

ESI

Geometries and Vibrational Frequencies at BB1K/6-311++G(2df,2p) Level
Gaussian-03 Input: BB95 Iop(3/76=0580004200)

***** OH // BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2
O,0,0.,0.,-0.1071096957
H,0,0.,0.,0.8568775658
Rotational constants (GHZ): 0.0000000 573.6228489 573.6228489
SCF Done: E(UB+HF-B95) = -75.7295757730 A.U. after 1 cycles
S**2 = 0.7529
Frequencies -- 3853.5047

***** O2 // BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,3
O,0,0.,0.,-0.5903923498
O,0,0.,0.,0.5903923498
Rotational constants (GHZ): 0.0000000 45.3235409 45.3235409
SCF Done: E(UB+HF-B95) = -150.316038889 A.U. after 1 cycles
S**2 = 2.0131
Frequencies -- 1789.4604

***** C10H8 // BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,1
C,0,0.,0.705689088,0.
C,0,0.,-0.705689088,0.
C,0,1.2304870312,1.3858634703,0.
C,0,1.2304870312,-1.3858634703,0.
C,0,-1.2304870312,1.3858634703,0.
C,0,-1.2304870312,-1.3858634703,0.
C,0,2.4039239065,0.7012738404,0.
C,0,2.4039239065,-0.7012738404,0.
C,0,-2.4039239065,0.7012738404,0.
C,0,-2.4039239065,-0.7012738404,0.
H,0,1.2269068059,2.4633259498,0.
H,0,1.2269068059,-2.4633259498,0.
H,0,-1.2269068059,2.4633259498,0.
H,0,-1.2269068059,-2.4633259498,0.
H,0,3.3394714519,1.2335466513,0.
H,0,3.3394714519,-1.2335466513,0.
H,0,-3.3394714519,1.2335466513,0.
H,0,-3.3394714519,-1.2335466513,0.
Rotational constants (GHZ): 3.1916674 1.2600228 0.9033813
E(RB+HF-B95) = -385.808645765
Frequencies -- 176.9650 190.8414 358.0299
Frequencies -- 405.7599 486.8741 499.7780
Frequencies -- 518.1104 525.2472 631.0080
Frequencies -- 653.0848 751.4024 797.3429
Frequencies -- 812.7690 816.9628 826.1727
Frequencies -- 877.8965 931.4810 964.1109
Frequencies -- 1002.5863 1023.3402 1033.1895
Frequencies -- 1039.3173 1063.4715 1073.8456
Frequencies -- 1172.2761 1180.4144 1194.6905
Frequencies -- 1201.3744 1261.5661 1292.3038
Frequencies -- 1314.3047 1430.3946 1446.1937
Frequencies -- 1457.6295 1526.4738 1528.0550
Frequencies -- 1597.2838 1678.8144 1700.3077
Frequencies -- 1738.3779 3234.6302 3235.3052
Frequencies -- 3239.0734 3241.0686 3253.4549
Frequencies -- 3254.0472 3266.3875 3267.0522

***** C10H8-1-OH (R1) // BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

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0,2

C,0,1.0931481307,1.2310840917,0.0152596102
C,0,2.1548162376,0.5319439214,0.7794156782
C,0,2.0644014684,-0.7726077388,1.1405622947
C,0,0.9583925162,-1.5470363124,0.8050291609
C,0,-1.2582590606,-1.7432132021,-0.2341502836
C,0,-2.3081641521,-1.1909579195,-0.9203809178
C,0,-2.2582699142,0.1391429612,-1.3048060575
C,0,-1.1525488445,0.9008895433,-0.9951553023
C,0,-0.0868594426,0.3593549731,-0.3056657985
C,0,-0.1300647801,-0.9833886806,0.0863985386
O,0,0.6969004505,2.4245704112,0.6711599362
H,0,1.5166273013,1.5960633506,-0.9210485675
H,0,3.0130935729,1.1229843524,1.0499338082
H,0,2.8662319365,-1.2217236812,1.7026982052
H,0,0.9067875305,-2.5799509323,1.1025677593
H,0,-1.2911692959,-2.776547426,0.0695732552
H,0,-3.1697989125,-1.7902219389,-1.159365793
H,0,-3.0803208015,0.5768403985,-1.8441014352
H,0,-1.1124133181,1.9388876501,-1.2804882339
H,0,0.3162054304,2.185835114,1.5119099754
Rotational constants (GHZ): 1.9933939 1.0974123 0.7349935
SCF Done: E(UB+HF-B95) = -461.579688937 A.U. after 1 cycles
S**2 = 0.7936

Frequencies --	53.9046	154.4913	207.0469
Frequencies --	268.1032	320.2804	391.5331
Frequencies --	416.1210	467.8540	488.1169
Frequencies --	517.1721	533.5990	575.9448
Frequencies --	641.8698	713.9984	746.3746
Frequencies --	786.3504	801.9320	824.2326
Frequencies --	836.5354	912.6785	925.1170
Frequencies --	1005.0919	1005.9499	1020.6634
Frequencies --	1033.7366	1079.1843	1092.7780
Frequencies --	1116.3765	1164.5743	1187.4425
Frequencies --	1192.5744	1241.9892	1250.8754
Frequencies --	1262.8690	1305.0462	1356.4180
Frequencies --	1387.8133	1416.0103	1426.6584
Frequencies --	1470.9338	1508.5105	1559.1677
Frequencies --	1601.9625	1660.8330	1692.2866
Frequencies --	3064.0685	3233.9995	3235.6505
Frequencies --	3243.4750	3253.2290	3254.6657
Frequencies --	3262.4269	3267.6421	3946.9005

***** TS C10H8 + OH --> C10H8-1-OH //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2

C,0,-0.1878608899,0.4677143819,-0.2732554903
C,0,-0.1416255576,-0.9328324844,-0.1539872587
C,0,1.0290806821,1.2035492243,-0.2578881458
C,0,1.1123698578,-1.5726903727,-0.0609402765
C,0,-1.427517588,1.1028847549,-0.3887051709
C,0,-1.3445919634,-1.655481865,-0.1458088384
C,0,2.2378276481,0.5313507577,-0.2307653463
C,0,2.2719817288,-0.856154508,-0.1037824827
C,0,-2.5821709679,0.3779894664,-0.383719821
C,0,-2.5401942177,-1.0139688425,-0.2590335443
H,0,1.0006585937,2.24755359,-0.5076101148
H,0,1.1388308547,-2.6457415188,0.0319663734
H,0,-1.4555618397,2.1762045672,-0.4700852833
H,0,-1.3063618222,-2.7280929366,-0.0514858468
H,0,3.1526027044,1.0944753779,-0.2726735555
H,0,3.2203750108,-1.3615650585,-0.0472639289
H,0,-3.5317553013,0.8767927401,-0.4720831134
H,0,-3.4573139977,-1.577237999,-0.2534499812
O,0,1.1806398012,1.873876408,1.6857002953
H,0,1.2296149942,1.0124368975,2.104401337

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Rotational constants (GHZ):	1.9540208	1.0269216	0.7575522
SCF Done: E(UB+HF-B95) =	-461.539855860	A.U. after	1 cycles
S**2 =	0.7997		
Frequencies --	-328.0632	93.1007	98.4485
Frequencies --	170.4008	188.2480	207.2971
Frequencies --	360.7793	386.3175	479.4738
Frequencies --	504.9338	517.5324	521.5658
Frequencies --	623.0294	634.2720	752.7350
Frequencies --	760.2296	795.5178	812.3813
Frequencies --	817.3177	826.1176	896.4283
Frequencies --	932.8849	961.9855	997.2621
Frequencies --	1017.8493	1026.9030	1038.8368
Frequencies --	1062.8811	1077.5300	1162.7027
Frequencies --	1183.1684	1186.7891	1199.5972
Frequencies --	1255.7914	1286.8107	1313.4376
Frequencies --	1419.6995	1434.6137	1443.0489
Frequencies --	1517.5530	1521.4571	1582.8483
Frequencies --	1651.2593	1668.1561	1719.7142
Frequencies --	3236.5979	3239.2249	3245.2296
Frequencies --	3256.3576	3258.0555	3268.2366
Frequencies --	3271.1172	3283.4986	3903.0058

***** C10H8-2-OH // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,0.719197232,1.2642206759,0.3582613445			
C,0,1.6496648516,0.6347725864,1.3168620086			
C,0,1.458860891,-0.8376794365,1.4245703917			
C,0,0.5862141619,-1.5087774384,0.6837547251			
C,0,-1.1623488759,-1.5662463595,-1.0531710057			
C,0,-1.9823080229,-0.9236874927,-1.9571253835			
C,0,-1.9126357775,0.4591242315,-2.0949776663			
C,0,-1.0336504331,1.1832366649,-1.3405344379			
C,0,-0.1791721459,0.5500447667,-0.4149990967			
C,0,-0.2633328823,-0.8600167408,-0.2802729543			
O,0,1.4918166269,1.2844224688,2.5693336397			
H,0,0.7590372133,2.3377547208,0.2816432597			
H,0,2.6745580163,0.8246100787,0.9705723464			
H,0,2.076610284,-1.3560039861,2.140887656			
H,0,0.4893124534,-2.5769045211,0.7955724649			
H,0,-1.2203788662,-2.6365667484,-0.9408655866			
H,0,-2.6765346273,-1.4899400227,-2.5529530739			
H,0,-2.5545141951,0.9601889821,-2.7990046153			
H,0,-0.978851019,2.2541036653,-1.4440658811			
H,0,2.2132937331,1.0374293365,3.1393367598			
Rotational constants (GHZ):	2.7061160	0.8408745	0.6615352
SCF Done: E(UB+HF-B95) =	-461.567954230	A.U. after	1 cycles
S**2 =	0.8013		
Frequencies --	68.1172	160.9816	202.2772
Frequencies --	221.4507	289.0000	368.7830
Frequencies --	408.5181	439.3862	481.0714
Frequencies --	511.1573	526.1204	611.9665
Frequencies --	630.1477	733.9681	736.2178
Frequencies --	777.0354	783.9078	813.1245
Frequencies --	842.0256	901.8344	928.5215
Frequencies --	942.6624	989.6719	1020.8892
Frequencies --	1031.1133	1071.4642	1083.7355
Frequencies --	1106.2919	1163.3931	1179.0757
Frequencies --	1192.9281	1219.1249	1233.0238
Frequencies --	1272.4891	1321.3470	1357.9120
Frequencies --	1379.9906	1434.3257	1452.0845
Frequencies --	1476.8622	1497.9475	1548.9429
Frequencies --	1622.4713	1660.1448	1737.9784
Frequencies --	2963.1165	3219.1153	3233.8477
Frequencies --	3238.9582	3240.5052	3248.5910
Frequencies --	3253.5461	3267.5084	3965.2346

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***** TS C10H8 + OH --> C10H8-2-OH //
BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,-0.3199165377,0.572995733,-0.2716255995
C,0,-0.3145785009,-0.8366542515,-0.1922623364
C,0,0.9035035223,1.2570664269,-0.3055562843
C,0,0.9281457738,-1.5174630881,-0.1498476417
C,0,-1.5509208804,1.2490755675,-0.3278538256
C,0,-1.5357058303,-1.5177426243,-0.1676950435
C,0,2.1056679179,0.5792726584,-0.1913918476
C,0,2.0954002293,-0.8427564345,-0.1643414925
C,0,-2.7242303144,0.5599399049,-0.3036336737
C,0,-2.7165597836,-0.8364037736,-0.2217206191
H,0,0.9060637019,2.3304229658,-0.3826024138
H,0,0.9209754231,-2.5940974316,-0.1081712592
H,0,-1.5485802736,2.3246375314,-0.3887215517
H,0,-1.5309817617,-2.593362964,-0.1064426808
H,0,3.0244849885,1.0916323765,-0.4031530068
H,0,3.0331533806,-1.3678324694,-0.126814373
H,0,-3.6613612162,1.0873123866,-0.3461005722
H,0,-3.6489926959,-1.3736306802,-0.2023376347
O,0,2.4486549372,1.0598393729,1.7176430201
H,0,1.6911653803,0.6122225892,2.0987695152
Rotational constants (GHZ): 2.3498643 0.8739099 0.7111746
SCF Done: E(UB+HF-B95) = -461.538136072 A.U. after 1 cycles
S**2 = 0.8010
Frequencies -- -394.2741 85.4393 114.3373
Frequencies -- 183.0021 209.4133 218.9936
Frequencies -- 366.2180 397.2331 463.2743
Frequencies -- 495.6675 517.1967 523.0493
Frequencies -- 626.2465 629.9416 768.6607
Frequencies -- 788.2250 794.8619 799.3553
Frequencies -- 832.7393 848.4786 877.8775
Frequencies -- 926.6460 962.5265 1001.9775
Frequencies -- 1011.3490 1027.4199 1037.7974
Frequencies -- 1054.3100 1073.7403 1164.1103
Frequencies -- 1182.7051 1187.2913 1199.9088
Frequencies -- 1253.1773 1290.1236 1316.9206
Frequencies -- 1422.1249 1442.0536 1459.4532
Frequencies -- 1508.6507 1523.6390 1582.9686
Frequencies -- 1648.8489 1689.5807 1708.7343
Frequencies -- 3237.2126 3239.5682 3242.4944
Frequencies -- 3255.5391 3258.8283 3268.1921
Frequencies -- 3268.3426 3287.7925 3903.5359

***** C10H8-10H-200-Syn (R1-200-s) //
BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,0.7340339488,1.0343720119,-0.4708437446
C,0,1.8506911934,0.2792432499,0.2150010189
C,0,1.9498951061,-1.1064887114,-0.3145657752
C,0,0.8527075181,-1.7448689948,-0.6988350772
C,0,-1.620577933,-1.8756570091,-0.7404398791
C,0,-2.8518953992,-1.2659077856,-0.629682159
C,0,-2.9267756577,0.0951592333,-0.4229067946
C,0,-1.7728367429,0.8523511098,-0.3424509057
C,0,-0.5443294748,0.247060089,-0.4524487164
C,0,-0.4604468037,-1.1292390853,-0.6408238997
O,0,0.5943908316,2.3462495568,-0.0360320205
O,0,1.5833080978,0.14751262,1.6374350874
O,0,1.7323177116,1.2598070541,2.2663557149
H,0,1.0535859235,1.0840577745,-1.5143543972
H,0,2.7746210797,0.838623016,0.1353791782
H,0,2.9092974769,-1.5922514813,-0.3114114079

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H,0,0.914350953,-2.7680198353,-1.0331102129			
H,0,-1.5532866378,-2.9401613546,-0.8935306201			
H,0,-3.7509592375,-1.8529454232,-0.7011399958			
H,0,-3.8868932215,0.5727195348,-0.3298208147			
H,0,-1.8185813875,1.9172691752,-0.1986734769			
H,0,0.8149373922,2.3960101,0.8925670878			
Rotational constants (GHZ): 1.4292323 0.7018330 0.5601687			
SCF Done: E(UB+HF-B95) = -611.915622205 A.U. after 1 cycles			
S**2 = 0.7563			
Frequencies --	52.1206	111.1491	133.6581
Frequencies --	199.8844	234.2498	267.4166
Frequencies --	279.2228	333.1630	396.7368
Frequencies --	422.5707	455.7098	489.8708
Frequencies --	505.9415	549.7761	565.1310
Frequencies --	595.1353	696.0789	729.0308
Frequencies --	759.0020	793.8022	821.4656
Frequencies --	842.7796	874.9833	930.2095
Frequencies --	989.3682	1012.2079	1025.0747
Frequencies --	1042.3669	1046.9416	1080.2400
Frequencies --	1082.4196	1145.0245	1185.0387
Frequencies --	1195.7989	1203.1526	1243.5690
Frequencies --	1264.4877	1289.2583	1312.5206
Frequencies --	1315.6781	1340.6720	1365.2119
Frequencies --	1384.5076	1402.1805	1442.7909
Frequencies --	1456.7768	1528.4043	1559.9707
Frequencies --	1677.4501	1710.2545	1748.8718
Frequencies --	3058.3979	3170.5669	3235.0584
Frequencies --	3237.8664	3249.4344	3265.1866
Frequencies --	3269.4063	3274.8593	3890.8423

***** C10H8-10H-200-Anti (R1-200-a) //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,0.4040095008,0.9654724038,-0.1188142503			
C,0,1.5477341967,0.2969006874,0.6120737626			
C,0,1.789153843,-1.0886114028,0.1363923008			
C,0,0.7922871912,-1.8281890739,-0.3190461415			
C,0,-1.6474546905,-2.1575849534,-0.5772015427			
C,0,-2.9306426615,-1.6541137404,-0.5905109253			
C,0,-3.1363393416,-0.3033744314,-0.4114572332			
C,0,-2.0610760315,0.5466824266,-0.233107222			
C,0,-0.7795721781,0.0471461651,-0.2222921124			
C,0,-0.566251137,-1.3172981647,-0.3845788564			
O,0,0.0084824299,2.1574225883,0.4811170975			
O,0,2.7729193815,1.0178400055,0.359973278			
O,0,2.7723163335,2.1944246554,0.8774392992			
H,0,0.7634662001,1.1498659332,-1.1378267564			
H,0,1.3824608772,0.3414898027,1.6874938766			
H,0,2.7903970578,-1.4733884541,0.2261452328			
H,0,0.9658170417,-2.8498356993,-0.6142093802			
H,0,-1.4769987816,-3.2136549917,-0.7062724721			
H,0,-3.7669415828,-2.3156932967,-0.735624455			
H,0,-4.1364150441,0.0944586914,-0.411777696			
H,0,-2.2126348532,1.6018501318,-0.0951530067			
H,0,0.7900117775,2.6652303916,0.690240582			
Rotational constants (GHZ): 1.8268721 0.5941758 0.4551877			
SCF Done: E(UB+HF-B95) = -611.916866381 A.U. after 1 cycles			
S**2 = 0.7561			
Frequencies --	46.5207	102.1580	127.6550
Frequencies --	195.2463	223.6346	289.2556
Frequencies --	314.1553	347.2941	409.7234
Frequencies --	427.2251	443.7360	470.2608
Frequencies --	514.1317	538.8739	543.8251
Frequencies --	592.4124	656.2464	729.6256
Frequencies --	741.8750	783.8608	827.0352
Frequencies --	857.0403	887.5847	932.2152

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Frequencies --	1007.9334	1029.2515	1035.9886
Frequencies --	1043.9954	1048.3124	1093.1557
Frequencies --	1112.2037	1144.5896	1188.1687
Frequencies --	1200.4274	1207.2869	1238.7865
Frequencies --	1267.8395	1272.5267	1300.4939
Frequencies --	1323.5560	1329.4820	1338.1992
Frequencies --	1371.0970	1417.7536	1433.2807
Frequencies --	1463.3397	1525.4166	1567.4378
Frequencies --	1678.0639	1709.4619	1764.1425
Frequencies --	3011.4277	3102.0572	3237.8180
Frequencies --	3240.1271	3250.4522	3264.5778
Frequencies --	3266.1696	3288.0897	3904.9973

***** C10H8-10H-400-Syn (R1-400-s) //
BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,0.7551503529,1.5894363112,0.2230824423			
C,0,1.9713845654,0.8804162755,0.7180579458			
C,0,2.0614130694,-0.431746866,0.7884172137			
C,0,0.932516399,-1.3030829663,0.3891454864			
C,0,-0.878492079,-1.4562159253,-1.3042604027			
C,0,-1.808370655,-0.8805633237,-2.1382255229			
C,0,-1.9025072805,0.4958252597,-2.2099071139			
C,0,-1.0666826026,1.2824617582,-1.4505759757			
C,0,-0.1298336628,0.710446242,-0.6095108767			
C,0,-0.0403298542,-0.6661911402,-0.5376932098			
O,0,0.0556234173,2.1497967866,1.3105028098			
O,0,-0.3017120657,-0.7620335671,2.2459688155			
O,0,0.2285170994,-1.7380323374,1.6131096657			
H,0,1.0598072228,2.4400604173,-0.3794242351			
H,0,2.771698205,1.5018018583,1.0854190695			
H,0,2.9291571693,-0.9100422805,1.2107102164			
H,0,1.2720194806,-2.255625694,0.0005260143			
H,0,-0.7993612273,-2.5292393809,-1.2421087222			
H,0,-2.4559806474,-1.4998982976,-2.7340031234			
H,0,-2.625273623,0.9539847753,-2.8627969519			
H,0,-1.1379416507,2.3562349808,-1.501834067			
H,0,-0.2390420531,1.4201628142,1.8556815526			
Rotational constants (GHZ):	1.2536090	0.8237175	0.6291307
SCF Done: E(UB+HF-B95) = -611.909407901	A.U. after	1	cycles
S**2 = 0.7562			
Frequencies --	92.4206	99.4476	144.3330
Frequencies --	171.8557	198.3889	256.2388
Frequencies --	336.4609	352.4888	378.9325
Frequencies --	434.0608	505.1385	521.1223
Frequencies --	530.1042	537.3720	575.0986
Frequencies --	637.1366	689.8579	752.1138
Frequencies --	795.3863	799.3915	808.0555
Frequencies --	848.7206	882.0454	927.0887
Frequencies --	963.2848	1009.7710	1017.9772
Frequencies --	1044.5275	1051.1275	1062.0484
Frequencies --	1094.6629	1109.2742	1167.7792
Frequencies --	1199.6583	1211.3772	1249.5644
Frequencies --	1256.9396	1258.5096	1287.4765
Frequencies --	1310.3316	1379.4158	1394.9127
Frequencies --	1408.5232	1420.3225	1442.7664
Frequencies --	1461.3572	1536.5534	1575.6418
Frequencies --	1695.7544	1716.6928	1785.3872
Frequencies --	3124.9221	3164.1247	3234.2204
Frequencies --	3234.8179	3240.9368	3254.2220
Frequencies --	3255.6982	3267.8825	3912.9022

***** C10H8-10H-400-Anti (R1-400-a) //
BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

ESI			
0,2			
C,0,-1.3972048801,0.8731718782,-0.3757317681			
C,0,-0.511915288,1.9844757995,-0.8236314058			
C,0,0.7981912886,1.8771547528,-0.9091585411			
C,0,1.4778173423,0.5974452429,-0.6017107791			
C,0,1.3866128796,-1.1986226856,1.1141370138			
C,0,0.6938738789,-2.0218244599,1.9719270641			
C,0,-0.679309225,-1.9113803104,2.0616639742			
C,0,-1.3487256378,-0.9801566517,1.299472089			
C,0,-0.6566770156,-0.1499147033,0.4369426278			
C,0,0.7188098651,-0.2646064494,0.3434140176			
O,0,-2.5377568694,1.3567769577,0.2858783443			
O,0,1.7093790486,-0.1323748457,-1.8582568214			
O,0,0.6092451158,-0.4567351911,-2.430334535			
H,0,-1.7792559064,0.383128358,-1.2698184195			
H,0,-1.0160030086,2.895446038,-1.10347309			
H,0,1.4019401073,2.6932160925,-1.2678908676			
H,0,2.4928760638,0.750510304,-0.2560926902			
H,0,2.458488396,-1.2786190353,1.0370909665			
H,0,1.2209769483,-2.7444679201,2.5701753963			
H,0,-1.2292024473,-2.5505250534,2.7308790082			
H,0,-2.4181441612,-0.8825260233,1.3698182772			
H,0,-2.2674536001,1.7580473942,1.1070697619			
Rotational constants (GHZ):	1.1143773	0.8810029	0.5846731
SCF Done: E(UB+HF-B95) = -611.908568530	A.U. after	1 cycles	
S**2 = 0.7561			
Frequencies --	66.4369	95.3183	122.0678
Frequencies --	169.2976	207.0637	270.3071
Frequencies --	298.4852	342.2050	374.3585
Frequencies --	421.4933	453.8588	480.4830
Frequencies --	492.6179	541.8410	574.9135
Frequencies --	630.4028	695.1075	734.6187
Frequencies --	768.2782	795.1711	802.5792
Frequencies --	863.8778	893.2670	938.0078
Frequencies --	943.0613	1014.6378	1024.8583
Frequencies --	1046.1653	1047.4480	1064.5006
Frequencies --	1089.4085	1131.2751	1168.4742
Frequencies --	1195.8724	1200.6456	1239.4449
Frequencies --	1248.6754	1250.9198	1264.9682
Frequencies --	1301.0124	1361.2199	1377.0276
Frequencies --	1391.9973	1412.2206	1419.0457
Frequencies --	1444.1507	1529.5648	1563.9817
Frequencies --	1687.4693	1712.4024	1778.2574
Frequencies --	3104.2726	3166.4894	3234.4902
Frequencies --	3237.2764	3247.8587	3257.3131
Frequencies --	3262.4142	3270.6696	3949.8129

***** C10H8-10H-500-Syn (R1-500-s) //
BB1k=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,-0.9231017704,1.7166903783,-0.4790596175			
C,0,-1.9365842997,1.1390462006,-1.326979709			
C,0,0.1177550978,0.9932261155,-0.0508744595			
C,0,-1.95439646,-0.1571043075,-1.6162419316			
C,0,1.1620328958,1.5883845118,0.851341722			
C,0,0.238731438,-0.3820705681,-0.4628411481			
C,0,1.4031030815,-1.0261019971,-0.3128683641			
C,0,-0.9488338746,-1.0705703158,-1.0305885959			
O,0,-1.6618467591,-1.792677179,0.0493094005			
C,0,2.4408668995,0.8229404668,0.8459329168			
O,0,0.6942490176,1.7148089551,2.1814548893			
C,0,2.5343195446,-0.3935220392,0.3219731102			
O,0,-1.0131047671,-2.8273938555,0.4340520117			
H,0,-1.0037826177,2.7559437551,-0.2070621367			
H,0,-2.6930888228,1.7889656228,-1.7334023067			
H,0,-2.721032479,-0.5824237403,-2.2395770414			

ESI			
H,0,1.3479786681,2.6113525512,0.5405945291			
H,0,1.4999110062,-2.040455626,-0.661158862			
H,0,-0.6509959512,-1.8558832514,-1.714443531			
H,0,3.2756546438,1.2772594804,1.3522214719			
H,0,0.5272539273,0.8417973094,2.5271356936			
H,0,3.460366379,-0.9399701383,0.3783982317			
Rotational constants (GHZ): 1.2038184 0.7490054 0.5717679			
SCF Done: E(UB+HF-B95) = -611.862810552 A.U. after 1 cycles			
S**2 = 0.7570			
Frequencies --	42.5432	73.1946	114.4527
Frequencies --	139.2543	191.4609	230.4667
Frequencies --	298.1172	319.6446	362.2940
Frequencies --	396.4955	433.8406	461.7997
Frequencies --	500.6124	528.9254	551.9473
Frequencies --	591.8422	633.6277	743.3597
Frequencies --	762.3510	786.9219	796.6178
Frequencies --	805.3607	895.8730	932.6356
Frequencies --	943.4934	971.9230	999.6955
Frequencies --	1039.6487	1042.9074	1051.7714
Frequencies --	1070.7101	1078.6118	1096.8836
Frequencies --	1198.0131	1206.0710	1219.2559
Frequencies --	1259.5205	1276.0920	1300.6624
Frequencies --	1324.5518	1335.3550	1387.4738
Frequencies --	1396.0743	1426.5161	1450.6354
Frequencies --	1475.4539	1499.3702	1677.1824
Frequencies --	1688.3518	1744.5166	1770.9699
Frequencies --	3131.9811	3160.7063	3238.6284
Frequencies --	3238.9461	3251.1820	3253.4322
Frequencies --	3263.6311	3269.1316	3944.8820

***** C10H8-10H-500-Anti (R1-500-a) //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,-1.078614441,1.4801640145,-0.5067866639			
C,0,-2.3351147007,0.773630331,-0.5615767337			
C,0,0.0334949809,0.8699240783,-0.0811470007			
C,0,-2.4240098252,-0.5308497236,-0.3275443075			
C,0,1.3521588461,1.5821958207,-0.0023635669			
C,0,-0.0328699045,-0.5075688491,0.3486604039			
C,0,0.9412916033,-1.0236669199,1.1069852582			
C,0,-1.2084869487,-1.3249544664,-0.0475825855			
O,0,-0.9006895624,-2.0356607511,-1.3112065885			
C,0,2.2783207051,0.9785188807,0.9999611277			
O,0,1.2113432162,2.9666952584,0.1706727084			
C,0,2.0935596933,-0.2406526459,1.4878060956			
O,0,-0.0704101114,-2.9921458592,-1.1220961308			
H,0,-1.0447201585,2.5177899882,-0.789540908			
H,0,-3.2231905351,1.335330527,-0.7984154921			
H,0,-3.3649667598,-1.0487971011,-0.3848006437			
H,0,1.8414994485,1.482605222,-0.9747778843			
H,0,0.8554582289,-2.0358418255,1.4649134527			
H,0,-1.383624038,-2.1246612007,0.6612368058			
H,0,3.1386742687,1.5702737838,1.264541209			
H,0,0.7375540579,3.1196982925,0.98391413			
H,0,2.8029870956,-0.667949993,2.1754972551			
Rotational constants (GHZ): 1.2751667 0.7300497 0.5199339			
SCF Done: E(UB+HF-B95) = -611.863337961 A.U. after 1 cycles			
S**2 = 0.7570			
Frequencies --	45.4968	78.8182	113.0694
Frequencies --	154.2890	204.5512	248.0381
Frequencies --	272.4700	322.3327	377.8652
Frequencies --	415.2784	437.2711	466.5538
Frequencies --	492.9275	525.0457	530.9653
Frequencies --	584.5780	651.9711	701.5747
Frequencies --	747.4773	781.5943	787.6623
Frequencies --	828.3625	886.0677	917.8875

		ESI	
Frequencies	--	955.6423	971.4866
Frequencies	--	1038.5428	1040.6809
Frequencies	--	1074.0123	1077.1860
Frequencies	--	1188.9385	1202.6143
Frequencies	--	1268.5422	1275.0052
Frequencies	--	1324.8677	1338.4400
Frequencies	--	1395.1986	1417.3475
Frequencies	--	1472.1040	1491.7687
Frequencies	--	1691.2480	1744.0336
Frequencies	--	3043.4830	3162.3466
Frequencies	--	3240.9401	3252.6110
Frequencies	--	3264.5961	3270.5155
			1007.4964
			1056.7298
			1145.4562
			1212.2979
			1300.9548
			1360.5557
			1445.9197
			1679.0304
			1770.2811
			3240.2423
			3264.3818
			3943.3646

***** C10H8-10H-700-Syn (R1-700-s)//
BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,-0.6445759938,-0.8856010183,0.4532673601			
C,0,-1.9305097551,-0.1596478395,0.4742762006			
C,0,0.5290127322,-0.2786298883,0.3120548639			
C,0,-1.8090535704,1.3055077289,0.3110896202			
O,0,-2.7396510774,-0.6968215574,-0.6229941985			
C,0,1.8124002288,-1.0680923916,0.3917666494			
C,0,0.5998785765,1.1562063585,0.1020392282			
O,0,-3.9892717075,-0.4640147832,-0.445449925			
C,0,1.7679773537,1.7336962924,-0.2158258148			
C,0,-0.6363297445,1.8979229342,0.1428734427			
C,0,2.9905722861,-0.344932622,-0.1636224943			
O,0,1.6800647668,-2.360449302,-0.1371925178			
C,0,2.9698485365,0.9597391104,-0.4022630881			
H,0,-0.6826915739,-1.9545551845,0.5811730983			
H,0,-2.5068695267,-0.4079939493,1.3628661189			
H,0,-2.7276776083,1.8666509451,0.3184409542			
H,0,2.0239836652,-1.2345776302,1.4496256102			
H,0,1.7997776616,2.7951566036,-0.3982300947			
H,0,-0.5806280568,2.9662926341,0.0110838511			
H,0,3.8817987749,-0.9328187132,-0.3045375204			
H,0,1.4331737591,-2.2871725319,-1.0552428636			
H,0,3.8546731498,1.4622909792,-0.7540218313			
Rotational constants (GHZ):	1.6017744	0.5653227	0.4385059
SCF Done: E(UB+HF-B95) = -611.867927601	A.U. after	1	cycles
S**2 = 0.7563			
Frequencies	--	38.9911	70.5211
Frequencies	--	148.3382	234.5242
Frequencies	--	279.9759	315.2224
Frequencies	--	411.9195	415.6936
Frequencies	--	500.4052	508.4997
Frequencies	--	598.0982	639.5447
Frequencies	--	760.0895	797.0342
Frequencies	--	843.4055	892.4139
Frequencies	--	949.2626	964.5860
Frequencies	--	1027.3349	1040.2342
Frequencies	--	1070.9000	1120.2185
Frequencies	--	1185.7817	1190.0833
Frequencies	--	1272.9497	1273.1848
Frequencies	--	1329.7937	1347.4847
Frequencies	--	1406.7976	1421.7361
Frequencies	--	1464.9500	1493.2007
Frequencies	--	1728.2728	1740.3011
Frequencies	--	3060.2063	3103.3881
Frequencies	--	3237.6755	3248.1187
Frequencies	--	3262.0649	3264.2266
			86.3543
			259.8441
			369.1311
			461.0888
			523.7935
			705.9791
			804.8913
			919.2597
			984.4374
			1043.0107
			1152.4491
			1215.4294
			1306.7214
			1361.5966
			1451.1460
			1682.3627
			1790.9230
			3234.2554
			3251.4950
			3946.9658

***** C10H8-10H-700-Anti (R1-700-a)//
BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

ESI			
0,2			
C,0,-0.6164869425,0.9477805177,-0.001248328			
C,0,-1.8932212546,0.3133087895,-0.3913644923			
C,0,0.4993723653,0.2581577638,0.20754653			
C,0,-1.7989213192,-1.1409079106,-0.64623869			
O,0,-2.3417932319,0.9879607259,-1.6084474734			
C,0,1.7871881678,0.9650134603,0.5531336258			
C,0,0.5109075684,-1.1881104696,0.0810503084			
O,0,-3.5972305053,0.8102475097,-1.8095225618			
C,0,1.5808327797,-1.8908689607,0.4813935473			
C,0,-0.6861639752,-1.8212334183,-0.415917681			
C,0,2.804155054,0.070010552,1.1728074386			
O,0,1.577149868,2.1334968771,1.2996005721			
C,0,2.7181870666,-1.2514992556,1.0951013343			
H,0,-0.6154758131,2.0191298968,0.1119266051			
H,0,-2.6801175833,0.5291703841,0.3291855031			
H,0,-2.6899732351,-1.6214420911,-1.0121904314			
H,0,2.2164440183,1.3214393636,-0.3852523926			
H,0,1.5692784021,-2.965152615,0.3993670466			
H,0,-0.6543419387,-2.8855507557,-0.583233196			
H,0,3.6448242091,0.558009509,1.636534006			
H,0,1.1722097408,1.8927666634,2.1283880926			
H,0,3.4970460921,-1.8719176681,1.5046489135			
Rotational constants (GHZ):	1.6603540	0.5514628	0.4263869
SCF Done: E(UB+HF-B95) = -611.867886926	A.U. after	1 cycles	
S**2 = 0.7562			
Frequencies --	40.2672	71.9305	93.3176
Frequencies --	158.5128	205.3222	239.0403
Frequencies --	311.1023	323.2835	366.0449
Frequencies --	411.5493	417.5463	454.4115
Frequencies --	498.1574	518.2807	528.2715
Frequencies --	599.3029	646.4514	702.1352
Frequencies --	753.6572	790.0289	807.3094
Frequencies --	842.3021	884.9503	928.6991
Frequencies --	951.9525	966.5754	982.2252
Frequencies --	1027.7242	1040.9431	1042.7617
Frequencies --	1070.2126	1122.2995	1151.4905
Frequencies --	1183.7919	1188.3518	1213.7060
Frequencies --	1268.9998	1274.1993	1307.7139
Frequencies --	1325.9757	1343.7988	1356.7960
Frequencies --	1400.7987	1420.6201	1449.9835
Frequencies --	1463.7229	1493.7109	1681.8848
Frequencies --	1728.3345	1739.2073	1792.7170
Frequencies --	3059.6403	3093.0994	3234.5567
Frequencies --	3237.0881	3247.1664	3250.5108
Frequencies --	3262.6758	3263.1723	3947.6513

***** C10H8-10H-900-Syn (R1-900-s)//
BB1k=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,-1.2427242853,1.0941065181,-0.5017973712			
C,0,-2.407372628,0.53779492,-0.8106551982			
C,0,-0.1153636523,0.2616878909,-0.0141642077			
C,0,-2.6086191777,-0.8913157825,-0.7645364966			
C,0,1.2286424307,0.7624717526,-0.5033030588			
C,0,-0.2681497833,-1.2052284806,-0.2865577445			
O,0,-0.1253872468,0.2873179816,1.4817288595			
C,0,0.8182768817,-1.9830196824,-0.1718664295			
O,0,-0.0185286639,1.4673475477,1.9717754127			
C,0,-1.5833566955,-1.7156108937,-0.5338820165			
C,0,2.340377565,-0.1342377134,-0.0725089653			
O,0,1.460211372,2.1091502853,-0.2435733071			
C,0,2.1326968488,-1.4391262852,0.0580973101			
H,0,-1.0799275805,2.1551453384,-0.559725947			
H,0,-3.2270595273,1.1592789262,-1.1299329495			
H,0,-3.589645406,-1.2848044505,-0.964508529			

ESI			
H,0,1.1648946191,0.6733346649,-1.5935365666			
H,0,0.706063656,-3.0521364262,-0.2554230334			
H,0,-1.7143294808,-2.784565316,-0.558790653			
H,0,3.3139734415,0.3115297927,0.0364916507			
H,0,1.1890825994,2.2951348482,0.6545595862			
H,0,2.9401389633,-2.1085773568,0.2984637906			
Rotational constants (GHZ):	1.2293006	0.9011542	0.6672836
SCF Done: E(UB+HF-B95) = -611.863321937	A.U. after	1 cycles	
S**2 = 0.7574			
Frequencies -- 62.8607	133.6915	149.8477	
Frequencies -- 189.8556	219.1951	258.0370	
Frequencies -- 302.7861	367.6203	410.3784	
Frequencies -- 429.7804	440.1745	466.4069	
Frequencies -- 475.6533	507.1292	547.5462	
Frequencies -- 578.7457	639.7399	674.4280	
Frequencies -- 711.5986	752.7395	782.0676	
Frequencies -- 810.5249	842.5695	874.5223	
Frequencies -- 951.1109	968.9543	1013.0006	
Frequencies -- 1025.7772	1030.5351	1042.8868	
Frequencies -- 1047.2262	1073.7003	1147.5958	
Frequencies -- 1165.5155	1199.0916	1200.3409	
Frequencies -- 1211.8412	1252.7477	1289.4177	
Frequencies -- 1303.2437	1321.3524	1345.3070	
Frequencies -- 1424.0627	1438.5177	1451.6301	
Frequencies -- 1459.2339	1492.3373	1651.0320	
Frequencies -- 1681.7686	1737.2223	1766.2832	
Frequencies -- 3027.0648	3233.9930	3239.8423	
Frequencies -- 3245.7721	3252.4061	3268.2139	
Frequencies -- 3271.5568	3280.5285	3898.3101	

***** TS R1 + O2 - R1-200-s // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,0.7576518844,1.0733449965,-0.5777686974			
C,0,1.9380445741,0.2934468539,-0.1267937716			
C,0,1.9988575273,-1.0718233479,-0.4350051338			
C,0,0.8617482399,-1.7560404539,-0.7079813116			
C,0,-1.5986783674,-1.8679894707,-0.7221596695			
C,0,-2.8236473734,-1.2527438532,-0.6186691931			
C,0,-2.8922346764,0.117697436,-0.4607203098			
C,0,-1.7357922914,0.8718601962,-0.4225079036			
C,0,-0.5069049595,0.2627829485,-0.5254837579			
C,0,-0.426961743,-1.1232541692,-0.6681814842			
O,0,0.6512542009,2.3306734512,0.0115059127			
O,0,1.4910566127,0.1261781095,1.9040963669			
O,0,1.4996537496,1.166210576,2.540661186			
H,0,0.9409486013,1.2781518515,-1.6402704153			
H,0,2.8387454791,0.8545397826,0.0515240375			
H,0,2.9393404968,-1.590075242,-0.3666713198			
H,0,0.9003190451,-2.8164563841,-0.8938798866			
H,0,-1.5355098539,-2.9377551093,-0.8342222727			
H,0,-3.7254797763,-1.8387851075,-0.6549838461			
H,0,-3.8494442426,0.601509735,-0.3705186044			
H,0,-1.7798447197,1.9408523434,-0.3096139572			
H,0,0.7027115773,2.2398342195,0.9601559337			
Rotational constants (GHZ):	1.2955601	0.6852544	0.5697602
SCF Done: E(UB+HF-B95) = -611.881385746	A.U. after	1 cycles	
S**2 = 1.2623			
Frequencies -- -458.6945	26.8172	77.4044	
Frequencies -- 90.2514	176.6513	184.1526	
Frequencies -- 234.3855	268.7418	309.9463	
Frequencies -- 382.1712	420.0384	451.1094	
Frequencies -- 464.8911	470.2421	515.2582	
Frequencies -- 549.3648	568.5685	657.9810	
Frequencies -- 732.8287	762.2410	792.8207	
Frequencies -- 809.5789	839.9739	890.0609	
Frequencies -- 931.3589	935.0894	1008.7364	

ESI			
Frequencies --	1014.5668	1028.4648	1044.4544
Frequencies --	1085.5959	1109.7198	1145.2725
Frequencies --	1182.2094	1190.8203	1195.5191
Frequencies --	1244.5327	1260.4407	1269.3282
Frequencies --	1306.3563	1342.1202	1376.4556
Frequencies --	1409.0067	1413.1794	1448.0340
Frequencies --	1492.7371	1517.3036	1562.9934
Frequencies --	1598.2612	1680.0996	1703.0700
Frequencies --	2990.6855	3238.4207	3241.5929
Frequencies --	3250.0667	3256.5684	3264.2045
Frequencies --	3269.3335	3273.5734	3922.3783

***** TS R1 + O2 - R1-200-a // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,0.375693729,0.972644874,0.4374214638			
C,0,1.6195985955,0.2871877024,0.8284644613			
C,0,1.8044253287,-1.0735255933,0.541043226			
C,0,0.8029026156,-1.8081739884,0.0089222988			
C,0,-1.5781864782,-2.0989999314,-0.5318182417			
C,0,-2.8586998021,-1.6078452329,-0.5910214926			
C,0,-3.1009440196,-0.2855691191,-0.2660593165			
C,0,-2.0601641763,0.5427172301,0.0954524009			
C,0,-0.7699542678,0.0591650929,0.1468419602			
C,0,-0.5203576319,-1.2791575643,-0.1533217093			
O,0,-0.0015715524,1.9879192188,1.3302212363			
O,0,2.9269200113,1.1809260121,-0.5520582323			
O,0,2.3389860734,1.9367048355,-1.3016503786			
H,0,0.6211830255,1.441452799,-0.5380624219			
H,0,2.2267139052,0.7644609955,1.5760252911			
H,0,2.7491171018,-1.5335825048,0.7739933601			
H,0,0.9602652739,-2.8495598207,-0.2181661793			
H,0,-1.3807491718,-3.1320479341,-0.7657585386			
H,0,-3.6713453632,-2.2513503175,-0.8800036101			
H,0,-4.1050470591,0.1010481983,-0.2959530205			
H,0,-2.2421643816,1.5709554634,0.3528944145			
H,0,0.4414670534,2.7935617698,1.0873793957			
Rotational constants (GHZ): 1.4615215 0.5960832 0.4944227			
SCF Done: E(UB+HF-B95) = -611.881491497 A.U. after 1 cycles			
S**2 = 1.1669			
Frequencies --	-380.2802	45.3045	71.1501
Frequencies --	120.8992	132.1964	205.1289
Frequencies --	225.1186	235.9706	284.8394
Frequencies --	398.0134	423.3954	444.9677
Frequencies --	467.7959	492.7297	519.9643
Frequencies --	544.8910	583.6169	661.7428
Frequencies --	739.6151	769.1464	795.5230
Frequencies --	810.0240	842.5077	887.5376
Frequencies --	904.0528	927.9314	1003.3733
Frequencies --	1014.4018	1040.4299	1041.3957
Frequencies --	1091.9930	1118.7154	1146.0261
Frequencies --	1184.0360	1196.5696	1197.4810
Frequencies --	1231.1362	1256.1425	1268.9343
Frequencies --	1303.5191	1342.7162	1381.9719
Frequencies --	1404.3395	1441.7618	1479.8021
Frequencies --	1505.9470	1523.7950	1569.5211
Frequencies --	1612.4845	1684.2893	1706.6985
Frequencies --	2826.2417	3237.3766	3240.2361
Frequencies --	3248.7420	3257.9334	3263.8658
Frequencies --	3273.3680	3275.9684	3986.1212

***** TS R1 + O2 - R1-400-s // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,0.8324915203,1.5233786603,0.1588002895			
C,0,1.9313244311,0.786792122,0.834609123			

ESI
C,0,2.0704380298,-0.541559701,0.7931522195
C,0,1.0695109088,-1.3469192356,0.1997123576
C,0,-0.7945126009,-1.5317408233,-1.3931152982
C,0,-1.7846984907,-0.9528388322,-2.1438679371
C,0,-1.9329519106,0.4244049882,-2.1408127069
C,0,-1.0847323483,1.2077051256,-1.3930161191
C,0,-0.0774565547,0.6367528353,-0.6383365945
C,0,0.0699659219,-0.7464901373,-0.6349244813
O,0,0.1203938412,2.3147384757,1.0802070238
O,0,-0.3517306054,-0.4664185303,2.3392346099
O,0,-0.0837807782,-1.5580605582,1.8766438422
H,0,1.2811479676,2.2469223211,-0.5219447139
H,0,2.6374172989,1.395555562,1.3749431206
H,0,2.8846125053,-1.0206789862,1.3091918683
H,0,1.2261069295,-2.4077846143,0.1146518867
H,0,-0.6769757973,-2.6026074194,-1.3798624685
H,0,-2.4464807456,-1.566452549,-2.7299691961
H,0,-2.7116927856,0.8826467712,-2.7256782453
H,0,-1.2026360119,2.2781872315,-1.379605535
H,0,-0.2668324606,1.7152265735,1.7163843604
Rotational constants (GHZ): 1.2117903 0.8018290 0.6346925
SCF Done: E(UB+HF-B95) = -611.887913016 A.U. after 1 cycles
S**2 = 1.1139
Frequencies -- -434.5005 79.8621 105.9341
Frequencies -- 135.6793 162.3998 171.3623
Frequencies -- 229.8896 291.1251 362.7601
Frequencies -- 394.0461 401.9662 480.8727
Frequencies -- 501.3840 507.5353 532.0017
Frequencies -- 543.4124 598.6294 650.0323
Frequencies -- 752.1256 785.4756 799.2241
Frequencies -- 803.1990 838.0259 914.9466
Frequencies -- 933.9898 946.2438 1010.6460
Frequencies -- 1022.5108 1041.3838 1042.3296
Frequencies -- 1084.6481 1098.8967 1118.2049
Frequencies -- 1169.4183 1197.1491 1206.0187
Frequencies -- 1247.4445 1259.6265 1272.3738
Frequencies -- 1307.8073 1382.1216 1399.5297
Frequencies -- 1433.4749 1446.8209 1449.5165
Frequencies -- 1487.0441 1542.4929 1560.4308
Frequencies -- 1661.0885 1692.7102 1707.0711
Frequencies -- 3077.2877 3239.1605 3239.7346
Frequencies -- 3245.8088 3255.6086 3257.4502
Frequencies -- 3267.1504 3269.5775 3927.3543

***** TS R1 + O2 - R1-400-a // BB1k=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,0.3850391909,1.358964128,0.8923820947
C,0,1.4796907541,0.5673782795,1.5127663698
C,0,1.6570679126,-0.7416675922,1.3107881614
C,0,0.8759773628,-1.4278090156,0.3502052514
C,0,-1.2750012695,-1.5802369388,-0.8341435457
C,0,-2.4310477086,-1.0026169898,-1.2939804774
C,0,-2.6737339437,0.3378282761,-1.0480083859
C,0,-1.7576107794,1.0871126228,-0.3452436424
C,0,-0.5886401176,0.5167446563,0.1210399098
C,0,-0.3443397795,-0.8322218879,-0.1197720033
O,0,-0.2646088276,2.1576787647,1.8587780102
H,0,0.8314022688,2.0804194056,0.2116057467
H,0,2.1203590687,1.1146302623,2.1843415704
H,0,2.4641405203,-1.2629122391,1.7960562832
H,0,0.9877334732,-2.4921689657,0.2426248637
H,0,-1.0770374923,-2.6228272294,-1.0200642056
H,0,-3.1463479132,-1.5904039741,-1.8425625228
H,0,-3.5799916797,0.7951879247,-1.4057798437
H,0,-1.9455965431,2.1273644598,-0.1410377988
H,0,-0.7137784018,1.5824572343,2.4721051092

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                                ESI
O,0,2.0248910108,-1.0143524822,-1.2688888518
O,0,2.2515561875,0.1775987039,-1.3115756081
Rotational constants (GHZ):      1.1019866      0.8395408      0.5913451
SCF Done: E(UB+HF-B95) = -611.885632316      A.U. after      1 cycles
                                S**2 = 1.1288
Frequencies -- -469.0569      61.5279      101.9419
Frequencies -- 115.1212      146.6014      164.3969
Frequencies -- 241.9580      274.1227      330.7064
Frequencies -- 353.5663      411.5586      444.6626
Frequencies -- 473.9443      487.4291      530.3715
Frequencies -- 563.1143      582.2773      655.9896
Frequencies -- 746.1745      782.6181      798.1378
Frequencies -- 801.2800      841.1371      905.8903
Frequencies -- 929.0960      947.6551      1011.5792
Frequencies -- 1031.7573      1032.2827      1042.0968
Frequencies -- 1082.2594      1098.4467      1115.2393
Frequencies -- 1168.1237      1195.1333      1201.3463
Frequencies -- 1247.4247      1256.1073      1259.4420
Frequencies -- 1303.9904      1374.4218      1387.4995
Frequencies -- 1420.6228      1436.5318      1457.1991
Frequencies -- 1487.7187      1539.7740      1557.9908
Frequencies -- 1661.1865      1694.2231      1706.2073
Frequencies -- 3105.4198      3237.6385      3240.5936
Frequencies -- 3246.4976      3256.4072      3258.5301
Frequencies -- 3267.9995      3269.0109      3946.9240

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***** TS R1 + O2 - R1-500-s // BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

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O,2
C,0,-0.1244856491,1.947968862,0.1433247298
C,0,-1.5223247973,2.1049000483,-0.0784501131
C,0,0.4967732789,0.7916659467,-0.1639122325
C,0,-2.2835767071,1.090264085,-0.5209032432
C,0,1.9892943099,0.6537404275,-0.0265054877
C,0,-0.2667542852,-0.3078440724,-0.6657296315
C,0,0.3157774266,-1.5130224784,-0.8879393466
C,0,-1.6994366564,-0.2076742219,-0.6841084684
O,0,-2.1504292618,-1.0510897415,0.8259679939
C,0,2.4686803462,-0.7516912588,-0.1337018539
O,0,2.4788142866,1.2883298506,1.1281430098
C,0,1.6950517251,-1.7426501299,-0.5655678989
O,0,-1.4755925526,-2.0725753414,1.0083727862
H,0,0.4504311241,2.7736013219,0.5258943379
H,0,-1.9653120472,3.0709919748,0.0953926671
H,0,-3.3344831844,1.2235399831,-0.7054433565
H,0,2.4530028129,1.2047477955,-0.8469815992
H,0,-0.2692803982,-2.3200605848,-1.2913152221
H,0,-2.2152807591,-0.909839876,-1.3182507666
H,0,3.5022129718,-0.9148569343,0.1221396174
H,0,2.0521637642,0.8992147717,1.8869762385
H,0,2.090211988,-2.7385998417,-0.6673209602
Rotational constants (GHZ):      1.1759726      0.8076483      0.5698333
SCF Done: E(UB+HF-B95) = -611.855601570      A.U. after      1 cycles
                                S**2 = 0.8626
Frequencies -- -546.3316      42.5236      85.8115
Frequencies -- 125.0045      134.6136      212.2605
Frequencies -- 216.5413      279.6412      330.3979
Frequencies -- 377.4542      422.2543      448.3585
Frequencies -- 468.3094      483.9275      527.9822
Frequencies -- 548.9827      579.3055      635.7764
Frequencies -- 740.0797      765.3871      793.5828
Frequencies -- 798.3270      838.0289      907.1501
Frequencies -- 923.5119      951.3639      1007.7453
Frequencies -- 1035.5359      1040.0798      1059.8640
Frequencies -- 1070.0795      1096.3963      1112.3128
Frequencies -- 1140.4243      1193.0784      1211.3765
Frequencies -- 1218.0227      1264.4229      1269.7904

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		ESI	
Frequencies --	1322.4298	1354.8663	1387.4220
Frequencies --	1418.2366	1422.6261	1453.4074
Frequencies --	1492.6205	1504.0230	1610.4704
Frequencies --	1625.1733	1707.9911	1741.9115
Frequencies --	3056.7801	3227.7945	3242.4788
Frequencies --	3242.9644	3259.3011	3260.9224
Frequencies --	3271.9771	3273.5935	3946.0201

***** TS R1 + O2 - R1-500-a // BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2

C,0,-0.2058127779,1.9127208693,0.2368646694			
C,0,1.0937306128,2.3307733968,-0.1655879809			
C,0,-0.5959113288,0.6300492068,0.0931455199			
C,0,2.0009091377,1.4548584581,-0.6313377826			
C,0,-1.9768761512,0.1980605851,0.503863772			
C,0,0.3099768542,-0.3199457778,-0.4732225143			
C,0,-0.0784994048,-1.5984386706,-0.7043656797			
C,0,1.6811445662,0.0605603692,-0.671999686			
O,0,2.4639022195,-0.6121661224,0.7977119475			
C,0,-2.300476251,-1.2066949829,0.131900492			
O,0,-2.9725457746,1.0894259128,0.0559995761			
C,0,-1.4111297858,-2.0367900309,-0.4060742248			
O,0,2.0813611979,-1.7662823595,1.0264088994			
H,0,-0.8968563777,2.636892861,0.6333664981			
H,0,1.3424770621,3.3765452035,-0.1016947856			
H,0,2.9792201205,1.779571293,-0.9377858439			
H,0,-2.0387780198,0.2647260612,1.590558903			
H,0,0.6085246282,-2.2845939614,-1.1668607825			
H,0,2.2539328712,-0.5611761549,-1.3400074022			
H,0,-3.3086718149,-1.5244526558,0.339028184			
H,0,-2.9369309752,1.1242745207,-0.8959506477			
H,0,-1.6869914649,-3.0505271523,-0.6407370181			
Rotational constants (GHZ):	1.2196946	0.7802266	0.5356190
SCF Done: E(UB+HF-B95) = -611.855042170	A.U. after	2	cycles
S**2 =	0.9124		
Frequencies --	-646.7958	34.0171	81.8309
Frequencies --	116.0283	135.3960	204.5242
Frequencies --	218.2502	272.2955	314.9711
Frequencies --	370.9874	414.3258	433.4624
Frequencies --	478.5604	500.6951	533.4214
Frequencies --	541.0720	563.4810	664.6407
Frequencies --	718.3005	765.8600	794.6187
Frequencies --	799.4320	836.9450	912.1892
Frequencies --	930.0812	953.3163	1005.6544
Frequencies --	1034.5530	1041.4766	1066.2990
Frequencies --	1072.8919	1099.2234	1114.6784
Frequencies --	1132.5339	1197.3918	1212.5328
Frequencies --	1221.8823	1260.8503	1274.6626
Frequencies --	1326.6581	1355.3294	1387.0166
Frequencies --	1419.2655	1422.3272	1455.5230
Frequencies --	1491.5437	1508.4459	1609.0923
Frequencies --	1627.0808	1708.6100	1741.4658
Frequencies --	3070.1597	3229.2468	3241.0098
Frequencies --	3243.4359	3257.6785	3259.1139
Frequencies --	3271.7731	3272.4297	3949.0491

***** TS R1 + O2 - R1-700-s // BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2

C,0,-0.7309011661,-0.8316549851,0.603387661		
C,0,-1.9407089758,-0.0738950626,0.522731712		
C,0,0.4726115179,-0.2522072732,0.4438937866		
C,0,-1.8270632905,1.3531888665,0.501006234		
O,0,-2.5428189287,-0.457872201,-1.1675319915		
C,0,1.7327018116,-1.0728306872,0.51232097		

ESI
C,0,0.5671705018,1.1668176994,0.247445332
O,0,-3.7085561335,-0.8675585646,-1.1751821621
C,0,1.7659345772,1.7337704328,-0.0604783715
C,0,-0.6319193374,1.9367564701,0.3306002367
C,0,2.9265124997,-0.372270659,-0.0339663516
O,0,1.5703752549,-2.3557839386,-0.0328816634
C,0,2.9385057977,0.9418746067,-0.2569749514
H,0,-0.7936774708,-1.8965591491,0.7475054468
H,0,-2.8253399283,-0.4996635238,0.9646440307
H,0,-2.7239853183,1.9436503267,0.5660330738
H,0,1.9411628458,-1.2596097352,1.5687179568
H,0,1.818081936,2.7978002541,-0.2200348946
H,0,-0.5512653675,3.0084527115,0.2528746655
H,0,3.8019893526,-0.9802437983,-0.1870686426
H,0,1.3074531776,-2.2662840711,-0.9451672712
H,0,3.8365156153,1.4248781676,-0.6025353752
Rotational constants (GHZ): 1.4344520 0.5829181 0.4573513
SCF Done: E(UB+HF-B95) = -611.852660488 A.U. after 1 cycles
S**2 = 1.1182
Frequencies -- -864.5924 25.4951 46.7121
Frequencies -- 81.7940 137.2152 225.1610
Frequencies -- 249.5430 270.1360 319.2192
Frequencies -- 342.9221 406.0792 424.1194
Frequencies -- 452.3311 478.0370 497.8384
Frequencies -- 521.5634 574.6764 637.3103
Frequencies -- 720.3674 754.3092 801.4117
Frequencies -- 808.8454 846.1555 902.0592
Frequencies -- 930.8641 954.2796 994.7729
Frequencies -- 1026.0592 1028.9779 1042.5415
Frequencies -- 1073.2630 1116.7781 1127.3356
Frequencies -- 1157.3547 1192.3454 1202.6365
Frequencies -- 1214.5862 1268.9074 1279.1026
Frequencies -- 1325.2333 1335.0573 1369.4421
Frequencies -- 1420.0828 1432.8004 1457.6114
Frequencies -- 1484.2291 1503.4723 1573.1544
Frequencies -- 1631.4754 1685.0585 1717.3740
Frequencies -- 3043.6491 3236.7589 3239.2495
Frequencies -- 3241.6295 3250.2960 3260.3199
Frequencies -- 3265.1254 3267.0910 3944.5397

***** TS R1 + O2 - R1-700-a // BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,0.7179975409,-0.8718451455,0.3625957175
C,0,1.9194179478,-0.1155199784,0.5308388131
C,0,-0.4615225513,-0.2770580904,0.1042422193
C,0,1.796437688,1.3085181303,0.6234740709
O,0,2.7689476319,-0.3441370191,-1.0748148647
C,0,-1.6802485654,-1.1150009299,-0.1838211417
C,0,-0.5593419944,1.1540936934,0.1076659197
O,0,3.7931436799,-1.0286369586,-0.9750446908
C,0,-1.7681321918,1.7564870312,-0.0658110481
C,0,0.6217928478,1.9077128042,0.3821966362
C,0,-2.9454547149,-0.3360480704,-0.2343395779
O,0,-1.7814600183,-2.2228668302,0.677949543
C,0,-2.9688182714,0.9969529006,-0.2099024957
H,0,0.7742594721,-1.9466214127,0.3948767818
H,0,2.7329216977,-0.584625794,1.0574691801
H,0,2.6730418977,1.8889740619,0.851601101
H,0,-1.5424406541,-1.5633558934,-1.1690190048
H,0,-1.8271680973,2.8318380938,-0.0448259861
H,0,0.5377186098,2.9813453028,0.4203004175
H,0,-3.8503976648,-0.9125419617,-0.3261108945
H,0,-1.8699263556,-1.9019773382,1.5712029535
H,0,-3.9058256647,1.5223373342,-0.283049128
Rotational constants (GHZ): 1.4818013 0.5608236 0.4457710
SCF Done: E(UB+HF-B95) = -611.852034533 A.U. after 1 cycles

ESI			
S**2 = 1.1210			
Frequencies --	-873.9813	20.1218	38.9102
Frequencies --	86.2593	141.8873	200.6976
Frequencies --	221.1713	296.0791	320.0498
Frequencies --	341.5673	404.3358	419.2187
Frequencies --	450.9164	476.4770	494.5838
Frequencies --	532.6318	579.1804	644.8876
Frequencies --	716.2203	760.4941	802.3887
Frequencies --	805.7718	841.8229	910.8510
Frequencies --	930.2090	948.7686	997.3114
Frequencies --	1029.1610	1030.3692	1039.9511
Frequencies --	1073.9774	1115.9744	1122.9571
Frequencies --	1155.2274	1194.0466	1202.1142
Frequencies --	1220.0822	1262.6705	1279.3724
Frequencies --	1323.4338	1333.5215	1373.1022
Frequencies --	1420.2984	1431.5051	1459.7002
Frequencies --	1484.5137	1502.9445	1572.4316
Frequencies --	1631.4695	1684.2392	1718.4420
Frequencies --	3062.5629	3236.4638	3237.8482
Frequencies --	3241.2511	3249.7014	3256.8165
Frequencies --	3263.2668	3266.0827	3948.8557

***** TS R1 + O2 - R1-900-s // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,1.0166271857,-1.2628048922,-0.6280492012			
C,0,2.3379227239,-1.0505026378,-0.5126481941			
C,0,0.0917281419,-0.2215809241,-0.2974665473			
C,0,2.856986303,0.2235093813,-0.135198321			
C,0,-1.2804764455,-0.3021683874,-0.8913995003			
C,0,0.6210229699,1.1098622715,-0.0734993987			
O,0,-0.3170127496,-0.5495852731,1.4831262709			
C,0,-0.2577208051,2.1263258853,0.1352173195			
O,0,-0.7286624481,-1.7006176544,1.7263198799			
C,0,2.0291220924,1.264308453,0.0626710705			
C,0,-2.1715981442,0.7807361682,-0.3923947742			
O,0,-1.8432378473,-1.573081704,-0.820573287			
C,0,-1.6697891075,1.9343981262,0.0507359824			
H,0,0.6201074156,-2.2147318629,-0.9321898348			
H,0,3.0282539762,-1.8482590356,-0.7279597952			
H,0,3.9208473987,0.3484673014,-0.0360174028			
H,0,-1.1420731376,-0.1046000761,-1.9629775294			
H,0,0.1230190442,3.09801859,0.4039632935			
H,0,2.4143075016,2.2380673673,0.3147611438			
H,0,-3.2310088555,0.6191390881,-0.4945126037			
H,0,-1.7429813621,-1.9014128135,0.0736823345			
H,0,-2.3221171074,2.7390878293,0.34245687			
Rotational constants (GHZ):	1.2012946	0.8772822	0.6668085
SCF Done: E(UB+HF-B95) = -611.853629744	A.U. after	1 cycles	
S**2 = 0.9983			
Frequencies --	-712.9343	58.9584	125.4002
Frequencies --	141.6967	152.5520	217.0535
Frequencies --	226.3566	276.1510	349.3162
Frequencies --	409.2398	422.1697	453.7577
Frequencies --	463.8522	479.2239	507.5284
Frequencies --	543.7267	567.5371	657.3517
Frequencies --	689.5193	722.1533	775.4294
Frequencies --	786.1254	823.4284	867.2632
Frequencies --	904.6210	951.5111	1019.1014
Frequencies --	1023.0135	1032.4169	1039.9114
Frequencies --	1049.7149	1083.8206	1143.8768
Frequencies --	1179.7259	1188.5214	1207.3378
Frequencies --	1217.3469	1255.5886	1264.2393
Frequencies --	1286.4161	1340.2602	1357.7341
Frequencies --	1442.7634	1448.2692	1461.7986
Frequencies --	1477.8381	1511.1469	1529.0311
Frequencies --	1627.9528	1700.1607	1728.6059

		ESI	
Frequencies --	2988.0616	3239.7433	3242.0723
Frequencies --	3249.9003	3252.7676	3267.3334
Frequencies --	3269.8263	3277.6679	3851.8463

***** TS R1 + O2 - R1-900-a // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,-1.1368241832,1.2777361151,-0.0657889459			
C,0,-2.335607148,0.7882430263,-0.4129396851			
C,0,-0.0151143203,0.3956080249,0.0707794288			
C,0,-2.4991794573,-0.5763781149,-0.80866515			
C,0,1.3525660091,1.0450371915,0.1460281615			
C,0,-0.1351974247,-0.9224839404,-0.5351336147			
O,0,-0.0831071405,-0.0586397023,1.8054358672			
C,0,0.9776892091,-1.6839123653,-0.6810104643			
O,0,-1.2053301726,-0.4037596002,2.1929129595			
C,0,-1.4334766475,-1.3870593533,-0.8944721477			
C,0,2.4736600944,0.0854976077,-0.0135457337			
O,0,1.4876904383,2.1235639499,-0.749302164			
C,0,2.2822924647,-1.179697272,-0.3868333274			
H,0,-1.0051219441,2.3136970593,0.190985497			
H,0,-3.1933565645,1.4389594738,-0.4334817731			
H,0,-3.478626444,-0.9306120312,-1.0777195207			
H,0,1.4128383758,1.4990547115,1.1334480957			
H,0,0.880038499,-2.688531921,-1.0576270361			
H,0,-1.5322302109,-2.3990915294,-1.2496090238			
H,0,3.4641260186,0.4789088067,0.1395333369			
H,0,1.5474950781,1.7797133866,-1.6361104959			
H,0,3.1259606133,-1.8369606527,-0.5123035104			
Rotational constants (GHZ):	1.2398009	0.7894232	0.7211344
SCF Done: E(UB+HF-B95) = -611.851171658	A.U. after	30 cycles	
S**2 =	1.0245		
Frequencies --	-763.9624	58.2709	97.7670
Frequencies --	155.3110	167.1217	182.3362
Frequencies --	213.5898	284.6583	327.2720
Frequencies --	374.9677	397.6238	430.8645
Frequencies --	450.5994	487.6631	511.2709
Frequencies --	538.9302	585.3262	637.8049
Frequencies --	727.1876	736.4171	762.6882
Frequencies --	786.5414	809.6119	866.4642
Frequencies --	921.4097	933.4994	1015.2983
Frequencies --	1018.6277	1032.9100	1035.4289
Frequencies --	1038.9364	1079.1579	1116.2367
Frequencies --	1179.6171	1185.8275	1209.2947
Frequencies --	1221.3128	1254.5249	1259.8930
Frequencies --	1298.3395	1340.3081	1376.1271
Frequencies --	1427.4935	1444.4688	1459.1979
Frequencies --	1475.9917	1510.3330	1519.6222
Frequencies --	1632.0950	1709.8476	1732.2697
Frequencies --	3099.6716	3237.1938	3241.4572
Frequencies --	3247.8185	3249.1290	3263.7436
Frequencies --	3267.6947	3274.4730	3953.5339

***** c10H8-10H-2300-Syn (R1-2300-s) // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,-2.0412288764,0.02638878,0.6029057424			
C,0,-2.5299097341,-1.0941865563,1.24989978			
C,0,-0.8307386582,-0.0044639166,-0.0458567283			
C,0,-1.8025026032,-2.2737084704,1.2352382494			
C,0,-0.3851997617,1.1764269578,-0.8580290999			
C,0,-0.0614571276,-1.1857820203,-0.0372628732			
C,0,-0.5914983726,-2.3211323991,0.6004246022			
C,0,1.1092140764,1.2733162034,-1.0053722096			
O,0,-0.8712468456,2.3915828957,-0.3650573358			

ESI			
O,0,1.7188983835,1.6656419456,0.2221503418			
C,0,1.9258607691,0.0033830575,-0.9818690687			
C,0,1.206892292,-1.2242472637,-0.6266937539			
O,0,2.6306881046,0.5594653484,0.1615602102			
H,0,-2.6125880702,0.9383379616,0.5875044117			
H,0,-3.4800878537,-1.0510733268,1.7530801218			
H,0,-2.1856081809,-3.149615242,1.7295429856			
H,0,-0.8078064187,1.0747363685,-1.8565754545			
H,0,-0.0115165908,-3.2287713756,0.6022838185			
H,0,1.364126648,1.9720719983,-1.7955180006			
H,0,-0.4587642233,2.5466332369,0.4828622888			
H,0,2.6208402075,-0.1368987628,-1.8008400767			
H,0,1.7480953202,-2.1549086095,-0.6518736667			
Rotational constants (GHZ): 1.4771271 0.7546362 0.5577408			
SCF Done: E(UB+HF-B95) = -611.896362112 A.U. after 1 cycles			
S**2 = 0.7892			
Frequencies --	51.4645	71.6959	137.4238
Frequencies --	198.0946	247.4070	276.2350
Frequencies --	367.0483	412.1729	436.9818
Frequencies --	445.8091	471.5459	517.6590
Frequencies --	538.9143	565.3413	671.7093
Frequencies --	696.1981	727.6709	752.7293
Frequencies --	800.8163	809.7691	839.1055
Frequencies --	908.9387	914.7953	953.1238
Frequencies --	958.4503	1003.7779	1012.6948
Frequencies --	1031.9447	1062.4732	1076.2012
Frequencies --	1105.6329	1126.2329	1164.7672
Frequencies --	1180.2192	1189.1265	1229.9897
Frequencies --	1259.8943	1269.9991	1298.4213
Frequencies --	1310.1959	1341.8894	1363.1349
Frequencies --	1385.6323	1405.6493	1425.0288
Frequencies --	1445.9744	1469.3329	1515.6435
Frequencies --	1544.8492	1639.4533	1666.0936
Frequencies --	3093.5508	3133.6418	3156.8849
Frequencies --	3239.1519	3246.1899	3249.7121
Frequencies --	3259.9372	3269.8006	3918.6379

***** C10H8-10H-2300-Anti (R1-2300-a) //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,-2.1551230792,0.1729319137,0.3153831221			
C,0,-2.8342507146,-1.0054463285,0.5715156987			
C,0,-0.7837248388,0.2006965136,0.2390389968			
C,0,-2.121271651,-2.1784000419,0.7592451605			
C,0,-0.0682899901,1.5071967983,0.1168128681			
C,0,-0.0482580954,-0.9933114235,0.3880778018			
C,0,-0.7548447733,-2.1750493783,0.6697450337			
C,0,1.2674151513,1.390964979,-0.5558144435			
O,0,0.2211610414,2.0511897368,1.3867101841			
O,0,1.1667770752,1.0556436739,-1.932449537			
C,0,2.0711244361,0.13358703,-0.3337621051			
C,0,1.341143551,-1.0038680235,0.2389476619			
O,0,2.1612762313,0.0306694348,-1.7803093574			
H,0,-2.7073476658,1.0889058688,0.1757795508			
H,0,-3.9086842458,-1.0086165489,0.6256046258			
H,0,-2.6429609119,-3.0972892597,0.9640636082			
H,0,-0.6827691761,2.1999270049,-0.4597877346			
H,0,-0.2005310355,-3.0901983545,0.7938010754			
H,0,1.8299584312,2.3074510672,-0.4067241973			
H,0,-0.5070457605,1.8719947467,1.9726106014			
H,0,3.0616167745,0.2538550612,0.0868160344			
H,0,1.8805288314,-1.9218645847,0.4010873496			
Rotational constants (GHZ): 1.4922667 0.7101048 0.5868143			
SCF Done: E(UB+HF-B95) = -611.894297111 A.U. after 1 cycles			
S**2 = 0.7904			
Frequencies --	62.1532	87.5709	126.7790

ESI			
Frequencies	--	188.5393	214.5357
Frequencies	--	321.5030	340.9055
Frequencies	--	446.8615	482.4299
Frequencies	--	527.0618	584.0775
Frequencies	--	716.5348	753.3216
Frequencies	--	794.3133	801.1950
Frequencies	--	896.7560	908.7925
Frequencies	--	962.6031	995.8083
Frequencies	--	1029.7982	1070.6404
Frequencies	--	1111.0813	1136.8482
Frequencies	--	1159.9301	1190.1245
Frequencies	--	1234.2633	1261.0340
Frequencies	--	1310.5787	1335.0451
Frequencies	--	1375.3231	1410.5750
Frequencies	--	1456.3651	1479.7750
Frequencies	--	1545.4961	1636.2637
Frequencies	--	3068.5146	3131.9344
Frequencies	--	3227.8304	3241.5676
Frequencies	--	3256.3560	3270.3069
			245.0781
			407.9920
			508.0399
			622.6606
			771.1916
			845.7891
			950.7372
			1027.5894
			1077.5376
			1143.6978
			1228.0083
			1289.2968
			1359.1827
			1429.9171
			1522.5446
			1664.9479
			3162.6189
			3246.0200
			3975.4986

***** C10H8-10H-2400-Syn (R1-2400-s) //
BB1k=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,0.7123409767,	1.3285602137,-0.5438493856		
C,0,1.9360416093,	0.5905304694,0.0062667061		
C,0,1.9749664778,-0.7714530102,-0.538930039			
C,0,0.9602707286,-1.4147985303,0.3184146881			
C,0,-1.5116968578,-1.710977718,-0.0888492834			
C,0,-2.7414410111,-1.2008569778,-0.4422801835			
C,0,-2.8543663582,0.1272202298,-0.8019414721			
C,0,-1.7384798681,0.9350615244,-0.8190868928			
C,0,-0.4974206406,0.4279550758,-0.4845482348			
C,0,-0.3917317328,-0.9030550632,-0.1018480363			
O,0,0.5132552347,2.5240772914,0.1466535287			
O,0,1.717430339,0.4149474323,1.3973484964			
O,0,1.2993177296,-0.9346394344,1.6014929408			
H,0,0.9081867251,1.609417719,-1.5753127774			
H,0,2.8331458383,1.1876290397,-0.1134173207			
H,0,2.1736781062,-1.017494246,-1.5638008694			
H,0,0.9960511762,-2.4954377256,0.3806788764			
H,0,-1.4177506303,-2.7422472229,0.2094544805			
H,0,-3.6109857387,-1.8350215599,-0.4305076658			
H,0,-3.8143885143,0.5320227402,-1.0721197453			
H,0,-1.8224031185,1.973587435,-1.0915422932			
H,0,0.4235397863,2.303344225,1.0725203872			
Rotational constants (GHZ):	1.4622160	0.8359685	0.6169072
SCF Done: E(UB+HF-B95) = -611.899041652	A.U. after	1 cycles	
S**2	=	0.7545	
Frequencies	--	78.1980	121.7937
Frequencies	--	233.4316	259.4455
Frequencies	--	362.7960	377.9925
Frequencies	--	459.5232	497.7617
Frequencies	--	565.7917	594.0231
Frequencies	--	697.8625	748.8985
Frequencies	--	811.8920	826.0138
Frequencies	--	897.1215	915.2252
Frequencies	--	978.0365	1000.1326
Frequencies	--	1028.6148	1044.3868
Frequencies	--	1090.5709	1095.6831
Frequencies	--	1161.0333	1197.9635
Frequencies	--	1239.2211	1247.3226
Frequencies	--	1283.6044	1307.3844
Frequencies	--	1346.3466	1355.7295
Frequencies	--	1385.2778	1444.4787
Frequencies	--	1559.0291	1681.7923
Frequencies	--	3119.7435	3156.1288
			164.8833
			341.1449
			415.7963
			521.3915
			656.5673
			786.4145
			849.6999
			935.8078
			1010.2581
			1067.4065
			1129.7488
			1211.8493
			1260.0177
			1329.3738
			1375.9700
			1523.4972
			1709.6940
			3176.2241

		ESI	
Frequencies --	3235.2595	3244.5902	3255.5572
Frequencies --	3267.6105	3305.3047	3912.3140

***** C10H8-10H-2400-Anti (R1-2400-a) //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,0.7681023649,	1.3685277693,-0.2715143632		
C,0,1.9690319225,	0.4429331753,-0.0354649719		
C,0,1.7083457877,	-0.3948543184,1.1421497114		
C,0,0.815358232,	-1.403002406,0.5397610546		
C,0,-1.7004145926,	-1.4300980911,0.3746237343		
C,0,-2.8953564445,	-0.8115179022,0.0791980189		
C,0,-2.9009484924,	0.5010280271,-0.3478495916		
C,0,-1.7136512797,	1.1889932975,-0.4737383192		
C,0,-0.5103487998,	0.5788039675,-0.1740461372		
C,0,-0.5082370229,	-0.7441986985,0.2489561469		
O,0,0.7838826504,	2.462618929,0.6045319472		
O,0,1.491615272,	-1.7144673763,-0.6581366946		
O,0,2.0090568833,	-0.4684702261,-1.1194669418		
H,0,0.8686123175,	1.7843663745,-1.2692096433		
H,0,2.8923986324,	1.0103616034,-0.0189720388		
H,0,1.7035093649,	-0.0654911804,2.1623176646		
H,0,0.7035390218,	-2.3354027142,1.0790837928		
H,0,-1.6886776889,	-2.4566103116,0.702416227		
H,0,-3.8207459772,	-1.3520803626,0.1783168463		
H,0,-3.8313374296,	0.9878140329,-0.5841385664		
H,0,-1.7136742923,	2.2158486867,-0.7999994831		
H,0,0.4186475541,	2.1940543352,1.4423070164		
Rotational constants (GHZ):	1.4026824	0.8378514	0.6149284
SCF Done: E(UB+HF-B95) =	-611.894897136	A.U. after	1 cycles
S**2 =	0.7546		
Frequencies --	81.0781	117.8641	168.1503
Frequencies --	208.3585	261.7499	280.1284
Frequencies --	319.3071	346.6034	375.6869
Frequencies --	432.8697	476.1344	500.2032
Frequencies --	557.9611	581.2279	635.3044
Frequencies --	708.3192	752.1871	775.8209
Frequencies --	803.6139	828.6382	845.6292
Frequencies --	901.6444	926.4765	934.0591
Frequencies --	973.2495	1008.0021	1010.1893
Frequencies --	1043.1197	1048.1417	1070.4787
Frequencies --	1088.1770	1095.7112	1117.8334
Frequencies --	1156.8395	1197.1933	1215.5143
Frequencies --	1222.9559	1250.3966	1263.7518
Frequencies --	1269.3854	1301.0870	1321.5655
Frequencies --	1345.3890	1352.0963	1377.5174
Frequencies --	1404.8248	1431.8015	1522.2899
Frequencies --	1560.1762	1681.5966	1708.0276
Frequencies --	3135.2797	3160.2111	3177.7222
Frequencies --	3235.1317	3241.6479	3254.3397
Frequencies --	3268.1662	3309.3997	3958.8558

***** C10H8-10H-2900-Syn (R1-2900-s) //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2	
C,0,-1.4449169225,	0.9578301655,-0.6578018538
C,0,-2.5852297996,	0.2832431235,-0.8706441413
C,0,-0.2543530656,	0.3037713181,-0.0809996777
C,0,-2.6965536391,	-1.0981789076,-0.583931972
C,0,1.064435647,	0.5890527087,-0.8109887523
C,0,-0.406876964,	-1.1694107094,0.1242689261
O,0,0.0022774884,	0.9296290875,1.1993037724
C,0,-1.6096371292,	-1.7940946483,-0.0987039627
C,0,1.980023454,	0.2556406203,0.3477780137

ESI
O,0,1.1888824347,1.9131716037,-1.1900476736
C,0,1.9209947742,-1.1869033696,0.7042191557
O,0,1.4178835641,1.0815519156,1.3489674119
C,0,0.7590177341,-1.8413887717,0.5797476781
H,0,-1.354263013,2.0047160248,-0.8839477275
H,0,-3.4382708109,0.8016593758,-1.2744902686
H,0,-3.6310282339,-1.6028892485,-0.7517462781
H,0,1.1969587373,-0.0418181344,-1.6780693647
H,0,-1.6943444219,-2.848242798,0.1092006318
H,0,2.9878210791,0.6218772346,0.1959414401
H,0,1.2033734371,2.4382651862,-0.3904529048
H,0,2.8070806795,-1.6764198946,1.0671385695
H,0,0.6889001138,-2.889337778,0.8229773327
Rotational constants (GHZ): 1.4872662 0.8842405 0.6694275
SCF Done: E(UB+HF-B95) = -611.899522432 A.U. after 1 cycles
S**2 = 0.8157
Frequencies -- 89.6500 154.7435 208.6213
Frequencies -- 225.3206 291.1169 316.2714
Frequencies -- 379.9604 408.5052 434.6859
Frequencies -- 459.0446 484.3377 494.1277
Frequencies -- 544.1673 579.0727 661.4633
Frequencies -- 676.4570 703.8478 737.2157
Frequencies -- 773.9226 835.1675 840.2808
Frequencies -- 854.5326 888.0085 924.8240
Frequencies -- 955.2341 966.3804 1012.8886
Frequencies -- 1020.4453 1021.4743 1034.0012
Frequencies -- 1055.2712 1059.3656 1104.7384
Frequencies -- 1132.9635 1153.8361 1187.1506
Frequencies -- 1195.8827 1244.6415 1265.2095
Frequencies -- 1285.2700 1303.3528 1330.5258
Frequencies -- 1356.5163 1369.4682 1430.0960
Frequencies -- 1447.5486 1455.2997 1480.1730
Frequencies -- 1563.7285 1648.2300 1672.1606
Frequencies -- 3178.4331 3208.2826 3233.9865
Frequencies -- 3236.4416 3245.7078 3268.3734
Frequencies -- 3270.7104 3280.4900 3905.3004

***** C10H8-10H-2900-Anti (R1-2900-a) //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,-1.541837687,0.8969875347,0.7758351749
C,0,-2.5983235893,0.0799761893,0.9040170054
C,0,-0.3108360143,0.4735085513,0.0843593961
C,0,-2.5812899056,-1.2380304494,0.3874264862
C,0,0.9949044947,0.7215964084,0.8593256813
O,0,-0.1398534067,1.3200043685,-1.0589001996
C,0,-0.3278618366,-0.9520303195,-0.3739396553
C,0,0.8899831469,-1.4108693878,-0.9514182299
C,0,1.9146871585,0.726403049,-0.3497137227
O,0,1.2761449997,-0.1823906628,1.8590377103
C,0,-1.4537176381,-1.7257589929,-0.2412138767
O,0,1.2531744719,1.6377460794,-1.185827874
C,0,1.986360494,-0.6365384746,-0.9557754815
H,0,-1.56207059,1.9073985455,1.146826276
H,0,-3.4849367307,0.4320996698,1.4030803571
H,0,-3.4541949931,-1.8580443072,0.4865975117
H,0,0.9729084548,1.7098887493,1.3012520989
H,0,0.9151059455,-2.3994841191,-1.3817132852
H,0,2.888210741,1.1540748339,-0.146404265
H,0,1.3206014002,-1.0581354936,1.4797870984
H,0,-1.4483846736,-2.7298610002,-0.6334024147
H,0,2.9046201876,-0.9722798101,-1.4039171365
Rotational constants (GHZ): 1.5036315 0.8244184 0.7561664
SCF Done: E(UB+HF-B95) = -611.895333729 A.U. after 2 cycles
S**2 = 0.8156
Frequencies -- 86.5708 153.1175 207.0362

ESI			
Frequencies	--	229.5603	278.4050
Frequencies	--	352.0593	365.8299
Frequencies	--	455.7359	495.0472
Frequencies	--	557.4426	576.8855
Frequencies	--	679.7282	708.1639
Frequencies	--	752.4907	787.5539
Frequencies	--	845.3513	900.6283
Frequencies	--	952.9260	968.8512
Frequencies	--	1019.9181	1030.0639
Frequencies	--	1052.2471	1100.4431
Frequencies	--	1145.4312	1165.1742
Frequencies	--	1201.8302	1232.3885
Frequencies	--	1302.9198	1310.2522
Frequencies	--	1356.9954	1380.2836
Frequencies	--	1441.0728	1457.8118
Frequencies	--	1564.9995	1639.4860
Frequencies	--	3172.7634	3183.5120
Frequencies	--	3234.2454	3244.2711
Frequencies	--	3266.7804	3273.2445
			321.6634
			413.8633
			509.9205
			631.1576
			723.2593
			833.8975
			929.0314
			1014.9310
			1038.0101
			1131.2975
			1192.7353
			1259.9382
			1326.3017
			1436.1715
			1477.2690
			1670.1945
			3229.8823
			3261.1928
			3920.6346

***** C10H8-10H-2-10-00-Syn (R1-2-10-00-s) //
BB1k=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,-0.9221840821,0.5744872786,-1.7415953918			
C,0,-1.8972284179,-0.3750918304,-2.0623278857			
C,0,-0.084020989,0.3779967858,-0.7011849371			
C,0,-2.0295543448,-1.5382264953,-1.2823415872			
C,0,0.9324421942,1.3628886896,-0.2100496528			
C,0,-0.1605741269,-0.8346755944,0.1591879412			
O,0,-0.4981004548,-0.3801120748,1.498851			
C,0,-1.2297765635,-1.7777116739,-0.2254225045			
C,0,1.522577166,0.7332401309,1.0453136537			
O,0,0.3826012628,2.6161311243,0.0674386054			
C,0,2.1085439283,-0.5942987443,0.7333911261			
O,0,0.4437157789,0.5830828746,1.963525063			
C,0,1.2118820936,-1.4372241269,0.2585307998			
H,0,-0.8457998522,1.482830687,-2.3164256341			
H,0,-2.5553174885,-0.2124769703,-2.8967288486			
H,0,-2.7908709209,-2.2550337277,-1.539727272			
H,0,1.7164608754,1.5279313974,-0.9431947943			
H,0,-1.3399645681,-2.6643903346,0.3748148413			
H,0,2.1933437716,1.4189523637,1.5456852746			
H,0,-0.2492684125,2.4970666246,0.774970652			
H,0,3.1397556957,-0.8313407298,0.9246039847			
H,0,1.3932870565,-2.464661222,-0.0035249207			
Rotational constants (GHZ):	1.4448773	0.8948250	0.6976870
SCF Done: E(UB+HF-B95) = -611.873056956	A.U. after	2 cycles	
S**2 = 0.7986			
Frequencies	--	62.1470	151.5610
Frequencies	--	230.5280	259.0264
Frequencies	--	365.2049	392.6431
Frequencies	--	441.2114	494.6844
Frequencies	--	556.8820	583.0978
Frequencies	--	673.6646	693.7318
Frequencies	--	759.3471	780.8645
Frequencies	--	824.9444	889.7953
Frequencies	--	970.2082	983.0497
Frequencies	--	1013.6433	1018.7928
Frequencies	--	1047.2893	1078.0162
Frequencies	--	1134.3306	1140.5681
Frequencies	--	1192.0146	1209.1934
Frequencies	--	1282.7465	1308.3521
Frequencies	--	1360.0157	1375.8409
Frequencies	--	1437.8432	1450.0619
Frequencies	--	1595.4831	1665.4589
Frequencies	--	3128.4347	3189.9871
			199.1265
			350.2321
			405.4100
			509.4977
			604.9520
			715.4632
			815.7271
			937.7196
			1012.1708
			1031.3458
			1117.8695
			1158.2700
			1264.0273
			1349.0238
			1416.5798
			1469.3319
			1735.1232
			3240.0372

		ESI	
Frequencies --	3243.5863	3255.8161	3261.2937
Frequencies --	3273.8957	3279.3038	3913.3037

***** C10H8-10H-2-10-OO-Anti (R1-2-10-OO-a) //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2

C,0,-1.3311743621,1.2632733817,-0.9167516111		
C,0,-2.3076178285,0.4956208661,-1.5621919037		
C,0,-0.2929199169,0.6711119654,-0.2880089031		
C,0,-2.1998038729,-0.9065557772,-1.5824780586		
C,0,0.8235894264,1.3733902852,0.4118815103		
C,0,-0.1644527605,-0.8125711855,-0.1970786562		
C,0,-0.107187239,-1.1677000462,1.2648160402		
O,0,1.1086118914,-1.1920240415,-0.7586374028		
C,0,-1.1907829135,-1.5491074225,-0.9637714908		
C,0,1.7054927113,0.266137429,0.9835113492		
O,0,0.3981947885,2.2825693376,1.3880891804		
C,0,0.9015035005,-0.5927951926,1.8935640357		
O,0,2.1751964257,-0.5055350277,-0.1110204793		
H,0,-1.3997404611,2.3387162541,-0.9275921857		
H,0,-3.1271449618,0.9771723475,-2.0643234965		
H,0,-2.944041809,-1.4792698357,-2.1094929031		
H,0,1.4184639301,1.9416149284,-0.2966639315		
H,0,-0.809249029,-1.8572405333,1.6998879461		
H,0,-1.1041042758,-2.6216375059,-0.9899996566		
H,0,2.6024853521,0.6701177212,1.4326497355		
H,0,-0.2682473305,1.8561025163,1.9206117495		
H,0,1.1556732717,-0.7504838609,2.9265184844		
Rotational constants (GHZ):	1.4247275	0.8915170
SCF Done: E(UB+HF-B95) = -611.870887459	A.U. after	1 cycles
S**2 =	0.7983	
Frequencies --	66.3258	156.0995
Frequencies --	208.4520	269.8506
Frequencies --	362.2879	378.7341
Frequencies --	419.3966	480.7546
Frequencies --	558.7535	571.4717
Frequencies --	665.6575	691.7801
Frequencies --	766.6598	794.3560
Frequencies --	828.1865	902.7843
Frequencies --	969.0339	999.1329
Frequencies --	1015.8244	1027.4253
Frequencies --	1071.4818	1076.7362
Frequencies --	1126.9607	1139.9164
Frequencies --	1188.5523	1214.5237
Frequencies --	1273.3891	1306.3626
Frequencies --	1366.2569	1371.4589
Frequencies --	1429.3652	1445.8028
Frequencies --	1595.0408	1665.0704
Frequencies --	3134.2335	3194.3103
Frequencies --	3243.7294	3253.2861
Frequencies --	3274.0169	3276.7201
		3944.0040

***** C10H8-10H-3400-Syn (R1-3400-s) //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2

C,0,-2.2013424584,0.4502446224,-0.5893193686	
C,0,-3.0050795906,-0.6647298854,-0.4749620584	
C,0,-0.8425609218,0.3614942149,-0.3671244458	
C,0,-2.4536665599,-1.8848334256,-0.1435658476	
C,0,0.0406475841,1.5707423087,-0.4777756923	
C,0,-0.2900763183,-0.8668089401,-0.0317712536	
C,0,-1.0961990977,-1.9829032235,0.0752666427	
C,0,1.3590162667,1.1988678677,-1.0520240658	
O,0,0.1939652314,2.2245095075,0.7675161541	

ESI
C,0,2.0640905622,0.0313680761,-0.5179226078
C,0,1.1658195323,-0.9488082652,0.2121242903
O,0,2.6777627422,0.3171937253,0.7711754436
O,0,1.5743455173,-0.3172025479,1.4400310701
H,0,-2.6322324171,1.4019775256,-0.8523776383
H,0,-4.0641474148,-0.5823167995,-0.6488168637
H,0,-3.0783815656,-2.7567525219,-0.0578508061
H,0,-0.4438654803,2.3007543857,-1.1156051997
H,0,-0.6549898414,-2.9322219622,0.3312743694
H,0,1.901048305,1.9136308683,-1.6462020685
H,0,0.6303870795,1.619662922,1.3674762783
H,0,2.8016510818,-0.3769683075,-1.1968996587
H,0,1.5280483341,-1.9715716887,0.1916666864
Rotational constants (GHZ): 1.6091983 0.7396411 0.5898218
SCF Done: E(UB+HF-B95) = -611.879552488 A.U. after 1 cycles
S**2 = 0.7555
Frequencies -- 95.9920 118.7340 145.8583
Frequencies -- 185.2400 262.5427 295.7693
Frequencies -- 309.4788 374.3323 384.0175
Frequencies -- 449.3525 478.6847 503.0739
Frequencies -- 534.3260 601.2263 642.1571
Frequencies -- 673.7458 725.1265 773.3003
Frequencies -- 798.5826 815.3516 883.9161
Frequencies -- 915.4001 925.9535 934.3369
Frequencies -- 953.2442 1005.9391 1012.5554
Frequencies -- 1035.7803 1045.9538 1068.8851
Frequencies -- 1073.2511 1093.3071 1133.5984
Frequencies -- 1162.8087 1200.4777 1249.3319
Frequencies -- 1251.6974 1275.8711 1280.4651
Frequencies -- 1309.0278 1322.5674 1348.3851
Frequencies -- 1390.5665 1400.2422 1425.7663
Frequencies -- 1444.6115 1461.0168 1540.4437
Frequencies -- 1572.4787 1693.9267 1717.1475
Frequencies -- 3133.7470 3149.9840 3170.4017
Frequencies -- 3236.6120 3241.8819 3254.6951
Frequencies -- 3258.0013 3268.3620 3896.2045

***** C10H8-10H-3400-Anti (R1-3400-a) //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,-2.0423779719,0.228577221,0.7901025171
C,0,-2.6529142251,-0.9758461996,1.0778427914
C,0,-0.7603559711,0.2552928559,0.2844353162
C,0,-1.984381301,-2.1626375894,0.8683583901
C,0,-0.0699629177,1.5622696422,-0.0185707144
C,0,-0.0880145663,-0.939607067,0.0653255289
C,0,-0.7020123776,-2.1395688072,0.3619577241
C,0,1.3716891147,1.4633874218,0.3122405157
O,0,-0.6847703718,2.6559673209,0.5987834018
C,0,2.1309424465,0.3178849571,-0.1851162023
C,0,1.2773927814,-0.896730162,-0.4998824082
O,0,2.3781057022,0.4275342055,-1.6123472884
O,0,1.305574364,-0.4906229384,-1.8762342251
H,0,-2.5615981808,1.1569478391,0.9509109717
H,0,-3.6559782326,-0.9852115967,1.4686150463
H,0,-2.4585755089,-3.1012991867,1.0960196368
H,0,-0.1638362767,1.7495778684,-1.0918554056
H,0,-0.1685058697,-3.0604973629,0.1925992505
H,0,1.8786077526,2.3500100173,0.6522445538
H,0,-0.5991078723,2.5603328282,1.5434094884
H,0,3.0593280583,0.1505857489,0.345221602
H,0,1.7983585031,-1.8416084964,-0.3789410038
Rotational constants (GHZ): 1.3466667 0.7931154 0.5456843
SCF Done: E(UB+HF-B95) = -611.878355028 A.U. after 1 cycles
S**2 = 0.7552
Frequencies -- 90.8186 113.9660 137.2879

ESI		
Frequencies --	173.9487	269.0571
Frequencies --	331.5207	347.3228
Frequencies --	403.3563	454.5689
Frequencies --	534.3795	568.0058
Frequencies --	667.7603	693.9973
Frequencies --	802.1963	828.9152
Frequencies --	886.1760	919.2097
Frequencies --	966.5919	1010.5399
Frequencies --	1047.5506	1050.1723
Frequencies --	1091.2353	1122.2840
Frequencies --	1169.4823	1196.7892
Frequencies --	1248.2955	1261.9212
Frequencies --	1299.5040	1315.9736
Frequencies --	1363.5828	1394.0770
Frequencies --	1432.0951	1448.7959
Frequencies --	1560.5242	1687.9123
Frequencies --	3040.4782	3126.1382
Frequencies --	3237.1858	3247.8477
Frequencies --	3265.0688	3272.8361
		284.8503
		388.5696
		493.3416
		598.0821
		765.3909
		875.4867
		933.0158
		1020.0413
		1079.8425
		1138.8381
		1234.6179
		1278.9210
		1323.4537
		1403.1671
		1532.0815
		1712.5372
		3172.7254
		3257.4980
		3946.5828

***** C10H8-10H-4500-Syn (R1-4500-s) //
BB1k=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2		
C,0,-0.3623460745,2.0423874679,0.1173566879		
C,0,0.9576842751,2.4387286799,-0.1660047848		
C,0,-0.634589542,0.6943319936,0.4088174241		
C,0,1.9986795009,1.5773916354,-0.1418804805		
C,0,-2.0246642071,0.1252349555,0.3547225437		
C,0,0.3963851653,-0.1496533864,0.5773793735		
C,0,1.8059557639,0.1878714632,0.3173080902		
C,0,-1.9875681035,-1.2586009572,-0.2289278382		
O,0,-2.9100831761,0.9492022027,-0.354294577		
C,0,-0.9223441532,-2.0366878778,-0.2292959014		
O,0,2.0997828595,-0.7804206843,-0.6898010852		
C,0,0.3182716517,-1.6196408718,0.4827914004		
O,0,1.5462271873,-1.9750232102,-0.1487788167		
H,0,-1.1734124273,2.7416512568,0.0252255669		
H,0,1.1351001757,3.4645628163,-0.442308799		
H,0,2.9927993231,1.8990676991,-0.3971364053		
H,0,-2.4434775932,0.0755087271,1.3581305044		
H,0,2.4491029735,-0.0284493953,1.1769786041		
H,0,-2.9165413868,-1.5910482965,-0.6632428995		
H,0,-2.613116906,1.0088172996,-1.2583668612		
H,0,-0.9420549517,-3.019924035,-0.6681379755		
H,0,0.3514001684,-2.1084311507,1.458255007		
Rotational constants (GHZ):	1.2147980	0.9508938
SCF Done: E(UB+HF-B95) = -611.874659115	A.U. after	1 cycles
S**2 = 0.7993		
Frequencies --	71.2711	134.5654
Frequencies --	213.2661	277.8043
Frequencies --	330.8200	392.6192
Frequencies --	473.5370	482.2780
Frequencies --	538.9278	583.7949
Frequencies --	685.8902	707.5034
Frequencies --	746.0100	809.3955
Frequencies --	876.4445	885.5300
Frequencies --	986.0559	1012.6795
Frequencies --	1035.3302	1049.1229
Frequencies --	1076.2493	1104.7177
Frequencies --	1174.1704	1188.9713
Frequencies --	1200.1684	1250.4539
Frequencies --	1312.9954	1340.1219
Frequencies --	1361.6688	1386.8205
Frequencies --	1439.3561	1445.7521
Frequencies --	1604.5285	1679.5473
Frequencies --	3008.6038	3055.2714
		183.3002
		305.7853
		419.5410
		511.2603
		586.4524
		736.2160
		823.7537
		962.6887
		1014.2581
		1051.6799
		1130.5735
		1195.4084
		1284.4894
		1344.8658
		1417.5852
		1473.1545
		1759.1165
		3098.4492

		ESI	
Frequencies --	3234.2097	3241.4649	3258.9662
Frequencies --	3267.6403	3278.2933	3945.6397

***** C10H8-10H-4500-Anti (R1-4500-a) //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,-1.3696123698,1.6259107355,-0.2774972698
C,0,-2.5375189136,0.942521807,0.0967150578
C,0,-0.1144459971,0.9995754287,-0.1356916444
C,0,-2.5129039325,-0.3033825142,0.6241241821
C,0,1.1096583159,1.5040059149,-0.8381743674
C,0,-0.0550265971,-0.1687865492,0.5204686621
C,0,1.0527534235,-1.1361474955,0.4465036928
C,0,-1.2272259831,-0.9524839073,0.9470267062
C,0,2.0214527029,0.3743595877,-1.21409064
O,0,-1.0003941579,-2.1394873694,0.1870861668
O,0,1.7979611082,2.5058867556,-0.1211632688
C,0,1.9770007987,-0.8321919473,-0.6789735731
O,0,0.3865387538,-2.3978506609,0.3875561298
H,0,-1.4376979809,2.5911419087,-0.7478821323
H,0,-3.4882717167,1.4188812141,-0.0737656352
H,0,-3.4232658555,-0.8221343882,0.8669919541
H,0,0.7919441215,2.003540972,-1.7484592017
H,0,1.6342376636,-1.1676818268,1.3708226807
H,0,-1.1839382972,-1.2245666694,2.0065748503
H,0,2.7679537835,0.6064754895,-1.956254411
H,0,2.1299160004,2.1262513977,0.6871483811
H,0,2.6714879618,-1.6005842612,-0.975473545
Rotational constants (GHZ): 1.2321479 0.9211347 0.5736036
SCF Done: E(UB+HF-B95) = -611.871433849 A.U. after 2 cycles
S**2 = 0.7990
Frequencies -- 62.9302 125.5820 169.2149
Frequencies -- 206.2205 222.5321 284.9177
Frequencies -- 314.3865 374.9065 424.4652
Frequencies -- 464.5013 472.9783 504.0807
Frequencies -- 541.7483 596.6798 661.3222
Frequencies -- 667.9161 690.1717 722.2648
Frequencies -- 771.2030 798.4405 833.8007
Frequencies -- 871.1494 893.0736 965.6068
Frequencies -- 978.2253 1012.4902 1013.6007
Frequencies -- 1042.1805 1045.5574 1052.7815
Frequencies -- 1085.1229 1099.3637 1109.0299
Frequencies -- 1184.6518 1185.4938 1197.4564
Frequencies -- 1221.9228 1239.0909 1274.7464
Frequencies -- 1312.3576 1345.9098 1364.3853
Frequencies -- 1395.0785 1398.7194 1425.5865
Frequencies -- 1445.9041 1461.9734 1478.0480
Frequencies -- 1601.6890 1693.8918 1761.0491
Frequencies -- 3012.8824 3044.0825 3127.8570
Frequencies -- 3231.9610 3242.4100 3254.0634
Frequencies -- 3260.8718 3270.1940 3959.1433

***** C10H8-10H-4900-Syn (R1-4900-s) //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,-1.5042672401,1.1848434842,-0.1235988036
C,0,-2.5786426013,0.5236636638,-0.6056385534
C,0,-0.2337666732,0.4638606239,0.0902311216
C,0,-2.572250176,-0.867913213,-0.8146062512
C,0,0.861896134,0.9140562857,-0.9041664633
C,0,-0.3710941614,-1.0019610994,0.0439176542
O,0,0.3412867821,0.7058013169,1.3875125678
C,0,-1.4611885372,-1.6330542104,-0.4222476355
C,0,2.0337250026,-0.0124681831,-0.8241502446

ESI
O,0,1.2433459693,2.2265933657,-0.6207804824
C,0,2.0496967164,-1.0876104753,-0.0584892755
C,0,0.8454030802,-1.4130726497,0.7739285972
O,0,0.7769213311,-0.5548738493,1.9030691524
H,0,-1.5139058839,2.2490498483,0.0299251313
H,0,-3.4777442949,1.0737623865,-0.8263432426
H,0,-3.449142257,-1.353642884,-1.2026695627
H,0,0.4512126639,0.9245179914,-1.9095469304
H,0,-1.5094451267,-2.7086723888,-0.4477361261
H,0,2.8980194757,0.273527238,-1.401832918
H,0,1.5305068682,2.2372321281,0.2916946134
H,0,2.9206357959,-1.7171051887,0.010889575
H,0,0.8403608353,-2.4209011579,1.1661286823
Rotational constants (GHZ): 1.3368611 0.9182746 0.7350997
SCF Done: E(UB+HF-B95) = -611.875143830 A.U. after 1 cycles
S**2 = 0.7968
Frequencies -- 92.3502 116.4032 192.7882
Frequencies -- 254.3830 282.7933 305.8179
Frequencies -- 348.7597 393.5510 458.0771
Frequencies -- 500.1672 510.8017 533.7931
Frequencies -- 543.0006 563.7556 641.5004
Frequencies -- 650.5362 704.7292 728.2514
Frequencies -- 773.4525 812.4673 814.6416
Frequencies -- 865.2880 919.1258 937.5168
Frequencies -- 949.4222 972.6974 1004.0828
Frequencies -- 1010.0657 1021.1678 1033.7684
Frequencies -- 1047.8818 1074.8307 1095.7102
Frequencies -- 1128.3665 1139.4773 1174.3937
Frequencies -- 1186.2042 1197.7935 1268.3558
Frequencies -- 1286.1370 1322.9229 1340.0013
Frequencies -- 1359.0351 1383.9803 1420.1272
Frequencies -- 1443.5640 1448.2436 1465.6750
Frequencies -- 1593.2484 1689.1079 1754.9834
Frequencies -- 3130.8260 3194.4193 3233.1050
Frequencies -- 3243.1021 3246.8540 3257.5060
Frequencies -- 3271.0493 3277.1060 3902.5952

***** C10H8-10H-4900-Anti (R1-4900-a) //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,-1.4498985035,1.2869002471,0.0286408224
C,0,-2.5052617178,0.6025420305,-0.4620176792
C,0,-0.1616098657,0.6002365457,0.2409431243
C,0,-2.4608174894,-0.7875663185,-0.6714629823
C,0,0.9008782079,1.0002465524,-0.8180505526
C,0,-0.2732995506,-0.8697595812,0.2307093802
O,0,0.4507394821,0.8936982777,1.5013197728
C,0,0.9474208371,-1.2383483324,0.9768941192
C,0,-1.3381353067,-1.5282665243,-0.2546688249
C,0,2.122205229,0.1531551848,-0.6401405667
O,0,0.4146572817,0.9244933323,-2.1246810288
O,0,0.8448954521,-0.3485851849,2.0795481239
C,0,2.1529896774,-0.9025506141,0.1523157857
H,0,-1.49488636,2.3493134665,0.1944551751
H,0,-3.417621441,1.1287218431,-0.6858350502
H,0,-3.3197521827,-1.2957650143,-1.0709339798
H,0,1.1439047304,2.0450094611,-0.6475980266
H,0,0.9615602129,-2.2351461976,1.3958052977
H,0,-1.3650439633,-2.6050881711,-0.2716185448
H,0,2.9859706661,0.4354373097,-1.2201096673
H,0,0.1731423169,0.0188821565,-2.3053669812
H,0,3.043559188,-1.4977513952,0.2627310766
Rotational constants (GHZ): 1.3499857 0.9174377 0.7880076
SCF Done: E(UB+HF-B95) = -611.871825001 A.U. after 1 cycles
S**2 = 0.7964
Frequencies -- 85.1978 118.3221 199.3500

ESI			
Frequencies	--	233.5467	265.2013
Frequencies	--	352.9385	376.8885
Frequencies	--	442.7904	462.9014
Frequencies	--	544.5212	565.7519
Frequencies	--	682.0743	706.5102
Frequencies	--	785.2272	791.4763
Frequencies	--	837.5759	931.6796
Frequencies	--	951.6234	970.5766
Frequencies	--	1010.7990	1021.1751
Frequencies	--	1037.9590	1067.5365
Frequencies	--	1130.9608	1139.7119
Frequencies	--	1190.7699	1196.4579
Frequencies	--	1281.8870	1315.9031
Frequencies	--	1354.5915	1386.0902
Frequencies	--	1439.4860	1454.3620
Frequencies	--	1594.1926	1691.8368
Frequencies	--	3132.6100	3196.4804
Frequencies	--	3240.9841	3245.1613
Frequencies	--	3262.7118	3274.4351
			331.8972
			432.1690
			509.6477
			613.7931
			732.1111
			814.8235
			939.9505
			1004.9251
			1034.9325
			1113.4141
			1175.4975
			1258.0202
			1337.6993
			1416.3311
			1465.9129
			1755.5706
			3232.4382
			3256.7958
			3931.6849

***** C10H8-10H-4-10-00-Syn (R1-4-10-00-s) //
BB1k=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,-1.7761961159,1.2215983737,-0.033227734			
C,0,-2.6773411786,0.5757273537,-0.883969899			
C,0,-0.5560682829,0.7006803843,0.2369783625			
C,0,-2.3251339925,-0.6460964544,-1.4784960988			
C,0,0.427925839,1.3729104899,1.1316042729			
C,0,-0.1244363239,-0.5659060487,-0.3715508793			
O,0,0.3597770648,-1.5286098526,0.6334295481			
C,0,-1.1195830346,-1.2034186704,-1.2476339469			
C,0,1.79570347,1.3610958502,0.5230823479			
O,0,0.4639260333,0.7989687862,2.4190340691			
C,0,2.184491026,0.4943065683,-0.3926463612			
C,0,1.316106521,-0.5945625414,-0.8990709424			
O,0,1.5250663115,-1.8023586302,-0.1590247878			
H,0,-2.0566725065,2.1579856174,0.4209135316			
H,0,-3.6431621357,1.0084542661,-1.0733712403			
H,0,-3.0316930279,-1.146018257,-2.1187344524			
H,0,0.113277297,2.3993458695,1.2885563687			
H,0,-0.8419114697,-2.1508156129,-1.678059304			
H,0,2.4960396321,2.082402981,0.9124012751			
H,0,0.6701139975,-0.128751992,2.3095380687			
H,0,3.1992403389,0.5071815343,-0.757118676			
H,0,1.4318050319,-0.7717986638,-1.9620509366			
Rotational constants (GHZ):	1.2949941	0.8992922	0.6712275
SCF Done: E(UB+HF-B95) =	-611.861410060	A.U. after	1 cycles
S**2 =	0.7961		
Frequencies	--	90.6688	105.0099
Frequencies	--	221.1316	251.3256
Frequencies	--	337.4190	376.2852
Frequencies	--	464.5981	486.6552
Frequencies	--	533.1515	572.7000
Frequencies	--	651.7080	698.6520
Frequencies	--	782.5353	787.9637
Frequencies	--	868.4624	912.7181
Frequencies	--	976.9708	993.0636
Frequencies	--	1016.6527	1038.7890
Frequencies	--	1053.0303	1070.7926
Frequencies	--	1140.8050	1150.0721
Frequencies	--	1193.3824	1231.1505
Frequencies	--	1302.9145	1311.7371
Frequencies	--	1390.0837	1398.8482
Frequencies	--	1460.9552	1470.9115
Frequencies	--	1594.3082	1660.6879
Frequencies	--	3137.1892	3153.5111
			169.5175
			307.1111
			407.9503
			506.5864
			593.9449
			739.4696
			842.3107
			965.9381
			1006.8834
			1047.4697
			1098.7961
			1164.4515
			1277.5515
			1358.3943
			1438.0769
			1475.8228
			1772.5491
			3223.1713

		ESI	
Frequencies --	3236.8820	3244.1187	3244.9051
Frequencies --	3259.8085	3274.7382	3912.8048

***** C10H8-10H-4-10-OO-Anti (R1-4-10-OO-a) //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,1.0434416521,-0.669594113,1.6080145188
C,0,1.9887107823,-1.5857084163,1.1339066513
C,0,0.1148107013,-0.1233266259,0.7889542085
C,0,1.9865727859,-1.958034856,-0.2181902057
C,0,-0.8845712617,0.8819706072,1.2614596252
C,0,0.0552524814,-0.4773718322,-0.6372422771
C,0,-0.1885586875,0.6738970765,-1.6182790824
O,0,-1.2779161462,-0.9430403943,-1.0383185516
C,0,1.0803669027,-1.4411003855,-1.0719317135
C,0,-1.0231517368,1.9991774848,0.2765909263
O,0,-0.6058538973,1.3702889365,2.5442267958
O,0,-1.25403659,-0.0880664898,-2.19219628
C,0,-0.6862980589,1.9218843003,-0.995934756
H,0,1.0424788628,-0.3932626255,2.6484018565
H,0,2.7079663316,-2.011701452,1.8101168668
H,0,2.7097464561,-2.6725824438,-0.5725911703
H,0,-1.8556800265,0.3947989109,1.3493619754
H,0,0.5933851824,0.8495560623,-2.3482543802
H,0,1.0470109545,-1.7354471925,-2.107351906
H,0,-1.4462326261,2.906128287,0.6791769533
H,0,0.2173671657,1.8503377621,2.5150752749
H,0,-0.8330425976,2.7679568326,-1.6477185572
Rotational constants (GHZ): 1.1242719 1.0021558 0.6073389
SCF Done: E(UB+HF-B95) = -611.860313096 A.U. after 1 cycles
S**2 = 0.7953
Frequencies -- 79.6145 99.8340 171.5824
Frequencies -- 227.8980 241.2261 287.6785
Frequencies -- 328.6304 380.9459 405.0668
Frequencies -- 438.4428 458.0997 480.7040
Frequencies -- 511.4590 554.5304 607.9006
Frequencies -- 655.4495 690.5908 737.2004
Frequencies -- 766.2698 795.1558 832.5118
Frequencies -- 860.6527 919.5075 959.6097
Frequencies -- 992.0623 995.4174 1007.9336
Frequencies -- 1015.3839 1044.7636 1048.9667
Frequencies -- 1056.9184 1076.3917 1111.5836
Frequencies -- 1148.1584 1160.3528 1169.6812
Frequencies -- 1185.0947 1214.4846 1271.9757
Frequencies -- 1297.0452 1314.2142 1350.7500
Frequencies -- 1373.1826 1391.3426 1425.6096
Frequencies -- 1443.7889 1463.0883 1471.3721
Frequencies -- 1593.0479 1659.5415 1774.8845
Frequencies -- 3085.2124 3150.5742 3222.9850
Frequencies -- 3242.4838 3244.2190 3256.5714
Frequencies -- 3261.6643 3275.1398 3943.6665

***** TS R1-200-s --> R1-2300-s //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,-1.6475800558,1.3016053877,0.2109506853
C,0,-2.8665740838,0.7018573149,0.4644683863
C,0,-0.5773842635,0.5551152217,-0.2228904625
C,0,-3.0260369643,-0.6563625,0.2697545822
C,0,0.7256925459,1.2152933525,-0.5810193896
C,0,-0.7252751742,-0.8235922887,-0.4068260688
C,0,-1.9639450904,-1.410841744,-0.1657878645
C,0,1.8845259936,0.2905715768,-0.3320823577
O,0,0.9211477145,2.4278660117,0.0844337018

ESI
O,0,1.9593321596,0.0391383141,1.0551443754
C,0,1.6659321674,-1.1263245346,-0.8008089476
C,0,0.3865339904,-1.6069683078,-0.8479595294
O,0,2.2360875892,-1.3233423495,0.9771509578
H,0,-1.522570602,2.3620452845,0.3439042042
H,0,-3.6943086574,1.297901638,0.808069314
H,0,-3.9764492201,-1.1229384463,0.4618066505
H,0,0.7111168377,1.456166742,-1.6435542957
H,0,-2.0755088063,-2.4722494097,-0.3123028561
H,0,2.8087803574,0.726649919,-0.7004741824
H,0,1.0063329495,2.2417314645,1.0173543891
H,0,2.4613813062,-1.651732428,-1.2947838994
H,0,0.213351737,-2.6289914456,-1.140645806
Rotational constants (GHZ): 1.4184228 0.7685779 0.5764521
SCF Done: E(UB+HF-B95) = -611.872182539 A.U. after 1 cycles
S**2 = 0.8016
Frequencies -- -855.4564 77.7193 116.0004
Frequencies -- 139.3692 208.1898 238.3771
Frequencies -- 276.3143 350.3680 400.9756
Frequencies -- 429.6484 446.6431 465.4075
Frequencies -- 519.6572 556.1399 559.0172
Frequencies -- 657.0523 699.9873 745.8504
Frequencies -- 782.6418 806.5262 833.4512
Frequencies -- 845.6508 896.1089 913.7357
Frequencies -- 929.9211 978.8321 1011.7468
Frequencies -- 1030.3263 1041.4463 1048.5307
Frequencies -- 1083.3901 1106.3070 1158.4539
Frequencies -- 1170.3875 1183.4705 1194.8230
Frequencies -- 1242.4796 1260.4908 1279.0146
Frequencies -- 1310.8682 1343.3574 1370.3680
Frequencies -- 1391.4633 1394.5058 1444.9192
Frequencies -- 1455.3647 1511.6541 1543.7005
Frequencies -- 1572.5324 1672.6033 1693.0211
Frequencies -- 3091.9041 3126.0687 3239.7803
Frequencies -- 3246.2262 3248.9065 3262.5560
Frequencies -- 3270.6155 3282.3877 3925.9367

***** TS R1-200-a --> R1-2300-a //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,0.1673550087,-1.9946803828,0.8494973762
C,0,1.3977137253,-2.596380403,0.6771051035
C,0,-0.0244897208,-0.67647826,0.504569042
C,0,2.4558574963,-1.8684932909,0.1656580322
C,0,-1.3228737425,0.0164101687,0.7852189283
C,0,1.0379340384,0.062812424,-0.0253183869
C,0,2.2785926704,-0.5507099308,-0.1778128178
C,0,-1.5955267161,1.0899199769,-0.2381375844
O,0,-1.3448459914,0.5739262535,2.0765631278
O,0,-1.7185796994,0.4962462304,-1.5087253638
C,0,-0.403670994,1.9711673376,-0.5298315776
C,0,0.8469425664,1.4369883453,-0.3806173765
O,0,-0.9967856219,1.4487631739,-2.2216960513
H,0,-0.6551523794,-2.5564630925,1.2600355535
H,0,1.5321164431,-3.630381614,0.9432488934
H,0,3.4164880294,-2.3349351013,0.0326936124
H,0,-2.1352710952,-0.7019103446,0.7507249401
H,0,3.0974960757,0.0192772214,-0.5839087889
H,0,-2.4799810246,1.6570001298,0.0376615714
H,0,-0.5030158785,0.9883986037,2.2450992393
H,0,-0.5314784189,3.0337538665,-0.6168681038
H,0,1.713482757,2.0304391584,-0.619805054
Rotational constants (GHZ): 1.4268410 0.7249769 0.6100499
SCF Done: E(UB+HF-B95) = -611.869758867 A.U. after 2 cycles
S**2 = 0.8009
Frequencies -- -855.5606 70.3285 110.7106

ESI			
Frequencies	--	137.6739	204.1832
Frequencies	--	262.4110	308.5328
Frequencies	--	380.6011	442.8295
Frequencies	--	510.3230	537.3026
Frequencies	--	626.9956	722.2591
Frequencies	--	781.2099	802.5444
Frequencies	--	840.2383	894.9281
Frequencies	--	940.9645	952.7801
Frequencies	--	1032.1529	1038.9872
Frequencies	--	1098.7164	1115.6836
Frequencies	--	1163.7260	1187.0123
Frequencies	--	1249.7023	1256.9687
Frequencies	--	1309.9678	1338.6623
Frequencies	--	1398.2665	1407.3378
Frequencies	--	1468.6080	1509.7897
Frequencies	--	1572.0802	1668.1258
Frequencies	--	3125.5884	3145.4552
Frequencies	--	3243.6238	3245.2149
Frequencies	--	3269.9373	3280.5493
			212.2558
			346.3483
			500.6942
			593.4002
			760.7163
			818.6551
			924.4507
			1005.0533
			1085.5342
			1122.5210
			1197.7025
			1262.8038
			1362.4869
			1434.9190
			1546.6802
			1694.9260
			3239.2050
			3256.6720
			3949.1213

***** TS R1-200-s --> R1-2400-s //
BB1k=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,0.7209320416,	1.2287870618,-0.5816043502		
C,0,1.9514898276,	0.5910185247,0.0487028358		
C,0,2.0607398021,-	0.8690473571,-0.2270229726		
C,0,0.9164810464,-	1.5033072674,0.2061161376		
C,0,-1.5099735613,-	1.800926405,-0.1833535573		
C,0,-2.7384288703,-	1.2870448883,-0.5404440646		
C,0,-2.8478330462,	0.041738023,-0.8915669197		
C,0,-1.7301987049,	0.8534025162,-0.892466076		
C,0,-0.4980437309,	0.344778647,-0.5468683737		
C,0,-0.3914695033,-	0.9909910985,-0.1866926721		
O,0,0.4910738404,	2.479651205,-0.0075264414		
O,0,1.8863860245,	0.6059976915,1.4639554036		
O,0,0.9716214874,-	0.3743716362,1.8107779429		
H,0,0.9648826731,	1.4227667409,-1.6242451095		
H,0,2.8305676798,	1.1715751919,-0.1996449525		
H,0,3.0219207083,-	1.349503616,-0.2529611145		
H,0,0.9651935276,-	2.5358416753,0.5125941035		
H,0,-1.416252344,-	2.8340861194,0.1072199093		
H,0,-3.6087098205,-	1.9199326121,-0.5357742946		
H,0,-3.8059305984,	0.4501821166,-1.1630182496		
H,0,-1.812462046,	1.8953211911,-1.1509769633		
H,0,0.465967597,	2.3588541611,0.9403515079		
Rotational constants (GHZ):	1.5108766	0.7940394	0.6078866
SCF Done: E(UB+HF-B95) =	-611.858014378	A.U. after	1 cycles
S**2 =	0.8187		
Frequencies	--	-804.6335	74.8545
Frequencies	--	151.5187	232.4384
Frequencies	--	306.3250	373.0872
Frequencies	--	426.3371	432.1029
Frequencies	--	521.8456	554.4240
Frequencies	--	630.7518	702.5718
Frequencies	--	770.0016	795.6830
Frequencies	--	845.8342	885.9659
Frequencies	--	927.5696	958.6502
Frequencies	--	1007.5658	1021.9223
Frequencies	--	1082.6076	1092.4907
Frequencies	--	1154.2684	1169.8689
Frequencies	--	1247.6174	1262.9768
Frequencies	--	1306.2558	1328.7952
Frequencies	--	1381.3920	1394.7235
Frequencies	--	1444.7452	1485.5107
Frequencies	--	1569.4498	1692.8248
Frequencies	--	3102.0196	3183.1086
			132.4749
			250.3284
			389.0814
			484.4781
			577.4989
			730.3315
			816.1643
			917.0580
			1005.0331
			1043.5821
			1139.9792
			1198.3894
			1283.1818
			1350.2137
			1416.5824
			1547.8687
			1711.2080
			3236.7901

		ESI	
Frequencies --	3238.6929	3247.6665	3258.9069
Frequencies --	3269.4173	3273.4954	3917.2349

***** TS R1-200-a --> R1-2400-a //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,0.7453631316,	1.3066526187,	-0.2339098838	
C,0,1.9807588149,	0.4328145127,	-0.0456578144	
C,0,1.8093475888,	-0.6084285663,	1.0084282056	
C,0,0.721676257,	-1.3912294861,	0.689882075	
C,0,-1.7469876647,	-1.4334516051,	0.5003430341	
C,0,-2.9386634448,	-0.8080808357,	0.2038606417	
C,0,-2.9371177675,	0.5001261745,	-0.2337403255	
C,0,-1.7432761394,	1.1771257382,	-0.3796464857	
C,0,-0.546338555,	0.5576911791,	-0.0893534915	
C,0,-0.5514840329,	-0.7550401986,	0.3607295897	
O,0,0.7983399701,	2.4037706171,	0.646027345	
O,0,1.3217050706,	-1.3849979415,	-1.1639689811	
O,0,2.2586245073,	-0.3705206001,	-1.1787736349	
H,0,0.8121750511,	1.7234780361,	-1.2345067569	
H,0,2.8416945987,	1.074977506,	0.0843158916	
H,0,2.6534989922,	-0.9752186323,	1.5631374525	
H,0,0.6805994241,	-2.4132987656,	1.0304356251	
H,0,-1.739103709,	-2.4549023847,	0.8427121	
H,0,-3.8668992148,	-1.3419152747,	0.3112237462	
H,0,-3.8652867598,	0.9910819907,	-0.4695796298	
H,0,-1.7375372036,	2.1974268969,	-0.7254918332	
H,0,0.43183331,	2.1432768361,	1.4858623015	
Rotational constants (GHZ):	1.4397907	0.7840573	0.6093635
SCF Done: E(UB+HF-B95) =	-611.854420393	A.U. after	1 cycles
S**2 =	0.8202		
Frequencies --	-857.6902	61.6584	125.3035
Frequencies --	148.4409	228.0380	246.4590
Frequencies --	274.2979	303.4289	366.0761
Frequencies --	388.8823	444.8425	496.2140
Frequencies --	516.2141	538.7187	562.6916
Frequencies --	642.2660	670.2601	757.7519
Frequencies --	772.4062	794.7075	816.4999
Frequencies --	828.7053	905.4741	915.2013
Frequencies --	927.6989	978.7085	997.0064
Frequencies --	1004.3145	1015.3230	1042.5088
Frequencies --	1085.7769	1096.2884	1114.5759
Frequencies --	1151.0981	1164.1299	1197.4470
Frequencies --	1245.7402	1253.5144	1264.6558
Frequencies --	1295.4808	1329.5553	1345.4989
Frequencies --	1380.0918	1386.0988	1422.8705
Frequencies --	1436.6732	1485.8982	1546.5756
Frequencies --	1568.1358	1689.7452	1709.2565
Frequencies --	3132.2284	3189.3821	3238.0628
Frequencies --	3239.4460	3244.2043	3256.0699
Frequencies --	3269.3548	3277.0581	3959.6444

***** TS R1-200-s --> R1-2900-s //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2		
C,0,-1.457343534,	0.9337515171,	-0.679866733
C,0,-2.6222208153,	0.2443416719,	-0.854991101
C,0,-0.2719944776,	0.249994423,	-0.3320340863
C,0,-2.6454165314,	-1.1451298536,	-0.7614733287
C,0,1.0739464568,	0.8623298602,	-0.6215864804
C,0,-0.3031070578,	-1.1808366732,	-0.2756156181
O,0,-0.0337733876,	0.5139283861,	1.5290394711
C,0,-1.4869258822,	-1.8467810478,	-0.4825829529
C,0,1.9380171771,	0.3532567032,	0.5168020369

ESI
O,0,1.0456831522,2.2454046488,-0.6556878204
C,0,1.9700746663,-1.1349841051,0.5310194162
O,0,1.2758260299,0.9302936688,1.625634304
C,0,0.9115089759,-1.8351166315,0.1272633442
H,0,-1.4117198811,2.0008007294,-0.8001726646
H,0,-3.5276403811,0.7760465744,-1.0913107777
H,0,-3.5693442147,-1.6752746236,-0.9127772066
H,0,1.4378616845,0.5057582073,-1.5793116329
H,0,-1.5101494179,-2.9209161981,-0.4061755081
H,0,2.927936293,0.7928178993,0.5035813929
H,0,0.932249732,2.541099399,0.2478550613
H,0,2.8548655193,-1.6296023947,0.8918081436
H,0,0.9248204427,-2.912698408,0.1530085733
Rotational constants (GHZ): 1.4777597 0.8593718 0.6640386
SCF Done: E(UB+HF-B95) = -611.880358232 A.U. after 1 cycles
S**2 = 0.8183
Frequencies -- -581.7427 122.2952 144.4975
Frequencies -- 213.2809 247.5162 279.7060
Frequencies -- 332.5299 374.9704 419.0738
Frequencies -- 432.8951 464.2036 476.0866
Frequencies -- 505.8623 549.7326 586.2480
Frequencies -- 647.3465 700.7704 712.7621
Frequencies -- 764.6528 793.9137 817.0185
Frequencies -- 840.1170 891.4941 904.8053
Frequencies -- 958.1201 987.4628 996.6841
Frequencies -- 1026.3390 1033.8392 1047.9034
Frequencies -- 1064.0991 1071.4706 1127.3812
Frequencies -- 1167.3769 1175.6876 1193.3196
Frequencies -- 1217.8220 1256.7048 1270.0655
Frequencies -- 1299.6525 1315.1321 1353.3707
Frequencies -- 1358.9947 1377.0049 1447.7874
Frequencies -- 1452.3627 1484.8437 1519.4374
Frequencies -- 1602.9078 1652.1077 1702.4202
Frequencies -- 3155.0799 3175.8037 3235.4143
Frequencies -- 3242.5558 3251.8185 3264.5983
Frequencies -- 3268.5237 3284.7044 3893.0613

***** TS R1-200-a --> R1-2900-a //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,-1.557866032,0.8311267877,0.8112628341
C,0,-2.6792870731,0.0498761099,0.8189833775
C,0,-0.3434810983,0.3316088578,0.3007990525
C,0,-2.62444274,-1.2670750452,0.3750321078
C,0,0.981223982,0.8910357313,0.7677256601
O,0,-0.1238514811,1.0816791068,-1.4024237161
C,0,-0.2957267162,-1.0358293959,-0.12185647
C,0,0.9490229084,-1.4841980888,-0.6940621698
C,0,1.8547418742,0.7868910604,-0.4716416662
O,0,1.4856041022,0.2402666861,1.8868680119
C,0,-1.433481442,-1.8022953517,-0.0871815099
O,0,1.1446739805,1.6063750324,-1.370209326
C,0,1.9614760921,-0.640903941,-0.9000072671
H,0,-1.58490148,1.8412011839,1.1818713061
H,0,-3.6085278279,0.4487782767,1.1870214034
H,0,-3.5125750704,-1.8741011584,0.3909253741
H,0,0.8708690976,1.9361319164,1.0279053076
H,0,1.0206413032,-2.5122017272,-1.0113450541
H,0,2.8246176838,1.2486718852,-0.3354809217
H,0,1.6012835311,-0.6840586214,1.6760285405
H,0,-1.4002374634,-2.8183756452,-0.4436868681
H,0,2.8643388817,-0.9740330596,-1.381442541
Rotational constants (GHZ): 1.4706869 0.7852105 0.7442757
SCF Done: E(UB+HF-B95) = -611.872595390 A.U. after 1 cycles
S**2 = 0.8219
Frequencies -- -674.9396 115.3844 150.7984

ESI			
Frequencies	--	209.2214	246.0678
Frequencies	--	321.8798	352.0840
Frequencies	--	398.6340	449.4072
Frequencies	--	518.9340	542.1262
Frequencies	--	627.1711	667.0333
Frequencies	--	764.5357	765.6527
Frequencies	--	833.1103	890.3292
Frequencies	--	954.3656	978.1362
Frequencies	--	1022.5660	1034.6740
Frequencies	--	1068.4233	1088.3944
Frequencies	--	1164.5885	1176.3013
Frequencies	--	1227.5937	1246.2746
Frequencies	--	1297.1762	1321.7591
Frequencies	--	1358.6673	1391.6268
Frequencies	--	1451.0919	1486.1196
Frequencies	--	1606.2803	1651.7791
Frequencies	--	3173.4836	3180.9617
Frequencies	--	3241.0648	3249.7317
Frequencies	--	3263.0099	3272.3161
			287.1096
			369.6644
			503.9537
			571.8073
			737.7512
			810.0798
			914.5904
			987.0101
			1061.9513
			1153.3025
			1185.0335
			1270.5656
			1342.4042
			1445.8445
			1521.2016
			1695.6539
			3233.0264
			3261.7890
			3926.1730

***** TS R1-200-s --> R1-2-10-00-s //
BB1k=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,-1.3340030298,1.4743304439,-0.2017290854			
C,0,-2.597549052,0.9982265085,0.1102676632			
C,0,-0.3016022502,0.6075231522,-0.4135083544			
C,0,-2.8218177603,-0.3746871894,0.2164432893			
C,0,1.1147195995,1.0452564007,-0.6120652677			
C,0,-0.4837445332,-0.8082740607,-0.2396123384			
O,0,0.3330557318,-0.8988043304,1.3486753158			
C,0,-1.8126519636,-1.263140791,0.0182701226			
C,0,1.9758604423,-0.1052558037,-0.0972539468			
O,0,1.4001606635,2.2330137501,0.0567118228			
C,0,1.7331229315,-1.3234691404,-0.8973680686			
O,0,1.5728602337,-0.2792486043,1.2638523612			
C,0,0.4631818895,-1.6832410711,-0.9479539934			
H,0,-1.1464397666,2.5322874769,-0.2684914011			
H,0,-3.4090862025,1.6869442089,0.2657341536			
H,0,-3.8125125508,-0.7341722794,0.4357786402			
H,0,1.3362748437,1.2137057239,-1.6631970541			
H,0,-1.991031376,-2.3233241427,0.0694825395			
H,0,3.0134605711,0.1947383988,-0.0385739718			
H,0,1.3042264445,2.0551191962,0.9916339545			
H,0,2.5364772239,-1.8894929423,-1.3326552372			
H,0,0.1069201397,-2.5791028593,-1.4265677456			
Rotational constants (GHZ):	1.4187330	0.9079632	0.6922704
SCF Done: E(UB+HF-B95) = -611.861606649	A.U. after	1 cycles	
S**2 = 0.8066			
Frequencies	--	-614.6825	97.1647
Frequencies	--	179.2776	246.2571
Frequencies	--	335.7367	389.3337
Frequencies	--	423.3989	460.8088
Frequencies	--	499.0286	565.7300
Frequencies	--	619.3219	653.5149
Frequencies	--	752.3157	774.2783
Frequencies	--	811.8340	874.3720
Frequencies	--	936.8741	994.2119
Frequencies	--	1014.5300	1026.3849
Frequencies	--	1058.5089	1064.8813
Frequencies	--	1162.6408	1164.6461
Frequencies	--	1210.9635	1236.4274
Frequencies	--	1269.9904	1313.3191
Frequencies	--	1366.3983	1380.0075
Frequencies	--	1441.5064	1493.5544
Frequencies	--	1601.4724	1657.4640
Frequencies	--	3114.8647	3190.7894
			162.2655
			254.3796
			408.1468
			473.7196
			578.0981
			708.3775
			804.2662
			886.0022
			1010.1531
			1047.6056
			1118.6739
			1188.5356
			1268.4013
			1356.4413
			1434.3110
			1508.1478
			1741.1932
			3244.2689

		ESI	
Frequencies --	3253.0012	3253.7418	3261.7651
Frequencies --	3272.4172	3280.2713	3906.3042

***** TS R1-200-a --> R1-2-10-00-a //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,-1.3753195303,1.4286779764,-0.5426345119
C,0,-2.65293487,0.8982413841,-0.4467137026
C,0,-0.2950126347,0.722257938,-0.1020663195
C,0,-2.8427412265,-0.3701060482,0.1006791927
C,0,1.1225652964,1.1692162759,-0.2575692285
C,0,-0.4527654225,-0.6105153878,0.4152204194
C,0,0.595918873,-1.081853145,1.3349307964
O,0,0.2024685677,-1.474089709,-1.0099405129
C,0,-1.7870850474,-1.0996028928,0.5510621053
C,0,1.9537747105,-0.1128367594,-0.3155333926
O,0,1.5614717782,2.0478374059,0.7421420324
C,0,1.843289323,-0.8246359753,0.9775068288
O,0,1.387044769,-0.8724451932,-1.3869260253
H,0,-1.2276154109,2.4063923729,-0.9698781676
H,0,-3.4991839857,1.4658541074,-0.7912450171
H,0,-3.8400348222,-0.7655031588,0.1886636912
H,0,1.2391560092,1.6959052153,-1.1974814731
H,0,0.3228719072,-1.6447991622,2.2112183928
H,0,-1.9370263334,-2.0644886708,1.0041002239
H,0,2.9711329838,0.0909803947,-0.6195206652
H,0,1.3999278737,1.6402508599,1.5895931162
H,0,2.704754031,-1.1480721833,1.5330528202
Rotational constants (GHZ): 1.4335326 0.8542519 0.7099819
SCF Done: E(UB+HF-B95) = -611.856576049 A.U. after 1 cycles
S**2 = 0.8114
Frequencies -- -679.9574 97.7284 157.6217
Frequencies -- 178.2405 221.9050 283.6907
Frequencies -- 322.3618 362.1686 371.6759
Frequencies -- 395.8156 423.4351 475.1355
Frequencies -- 514.5267 536.0422 584.5864
Frequencies -- 626.2387 671.7530 713.5298
Frequencies -- 744.8357 778.0980 784.2052
Frequencies -- 828.8889 875.7949 904.6493
Frequencies -- 931.4099 985.2682 995.3116
Frequencies -- 1016.6425 1025.4348 1041.6097
Frequencies -- 1063.3149 1091.2552 1125.0395
Frequencies -- 1153.1273 1162.7533 1188.2538
Frequencies -- 1229.4018 1233.0915 1264.0444
Frequencies -- 1269.5851 1313.7715 1339.3273
Frequencies -- 1377.8070 1386.3189 1434.0521
Frequencies -- 1449.0131 1495.0972 1512.2197
Frequencies -- 1604.3957 1660.5640 1732.1605
Frequencies -- 3158.6530 3194.9477 3242.0851
Frequencies -- 3247.2357 3249.4526 3259.5519
Frequencies -- 3270.7922 3278.3091 3933.8839

***** TS R1-400-s --> R1-2400-s //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,0.6617838473,1.4725664503,0.2726023567
C,0,1.7322104438,0.6868904344,0.9697345738
C,0,2.1092585978,-0.5498851712,0.5268760712
C,0,0.9016030912,-1.4130934129,0.3555308384
C,0,-0.9208618166,-1.5566725574,-1.3484016864
C,0,-1.8861132558,-0.969525606,-2.1332589895
C,0,-2.0376284283,0.4039565882,-2.1201805284
C,0,-1.2159940032,1.1795140875,-1.3346889276
C,0,-0.2351887953,0.5966499404,-0.5533063776

ESI
C,0,-0.0977073065,-0.7804987135,-0.5533071353
O,0,-0.0470910704,2.286869464,1.1564518292
O,0,0.3874047473,-0.185918668,2.1301367763
O,0,0.4258683416,-1.4819995061,1.6998057723
H,0,1.1751673795,2.1638194059,-0.3951995922
H,0,2.4028565314,1.2768560552,1.5744794549
H,0,3.0686194628,-0.9878111683,0.7360729404
H,0,1.113390741,-2.4366100334,0.0757676022
H,0,-0.806281999,-2.6281429474,-1.3415514473
H,0,-2.5236923588,-1.5790128416,-2.7498558786
H,0,-2.7958436822,0.868252742,-2.7268774453
H,0,-1.3321250955,2.2501387031,-1.3153186785
H,0,-0.4997213741,1.7014875267,1.7617268497
Rotational constants (GHZ): 1.4136075 0.8338832 0.6222416
SCF Done: E(UB+HF-B95) = -611.858296554 A.U. after 1 cycles
S**2 = 0.8097
Frequencies -- -847.7653 101.7183 127.1174
Frequencies -- 202.8562 240.6235 262.4057
Frequencies -- 361.0493 370.9509 383.8510
Frequencies -- 435.7446 493.5440 508.1767
Frequencies -- 529.1935 544.3447 583.8839
Frequencies -- 635.8025 680.4168 756.0431
Frequencies -- 773.8162 792.9963 814.5566
Frequencies -- 822.2530 887.6505 926.3592
Frequencies -- 933.9800 950.9500 998.4362
Frequencies -- 1011.1474 1032.0427 1044.8381
Frequencies -- 1045.8411 1090.4367 1135.7640
Frequencies -- 1158.2771 1174.2817 1197.9557
Frequencies -- 1235.5039 1247.3818 1279.8943
Frequencies -- 1296.9281 1329.8773 1357.9790
Frequencies -- 1382.3713 1393.2103 1396.2076
Frequencies -- 1446.9857 1518.6002 1527.9089
Frequencies -- 1568.0901 1686.6145 1711.9792
Frequencies -- 3087.2442 3185.9533 3233.7052
Frequencies -- 3236.7458 3244.6694 3256.3532
Frequencies -- 3268.8532 3270.0913 3915.2016

***** TS R1-400-a --> R1-2400-a //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,-1.3536033666,0.7497164174,-0.3959566163
C,0,-0.4204618629,1.741167774,-1.0308678236
C,0,0.8637571878,1.9019376641,-0.5814117654
C,0,1.5320718897,0.5682793077,-0.5220060756
C,0,1.424401249,-1.3347393822,1.0934615383
C,0,0.714449411,-2.2177577513,1.874470222
C,0,-0.6640337348,-2.1429064676,1.9115060602
C,0,-1.3219704036,-1.1867535003,1.1704792411
C,0,-0.6137599001,-0.297590008,0.3830953636
C,0,0.7676683855,-0.3745619482,0.3460380871
O,0,-2.3031525213,1.4220248115,0.393902671
O,0,1.4902745093,0.1859591384,-1.8975191793
O,0,0.1890226005,0.3763427916,-2.268885412
H,0,-1.9253863524,0.275933718,-1.1864487697
H,0,-0.9152557741,2.5488489742,-1.5460336598
H,0,1.4379553654,2.7986293631,-0.7285923655
H,0,2.5816457678,0.5953094145,-0.2609795528
H,0,2.5001473361,-1.3874248022,1.0592839472
H,0,1.2321343137,-2.9621795929,2.4541064446
H,0,-1.2258674601,-2.8301052728,2.5203731578
H,0,-2.3959997102,-1.1138983339,1.2025174706
H,0,-1.8696433244,1.7595199666,1.1729393019
Rotational constants (GHZ): 1.3189330 0.8522387 0.6039595
SCF Done: E(UB+HF-B95) = -611.855735182 A.U. after 1 cycles
S**2 = 0.8105
Frequencies -- -876.7957 91.3359 127.8782

ESI		
Frequencies --	180.9106	240.8162
Frequencies --	319.2614	354.1370
Frequencies --	392.1887	439.2235
Frequencies --	520.6719	554.5338
Frequencies --	635.3043	683.3888
Frequencies --	775.5229	798.9447
Frequencies --	848.3523	910.3637
Frequencies --	932.2544	961.7676
Frequencies --	1011.4461	1022.8596
Frequencies --	1044.5458	1088.3788
Frequencies --	1159.8033	1166.2479
Frequencies --	1236.5180	1248.0836
Frequencies --	1294.4238	1327.8825
Frequencies --	1381.9658	1393.2059
Frequencies --	1426.3260	1511.1296
Frequencies --	1568.0597	1689.9188
Frequencies --	3146.3585	3186.8958
Frequencies --	3237.8172	3244.0237
Frequencies --	3268.2210	3273.7247
		266.3440
		366.3212
		492.9592
		583.7193
		745.8461
		804.6691
		921.5949
		1007.5418
		1039.5211
		1112.5897
		1196.3267
		1259.5017
		1357.1554
		1396.7739
		1528.8477
		1712.1119
		3235.8256
		3255.9023
		3949.6383

***** TS R1-400-s --> R1-3400-s //
BB1k=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2		
C,0,1.4767519748,-0.5315905963,0.4897113977		
C,0,0.7597338571,-1.8063595285,0.7898272229		
C,0,-0.5051794192,-2.0175465006,0.3246469163		
C,0,-1.2001892697,-0.8711581361,-0.3762136666		
C,0,-1.6583575015,1.5377186837,0.1237956107		
C,0,-1.22966462,2.7770361922,0.550139062		
C,0,0.0767185885,2.9451619473,0.9591583473		
C,0,0.9493847825,1.8767952484,0.9458158148		
C,0,0.528636628,0.6344593484,0.5186246038		
C,0,-0.7851485648,0.4698536586,0.1078941422		
O,0,-0.654162652,-1.1033062305,-1.6691489097		
O,0,-0.2782637178,-2.4384314289,-1.4642332454		
H,0,1.3010831184,-2.60303702,1.2701837079		
H,0,-1.0777207606,-2.8643289403,0.655908038		
H,0,-2.2798938421,-0.9843053073,-0.395927724		
H,0,-2.6771406522,1.3960138055,-0.197373244		
H,0,-1.9129009164,3.6082409343,0.5651658548		
H,0,0.4161096465,3.9102792085,1.2937185113		
H,0,1.9690374631,2.0084440776,1.2680206124		
O,0,2.1807548613,-0.6245430352,-0.7274830431		
H,0,1.5560114233,-0.8568593085,-1.4136287873		
H,0,2.2426678537,-0.3704237966,1.2404579097		
Rotational constants (GHZ):	1.5666132	0.7425735
SCF Done: E(UB+HF-B95) = -611.859798182	A.U. after	0.5933272
S**2 = 0.7898	2 cycles	
Frequencies --	-779.3979	53.8449
Frequencies --	138.5233	121.4387
Frequencies --	276.4683	233.2622
Frequencies --	386.6018	366.3974
Frequencies --	526.2643	479.1892
Frequencies --	651.7163	603.6711
Frequencies --	782.3517	775.1064
Frequencies --	836.1048	818.6376
Frequencies --	945.9709	928.5673
Frequencies --	1026.1567	1007.9868
Frequencies --	1074.6573	1035.4848
Frequencies --	1163.6839	1093.5790
Frequencies --	1248.9690	1183.2560
Frequencies --	1312.7130	1258.2997
Frequencies --	1399.1721	1331.5436
Frequencies --	1459.3325	1418.2171
Frequencies --	1576.0141	1433.0357
Frequencies --	3127.7322	1539.6336
		1550.7054
		1696.2016
		1717.4418
		3140.6828
		3236.8518

		ESI	
Frequencies --	3241.8765	3254.2758	3254.3509
Frequencies --	3268.0257	3276.8291	3891.6805

***** TS R1-400-a --> R1-3400-a //
BB1K=BB95-IOP(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,-1.3337988832,0.6869003937,-0.4228811611
C,0,-0.4661666934,1.8762735413,-0.6478090838
C,0,0.8764276012,1.7296080485,-0.8407284874
C,0,1.4514255348,0.3420144491,-0.6652143351
C,0,1.3973089219,-1.3684556676,1.1637562076
C,0,0.6967085267,-2.1179909402,2.085897584
C,0,-0.6692028968,-1.9664481074,2.1902443611
C,0,-1.334547795,-1.0660728257,1.3819915288
C,0,-0.636260092,-0.3127009527,0.4629862286
C,0,0.7374449151,-0.4684595211,0.3538699287
O,0,-2.6010619528,1.0432237715,0.0482709534
O,0,1.1466848606,-0.1268991601,-1.9695343781
O,0,1.0223842008,1.1315267937,-2.57000133
H,0,-1.5059822266,0.2144537756,-1.3915669034
H,0,-0.9527438592,2.8293140261,-0.7657980557
H,0,1.5264328901,2.5849567616,-0.8462283534
H,0,2.5252408343,0.3494191179,-0.5018130047
H,0,2.464954275,-1.4805698782,1.0703777701
H,0,1.2148883045,-2.8182499689,2.7175420687
H,0,-1.2222730842,-2.552031145,2.9043890112
H,0,-2.4016512985,-0.9498480986,1.4566593367
H,0,-2.5089575404,1.4317336622,0.9138795389
Rotational constants (GHZ): 1.3334377 0.7915428 0.5496985
SCF Done: E(UB+HF-B95) = -611.859407238 A.U. after 1 cycles
S**2 = 0.7893
Frequencies -- -804.0547 70.0431 127.6783
Frequencies -- 144.8007 199.3709 264.1358
Frequencies -- 278.1012 326.6665 348.5489
Frequencies -- 400.8444 454.6745 466.3361
Frequencies -- 500.9775 540.3122 588.9542
Frequencies -- 630.1523 675.6851 738.1229
Frequencies -- 765.9924 802.7669 823.0910
Frequencies -- 844.4531 894.5713 928.3676
Frequencies -- 935.9796 995.2740 1010.7400
Frequencies -- 1024.6977 1045.5268 1046.8650
Frequencies -- 1078.9423 1089.9413 1131.1091
Frequencies -- 1163.8801 1168.6228 1196.4413
Frequencies -- 1228.7926 1250.5064 1263.9001
Frequencies -- 1301.3435 1320.5820 1333.2357
Frequencies -- 1369.2632 1399.8543 1410.7097
Frequencies -- 1430.6417 1528.4346 1539.1054
Frequencies -- 1567.0892 1689.7688 1712.8177
Frequencies -- 3071.1589 3122.4906 3238.2167
Frequencies -- 3248.1139 3256.2224 3263.6574
Frequencies -- 3271.3444 3278.8708 3945.8077

***** TS R1-400-s --> R1-4500-s //
BB1K=BB95-IOP(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,-0.3589230642,2.0416957589,0.020846195
C,0,0.9415580099,2.4926169248,-0.1686456962
C,0,-0.6025295833,0.7113890773,0.3600040788
C,0,2.0104919789,1.656512168,0.0022630753
C,0,-1.9945111399,0.1435565245,0.3418590605
C,0,0.4540567689,-0.1161023938,0.580438739
C,0,1.7982144164,0.3093752005,0.3754572074
C,0,-1.972819558,-1.2726277152,-0.1431118219
O,0,-2.8785987364,0.9240486977,-0.4177032461

ESI
C,0,-0.9085921231,-2.0483653299,-0.0972988618
O,0,1.9120826304,-0.9504487414,-0.9312739909
C,0,0.3524013757,-1.6022109546,0.5533574442
O,0,1.5419457567,-2.0042766567,-0.1131630825
H,0,-1.1931732422,2.7001302039,-0.1444979897
H,0,1.1060009192,3.5203009075,-0.443887768
H,0,3.0156924236,2.0190040102,-0.1193133803
H,0,-2.4096144071,0.1681195935,1.3480302332
H,0,2.5883415883,-0.195906533,0.9060316683
H,0,-2.9064842358,-1.6325141236,-0.5443362443
H,0,-2.6090050448,0.8868751626,-1.3315734734
H,0,-0.9341711998,-3.059857571,-0.4667853014
H,0,0.4228935059,-2.0557736108,1.5424382901
Rotational constants (GHZ): 1.1592143 0.9712090 0.5734548
SCF Done: E(UB+HF-B95) = -611.854534901 A.U. after 1 cycles
S**2 = 0.8139
Frequencies -- -706.9326 68.5121 140.3067
Frequencies -- 193.9605 231.3702 290.1910
Frequencies -- 332.9341 356.4013 400.3497
Frequencies -- 427.2647 474.5535 482.7306
Frequencies -- 529.7280 534.5593 569.8132
Frequencies -- 609.9988 673.1247 721.6892
Frequencies -- 743.2652 778.6478 819.9092
Frequencies -- 862.0872 913.3356 935.2624
Frequencies -- 962.5830 981.9804 1022.8680
Frequencies -- 1029.4758 1039.3704 1046.3899
Frequencies -- 1082.0033 1098.7899 1120.1584
Frequencies -- 1158.6830 1183.0321 1196.9955
Frequencies -- 1199.2392 1222.1264 1262.2013
Frequencies -- 1293.3766 1346.4947 1351.0798
Frequencies -- 1366.5482 1384.1006 1423.1686
Frequencies -- 1441.4401 1479.3989 1535.1647
Frequencies -- 1617.2718 1658.7685 1769.6580
Frequencies -- 3074.6681 3094.4420 3224.9728
Frequencies -- 3232.5953 3247.4563 3256.6942
Frequencies -- 3269.6039 3276.3737 3944.4110

***** TS R1-400-a --> R1-4500-a //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,-0.2190863938,2.0948409981,-0.3234766517
C,0,-1.5979995362,2.2113098905,-0.234430742
C,0,0.4175670688,0.8924995334,-0.0052193022
C,0,-2.3651513735,1.1602115832,0.1928666046
C,0,1.8670157297,0.6866653828,-0.3240760364
C,0,-0.3292725901,-0.1349393789,0.4771304289
C,0,0.132130103,-1.5481397862,0.4942630551
C,0,-1.7515399358,-0.0617397697,0.549032369
C,0,2.1632341613,-0.7461221467,-0.6303291539
O,0,-1.7824325594,-1.39189986,-0.6906810541
O,0,2.7302686831,1.1920571757,0.6729455583
C,0,1.3706671203,-1.748661013,-0.3031210832
O,0,-1.0079202803,-2.2741958884,0.0436657167
H,0,0.367494765,2.9204526281,-0.6895983344
H,0,-2.0678104341,3.1425155234,-0.5004785415
H,0,-3.4324418951,1.2602069521,0.2795490524
H,0,2.1048177238,1.2812894433,-1.2008727113
H,0,0.3096819605,-1.9213871402,1.5039142575
H,0,-2.2709448958,-0.7031898775,1.2415128241
H,0,3.0993298018,-0.9367487094,-1.1294989739
H,0,2.6085430711,0.6804599246,1.4674511577
H,0,1.6366170319,-2.7668419239,-0.5352574277
Rotational constants (GHZ): 1.1762419 0.9453092 0.5758009
SCF Done: E(UB+HF-B95) = -611.851298613 A.U. after 2 cycles
S**2 = 0.8147
Frequencies -- -709.9447 62.4635 133.5145

ESI			
Frequencies	--	173.7215	209.0897
Frequencies	--	306.3731	314.9149
Frequencies	--	444.2066	449.8053
Frequencies	--	521.5660	546.1055
Frequencies	--	650.3412	686.4798
Frequencies	--	764.8245	791.3845
Frequencies	--	873.5524	916.1412
Frequencies	--	964.2696	979.6458
Frequencies	--	1026.9623	1035.8930
Frequencies	--	1078.1948	1101.0365
Frequencies	--	1142.6746	1193.2719
Frequencies	--	1201.3970	1244.7199
Frequencies	--	1281.2304	1350.1455
Frequencies	--	1391.2005	1406.6065
Frequencies	--	1447.8007	1487.7470
Frequencies	--	1618.5320	1666.8261
Frequencies	--	3067.1567	3127.8998
Frequencies	--	3230.7294	3244.2446
Frequencies	--	3257.8132	3271.7575
			250.4369
			383.4102
			483.9738
			561.7266
			700.7391
			807.5571
			921.3320
			1018.6199
			1048.7090
			1104.3065
			1198.3036
			1255.6540
			1372.6784
			1430.2301
			1543.1606
			1768.8512
			3229.0645
			3252.2650
			3958.5348

***** TS R1-400-s --> R1-4900-s //
BB1k=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,-1.3847083407,1.3290658362,0.1797732951			
C,0,-2.643237087,0.8003329124,0.1066115502			
C,0,-0.2531048807,0.5183219968,-0.0857666917			
C,0,-2.8363937671,-0.5307123896,-0.244638059			
C,0,0.9511324156,1.1889289801,-0.7172834656			
C,0,-0.4850083915,-0.8582630856,-0.3524764174			
O,0,0.7077297043,0.0858227438,1.4620202746			
C,0,-1.7423613083,-1.3687201717,-0.4392592594			
C,0,2.023583963,0.202706378,-1.0371180576			
O,0,1.4277655533,2.2318131366,0.0786716767			
C,0,1.940535429,-1.0795185657,-0.7406425034			
C,0,0.7569331766,-1.5997290664,0.0025105416			
O,0,0.8470120457,-1.2833234276,1.3914913737			
H,0,-1.2291525329,2.3747944753,0.3811564384			
H,0,-3.4975061498,1.4274060573,0.2946253104			
H,0,-3.8338056463,-0.9286357436,-0.3110703554			
H,0,0.6186345241,1.6604060289,-1.6405300783			
H,0,-1.8902071406,-2.4254651039,-0.5865939912			
H,0,2.9010552659,0.6077505764,-1.5150215505			
H,0,1.7016291781,1.8296992488,0.9030345661			
H,0,2.7445849145,-1.7586916555,-0.9674818948			
H,0,0.6604819078,-2.6762404535,-0.0458506412			
Rotational constants (GHZ):	1.3711252	0.8961290	0.6955379
SCF Done: E(UB+HF-B95) = -611.853803623	A.U. after	1 cycles	
S**2 =	0.8111		
Frequencies	--	-661.1745	124.5075
Frequencies	--	189.1103	257.7290
Frequencies	--	313.9789	350.4584
Frequencies	--	442.2761	486.3587
Frequencies	--	546.0209	566.5002
Frequencies	--	646.1516	652.6272
Frequencies	--	760.6617	785.6470
Frequencies	--	829.5355	889.3068
Frequencies	--	949.1972	965.0661
Frequencies	--	1012.4193	1027.2830
Frequencies	--	1051.3636	1061.7350
Frequencies	--	1157.0359	1174.1902
Frequencies	--	1202.5702	1222.4625
Frequencies	--	1285.5132	1331.1350
Frequencies	--	1376.6993	1393.7290
Frequencies	--	1452.1276	1488.7271
Frequencies	--	1604.9170	1662.5554
Frequencies	--	3097.8799	3186.1159
			136.5065
			285.0835
			394.4983
			521.7213
			569.2612
			727.5032
			803.2649
			939.1788
			985.0060
			1040.5502
			1129.4526
			1191.0094
			1272.0351
			1357.1286
			1429.3703
			1511.0056
			1767.0681
			3232.1941

		ESI	
Frequencies --	3242.4082	3249.8476	3256.9469
Frequencies --	3263.0575	3271.9227	3886.6702

***** TS R1-400-a --> R1-4900-a //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,-1.5903308508,	0.5773572255,	0.9002476723	
C,0,-2.676987095,	-0.0950990873,	0.4156778177	
C,0,-0.2965390925,	0.3315812224,	0.3732413558	
C,0,-2.5419319357,	-1.0120007299,	-0.6200512619	
C,0,0.6709399633,	1.4988930518,	0.3422109899	
C,0,-0.1896748489,	-0.6678413131,	-0.6354084707	
O,0,0.80987169,	-0.6116978396,	1.5011116111	
C,0,1.2119428759,	-1.1684159326,	-0.6138132048	
C,0,-1.2791489841,	-1.3190113807,	-1.1210350459	
C,0,1.9408907631,	1.1396559054,	-0.3491519833	
O,0,0.0873412947,	2.6407192485,	-0.2344633272	
O,0,1.2679262686,	-1.6543831126,	0.7313653493	
C,0,2.1897597649,	-0.0651460449,	-0.8259587546	
H,0,-1.7084871779,	1.3477541806,	1.6427100474	
H,0,-3.6536179357,	0.1088394884,	0.8192849767	
H,0,-3.408493814,	-1.5243887215,	-0.9996283249	
H,0,0.8826562425,	1.7743803437,	1.3708385239	
H,0,1.389587736,	-2.0281395345,	-1.2456689398	
H,0,-1.1617882644,	-2.115723791,	-1.836587517	
H,0,2.6563656265,	1.9390298942,	-0.45631271	
H,0,-0.0725445595,	2.4711323682,	-1.1586267566	
H,0,3.1216847585,	-0.2898280976,	-1.3158730522	
Rotational constants (GHZ):	1.2760824	0.9248549	0.7042528
SCF Done: E(UB+HF-B95) =	-611.850240163	A.U. after	1 cycles
S**2 =	0.8134		
Frequencies --	-716.0242	117.9722	122.9022
Frequencies --	201.8520	229.8933	287.7162
Frequencies --	322.3856	342.3916	361.9310
Frequencies --	417.1654	439.4462	469.9138
Frequencies --	517.0924	549.5900	589.1055
Frequencies --	607.6711	667.5649	751.8474
Frequencies --	759.9900	786.4391	814.5286
Frequencies --	816.8757	882.5557	934.4246
Frequencies --	943.5380	960.7785	982.2236
Frequencies --	1011.7223	1022.0821	1037.7631
Frequencies --	1048.0939	1063.3654	1120.5450
Frequencies --	1154.9719	1180.1634	1190.2683
Frequencies --	1212.6967	1224.3113	1254.5615
Frequencies --	1280.9511	1329.3724	1355.2207
Frequencies --	1374.8894	1395.3752	1416.1694
Frequencies --	1443.6086	1494.6045	1517.7590
Frequencies --	1606.5329	1664.6257	1763.7186
Frequencies --	3135.7092	3189.8033	3232.8453
Frequencies --	3240.4928	3247.9696	3258.5521
Frequencies --	3260.2536	3270.7859	3951.5244

***** TS R1-400-s --> R1-4-10-00-s //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2		
C,0,-1.5087078068,	1.5518513553,	-0.1460617036
C,0,-2.7306362237,	0.900414157,	-0.0690981002
C,0,-0.3398195756,	0.846044514,	-0.2186419699
C,0,-2.7860931079,	-0.4908874193,	-0.0614186288
C,0,0.9883432579,	1.5308970254,	-0.1876532656
C,0,-0.3706188777,	-0.5735137192,	-0.1702214745
O,0,0.4295860072,	-1.0507495134,	1.3682105977
C,0,-1.6378871034,	-1.2169202736,	-0.1356907521
C,0,2.0541953804,	0.7422466948,	-0.8726650685

ESI
O,0,1.3710555028,1.788040164,1.1456540289
C,0,1.9824627671,-0.5592466734,-1.0679025674
C,0,0.8242541942,-1.3824972347,-0.639816163
O,0,1.0791040504,-2.0400604405,0.5862930506
H,0,-1.474219627,2.6285077778,-0.1426703278
H,0,-3.6397249803,1.4737035947,-0.0168655386
H,0,-3.7381035684,-0.989190379,-0.0063029008
H,0,0.8960005487,2.5078250632,-0.6507641973
H,0,-1.6562495181,-2.2933938404,-0.1354139012
H,0,2.9486848584,1.2818070225,-1.1383836912
H,0,1.3962058333,0.9401863466,1.5919766351
H,0,2.8134706414,-1.0944984183,-1.4977673612
H,0,0.5630139021,-2.1231194066,-1.3900519728
Rotational constants (GHZ): 1.2876652 0.8994365 0.6602301
SCF Done: E(UB+HF-B95) = -611.850646134 A.U. after 1 cycles
S**2 = 0.8094
Frequencies -- -623.9995 75.2382 114.5173
Frequencies -- 148.0515 199.7320 219.2969
Frequencies -- 296.6093 330.9042 366.2119
Frequencies -- 399.2539 467.3967 507.5549
Frequencies -- 535.0517 539.5836 574.1906
Frequencies -- 611.0414 677.8025 749.7101
Frequencies -- 767.0021 776.6752 788.5085
Frequencies -- 848.2832 896.2581 942.9544
Frequencies -- 991.3546 995.3886 1000.4461
Frequencies -- 1029.1640 1046.6100 1050.1133
Frequencies -- 1069.8290 1087.6896 1099.5887
Frequencies -- 1156.3750 1182.8823 1201.5288
Frequencies -- 1210.1740 1241.7099 1277.4179
Frequencies -- 1305.6412 1344.1294 1359.9499
Frequencies -- 1400.6229 1412.8991 1442.7685
Frequencies -- 1462.8232 1498.0863 1527.6175
Frequencies -- 1609.6547 1660.5985 1782.1542
Frequencies -- 3125.3575 3135.8654 3227.7603
Frequencies -- 3243.2403 3248.9874 3250.5846
Frequencies -- 3261.5763 3272.6599 3853.2558

***** TS R1-400-a --> R1-4-10-00-a //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,1.2538269956,1.6307282119,0.1700480797
C,0,2.5493708644,1.164897697,-0.0025536462
C,0,0.1847880459,0.7807445372,0.0892803441
C,0,2.7824033606,-0.1796143745,-0.2705499662
C,0,-1.2076599347,1.2738637958,0.3300317204
C,0,0.4005124903,-0.6068831164,-0.1322008671
C,0,-0.7239868812,-1.5002785677,-0.620607068
O,0,-0.0843250075,-1.482312053,1.3468427166
C,0,1.7343518639,-1.0434048516,-0.3641788801
C,0,-2.2409316489,0.4189664718,-0.3178509949
O,0,-1.3639011189,2.6264129598,-0.012862607
O,0,-0.7006782062,-2.4054109942,0.4638264507
C,0,-2.0292985395,-0.8084907733,-0.7473498089
H,0,1.0747055275,2.6726118434,0.3705639679
H,0,3.3763234267,1.849677551,0.0688400618
H,0,3.78842075,-0.534187036,-0.4119186057
H,0,-1.3856605928,1.2402218192,1.4052162106
H,0,-0.473547618,-2.0357316282,-1.5321773509
H,0,1.8886756943,-2.0880917481,-0.573760241
H,0,-3.2199546771,0.8659328721,-0.3882412521
H,0,-1.2405920583,2.7184837984,-0.9535474599
H,0,-2.8373954903,-1.3816109544,-1.1718412899
Rotational constants (GHZ): 1.1107957 0.9921495 0.5932098
SCF Done: E(UB+HF-B95) = -611.849227530 A.U. after 2 cycles
S**2 = 0.8104
Frequencies -- -674.6162 65.0515 114.3988

			ESI	
Frequencies	--	156.4331	191.9351	233.8667
Frequencies	--	268.9780	331.4514	368.4118
Frequencies	--	399.4429	449.3408	458.7512
Frequencies	--	471.0981	501.5757	560.3680
Frequencies	--	633.9186	684.4847	700.5408
Frequencies	--	769.1350	774.2607	801.0696
Frequencies	--	836.6975	902.4955	926.7142
Frequencies	--	990.1536	995.6536	1007.1905
Frequencies	--	1028.9319	1047.3165	1055.7336
Frequencies	--	1067.1413	1094.4858	1128.4792
Frequencies	--	1162.4312	1180.1483	1196.2979
Frequencies	--	1211.0357	1228.8240	1268.4790
Frequencies	--	1292.2741	1347.1933	1362.5004
Frequencies	--	1373.7064	1403.1423	1418.4277
Frequencies	--	1447.6855	1491.5445	1525.2939
Frequencies	--	1610.9546	1657.9221	1781.2206
Frequencies	--	3080.7229	3120.3039	3226.5887
Frequencies	--	3245.6399	3248.1135	3255.1458
Frequencies	--	3264.3659	3272.2111	3949.4400

***** TS R1-200-s --> R1-P201-s //
BB1k=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,0.6723302391,1.0477375004,-0.4343718549			
C,0,1.8787932688,0.2701309417,0.2663713464			
C,0,1.9513420112,-1.1296995265,-0.213759738			
C,0,0.8679258851,-1.7721506761,-0.6262903229			
C,0,-1.5934893984,-1.9332312898,-0.7747106472			
C,0,-2.8383161271,-1.3461069141,-0.7077573733			
C,0,-2.9461798113,0.0134692235,-0.5005699641			
C,0,-1.8098266352,0.7891569578,-0.3802831434			
C,0,-0.5656965975,0.2077954668,-0.4586671889			
C,0,-0.4499783541,-1.1661128879,-0.63752651			
O,0,0.5576672725,2.244047295,0.1339356428			
O,0,1.6175025606,0.3014473451,1.6239577913			
O,0,1.7204901285,1.5867296626,2.0473051599			
H,0,1.0753282048,1.1250696829,-1.4550887965			
H,0,2.7669930886,0.8568749696,0.059380881			
H,0,2.9116395659,-1.614630767,-0.1880700428			
H,0,0.9465284946,-2.8004746109,-0.9405924627			
H,0,-1.5024083624,-2.9972285358,-0.9180927156			
H,0,-3.7234731406,-1.9494141104,-0.8103538148			
H,0,-3.9173922385,0.4731851468,-0.4388892012			
H,0,-1.878076076,1.8521398264,-0.2275734161			
H,0,1.1541538872,2.1107512023,1.2830831957			
Rotational constants (GHZ): 1.5171185 0.6995483 0.5444405			
SCF Done: E(UB+HF-B95) = -611.875437455 A.U. after 1 cycles			
S**2 = 0.7599			
Frequencies	--	-1514.8511	73.4748 111.8549
Frequencies	--	195.1208	255.9360 280.8812
Frequencies	--	297.9537	406.3122 435.5436
Frequencies	--	465.4018	479.9868 526.5410
Frequencies	--	547.2679	559.3734 594.0416
Frequencies	--	681.6965	694.8460 722.2066
Frequencies	--	766.7992	794.1714 806.5537
Frequencies	--	824.7355	858.2396 873.1451
Frequencies	--	918.4416	936.5509 1007.8457
Frequencies	--	1021.3531	1042.0755 1047.0057
Frequencies	--	1068.7771	1089.5032 1144.5333
Frequencies	--	1167.5190	1197.3305 1200.7941
Frequencies	--	1208.9543	1236.8281 1267.0134
Frequencies	--	1276.4219	1319.4393 1327.2102
Frequencies	--	1376.1261	1379.9451 1398.9221
Frequencies	--	1457.1526	1525.4085 1565.8828
Frequencies	--	1676.4480	1708.2688 1752.8047
Frequencies	--	1845.0521	2964.3409 3150.3671

		ESI	
Frequencies --	3233.8393	3238.2502	3249.8183
Frequencies --	3260.9262	3263.4824	3271.8740

***** TS R1-200-a --> R1-P201-a //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,0.4601359927,0.9673593951,-0.3684901062			
C,0,1.5282944152,0.2494015741,0.6086676176			
C,0,1.8455912494,-1.078549789,0.049743748			
C,0,0.8539371792,-1.823174492,-0.4211676266			
C,0,-1.6004468204,-2.17281496,-0.5232889785			
C,0,-2.8814935007,-1.668677422,-0.4706923361			
C,0,-3.0844218656,-0.3099088847,-0.3356987571			
C,0,-2.0062511732,0.5495384501,-0.2707164851			
C,0,-0.7259990038,0.0489955115,-0.3325779619			
C,0,-0.5099799427,-1.32429945,-0.436556208			
O,0,0.2688051773,2.1985748154,0.0725321522			
O,0,2.6069459144,1.080560287,0.6527933906			
O,0,2.2430295422,2.2093007631,1.3155253636			
H,0,0.9398867681,0.9176214574,-1.3530267683			
H,0,1.0305073115,0.2170193526,1.5765129977			
H,0,2.8687394994,-1.4115451678,0.0653259238			
H,0,1.0415441311,-2.8220192633,-0.7779329693			
H,0,-1.4382473727,-3.2341104603,-0.6127713211			
H,0,-3.7230231297,-2.3367237703,-0.530796842			
H,0,-4.0855485445,0.0826351522,-0.2919135774			
H,0,-2.144654167,1.6125971703,-0.1813740967			
H,0,1.2843512507,2.4398190074,0.7838319668			
Rotational constants (GHZ):	1.7666520	0.6241193	0.4789599
SCF Done: E(UB+HF-B95) = -611.875585042	A.U. after	2 cycles	
S**2 =	0.7589		
Frequencies --	-1719.7579	84.3731	128.1482
Frequencies --	203.2207	238.3227	269.0515
Frequencies --	350.6199	374.8535	422.8137
Frequencies --	443.4428	491.5757	512.4715
Frequencies --	542.7675	548.8752	585.7637
Frequencies --	646.6201	691.2483	719.1288
Frequencies --	733.1728	781.9994	796.7164
Frequencies --	829.1714	872.2393	893.3613
Frequencies --	932.8413	951.0471	1011.5075
Frequencies --	1025.0015	1047.3611	1089.7896
Frequencies --	1093.7469	1126.0666	1140.4299
Frequencies --	1157.0544	1193.6613	1200.2473
Frequencies --	1220.5289	1239.4961	1257.9934
Frequencies --	1267.2588	1321.8468	1331.4082
Frequencies --	1358.3543	1382.0149	1402.9352
Frequencies --	1454.4987	1525.7055	1558.0918
Frequencies --	1667.5592	1704.9627	1734.9695
Frequencies --	1837.5186	3008.2523	3101.0571
Frequencies --	3239.7093	3245.4832	3251.6185
Frequencies --	3265.6196	3269.8298	3274.8965

***** TS R1-200-a --> R1-P2C1 // BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,0.394816744,0.9820725739,0.2588856028			
C,0,1.6704472386,0.359641288,0.8246434674			
C,0,1.8385936943,-1.0419628027,0.3638692318			
C,0,0.8221839839,-1.7606508461,-0.0850033307			
C,0,-1.599452928,-2.0564466442,-0.4764617059			
C,0,-2.8788672156,-1.5461569696,-0.5425495396			
C,0,-3.099908071,-0.2009536717,-0.3192345155			
C,0,-2.0414539958,0.6344188457,-0.0397974973			
C,0,-0.7546373564,0.1276440284,0.0268358733			
C,0,-0.5265009536,-1.2352515084,-0.1865836148			

ESI			
O,0,0.09254003,2.197129244,0.7900278259			
O,0,2.6488296709,1.2369075223,0.3217025043			
O,0,2.3816861794,1.2875947111,-1.0252650367			
H,0,1.0568040443,1.1783070582,-0.8173913802			
H,0,1.7282535159,0.440365176,1.9096150872			
H,0,2.8297167683,-1.4565005583,0.4370729554			
H,0,0.9756074879,-2.7867504059,-0.376839156			
H,0,-1.4275458031,-3.1066667249,-0.6434879112			
H,0,-3.7053078247,-2.1982459019,-0.7659759433			
H,0,-4.098719626,0.1967283514,-0.3649972534			
H,0,-2.1984106214,1.6844150826,0.1309318079			
H,0,0.9038281742,2.7011703431,0.8517256163			
Rotational constants (GHZ): 1.6781962 0.6543198 0.5132340			
SCF Done: E(UB+HF-B95) = -611.873879172 A.U. after 1 cycles			
S**2 = 0.7746			
Frequencies --	-2090.8494	80.9439	119.9138
Frequencies --	200.7808	219.3915	268.9546
Frequencies --	306.5892	336.2384	406.8113
Frequencies --	410.8832	465.7190	511.0375
Frequencies --	520.9604	531.0792	548.1447
Frequencies --	597.1107	676.8102	717.3451
Frequencies --	733.0135	764.9167	801.7058
Frequencies --	828.4547	876.8851	929.0194
Frequencies --	943.2402	985.7117	1006.4120
Frequencies --	1022.0984	1035.3951	1043.8083
Frequencies --	1056.7545	1084.9919	1099.6220
Frequencies --	1142.3424	1184.8212	1196.4414
Frequencies --	1222.9648	1255.2765	1263.5484
Frequencies --	1270.3343	1305.8575	1343.0190
Frequencies --	1364.6590	1391.8508	1443.0680
Frequencies --	1467.9695	1533.8623	1558.2539
Frequencies --	1667.5035	1695.6804	1759.0677
Frequencies --	1781.4848	3099.9362	3234.7906
Frequencies --	3239.7075	3251.8230	3259.1449
Frequencies --	3265.5120	3275.7255	3899.5803

***** TS R1-400-s --> R1-P401-s //
BB1K=BB95-IOP(3/76=0580004200)/6-311++G(2df,2p)

O,2			
C,0,0.7261577551,1.5353954723,0.2761614361			
C,0,2.0432725722,0.8808037535,0.546759248			
C,0,2.1029578269,-0.4352362649,0.6548854058			
C,0,0.876638298,-1.2632884874,0.4859809268			
C,0,-0.8972309223,-1.4741671777,-1.2660306212			
C,0,-1.7646986897,-0.9058770902,-2.1760298638			
C,0,-1.8175662356,0.4647554431,-2.3100867869			
C,0,-1.0060519684,1.2665083559,-1.5323685971			
C,0,-0.1380520649,0.7013537057,-0.6247644223			
C,0,-0.0830031659,-0.676214268,-0.4922384032			
O,0,0.1471444638,1.7238513623,1.52803792			
O,0,-0.6156488633,-0.4686692734,2.0875206492			
O,0,0.331794183,-1.3914554918,1.8218448011			
H,0,0.8576921212,2.5328809924,-0.144494131			
H,0,2.8942118769,1.5032367143,0.7653342779			
H,0,3.0111662799,-0.929640065,0.9553794951			
H,0,1.1175975648,-2.2856527965,0.22131669			
H,0,-0.8517740595,-2.5451688377,-1.1578382422			
H,0,-2.3953771258,-1.532652833,-2.78213057			
H,0,-2.4901151229,0.912027642,-3.0214546391			
H,0,-1.049952197,2.3386118042,-1.6318242141			
H,0,-0.2543080392,0.5323439483,1.9228744372			
Rotational constants (GHZ): 1.3795200 0.8012050 0.6715608			
SCF Done: E(UB+HF-B95) = -611.847523182 A.U. after 1 cycles			
S**2 = 0.7640			
Frequencies --	-2803.7071	45.7384	109.5634
Frequencies --	136.2123	223.1459	265.9189

ESI			
Frequencies	--	335.2698	348.5569
Frequencies	--	424.5469	487.4715
Frequencies	--	552.5756	562.9632
Frequencies	--	648.1022	687.8379
Frequencies	--	782.2979	791.2842
Frequencies	--	836.9971	903.9906
Frequencies	--	952.4910	972.3627
Frequencies	--	1008.0009	1029.6818
Frequencies	--	1048.5780	1069.6066
Frequencies	--	1161.2680	1174.6988
Frequencies	--	1200.4054	1230.0597
Frequencies	--	1279.6856	1295.2443
Frequencies	--	1354.4794	1380.3435
Frequencies	--	1427.1253	1531.7053
Frequencies	--	1569.2494	1691.0071
Frequencies	--	1744.5048	3073.9013
Frequencies	--	3235.7265	3240.9914
Frequencies	--	3253.8507	3263.7270
			361.5509
			515.6040
			592.6095
			765.8091
			821.6293
			928.6144
			997.0446
			1042.9131
			1091.2568
			1196.1138
			1249.2697
			1349.4396
			1411.4988
			1541.1215
			1716.5789
			3162.5326
			3241.9799
			3267.8072

***** TS R1-400-a --> R1-P4C1 // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,-1.1573885415,0.9017613298,-0.2954150928			
C,0,-0.3325136497,2.0892144362,-0.4886393644			
C,0,0.9733493471,1.9221970571,-0.6715866214			
C,0,1.4619299188,0.5153167288,-0.7631398314			
C,0,1.5210768012,-1.3037803907,0.9843891429			
C,0,0.8645078166,-2.0578625707,1.9370565753			
C,0,-0.4803706356,-1.8554554919,2.1709037784			
C,0,-1.1794872674,-0.9006872968,1.4612831537			
C,0,-0.5151685768,-0.1352537265,0.5277056543			
C,0,0.834216742,-0.3445484178,0.2767504205			
O,0,-2.4907610156,1.0683071642,-0.0313722647			
O,0,1.0838364677,0.1431831196,-2.1165599049			
O,0,-0.1314066282,-0.4377342479,-2.1617774391			
H,0,-0.9087466529,0.2961427898,-1.4162308539			
H,0,-0.8057064125,3.0570574704,-0.5424722499			
H,0,1.6398260601,2.7397529184,-0.8779819888			
H,0,2.5408135714,0.4406994096,-0.7574649731			
H,0,2.5675874224,-1.4676439982,0.7876822992			
H,0,1.4016549656,-2.8073323711,2.491754245			
H,0,-0.9887313918,-2.4452550097,2.9141212281			
H,0,-2.2280176251,-0.7359124722,1.6336885746			
H,0,-2.8529422564,1.7470330319,-0.5912663015			
Rotational constants (GHZ):	1.2476704	0.8561309	0.6374119
SCF Done: E(UB+HF-B95) = -611.865163944	A.U. after	1	cycles
S**2 = 0.7681			
Frequencies	--	-2086.8826	117.1269
Frequencies	--	207.6377	252.8200
Frequencies	--	290.9824	308.5436
Frequencies	--	403.9654	434.4523
Frequencies	--	504.6443	526.8607
Frequencies	--	571.1900	666.3037
Frequencies	--	725.7541	770.9642
Frequencies	--	810.3677	843.0321
Frequencies	--	927.3750	939.7486
Frequencies	--	1003.0861	1017.9341
Frequencies	--	1060.6992	1089.9650
Frequencies	--	1152.0255	1174.7460
Frequencies	--	1202.5964	1217.4596
Frequencies	--	1291.1344	1321.5677
Frequencies	--	1366.1756	1401.3468
Frequencies	--	1436.7278	1537.2134
Frequencies	--	1601.5374	1677.3346
Frequencies	--	1715.4965	3186.1976
Frequencies	--	3239.5919	3249.9609
Frequencies	--	3277.5712	3278.5427
			155.2160
			263.4641
			384.5643
			461.0014
			565.5327
			667.6696
			792.5360
			898.5351
			1000.1639
			1042.0640
			1117.0621
			1198.7358
			1241.8308
			1342.3403
			1425.8075
			1554.7169
			1704.0869
			3230.7190
			3265.9231
			3981.6675

ESI

***** R1-2O-s (C10H8-10H-2O-Syn) //
BB1K=BB95-IOP(3/76=0580004200)/6-311++G(2df,2p)

0,2

C,0,0.8263533093,0.9313893792,-0.7688356175
C,0,2.06651473,0.2289892375,-0.2218744926
C,0,1.943837017,-1.2616572292,-0.2449168719
C,0,0.7489494906,-1.8275730673,-0.1593671151
C,0,-1.6629561788,-1.6530450711,0.352912884
C,0,-2.7974414044,-0.8946776846,0.5481229761
C,0,-2.7486927604,0.4705017723,0.3623656873
C,0,-1.5713899518,1.0743872184,-0.036440692
C,0,-0.4396871837,0.3193387844,-0.2424007441
C,0,-0.4756606078,-1.0553358198,-0.031054468
O,0,0.917225562,2.3008185843,-0.54741272
O,0,2.4247099906,0.6848010189,1.009796484
H,0,0.8318583355,0.785576641,-1.8482309784
H,0,2.9127161205,0.547056913,-0.8487226574
H,0,2.8454690403,-1.8482820788,-0.2580998922
H,0,0.6647753534,-2.9023584722,-0.128811575
H,0,-1.6895719716,-2.718389916,0.5129225509
H,0,-3.7155204125,-1.3676551268,0.8507878614
H,0,-3.6298685487,1.068276933,0.5201188603
H,0,-1.5246085072,2.1370381664,-0.1986248772
H,0,1.2303074102,2.4198749965,0.3485213185
Rotational constants (GHZ): 1.7111340 0.8730369 0.6338020
SCF Done: E(UB+HF-B95) = -536.759960362 A.U. after 1 cycles
S**2 = 0.7551
Frequencies -- 82.2950 117.7587 195.1408
Frequencies -- 245.1633 268.0736 287.1943
Frequencies -- 407.1558 427.7178 454.4306
Frequencies -- 463.1020 486.5139 536.9753
Frequencies -- 571.8047 585.5178 695.1622
Frequencies -- 728.0236 767.9062 780.2914
Frequencies -- 825.4590 844.7818 889.6730
Frequencies -- 914.1720 937.8729 1009.3114
Frequencies -- 1035.9546 1044.1183 1051.4720
Frequencies -- 1082.5084 1095.9134 1144.5242
Frequencies -- 1167.4084 1170.2420 1194.3854
Frequencies -- 1211.4002 1244.2556 1266.7327
Frequencies -- 1270.3098 1302.3524 1321.2612
Frequencies -- 1372.0755 1381.4943 1435.7731
Frequencies -- 1445.5624 1525.8585 1563.8571
Frequencies -- 1678.8892 1710.0003 1751.2258
Frequencies -- 2971.2750 3092.2724 3228.5182
Frequencies -- 3235.4916 3246.1866 3260.7630
Frequencies -- 3265.6409 3268.9785 3899.0863

***** R1-2O-a (C10H8-10H-2O-Anti) //
BB1K=BB95-IOP(3/76=0580004200)/6-311++G(2df,2p)

0,2

C,0,0.8855057769,1.2235706842,0.0801706977
C,0,2.1139276336,0.3291885538,0.0061001582
C,0,1.9011881262,-0.9902722237,0.7044886159
C,0,0.6830605111,-1.5122880687,0.7719681241
C,0,-1.6871289779,-1.5190302677,0.08476142
C,0,-2.7798066511,-0.8878478526,-0.4667760162
C,0,-2.6789013791,0.4249269924,-0.8784438521
C,0,-1.4856276913,1.1036543372,-0.7300591667
C,0,-0.3879333446,0.4800098325,-0.180718352
C,0,-0.484004965,-0.8472615886,0.224227736
O,0,0.8505000619,1.864630966,1.3323709424
O,0,2.4095257801,-0.1182111285,-1.2402032369
H,0,1.0053249137,2.0145763862,-0.6520564986

ESI
H,0,2.9518813455,0.8560856659,0.4678824186
H,0,2.7703573759,-1.5157829335,1.0550074737
H,0,0.5365099682,-2.4749642591,1.2360373277
H,0,-1.758142671,-2.5467492203,0.4006495847
H,0,-3.7090640065,-1.418982215,-0.5784191616
H,0,-3.529037676,0.9223818369,-1.3121798417
H,0,-1.4068579183,2.1326355795,-1.0395650848
H,0,0.5771477002,1.2315380665,1.9909859486
Rotational constants (GHZ): 1.7386192 0.8270486 0.6943109
SCF Done: E(UB+HF-B95) = -536.756758875 A.U. after 1 cycles
S**2 = 0.7591
Frequencies -- 76.8661 103.8937 163.8852
Frequencies -- 198.5823 260.0322 289.1366
Frequencies -- 329.9636 364.5159 419.7471
Frequencies -- 501.1280 503.1343 523.0675
Frequencies -- 555.7489 601.5329 638.2063
Frequencies -- 759.0427 771.0466 791.6870
Frequencies -- 811.0401 838.3327 909.4843
Frequencies -- 930.1223 933.1189 1005.3889
Frequencies -- 1027.9986 1042.7402 1076.0028
Frequencies -- 1092.0432 1112.1457 1142.4194
Frequencies -- 1162.2448 1193.1117 1198.8210
Frequencies -- 1248.9908 1254.3551 1260.7563
Frequencies -- 1285.1765 1309.5584 1358.8396
Frequencies -- 1382.8923 1397.5005 1433.1977
Frequencies -- 1443.8392 1525.5860 1569.1419
Frequencies -- 1670.5683 1708.8392 1724.9101
Frequencies -- 3055.7331 3148.4012 3227.8911
Frequencies -- 3237.2734 3242.3366 3255.1248
Frequencies -- 3268.9087 3281.7782 3947.9495

***** R1-230-s // BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,0.8263668139,1.1886221678,-0.5464233223
C,0,2.0956077112,0.5415329563,-0.0923853136
C,0,2.1277045695,-0.8789653596,0.232760027
C,0,0.9187377469,-1.6653131896,0.0957329803
C,0,-1.5160888489,-1.7684924311,0.022337031
C,0,-2.7334708918,-1.1546653215,-0.0857462555
C,0,-2.8004209526,0.2142467307,-0.2943740355
C,0,-1.6369355159,0.9494945005,-0.4102222508
C,0,-0.4019397049,0.3497178598,-0.3148398229
C,0,-0.3204748555,-1.036123372,-0.0737460839
O,0,0.7077296106,2.4633548599,0.0311801687
O,0,2.1096171569,0.1348351101,1.2477365778
H,0,0.918067429,1.3722996048,-1.6152665265
H,0,3.0005181302,1.0283331616,-0.4256518664
H,0,3.0710398984,-1.3958922373,0.1714340477
H,0,0.9671463902,-2.7330357965,0.2182689707
H,0,-1.4562995539,-2.8289836494,0.2021588972
H,0,-3.6373998135,-1.7330448483,-0.002573476
H,0,-3.7554391942,0.703577135,-0.3747282659
H,0,-1.6814389534,2.0113996129,-0.5820479807
H,0,0.6805150957,2.3495000097,0.9785145063
Rotational constants (GHZ): 1.7635912 0.9090265 0.6401206
SCF Done: E(UB+HF-B95) = -536.771702056 A.U. after 1 cycles
S**2 = 0.7869
Frequencies -- 63.1743 144.9683 175.8414
Frequencies -- 252.1918 293.7690 373.0468
Frequencies -- 399.0335 422.6327 453.9392
Frequencies -- 470.1976 505.8605 550.5827
Frequencies -- 586.3715 674.1086 695.2470
Frequencies -- 735.6256 761.3753 798.7426
Frequencies -- 816.8309 834.7480 897.0384
Frequencies -- 911.0399 924.6712 1005.9342
Frequencies -- 1012.8695 1032.1007 1074.3036

ESI			
Frequencies --	1085.8143	1104.8573	1135.3011
Frequencies --	1164.8019	1183.8162	1191.4575
Frequencies --	1229.7227	1256.6977	1279.4864
Frequencies --	1303.4920	1313.0620	1366.3135
Frequencies --	1388.8250	1404.1921	1444.5834
Frequencies --	1460.4405	1492.9257	1528.7840
Frequencies --	1546.2148	1637.4034	1669.5405
Frequencies --	3101.6897	3195.2754	3226.9457
Frequencies --	3237.9130	3248.9128	3258.8915
Frequencies --	3261.0688	3269.8461	3933.3412

***** R1-230-a // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,0.8150450007,	1.0737115549,-0.7697114211		
C,0,1.8787052776,	0.0683218769,-1.0889085099		
C,0,1.8878422952,-	1.2256843608,-0.4112696951		
C,0,0.8298742068,-	1.5354719997,0.5282398599		
C,0,-1.4502527234,-	1.1581638846,1.3143898643		
C,0,-2.595137616,-	0.4097269329,1.338535218		
C,0,-2.6591989549,	0.7844554888,0.6362792917		
C,0,-1.5571823533,	1.2198502319,-0.0715951415		
C,0,-0.392543394,	0.486795225,-0.1032201044		
C,0,-0.3247053129,-	0.7413231195,0.584385017		
O,0,1.3812780872,	2.1062408568,0.0081736692		
O,0,1.4825883041,-	1.07493971,-1.7792046742		
H,0,0.5097186622,	1.5542137874,-1.6954499393		
H,0,2.8173412036,	0.5035626356,-1.4007910786		
H,0,2.8257714131,-	1.7441460559,-0.3014553435		
H,0,0.8931863178,-	2.4303962865,1.1221146159		
H,0,-1.4020218561,-	2.0935435322,1.8466115668		
H,0,-3.44873243,-	0.7513516535,1.8982518227		
H,0,-3.5603064142,	1.3722663425,0.6468271172		
H,0,-1.5946837459,	2.1587591777,-0.5993778305		
H,0,1.4541171642,	1.8036419303,0.9087708346		
Rotational constants (GHZ):	1.7531368	0.8737836	0.6685172
SCF Done: E(UB+HF-B95) =	-536.769579072	A.U. after	1 cycles
S**2 =	0.7863		
Frequencies --	59.5325	133.5837	180.7644
Frequencies --	236.9072	278.6313	324.0107
Frequencies --	372.8491	399.4975	459.2767
Frequencies --	488.5728	510.9775	558.1373
Frequencies --	577.5351	634.8086	689.5167
Frequencies --	751.6902	780.9350	791.9734
Frequencies --	805.1313	833.0097	888.8698
Frequencies --	908.7993	939.2605	1001.1681
Frequencies --	1030.9162	1049.5261	1075.9619
Frequencies --	1092.2815	1102.8311	1115.4075
Frequencies --	1163.3897	1187.8725	1192.0397
Frequencies --	1233.6152	1257.9701	1262.4667
Frequencies --	1299.3108	1311.9288	1367.7828
Frequencies --	1397.5275	1413.7773	1430.0238
Frequencies --	1458.4379	1500.3862	1531.5210
Frequencies --	1551.2419	1642.4025	1674.2783
Frequencies --	3118.6699	3192.8571	3227.8295
Frequencies --	3236.1759	3240.8897	3254.2425
Frequencies --	3259.3401	3267.9050	3955.6330

***** TS R1-20-s --> R1-230-s // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,0.8388392121,	1.1500182199,-0.5618209787		
C,0,2.0749828084,	0.5261831506,0.0380373923		
C,0,2.1164547698,-	0.9466562388,0.0926433715		
C,0,0.9638201133,-	1.6697101076,0.0389868334		
C,0,-1.4826531927,-	1.7909767997,0.0228281912		

ESI
C,0,-2.7141231357,-1.1872063587,-0.0564144451
C,0,-2.7930658243,0.1763797041,-0.2616570646
C,0,-1.6405480212,0.9258228335,-0.3992340391
C,0,-0.4017299692,0.3304327059,-0.3331250932
C,0,-0.3149449599,-1.0454187517,-0.1059223601
O,0,0.7013367864,2.4585294111,-0.0832231649
O,0,2.030353575,0.3739722269,1.3930167781
H,0,0.9929356004,1.243354945,-1.635437028
H,0,2.9787934995,1.0026140826,-0.3337091339
H,0,3.0703776273,-1.412895867,0.2462515261
H,0,1.0010332198,-2.7396485053,0.1598588739
H,0,-1.4078648218,-2.8510608977,0.2005398456
H,0,-3.6105202729,-1.7733531589,0.0475917365
H,0,-3.7541626316,0.6575987786,-0.3192721539
H,0,-1.6970650558,1.9882414192,-0.5610471174
H,0,0.6907591406,2.4119259557,0.8709436999
Rotational constants (GHZ): 1.7363203 0.9065140 0.6454094
SCF Done: E(UB+HF-B95) = -536.755339214 A.U. after 1 cycles
S**2 = 0.8059
Frequencies -- -424.5258 75.1846 134.7984
Frequencies -- 175.5702 255.1388 290.7350
Frequencies -- 369.1558 412.6266 437.7169
Frequencies -- 445.0391 470.7552 522.5386
Frequencies -- 555.3733 578.0411 693.8135
Frequencies -- 731.5772 775.9111 785.8858
Frequencies -- 839.3264 840.2956 882.0404
Frequencies -- 929.0071 949.5506 1002.6105
Frequencies -- 1010.3306 1021.8239 1043.3020
Frequencies -- 1092.4970 1116.0145 1166.6730
Frequencies -- 1174.2091 1191.2841 1198.3395
Frequencies -- 1245.7113 1258.7476 1278.6529
Frequencies -- 1300.2518 1316.5739 1368.6316
Frequencies -- 1388.8857 1411.5678 1443.5515
Frequencies -- 1452.5078 1503.8888 1545.7253
Frequencies -- 1570.2662 1670.5647 1694.0005
Frequencies -- 3096.5639 3112.5901 3238.2141
Frequencies -- 3242.4838 3248.9086 3264.0984
Frequencies -- 3272.2651 3301.9925 3921.3055

***** TS R1-20-a --> R1-230-a // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,0.8188803045,1.0712448552,-0.7419980399
C,0,1.8164962201,0.0146458447,-1.1540325803
C,0,1.9287341754,-1.1556140788,-0.2564405129
C,0,0.8891597566,-1.4938217551,0.5542292676
C,0,-1.4270282278,-1.1820049652,1.2994184963
C,0,-2.594088667,-0.4579181932,1.3219464182
C,0,-2.6699498724,0.7446084458,0.6450674683
C,0,-1.5716176402,1.2158881753,-0.0448278001
C,0,-0.3946590268,0.5013052388,-0.0736986296
C,0,-0.3160118969,-0.7195191575,0.6007228796
O,0,1.450399428,2.0282074655,0.076681279
O,0,1.3680197924,-0.9475269741,-2.0011435772
H,0,0.5172865985,1.6071268896,-1.6367113634
H,0,2.765963448,0.4740735554,-1.4215749106
H,0,2.8177215516,-1.7528764694,-0.3183724902
H,0,0.9429099647,-2.3907618178,1.1486543061
H,0,-1.3645670983,-2.1251532381,1.8165032877
H,0,-3.4479394684,-0.8285810205,1.8619651244
H,0,-3.5829055271,1.3143478771,0.6556846256
H,0,-1.6250015287,2.1578769212,-0.5650841814
H,0,1.5496875437,1.6656169125,0.9523121844
Rotational constants (GHZ): 1.7467779 0.8573134 0.6822048
SCF Done: E(UB+HF-B95) = -536.753248961 A.U. after 1 cycles
S**2 = 0.8060
Frequencies -- -446.1803 71.7484 125.2998

ESI			
Frequencies	--	178.8259	232.7301
Frequencies	--	313.1277	370.8456
Frequencies	--	473.5094	508.9627
Frequencies	--	539.6317	591.2854
Frequencies	--	758.9631	773.5890
Frequencies	--	810.2666	835.6317
Frequencies	--	923.8833	935.7471
Frequencies	--	1007.8996	1040.7448
Frequencies	--	1090.5523	1109.0590
Frequencies	--	1176.1674	1184.2324
Frequencies	--	1245.1660	1254.6603
Frequencies	--	1289.4030	1312.0763
Frequencies	--	1397.6661	1409.0607
Frequencies	--	1456.8308	1506.8806
Frequencies	--	1573.4086	1675.7807
Frequencies	--	3101.7051	3136.0453
Frequencies	--	3241.7381	3243.4367
Frequencies	--	3268.7779	3301.2022
			271.1974
			391.8724
			516.3747
			635.3373
			795.6688
			908.9171
			994.7749
			1065.7517
			1163.9821
			1197.7065
			1262.4738
			1371.3513
			1434.0613
			1549.0511
			1698.9070
			3237.6396
			3255.3482
			3954.2918

***** TS R1-20-s (C1-C2-Cleavage) //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,0.7399343392,	0.9754413806,	-0.9137438559	
C,0,2.2764776279,	0.1311718783,	0.0962171163	
C,0,1.9720436609,	-1.2960779536,	-0.2291046098	
C,0,0.7525044457,	-1.8051364588,	-0.3186767724	
C,0,-1.622228805,	-1.6211330744,	0.3215398733	
C,0,-2.7352728677,	-0.8627957004,	0.6193569623	
C,0,-2.695749313,	0.5070472332,	0.4668586602	
C,0,-1.5528729139,	1.1128737986,	-0.0113423209	
C,0,-0.44249982,	0.3547054384,	-0.334080073	
C,0,-0.4603415713,	-1.025360063,	-0.1303532039	
O,0,0.9248240032,	2.2913822084,	-0.7640739306	
O,0,2.1530388296,	0.5808585323,	1.2366849799	
H,0,1.0564450887,	0.6259400845,	-1.8851302475	
H,0,2.9842091622,	0.6105480876,	-0.5937811097	
H,0,2.8314681327,	-1.9376141157,	-0.3555664766	
H,0,0.6314938519,	-2.8640467438,	-0.484453208	
H,0,-1.6415205137,	-2.6882059805,	0.468381371	
H,0,-3.6294399666,	-1.3411753417,	0.9793993088	
H,0,-3.5599900927,	1.1031213275,	0.7029310228	
H,0,-1.5316236804,	2.1764435243,	-0.1770406493	
H,0,0.8440866582,	2.5126443589,	0.1643409367	
Rotational constants (GHZ):	1.5919261	0.8854393	0.6519077
SCF Done: E(UB+HF-B95) =	-536.743879317	A.U. after	1 cycles
S**2 =	0.7717		
Frequencies	--	-296.4115	80.7620
Frequencies	--	141.9655	227.2938
Frequencies	--	294.3225	343.1219
Frequencies	--	432.8297	457.5922
Frequencies	--	511.2965	554.1646
Frequencies	--	640.3332	705.3619
Frequencies	--	789.5454	802.0464
Frequencies	--	876.6229	907.4080
Frequencies	--	951.8205	1005.8333
Frequencies	--	1040.6924	1057.7708
Frequencies	--	1140.1788	1196.0842
Frequencies	--	1203.4592	1247.7362
Frequencies	--	1331.9560	1360.7918
Frequencies	--	1403.3550	1441.3450
Frequencies	--	1519.1361	1562.0848
Frequencies	--	1669.4521	1695.0620
Frequencies	--	2981.7287	3209.4435
Frequencies	--	3233.5558	3240.1235
Frequencies	--	3259.4301	3270.9707
			117.5264
			256.5451
			407.9290
			508.0716
			614.3655
			776.1846
			818.0468
			938.8734
			1032.2867
			1095.6016
			1201.9671
			1268.7881
			1379.4178
			1465.7041
			1604.4481
			1745.3864
			3212.3063
			3248.6004
			3885.2217

ESI

***** TS R1-20-a (C1-C2-Cleavage) //
BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,0.7204110846,1.3782114618,0.2347070941
C,0,2.2898966771,0.127284326,-0.2289465839
C,0,1.9087936627,-0.9897534916,0.6947195717
C,0,0.6689306072,-1.3881031629,0.9362156522
C,0,-1.659990501,-1.4890764817,0.1247332344
C,0,-2.7256476131,-0.9356390351,-0.5532065408
C,0,-2.6443975609,0.3553066849,-1.029516526
C,0,-1.5069719004,1.1017249536,-0.7972192249
C,0,-0.4489484395,0.5621870149,-0.0935394737
C,0,-0.5045576161,-0.7610204994,0.340188411
O,0,0.9559544726,1.6706399082,1.5253141208
O,0,2.2747587098,-0.0322819857,-1.4467286106
H,0,0.9599147979,2.2071459355,-0.4093799834
H,0,2.9570684312,0.874132919,0.2214434041
H,0,2.7368748707,-1.5214180828,1.139485784
H,0,0.4992833188,-2.2581946046,1.5508703645
H,0,-1.7094043286,-2.5100517983,0.464850689
H,0,-3.6147397829,-1.5180610183,-0.7217037304
H,0,-3.4680391292,0.7870636003,-1.5708092069
H,0,-1.4464655032,2.1188026283,-1.1460324962
H,0,0.6546914638,0.9469864177,2.0737774089
Rotational constants (GHZ): 1.6562255 0.7976031 0.7127501
SCF Done: E(UB+HF-B95) = -536.738894174 A.U. after 1 cycles
S**2 = 0.7718
Frequencies -- -309.1684 75.2711 112.8586
Frequencies -- 181.6859 199.8631 292.6692
Frequencies -- 309.9702 332.1710 393.8407
Frequencies -- 419.2407 448.0064 493.2092
Frequencies -- 524.4332 567.1471 614.0676
Frequencies -- 638.9893 711.8484 771.3534
Frequencies -- 784.7165 806.7543 821.0215
Frequencies -- 900.2955 905.3286 924.4813
Frequencies -- 956.7476 1003.3878 1032.2736
Frequencies -- 1040.6297 1053.8220 1091.2460
Frequencies -- 1147.7930 1188.7708 1196.3097
Frequencies -- 1199.6841 1259.6058 1265.6975
Frequencies -- 1310.8164 1348.8212 1375.7887
Frequencies -- 1391.8495 1438.8248 1466.8855
Frequencies -- 1527.0035 1566.1442 1604.8156
Frequencies -- 1674.9845 1701.2085 1745.6180
Frequencies -- 2989.0389 3209.4988 3232.0277
Frequencies -- 3239.1952 3245.5862 3251.5284
Frequencies -- 3256.7745 3269.5123 3908.4270

***** R1-230-40-ss // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,1.8337002822,-1.0788464265,-0.0762182163
C,0,2.8994886689,-0.2196118069,0.0698639372
C,0,2.6906327527,1.1435518809,0.0470927835
C,0,1.4167857936,1.6356798223,-0.1259501087
C,0,0.3469057838,0.7768896342,-0.2832083244
C,0,0.5504633447,-0.5940912843,-0.2557266849
C,0,-0.5821392361,-1.5703694703,-0.4211170206
C,0,-1.8962029526,-0.9945994168,0.0061502948
O,0,-0.344339668,-2.7801009819,0.245895298
O,0,-1.8784329821,-0.2452694991,1.1997723731
C,0,-2.120710193,0.4348492347,-0.0019399508
C,0,-1.0298495035,1.3481786708,-0.4889218795
O,0,-1.190077288,2.6214387378,-0.0628372708
H,0,1.9857785697,-2.14365328,-0.0505581415
H,0,3.8917969725,-0.614059024,0.2048817041

ESI
H,0,3.5167812181,1.8226190057,0.168392273
H,0,1.232402941,2.695596038,-0.1286223878
H,0,-0.6718789876,-1.8451834553,-1.4707419461
H,0,-2.7370814919,-1.6640486404,-0.0916919261
H,0,-0.2434488693,-2.5924970632,1.1760127813
H,0,-3.1198576805,0.8263168201,-0.1141401338
H,0,-1.2061416119,1.4565785175,-1.5763244074
Rotational constants (GHZ): 1.1533516 0.9293414 0.5536836
SCF Done: E(UB+HF-B95) = -611.959869341 A.U. after 1 cycles
S**2 = 0.7550
Frequencies -- 56.7642 121.4932 170.5271
Frequencies -- 194.3659 265.5657 286.0699
Frequencies -- 336.6453 374.9827 405.4062
Frequencies -- 436.8630 473.0232 490.5050
Frequencies -- 532.0378 573.9070 649.6885
Frequencies -- 686.9555 703.2147 761.1475
Frequencies -- 788.9157 816.8795 836.5482
Frequencies -- 913.9223 924.6113 955.6903
Frequencies -- 1008.8818 1024.7189 1049.6436
Frequencies -- 1058.9957 1094.9490 1108.5509
Frequencies -- 1121.5892 1140.7452 1155.8444
Frequencies -- 1166.8066 1188.0466 1198.5798
Frequencies -- 1218.0166 1248.4500 1278.4682
Frequencies -- 1284.5931 1308.1034 1330.0500
Frequencies -- 1371.2154 1384.0207 1389.4283
Frequencies -- 1444.1666 1521.8224 1531.4641
Frequencies -- 1566.4021 1687.4731 1711.7306
Frequencies -- 2902.1587 3099.5082 3207.1405
Frequencies -- 3218.4176 3244.4170 3258.4025
Frequencies -- 3269.2173 3275.5161 3938.2804

***** R1-230-40-sa // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,-1.3067155748,0.7909190106,-1.4665542119
C,0,-2.4257925267,0.0118231321,-1.6444316986
C,0,-2.5414645793,-1.1905134197,-0.9751568583
C,0,-1.5347647423,-1.5934983226,-0.1306257841
C,0,-0.4051098001,-0.8160187122,0.0487036876
C,0,-0.2823392045,0.3859139656,-0.6257218123
C,0,0.9355355989,1.2630769843,-0.5104531118
C,0,1.737416177,0.9969988824,0.7205120193
O,0,0.6104824082,2.6263582374,-0.5843108096
O,0,0.9977630807,0.931154879,1.9224202653
C,0,1.6042160309,-0.2434689642,1.454650229
C,0,0.6771004846,-1.3167853583,0.9632953139
O,0,1.3652483023,-2.3812672629,0.4754151896
H,0,-1.2107391089,1.7306905207,-1.9816886475
H,0,-3.2094050382,0.3407664048,-2.3049136109
H,0,-3.4144433946,-1.8058846409,-1.1067401998
H,0,-1.6161389794,-2.5279685059,0.400127875
H,0,1.5802157347,1.0830294707,-1.3681055269
H,0,2.6562800413,1.5576462666,0.7953556752
H,0,0.0529314035,2.8386557622,0.1604098822
H,0,2.4360981957,-0.6057198388,2.0391167053
H,0,0.1887596343,-1.7518654558,1.8529340481
Rotational constants (GHZ): 1.1949430 0.8755204 0.5662216
SCF Done: E(UB+HF-B95) = -611.958612183 A.U. after 1 cycles
S**2 = 0.7551
Frequencies -- 40.3585 105.7423 156.8008
Frequencies -- 177.1061 250.0166 300.5461
Frequencies -- 309.6747 378.3682 422.1299
Frequencies -- 444.1995 455.0786 493.6016
Frequencies -- 535.1204 567.3380 607.1793
Frequencies -- 692.3931 731.5186 757.1547
Frequencies -- 797.6314 816.9358 835.7033
Frequencies -- 913.6204 924.3557 948.4287

ESI			
Frequencies	--	1013.6905	1043.1101
Frequencies	--	1061.4115	1090.9783
Frequencies	--	1124.0562	1128.4188
Frequencies	--	1182.6951	1193.7857
Frequencies	--	1230.0451	1248.5749
Frequencies	--	1280.2285	1300.9466
Frequencies	--	1375.8621	1393.1357
Frequencies	--	1444.6198	1520.6867
Frequencies	--	1569.3972	1689.7357
Frequencies	--	2929.5691	3108.9636
Frequencies	--	3217.7139	3235.7968
Frequencies	--	3262.6254	3270.8728
			1045.7222
			1097.3879
			1167.4756
			1199.7359
			1273.3773
			1327.2241
			1398.3266
			1541.0733
			1711.4509
			3206.3457
			3247.2534
			3937.9915

***** R1-230-40-as // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,	1.6871616262,-1.3678234663,-0.1796503986		
C,0,	2.884103947,-0.6937717794,-0.2182128885		
C,0,	2.8939884689,0.6872086038,-0.1676909566		
C,0,	1.7059214837,1.3729263043,-0.082565301		
C,0,	0.499685151,0.6975399137,-0.0380188404		
C,0,	0.4857350324,-0.6850486975,-0.0843809662		
C,0,	-0.7815323685,-1.4786020632,0.0224711549		
C,0,	-1.9977351857,-0.7038157797,-0.3787991234		
O,0,	-0.9717947534,-2.0027692329,1.3158197947		
O,0,	-1.9042293926,0.0573439806,-1.5571792088		
C,0,	-2.0025960073,0.7459597908,-0.3401655705		
C,0,	-0.7723695792,1.4901041244,0.0947210904		
O,0,	-0.9422379103,2.0524866634,1.3197140099		
H,0,	1.6714627953,-2.4446137118,-0.2156587264		
H,0,	3.8085347002,-1.2398143316,-0.2923259406		
H,0,	3.8256077768,1.2249021186,-0.2017669245		
H,0,	1.7059016384,2.4499734915,-0.0438752098		
H,0,	-0.7009163289,-2.3484614183,-0.6229394176		
H,0,	-2.9296523797,-1.231675037,-0.2454413491		
H,0,	-0.836280654,-1.3089632593,1.9550951885		
H,0,	-2.9283344666,1.2746206831,-0.1723058745		
H,0,	-0.6844020416,2.3794784705,-0.5538677138		
Rotational constants (GHZ):			
	1.2628005	0.8010246	0.6137308
SCF Done: E(UB+HF-B95) = -611.956237428 A.U. after 1 cycles			
S**2 = 0.7551			
Frequencies	--	27.4938	104.7029
Frequencies	--	180.6705	253.1786
Frequencies	--	286.2362	346.9899
Frequencies	--	441.3195	477.7035
Frequencies	--	521.6777	565.3344
Frequencies	--	636.3464	748.0929
Frequencies	--	800.6030	804.6218
Frequencies	--	890.6526	922.7037
Frequencies	--	1009.5711	1045.1019
Frequencies	--	1062.7481	1089.5529
Frequencies	--	1105.7198	1134.6304
Frequencies	--	1179.2736	1188.1698
Frequencies	--	1219.5013	1251.0450
Frequencies	--	1265.9455	1307.1812
Frequencies	--	1373.9258	1395.6176
Frequencies	--	1435.7287	1521.3897
Frequencies	--	1571.3994	1687.5960
Frequencies	--	2928.6547	3126.3562
Frequencies	--	3217.4561	3235.7700
Frequencies	--	3254.9386	3268.9209
			140.8177
			259.8878
			364.7813
			511.2511
			599.8123
			775.9638
			861.5874
			966.6345
			1053.2509
			1091.6389
			1164.1769
			1199.7609
			1262.9640
			1319.8011
			1416.3244
			1543.5591
			1711.9104
			3206.3496
			3240.9637
			3951.6115

***** R1-230-40-aa // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,	1.6798219103,-1.3585664951,-0.3730012331		

ESI
C,0,2.8618354128,-0.6556162464,-0.3698224166
C,0,2.850669757,0.6950572791,-0.0847809065
C,0,1.6613755466,1.3275029641,0.197075999
C,0,0.473835318,0.6206373928,0.2067928745
C,0,0.4787148281,-0.7349529071,-0.0822323874
C,0,-0.7737444171,-1.5544530624,-0.0639727046
C,0,-2.0025700616,-0.7382588076,-0.329859396
O,0,-0.9417845114,-2.263700531,1.1438814891
O,0,-1.9100490476,0.2131023408,-1.3580845366
C,0,-2.0258433436,0.6819268894,-0.041255637
C,0,-0.8065604745,1.3425198004,0.538427005
O,0,-0.7796385811,2.6756437365,0.3066237884
H,0,1.677045204,-2.4106131151,-0.6057780716
O,0,3.7873561227,-1.1552313576,-0.5978086948
H,0,3.7686876243,1.2568963063,-0.0894850392
H,0,1.6376210363,2.383429601,0.4011269231
H,0,-0.6997930223,-2.3179578227,-0.8329436078
H,0,-2.9283240163,-1.2922057727,-0.2928244216
H,0,-0.6662920802,-1.7119296112,1.8691741187
H,0,-2.9575192171,1.1745462616,0.1897656658
H,0,-0.9522113868,1.3179202968,1.6351800157
Rotational constants (GHZ): 1.1972449 0.8630193 0.5812825
SCF Done: E(UB+HF-B95) = -611.956475023 A.U. after 1 cycles
S**2 = 0.7550
Frequencies -- 48.3801 111.2575 150.1180
Frequencies -- 175.1715 197.3686 257.1215
Frequencies -- 298.1902 328.6954 413.1345
Frequencies -- 439.9960 451.4988 489.7936
Frequencies -- 541.8343 557.4949 612.3290
Frequencies -- 683.8996 715.5260 768.4620
Frequencies -- 800.8238 814.5847 839.5580
Frequencies -- 905.2077 927.5884 952.3307
Frequencies -- 1014.6474 1044.7040 1047.9605
Frequencies -- 1058.4919 1095.6841 1103.8176
Frequencies -- 1111.9695 1134.7276 1156.1970
Frequencies -- 1166.3395 1191.2574 1200.6971
Frequencies -- 1219.9065 1251.9822 1262.1021
Frequencies -- 1282.1372 1315.5856 1326.8817
Frequencies -- 1371.3625 1393.4900 1412.2741
Frequencies -- 1435.3544 1523.1652 1538.9171
Frequencies -- 1569.9910 1686.4567 1712.2488
Frequencies -- 2903.7908 3125.3191 3205.7433
Frequencies -- 3218.3369 3238.3827 3249.8375
Frequencies -- 3265.1316 3276.3170 3966.8064

***** TS R1-230-40-ss (C3-C4 cleavage) //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2
C,0,1.738422537,-1.0518039987,0.0820992714
C,0,2.7923369432,-0.2109712301,0.3766208002
C,0,2.6282125103,1.1563131927,0.3143869083
C,0,1.4115625294,1.6760243605,-0.0645030024
C,0,0.359431723,0.8381735782,-0.3821988784
C,0,0.5117056636,-0.5410145637,-0.2897935509
C,0,-0.6503540837,-1.4658765672,-0.5350986685
C,0,-1.86815425,-1.0521450038,0.2512827809
O,0,-0.3556546247,-2.8071417778,-0.2789353101
O,0,-1.628490751,-0.3467160422,1.4940991116
C,0,-2.175913025,0.3223245975,0.4782428242
C,0,-0.9009983629,1.4524301502,-0.8553896713
O,0,-1.1702647694,2.6285800577,-0.6848151154
H,0,1.8776724814,-2.117384619,0.1260284203
H,0,3.7438861376,-0.6292733709,0.6562997894
H,0,3.4471655663,1.8132449279,0.5506718961
H,0,1.2497460423,2.7377280104,-0.1341493446
H,0,-0.9319290752,-1.436529417,-1.5865402948

ESI			
H,0,-2.6305452348,-1.8122558149,0.328144854			
H,0,-0.0945296469,-2.8969419947,0.6339736259			
H,0,-3.0646485276,0.9235367913,0.554768251			
H,0,-1.4390496924,0.8793704909,-1.6258795672			
Rotational constants (GHZ): 1.0714136 0.9135879 0.5704576			
SCF Done: E(UB+HF-B95) = -611.928660108 A.U. after 1 cycles			
S**2 = 0.7695			
Frequencies --	-204.5787	78.6946	132.2782
Frequencies --	157.0641	177.2950	250.9517
Frequencies --	280.4935	327.0372	366.7672
Frequencies --	400.2670	436.3616	445.8351
Frequencies --	483.4442	520.7530	542.5845
Frequencies --	596.2261	666.6568	688.0013
Frequencies --	762.0803	783.1063	797.9256
Frequencies --	838.0951	860.9649	887.7241
Frequencies --	937.7463	979.7957	1022.4447
Frequencies --	1030.5231	1049.9538	1072.1720
Frequencies --	1100.3326	1117.7306	1131.6921
Frequencies --	1160.6064	1198.5736	1218.1063
Frequencies --	1234.3732	1255.9620	1286.4163
Frequencies --	1303.3913	1331.1404	1357.7334
Frequencies --	1374.7708	1411.6613	1443.8336
Frequencies --	1512.6556	1525.8757	1559.6492
Frequencies --	1659.7805	1688.5448	1710.5943
Frequencies --	2958.5080	3101.0926	3213.6577
Frequencies --	3244.5271	3258.1869	3262.8755
Frequencies --	3267.9541	3273.2981	3941.2242

***** TS R1-230-40-sa (C3-C4 cleavage) //
BB1K=BB95-Iop(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,-1.3063888377,0.8086157134,-1.2879489911			
C,0,-2.5186105702,0.1476957428,-1.335400493			
C,0,-2.6700144954,-1.0693712445,-0.7098533841			
C,0,-1.5931186058,-1.6316312686,-0.0584125232			
C,0,-0.3692937925,-0.9942040383,-0.0449933581			
C,0,-0.2244101339,0.2537093329,-0.6386106481			
C,0,1.0660140572,1.0148583683,-0.5059926555			
C,0,1.5383187865,1.047532753,0.92475658			
O,0,0.9867955155,2.31881069,-1.0048660761			
O,0,0.504753915,1.024417454,1.9540775268			
C,0,1.3160526956,-0.0275066083,1.8293082748			
C,0,0.7780881205,-1.6933106266,0.5758433352			
O,0,1.8704317512,-1.7907146352,0.034748658			
H,0,-1.1979450229,1.7629114779,-1.7722888264			
H,0,-3.3478990476,0.5945542977,-1.8561328767			
H,0,-3.6169298356,-1.5799016063,-0.7320111394			
H,0,-1.6927775308,-2.5871812556,0.4306049875			
H,0,1.8443820598,0.5197354916,-1.0781164394			
H,0,2.3125307152,1.7728317482,1.12051032			
H,0,0.3255515987,2.7990005211,-0.5133934681			
H,0,1.8698924403,-0.4695286929,2.6392770346			
H,0,0.5075218236,-2.370858797,1.3976927181			
Rotational constants (GHZ): 1.1935267 0.8364594 0.6244068			
SCF Done: E(UB+HF-B95) = -611.928057632 A.U. after 2 cycles			
S**2 = 0.7706			
Frequencies --	-261.2618	90.4598	135.9880
Frequencies --	159.0366	183.5698	243.3084
Frequencies --	280.2255	339.5225	349.6203
Frequencies --	402.5097	440.2839	457.3868
Frequencies --	475.1144	512.5951	559.7804
Frequencies --	589.4603	664.5930	691.6324
Frequencies --	752.8314	779.5281	799.1097
Frequencies --	847.0504	877.3949	888.9340
Frequencies --	931.4962	964.7784	1011.2780
Frequencies --	1038.4374	1045.4375	1073.9914

ESI			
Frequencies --	1100.7166	1124.7201	1127.6764
Frequencies --	1169.7770	1201.6631	1213.6938
Frequencies --	1238.5113	1259.1702	1291.2156
Frequencies --	1306.3706	1326.9727	1366.4302
Frequencies --	1377.9320	1416.2125	1465.5923
Frequencies --	1512.7752	1526.3457	1563.9037
Frequencies --	1643.9910	1692.9508	1710.5470
Frequencies --	2990.6015	3153.3510	3220.1570
Frequencies --	3233.6250	3248.7413	3255.8748
Frequencies --	3264.8195	3273.8118	3942.4489

***** TS R1-230-40-as (C3-C4 cleavage) //
BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,-1.6885326059,	1.2436925798,	0.4347046569	
C,0,-2.8854796413,	0.6537630367,	0.0775589749	
C,0,-0.4900808738,	0.6775258598,	0.056411934	
C,0,-2.8914953049,	-0.5116475824,	-0.6580438786	
C,0,0.829267487,	1.2390163224,	0.5102082816	
C,0,-0.4979859809,	-0.4809352928,	-0.71428549	
C,0,-1.6977111676,	-1.0732322295,	-1.0559904006	
C,0,1.5985051625,	0.1669351001,	1.2510634234	
O,0,0.7256947896,	2.4033791892,	1.2670087838	
C,0,1.8343452974,	-1.0919440599,	0.6255207139	
O,0,2.8655152718,	-0.2413187046,	0.6887442708	
C,0,0.756493772,	-1.0708818916,	-1.2518647852	
O,0,0.8057065586,	-2.2104028819,	-1.6821353115	
H,0,-1.6935029394,	2.161896905,	0.9964561487	
H,0,-3.8135912411,	1.1096784575,	0.3764895476	
H,0,-3.8238114617,	-0.9737858178,	-0.9323513278	
H,0,1.430457122,	1.5056006226,	-0.3556182062	
H,0,-1.668835338,	-1.9711494984,	-1.6486840357	
H,0,1.6193237784,	0.2668845874,	2.3266118655	
H,0,0.1589529667,	2.2465983202,	2.0168013549	
H,0,1.878817147,	-2.1277878124,	0.9120920134	
H,0,1.5329001396,	-0.3449476413,	-1.5324398876	
Rotational constants (GHZ):	1.1619742	0.8216196	0.5150405
SCF Done: E(UB+HF-B95) =	-611.925092655	A.U. after	1 cycles
S**2 =	0.7693		
Frequencies --	-219.7281	85.9857	132.9883
Frequencies --	162.8517	186.7292	249.3136
Frequencies --	278.1286	288.0483	335.8498
Frequencies --	365.2656	376.0972	420.3886
Frequencies --	465.3945	507.1189	529.4160
Frequencies --	586.7128	649.1546	679.0691
Frequencies --	771.3924	789.8802	824.6485
Frequencies --	831.9637	853.5104	878.9112
Frequencies --	931.6105	980.0075	1017.8372
Frequencies --	1048.2193	1051.5755	1074.7356
Frequencies --	1096.5841	1115.0366	1131.8917
Frequencies --	1177.5196	1199.0603	1212.1762
Frequencies --	1228.3283	1254.2965	1265.0830
Frequencies --	1313.9100	1327.7540	1344.9428
Frequencies --	1378.9973	1412.3868	1469.8822
Frequencies --	1514.1004	1525.2313	1557.4752
Frequencies --	1654.0379	1687.5584	1708.5038
Frequencies --	2982.1430	3122.7655	3198.3944
Frequencies --	3243.2173	3254.1509	3263.2131
Frequencies --	3264.2778	3272.5911	3950.6648

***** TS R1-230-40-aa (C3-C4 cleavage) //
BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

0,2			
C,0,1.6189263324,	-1.3538805544,	0.0948565978	

ESI
C,0,2.8523777031,-0.7888455414,0.366889112
C,0,0.5228807709,-0.5574447243,-0.1454177102
C,0,2.992054317,0.5788199101,0.4141566666
C,0,-0.8600284319,-1.12205079,-0.3293981025
C,0,0.6749334834,0.8252310702,-0.1385771963
C,0,1.897727097,1.3839532576,0.1620167151
C,0,-1.7544999578,-0.5136180259,0.7282153196
O,0,-0.9137650598,-2.5144954303,-0.2935732621
C,0,-1.8487697617,0.9035300373,0.8631826339
O,0,-2.8808399547,0.2786902985,0.2962404555
C,0,-0.4459691978,1.7193467755,-0.5464618267
H,0,1.519747189,-2.4250899754,0.0557612845
H,0,3.7016800576,-1.424732015,0.5479800415
H,0,3.947782075,1.0206494358,0.6359687701
H,0,-1.2483533703,-0.8179916806,-1.2943035045
H,0,1.9990229907,2.4572437444,0.1760667208
H,0,-1.9818868082,-1.1583524488,1.5657260565
H,0,-0.5414870099,-2.8284691323,0.5254344328
H,0,-1.9446801271,1.6060796628,1.6743033366
H,0,-0.4423298332,2.7099522462,-0.0703611651
O,0,-1.068806147,1.5371128411,-1.581835847
Rotational constants (GHZ): 1.3237849 0.7653983 0.5622999
SCF Done: E(UB+HF-B95) = -611.920433203 A.U. after 1 cycles
S**2 = 0.7715
Frequencies -- -296.6613 91.2033 129.9214
Frequencies -- 154.4631 176.7678 235.0303
Frequencies -- 268.9014 296.5557 328.3759
Frequencies -- 368.7881 387.3210 426.1498
Frequencies -- 446.8629 487.5949 540.4780
Frequencies -- 587.7771 651.9256 674.8534
Frequencies -- 771.1114 795.7845 824.2336
Frequencies -- 838.3006 873.1055 880.5140
Frequencies -- 927.7544 970.8498 1005.4442
Frequencies -- 1042.8090 1044.4421 1076.7979
Frequencies -- 1092.7386 1113.9968 1137.6160
Frequencies -- 1172.9020 1198.4698 1218.3634
Frequencies -- 1223.3900 1250.3628 1267.4663
Frequencies -- 1318.7242 1324.5748 1351.5086
Frequencies -- 1380.4630 1410.6135 1422.2180
Frequencies -- 1516.2971 1523.5951 1558.5755
Frequencies -- 1637.6351 1693.2912 1709.7716
Frequencies -- 2985.2345 3175.3971 3189.4132
Frequencies -- 3231.8451 3236.9560 3245.0428
Frequencies -- 3257.3429 3269.2733 3949.0107

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

ESI

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)^{ESI}

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

***** // BB1K=BB95-IOp(3/76=0580004200)/6-311++G(2df,2p)

ESI