384,
	6	-3.839926000	-0.414095000	0.261592000	3165.2957,	3165.542,	3206.7525,
	1	-4.408338000	-1.343585000	0.169594000	3342.1396,	3605.747,	3870.8652
	1	-4.271579000	0.315027000	-0.431812000			
	1	-3.978379000	-0.033519000	1.278808000			
PC3c	6	-0.720868000	-1.729414000	-0.304733000	18.0373,	48.9032,	69.5,
	6	0.254275000	-0.683897000	0.190210000	101.5407,	126.1152,	127.8242,
	1	-0.233631000	-2.577978000	-0.786326000	197.4563,	213.4447,	237.2348,
	1	-1.408875000	-1.237143000	-0.996516000	306.6917,	326.3753,	439.369,
	1	-1.311737000	-2.071504000	0.549073000	529.7933,	610.5508,	674.3073,
	6	1.687751000	-0.906735000	-0.027704000	753.5226,	769.3665,	873.1763,
	8	-0.131803000	0.322918000	0.756520000	935.8681,	945.5097,	1016.9489,
	6	2.668963000	0.122040000	0.406960000	1038.0967,	1061.6898,	1107.0391,
	1	2.007482000	-1.786693000	-0.577439000	1153.878,	1228.3621,	1311.8761,
	1	3.649987000	-0.337920000	0.557556000	1320.1167,	1345.0312,	1406.3918,
	1	2.328171000	0.549554000	1.354338000	1413.7474,	1463.0225,	1493.5653,
	1	-3.747547000	0.113063000	-0.869320000	1495.7217,	1511.4401,	1519.7695,
	8	-2.985252000	0.694781000	-0.795565000	1527.9951,	1583.1069,	1999.432,
	8	-2.858561000	0.700770000	0.652582000	3081.3959,	3090.3102,	3096.969,
	1	-1.887258000	0.622106000	0.721985000	3157.2097,	3173.0385,	3183.0741,
	6	2.776512000	1.257964000	-0.632593000	3190.357,	3204.4703,	3236.9895,
	1	1.808100000	1.749135000	-0.746082000	3602.0771,	3876.6919	
	1	3.092100000	0.869304000	-1.604773000			
	1	3.508339000	2.000582000	-0.303632000			
PC4c	6	2.866020000	0.979008000	-0.361959000	26.7751,	34.4322,	69.0739,
	6	1.489258000	0.481725000	0.023805000	89.6995,	92.1414,	101.6966,
	6	1.380091000	-0.951396000	0.343287000	128.1282,	192.7555,	228.1264,
	6	0.065182000	-1.566387000	0.666604000	249.167,	298.9063,	323.4014,
	6	-0.687556000	-1.971790000	-0.619003000	432.4311,	514.2402,	606.8206,
	8	0.533192000	1.226269000	0.059249000	655.5032,	715.7598,	773.8785,
	1	2.836167000	2.058799000	-0.501574000	867.5266,	938.6967,	943.5687,
	1	3.178043000	0.490437000	-1.290725000	983.1421,	1034.6933,	1060.7237,
	1	3.591789000	0.713125000	0.412400000	1107.4331,	1164.8186,	1232.2501,
	1	-3.166557000	-0.067441000	-0.370356000	1314.303,	1335.6112,	1344.0902,
	1	2.268349000	-1.570352000	0.249341000	1394.0086,	1418.1754,	1468.3797,
	1	-0.547550000	-0.847162000	1.215402000	1484.4506,	1494.8204,	1507.739,

	1	0.217359000	-2.448164000	1.296474000	1523.2006,	1530.5672,	1543.8815,
	1	-0.906509000	-1.087815000	-1.220384000	2032.0373,	3078.1559,	3081.8216,
	1	-0.095874000	-2.672829000	-1.214262000	3100.024,	3160.5443,	3166.8531,
	1	-1.633054000	-2.457054000	-0.358997000	3169.7834,	3193.3497,	3217.3196,
	1	-1.245350000	1.190067000	0.429908000	3225.6124,	3685.9553,	3871.7773
	8	-2.183320000	1.118218000	0.679287000			
	8	-2.746720000	0.764441000	-0.608990000			
PC5c	6	2.395164000	-0.619998000	-0.704127000	30.7472,	51.0335,	78.8112,
	6	1.188145000	-0.710795000	0.203289000	87.6459,	90.5446,	119.7641,
	6	-1.332516000	-0.849835000	0.363382000	131.2354,	145.0667,	177.0486,
	8	1.254800000	-0.520446000	1.403362000	202.9251,	263.3791,	351.0083,
	1	2.286587000	0.269728000	-1.332252000	390.0339,	448.591,	510.9282,
	1	2.447769000	-1.490800000	-1.364672000	559.1301,	603.6794,	808.2436,
	1	3.304386000	-0.543650000	-0.106680000	846.6918,	934.183,	943.3188,
	1	-1.109623000	1.248011000	0.351799000	982.3034,	986.8345,	1057.0736,
	1	-1.213619000	-0.991563000	1.432678000	1131.8689,	1171.113,	1196.7103,
	1	0.913554000	2.347072000	0.434964000	1217.8994,	1322.0809,	1368.1366,
	8	0.440683000	2.040035000	-0.347222000	1394.9594,	1416.6936,	1437.0287,
	8	-0.923363000	2.168862000	0.105513000	1456.8345,	1468.6949,	1490.425,
	6	-0.125218000	-1.067406000	-0.485759000	1499.1706,	1500.1734,	1506.0163,
	1	-0.045286000	-2.128952000	-0.786098000	1792.9894,	2992.2906,	3028.7329,
	1	-0.191813000	-0.503199000	-1.424714000	3079.4013,	3099.4849,	3112.4999,
	6	-2.693736000	-0.906431000	-0.250158000	3166.166,	3166.6733,	3201.477,
	1	-2.956567000	-1.935803000	-0.538992000	3237.1213,	3683.6512,	3841.6591
	1	-3.463129000	-0.553556000	0.441049000			
	1	-2.740258000	-0.298112000	-1.160066000			
PC6c	6	-2.445824000	-1.397776000	0.025900000	16.6273,	42.5505,	73.6363,
	6	-0.990434000	-1.006569000	0.096852000	80.0007,	102.617,	124.7561,
	6	-0.665418000	0.339991000	0.727949000	126.7895,	163.1546,	192.3881,
	6	-0.399600000	1.330580000	-0.369575000	218.5943,	240.4207,	348.6504,
	6	-0.863647000	2.744932000	-0.258449000	379.0359,	490.2864,	536.0429,
	8	-0.108943000	-1.713848000	-0.368065000	593.4396,	699.4004,	814.8731,
	1	-2.827829000	-1.552428000	1.040658000	904.5144,	919.3772,	938.9968,
	1	-2.562790000	-2.310395000	-0.558711000	981.995,	1010.0076,	1046.4256,
	1	-3.021160000	-0.580223000	-0.419819000	1130.6752,	1175.1447,	1195.3487,
	1	-1.491886000	0.681102000	1.359575000	1263.0718,	1321.5667,	1339.2637,
	1	0.229927000	0.204525000	1.350743000	1400.0555,	1408.2513,	1440.0376,
	1	0.365062000	1.062862000	-1.091371000	1480.048,	1489.5213,	1496.8554,
	1	2.678434000	0.895058000	0.477673000	1497.1339,	1505.8097,	1541.6544,
	1	-1.920927000	2.793554000	0.026108000	1771.2166,	3025.1676,	3053.5174,
	1	-0.303925000	3.293115000	0.515338000	3076.5042,	3105.3489,	3136.5805,
	1	-0.735809000	3.283488000	-1.200501000	3160.1476,	3166.627,	3206.4448,
	1	1.627425000	-1.056992000	-0.494372000	3236.8609,	3684.2521,	3860.6109
	8	2.472042000	-0.592770000	-0.625895000			
	8	2.656029000	-0.040957000	0.701287000			
PC7c	6	2.298004000	-0.946654000	-0.733121000	29.0583,	49.3041,	68.7367,
	6	1.589850000	0.163347000	0.013790000	95.0503,	128.4492,	129.869,
	6	0.354895000	0.732362000	-0.664827000	153.0148,	163.9386,	176.1086,

	6	-0.559078000	1.473187000	0.310605000	207.0304,	227.879,	353.0903,
	6	-1.906705000	1.767441000	-0.264585000	391.7977,	473.9035,	508.5619,
	8	1.967795000	0.566662000	1.098988000	575.6042,	606.445,	750.4946,
	1	3.270352000	-1.143131000	-0.279980000	834.1168,	916.2501,	931.324,
	1	2.412509000	-0.692486000	-1.791245000	936.2096,	983.8672,	1058.9556,
	1	1.672147000	-1.843426000	-0.673079000	1118.8802,	1140.8462,	1185.0222,
	1	0.694593000	1.405239000	-1.465080000	1203.5243,	1307.9333,	1329.0816,
	1	-0.178342000	-0.087080000	-1.156054000	1341.6472,	1394.2093,	1423.9157,
	1	-0.065703000	2.401991000	0.633169000	1459.2406,	1483.1998,	1486.8008,
	1	-0.657332000	0.874647000	1.222799000	1491.0593,	1495.3863,	1499.5042,
	1	-2.701153000	2.135092000	0.376129000	1783.814,	3046.3411,	3067.2234,
	1	-2.024129000	1.911900000	-1.333608000	3076.7922,	3116.4213,	3143.7258,
	1	-2.242734000	-0.542989000	-0.167633000	3162.9303,	3183.1386,	3201.2643,
	1	-1.459413000	-2.292398000	1.265202000	3294.6561,	3759.8499,	3857.3295
	8	-1.020569000	-1.729477000	0.618322000			
	8	-2.120050000	-1.495367000	-0.292534000			
P1c	6	2.342871000	-0.820562000	-0.000091000	57.1196,	97.0566,	176.0158,
	6	1.186158000	0.107705000	0.000051000	250.6865,	260.6701,	344.5103,
	6	-0.183798000	-0.555880000	0.000131000	398.2314,	499.2593,	602.1402,
	6	-1.336303000	0.439321000	-0.000178000	625.301,	760.2406,	839.1064,
	6	-2.696890000	-0.256399000	0.000026000	894.9253,	938.5491,	973.3513,
	8	1.332431000	1.296166000	0.000071000	1085.4527,	1111.4419,	1147.8102,
	1	3.337385000	-0.392803000	-0.000113000	1194.9023,	1262.3818,	1335.5062,
	1	2.212252000	-1.895911000	-0.000225000	1338.0714,	1418.5825,	1431.9557,
	1	-0.232887000	-1.217972000	-0.875860000	1465.1086,	1474.7287,	1507.5503,
	1	-0.232953000	-1.217449000	0.876518000	1521.9186,	1527.0658,	2119.2762,
	1	-1.239657000	1.089486000	-0.874735000	3056.4065,	3068.6058,	3102.8097,
	1	-1.239662000	1.089984000	0.873975000	3103.7801,	3142.259,	3163.1755,
	1	-2.811808000	-0.891184000	-0.884734000	3164.7941,	3202.1031,	3335.9483
	1	-2.811811000	-0.890632000	0.885183000			
	1	-3.512539000	0.472034000	-0.000201000			
P2c	6	-2.311420000	-0.425303000	-0.325118000	60.2195,	81.8541,	97.1243,
	6	-0.968047000	0.154644000	0.079240000	213.4214,	288.308,	317.1848,
	6	0.134456000	-0.820419000	0.241920000	420.84,	499.4268,	606.8892,
	6	1.494211000	-0.331770000	0.597444000	641.3563,	759.1471,	857.2918,
	6	2.242437000	0.192466000	-0.645408000	937.0773,	973.5396,	1037.4638,
	8	-0.794758000	1.330644000	0.255710000	1064.5144,	1101.6166,	1159.1649,
	1	-2.218838000	-0.914121000	-1.300154000	1219.5422,	1311.7443,	1346.4248,
	1	-3.050751000	0.373184000	-0.375913000	1388.4185,	1412.5412,	1453.1167,
	1	-2.621515000	-1.185256000	0.398567000	1484.7023,	1494.9244,	1496.0722,
	1	-0.042796000	-1.868194000	0.015256000	1518.2648,	1528.2127,	2104.2863,
	1	2.071416000	-1.134158000	1.066869000	3078.8401,	3081.1634,	3093.3343,
	1	1.390283000	0.491366000	1.310717000	3152.6678,	3167.0068,	3168.9279,
	1	2.347603000	-0.593923000	-1.398289000	3188.1106,	3214.7944,	3225.9352
	1	1.691237000	1.027589000	-1.082307000			
	1	3.241606000	0.540651000	-0.368893000			
P3c	6	-2.309928000	-0.757241000	-0.085698000	61.5973,	76.4053,	130.9375,
	6	-1.107411000	0.159395000	0.028141000	142.5395,	181.2584,	346.7502,

	6	0.244158000	-0.537604000	0.145827000	367.8718,	400.3582,	464.5843,
	6	1.414690000	0.351644000	-0.099089000	602.5275,	804.9395,	846.0896,
	6	2.797644000	-0.207888000	-0.048533000	934.8376,	981.9861,	990.1399,
	8	-1.215163000	1.370445000	0.027871000	1047.0699,	1131.3632,	1177.8552,
	1	-2.334379000	-1.184374000	-1.094234000	1195.8962,	1205.0249,	1319.5897,
	1	-3.225423000	-0.190496000	0.086728000	1397.8965,	1419.1807,	1441.2046,
	1	-2.234956000	-1.588061000	0.621979000	1456.948,	1486.7027,	1498.1601,
	1	0.275545000	-0.970649000	1.163623000	1499.5295,	1508.3437,	1799.7057,
	1	0.253133000	-1.410313000	-0.524158000	2986.9851,	3023.1155,	3062.6896,
	1	1.251100000	1.420268000	-0.035293000	3076.8652,	3102.7589,	3160.9298,
	1	3.105389000	-0.432655000	0.984870000	3162.9506,	3202.6358,	3258.4981
	1	2.866563000	-1.147768000	-0.608518000			
	1	3.529413000	0.490656000	-0.461849000			
P4c	6	-2.287397000	-0.753005000	0.023763000	59.3907,	102.419,	109.1526,
	6	-1.066989000	0.147076000	-0.020768000	148.5427,	178.9887,	349.1333,
	6	0.279422000	-0.556873000	-0.087621000	389.9442,	464.149,	474.4876,
	6	1.467207000	0.391355000	0.058929000	601.9788,	730.9111,	840.7326,
	6	2.780012000	-0.317121000	-0.015508000	880.8299,	948.6937,	972.0235,
	8	-1.158279000	1.361089000	0.003194000	1055.7649,	1120.2426,	1140.8532,
	1	-2.211414000	-1.547654000	-0.724123000	1183.0279,	1204.8158,	1314.185,
	1	-3.188728000	-0.161500000	-0.140356000	1325.5169,	1396.901,	1418.7359,
	1	-2.342715000	-1.231204000	1.007799000	1469.2961,	1487.3128,	1488.4395,
	1	0.302706000	-1.337687000	0.684512000	1496.109,	1498.7166,	1779.3878,
	1	0.329973000	-1.087198000	-1.048430000	3033.4674,	3062.0037,	3077.5193,
	1	1.366929000	0.925038000	1.016926000	3106.1784,	3131.0497,	3161.4761,
	1	1.402920000	1.167797000	-0.709572000	3195.5864,	3202.0186,	3308.9946
	1	2.891485000	-1.304176000	0.418863000			
	1	3.681545000	0.219278000	-0.283933000			
iPMK	6	1.911137000	0.604967000	0.238533000	61.1475,	140.9111,	215.4885,
	6	0.733284000	-0.331712000	0.025294000	235.4786,	263.1662,	315.8307,
	6	-0.646874000	0.200481000	0.396999000	353.1597,	434.6275,	559.2944,
	6	-1.723391000	-0.858849000	0.189062000	621.532,	737.2735,	920.7214,
	8	0.890598000	-1.445063000	-0.443643000	938.5173,	976.3796,	982.1957,
	1	2.824486000	0.014892000	0.326643000	1005.6896,	1130.3659,	1161.8604,
	1	1.774978000	1.233761000	1.122449000	1184.3764,	1234.0217,	1330.8853,
	1	2.006189000	1.263327000	-0.631545000	1376.1878,	1401.7802,	1418.3784,
	1	-2.697636000	-0.477792000	0.509751000	1435.3451,	1487.9005,	1497.4425,
	1	-1.495404000	-1.766720000	0.751922000	1506.2812,	1509.5829,	1525.3392,
	1	-1.784314000	-1.132894000	-0.867716000	1529.462,	1770.9239,	3059.6076,
	6	-0.948995000	1.478638000	-0.401008000	3069.8468,	3079.1009,	3080.3519,
	1	-0.927878000	1.267070000	-1.475679000	3157.0572,	3164.4132,	3169.0685,
	1	-0.230876000	2.276204000	-0.192177000	3169.8843,	3179.7098,	3198.6116
	1	-1.947103000	1.848922000	-0.149413000			
	1	-0.598194000	0.472588000	1.461627000			
RC1d	6	-0.205039000	2.015431000	-0.417718000	16.7434,	38.7701,	69.4568,
	6	-0.315572000	0.653981000	0.223776000	87.958,	138.2875,	171.6882,
	1	-1.178581000	2.366498000	-0.770007000	213.4885,	238.4701,	251.1561,
	1	0.230245000	2.728073000	0.283878000	259.4741,	301.3937,	335.2344,

	6	-1.237584000	-0.352993000	-0.439212000	437.2073,	496.0438,	599.7488,
	8	0.284030000	0.378427000	1.257841000	605.4783,	759.6875,	918.9262,
	6	-2.654217000	-0.121990000	0.117172000	943.8473,	982.5848,	987.2297,
	1	-1.246553000	-0.141679000	-1.515675000	1024.5965,	1130.7265,	1151.9117,
	1	-3.358550000	-0.809577000	-0.359756000	1189.8217,	1236.288,	1321.3217,
	1	-3.004092000	0.899829000	-0.058505000	1334.424,	1384.2879,	1405.8502,
	1	-2.663283000	-0.310820000	1.195285000	1421.4932,	1431.3297,	1482.2237,
	1	0.452261000	1.916082000	-1.287733000	1497.566,	1508.3814,	1509.9139,
	8	2.281532000	-0.212159000	-0.847070000	1524.1071,	1533.9795,	1534.9991,
	8	2.679153000	-0.472532000	0.363610000	1757.2548,	3070.7618,	3082.121,
	1	1.917385000	-0.220825000	0.930359000	3083.0305,	3090.5874,	3162.9129,
	6	-0.774765000	-1.785854000	-0.190240000	3165.7171,	3171.0012,	3173.6894,
	1	-0.742278000	-1.986249000	0.883656000	3185.0608,	3202.8694,	3516.0888
	1	0.224284000	-1.949949000	-0.600215000			
	1	-1.465497000	-2.492726000	-0.659003000			
RC2d	6	-0.261179000	1.538547000	-0.319265000	26.7689,	37.695,	67.1154,
	6	0.336750000	0.158517000	-0.159542000	91.6205,	130.3512,	161.7165,
	1	-0.283420000	2.019807000	0.665038000	215.8867,	219.1107,	240.3883,
	1	0.333400000	2.162076000	-0.989983000	273.9701,	328.3187,	353.473,
	6	1.832181000	0.007046000	-0.365795000	445.4945,	571.6369,	632.057,
	8	-0.352795000	-0.802575000	0.164989000	699.8064,	749.9731,	922.6576,
	6	2.269780000	-1.451933000	-0.304729000	940.2224,	982.4555,	999.7159,
	1	2.050163000	0.420660000	-1.360721000	1016.7904,	1134.0481,	1163.5886,
	1	3.342947000	-1.530159000	-0.500989000	1187.9574,	1240.7245,	1323.6726,
	1	1.732887000	-2.056518000	-1.039377000	1327.259,	1387.5758,	1411.6856,
	1	2.063287000	-1.869091000	0.684374000	1421.3522,	1437.1615,	1488.3306,
	1	-1.288950000	1.453319000	-0.675914000	1502.9386,	1509.5448,	1512.0792,
	8	-3.420528000	0.275472000	-0.299063000	1525.7803,	1530.4956,	1594.7329,
	8	-3.060458000	-0.695599000	0.492007000	1752.3809,	3067.7811,	3073.5228,
	1	-2.081630000	-0.749867000	0.396386000	3079.5537,	3082.763,	3162.1439,
	6	2.572869000	0.866519000	0.673700000	3167.6591,	3172.9435,	3174.1372,
	1	3.652626000	0.765328000	0.533886000	3179.9205,	3203.659,	3454.1255
	1	2.328547000	0.527495000	1.686013000			
	1	2.317983000	1.926390000	0.591601000			
RC3d	6	2.089745000	1.433355000	0.080435000	37.4237,	45.1247,	74.676,
	6	0.723946000	0.805454000	-0.064075000	85.0609,	144.4439,	177.2361,
	1	2.660962000	1.290323000	-0.842050000	222.857,	225.0217,	242.6521,
	1	2.649615000	0.951745000	0.887775000	281.0152,	293.148,	342.5694,
	1	1.977406000	2.498646000	0.282122000	500.3001,	537.8437,	598.4396,
	6	0.614607000	-0.706261000	-0.139801000	723.1042,	750.2514,	925.301,
	8	-0.280989000	1.510341000	-0.069504000	949.8467,	972.1248,	986.4743,
	6	0.435682000	-1.233298000	1.294839000	1031.5304,	1114.0012,	1158.7331,
	1	-0.307732000	-0.918598000	-0.689064000	1205.904,	1295.8364,	1317.4493,
	1	0.309585000	-2.319517000	1.274731000	1350.2396,	1389.6663,	1404.7626,
	1	-0.450910000	-0.794522000	1.760195000	1414.1805,	1437.7699,	1479.288,
	1	1.310533000	-1.003099000	1.912751000	1495.3256,	1506.4028,	1513.9016,
	8	-2.746611000	-0.657244000	-0.515894000	1527.2914,	1530.2747,	1593.7064,
	8	-2.786148000	0.469109000	0.141095000	1749.5853,	3069.8519,	3071.8802,

	1	-1.889975000	0.864072000	0.024269000	3083.1082, 3122.0982, 3159.2179,
	6	1.797417000	-1.377120000	-0.839399000	3162.136, 3165.3566, 3167.2056,
	1	2.728066000	-1.234917000	-0.281351000	3173.929, 3207.1031, 3430.4998
	1	1.939584000	-0.991555000	-1.853684000	
	1	1.614458000	-2.453008000	-0.913267000	
RC4d (identified as RC3d in PES)	6	-2.089479000	-1.433568000	0.079859000	37.5388, 44.9804, 74.7227,
	6	-0.723688000	-0.805479000	-0.063944000	85.1627, 144.543, 177.2585,
	1	-2.660231000	-1.290631000	-0.842928000	222.8729, 225.0237, 242.6558,
	1	-2.649838000	-0.952009000	0.886890000	281.0171, 293.1603, 342.5686,
	1	-1.977109000	-2.498841000	0.281625000	500.3062, 537.8437, 598.4559,
	6	-0.614592000	0.706235000	-0.139560000	723.3702, 750.27, 925.2989,
	8	0.281357000	-1.510246000	-0.068890000	949.8326, 972.1265, 986.4713,
	6	-0.436307000	1.233240000	1.295165000	1031.5258, 1114.0073, 1158.7382,
	1	0.307876000	0.918680000	-0.688509000	1205.8962, 1295.8653, 1317.4854,
	1	-0.310414000	2.319486000	1.275153000	1350.2498, 1389.6544, 1404.7614,
	1	0.450192000	0.794604000	1.760831000	1414.1754, 1437.7669, 1479.2846,
	1	-1.311339000	1.002850000	1.912750000	1495.3266, 1506.4016, 1513.9018,
	8	2.745888000	0.657362000	-0.516325000	1527.2929, 1530.2731, 1593.7266,
	8	2.786468000	-0.468712000	0.141060000	1749.5033, 3069.8449, 3071.8763,
	1	1.890377000	-0.864275000	0.025269000	3083.1102, 3122.3379, 3159.2108,
	6	-1.797234000	1.376926000	-0.839609000	3162.1292, 3165.3662, 3167.2121,
	1	-2.728082000	1.234640000	-0.281917000	3173.9196, 3207.1015, 3429.9099
	1	-1.938969000	0.991307000	-1.853936000	
	1	-1.614367000	2.452832000	-0.913454000	
RC5d (identified as RC2d in PES)	6	0.260724000	1.538861000	-0.318984000	26.7945, 37.7479, 67.1284, 91.61,
	6	-0.336839000	0.158655000	-0.159438000	130.3311, 161.698, 215.8275,
	6	-1.832211000	0.006810000	-0.365828000	219.1197, 240.3863, 273.9883,
	6	-2.269469000	-1.452257000	-0.304509000	328.3155, 353.4869, 445.485,
	8	0.352923000	-0.802278000	0.165093000	571.6049, 632.056, 699.7565,
	1	-0.333714000	2.162110000	-0.990094000	749.9691, 922.6598, 940.2221,
	1	1.288725000	1.453986000	-0.675029000	982.4519, 999.6992, 1016.7713,
	1	0.282200000	2.020234000	0.665280000	1134.0486, 1163.6047, 1187.9616,
	1	-2.050149000	0.420143000	-1.360883000	1240.728, 1323.6776, 1327.262,
	1	-1.732309000	-2.056886000	-1.038924000	1387.5634, 1411.688, 1421.3549,
	1	-3.342583000	-1.530784000	-0.500941000	1437.1651, 1488.3231, 1502.9364,
	1	-2.063057000	-1.869142000	0.684725000	1509.5488, 1512.0722, 1525.7834,
	8	3.420593000	0.276242000	-0.298389000	1530.4959, 1594.7004, 1752.3965,
	8	3.060955000	-0.696293000	0.491069000	3067.7587, 3073.5207, 3079.5625,
	1	2.082062000	-0.750336000	0.395919000	3082.7634, 3162.1409, 3167.6573,
	6	-2.573261000	0.866355000	0.673351000	3172.9476, 3174.132, 3179.926,
	1	-2.328922000	0.527721000	1.685790000	3203.6905, 3454.1387
	1	-3.652974000	0.764769000	0.533475000	
	1	-2.318717000	1.926283000	0.590948000	
RC6d	6	-2.016352000	-1.707384000	0.272413000	31.4587, 54.4204, 79.4921,
	6	-0.868122000	-0.734361000	0.103162000	89.8263, 131.679, 141.4505,
	6	-1.145108000	0.730593000	0.392150000	212.4851, 220.9076, 262.7825,
	6	0.107351000	1.589867000	0.266113000	275.8802, 323.5944, 357.1709,
	8	0.220319000	-1.137845000	-0.284593000	444.1327, 562.8874, 617.3966,

	1	-2.694210000	-1.399518000	1.071868000	642.2374,	745.8425,	923.6544,
	1	-1.616861000	-2.703167000	0.468550000	939.9571,	981.6024,	991.6819,
	1	-2.587439000	-1.742028000	-0.661589000	1011.0971,	1134.4924,	1162.5232,
	1	-1.517289000	0.770338000	1.426069000	1186.8377,	1238.7264,	1303.2918,
	1	0.905137000	1.237445000	0.922548000	1326.1745,	1383.3319,	1407.8958,
	1	-0.125434000	2.626589000	0.524928000	1421.6186,	1441.4328,	1485.8437,
	1	0.483030000	1.570612000	-0.761085000	1498.1116,	1512.1555,	1515.2837,
	1	1.879073000	-0.541724000	-0.519247000	1528.2106,	1535.5685,	1573.1375,
	8	2.821105000	-0.299020000	-0.643094000	1763.1849,	3065.0018,	3073.1985,
	8	3.217288000	0.117557000	0.529528000	3082.7131,	3082.9382,	3161.541,
	6	-2.270411000	1.228295000	-0.531699000	3169.334,	3169.5428,	3173.6922,
	1	-1.969561000	1.130907000	-1.580341000	3189.3361,	3204.3194,	3548.7235
	1	-2.467092000	2.285503000	-0.333920000			
	1	-3.203199000	0.677456000	-0.385348000			
TS1d	6	-0.623120000	-1.586967000	-0.111405000	1894.433i,	45.9889,	50.481,
	6	0.168907000	-0.432862000	0.437808000	102.2374,	136.8464,	205.059,
	1	-0.293335000	-2.034173000	-1.047560000	214.2097,	246.8127,	264.277,
	1	-0.982148000	-2.279039000	0.648194000	301.9026,	344.983,	415.0453,
	6	1.240005000	0.143049000	-0.470492000	436.8472,	547.663,	606.2925,
	8	-0.058764000	0.002908000	1.541758000	646.3428,	741.0899,	755.0815,
	6	2.486263000	-0.749656000	-0.338478000	921.1895,	944.2376,	980.7773,
	1	0.869923000	0.076777000	-1.501462000	993.8549,	1029.1687,	1115.0564,
	1	3.274846000	-0.389999000	-1.005345000	1126.9555,	1151.1104,	1185.2162,
	1	2.273414000	-1.792522000	-0.593777000	1189.2362,	1235.6852,	1328.8613,
	1	2.860164000	-0.714563000	0.689580000	1396.7024,	1418.1247,	1431.2496,
	1	-1.721024000	-0.908057000	-0.409032000	1436.1752,	1474.1466,	1482.4199,
	8	-2.623294000	-0.188163000	-0.441357000	1506.2713,	1507.3671,	1522.6411,
	8	-2.070521000	1.083383000	-0.320317000	1531.2185,	2205.6696,	3070.3298,
	1	-2.000861000	1.189254000	0.640109000	3082.0966,	3087.7105,	3151.4744,
	6	1.542751000	1.593732000	-0.115170000	3161.5568,	3167.6233,	3173.1585,
	1	1.870561000	1.664324000	0.924493000	3184.1929,	3262.4082,	3772.1642
	1	0.649964000	2.212593000	-0.234508000			
	1	2.330286000	1.986599000	-0.764936000			
TS2d	6	0.623537000	1.375530000	0.069750000	1896.8212i,	27.0049,	54.2349,
	6	-0.187892000	0.158924000	-0.263408000	142.1266,	159.0619,	207.8574,
	1	1.189887000	1.782323000	-0.766878000	212.9433,	237.1782,	251.3339,
	1	0.195954000	2.101503000	0.757917000	307.033,	340.587,	433.1538,
	6	-1.524988000	0.011757000	0.438700000	550.4338,	586.3769,	600.402,
	8	0.224422000	-0.671861000	-1.052126000	656.088,	728.6469,	759.137,
	6	-2.007853000	-1.433809000	0.421256000	911.6765,	932.7125,	951.4467,
	1	-1.389448000	0.354003000	1.473443000	988.6222,	1003.9597,	1116.9094,
	1	-2.970808000	-1.516691000	0.933608000	1129.3974,	1152.7411,	1190.4524,
	1	-1.289250000	-2.092713000	0.915373000	1236.5435,	1251.5085,	1327.7194,
	1	-2.123457000	-1.778151000	-0.608994000	1395.3157,	1419.0432,	1434.8234,
	1	1.619928000	0.759031000	0.690953000	1470.1295,	1492.7021,	1503.9426,
	8	2.398954000	-0.062963000	0.906004000	1507.8965,	1522.3055,	1528.6397,
	8	2.951151000	-0.350931000	-0.333463000	1531.9376,	2046.0316,	3071.2426,
	1	2.245528000	-0.875824000	-0.749713000	3078.1493,	3082.2146,	3151.7567,

TS3d	6	-2.524806000	0.954786000	-0.253621000	3163.4021,	3167.5405,	3172.9486,
	1	-3.494747000	0.902791000	0.248775000	3182.513,	3263.4246,	3696.0928
	1	-2.660457000	0.651152000	-1.296509000			
	1	-2.187333000	1.995493000	-0.237362000			
	6	-0.051154000	2.047865000	0.593780000	1945.77i,	54.9806,	76.4372,
	6	-0.154906000	0.919371000	-0.407647000	109.2197,	132.6221,	175.5067,
	1	0.553624000	1.711066000	1.441669000	185.441,	221.7411,	229.9998,
	1	-1.037145000	2.332696000	0.971739000	279.5295,	293.4332,	359.1356,
	1	0.430834000	2.899294000	0.113086000	434.1189,	515.2067,	552.0295,
	6	-0.808367000	-0.374329000	0.042781000	571.2814,	634.4055,	736.0283,
	8	0.328438000	1.003199000	-1.517324000	939.5401,	956.7408,	987.1477,
	6	-1.370584000	-1.194840000	-1.098269000	1011.5547,	1031.1986,	1133.1889,
	1	0.268102000	-0.962902000	0.338160000	1155.4653,	1191.4827,	1205.7629,
	1	-1.580543000	-2.216808000	-0.770067000	1281.7178,	1314.9263,	1396.2688,
	1	-0.670456000	-1.216782000	-1.933932000	1411.69,	1427.3492,	1434.0614,
	1	-2.309560000	-0.749585000	-1.451927000	1473.9015,	1481.7855,	1496.2888,
TS4d	8	1.384627000	-1.456863000	0.429707000	1499.5391,	1503.5434,	1518.8411,
	8	2.261106000	-0.390677000	0.388225000	1525.1788,	2080.2516,	3055.4451,
	1	2.397641000	-0.262311000	-0.561568000	3062.7423,	3082.0916,	3141.9658,
	6	-1.650546000	-0.351565000	1.300918000	3147.7754,	3171.0451,	3177.9311,
	1	-2.586492000	0.196364000	1.126902000	3197.6923,	3207.3254,	3777.5392
	1	-1.130755000	0.116788000	2.139658000			
	1	-1.915273000	-1.372096000	1.592047000			
	6	-1.667183000	1.523351000	0.420821000	2016.1018i,	48.5724,	106.1083,
	6	-0.643094000	0.751825000	-0.383248000	132.5281,	156.427,	161.1474,
	1	-1.393881000	1.488531000	1.480493000	193.9695,	214.2265,	239.1889,
	1	-2.661349000	1.079138000	0.317405000	276.6488,	313.6732,	363.2274,
	1	-1.678695000	2.557823000	0.077265000	434.1134,	499.738,	528.8459,
	6	-0.437977000	-0.710827000	-0.063068000	554.6207,	638.0577,	723.163,
	8	0.065750000	1.304297000	-1.207744000	937.096,	966.93,	987.7545,
	6	0.172821000	-1.502266000	-1.197346000	1008.7463,	1018.5779,	1107.0237,
	1	0.539779000	-0.486477000	0.720983000	1164.7082,	1191.6661,	1244.0091,
TS5d	1	0.435099000	-2.509624000	-0.863505000	1272.9457,	1337.593,	1398.268,
	1	1.065612000	-1.006013000	-1.579425000	1413.0491,	1430.1884,	1459.9494,
	1	-0.546247000	-1.584669000	-2.022852000	1479.6154,	1492.1916,	1500.205,
	8	1.510508000	0.033157000	1.247985000	1500.9352,	1514.5335,	1518.0862,
	8	2.417885000	0.223697000	0.230190000	1534.1038,	1933.3434,	3055.0378,
	1	2.105767000	1.041323000	-0.189212000	3062.4689,	3080.2135,	3141.9389,
	6	-1.504254000	-1.428206000	0.737737000	3151.2298,	3166.8311,	3176.6008,
	1	-2.401204000	-1.587115000	0.123838000	3197.228,	3206.4828,	3738.8642
	1	-1.799741000	-0.874519000	1.631980000			
	1	-1.140170000	-2.410876000	1.050210000			
	6	0.927307000	-1.935318000	-0.575422000	2087.9218i,	70.1302,	73.2823,
	6	0.630671000	-0.730661000	0.289066000	95.9692,	122.9301,	154.5151,
	6	0.745342000	0.632352000	-0.389104000	195.5128,	228.6201,	253.548,
	6	-0.169927000	1.643845000	0.254377000	283.3609,	346.6696,	422.4506,
	8	0.340565000	-0.827042000	1.469295000	458.3798,	540.9487,	595.7541,
	1	1.816678000	-1.769797000	-1.190136000	616.0224,	641.7362,	753.2294,

	1	0.077718000	-2.078525000	-1.250882000	928.7888,	968.1349,	976.8834,
	1	1.056930000	-2.820638000	0.048475000	1011.9813,	1031.6661,	1125.5177,
	1	0.488694000	0.516537000	-1.448858000	1143.0575,	1163.8132,	1181.4518,
	1	-1.360773000	1.215042000	0.051187000	1203.8602,	1233.3374,	1321.9104,
	1	-0.165431000	2.626360000	-0.220992000	1384.9387,	1408.8426,	1415.8997,
	1	-0.087302000	1.682716000	1.340879000	1418.8105,	1466.2017,	1487.8,
	8	-2.413336000	0.699409000	-0.178183000	1498.0638,	1508.9289,	1515.4851,
	8	-2.114674000	-0.644522000	-0.394835000	1520.8056,	1778.5399,	3071.0921,
	1	-2.166799000	-1.014193000	0.496792000	3080.2639,	3097.662,	3127.9018,
	6	2.216682000	1.090037000	-0.284022000	3162.6708,	3168.5124,	3171.1973,
	1	2.495590000	1.201486000	0.767894000	3200.7769,	3226.8404,	3797.9081
	1	2.351664000	2.052215000	-0.785666000			
	1	2.892138000	0.364513000	-0.748285000			
TS6d	6	-1.913734000	-1.608261000	0.428022000	2185.7273j,	49.3373,	64.8061,
	6	-0.769220000	-0.742527000	-0.061777000	135.7501,	148.1899,	171.4696,
	6	-0.820610000	0.736167000	0.308595000	177.4372,	224.0758,	263.0953,
	6	0.403363000	1.487469000	-0.153521000	303.1381,	326.8263,	433.9848,
	8	0.119839000	-1.217219000	-0.749899000	542.4951,	549.8785,	592.1439,
	1	-2.300554000	-1.264398000	1.390360000	627.8931,	675.2097,	744.0993,
	1	-1.572356000	-2.641711000	0.500575000	927.0566,	959.3796,	974.4939,
	1	-2.729384000	-1.564398000	-0.301620000	989.1516,	1009.3559,	1116.7964,
	1	-0.886123000	0.781136000	1.404909000	1137.5334,	1158.0586,	1165.9978,
	1	1.420639000	0.914080000	0.415341000	1227.3882,	1259.1404,	1313.8956,
	1	0.440634000	2.529275000	0.167987000	1386.3063,	1408.2936,	1418.6786,
	1	0.653256000	1.348960000	-1.206502000	1468.085,	1473.6237,	1486.1648,
	1	2.145664000	-0.989013000	-0.606977000	1498.0987,	1514.8322,	1521.442,
	8	2.817847000	-0.349322000	-0.328672000	1522.1256,	1771.2002,	3069.5397,
	8	2.233713000	0.178198000	0.819341000	3074.2107,	3081.8146,	3127.4519,
	6	-2.110142000	1.362800000	-0.264679000	3166.2389,	3168.2718,	3172.397,
	1	-2.120406000	1.273951000	-1.355684000	3202.352,	3225.3683,	3765.3457
	1	-2.153421000	2.424521000	-0.007991000			
	1	-3.007075000	0.880443000	0.133605000			
PC1d	6	0.297403000	1.425094000	-0.556812000	24.4278,	36.3725,	54.04,
	6	-0.348031000	0.201066000	-0.057793000	100.2192,	122.5112,	190.4651,
	1	-0.244017000	2.117573000	-1.189031000	211.4808,	233.3641,	240.4117,
	1	1.328890000	1.617165000	-0.290848000	258.6679,	303.5601,	328.2471,
	6	-1.812525000	0.006907000	-0.414777000	343.4625,	452.2683,	609.0928,
	8	0.241585000	-0.600292000	0.638366000	630.2209,	754.0593,	792.1246,
	6	-2.637694000	0.871230000	0.555522000	819.0535,	928.2549,	940.1874,
	1	-1.966270000	0.386624000	-1.432899000	945.0562,	985.6836,	1003.456,
	1	-3.703096000	0.765385000	0.332908000	1117.6392,	1154.6151,	1199.379,
	1	-2.376741000	1.931517000	0.485017000	1246.2128,	1333.5535,	1350.6826,
	1	-2.464040000	0.539569000	1.583834000	1400.0418,	1422.597,	1434.5949,
	1	3.833144000	-0.978537000	-0.534237000	1487.0545,	1504.3336,	1507.8308,
	8	3.190108000	-0.270968000	-0.638888000	1522.1645,	1530.127,	1542.7668,
	8	2.916904000	0.016977000	0.753937000	2017.988,	3071.9657,	3082.5387,
	1	1.995972000	-0.305305000	0.805998000	3085.7094,	3164.9064,	3169.5165,
	6	-2.210447000	-1.462576000	-0.334865000	3172.2479,	3187.1661,	3207.1006,

PC2d	1	-2.039027000	-1.841063000	0.674907000	3341.7015, 3597.0973, 3870.5928		
	1	-1.617208000	-2.068868000	-1.024328000			
	1	-3.268622000	-1.580120000	-0.586288000			
	6	-0.414293000	2.047112000	0.243475000	45.9786,	72.4061,	74.5274,
	6	-0.347241000	0.690726000	-0.324020000	94.9004,	172.6785,	208.1741,
	1	0.072284000	2.849826000	-0.296148000	223.698,	231.9979,	245.5827,
	1	-0.900101000	2.244056000	1.190761000	256.1877,	291.5516,	311.7517,
	6	-1.105576000	-0.395334000	0.418862000	354.3138,	439.459,	584.4389,
	8	0.250732000	0.480123000	-1.364373000	602.5086,	645.8691,	740.4678,
	6	-0.679358000	-1.787110000	-0.033166000	776.4363,	928.2383,	936.1921,
	1	-0.891877000	-0.265930000	1.487164000	945.2044,	982.4476,	997.1797,
	1	-1.256295000	-2.546513000	0.502989000	1113.2684,	1155.2299,	1196.9733,
	1	0.382279000	-1.954160000	0.155733000	1243.9058,	1324.406,	1340.7626,
	1	-0.856977000	-1.901845000	-1.105505000	1396.9631,	1421.1402,	1436.8621,
	1	2.740714000	0.686297000	1.074904000	1479.4169,	1505.7554,	1509.9062,
	8	2.053260000	0.024203000	0.946474000	1514.375,	1525.1366,	1536.2701,
	8	2.541715000	-0.604399000	-0.261096000	1976.6982,	3070.8368,	3084.7255,
	1	1.840090000	-0.324703000	-0.876213000	3091.103,	3162.5974,	3166.7784,
	6	-2.609210000	-0.162380000	0.183917000	3173.3107,	3194.8824,	3205.4584,
	1	-3.187715000	-0.927445000	0.709254000	3337.1882,	3669.9473,	3856.2853
PC3d	1	-2.835213000	-0.235573000	-0.884730000			
	1	-2.938779000	0.818489000	0.539333000			
	6	-0.245014000	1.448450000	0.735180000	17.4368,	56.1738,	61.5881,
	6	0.293161000	0.046820000	0.524834000	72.334,	84.229,	118.1352,
	1	-0.256966000	1.995808000	-0.210864000	153.2175,	205.0531,	212.6524,
	1	0.394857000	1.992381000	1.436847000	236.8002,	293.4624,	301.0402,
	1	-1.254847000	1.377715000	1.135383000	367.2616,	452.3127,	566.3209,
	6	1.639053000	-0.098795000	-0.045937000	586.9373,	704.9478,	741.9593,
	8	-0.362012000	-0.936057000	0.829375000	933.3805,	942.526,	956.9405,
	6	2.167462000	-1.472770000	-0.277329000	985.3537,	1007.352,	1016.444,
	1	-2.973448000	0.974037000	-1.057830000	1067.9766,	1180.5746,	1314.5928,
	1	2.405640000	-1.611298000	-1.339701000	1326.2241,	1377.1921,	1408.5799,
	1	1.438943000	-2.220983000	0.032286000	1416.1712,	1429.6199,	1480.8269,
	1	3.101778000	-1.618821000	0.279383000	1486.1658,	1500.3421,	1504.4815,
	8	-2.513012000	0.132505000	-1.126964000	1513.3183,	1519.3499,	1564.5754,
	8	-2.960512000	-0.467042000	0.118533000	1943.7652,	3045.461,	3053.9833,
	1	-2.090314000	-0.735783000	0.471102000	3086.5327,	3117.3211,	3127.2145,
	6	2.457875000	1.064661000	-0.502008000	3173.0168,	3187.6259,	3207.6163,
	1	3.521606000	0.867048000	-0.335877000	3221.1924,	3607.8904,	3873.9194
	1	2.194173000	1.998342000	-0.003154000			
PC4d	1	2.327658000	1.216108000	-1.583567000			
	6	-1.374221000	-1.847809000	-0.358017000	20.0236,	51.2674,	66.7102,
	6	-0.573917000	-0.785250000	0.366120000	73.0929,	101.9226,	110.5222,
	1	-1.146969000	-1.793093000	-1.428087000	159.0865,	173.5997,	221.9002,
	1	-2.450298000	-1.701245000	-0.233217000	256.4681,	285.4083,	289.2549,
	1	-1.077012000	-2.823696000	0.023791000	369.7912,	452.345,	556.4994,
	6	-0.951060000	0.618206000	0.160457000	580.6398,	666.0497,	708.235,
	8	0.360092000	-1.099161000	1.089518000	933.6499,	938.5704,	952.3828,

	6	-0.204403000	1.677278000	0.896387000	997.2565,	1003.7854,	1016.8737,
	1	2.065655000	1.210268000	-1.158183000	1067.8887,	1174.7881,	1314.1791,
	1	0.080734000	2.484871000	0.212474000	1331.1797,	1373.8606,	1411.7506,
	1	0.685075000	1.268893000	1.373302000	1416.9512,	1425.4502,	1479.1674,
	1	-0.844729000	2.126113000	1.668212000	1489.1637,	1499.0133,	1501.9852,
	8	1.896669000	0.263140000	-1.166073000	1512.2822,	1517.014,	1540.9363,
	8	2.671340000	-0.117027000	-0.000516000	1923.7631,	3043.3924,	3052.0869,
	1	1.956778000	-0.523700000	0.523137000	3081.844,	3118.516,	3131.9245,
	6	-2.124666000	1.008092000	-0.679836000	3167.9206,	3177.0014,	3212.0735,
	1	-3.056503000	0.953221000	-0.097934000	3214.7858,	3650.3382,	3868.9453
	1	-2.246828000	0.359942000	-1.550938000			
	1	-2.021111000	2.039712000	-1.026647000			
PC5d	6	-0.637341000	1.970689000	-0.550828000	31.2255,	56.2074,	86.2942,
	6	-0.582609000	0.713539000	0.286536000	91.2236,	113.4507,	115.0493,
	6	-0.997556000	-0.580279000	-0.413178000	165.238,	223.0246,	241.0372,
	6	-0.290403000	-1.768004000	0.149056000	246.3501,	283.4967,	304.3672,
	8	-0.255620000	0.721086000	1.460293000	332.5301,	431.0456,	512.7457,
	1	-1.550054000	2.004529000	-1.152456000	597.1402,	598.6656,	654.8507,
	1	0.216194000	1.951220000	-1.236236000	746.7148,	922.3318,	942.5247,
	1	-0.573504000	2.850287000	0.091177000	967.5363,	976.7562,	1020.3245,
	1	-0.788768000	-0.483313000	-1.485831000	1070.1714,	1120.242,	1167.7429,
	1	1.907942000	-1.316523000	-0.249193000	1210.0571,	1309.0472,	1370.9208,
	1	-0.343547000	-2.716060000	-0.375265000	1384.022,	1406.2624,	1416.3453,
	1	-0.033341000	-1.766764000	1.201858000	1452.7522,	1472.61,	1487.8111,
	8	2.737982000	-0.830086000	-0.146489000	1499.6934,	1514.8159,	1518.3772,
	8	2.258783000	0.517638000	-0.338800000	1783.9629,	3072.599,	3079.9824,
	1	2.194145000	0.811578000	0.577798000	3088.4699,	3164.5254,	3169.1187,
	6	-2.531819000	-0.722827000	-0.237687000	3176.7496,	3190.3843,	3200.3395,
	1	-2.772393000	-0.807233000	0.825519000	3312.1382,	3762.7827,	3836.8582
	1	-2.889227000	-1.619417000	-0.750741000			
	1	-3.058237000	0.143890000	-0.650056000			
PC6d	6	-0.364296000	1.994357000	-0.529397000	45.0266,	52.5334,	97.6059,
	6	-0.396001000	0.692018000	0.231581000	121.3623,	146.3762,	152.9392,
	6	-1.158221000	-0.460733000	-0.415107000	193.2439,	224.0836,	241.7163,
	6	-0.546458000	-1.784913000	-0.096526000	249.6484,	273.766,	291.7036,
	8	0.123665000	0.562232000	1.329354000	326.5398,	427.8307,	535.0706,
	1	0.364035000	1.881433000	-1.339002000	579.92,	603.3518,	614.9802,
	1	-0.052004000	2.805554000	0.129277000	750.6336,	921.9001,	940.799,
	1	-1.338219000	2.214602000	-0.975634000	967.261,	980.8205,	1023.3105,
	1	-1.179823000	-0.302377000	-1.500903000	1073.5146,	1118.7875,	1167.3025,
	1	1.698595000	-1.117001000	-0.986585000	1212.2395,	1310.3818,	1374.8121,
	1	-0.877581000	-2.667778000	-0.631099000	1384.4799,	1406.3643,	1418.6265,
	1	-0.016309000	-1.906858000	0.840006000	1473.4371,	1475.1325,	1485.2359,
	1	2.003157000	0.057913000	0.977741000	1499.0808,	1514.706,	1518.254,
	8	2.674941000	-0.362792000	0.421089000	1775.7975,	3072.084,	3079.8494,
	8	2.052604000	-0.225834000	-0.873139000	3082.982,	3163.8405,	3169.6777,
	6	-2.617197000	-0.382687000	0.103969000	3178.4354,	3197.3783,	3202.6191,
	1	-2.626493000	-0.525219000	1.187752000	3319.1604,	3767.3857,	3813.0945

P1d	1	-3.223979000	-1.165160000	-0.358914000			
	1	-3.068023000	0.587781000	-0.128190000			
	6	-1.918406000	0.607776000	-0.421378000	51.5163,	203.9754,	222.0841,
	6	-0.788079000	-0.254798000	-0.003479000	243.2242,	277.2502,	302.1926,
	1	-2.916221000	0.320768000	-0.114056000	340.1433,	437.6429,	576.6402,
	1	-1.769947000	1.495228000	-1.024334000	603.4357,	738.9205,	786.4346,
	6	0.602039000	0.228024000	-0.406952000	925.5531,	942.9289,	964.7423,
	8	-0.965446000	-1.252477000	0.636423000	995.6104,	1115.1451,	1154.3373,
	6	1.610939000	-0.913206000	-0.359987000	1186.4601,	1231.8647,	1332.5822,
	1	0.537201000	0.635211000	-1.424584000	1394.0198,	1419.0433,	1434.1952,
	1	2.605668000	-0.552201000	-0.638184000	1473.4038,	1503.868,	1507.4834,
	1	1.325851000	-1.718199000	-1.042154000	1522.3397,	1528.8988,	2104.8016,
	1	1.651550000	-1.331942000	0.647812000	3070.6309,	3078.7969,	3082.2939,
	6	0.992787000	1.369203000	0.547483000	3162.8162,	3166.8165,	3171.3734,
	1	1.986637000	1.747470000	0.291820000	3185.3844,	3202.2873,	3335.2844
	1	1.019733000	0.996930000	1.576404000			
	1	0.287412000	2.204556000	0.501768000			
P2d	6	-1.798206000	0.815349000	-0.000620000	61.7128,	80.1143,	94.5817,
	6	-0.769879000	-0.306072000	-0.004549000	182.1279,	273.9392,	282.3617,
	1	-1.743570000	1.378129000	-0.937723000	359.2601,	444.6597,	556.2637,
	1	-1.612946000	1.514395000	0.820000000	580.6123,	692.7421,	943.1238,
	1	-2.787202000	0.370420000	0.101471000	953.3903,	985.5058,	992.5588,
	6	0.658374000	0.084075000	-0.033546000	1013.5287,	1066.5734,	1170.4547,
	8	-1.105519000	-1.462174000	0.011252000	1312.9054,	1356.2856,	1403.2696,
	6	1.682257000	-0.998818000	0.000693000	1409.4543,	1425.5274,	1481.3487,
	1	2.329839000	-0.942094000	-0.883593000	1486.9432,	1498.772,	1503.5729,
	1	1.199551000	-1.975181000	0.033733000	1512.6655,	1515.6646,	2036.8157,
	1	2.332528000	-0.882492000	0.877636000	3040.5185,	3050.0796,	3082.6143,
	6	1.119641000	1.505549000	0.006529000	3112.3172,	3123.2391,	3168.2477,
	1	1.341548000	1.809142000	1.040489000	3181.8869,	3202.3238,	3214.2122
	1	0.382908000	2.205775000	-0.391084000			
	1	2.048370000	1.618799000	-0.561980000			
P3d	6	1.815337000	0.720654000	-0.231538000	45.3549,	148.9626,	151.4935,
	6	0.719591000	-0.312400000	-0.030134000	230.0909,	276.8699,	303.2169,
	6	-0.701976000	0.124252000	-0.389567000	343.3005,	404.5858,	457.5322,
	6	-1.691508000	-0.975583000	-0.204476000	553.8984,	627.0891,	732.6191,
	8	0.971184000	-1.417049000	0.413454000	921.6664,	971.3267,	974.2201,
	1	1.620701000	1.356708000	-1.098995000	995.6981,	1081.2015,	1121.6913,
	1	2.771314000	0.207033000	-0.341904000	1169.8383,	1197.5179,	1300.6192,
	1	1.867363000	1.363721000	0.653387000	1369.0115,	1402.7509,	1417.0665,
	1	-0.666500000	0.425812000	-1.450475000	1470.0522,	1487.7281,	1498.5221,
	1	-2.736449000	-0.799434000	-0.426942000	1518.6345,	1523.5467,	1789.4593,
	1	-1.368569000	-1.949342000	0.134207000	3014.1452,	3074.6759,	3080.2361,
	6	-1.087557000	1.384706000	0.416813000	3165.8376,	3168.329,	3171.0152,
	1	-1.049587000	1.170745000	1.489164000	3200.0418,	3213.3308,	3340.3412
	1	-2.108379000	1.685802000	0.166711000			
	1	-0.422683000	2.225568000	0.200632000			

iBMK	6	2.593260000	0.561763000	-0.467077000	53.6953,	97.4693,	132.0304,
	6	1.350695000	-0.022188000	0.176847000	174.222,	225.3301,	265.5088,
	6	0.052743000	0.732859000	-0.074279000	315.0541,	348.7066,	415.1814,
	6	-1.209759000	-0.061223000	0.255558000	432.2618,	473.9066,	603.9957,
	8	1.390772000	-1.027304000	0.863491000	816.2008,	845.6487,	864.16,
	1	3.484122000	0.089145000	-0.051806000	941.4514,	973.7544,	987.1173,
	1	2.632109000	1.645440000	-0.320998000	994.2739,	1022.4873,	1151.1325,
	1	2.553019000	0.377426000	-1.546336000	1162.3967,	1206.2452,	1219.0961,
	1	0.032292000	1.077983000	-1.117894000	1267.5085,	1325.7719,	1377.1634,
	1	0.103736000	1.643752000	0.541617000	1394.9227,	1414.3719,	1416.1953,
	1	-1.076794000	-0.484287000	1.257856000	1431.3282,	1461.7169,	1485.7968,
	6	-2.432735000	0.856912000	0.257890000	1498.3533,	1506.6677,	1513.8153,
	6	-1.397999000	-1.215866000	-0.730221000	1524.1714,	1532.7576,	1778.5003,
	1	-3.341354000	0.295378000	0.497759000	3044.0557,	3058.3467,	3061.9639,
	1	-2.570621000	1.314521000	-0.728866000	3075.2581,	3089.7147,	3103.9343,
	1	-2.324965000	1.661351000	0.993062000	3143.2714,	3149.1932,	3154.3833,
	1	-0.545038000	-1.898684000	-0.707704000	3159.2804,	3171.7455,	3200.8416
	1	-2.298059000	-1.789613000	-0.487120000			
	1	-1.511856000	-0.827530000	-1.749811000			
RC1e	6	-1.064316000	1.749443000	-0.488339000	28.0867,	39.3806,	59.9819,
	6	-0.215249000	0.606966000	0.012147000	74.3822,	106.1032,	120.3633,
	1	-0.908526000	1.837384000	-1.569981000	155.8081,	193.3452,	224.3135,
	1	-2.120145000	1.563232000	-0.289726000	227.1022,	270.1403,	320.1316,
	6	1.269815000	0.871323000	0.156329000	360.5619,	420.4878,	437.9548,
	8	-0.687349000	-0.487194000	0.299980000	477.8142,	617.0722,	686.5681,
	1	1.376097000	1.479112000	1.068199000	816.3279,	858.0185,	867.2086,
	1	1.598814000	1.515186000	-0.671182000	942.4931,	987.7794,	987.8621,
	1	-0.741070000	2.690912000	-0.035485000	1000.7996,	1027.0594,	1153.4844,
	8	-3.950736000	-0.035424000	0.097710000	1169.1707,	1214.777,	1224.6311,
	8	-3.333306000	-1.174367000	0.236002000	1268.3053,	1324.2979,	1333.704,
	1	-2.376742000	-0.943150000	0.254261000	1378.0999,	1404.4421,	1417.8354,
	6	2.137039000	-0.383226000	0.246678000	1423.0573,	1433.464,	1458.3006,
	1	1.691365000	-1.036903000	1.005021000	1486.5744,	1506.0887,	1509.9605,
	6	3.557201000	-0.014401000	0.677730000	1514.2755,	1524.9517,	1532.1057,
	1	4.015211000	0.664617000	-0.050911000	1592.2017,	1761.3744,	3046.1304,
	1	3.560772000	0.481363000	1.653991000	3060.6203,	3063.9786,	3074.5979,
	1	4.186160000	-0.907378000	0.746600000	3093.0212,	3106.7286,	3146.373,
	6	2.150042000	-1.131256000	-1.087927000	3152.0888,	3157.8414,	3159.5102,
	1	2.762156000	-2.035718000	-1.017524000	3169.3705,	3206.7658,	3468.9328
RC2e (identified as RC1e in PES)	1	1.142453000	-1.429707000	-1.389199000			
	1	2.577398000	-0.496161000	-1.873306000			
	6	1.064244000	-1.749654000	0.488084000	28.0793,	39.3762,	59.9682,
	6	0.215138000	-0.607548000	-0.013170000	74.3861,	106.0881,	120.3686,
	1	0.908836000	-1.836617000	1.569857000	155.7428,	193.3334,	224.316,
	1	0.740633000	-2.691466000	0.036195000	227.0402,	270.1334,	320.1324,
	6	-1.270163000	-0.871589000	-0.155614000	360.5614,	420.4777,	437.9414,
	8	0.687316000	0.486032000	-0.303058000	477.8442,	617.0567,	686.5881,
	1	-1.598610000	-1.514383000	0.672944000	816.3171,	858.0232,	867.2052,

	1	-1.377525000	-1.480365000	-1.066697000	942.4945,	987.754,	987.8603,
	1	2.120028000	-1.563782000	0.288949000	1000.7856,	1027.0532,	1153.4836,
	8	3.950448000	0.035759000	-0.095943000	1169.1724,	1214.7766,	1224.634,
	8	3.332996000	1.174525000	-0.235580000	1268.301,	1324.2857,	1333.6969,
	1	2.376625000	0.942831000	-0.257924000	1378.1019,	1404.4306,	1417.8379,
	6	-2.137037000	0.383162000	-0.246577000	1423.0499,	1433.466,	1458.3156,
	1	-1.691895000	1.035778000	-1.006145000	1486.5825,	1506.086,	1509.909,
	6	-2.148419000	1.132777000	1.087153000	1514.2752,	1524.9523,	1532.1041,
	1	-2.575198000	0.498764000	1.873718000	1592.1569,	1761.3935,	3046.1377,
	1	-1.140420000	1.431230000	1.387051000	3060.6193,	3063.9776,	3074.616,
	1	-2.760285000	2.037372000	1.016301000	3093.0371,	3106.7422,	3146.3723,
	6	-3.557765000	0.014335000	-0.675756000	3152.0888,	3157.8388,	3159.498,
	1	-4.186472000	0.907455000	-0.745056000	3169.3619,	3206.8251,	3468.9007
	1	-3.562499000	-0.482592000	-1.651421000			
	1	-4.015283000	-0.663650000	0.054155000			
RC3e (identified as RC1e in PES)	6	-1.997340000	-1.998089000	-0.396032000	45.3311,	57.0643,	67.9083,
	6	-0.706299000	-1.250484000	-0.184733000	78.201,	115.5525,	141.2888,
	1	-2.106733000	-2.225666000	-1.462067000	165.8871,	176.7622,	232.1041,
	1	-2.840455000	-1.358628000	-0.115738000	234.949,	274.2601,	321.1179,
	1	-2.004109000	-2.919518000	0.186727000	374.5551,	400.9743,	423.2839,
	6	-0.545940000	0.099440000	-0.849590000	538.2044,	605.4018,	727.3955,
	8	0.185727000	-1.716359000	0.517847000	819.976,	858.4886,	898.0705,
	1	-1.391778000	0.306180000	-1.515550000	943.1505,	982.667,	989.962,
	1	0.374288000	0.067138000	-1.442830000	1000.6674,	1035.3956,	1146.0911,
	8	2.755624000	0.007793000	-0.516085000	1171.9512,	1209.6227,	1235.4731,
	8	2.651641000	-0.576761000	0.646236000	1279.7087,	1314.29,	1335.307,
	1	1.760057000	-1.000105000	0.635494000	1380.2429,	1388.0861,	1405.866,
	6	-0.421158000	1.224822000	0.194691000	1418.3016,	1433.9928,	1479.9626,
	1	0.424377000	0.974207000	0.844662000	1493.7143,	1497.0653,	1506.4707,
	6	-1.682990000	1.325580000	1.053607000	1514.131,	1523.1553,	1530.4724,
	1	-2.558795000	1.528677000	0.425585000	1595.8606,	1755.6301,	3058.0351,
	1	-1.868109000	0.404117000	1.616155000	3062.9209,	3075.149,	3080.3326,
	1	-1.591202000	2.141410000	1.777180000	3107.4655,	3144.1241,	3147.5442,
	6	-0.115745000	2.550021000	-0.501798000	3152.3424,	3156.2163,	3158.6756,
	1	-0.007821000	3.355673000	0.231292000	3165.3209,	3205.8285,	3416.7224
	1	0.812432000	2.481175000	-1.076571000			
	1	-0.929251000	2.820211000	-1.185199000			
RC4e (identified as RC1e in PES)	6	-1.995374000	-1.999945000	-0.396364000	45.2401,	57.0711,	67.8435,
	6	-0.705223000	-1.250926000	-0.184603000	78.1836,	115.6184,	141.3173,
	6	-0.546122000	0.099092000	-0.849553000	165.9532,	176.7469,	232.0006,
	8	0.186981000	-1.715741000	0.518453000	234.9457,	274.258,	321.1254,
	1	-2.104467000	-2.227200000	-1.462496000	374.5693,	400.9621,	423.2976,
	1	-2.839214000	-1.361532000	-0.115834000	538.1588,	605.4158,	727.1046,
	1	-2.001162000	-2.921602000	0.186045000	819.9617,	858.4905,	898.062,
	1	0.374057000	0.067508000	-1.442928000	943.1441,	982.6645,	989.97,
	1	-1.392265000	0.305066000	-1.515372000	1000.6728,	1035.3871,	1146.111,
	1	1.761026000	-0.998423000	0.636305000	1171.9438,	1209.6412,	1235.4708,
	8	2.652369000	-0.574637000	0.646217000	1279.6959,	1314.2838,	1335.3221,

	8	2.755145000	0.009227000	-0.516554000	1380.2275,	1388.0997,	1405.8686,
	6	-0.422094000	1.224644000	0.194617000	1418.3,	1433.9925,	1479.9606,
	1	0.423869000	0.974839000	0.844329000	1493.709,	1497.0456,	1506.4669,
	6	-1.683750000	1.324278000	1.053925000	1514.1276,	1523.1576,	1530.471,
	1	-2.559934000	1.526545000	0.426163000	1595.7457,	1755.6338,	3058.0267,
	1	-1.867848000	0.402664000	1.616564000	3062.9069,	3075.1262,	3080.2725,
	1	-1.592489000	2.140222000	1.777435000	3107.529,	3144.109,	3147.4927,
	6	-0.118179000	2.550117000	-0.502008000	3152.3273,	3156.2087,	3158.6526,
	1	-0.010641000	3.355869000	0.231031000	3165.2957,	3205.8105,	3417.2579
	1	0.809794000	2.482112000	-1.077217000			
	1	-0.932241000	2.819580000	-1.185038000			
RC5e	6	-2.463768000	-1.908307000	-0.152099000	20.1114,	33.3321,	48.2818,
	6	-1.790079000	-0.579765000	0.137445000	55.6586,	78.1931,	100.5106,
	6	-0.371150000	-0.443935000	-0.396703000	109.4638,	140.6577,	197.8823,
	6	0.270305000	0.945257000	-0.308036000	218.0328,	242.8042,	272.7894,
	8	-2.362218000	0.304752000	0.750154000	299.7521,	361.318,	400.2083,
	1	-1.783955000	-2.742402000	0.044081000	459.5689,	469.749,	646.3193,
	1	-2.734006000	-1.945889000	-1.213148000	790.2656,	823.9289,	853.9552,
	1	-3.366398000	-2.001817000	0.452647000	947.1104,	963.4223,	988.2175,
	1	-0.374319000	-0.789331000	-1.440012000	1022.9757,	1026.62,	1125.05,
	1	0.241517000	-1.180003000	0.144377000	1153.5239,	1197.9587,	1231.8032,
	1	1.260651000	0.840105000	-0.774571000	1251.9396,	1283.3996,	1361.937,
	1	2.516045000	0.026976000	0.665387000	1392.4567,	1396.0511,	1411.121,
	8	3.093461000	-0.753622000	0.626483000	1421.4615,	1433.1826,	1457.4701,
	8	3.164927000	-1.057361000	-0.645385000	1465.574,	1486.0191,	1498.1731,
	6	0.454614000	1.415474000	1.141357000	1505.1703,	1521.2058,	1528.1108,
	1	-0.509691000	1.670582000	1.583300000	1546.6904,	1776.7924,	3048.5935,
	1	0.898871000	0.633683000	1.771392000	3054.1891,	3059.9181,	3071.185,
	1	1.100268000	2.299574000	1.181108000	3077.215,	3100.0652,	3134.4938,
	6	-0.494737000	1.986036000	-1.130538000	3152.9248,	3161.9099,	3180.1113,
	1	0.041684000	2.940350000	-1.132471000	3187.1458,	3202.435,	3715.0318
	1	-0.601739000	1.657835000	-2.169943000			
	1	-1.489395000	2.151613000	-0.710719000			
RC6e	6	2.861266000	-1.268377000	-0.012828000	28.9342,	63.656,	69.0844,
	6	1.438412000	-0.767175000	-0.109473000	75.9533,	108.823,	120.9667,
	6	1.262799000	0.722776000	-0.322939000	133.6323,	172.06,	205.0729,
	6	-0.144956000	1.261376000	-0.077253000	215.806,	265.2583,	319.6087,
	8	0.495944000	-1.543009000	-0.027819000	345.435,	417.8632,	435.9283,
	1	3.491882000	-0.792621000	-0.768963000	473.6077,	603.6683,	632.4243,
	1	2.884023000	-2.353154000	-0.119601000	814.5317,	850.3381,	869.265,
	1	3.260374000	-0.991819000	0.969450000	947.9371,	982.876,	988.4554,
	1	1.568256000	0.911214000	-1.363851000	997.0241,	1024.1858,	1152.9873,
	1	1.997431000	1.252285000	0.300591000	1165.4789,	1213.2889,	1222.6718,
	1	-0.848141000	0.654622000	-0.656034000	1270.4174,	1304.7577,	1342.5885,
	1	-1.278332000	-1.560039000	0.107115000	1388.2684,	1400.6007,	1419.4665,
	8	-2.245342000	-1.659412000	0.237561000	1423.9885,	1434.54,	1455.9196,
	8	-2.792071000	-0.890536000	-0.665218000	1483.9374,	1497.952,	1506.2917,
	6	-0.244378000	2.707663000	-0.565417000	1512.8102,	1524.5156,	1531.0714,

	1	-0.024411000	2.781562000	-1.635505000	1564.0304,	1770.7415,	3044.107,
	1	0.464668000	3.346379000	-0.025444000	3059.9655,	3064.9661,	3078.7433,
	1	-1.250849000	3.102586000	-0.397195000	3092.0239,	3122.29,	3146.7662,
	6	-0.519947000	1.167078000	1.403355000	3155.0908,	3159.7734,	3163.692,
	1	-0.460065000	0.141195000	1.775781000	3170.9601,	3206.4028,	3547.5878
	1	-1.543882000	1.518131000	1.561564000			
	1	0.151633000	1.793268000	2.003229000			
RC7e (identified as RC1e in PES)	6	-1.995327000	2.000028000	-0.396327000	45.3232,	57.0818,	67.848,
	6	-0.705189000	1.250968000	-0.184655000	78.1875,	115.5609,	141.3043,
	6	-0.546101000	-0.099067000	-0.849573000	165.9131,	176.7549,	232.0359,
	6	-0.422321000	-1.224601000	0.194664000	234.9547,	274.2593,	321.1213,
	6	-0.118340000	-2.550097000	-0.501884000	374.5623,	400.9608,	423.2933,
	8	0.187064000	1.715722000	0.518357000	538.175,	605.4034,	727.2206,
	1	-2.001162000	2.921532000	0.186324000	819.9716,	858.4893,	898.0813,
	1	-2.839208000	1.361552000	-0.116073000	943.1524,	982.6669,	989.9604,
	1	-2.104289000	2.227579000	-1.462409000	1000.6703,	1035.3928,	1146.1093,
	1	-1.392155000	-0.305011000	-1.515510000	1171.9472,	1209.6312,	1235.473,
	1	0.374176000	-0.067574000	-1.442811000	1279.7109,	1314.2489,	1335.3182,
	1	0.423560000	-0.974833000	0.844522000	1380.2428,	1388.0944,	1405.8686,
	1	-0.010967000	-3.355840000	0.231189000	1418.3033,	1433.9932,	1479.9622,
	1	-0.932293000	-2.819535000	-1.185052000	1493.7126,	1497.0551,	1506.4687,
	1	0.809739000	-2.482138000	-1.076928000	1514.1298,	1523.1575,	1530.471,
	1	1.761031000	0.998203000	0.636062000	1595.7741,	1755.6923,	3058.0317,
	8	2.652514000	0.574674000	0.646171000	3062.9096,	3075.1333,	3080.2623,
	8	2.755615000	-0.009625000	-0.516364000	3107.398,	3144.1109,	3147.4768,
	6	-1.684130000	-1.324110000	1.053757000	3152.3194,	3156.2046,	3158.6625,
	1	-1.868245000	-0.402467000	1.616340000	3165.3025,	3205.8156,	3417.0405
	1	-1.593061000	-2.140044000	1.777304000			
	1	-2.560222000	-1.526319000	0.425848000			
RC8e	6	1.945511000	-0.344468000	0.268022000	18.982,	35.6412,	64.3997,
	6	1.480104000	-1.507303000	-0.611545000	86.9996,	93.7879,	138.6111,
	1	1.684555000	-0.569231000	1.308125000	169.7412,	179.0704,	227.446,
	1	0.398893000	-1.657517000	-0.544049000	241.8938,	274.21,	319.2393,
	1	1.970262000	-2.438822000	-0.312018000	360.9129,	415.5093,	436.3372,
	1	1.737853000	-1.313208000	-1.659757000	491.7856,	608.5525,	705.1243,
	1	-2.333224000	-0.350411000	0.924053000	813.7391,	862.4468,	863.7103,
	8	-3.168717000	-0.714202000	0.549827000	944.3609,	985.5099,	990.2444,
	8	-2.857449000	-1.012403000	-0.682592000	999.7067,	1024.252,	1151.7121,
	6	3.458079000	-0.149338000	0.162350000	1167.4275,	1213.8327,	1224.4753,
	1	3.740607000	0.111256000	-0.864298000	1265.0113,	1307.6624,	1333.9293,
	1	3.987344000	-1.068218000	0.433234000	1378.8057,	1400.7165,	1419.1955,
	1	3.803614000	0.651432000	0.824481000	1421.4682,	1435.4397,	1462.3518,
	6	1.213239000	0.940968000	-0.118144000	1478.2042,	1501.2683,	1506.7494,
	1	1.352979000	1.162110000	-1.184779000	1514.3592,	1525.5231,	1531.5585,
	1	1.626171000	1.801190000	0.430816000	1575.0438,	1761.7894,	3048.1591,
	6	-0.268494000	0.913887000	0.196152000	3060.1856,	3063.0745,	3081.8227,
	8	-0.700373000	0.207967000	1.100376000	3097.1345,	3110.7738,	3145.7931,
	6	-1.165042000	1.788275000	-0.644796000	3151.836,	3157.1379,	3166.9975,

	1	-1.311723000	1.289379000	-1.608654000	3168.9436, 3205.6098, 3447.4089
	1	-0.689351000	2.754820000	-0.832354000	
	1	-2.136061000	1.924203000	-0.167934000	
TS1e	6	1.628553000	-1.134152000	1.024504000	1897.2724 <i>i</i> , 30.4531 , 48.1502 ,
	6	0.478682000	-0.794200000	0.116206000	95.2052 , 113.8669 , 131.2195,
	1	1.495441000	-0.974993000	2.093394000	182.0589, 225.3688 , 248.3413,
	1	2.156974000	-2.042593000	0.740764000	267.9551 , 314.3155, 341.9861,
	6	-0.653741000	-0.016257000	0.753455000	404.6903, 417.0968, 438.7773,
	8	0.518728000	-1.069581000	-1.060324000	514.5707, 574.4776 , 616.5458,
	1	-0.187911000	0.901504000	1.142700000	648.0194, 841.2952, 867.8457,
	1	-1.012880000	-0.571347000	1.632561000	886.1319, 941.02, 983.148,
	1	2.460731000	-0.188621000	0.618941000	990.2394, 1003.4707, 1029.1101,
	8	3.074055000	0.600481000	0.039346000	1121.4296, 1131.2876, 1163.7773,
	8	2.125779000	1.371112000	-0.626158000	1189.1209, 1209.402, 1220.7219,
	1	1.990068000	0.871159000	-1.444375000	1271.0432, 1330.1049, 1374.9279,
	6	-1.806892000	0.315339000	-0.189567000	1412.9606, 1415.1947, 1430.8191,
	1	-1.369009000	0.713415000	-1.112475000	1435.7468, 1448.1053, 1474.2294,
	6	-2.707602000	1.383083000	0.433229000	1484.8599, 1507.0566, 1513.6408,
	1	-3.135931000	1.021156000	1.375317000	1523.6761, 1534.7418, 2181.7845,
	1	-2.149226000	2.301153000	0.643534000	3047.1524, 3059.478, 3062.7837,
	1	-3.535236000	1.632669000	-0.238236000	3090.9468, 3102.9504, 3144.026,
	6	-2.607978000	-0.940338000	-0.538767000	3149.7463, 3150.5135, 3156.592,
	1	-3.426379000	-0.697959000	-1.224242000	3179.9045, 3261.0797, 3776.4937
	1	-1.974068000	-1.691520000	-1.014694000	
	1	-3.047203000	-1.370963000	0.369547000	
TS2e	6	-1.460830000	-0.582305000	-1.311438000	1937.8546 <i>i</i> , 24.9139, 52.3279 ,
	6	-0.384145000	0.066705000	-0.492476000	104.2211 , 114.6134, 157.2627,
	1	-2.091233000	0.121160000	-1.853857000	196.2025, 223.5569 , 228.812,
	1	-1.212165000	-1.502628000	-1.836112000	267.6239 , 313.7153, 345.7709,
	6	0.930534000	-0.680194000	-0.398539000	412.8423, 432.7967, 495.5992,
	8	-0.595016000	1.102026000	0.112723000	555.5668, 583.0709, 655.0024,
	1	1.277389000	-0.904718000	-1.417830000	662.1304, 826.6764, 853.2493,
	1	0.685800000	-1.654268000	0.052898000	874.1913, 940.647, 953.4484,
	1	-2.300596000	-0.876508000	-0.331122000	990.0374, 995.1081, 1015.5354,
	8	-2.882143000	-0.750513000	0.656690000	1129.15, 1133.4412, 1163.7196,
	8	-3.345258000	0.556504000	0.622991000	1209.9512, 1219.4938, 1246.4389,
	1	-2.538357000	1.059386000	0.827128000	1268.3914, 1331.5808, 1375.591,
	6	2.018516000	0.034088000	0.399556000	1414.1284, 1415.9578, 1431.6061,
	1	1.566820000	0.376564000	1.337821000	1449.832, 1469.396, 1490.2677,
	6	2.538035000	1.256764000	-0.359399000	1506.7511, 1513.7026, 1524.0292,
	1	2.985763000	0.946740000	-1.311578000	1531.5676, 1534.1896, 2016.3684,
	1	1.733351000	1.966708000	-0.562776000	3042.8646, 3059.9615, 3063.5602,
	1	3.309408000	1.771876000	0.221777000	3088.1493, 3102.6125, 3145.0322,
	6	3.158934000	-0.933796000	0.719404000	3150.1322, 3150.4806, 3157.1511,
	1	3.943213000	-0.432225000	1.294906000	3178.6893, 3260.9483, 3705.0008
	1	2.803556000	-1.790347000	1.301679000	
	1	3.610125000	-1.313436000	-0.204814000	
TS3e	6	1.679900000	1.740170000	0.887790000	1907.5216 <i>i</i> , 56.1306, 60.3533 ,

	6	0.768133000	0.999335000	-0.060373000	78.2144,	113.0164,	117.9394,
	1	2.148162000	1.018447000	1.564440000	130.9409,	176.3987,	226.0288,
	1	1.092167000	2.436845000	1.494653000	232.6094,	271.5001,	312.9624,
	1	2.441748000	2.279250000	0.324434000	341.1956,	414.7185,	424.3341,
	6	-0.276514000	0.115274000	0.572013000	512.4487,	561.8135,	609.8614,
	8	0.880010000	1.057304000	-1.265711000	683.2084,	827.775,	874.1204,
	1	-0.430728000	0.270345000	1.644970000	885.002,	944.8921,	978.9279,
	1	0.385151000	-0.986348000	0.493739000	987.6958,	1001.5182,	1059.5264,
	8	1.022958000	-1.930169000	0.131104000	1151.3757,	1160.6185,	1181.047,
	8	2.252590000	-1.416855000	-0.247784000	1215.3919,	1219.0104,	1226.1298,
	1	2.101748000	-1.162328000	-1.169717000	1320.5811,	1360.7468,	1393.5947,
	6	-1.531033000	-0.129709000	-0.233304000	1409.7863,	1423.1356,	1430.5375,
	1	-1.213792000	-0.349021000	-1.258554000	1436.5477,	1478.7378,	1481.6077,
	6	-2.389971000	1.142584000	-0.259826000	1496.5583,	1505.1556,	1512.9876,
	1	-2.695701000	1.419433000	0.755574000	1523.5328,	1530.9782,	2119.3942,
	1	-1.840810000	1.978444000	-0.702874000	3061.7309,	3063.8654,	3077.3013,
	1	-3.294614000	0.976255000	-0.853748000	3107.4465,	3133.6471,	3149.042,
	6	-2.315100000	-1.319318000	0.322675000	3155.035,	3162.8546,	3164.2146,
	1	-3.220531000	-1.492044000	-0.267434000	3164.9225,	3207.7642,	3776.7213
	1	-1.712233000	-2.232183000	0.300936000			
	1	-2.617518000	-1.129345000	1.358870000			
TS4e	6	-2.222028000	-1.481512000	0.716555000	1959.6358 <i>j</i> ,	37.8209,	59.6052,
	6	-1.195711000	-0.705696000	-0.074506000	100.3571,	123.5956,	145.2782,
	6	0.070324000	-0.330682000	0.643471000	151.8318,	177.646,	225.8505,
	8	-1.387637000	-0.348096000	-1.223759000	235.9767,	273.4948,	314.0969,
	1	-2.456368000	-0.936437000	1.636840000	377.7293,	418.0796,	430.3172,
	1	-1.801956000	-2.450377000	1.006209000	517.8404,	528.2205,	609.3727,
	1	-3.124071000	-1.623883000	0.121088000	670.5939,	844.3911,	878.1149,
	1	-0.245024000	0.912105000	0.830242000	912.2426,	945.2881,	978.8409,
	1	0.180543000	-0.750850000	1.648218000	985.9334,	1006.5364,	1069.0689,
	1	-1.002070000	1.814573000	-1.172789000	1113.8331,	1161.6776,	1179.7268,
	8	-0.355364000	2.318417000	-0.651714000	1199.2329,	1214.7875,	1226.1441,
	8	-0.699034000	1.998005000	0.647727000	1331.693,	1358.5405,	1395.4661,
	6	1.335562000	-0.285906000	-0.180289000	1408.8026,	1428.7789,	1432.1898,
	1	1.110053000	0.281364000	-1.089122000	1470.6996,	1479.9013,	1494.3788,
	6	1.740188000	-1.710378000	-0.590458000	1503.5319,	1511.3982,	1522.2054,
	1	1.939588000	-2.323357000	0.295760000	1524.1401,	1529.694,	1969.016,
	1	0.953602000	-2.190220000	-1.180568000	3061.4927,	3064.0145,	3075.6088,
	1	2.651067000	-1.682655000	-1.197199000	3113.6392,	3136.7918,	3149.2739,
	6	2.456441000	0.418258000	0.584050000	3155.7292,	3160.5581,	3161.3179,
	1	3.367087000	0.460656000	-0.021467000	3167.7785,	3206.4162,	3725.433
	1	2.166142000	1.440479000	0.842974000			
	1	2.689031000	-0.122516000	1.508844000			
TS5e	6	-2.846044000	-1.430306000	-0.219325000	1983.2588 <i>j</i> ,	34.939,	48.7995,
	6	-1.896682000	-0.282562000	0.069890000	73.4698,	91.2028,	101.6733,
	6	-0.435045000	-0.541416000	-0.282996000	135.3057,	191.2258,	214.9526,
	6	0.494051000	0.645313000	-0.111378000	230.4474,	240.8215,	302.2573,
	8	-2.287360000	0.771457000	0.539048000	357.7266,	382.757,	418.2088,

	1	-2.443029000	-2.371776000	0.164789000	467.9587,	483.714,	580.0129,
	1	-2.957595000	-1.537926000	-1.303647000	696.7896,	799.9329,	828.5206,
	1	-3.819323000	-1.222380000	0.226490000	855.4826,	956.932,	965.1664,
	1	-0.400575000	-0.903574000	-1.319922000	999.6782,	1034.9419,	1038.4052,
	1	-0.084187000	-1.381451000	0.333242000	1134.9437,	1171.8811,	1193.2381,
	1	1.573992000	0.156149000	-0.444541000	1201.8402,	1225.1151,	1304.2052,
	1	3.228339000	-0.968717000	1.031117000	1329.3914,	1370.7085,	1400.4507,
	8	2.692976000	-1.417985000	0.364846000	1403.2234,	1409.7689,	1419.9263,
	8	2.640092000	-0.483488000	-0.655295000	1459.6373,	1486.2045,	1494.5979,
	6	0.711215000	1.071902000	1.327574000	1497.0261,	1506.1207,	1510.9099,
	1	-0.205026000	1.515369000	1.730773000	1521.0013,	1526.1688,	1776.0406,
	1	0.978699000	0.210940000	1.949538000	3057.1381,	3060.4184,	3063.209,
	1	1.514119000	1.813587000	1.392521000	3078.1084,	3106.1706,	3150.0581,
	6	0.253153000	1.786559000	-1.080604000	3153.0697,	3155.9825,	3159.2166,
	1	1.060664000	2.523020000	-1.022215000	3163.3746,	3202.6807,	3804.7377
	1	0.193727000	1.420988000	-2.110881000			
	1	-0.689352000	2.288957000	-0.835026000			
TS6e	6	-3.101174000	-0.168402000	-0.136447000	2101.5736 <i>i</i> ,	49.1293,	86.3702,
	6	-1.622393000	0.146673000	-0.054780000	120.6955,	127.9404,	141.1513,
	6	-0.688898000	-1.007150000	-0.392505000	154.4397,	177.4928,	196.7676,
	6	0.754097000	-0.876440000	0.056421000	222.0925,	231.182,	321.1962,
	8	-1.227814000	1.259869000	0.250027000	330.0129,	368.334,	423.1349,
	1	-3.324491000	-0.747522000	-1.037138000	470.2179,	572.8294,	601.6298,
	1	-3.678835000	0.756218000	-0.123522000	624.8551,	808.7332,	849.6012,
	1	-3.378823000	-0.783128000	0.726967000	871.009,	961.6885,	983.1579,
	1	-0.732614000	-1.117770000	-1.486582000	999.2528,	1009.3242,	1036.0214,
	1	-1.125894000	-1.934060000	0.013961000	1136.7139,	1170.1155,	1181.3825,
	1	1.168684000	0.200754000	-0.471542000	1191.595,	1230.8447,	1284.1948,
	1	0.530612000	2.283885000	0.206066000	1301.5084,	1380.7648,	1407.191,
	8	1.484514000	2.129255000	0.133596000	1410.4456,	1426.2351,	1446.6562,
	8	1.532695000	1.245849000	-0.934201000	1466.4946,	1484.1696,	1493.4621,
	6	1.655184000	-1.938625000	-0.541951000	1498.1606,	1498.9103,	1509.7721,
	1	1.573393000	-1.961004000	-1.633351000	1517.9107,	1521.7926,	1779.3157,
	1	1.381615000	-2.932493000	-0.159742000	3028.0755,	3042.5918,	3045.8302,
	1	2.699766000	-1.750014000	-0.278409000	3077.295,	3081.0458,	3131.6051,
	6	0.937701000	-0.683281000	1.546618000	3142.7416,	3161.7609,	3165.8071,
	1	0.387001000	0.185074000	1.913299000	3185.0386,	3204.8617,	3762.0341
	1	1.994768000	-0.540698000	1.787386000			
	1	0.582555000	-1.575664000	2.083091000			
TS7e	6	-2.555063000	-1.318407000	0.659433000	2045.4353 <i>i</i> ,	24.8635,	47.0388,
	6	-1.705835000	-0.272527000	-0.034672000	75.9939,	100.3945,	125.5929,
	6	-0.478809000	0.193652000	0.732823000	150.9818,	186.1364,	218.6244,
	6	0.467203000	1.061003000	-0.098149000	256.6033,	308.7751,	371.2748,
	6	1.867177000	1.014650000	0.468044000	397.4986,	415.5019,	435.5243,
	8	-1.974253000	0.142800000	-1.148098000	471.1896,	543.141,	605.103,
	1	-3.504876000	-1.433279000	0.135943000	641.4773,	819.8571,	840.483,
	1	-2.724749000	-1.051470000	1.706636000	890.4476,	955.3089,	978.2796,
	1	-2.012520000	-2.269979000	0.644269000	991.9045,	1002.0757,	1074.0601,

	1	-0.822811000	0.743639000	1.621881000	1148.3895,	1159.8536,	1177.104,
	1	0.035122000	-0.699917000	1.105337000	1198.9356,	1210.7921,	1233.9974,
	1	0.485287000	0.645468000	-1.111801000	1271.5782,	1339.0302,	1359.0929,
	1	2.617705000	1.560721000	-0.108991000	1394.897,	1400.1441,	1408.8093,
	1	1.937610000	1.218167000	1.540184000	1419.3606,	1465.9207,	1481.4176,
	1	2.212058000	-0.212667000	0.378268000	1487.825,	1498.0581,	1501.2516,
	1	1.969819000	-1.748296000	-1.531717000	1514.3746,	1524.0051,	1778.8488,
	8	1.459043000	-1.803109000	-0.714435000	3054.2063,	3065.5609,	3076.6628,
	8	2.384092000	-1.399448000	0.247063000	3100.4811,	3106.962,	3123.9472,
	6	-0.036954000	2.508787000	-0.194530000	3153.9003,	3162.1407,	3175.608,
	1	-1.042781000	2.522838000	-0.621437000	3196.9267,	3201.419,	3811.8432
	1	0.617706000	3.111090000	-0.832186000			
	1	-0.064933000	2.968791000	0.799670000			
TS8e	6	1.476971000	-0.057412000	0.227659000	2138.1987 <i>i</i> ,	36.418,	66.2635,
	6	1.215380000	-1.246289000	-0.672649000	91.3914,	144.1345,	161.6608,
	1	1.146132000	-0.302175000	1.243078000	181.4526,	192.8305,	233.0473,
	1	-0.061919000	-1.430310000	-0.735456000	253.6621,	298.0955,	367.7117,
	1	1.573093000	-2.204802000	-0.290503000	394.5145,	416.3868,	487.8069,
	1	1.490552000	-1.082846000	-1.719113000	580.4173,	591.3743,	603.8248,
	1	-1.626807000	-1.150081000	1.073700000	669.7188,	814.1641,	865.79,
	8	-1.549392000	-1.969461000	0.557749000	876.1744,	961.1965,	975.301,
	8	-1.240287000	-1.482614000	-0.706556000	989.7539,	1003.1092,	1025.2249,
	6	2.981058000	0.252139000	0.258479000	1132.4189,	1150.7994,	1164.9412,
	1	3.328398000	0.565043000	-0.732254000	1188.5622,	1215.4744,	1255.6303,
	1	3.555697000	-0.629152000	0.558672000	1273.2054,	1325.692,	1375.4032,
	1	3.192465000	1.058943000	0.968029000	1394.0285,	1413.9093,	1418.5612,
	6	0.676565000	1.165664000	-0.232296000	1463.3816,	1476.6775,	1480.8074,
	1	0.743295000	1.288881000	-1.320259000	1482.142,	1497.6084,	1505.8468,
	1	1.101640000	2.075931000	0.216022000	1515.7728,	1519.3647,	1772.1038,
	6	-0.780790000	1.145781000	0.211358000	3053.7163,	3062.6634,	3078.2471,
	8	-1.095510000	0.684459000	1.298645000	3100.0935,	3106.4122,	3118.8633,
	6	-1.785350000	1.773485000	-0.721831000	3153.7293,	3160.8326,	3165.8686,
	1	-1.867388000	1.140501000	-1.610753000	3201.6456,	3203.7158,	3710.4892
	1	-1.439572000	2.761900000	-1.041348000			
	1	-2.757073000	1.848894000	-0.232847000			
PC1e	6	-2.210455000	-1.870777000	0.481843000	35.3781,	61.3303,	70.0823,
	6	-0.931687000	-1.206344000	0.193542000	76.9825,	116.1236,	135.4319,
	1	-2.947330000	-1.426985000	1.138601000	173.173,	203.6376,	222.697,
	1	-2.401007000	-2.828609000	0.013813000	234.8204,	269.8806,	277.7548,
	6	-0.650125000	0.127316000	0.855238000	325.913,	379.0903,	415.9193,
	8	-0.132380000	-1.717582000	-0.561683000	425.6183,	550.875,	614.1873,
	1	0.232119000	-0.025999000	1.487088000	725.0647,	739.9757,	859.6754,
	1	-1.488224000	0.446703000	1.485098000	876.6027,	901.7924,	932.9624,
	1	2.928217000	0.588775000	0.387545000	943.8822,	987.9727,	992.6851,
	8	2.611536000	-0.292653000	0.608343000	1004.2135,	1140.5472,	1166.247,
	8	2.490202000	-0.830107000	-0.735830000	1211.2944,	1238.0292,	1275.7037,
	1	1.573271000	-1.162849000	-0.691103000	1326.9974,	1344.7868,	1386.4921,
	6	-0.333224000	1.206643000	-0.192885000	1400.7297,	1418.3009,	1433.067,

	1	0.487788000	0.826624000	-0.807855000	1481.8159,	1487.8761,	1505.2176,
	6	0.120070000	2.491470000	0.498618000	1513.797,	1523.5375,	1529.4758,
	1	-0.674646000	2.884641000	1.143192000	1570.3162,	2034.174,	3058.1297,
	1	1.002372000	2.308432000	1.119903000	3061.5657,	3080.2945,	3123.7731,
	1	0.369097000	3.262259000	-0.237824000	3144.262,	3146.1594,	3154.596,
	6	-1.542150000	1.461105000	-1.094763000	3157.829,	3159.1083,	3207.5755,
	1	-1.314727000	2.231895000	-1.837556000	3341.6862,	3616.4483,	3869.1002
	1	-1.838497000	0.556245000	-1.635822000			
	1	-2.397873000	1.805120000	-0.501273000			
PC2e	6	2.004212000	-2.038737000	0.442169000	36.301,	49.6067,	57.0601,
	6	0.755314000	-1.301640000	0.202525000	95.2285,	117.1601,	132.8183,
	1	2.124343000	-3.003590000	-0.034914000	167.1054,	215.5555,	234.2394,
	1	2.791545000	-1.635464000	1.065699000	243.6601,	266.7963,	278.5717,
	6	0.582415000	0.050293000	0.859102000	325.5109,	380.1072,	421.5396,
	8	-0.100680000	-1.770974000	-0.520106000	422.7358,	554.7244,	614.6641,
	1	1.397480000	0.260604000	1.561059000	733.6434,	792.3757,	859.7518,
	1	-0.365603000	0.016847000	1.405616000	881.0607,	903.4112,	938.3576,
	1	-3.473639000	-0.457402000	0.760208000	945.7421,	987.2038,	991.2396,
	8	-2.652873000	0.002572000	0.558000000	1007.4927,	1142.2541,	1165.6733,
	8	-2.481637000	-0.404622000	-0.821392000	1209.0861,	1238.7352,	1280.8763,
	1	-1.668540000	-0.940550000	-0.734540000	1342.972,	1344.1918,	1386.2671,
	6	0.502980000	1.166032000	-0.200552000	1395.4835,	1418.0399,	1433.2137,
	1	-0.301346000	0.896647000	-0.891507000	1481.9755,	1496.077,	1505.5822,
	6	1.814844000	1.275743000	-0.979158000	1514.861,	1522.268,	1530.0652,
	1	2.645403000	1.508949000	-0.301656000	1559.1874,	2024.1546,	3055.6431,
	1	2.053615000	0.346226000	-1.507800000	3060.5869,	3082.7086,	3123.5067,
	1	1.753772000	2.074077000	-1.725128000	3141.4322,	3149.2222,	3154.3381,
	6	0.137605000	2.489419000	0.469549000	3158.4886,	3166.6844,	3206.9693,
	1	0.076027000	3.292256000	-0.272097000	3340.9711,	3590.7143,	3864.8759
	1	-0.831354000	2.408830000	0.970521000			
	1	0.895599000	2.770092000	1.210721000			
PC3e	6	-1.698391000	-2.093565000	0.645574000	36.3321,	56.424,	65.2493,
	6	-0.795918000	-1.160551000	-0.131337000	74.6782,	88.8681,	94.8364,
	1	-2.148211000	-1.515372000	1.460097000	158.4961,	182.8543,	226.9024,
	1	-1.136864000	-2.920601000	1.087164000	235.4758,	265.9524,	273.1602,
	1	-2.485163000	-2.466985000	-0.009406000	301.6172,	353.5661,	427.6038,
	6	0.487440000	-0.824499000	0.488250000	431.7129,	531.4531,	610.5136,
	8	-1.137681000	-0.703268000	-1.212126000	679.9039,	720.0107,	859.7953,
	1	0.719536000	-1.251510000	1.462381000	897.697,	933.7071,	949.9826,
	1	-2.450554000	2.051631000	0.678554000	981.3382,	987.9538,	1025.833,
	8	-1.574970000	1.653268000	0.635509000	1035.8754,	1120.9312,	1175.5197,
	8	-1.227435000	1.979645000	-0.732034000	1218.2925,	1237.0288,	1338.7178,
	1	-1.207404000	1.077621000	-1.104529000	1341.4073,	1352.7029,	1394.5618,
	6	1.481808000	0.079304000	-0.149997000	1407.5933,	1428.0963,	1476.236,
	1	1.036343000	0.477209000	-1.065122000	1488.9355,	1498.6509,	1504.3236,
	6	2.748643000	-0.712007000	-0.518989000	1510.481,	1524.0226,	1530.9266,
	1	3.209692000	-1.139941000	0.377938000	1534.2769,	1929.2037,	3063.9698,
	1	2.519593000	-1.525420000	-1.213395000	3066.2249,	3081.5084,	3135.0558,

	1	3.477490000	-0.047345000	-0.993558000	3150.6549, 3160.743, 3165.1147,		
	6	1.819197000	1.247443000	0.788916000	3169.9415, 3190.0923, 3205.4481,		
	1	2.536404000	1.917592000	0.304344000	3212.944, 3624.8011, 3858.0987		
	1	0.920735000	1.815817000	1.036019000			
	1	2.272428000	0.873390000	1.714212000			
PC4e	6	1.774712000	-1.949120000	-0.738908000	34.7023,	49.7125,	73.1496,
	6	0.800523000	-1.102766000	0.046802000	79.805,	90.5899,	94.2874,
	6	-0.465973000	-0.760723000	-0.608587000	159.4136,	185.9773,	221.322,
	8	1.062916000	-0.697879000	1.169344000	233.2551,	241.5939,	272.3696,
	1	2.270478000	-1.288483000	-1.458811000	302.9191,	338.6533,	413.9394,
	1	1.266000000	-2.740924000	-1.294313000	426.5597,	516.4458,	611.4213,
	1	2.521105000	-2.366793000	-0.063593000	634.066,	657.6528,	860.8825,
	1	0.774183000	2.253178000	-0.919990000	897.642,	931.8923,	942.6653,
	1	-0.693624000	-1.192312000	-1.580623000	980.4825,	988.5077,	1023.4074,
	1	1.376981000	1.091922000	1.126885000	1039.8758,	1131.5251,	1170.9648,
	8	1.501452000	1.992655000	0.776342000	1220.0266,	1230.6027,	1327.2993,
	8	1.494503000	1.679255000	-0.639815000	1342.4353,	1353.4055,	1394.8662,
	6	-1.452298000	0.132988000	0.059763000	1404.6693,	1429.184,	1472.1557,
	1	-0.888213000	0.852545000	0.662167000	1486.435,	1498.2187,	1505.3425,
	6	-2.324702000	-0.689711000	1.028243000	1510.6317,	1523.7448,	1531.7216,
	1	-2.888482000	-1.453754000	0.482618000	1534.9481,	1944.4763,	3064.5067,
	1	-1.700942000	-1.178572000	1.780171000	3067.4629,	3081.2162,	3114.5854,
	1	-3.037565000	-0.033129000	1.537490000	3152.3707,	3157.5077,	3161.898,
	6	-2.311261000	0.879626000	-0.962880000	3170.2622,	3178.8165,	3211.5386,
	1	-3.006993000	1.556880000	-0.458491000	3215.42,	3661.2325,	3863.5541
	1	-1.692270000	1.471105000	-1.644992000			
	1	-2.897625000	0.174324000	-1.562084000			
PC5e	6	-2.602369000	-1.724418000	-0.242770000	33.4093,	43.1938,	48.4982,
	6	-1.864062000	-0.436780000	0.066731000	66.7686,	87.6998,	100.0072,
	6	-0.377013000	-0.421648000	-0.308696000	105.1723,	156.913,	165.2061,
	6	0.274004000	0.910002000	-0.092185000	167.9654,	182.1404,	235.31,
	8	-2.416152000	0.522282000	0.572765000	304.0441,	370.5647,	380.0085,
	1	-2.041201000	-2.587021000	0.128019000	443.0201,	468.3162,	574.2759,
	1	-2.693838000	-1.833662000	-1.328724000	614.2791,	792.9184,	825.5476,
	1	-3.596208000	-1.695543000	0.205136000	836.2395,	939.6493,	943.723,
	1	-0.297066000	-0.739492000	-1.357742000	967.9744,	999.072,	1041.3501,
	1	0.120212000	-1.202554000	0.282620000	1043.5491,	1089.9264,	1189.4052,
	1	2.110001000	0.045342000	-0.566391000	1195.902,	1301.616,	1340.6264,
	1	3.492800000	-1.171575000	0.942200000	1351.5202,	1352.3401,	1398.0115,
	8	2.694224000	-1.407792000	0.458711000	1409.0274,	1419.1849,	1464.6349,
	8	2.853920000	-0.565072000	-0.705642000	1484.8076,	1486.1925,	1491.9909,
	6	0.621854000	1.292837000	1.313377000	1496.127,	1502.5332,	1508.8352,
	1	-0.285178000	1.609085000	1.850342000	1517.4962,	1789.7307,	3029.5619,
	1	1.056315000	0.447677000	1.855882000	3033.2463,	3057.7915,	3078.4034,
	1	1.329597000	2.128234000	1.336196000	3110.83,	3113.4645,	3116.5342,
	6	-0.032042000	2.001897000	-1.069390000	3154.7815,	3159.7062,	3163.5361,
	1	0.703387000	2.810824000	-1.010352000	3202.9333,	3658.1488,	3858.8151
	1	-0.057466000	1.626446000	-2.097633000			

PC6e	1	-1.019526000	2.435568000	-0.848637000			
	6	3.114283000	-0.513311000	-0.326661000	30.5396,	48.6286,	59.9143,
	6	1.634474000	-0.363457000	-0.051627000	86.6887,	99.9212,	108.7253,
	6	0.988713000	0.930096000	-0.539966000	112.6324,	130.5545,	164.5262,
	6	-0.370562000	1.191550000	0.023500000	183.7888,	187.8092,	245.5713,
	8	1.006348000	-1.231449000	0.531629000	301.2729,	315.714,	350.7901,
	1	3.354098000	-0.190194000	-1.343672000	426.7297,	463.7072,	599.1517,
	1	3.417347000	-1.549067000	-0.172261000	649.3239,	809.4354,	821.9382,
	1	3.667406000	0.133386000	0.363420000	841.9854,	938.684,	952.9114,
	1	0.954039000	0.857150000	-1.636339000	986.1411,	998.9391,	1014.9512,
	1	1.692816000	1.752715000	-0.321368000	1043.8072,	1077.2992,	1188.868,
	1	-2.701268000	-0.835394000	-0.849113000	1206.9529,	1302.9803,	1337.1112,
	1	-0.876542000	-1.399630000	0.618967000	1339.9596,	1378.5724,	1405.3474,
	8	-1.830495000	-1.580166000	0.619537000	1419.0266,	1427.5495,	1452.6347,
	8	-2.071670000	-1.561365000	-0.808802000	1484.091,	1493.3709,	1498.2011,
	6	-1.448576000	1.693735000	-0.881152000	1499.3122,	1507.1655,	1517.1678,
	1	-1.445846000	1.160706000	-1.837156000	1531.3205,	1778.6716,	3001.2651,
	1	-1.327054000	2.766907000	-1.103301000	3011.8678,	3017.4737,	3078.1165,
	1	-2.433407000	1.577297000	-0.415547000	3086.0339,	3101.1093,	3116.6451,
	6	-0.502499000	1.430478000	1.494107000	3152.7363,	3162.5382,	3166.1643,
	1	0.275060000	0.912275000	2.061587000	3206.3929,	3724.3025,	3875.3215
	1	-1.473640000	1.078245000	1.856347000			
	1	-0.431478000	2.504898000	1.730307000			
PC7e	6	-2.178037000	1.435299000	0.744244000	47.0456,	60.7819,	68.0085,
	6	-0.852753000	1.271698000	0.030804000	77.6417,	100.0893,	128.6639,
	6	0.202052000	0.475480000	0.784278000	149.2663,	154.9487,	178.029,
	6	1.368830000	0.023903000	-0.099223000	197.9158,	233.3495,	260.6274,
	6	2.045732000	-1.186723000	0.464581000	304.3009,	359.3109,	405.4476,
	8	-0.654871000	1.723668000	-1.082785000	434.9896,	470.1184,	530.1868,
	1	-2.777234000	2.199476000	0.247615000	606.473,	665.2114,	818.0069,
	1	-2.027986000	1.690426000	1.797520000	839.5615,	892.5783,	937.3976,
	1	-2.699096000	0.473109000	0.702583000	949.6138,	980.3995,	1002.0598,
	1	0.569747000	1.100369000	1.612251000	1008.7055,	1113.5397,	1163.5576,
	1	-0.302279000	-0.379274000	1.247336000	1173.5365,	1204.6388,	1266.4088,
	1	0.956146000	-0.223298000	-1.085056000	1326.0256,	1337.0043,	1347.3977,
	1	2.774514000	-1.720215000	-0.138808000	1391.8568,	1404.1773,	1417.4566,
	1	2.093850000	-1.330515000	1.540303000	1460.3188,	1476.8015,	1490.5154,
	1	0.130441000	-2.365364000	0.118627000	1491.6797,	1499.7569,	1512.9684,
	1	-1.626915000	-2.172876000	-1.471620000	1525.4275,	1782.5627,	3055.2223,
	8	-1.401079000	-1.649477000	-0.694858000	3068.1275,	3077.7481,	3088.7575,
	8	-0.790301000	-2.667960000	0.130122000	3129.939,	3157.6496,	3165.5686,
	6	2.380183000	1.168552000	-0.309595000	3170.6073,	3180.0082,	3200.364,
	1	1.870951000	2.031799000	-0.744294000	3282.9664,	3737.9873,	3854.0978
	1	3.184329000	0.860095000	-0.984499000			
	1	2.827499000	1.457175000	0.647671000			
PC8e	6	1.752060000	-0.174452000	0.305209000	47.0194,	72.0386,	92.5472,
	6	1.148162000	-1.539909000	0.170581000	105.212,	115.1665,	128.7847,
	1	1.782788000	0.077125000	1.374737000	159.6484,	168.0279,	183.568,

	1	-0.997465000	-1.591010000	-1.049867000	203.9053,	253.4581,	283.5591,
	1	0.274952000	-1.809523000	0.751510000	322.7493,	351.5004,	425.6547,
	1	1.684237000	-2.324093000	-0.353288000	439.758,	476.3085,	550.0669,
	1	-2.067543000	-0.811348000	0.843984000	581.3806,	612.2028,	829.2596,
	8	-2.333579000	-1.539924000	0.262507000	845.8929,	877.5997,	938.7903,
	8	-1.807065000	-1.066670000	-0.995224000	940.9014,	979.7022,	996.9357,
	6	3.174431000	-0.137314000	-0.259577000	1020.6249,	1102.4955,	1163.1684,
	1	3.164079000	-0.356730000	-1.332967000	1211.5203,	1212.5872,	1217.7289,
	1	3.807066000	-0.881122000	0.233463000	1322.288,	1366.3749,	1380.0265,
	1	3.629236000	0.847890000	-0.117444000	1386.1261,	1407.7338,	1425.2743,
	6	0.891879000	0.909492000	-0.364929000	1457.8152,	1476.4932,	1488.1377,
	1	0.724506000	0.678116000	-1.425546000	1490.8928,	1500.5376,	1517.0179,
	1	1.425072000	1.871703000	-0.344914000	1524.3125,	1768.8328,	3050.8542,
	6	-0.457412000	1.133155000	0.291013000	3061.8437,	3066.5447,	3083.3201,
	8	-0.760435000	0.574597000	1.335895000	3105.8693,	3154.2548,	3163.669,
	6	-1.397387000	2.084365000	-0.412372000	3174.4224,	3192.4896,	3200.579,
	1	-1.827952000	1.556640000	-1.268769000	3313.4419,	3752.7435,	3804.1436
	1	-0.862684000	2.963809000	-0.781766000			
	1	-2.198050000	2.382506000	0.265885000			
P1e	6	2.617969000	-0.633219000	0.421263000	52.8603,	100.6974,	176.843,
	6	1.402353000	0.012137000	-0.129529000	226.8636,	260.2188,	267.5332,
	1	3.573041000	-0.158066000	0.236021000	317.4224,	344.0777,	416.6965,
	1	2.568595000	-1.556174000	0.986046000	437.0224,	504.9064,	604.1707,
	6	0.096800000	-0.730065000	0.126484000	638.1893,	835.4023,	866.9496,
	8	1.461634000	1.033837000	-0.753136000	911.1651,	941.5059,	975.5376,
	1	0.058026000	-1.029766000	1.183408000	991.0843,	1005.589,	1126.7106,
	1	0.164003000	-1.665293000	-0.449763000	1158.8957,	1206.7425,	1220.3546,
	6	-1.152908000	0.056048000	-0.261002000	1262.6257,	1330.2272,	1376.7538,
	1	-0.984205000	0.460691000	-1.265169000	1414.3335,	1415.5461,	1431.0231,
	6	-1.374646000	1.228707000	0.696140000	1455.8375,	1474.4025,	1506.8471,
	1	-1.525920000	0.858826000	1.717933000	1513.8455,	1523.9412,	1534.8003,
	1	-0.519447000	1.907866000	0.688305000	2116.0711,	3047.2813,	3058.1911,
	1	-2.265358000	1.797152000	0.409977000	3061.6412,	3094.7742,	3108.5645,
	6	-2.373440000	-0.865096000	-0.288228000	3142.639,	3148.7228,	3155.1169,
	1	-3.273942000	-0.309367000	-0.568296000	3179.9651,	3202.129,	3336.0612
	1	-2.240421000	-1.682062000	-1.005375000			
	1	-2.544219000	-1.305575000	0.701223000			
P2e	6	2.612911000	-0.634115000	0.394545000	51.6378,	80.0798,	94.261,
	6	1.371247000	0.059672000	-0.136760000	172.0851,	232.8278,	270.6189,
	6	0.080748000	-0.582448000	0.199721000	302.135,	334.236,	411.1066,
	8	1.419090000	1.070012000	-0.786035000	420.7502,	508.8534,	614.1456,
	1	2.636060000	-1.672326000	0.049581000	646.6486,	848.3343,	887.1916,
	1	2.580970000	-0.648893000	1.488645000	941.1069,	967.1047,	987.4323,
	1	3.500046000	-0.101417000	0.053741000	1017.2403,	1046.2235,	1130.2205,
	1	0.070425000	-1.459595000	0.843649000	1170.2026,	1216.3935,	1220.6686,
	6	-1.199763000	0.031981000	-0.249147000	1330.6424,	1344.262,	1391.7561,
	1	-1.014117000	0.483678000	-1.230757000	1403.4645,	1429.7682,	1458.7263,
	6	-1.587564000	1.175683000	0.709530000	1485.0203,	1495.7503,	1505.7848,

	1	-1.742902000	0.789716000	1.722778000	1512.0693,	1523.9325,	1531.788,
	1	-0.802148000	1.934384000	0.733849000	2101.9551,	3064.7006,	3066.481,
	1	-2.518020000	1.645312000	0.374057000	3080.8084,	3097.7741,	3151.6015,
	6	-2.318771000	-1.005945000	-0.353939000	3156.2057,	3162.7144,	3166.7707,
	1	-3.241946000	-0.539601000	-0.711307000	3180.1783,	3208.61,	3214.5834
	1	-2.051693000	-1.809837000	-1.046415000			
	1	-2.522242000	-1.450493000	0.626758000			
P3e	6	-2.646761000	0.093455000	-0.278695000	43.0671,	79.6578,	102.3901,
	6	-1.204010000	-0.071952000	0.161166000	151.1991,	153.0986,	166.6567,
	6	-0.148268000	0.089786000	-0.941775000	300.433,	351.1898,	375.3147,
	6	1.257373000	0.082760000	-0.432312000	437.1858,	462.348,	610.5248,
	8	-0.904528000	-0.307763000	1.316276000	792.348,	819.3935,	835.4869,
	1	-2.840456000	-0.471794000	-1.194944000	944.6344,	967.5497,	996.5722,
	1	-2.833689000	1.150377000	-0.497614000	1037.7925,	1041.6889,	1079.8523,
	1	-3.314871000	-0.233869000	0.518636000	1185.69,	1191.056,	1296.6636,
	1	-0.376621000	1.021299000	-1.479300000	1347.4018,	1353.6346,	1397.0126,
	1	-0.315010000	-0.726569000	-1.659653000	1413.6549,	1422.0979,	1460.7666,
	6	1.868245000	-1.234945000	-0.073897000	1485.8713,	1489.6117,	1496.9847,
	1	1.515246000	-1.565936000	0.914845000	1503.0221,	1503.5859,	1519.7826,
	1	1.598384000	-2.011616000	-0.797246000	1794.3969,	3025.5755,	3029.2682,
	1	2.960466000	-1.168209000	-0.029809000	3045.6454,	3077.2522,	3097.7374,
	6	1.745277000	1.306140000	0.277796000	3108.8661,	3110.1457,	3149.8513,
	1	2.839200000	1.332041000	0.318887000	3152.1998,	3162.1689,	3201.9563
	1	1.396517000	2.221166000	-0.212737000			
	1	1.375921000	1.323755000	1.315030000			
P4e	6	-2.559234000	-0.551265000	0.435723000	56.575,	100.8092,	130.4339,
	6	-1.303093000	0.038282000	-0.175335000	132.6643,	178.1078,	253.886,
	6	-0.024660000	-0.761305000	0.032023000	304.0474,	345.525,	391.0764,
	6	1.256277000	0.017850000	-0.270005000	425.7919,	472.7644,	546.3359,
	6	2.437123000	-0.899528000	-0.325987000	606.098,	813.3383,	843.2364,
	8	-1.318607000	1.080143000	-0.805943000	876.1892,	945.717,	975.3298,
	1	-3.438338000	-0.035473000	0.047766000	993.9349,	1012.2947,	1114.5731,
	1	-2.515555000	-0.428075000	1.523526000	1162.0527,	1166.0589,	1205.0809,
	1	-2.623387000	-1.623872000	0.229581000	1266.6881,	1322.2067,	1350.0451,
	1	-0.005539000	-1.155396000	1.057774000	1395.7967,	1408.7213,	1417.8393,
	1	-0.098367000	-1.638529000	-0.627232000	1462.3904,	1485.8506,	1492.1424,
	1	1.126381000	0.502948000	-1.244397000	1498.4562,	1512.8886,	1525.0225,
	1	3.345635000	-0.587303000	-0.828500000	1778.3438,	3051.3494,	3067.1461,
	1	2.503686000	-1.739875000	0.357572000	3075.6267,	3092.8792,	3106.1625,
	6	1.471505000	1.130815000	0.774812000	3157.6635,	3159.6591,	3171.5512,
	1	0.629196000	1.827877000	0.773547000	3184.0959,	3201.3146,	3298.3165
	1	2.383525000	1.693675000	0.556248000			
	1	1.574118000	0.693785000	1.774271000			
P5e	6	1.240514000	0.118359000	-0.235719000	55.1325,	105.1788,	130.4445,
	6	1.363852000	1.235949000	0.752473000	146.9015,	172.527,	251.4864,
	1	1.102025000	0.553160000	-1.232893000	310.3416,	334.3381,	394.7609,
	1	0.748831000	2.121335000	0.659360000	419.6124,	474.3705,	496.9158,
	1	1.947173000	1.096331000	1.656498000	608.2962,	825.581,	848.9144,

	6	2.489176000	-0.767609000	-0.237237000	872.322,	929.7005,	974.0774,
	1	2.625775000	-1.236428000	0.743915000	993.2218,	1016.9605,	1112.3094,
	1	3.382977000	-0.177030000	-0.457680000	1157.9884,	1196.582,	1205.3693,
	1	2.407169000	-1.562342000	-0.985702000	1233.0738,	1319.2355,	1373.7134,
	6	-0.011471000	-0.727785000	0.050251000	1385.8956,	1404.2684,	1423.2529,
	1	0.015799000	-1.125320000	1.073538000	1460.1149,	1484.5617,	1486.2484,
	1	-0.038607000	-1.602303000	-0.618264000	1498.2794,	1516.8266,	1522.8446,
	6	-1.315865000	0.027252000	-0.159471000	1778.7792,	3043.9046,	3063.7571,
	8	-1.358562000	1.084786000	-0.761955000	3075.6289,	3088.8632,	3106.3795,
	6	-2.558808000	-0.620885000	0.418227000	3150.7588,	3159.9588,	3163.0852,
	1	-2.538733000	-0.512896000	1.508331000	3194.6076,	3201.1343,	3318.3482
	1	-2.578012000	-1.691693000	0.194669000			
	1	-3.450300000	-0.132784000	0.022729000			
H₂O₂	8	-0.713335000	-0.117508000	-0.052406000	367.169,	943.1713,	1310.4888,
	8	0.713335000	0.117507000	-0.052407000	1466.7615,	3871.1361,	3874.1596
	1	1.000400000	-0.670310000	0.419253000			
	1	-1.000397000	0.670311000	0.419253000			
