

Supplementary Material

Kinetic Properties Study of H-atom Abstraction by H atom from Alkyl Cyclohexanes

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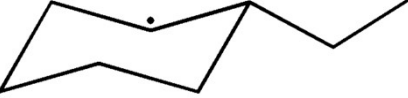
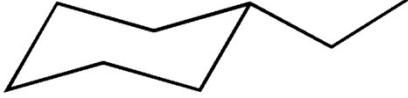

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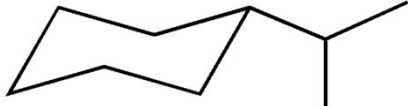

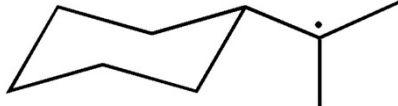

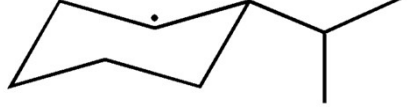
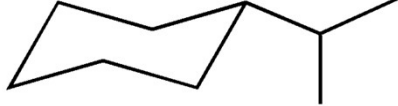
^c *Combustion Chemistry Centre, School of Biological and Chemical Sciences, MaREI, University of Galway,*

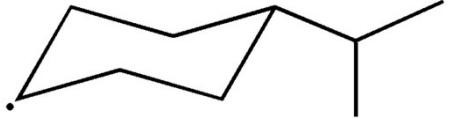

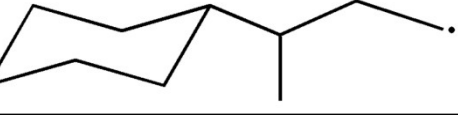
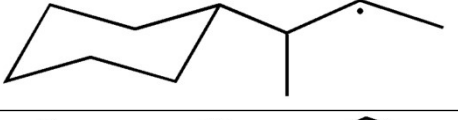
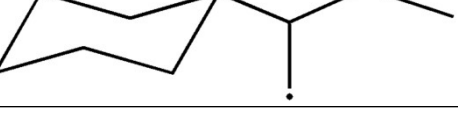
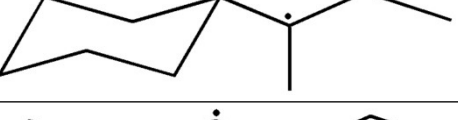



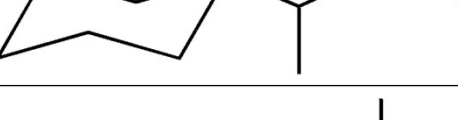
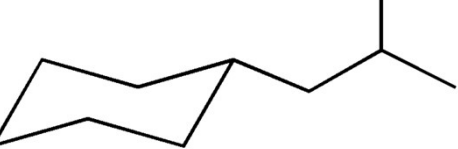
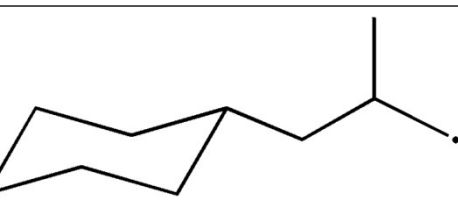
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Table S1. Structure for reactants and products studied in this work

Name	Structure
MCH	
MP1	
MP2	
MP3	
MP4	
MP5	
ECH	
EP1	
EP2	
EP3	
EP4	
EP5	
EP6	

$nPCH$	
$nP1$	
$nP2$	
$nP3$	
$nP4$	
$nP5$	
$nP6$	
$nP7$	
$iPCH$	
$iP1$	
$iP2$	
$iP3$	
$iP4$	
$iP5$	

<i>i</i> P6	
<i>s</i> BCH	
<i>s</i> BP1	
<i>s</i> BP2	
<i>s</i> BP3	
<i>s</i> BP4	
<i>s</i> BP5	
<i>s</i> BP6	
<i>s</i> BP7	
<i>s</i> BP8	
<i>i</i> BCH	
<i>i</i> BP1	

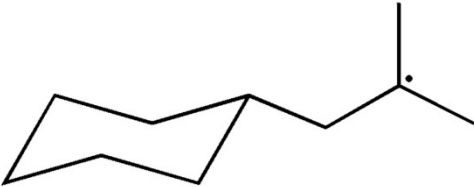

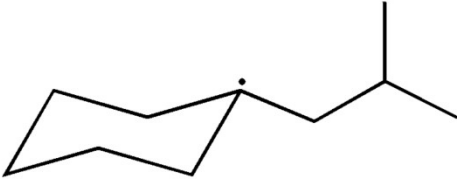


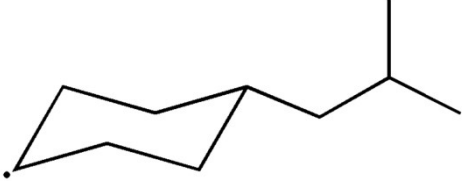
<i>i</i> BP2	
<i>i</i> BP3	
<i>i</i> BP4	
<i>i</i> BP5	
<i>i</i> BP6	
<i>i</i> BP7	

Table S2. T1 diagnostic values for the transition state, product and reactant calculated in this work.

Reactions	T1 diagnostic values		
	The transition state	The product (alkyl cyclohexyl radicals)	The reactant
$\text{MCH} + \dot{\text{H}} = \text{MP1} + \text{H}_2$	0.0106	0.0097	MCH:0.0087
$\text{MCH} + \dot{\text{H}} = \text{MP2} + \text{H}_2$	0.0099	0.0110	
$\text{MCH} + \dot{\text{H}} = \text{MP3} + \text{H}_2$	0.0099	0.0107	
$\text{MCH} + \dot{\text{H}} = \text{MP4} + \text{H}_2$	0.0098	0.0105	
$\text{MCH} + \dot{\text{H}} = \text{MP5} + \text{H}_2$	0.0097	0.0105	
$\text{ECH} + \dot{\text{H}} = \text{EP1} + \text{H}_2$	0.0101	0.0096	ECH:0.0087
$\text{ECH} + \dot{\text{H}} = \text{EP2} + \text{H}_2$	0.0096	0.0103	
$\text{ECH} + \dot{\text{H}} = \text{EP3} + \text{H}_2$	0.0099	0.0110	
$\text{ECH} + \dot{\text{H}} = \text{EP4} + \text{H}_2$	0.0098	0.0107	
$\text{ECH} + \dot{\text{H}} = \text{EP5} + \text{H}_2$	0.0097	0.0104	
$\text{ECH} + \dot{\text{H}} = \text{EP6} + \text{H}_2$	0.0109	0.0104	
$n\text{PCH} + \dot{\text{H}} = n\text{P1} + \text{H}_2$	0.0100	0.0096	<i>n</i> PCH:0.0088
$n\text{PCH} + \dot{\text{H}} = n\text{P2} + \text{H}_2$	0.0094	0.0094	
$n\text{PCH} + \dot{\text{H}} = n\text{P3} + \text{H}_2$	0.0096	0.0103	
$n\text{PCH} + \dot{\text{H}} = n\text{P4} + \text{H}_2$	0.0098	0.0109	
$n\text{PCH} + \dot{\text{H}} = n\text{P5} + \text{H}_2$	0.0097	0.0106	
$n\text{PCH} + \dot{\text{H}} = n\text{P6} + \text{H}_2$	0.0096	0.0102	
$n\text{PCH} + \dot{\text{H}} = n\text{P7} + \text{H}_2$	0.0095	0.0102	
$i\text{PCH} + \dot{\text{H}} = i\text{P1} + \text{H}_2$	0.0103	0.0098	<i>i</i> PCH:0.0087
$i\text{PCH} + \dot{\text{H}} = i\text{P2} + \text{H}_2$	0.0098	0.0106	
$i\text{PCH} + \dot{\text{H}} = i\text{P3} + \text{H}_2$	0.0098	0.0109	
$i\text{PCH} + \dot{\text{H}} = i\text{P4} + \text{H}_2$	0.0098	0.0104	
$i\text{PCH} + \dot{\text{H}} = i\text{P5} + \text{H}_2$	0.0097	0.0103	
$i\text{PCH} + \dot{\text{H}} = i\text{P6} + \text{H}_2$	0.0097	0.0103	
$s\text{BCH} + \dot{\text{H}} = s\text{BP1} + \text{H}_2$	0.0104	0.0098	<i>s</i> BCH:0.0089
$s\text{BCH} + \dot{\text{H}} = s\text{BP2} + \text{H}_2$	0.0097	0.0101	
$s\text{BCH} + \dot{\text{H}} = s\text{BP3} + \text{H}_2$	0.0103	0.0097	
$s\text{BCH} + \dot{\text{H}} = s\text{BP4} + \text{H}_2$	0.0099	0.0097	
$s\text{BCH} + \dot{\text{H}} = s\text{BP5} + \text{H}_2$	0.0097	0.0108	
$s\text{BCH} + \dot{\text{H}} = s\text{BP6} + \text{H}_2$	0.0098	0.0106	
$s\text{BCH} + \dot{\text{H}} = s\text{BP7} + \text{H}_2$	0.0096	0.0102	
$s\text{BCH} + \dot{\text{H}} = s\text{BP8} + \text{H}_2$	0.0097	0.0102	
$i\text{BCH} + \dot{\text{H}} = i\text{BP1} + \text{H}_2$	0.0102	0.0096	<i>i</i> BCH:0.0088
$i\text{BCH} + \dot{\text{H}} = i\text{BP2} + \text{H}_2$	0.0096	0.0105	
$i\text{BCH} + \dot{\text{H}} = i\text{BP3} + \text{H}_2$	0.0098	0.0103	
$i\text{BCH} + \dot{\text{H}} = i\text{BP4} + \text{H}_2$	0.0096	0.0108	
$i\text{BCH} + \dot{\text{H}} = i\text{BP5} + \text{H}_2$	0.0097	0.0106	
$i\text{BCH} + \dot{\text{H}} = i\text{BP6} + \text{H}_2$	0.0096	0.0102	
$i\text{BCH} + \dot{\text{H}} = i\text{BP7} + \text{H}_2$	0.0096	0.0102	

Table S3. Comparison of the frequencies used in the calculation of high-pressure limit rate constants. The optimized Cartesian coordinates and rotational constants of all alkyl cyclohexanes and the transition states are listed in the left column. The results of removing the torsional frequencies by visual inspection are listed in the middle column, and the bold numbers represent the torsional frequencies removed.

	Cartesian coordinates and rotational constants			Visual					
MCH	C	1.18829100	1.26062300	-0.21426700					
	C	-0.29282300	1.25582600	0.16972300					
	C	-1.01136100	0.00001400	-0.33470500					
	C	-0.29283400	-1.25581000	0.16971300					
	C	1.18828500	-1.26063500	-0.21426100					
	C	1.89195700	-0.00000500	0.29289900	158.18	925.29	1297.10	1501.32	3095.77
	H	-0.38357300	1.29367200	1.26391200	245.09	982.11	1336.39	1503.82	3099.98
	H	-0.79101500	2.14971500	-0.21892900	312.18	987.72	1336.43	1508.48	3117.29
	H	1.27599900	1.30564000	-1.30674100	336.60	994.41	1368.99	3014.14	3125.96
	H	1.67862000	2.15503500	0.17952300	410.29	1056.72	1383.29	3024.59	227.80
	H	-0.38358000	-1.29364600	1.26390100	446.46	1082.27	1387.07	3032.16	
	H	-0.79104300	-2.14969500	-0.21892900	450.67	1103.26	1387.89	3037.37	
	H	1.67859300	-2.15504300	0.17956400	548.04	1122.44	1405.19	3040.93	
	H	1.27602000	-1.30568300	-1.30673200	787.06	1142.93	1411.28	3045.60	
	H	1.88108000	-0.00000200	1.38985100	797.10	1189.51	1480.34	3048.19	
	H	2.94131600	-0.00000700	-0.01415000	860.23	1234.96	1487.46	3082.06	
	H	-0.95434800	0.00001200	-1.43234500	870.81	1279.02	1489.32	3085.02	
	C	-2.48117600	-0.00000500	0.07489300	891.13	1292.68	1493.98	3094.52	
	H	-2.57256900	-0.00072500	1.16568100					
	H	-2.99861500	0.88517500	-0.30369400					
H	-2.99892200	-0.88449400	-0.30488600						
	Rotational constants(GHz):								
	4.22278	2.19556	1.59622						
TS ₁ α	C	-1.23945200	-1.26095900	-0.19436600					
	C	0.25961900	-1.25979600	0.11037100					
	C	0.94622100	-0.00000700	-0.43201200	1400.91	862.31	1174.63	1458.85	3086.47
	C	0.25962500	1.25979300	0.11036200	151.05	874.26	1179.89	1483.37	3088.51
	C	-1.23944400	1.26096100	-0.19437900	240.00	890.67	1237.34	1487.18	3096.69
	C	-1.91295900	0.00000600	0.35173800	287.37	921.00	1259.34	1490.19	3097.14
	H	0.41150900	-1.29753900	1.19678500	312.14	962.06	1291.89	1495.15	3101.26
	H	0.73686400	-2.15116000	-0.30877600	353.00	987.57	1299.28	1508.85	3101.67
	H	-1.38632800	-1.30518800	-1.28056200	409.92	988.78	1321.66	1664.92	3185.50
	H	-1.70806400	-2.15507900	0.22515000	448.34	1056.80	1334.17	2968.29	164.96
	H	0.41151300	1.29754300	1.19677600	474.53	1079.88	1369.26	3034.73	
	H	0.73687800	2.15115000	-0.30879100	561.96	1103.07	1378.74	3037.24	
	H	-1.70805200	2.15508800	0.22512800	565.91	1104.81	1386.77	3039.80	
	H	-1.38631900	1.30518000	-1.28057600	790.07	1141.04	1388.88	3041.86	
	H	-1.84022100	0.00001200	1.44615400	797.09	1160.96	1402.14	3046.76	
	H	-2.97766100	0.00000700	0.10354400					

	H 0.81987900 -0.00000600 -1.52814700 C 2.42274900 -0.00001200 -0.13425100 H 2.50205400 0.00005000 1.24032200 H 2.96434100 -0.90919400 -0.39347700 H 2.96436600 0.90913000 -0.39356700 H 2.48108700 0.00008900 2.15524900 Rotational constants (GHZ): 4.01469 2.10117 1.57192	
TS ₁ α'	C -1.20073500 1.25801200 0.20391200 C 0.26806600 1.27013400 -0.22661800 C 0.99535800 0.00001200 0.16995900 C 0.26808200 -1.27010800 -0.22665700 C -1.20070400 -1.25802400 0.20392300 C -1.91149200 -0.00001700 -0.29771700 H 0.32550400 1.37093600 -1.32188200 H 0.78581900 2.13815300 0.19384300 H -1.25108400 1.28531600 1.29861500 H -1.70463700 2.15626500 -0.16177700 H 0.32547700 -1.37084000 -1.32192900 H 0.78586900 -2.13814100 0.19373300 H -1.70459600 -2.15629700 -0.16173100 H -1.25101800 -1.28530400 1.29862800 H -1.91834200 -0.00002300 -1.39496100 H -2.95530400 -0.00002600 0.02678600 H 0.93904900 -0.00002700 1.46846400 C 2.47344400 0.00000800 -0.14038300 H 2.96415800 0.88633400 0.26893800 H 2.96428300 -0.88593900 0.26961200 H 2.63290400 -0.00039800 -1.22567000 H 0.90980600 -0.00010900 2.45081400 Rotational constants (GHZ): 3.98820 2.12716 1.58506	1317.76i 859.22 1210.93 1469.35 3079.96 144.34 867.49 1228.74 1478.64 3080.96 222.43 899.44 1254.21 1489.66 3099.85 268.98 929.63 1282.45 1492.66 3101.37 297.01 978.55 1310.18 1494.07 3103.77 326.79 1000.30 1310.91 1499.60 3104.75 332.86 1001.36 1357.96 1506.62 3131.72 408.60 1054.50 1369.47 2995.36 196.02 426.95 1087.31 1382.14 2999.15 455.81 1106.76 1387.22 3034.64 551.05 1124.14 1398.88 3037.52 771.98 1150.56 1407.29 3049.57 792.81 1150.83 1434.87 3051.41

TS ₁ β'	C	-1.20051500	-1.23908100	-0.30508800					
	C	0.28708500	-1.22019100	-0.03571000					
	C	1.01005800	0.06102000	-0.39656100					
	C	0.27888500	1.27269200	0.19472800					
	C	-1.20460300	1.28110500	-0.17805700					
	C	-1.89067400	-0.00548500	0.28476000	1310.09	865.85	1205.36	1475.97	3090.48
	H	0.38783500	-1.28604900	1.30528200	152.60	870.08	1211.93	1487.65	3091.08
	H	0.81555600	-2.12751800	-0.33533200	210.73	891.18	1232.48	1492.38	3097.88
	H	-1.36323500	-1.25665200	-1.39309000	270.47	917.58	1271.37	1501.45	3105.10
	H	-1.64467800	-2.15619600	0.09163600	307.22	982.55	1286.34	1503.97	3108.63
	H	0.37808900	1.23966800	1.28744000	322.94	987.22	1319.26	1505.25	3124.85
	H	0.76566700	2.19301100	-0.14169300	339.48	1000.60	1331.34	1555.53	3129.56
	H	-1.69842200	2.15192600	0.26098100	415.27	1060.67	1359.64	2971.51	236.57
	H	-1.30458100	1.37431600	-1.26671100	456.35	1085.99	1367.36	3005.77	
	H	-1.84557600	-0.06174300	1.37851400	506.71	1100.34	1381.96	3035.29	
	H	-2.94768700	0.00151800	0.00710700	575.49	1115.58	1386.86	3040.99	
	H	0.97373100	0.15709400	-1.49476400	782.44	1144.26	1403.22	3051.80	
	C	2.47371500	0.02054100	0.03590900	807.76	1153.29	1411.45	3052.62	
	H	2.99717400	-0.82538800	-0.41632200					
	H	2.99321600	0.93694100	-0.25390300					
H	2.54476100	-0.08019200	1.12281600						
H	0.42444200	-1.28433700	2.24815400						
Rotational constants (GHZ):									
	3.98189	2.13650	1.58833						
TS ₁ γ'	C	-1.20051500	-1.23908100	-0.30508800					
	C	0.28708500	-1.22019100	-0.03571000					
	C	1.01005800	0.06102000	-0.39656100					
	C	0.27888500	1.27269200	0.19472800	1319.19	857.35	1201.24	1470.14	3079.79
	C	-1.20460300	1.28110500	-0.17805700	152.64	871.14	1221.50	1476.00	3086.44
	C	-1.89067400	-0.00548500	0.28476000	198.19	890.04	1246.84	1490.95	3092.37
	H	0.38783500	-1.28604900	1.30528200	268.12	918.28	1261.78	1500.55	3103.41
	H	0.81555600	-2.12751800	-0.33533200	290.04	979.45	1292.70	1502.85	3118.29
	H	-1.36323500	-1.25665200	-1.39309000	312.85	987.09	1317.84	1503.85	3121.52
	H	-1.64467800	-2.15619600	0.09163600	357.71	993.49	1336.10	1545.90	3127.90
	H	0.37808900	1.23966800	1.28744000	422.52	1061.73	1362.35	2989.84	239.35
	H	0.76566700	2.19301100	-0.14169300	437.94	1081.10	1372.32	3006.49	
	H	-1.69842200	2.15192600	0.26098100	471.11	1110.62	1382.34	3021.49	
	H	-1.30458100	1.37431600	-1.26671100	596.88	1122.47	1389.17	3035.16	
	H	-1.84557600	-0.06174300	1.37851400	785.07	1145.57	1405.40	3049.05	
	H	-2.94768700	0.00151800	0.00710700	813.44	1149.25	1413.68	3051.53	
	H	0.97373100	0.15709400	-1.49476400					
	C	2.47371500	0.02054100	0.03590900					
	H	2.99717400	-0.82538800	-0.41632200					
	H	2.99321600	0.93694100	-0.25390300					

	H 2.54476100 -0.08019200 1.12281600 H 0.42444200 -1.28433700 2.24815400 Rotational constants (GHZ): 3.98502 2.11981 1.57799	
TS ₁ δ'	C 1.14617700 1.27592600 -0.29297500 C -0.31852000 1.25352500 0.15265700 C -1.04875300 0.00000000 -0.33927700 C -0.31852000 -1.25352500 0.15265600 C 1.14617800 -1.27592500 -0.29297500 C 1.86047600 0.00000000 0.09150000 H -0.36112300 1.27399400 1.24937100 H -0.83346700 2.15108500 -0.20291700 H 1.18805800 1.38910600 -1.38649800 H 1.66281200 2.14192800 0.13002800 H -0.36112400 -1.27399500 1.24937000 H -0.83346600 -2.15108500 -0.20291900 H 1.66281200 -2.14192700 0.13003000 H 1.18805900 -1.38910700 -1.38649800 H 1.85398100 0.00000000 1.42935600 H 2.93085100 0.00000000 -0.11764400 H -1.01949900 0.00000000 -1.43830200 C -2.50731100 0.00000000 0.10892000 H -3.03440500 0.88480900 -0.25666000 H -3.03440500 -0.88481000 -0.25665900 H -2.56917100 0.00000000 1.20163800 H 1.80172600 -0.00000100 2.37526500 H -2.56917100 0.00000000 1.20163800 H 1.80172600 -0.00000100 2.37526500 Rotational constants (GHZ): 3.98569 2.11791 1.57923	1309.39i 863.76 1211.74 1472.94 3089.20 142.80 871.96 1220.00 1482.68 3090.02 218.07 898.41 1237.10 1485.14 3090.75 263.34 931.65 1253.12 1499.18 3092.37 282.67 972.13 1298.38 1502.36 3119.13 314.24 982.53 1328.09 1504.07 3122.58 346.04 998.18 1332.12 1545.45 3127.57 425.17 1055.39 1353.48 3005.65 238.69 460.07 1089.74 1377.81 3008.27 460.84 1106.90 1382.59 3013.67 602.27 1120.34 1389.15 3036.33 790.22 1145.86 1406.32 3041.12 791.27 1148.95 1411.59 3049.67

	Cartesian coordinates and rotational constants			Visual					
ECH	C	2.32508100	0.30952900	-0.22343300					
	C	1.34953600	1.41405800	0.18533900					
	C	-0.07609300	1.09937600	-0.27560000					
	C	-0.55919200	-0.26144900	0.23926400					
	C	0.43564500	-1.35711500	-0.16047500					
	C	1.85905600	-1.04736900	0.30650600					
	H	-0.75190300	1.89278100	0.05429700	131.87	904.66	1290.47	1489.40	3075.24
	H	1.35784400	1.51224200	1.27791200	220.16	935.87	1293.13	1491.50	3084.24
	H	1.67168800	2.37699100	-0.22032200	232.90	937.53	1310.02	1495.07	3093.98
	H	2.38249800	0.26712600	-1.31809700	334.98	1003.91	1320.32	1503.97	3094.64
	H	3.33136400	0.53624900	0.13921300	368.20	1033.40	1343.39	1509.24	3097.74
	H	-0.58478100	-0.21417800	1.33860200	431.25	1058.47	1366.93	1514.88	3100.32
	H	0.10392600	-2.32004700	0.24091600	445.20	1061.16	1377.71	3001.89	3127.73
	H	0.42841300	-1.45200700	-1.25491500	458.56	1081.57	1385.14	3023.26	3138.80
	H	1.88303700	-1.03230100	1.40305300	541.56	1109.48	1387.44	3028.72	83.72
	H	2.54257700	-1.83823100	-0.01425400	762.65	1126.25	1394.15	3036.60	246.92
	H	-0.10992400	1.08832500	-1.37411600	797.46	1145.71	1407.63	3039.90	
	C	-1.96739300	-0.60685200	-0.25274500	805.91	1190.12	1416.55	3041.07	
	H	-2.22363100	-1.60880700	0.10826000	858.87	1221.27	1480.35	3045.26	
	H	-1.95132700	-0.66956200	-1.34778800	890.28	1261.17	1486.08	3058.93	
C	-3.04853900	0.37824300	0.18942400						
H	-2.91570700	1.35892900	-0.27124500						
H	-4.04204300	0.01891000	-0.08592700						
H	-3.03063300	0.51305500	1.27473400						
	Rotational constants (GHZ):								
	3.83148	1.30334	1.05192						
TS ₂ β	C	-2.34214700	0.39769400	0.24110000					
	C	-1.32594100	1.43024000	-0.24904500	1361.44	821.58	1167.56	1393.77	3037.40
	C	0.09508000	1.06801100	0.18962600	203.58	860.92	1175.20	1412.44	3040.75
	C	0.49224500	-0.33986400	-0.26822900	215.50	898.19	1195.87	1458.37	3046.00
	C	-0.54087400	-1.36487200	0.21233600	237.57	906.52	1213.92	1472.91	3052.09
	C	-1.95977100	-1.00571400	-0.23228600	306.47	936.33	1241.48	1481.44	3083.50
	H	0.80238500	1.80731000	-0.19593400	333.38	940.30	1285.65	1488.03	3095.51
	H	-1.36153500	1.47492000	-1.34462300	372.16	998.30	1292.49	1489.02	3096.44
	H	-1.58776900	2.42688900	0.11604300	430.71	1010.66	1304.55	1494.12	3099.10
	H	-2.36929000	0.41186900	1.33761100	445.62	1059.16	1319.40	1508.00	3101.36
	H	-3.34629400	0.65672300	-0.10525000	460.89	1066.57	1342.64	1667.24	3104.91
	H	0.49057300	-0.34875000	-1.36867600	533.78	1077.41	1368.28	3004.88	3188.95
	H	-0.26895600	-2.36191500	-0.14893600	574.26	1102.73	1379.82	3018.33	92.82
	H	-0.50715400	-1.40556500	1.30950000	777.25	1119.30	1386.25	3024.90	130.33
	H	-2.01464300	-1.04321300	-1.32716100	797.55	1143.07	1389.06	3031.19	
	H	-2.67174000	-1.74425600	0.14589400					
	H	0.16375800	1.11261900	1.28548400					

	C 1.89542100 -0.73044200 0.20273900 H 2.10615000 -1.75421100 -0.13465300 H 1.90824400 -0.76942200 1.30018100 C 2.99465800 0.18229000 -0.28181900 H 4.01010400 -0.16959700 -0.10953900 H 2.86000000 0.60619500 -1.27712100 H 2.98142600 1.28775200 0.51949800 H 2.95271100 1.98859400 1.11114500 Rotational constants (GHZ): 3.64707 1.27778 1.02702	
TS ₂ α	C -2.38217800 -0.24650200 0.19761400 C -1.84074000 1.10623500 -0.26873600 C -0.41167200 1.32651800 0.22923100 C 0.52830400 0.19750700 -0.20810400 C -0.02679800 -1.16234800 0.25239300 C -1.45842700 -1.38327800 -0.24283400 H -0.02387700 2.28546200 -0.12734200 H -1.84891700 1.13882000 -1.36499100 H -2.48883600 1.91605800 0.07658900 H -2.45533800 -0.24629300 1.29213100 H -3.39239100 -0.40719700 -0.18824400 H 0.56210100 0.18629200 -1.30826900 H 0.62005100 -1.97063200 -0.09978700 H -0.01011700 -1.19289100 1.35016100 H -1.45287100 -1.43753100 -1.33828900 H -1.83502700 -2.34370200 0.11961600 H -0.41416200 1.37166000 1.32660200 C 1.93448700 0.42997100 0.29835300 H 1.97198400 0.66950000 1.36474500 H 2.27804600 1.58636300 -0.24790500 C 3.00845700 -0.53232200 -0.14827500 H 2.95690100 -0.69672100 -1.22806200 H 4.00333400 -0.15070400 0.09045600 H 2.90287400 -1.50482800 0.34328000 H 2.51765400 2.38165700 -0.71854800 Rotational constants (GHZ): 3.64160 1.27611 1.02200	1269.29i 831.44 1178.54 1404.89 3042.78 125.45 859.62 1203.33 1417.76 3046.83 187.42 893.45 1218.08 1480.94 3047.33 238.43 906.28 1224.11 1485.06 3089.94 280.24 937.92 1263.48 1487.68 3092.15 310.20 940.70 1292.03 1490.33 3094.22 366.99 1003.44 1299.34 1495.19 3095.99 378.60 1034.84 1309.86 1500.09 3097.23 433.95 1057.45 1334.81 1509.06 3101.28 449.89 1073.43 1365.15 1529.32 3111.56 465.56 1079.67 1374.73 3004.50 3132.78 540.52 1104.96 1379.17 3028.08 83.68 791.63 1122.65 1387.16 3033.99 212.27 800.71 1141.57 1389.09 3038.04

TS ₂ α'	C	2.32752400	0.32373700	-0.23860000					
	C	1.34416200	1.41689300	0.17938200					
	C	-0.07396700	1.11408100	-0.31340300					
	C	-0.54267700	-0.27009500	0.09315700					
	C	0.45910600	-1.36768500	-0.21349500					
	C	1.86757300	-1.03689700	0.28505400					
	H	-0.76619000	1.87320300	0.06019400	1297.22 <i>i</i>	795.39	1154.09	1415.81	3048.69
	H	1.33120700	1.48552700	1.27349100	125.77	858.54	1207.46	1446.55	3050.81
	H	1.66752000	2.39070400	-0.19718400	207.78	877.59	1218.58	1469.17	3062.25
	H	2.39056500	0.28960600	-1.33350600	221.50	913.81	1252.48	1475.12	3071.04
	H	3.33010700	0.55419200	0.13111900	271.97	936.00	1262.85	1483.86	3080.43
	H	-0.57214000	-0.22771600	1.39577300	296.85	947.68	1288.57	1489.69	3097.05
	H	0.11062800	-2.31214300	0.21678300	331.65	1005.05	1301.12	1493.08	3099.05
	H	0.48626300	-1.51197600	-1.30498500	371.77	1044.52	1318.70	1505.21	3100.20
	H	1.86264700	-1.01635100	1.38109000	416.99	1057.45	1355.23	1506.98	3103.76
	H	2.56458100	-1.82269100	-0.01715600	448.34	1066.81	1367.04	1514.61	3133.31
	H	-0.10088300	1.17726000	-1.41331500	462.63	1087.22	1380.55	2990.51	3140.52
	C	-1.96793400	-0.62753900	-0.28251800	546.92	1113.39	1383.59	2998.48	87.98
	H	-2.20747500	-1.59739300	0.16667800	752.55	1130.95	1387.51	3014.01	257.90
	H	-2.01235900	-0.77709700	-1.37110600	792.43	1144.48	1398.79	3036.51	
	C	-3.01545800	0.40212600	0.13853400					
	H	-4.02334200	0.02323500	-0.03936600					
	H	-2.92413400	0.63153400	1.20367300					
H	-2.91138000	1.33539400	-0.41781300						
H	-0.61558300	-0.22301500	2.37695800						
Rotational constants (GHZ):									
		3.62476	1.29146	1.05308					
TS ₂ β'	C	-2.32281400	0.29625000	0.19097600					
	C	-1.36499300	1.39599100	-0.27387500	1319.19 <i>i</i>	813.52	1159.48	1405.55	3046.81
	C	0.06823400	1.08289400	0.09517000	129.25	863.65	1202.76	1416.93	3051.47
	C	0.56580900	-0.29874000	-0.27865900	199.00	889.62	1208.68	1475.26	3059.32
	C	-0.43497100	-1.36798200	0.17871600	223.42	903.75	1220.68	1484.63	3082.64
	C	-1.85655400	-1.07387000	-0.30218200	276.17	931.11	1259.44	1491.69	3089.68
	H	0.76557400	1.89119200	-0.12673400	306.69	935.72	1281.15	1493.99	3091.27
	H	-1.43399200	1.49320700	-1.36769200	338.67	1002.33	1295.72	1503.54	3098.32
	H	-1.65658500	2.36392100	0.14331100	371.50	1035.43	1306.17	1504.52	3104.13
	H	-2.35515800	0.29090000	1.28664600	449.48	1060.13	1336.53	1515.49	3125.08
	H	-3.33617600	0.50787400	-0.15947700	452.81	1063.79	1362.09	1552.39	3130.20
	H	0.61708900	-0.33945400	-1.38129200	498.57	1085.88	1367.32	2956.54	3141.11
	H	-0.10462700	-2.34911000	-0.17546700	573.33	1108.15	1379.47	3005.28	69.95
	H	-0.42606400	-1.40505600	1.27582200	760.86	1118.70	1386.49	3034.65	241.37
	H	-1.88055100	-1.09262000	-1.39896600	799.22	1141.84	1389.75	3040.37	
	H	-2.53954400	-1.85438300	0.04325200					
	H	0.08046800	1.08033900	1.44196900					

	C 1.96726300 -0.59214400 0.26721900 H 2.22821100 -1.62116800 -0.00127200 H 1.92990200 -0.55716900 1.36213100 C 3.05356700 0.35270500 -0.24366500 H 4.04186100 0.02066500 0.07992800 H 3.05497000 0.39068300 -1.33678200 H 2.91481900 1.36985000 0.12756400 H 0.04656400 1.03970100 2.38485600 Rotational constants (GHZ): 3.63355 1.27922 1.04839	
TS ₂ γ'	C 2.31854600 0.24038400 -0.29730900 C 1.33934000 1.36312800 -0.04269800 C -0.10425400 1.06034500 -0.37737700 C -0.57853200 -0.26774700 0.22770400 C 0.40269800 -1.38904300 -0.12961100 C 1.82789900 -1.06994300 0.32320100 H -0.73877200 1.88471300 -0.04048000 H 1.34787400 1.52160700 1.28338700 H 1.67922600 2.34453600 -0.37573700 H 2.42867800 0.10508000 -1.38362900 H 3.30740200 0.50495900 0.08730900 H -0.57582400 -0.15365100 1.32163600 H 0.06428800 -2.32847900 0.31841800 H 0.39031600 -1.53527100 -1.21858600 H 1.84583800 -0.97614300 1.41511200 H 2.50435000 -1.88728600 0.06082500 H -0.21633200 1.00446100 -1.47268600 C -1.99977100 -0.62758300 -0.21171700 H -2.26155200 -1.59567100 0.22838600 H -2.00603600 -0.77202600 -1.29921000 C -3.05730800 0.40483200 0.17613100 H -4.06135400 0.03999600 -0.04870000 H -3.01210600 0.62354200 1.24676500 H -2.92231800 1.34468700 -0.36277900 H 1.33461300 1.58869900 2.23002400 Rotational constants (GHZ): 3.62329 1.27740 1.04341	1303.64i 814.23 1155.48 1409.34 3040.64 128.68 858.22 1196.25 1417.02 3051.32 196.19 890.91 1220.02 1471.22 3059.19 218.83 905.18 1236.46 1476.45 3077.47 273.15 927.84 1253.94 1487.46 3086.94 290.02 939.16 1277.82 1494.38 3091.80 354.96 999.06 1305.22 1500.51 3092.66 376.54 1034.45 1320.80 1504.41 3103.20 431.56 1058.62 1332.64 1515.71 3121.75 461.78 1065.51 1356.00 1539.52 3128.78 464.75 1083.95 1374.29 2985.97 3137.52 591.64 1116.94 1379.10 3006.56 87.46 764.44 1126.46 1385.43 3014.94 242.59 801.49 1146.32 1396.90 3027.32

TS ₂ δ'	C	-1.30451700	1.42123000	-0.26132500					
	C	0.10146400	1.09538000	0.25264600					
	C	0.59760200	-0.26395600	-0.25215300					
	C	-0.40101200	-1.35798100	0.14069800					
	C	-1.81143900	-1.07240700	-0.38101700					
	H	0.78873200	1.89052000	-0.04637600					
	H	-1.26031700	1.57669000	-1.34966200	1309.87	813.49	1155.81	1407.91	3037.20
	H	-1.66100600	2.35961900	0.17249700	124.51	859.44	1208.20	1417.03	3043.43
	H	-2.35031900	0.25430200	1.36439300	208.88	888.79	1221.63	1472.42	3059.16
	H	-3.31557200	0.52819500	-0.23222200	217.40	915.05	1227.69	1481.94	3077.34
	H	0.64332800	-0.22201300	-1.35133300	275.35	934.16	1241.62	1483.75	3089.59
	H	-0.05410300	-2.32815800	-0.22773500	280.71	939.27	1289.68	1491.19	3090.19
	H	-0.43141200	-1.42495900	1.23590000	343.92	995.60	1299.53	1499.87	3090.76
	H	-1.80896200	-1.13327700	-1.47951800	372.47	1032.53	1314.64	1505.66	3105.49
	H	-2.51238500	-1.83389100	-0.02793500	445.97	1057.17	1338.84	1514.91	3122.60
	H	0.08979200	1.07587700	1.35058100	451.51	1062.26	1354.67	1546.94	3128.27
	C	1.99699900	-0.60358400	0.26865200	469.56	1088.59	1372.14	2999.42	3139.30
	H	2.26118600	-1.60726800	-0.08137700	596.77	1112.10	1381.39	3004.57	80.61
	H	1.95995000	-0.65950400	1.36340600	762.60	1122.65	1384.01	3007.45	240.96
	C	3.08478100	0.38013100	-0.16000800	790.95	1145.70	1394.71	3035.55	
	H	4.07318900	0.02260400	0.13502100					
	H	3.08633400	0.50871400	-1.24621500					
H	2.94413400	1.36322000	0.29307100						
H	-2.35288500	0.20897300	2.31029900						
Rotational constants (GHZ):									
		3.63801	1.27025	1.04081					

	Cartesian coordinates and rotational constants			Visual					
<i>n</i> PCH	C	-2.35998300	-1.07360400	-0.28201700					
	C	-0.91999100	-1.35320900	0.15152900					
	C	0.04244000	-0.23657400	-0.27015500					
	C	-0.45785000	1.11425200	0.25564200					
	C	-1.90077600	1.39804900	-0.17031500					
	C	-2.84225300	0.27260000	0.26067700					
	H	-0.88556400	-1.44810400	1.24544400	129.04	913.63	1291.02	1489.71	3083.22
	H	-0.57727000	-2.30879100	-0.25803000	184.25	917.77	1298.13	1494.00	3090.69
	H	-2.40990300	-1.05799000	-1.37770200	232.62	943.35	1307.02	1497.55	3093.62
	H	-3.01893500	-1.87909600	0.05348300	295.98	989.57	1326.19	1504.84	3094.63
	H	-0.39658800	1.10505700	1.35299800	328.72	1039.80	1339.38	1508.38	3098.69
	H	0.19262300	1.92154900	-0.09114200	358.66	1058.48	1353.63	1512.45	3101.84
	H	-2.23343100	2.35367900	0.24410100	443.01	1060.59	1367.91	3003.13	3126.30
	H	-1.93770500	1.49675100	-1.26226300	445.61	1079.46	1382.73	3022.18	3132.17
	H	-2.87213300	0.22820900	1.35637700	472.68	1089.62	1385.94	3022.91	70.45
	H	-3.86163800	0.47805100	-0.07723600	571.56	1115.07	1389.45	3031.24	77.50
	H	0.04214200	-0.18964400	-1.36968700	741.21	1129.32	1403.08	3036.60	248.50
	C	1.46706500	-0.55370200	0.19102400	793.87	1143.62	1411.68	3040.48	
	H	1.73858000	-1.55142600	-0.17583800	802.47	1190.11	1414.05	3044.98	
	H	1.47961200	-0.61760800	1.28746600	848.82	1218.65	1479.15	3049.17	
	C	2.53199100	0.44250300	-0.26679500	861.02	1247.40	1485.50	3055.72	
	H	2.35266600	1.41851900	0.19291200	900.94	1284.27	1488.33	3059.92	
	H	2.44718700	0.58811000	-1.34979500					
	C	3.94357100	-0.02506800	0.08150000					
	H	4.69707600	0.69923100	-0.23415500					
	H	4.04872600	-0.16969000	1.16008900					
H	4.16926600	-0.97828500	-0.40355900						
	Rotational constants (GHZ):								
	3.74058	0.77490	0.67881						
TS ₃ γ	C	-2.42117400	-1.07075600	-0.24919700	1443.11	857.11	1178.38	1412.99	3040.74
	C	-0.96903500	-1.35384200	0.13898700	126.04	863.39	1185.89	1461.00	3045.63
	C	-0.01851200	-0.23780100	-0.31047900	190.32	901.46	1214.38	1476.59	3065.88
	C	-0.49968200	1.11310100	0.23300700	233.09	912.95	1222.92	1483.08	3082.96
	C	-1.95464900	1.39980700	-0.14754900	259.30	921.01	1280.38	1486.45	3088.08
	C	-2.88396600	0.27515000	0.31083000	328.65	943.00	1287.34	1489.62	3094.45
	H	-0.90057500	-1.45069200	1.23099300	333.89	989.86	1294.11	1492.62	3095.40
	H	-0.64096400	-2.30917100	-0.28290900	360.77	1026.35	1308.66	1496.36	3098.68
	H	-2.50540400	-1.05314400	-1.34274300	443.26	1058.18	1318.59	1509.06	3100.67
	H	-3.07039100	-1.87589900	0.10535700	445.80	1060.47	1336.57	1649.56	3107.80
	H	-0.40374500	1.10203700	1.32766800	474.82	1081.29	1354.96	3002.55	3192.18
	H	0.14005300	1.92080000	-0.13272000	549.81	1086.05	1367.87	3011.11	55.14
	H	-2.27224100	2.35519000	0.27886600	584.68	1111.23	1382.61	3024.85	75.86
	H	-2.02558000	1.50055900	-1.23762000	746.19	1126.74	1386.54	3028.63	159.89
	H	-2.87980900	0.22889500	1.40679700	794.21	1138.96	1389.60	3034.54	
	H	-3.91298100	0.48289300	0.00522000					

	H	-0.05179700	-0.18947900	-1.40950300	803.09	1159.92	1403.47	3037.39	
	C	1.41747900	-0.55957400	0.10894100					
	H	1.67761800	-1.55675900	-0.26656900					
	H	1.46675700	-0.62025600	1.20374200					
	C	2.46809200	0.43677500	-0.38342000					
	H	2.30431500	1.41887300	0.07020400					
	H	2.35209500	0.57709500	-1.46786200					
	C	3.87309800	-0.01690200	-0.08232500					
	H	4.67125700	0.67953900	-0.33207400					
	H	3.94643100	-0.05013500	1.28219000					
	H	4.10766700	-1.04595700	-0.35292300					
	H	3.92738300	-0.03012500	2.20111400					
	Rotational constants (GHZ):								
		3.57915	0.75290	0.66700					
TS ₃ β	C	1.89107800	1.39503700	-0.25435700					
	C	0.45621500	1.09532300	0.18638900					
	C	-0.00196700	-0.29532500	-0.26734800					
	C	0.98762600	-1.36253000	0.21393300					
	C	2.42007400	-1.06538500	-0.23323000					
	C	2.86272900	0.32109900	0.23707000					
	H	0.38994200	1.14567000	1.28211800					
	H	-0.21888100	1.86360700	-0.20025100	1285.86 <i>i</i>	855.46	1199.11	1415.82	3043.22
	H	1.92760100	1.43569500	-1.35011100	138.45	865.55	1212.84	1471.58	3043.77
	H	2.19582900	2.38040900	0.10806900	178.92	902.13	1223.45	1481.03	3045.90
	H	0.95375600	-1.39915100	1.31123400	236.81	914.54	1237.61	1487.09	3083.02
	H	0.67263300	-2.34788500	-0.14444100	288.66	924.01	1282.22	1488.92	3095.26
	H	3.10017600	-1.83316900	0.14543900	311.29	947.73	1291.09	1489.66	3095.98
	H	2.47189500	-1.10720500	-1.32811600	328.51	990.66	1298.41	1494.07	3097.05
	H	2.89146700	0.33619500	1.33352000	351.66	1034.08	1305.44	1495.24	3098.83
	H	3.87671700	0.53621000	-0.11073900	370.67	1057.89	1338.86	1508.02	3101.09
	H	-0.00208600	-0.30719700	-1.36774500	441.66	1068.53	1347.14	1545.27	3109.50
	C	-1.41897300	-0.62401500	0.20732300	446.85	1082.53	1368.32	3004.61	3137.19
	H	-1.43361000	-0.66320100	1.30579800	474.95	1095.28	1384.33	3006.25	78.78
	H	-1.67938300	-1.63760000	-0.13097900	570.65	1115.55	1386.77	3024.94	89.91
	C	-2.49120300	0.33075800	-0.26630800	786.94	1120.19	1389.52	3030.48	204.65
	H	-2.30765400	0.74525800	-1.26064400	797.37	1140.46	1401.89	3037.14	
	H	-2.38265300	1.40160300	0.50373300	813.74	1173.69	1410.24	3040.33	
	C	-3.91480000	-0.11738300	-0.03993800					
	H	-4.62992800	0.66555200	-0.29865900					
	H	-4.14488400	-0.99913700	-0.64791800					
	H	-4.07087400	-0.38875200	1.00770700					
	H	-2.35474300	2.10762500	1.14077800					
	Rotational constants (GHZ):								
		3.56982	0.76869	0.67023					

TS ₃ α	C	-1.97749900	-1.38110700	-0.22627900					
	C	-0.53091400	-1.16901500	0.22768200					
	C	0.01815600	0.18976000	-0.24360800					
	C	-0.90480400	1.32141100	0.22405500					
	C	-2.34849800	1.10960400	-0.23340400					
	C	-2.88275000	-0.24180100	0.24458000					
	H	-0.48234100	-1.20397300	1.32435000					
	H	0.10020400	-1.97971700	-0.14628600	1251.08	857.91	1199.55	1418.65	3046.72
	H	-2.00408800	-1.43154600	-1.32162600	130.15	867.05	1207.74	1481.18	3060.59
	H	-2.34782300	-2.34113100	0.14365200	159.23	903.29	1224.55	1483.91	3066.12
	H	-0.87576800	1.36245500	1.32122000	236.96	915.68	1247.96	1487.25	3085.33
	H	-0.52290500	2.27988000	-0.14003200	286.64	922.23	1288.54	1489.90	3090.55
	H	-2.98238000	1.92161900	0.13262100	296.05	944.93	1290.44	1494.86	3093.99
	H	-2.38791800	1.14545400	-1.32888400	322.26	991.52	1299.49	1503.72	3096.20
	H	-2.92355500	-0.24462600	1.34077500	364.11	1046.72	1304.71	1508.41	3097.40
	H	-3.90460400	-0.39655200	-0.11194000	376.64	1058.11	1336.49	1508.72	3101.29
	H	0.02083500	0.18342400	-1.34421000	445.76	1062.13	1346.01	1531.39	3130.75
	C	1.43765600	0.41895900	0.22495300	456.40	1083.18	1366.30	3006.34	3139.75
	H	1.50938900	0.65157800	1.29256400	476.79	1093.69	1374.21	3027.59	67.82
	H	1.76325000	1.57960000	-0.33514600	573.93	1112.71	1387.12	3029.78	80.49
	C	2.51563000	-0.52164800	-0.25987500	763.28	1127.33	1389.21	3033.74	227.26
	H	2.43967900	-0.62080800	-1.34880600	797.84	1138.25	1393.93	3038.12	
	H	2.34137200	-1.52331300	0.15298600	804.38	1179.68	1413.76	3042.45	
	C	3.91674200	-0.05201800	0.12827000					
	H	4.68115300	-0.74754600	-0.22228200					
	H	4.12767300	0.93006900	-0.30109000					
H	4.00926500	0.03103700	1.21411700						
H	1.97624600	2.35922400	-0.84023200						
Rotational constants (GHZ):									
		3.56066	0.76690	0.66821					
TS ₃ α'	C	-1.88459300	1.40056600	0.17150100	1297.45	850.41	1206.88	1445.86	3053.31
	C	-0.45341400	1.12849800	-0.30090400	133.24	860.76	1215.19	1468.31	3054.79
	C	0.03875900	-0.24642000	0.11059500	166.61	898.81	1249.37	1474.49	3057.46
	C	-0.93596000	-1.36462700	-0.20960000	218.60	909.74	1256.73	1481.50	3080.23
	C	-2.35761500	-1.06360800	0.26952600	267.64	920.86	1275.22	1489.70	3091.79
	C	-2.83855500	0.28716100	-0.26082300	291.22	942.79	1296.79	1492.97	3098.22
	H	-0.41122700	1.19435600	-1.40015000	301.68	989.72	1311.78	1497.19	3099.82
	H	0.21738800	1.90104300	0.08416200	325.51	1048.85	1323.91	1505.55	3102.09
	H	-1.88876100	1.46875300	1.26572300	364.35	1060.18	1333.39	1506.73	3103.62
	H	-2.22295400	2.36764300	-0.20926400	421.47	1066.80	1360.52	1511.68	3127.40
	H	-0.94516200	-1.50910900	-1.30134800	449.39	1084.54	1368.53	2990.59	3134.51
	H	-0.57363900	-2.30170600	0.22529000	473.71	1093.54	1383.05	2997.04	72.15
	H	-3.03386700	-1.86372200	-0.04215400	581.04	1119.68	1387.50	3002.79	81.79
	H	-2.36826500	-1.04301000	1.36553200	740.23	1134.01	1396.96	3036.55	248.47
	H	-2.88472100	0.25200700	-1.35654000	784.12	1147.50	1407.19	3048.48	
	H	-3.85105000	0.49652400	0.09414400					

	H	0.04935100	-0.20483700	1.41288700	794.35	1151.96	1415.03	3050.65	
	C	1.47498700	-0.57517700	-0.24592700					
	H	1.54094300	-0.72911500	-1.33417900					
	H	1.73243900	-1.53884300	0.21085100					
	C	2.50859800	0.46816300	0.17858100					
	H	2.35646200	0.71265400	1.23569900					
	H	2.35497600	1.39402100	-0.38284600					
	C	3.93723000	-0.02378900	-0.04055700					
	H	4.66983500	0.73322600	0.24537100					
	H	4.13448900	-0.92231000	0.54955200					
	H	4.10550400	-0.27332200	-1.09167800					
	H	0.08163400	-0.19886200	2.39459200					
	Rotational constants (GHZ):								
		3.54924	0.77204	0.68006					
TS ₃ β'	C	-2.36708400	-1.03393900	-0.35844400					
	C	-0.91185200	-1.31172700	-0.05889000					
	C	0.06171800	-0.18786800	-0.35106400					
	C	-0.43963100	1.12637600	0.26310400					
	C	-1.88678700	1.42811900	-0.13298900					
	C	-2.82085400	0.28664700	0.26930000					
	H	-0.86756500	-1.44339200	1.27850600					
	H	-0.56102400	-2.29381900	-0.38262400	1305.28 <i>i</i>	853.57	1203.69	1414.99	3051.83
	H	-2.50140200	-0.97898600	-1.44904600	130.33	865.73	1211.78	1476.98	3056.85
	H	-2.98908600	-1.86250000	-0.00847100	175.75	899.95	1221.55	1486.93	3066.40
	H	-0.36889900	1.04818800	1.35630400	208.51	911.67	1250.49	1487.10	3088.98
	H	0.20795700	1.95210400	-0.04174500	284.75	919.52	1268.03	1491.93	3093.05
	H	-2.21254300	2.36461000	0.32735200	294.05	941.79	1286.70	1497.82	3097.59
	H	-1.94023800	1.57343000	-1.21931600	317.45	987.55	1307.90	1503.76	3103.54
	H	-2.81308400	0.18357700	1.36055400	333.38	1038.84	1324.20	1505.84	3106.68
	H	-3.84951300	0.50963000	-0.02504600	356.64	1059.25	1333.00	1512.65	3109.60
	H	0.08734000	-0.05263000	-1.44688700	451.83	1064.00	1348.23	1551.74	3127.50
	C	1.47442400	-0.55842100	0.11066700	474.65	1077.58	1359.54	2959.52	3133.93
	H	1.74788700	-1.51997000	-0.34097700	514.81	1093.55	1367.93	3006.72	72.29
	H	1.45994000	-0.72100800	1.19600900	590.88	1115.40	1381.76	3029.86	79.81
	C	2.54980100	0.47086500	-0.23398300	743.76	1122.95	1388.27	3032.65	251.36
	H	2.36467200	1.39990700	0.31256200	797.82	1145.63	1402.81	3040.40	
	H	2.48547500	0.71801900	-1.29998100	806.41	1162.38	1409.88	3048.41	
	C	3.95277900	-0.03484500	0.09480200					
	H	4.71404100	0.71262700	-0.13670800					
	H	4.03653300	-0.28147000	1.15650400					
	H	4.18469900	-0.93873800	-0.47435900					
	H	-0.86027600	-1.48082800	2.22235200					
		Rotational constants (GHZ):							
			3.54924	0.76704	0.67633				

TS ₃ γ'	C	-1.87657500	1.34897400	-0.05280200					
	C	-0.42170100	1.07419000	-0.36168400					
	C	0.06749200	-0.24550100	0.25041100					
	C	-0.88650600	-1.38492300	-0.12397800					
	C	-2.32490100	-1.09307400	0.30440900					
	C	-2.82953600	0.20789100	-0.32457500					
	H	-0.28859300	1.02210200	-1.45481900					
	H	0.19086000	1.90994500	-0.01240900	1303.48	848.95	1196.76	1414.59	3051.24
	H	-1.91164900	1.50719700	1.27275900	128.06	861.72	1220.29	1471.70	3056.30
	H	-2.22903100	2.32382000	-0.39203600	180.57	900.40	1230.37	1476.07	3061.70
	H	-0.85274700	-1.52998000	-1.21264100	196.28	913.48	1247.34	1484.63	3085.48
	H	-0.53806200	-2.31813100	0.32926100	263.39	917.45	1269.89	1492.11	3089.19
	H	-2.98123500	-1.92294700	0.03047600	285.45	938.24	1296.62	1497.29	3091.63
	H	-2.36335700	-0.99995600	1.39585100	307.20	987.53	1301.71	1500.43	3097.76
	H	-2.91795100	0.07087800	-1.41265800	347.50	1038.60	1322.25	1505.55	3102.92
	H	-3.82986000	0.45348400	0.04260000	365.77	1060.45	1338.92	1512.27	3120.74
	H	0.04391600	-0.13294300	1.34412100	437.93	1064.09	1339.54	1539.29	3126.73
	C	1.50136600	-0.57964200	-0.16564600	462.68	1078.31	1363.80	2986.59	3133.00
	H	1.53153800	-0.72637600	-1.25383700	497.85	1095.09	1375.13	3006.78	72.14
	H	1.77709200	-1.54309700	0.28039400	609.08	1120.00	1384.31	3015.23	79.35
C	2.54705500	0.46214700	0.23100100	742.55	1129.12	1390.54	3022.67	250.39	
H	2.43958600	0.69277400	1.29696900	797.22	1145.99	1403.41	3031.39		
H	2.36658400	1.39628600	-0.30876600	811.72	1155.84	1412.74	3050.36		
C	3.96954800	-0.01519700	-0.05340600						
H	4.70913600	0.74120900	0.21621400						
H	4.19594800	-0.92323500	0.51134600						
H	4.09644300	-0.24505500	-1.11471700						
H	-1.91607500	1.57484200	2.21951400						
Rotational constants (GHZ):									
	3.54495	0.76394	0.67381						
TS ₃ δ'	C	-2.31260600	-1.09633000	-0.35143400	1307.15	855.07	1205.63	1414.36	3049.24
	C	-0.88229000	-1.35351700	0.12884700	126.83	861.03	1219.64	1472.39	3056.31
	C	0.08256700	-0.23896300	-0.29075200	170.79	904.56	1226.91	1481.60	3061.73
	C	-0.42694000	1.11003900	0.22919500	218.81	910.75	1235.00	1482.35	3089.06
	C	-1.85403900	1.40681400	-0.24245200	263.62	921.44	1275.11	1489.10	3089.93
	C	-2.79771600	0.27006600	0.07474500	279.55	946.12	1291.31	1496.06	3090.60
	H	-0.87984900	-1.42205500	1.22436100	296.88	984.04	1306.00	1501.13	3093.39
	H	-0.52642000	-2.31605500	-0.25081200	352.13	1036.65	1322.64	1504.91	3107.51
	H	-2.34064300	-1.15520400	-1.44970600	352.94	1057.31	1334.29	1512.47	3123.26
	H	-2.98730900	-1.87265100	0.01998000	445.52	1062.65	1349.58	1547.90	3127.08
	H	-0.40538800	1.09042300	1.32698500	454.31	1084.57	1357.12	3001.18	3132.82
	H	0.23461000	1.91910300	-0.08979500	512.13	1090.29	1377.84	3004.06	69.17
	H	-2.21660900	2.33738900	0.20301600	607.55	1117.61	1383.50	3007.03	74.50
	H	-1.84527800	1.56397900	-1.33142800	741.24	1126.38	1389.35	3025.07	247.44
	H	-2.82633200	0.21721200	1.41198200	789.53	1145.12	1404.00	3035.79	
	H	-3.84453200	0.47268600	-0.15463200					

H	0.09606100	-0.19605800	-1.39063500	804.92	1156.72	1412.58	3040.99
C	1.50141000	-0.55208700	0.19073700				
H	1.77847600	-1.55089800	-0.16860400				
H	1.49913900	-0.61149600	1.28733200				
C	2.57121600	0.44307500	-0.25791300				
H	2.38732000	1.42042100	0.19705700				
H	2.49908300	0.58542600	-1.34227600				
C	3.97848400	-0.02396200	0.10808400				
H	4.73554100	0.69959200	-0.20050100				
H	4.07090700	-0.16593000	1.18813000				
H	4.20971600	-0.97828400	-0.37210800				
H	-2.79899800	0.17160000	2.35731200				
Rotational constants (GHZ):							
	3.55501	0.76061	0.67227				

	Cartesian coordinates and rotational constants			Visual				
C	-1.92673200	1.25261900	0.25417900					
C	-0.47345500	1.25635600	-0.22548000					
C	0.29723400	-0.00009300	0.20702100					
C	-0.47357200	-1.25636100	-0.22579700					
C	-1.92682400	-1.25263400	0.25392800					
C	-2.66561700	0.00006700	-0.21310600					
H	-0.45416200	1.31600400	-1.32284900					
H	0.02344600	2.15369300	0.14907400	110.65	901.34	1224.39	1480.73	3045.30
H	-1.94158400	1.28802700	1.35056400	179.97	908.78	1262.42	1486.74	3048.62
H	-2.43679600	2.15370300	-0.09736300	227.49	929.76	1293.64	1488.18	3052.66
H	-0.45435400	-1.31566800	-1.32318400	312.52	942.72	1301.38	1490.45	3092.89
H	0.02327400	-2.15385700	0.14844700	353.03	968.00	1312.57	1493.68	3094.34
H	-2.43696600	-2.15361300	-0.09776700	398.38	977.08	1338.77	1506.21	3098.18
H	-1.94163800	-1.28824500	1.35030700	409.04	1017.42	1350.95	1506.29	3107.35
H	-2.72103500	0.00017400	-1.30869700	443.50	1067.57	1369.92	1509.32	3109.64
H	-3.69392300	0.00007200	0.15851100	446.71	1071.92	1371.32	1527.28	3115.47
H	0.35066800	-0.00022700	1.30764000	497.28	1098.19	1380.89	2991.85	3122.19
C	1.74483200	-0.00012200	-0.32455400	538.76	1116.15	1389.82	3020.40	3145.44
H	1.68958200	-0.00044400	-1.42201600	794.52	1126.53	1391.10	3021.50	3146.56
C	2.51675500	1.24866800	0.11312200	796.00	1154.74	1403.89	3030.29	50.84
H	3.56286700	1.17921400	-0.19395600	856.42	1190.67	1408.41	3036.76	229.28
H	2.10911800	2.16396000	-0.31713400	876.38	1199.23	1421.34	3040.47	264.28
H	2.49576400	1.34727100	1.20389000					
C	2.51693000	-1.24854600	0.11385300					
H	2.10920500	-2.16419700	-0.31555400					
H	3.56294600	-1.17930000	-0.19359900					
H	2.49627600	-1.34628400	1.20470300					
Rotational constants (GHZ):								
	3.54495	0.76394	0.67381					

TS ₄ β	C	-1.98175100	1.23280600	0.27857900					
	C	-0.54094400	1.27736200	-0.23483000					
	C	0.26834900	0.03653600	0.16980200					
	C	-0.47452100	-1.23510900	-0.26379100					
	C	-1.91819600	-1.27193700	0.24375900					
	C	-2.69813600	-0.03234800	-0.19022100					
	H	-0.55129800	1.34326100	-1.33181500	1351.85	857.18	1169.41	1412.54	3046.53
	H	-0.05710900	2.18477400	0.13243900	108.50	877.44	1180.18	1467.67	3056.55
	H	-1.97293900	1.25415300	1.37521900	125.90	900.98	1202.10	1482.62	3094.40
	H	-2.52152600	2.12492300	-0.05052100	229.04	909.01	1221.25	1487.50	3095.37
	H	-0.47239900	-1.28762700	-1.36191200	270.95	927.00	1252.90	1489.90	3099.26
	H	0.05062000	-2.12132800	0.09953800	330.52	941.99	1293.12	1494.33	3106.15
	H	-2.41253500	-2.18089200	-0.10969300	348.89	961.49	1299.69	1499.99	3109.79
	H	-1.90845600	-1.32275200	1.33943500	397.64	976.16	1308.27	1508.73	3119.18
	H	-2.77782900	-0.01864200	-1.28424800	429.52	1010.44	1325.47	1516.55	3124.96
	H	-3.71760400	-0.06430300	0.20350900	442.77	1065.51	1341.97	1661.88	3153.53
	H	0.34544700	0.02157900	1.26760900	445.35	1072.34	1357.95	2973.59	3200.43
	C	1.70726500	0.09555200	-0.39135900	520.14	1095.81	1369.73	3008.50	36.57
	H	1.61784700	0.22381800	-1.48307100	543.45	1103.41	1382.22	3020.91	195.04
	C	2.49553500	1.28406600	0.16856900	563.15	1125.52	1389.68	3029.94	125.90
	H	3.51810400	1.28123700	-0.21551500	794.72	1139.14	1391.39	3037.47	
	H	2.04768700	2.24160700	-0.09688400	797.96	1159.55	1405.68	3042.35	
	H	2.54684400	1.22017600	1.26017500					
	C	2.48309300	-1.17923600	-0.14735200					
	H	2.08919300	-2.09302400	-0.58555400					
	H	3.56294300	-1.09542200	-0.26072400					
	H	2.35235100	-1.42188500	1.20154300					
	H	2.21650000	-1.53580500	2.10152700					
Rotational constants (GHZ):									
	2.75931	1.02647	0.81354						
TS ₄ α	C	-1.95667800	-1.25262700	-0.24808800	1296.90	851.36	1182.48	1431.03	3040.43
	C	-0.48568500	-1.26031400	0.17251700	110.33	874.07	1212.51	1477.21	3046.84
	C	0.26409200	0.00006000	-0.28681700	226.92	901.37	1241.88	1483.82	3094.98
	C	-0.48574500	1.26032200	0.17273700	255.66	910.44	1271.94	1487.86	3096.64
	C	-1.95672700	1.25264500	-0.24790200	292.36	942.10	1287.03	1488.04	3099.99
	C	-2.67372400	-0.00004200	0.25213200	294.72	942.83	1295.72	1493.94	3104.80
	H	-0.41857500	-1.32400900	1.26703700	316.54	972.39	1304.24	1498.79	3106.49
	H	-0.00304300	-2.15391800	-0.22922900	352.35	990.53	1331.35	1500.29	3112.50
	H	-2.01716700	-1.28597900	-1.34306900	391.75	1018.26	1338.56	1508.42	3116.70
	H	-2.45216300	-2.15378900	0.12297400	411.66	1066.58	1367.14	1524.22	3144.19
	H	-0.41867100	1.32381400	1.26726900	444.41	1073.25	1375.11	2955.38	3145.98
	H	-0.00313500	2.15402400	-0.22882600	452.15	1096.09	1389.31	3029.61	64.39
	H	-2.45225500	2.15373300	0.12328300	494.73	1100.74	1390.68	3030.64	150.72
	H	-2.01719900	1.28615000	-1.34287900	539.76	1130.14	1399.75	3033.22	187.73
	H	-2.67980400	-0.00012100	1.34892500	788.58	1153.21	1404.41	3033.79	
	H	-3.71733800	-0.00004000	-0.07366500					

	H	0.27224900	0.00016400	-1.39205300	796.80	1162.35	1414.49	3038.68
	C	1.72311300	0.00004800	0.16549700				
	H	1.62964600	0.00023400	1.46272900				
	C	2.49687800	-1.26393600	-0.15311300				
	H	3.53796700	-1.16805600	0.16132200				
	H	2.07856900	-2.14089800	0.34271200				
	H	2.48953200	-1.45409000	-1.23418100				
	C	2.49702200	1.26383400	-0.15353100				
	H	2.07860200	2.14108300	0.34168600				
	H	3.53800900	1.16807900	0.16128100				
	H	2.49002900	1.45339600	-1.23470600				
	H	1.52947200	0.00028700	2.43880600				
	Rotational constants (GHZ):							
		2.76110	1.03172	0.81687				
	C	1.92389900	-1.24985600	0.24450100				
	C	0.48266700	-1.27021400	-0.27098700				
	C	-0.28571900	0.00000500	0.05452700				
	C	0.48267500	1.27021200	-0.27101500				
	C	1.92390600	1.24985900	0.24447500				
	C	2.66699700	-0.00000600	-0.22142400				
	H	0.48894600	-1.39572600	-1.36590800	1259.59	857.59	1183.83	1464.84 3055.01
	H	-0.03448300	-2.14010900	0.13947900	99.69	873.27	1206.42	1471.07 3058.15
	H	1.90831200	-1.26716300	1.34067000	186.11	892.54	1222.04	1478.84 3098.06
	H	2.44330200	-2.15489200	-0.08098700	214.77	919.95	1257.03	1489.23 3098.79
	H	0.48895700	1.39569700	-1.36594000	287.76	929.63	1267.01	1491.64 3102.42
	H	-0.03447100	2.14012100	0.13942700	291.73	941.73	1305.49	1493.27 3106.77
	H	2.44331300	2.15488500	-0.08103100	308.70	975.79	1305.53	1506.50 3107.71
	H	1.90831800	1.26718800	1.34064400	358.66	979.69	1340.13	1507.19 3123.88
	H	2.73306000	-0.00001700	-1.31666900	387.22	1028.07	1343.93	1509.42 3129.72
	H	3.69116000	-0.00000500	0.16074700	414.46	1068.59	1359.44	1528.49 3146.82
	H	-0.35851400	0.00001400	1.36805900	446.09	1082.59	1370.53	2982.13 3148.06
	C	-1.75112700	0.00000800	-0.37906500	448.78	1100.06	1386.54	2990.04 60.25
	C	-2.49792000	-1.25167400	0.09472200	503.89	1116.00	1391.00	2994.68 236.05
	H	-3.55789900	-1.17694200	-0.15695600	546.94	1133.63	1402.47	3036.78 266.89
	H	-2.11522300	-2.16382100	-0.36418000	773.03	1150.24	1403.05	3047.87
	H	-2.41633000	-1.35432600	1.18157300	792.02	1157.48	1419.69	3050.29
	C	-2.49793000	1.25166700	0.09476800				
	H	-2.11522500	2.16383600	-0.36408000				
	H	-3.55790300	1.17694600	-0.15693600				
	H	-2.41636200	1.35426600	1.18162600				
	H	-0.42992800	0.00001400	2.33876100				
	Rotational constants (GHZ):							
		2.75931	1.04041	0.82365				
TS ₄ α'	C	1.92389900	-1.24985600	0.24450100				
	C	0.48266700	-1.27021400	-0.27098700				
	C	-0.28571900	0.00000500	0.05452700				
	C	0.48267500	1.27021200	-0.27101500				
	C	1.92390600	1.24985900	0.24447500				
	C	2.66699700	-0.00000600	-0.22142400				
	H	0.48894600	-1.39572600	-1.36590800	1259.59	857.59	1183.83	1464.84 3055.01
	H	-0.03448300	-2.14010900	0.13947900	99.69	873.27	1206.42	1471.07 3058.15
	H	1.90831200	-1.26716300	1.34067000	186.11	892.54	1222.04	1478.84 3098.06
	H	2.44330200	-2.15489200	-0.08098700	214.77	919.95	1257.03	1489.23 3098.79
	H	0.48895700	1.39569700	-1.36594000	287.76	929.63	1267.01	1491.64 3102.42
	H	-0.03447100	2.14012100	0.13942700	291.73	941.73	1305.49	1493.27 3106.77
	H	2.44331300	2.15488500	-0.08103100	308.70	975.79	1305.53	1506.50 3107.71
	H	1.90831800	1.26718800	1.34064400	358.66	979.69	1340.13	1507.19 3123.88
	H	2.73306000	-0.00001700	-1.31666900	387.22	1028.07	1343.93	1509.42 3129.72
	H	3.69116000	-0.00000500	0.16074700	414.46	1068.59	1359.44	1528.49 3146.82
	H	-0.35851400	0.00001400	1.36805900	446.09	1082.59	1370.53	2982.13 3148.06
	C	-1.75112700	0.00000800	-0.37906500	448.78	1100.06	1386.54	2990.04 60.25
	C	-2.49792000	-1.25167400	0.09472200	503.89	1116.00	1391.00	2994.68 236.05
	H	-3.55789900	-1.17694200	-0.15695600	546.94	1133.63	1402.47	3036.78 266.89
	H	-2.11522300	-2.16382100	-0.36418000	773.03	1150.24	1403.05	3047.87
	H	-2.41633000	-1.35432600	1.18157300	792.02	1157.48	1419.69	3050.29
	C	-2.49793000	1.25166700	0.09476800				
	H	-2.11522500	2.16383600	-0.36408000				
	H	-3.55790300	1.17694600	-0.15693600				
	H	-2.41636200	1.35426600	1.18162600				
	H	-0.42992800	0.00001400	2.33876100				
	Rotational constants (GHZ):							
		2.75931	1.04041	0.82365				

TS ₄ β'	C	-1.94141500	-1.22749500	-0.30868100					
	C	-0.47366800	-1.22617400	0.05580500					
	C	0.31206200	0.03212800	-0.26596500					
	C	-0.46116800	1.27381300	0.20702700					
	C	-1.91565300	1.27902000	-0.26701500					
	C	-2.65313400	0.02614500	0.20009400					
	H	-0.46025100	-1.28419600	1.40009800					
	H	0.03290300	-2.15396600	-0.20674500	1308.12	858.28	1194.93	1422.94	3051.31
	H	-2.03316500	-1.27197900	-1.40425700	105.79	880.41	1206.97	1474.92	3053.36
	H	-2.41935000	-2.13116400	0.08007000	178.39	897.30	1208.85	1486.43	3088.27
	H	-0.43778000	1.29941900	1.30493700	194.97	909.04	1225.53	1489.72	3097.00
	H	0.03655600	2.17936600	-0.14496500	274.47	930.59	1260.44	1491.38	3104.15
	H	-2.42048200	2.17779500	0.09698400	303.27	937.86	1282.18	1502.32	3112.87
	H	-1.93845200	1.32445000	-1.36317400	327.09	965.54	1299.89	1507.01	3117.08
	H	-2.67441500	0.00720900	1.29590600	355.42	978.15	1330.52	1507.71	3123.20
	H	-3.69091600	0.03704300	-0.14248700	403.31	1016.90	1349.08	1527.55	3133.47
	H	0.39872200	0.09203200	-1.36675300	418.52	1066.70	1353.92	1548.96	3146.10
	C	1.74729800	-0.01239800	0.30092200	445.81	1073.58	1368.15	2946.11	3150.83
	H	1.66254800	-0.07711300	1.39367100	468.05	1098.28	1370.98	3005.07	228.93
	C	2.52283900	-1.23722200	-0.19325200	517.08	1104.41	1383.46	3030.53	260.52
	H	3.56225100	-1.18890100	0.13908700	576.75	1131.55	1390.79	3034.78	41.12
	H	2.10690900	-2.17451300	0.17783000	790.05	1153.69	1405.50	3040.19	
	H	2.52484800	-1.27372900	-1.28806300	808.13	1165.22	1407.81	3048.58	
	C	2.53129600	1.25672800	-0.04549500					
	H	2.11273700	2.14675900	0.42538000					
	H	3.56810300	1.16654000	0.28610300					
	H	2.54071100	1.41701800	-1.12916900					
	H	-0.48221100	-1.27934400	2.34490300					
Rotational constants (GHZ):									
	2.76047	1.03309	0.81836						
TS ₄ γ'	C	1.90729600	-1.21116000	0.06868700	1314.71	855.55	1195.92	1423.01	3051.65
	C	0.44192700	-1.23334300	-0.30277200	108.87	878.35	1199.09	1471.04	3053.65
	C	-0.31997400	0.01422500	0.17344900	178.89	900.99	1222.41	1477.07	3090.97
	C	0.43895700	1.28011300	-0.24930000	192.11	907.35	1241.22	1488.71	3101.37
	C	1.88871700	1.28111500	0.23881800	255.73	930.28	1255.04	1491.27	3101.53
	C	2.64997900	0.05808100	-0.27265000	283.17	935.17	1280.26	1499.74	3111.50
	H	0.35059000	-1.30029300	-1.39944700	335.25	969.12	1308.32	1506.79	3117.28
	H	-0.01457500	-2.13881000	0.10356900	362.11	977.57	1333.24	1508.42	3120.92
	H	1.91321100	-1.25562000	1.40304000	391.55	1012.09	1348.64	1527.76	3123.80
	H	2.44054800	-2.13064600	-0.17609000	410.31	1069.41	1357.17	1537.37	3143.26
	H	0.42133900	1.35176900	-1.34613100	449.55	1073.44	1370.59	2984.64	3146.63
	H	-0.06567200	2.16881200	0.13464900	468.39	1099.52	1376.98	3003.85	231.90
	H	2.39148100	2.19893900	-0.07656100	498.85	1111.58	1381.21	3005.87	272.36
	H	1.89687100	1.27218800	1.33492800	589.46	1131.30	1392.55	3019.32	52.20
	H	2.75430100	0.12760800	-1.36572500	790.43	1155.42	1404.98	3028.77	
	H	3.66278900	0.02999200	0.13865800					

	H	-0.34512600	-0.01129800	1.27398800	813.34	1162.84	1409.01	3049.78	
	C	-1.77830700	0.01598200	-0.32596500					
	H	-1.74837100	0.06839500	-1.42327400					
	C	-2.52038100	-1.26451000	0.06988600					
	H	-3.57487400	-1.19655300	-0.20701200					
	H	-2.11086200	-2.15125500	-0.41550700					
	H	-2.46888800	-1.41598000	1.15344200					
	C	-2.55733500	1.23014000	0.18912500					
	H	-2.16797400	2.17238000	-0.19767400					
	H	-3.60709200	1.16369700	-0.10571600					
	H	-2.52058900	1.27027100	1.28300000					
	H	1.88762200	-1.24745300	2.35219400					
	Rotational constants (GHZ):								
		2.75829	1.02727	0.81503					
TS ₄ δ'	C	-1.87944200	-1.26787000	-0.32855800					
	C	-0.44312800	-1.25346100	0.20287700					
	C	0.33497800	-0.00004700	-0.22338600					
	C	-0.44307600	1.25348500	0.20261900					
	C	-1.87939300	1.26781900	-0.32881400					
	C	-2.61945100	0.00002400	0.02134100					
	H	-0.46529600	-1.29233500	1.30018100					
	H	0.06648300	-2.15601000	-0.13912100	1315.95 <i>i</i>	855.67	1194.93	1421.97	3049.02
	H	-1.85508600	-1.37044700	-1.42388100	103.38	877.74	1208.60	1471.99	3053.14
	H	-2.41464300	-2.14158500	0.05364600	178.52	897.33	1220.55	1481.90	3089.51
	H	-0.46522200	1.29261800	1.29991500	214.94	919.16	1232.66	1483.88	3090.04
	H	0.06655700	2.15593400	-0.13961000	256.71	929.98	1244.19	1490.83	3113.46
	H	-2.41456700	2.14163400	0.05320000	281.93	944.98	1294.83	1498.65	3115.46
	H	-1.85502900	1.37016200	-1.42415900	336.20	964.84	1305.15	1506.36	3116.81
	H	-2.68231100	0.00016000	1.35987300	354.71	977.47	1323.33	1508.40	3123.24
	H	-3.67709100	0.00001900	-0.24469000	397.58	1008.71	1350.60	1527.22	3123.95
	H	0.40622000	-0.00014400	-1.32326900	409.31	1065.52	1362.22	1550.73	3146.43
	C	1.77378900	-0.00006200	0.33229200	453.20	1080.91	1371.65	2989.73	3147.52
	H	1.70022800	-0.00022800	1.42851300	465.89	1094.93	1375.63	3003.14	261.89
	C	2.55294000	-1.24843400	-0.09405800	499.76	1107.28	1385.58	3006.15	219.05
	H	3.59418900	-1.17755500	0.22848100	592.16	1129.87	1387.21	3024.67	46.21
	H	2.14102400	-2.16435900	0.33061700	789.22	1153.23	1404.87	3035.49	
	H	2.54847200	-1.34711800	-1.18501200	802.37	1161.66	1408.76	3041.12	
	C	2.55287100	1.24848800	-0.09365100					
	H	2.14096600	2.16423300	0.33142400					
	H	3.59414600	1.17750300	0.22878200					
	H	2.54831700	1.34760200	-1.18456700					
	H	-2.67788100	0.00025500	2.30570200					
		Rotational constants (GHZ):							
			2.76524	1.02403	0.81320				

	Cartesian coordinates and rotational constants				Visual					
sBCH	C	1.97117300	-1.44321700	0.08397200						
	C	0.59590200	-1.12361400	-0.50650700						
	C	-0.01167000	0.16096800	0.07517600						
	C	0.98487700	1.32121600	-0.07131700						
	C	2.35857600	0.99515300	0.51890100						
	C	2.94084900	-0.27644000	-0.09591500	125.21	909.87	1294.99	1499.18	3094.07	
	H	0.68631000	-1.00508200	-1.59548700	190.79	939.65	1305.06	1501.59	3097.78	
	H	-0.07313000	-1.97106400	-0.33723700	238.17	945.59	1313.05	1507.09	3103.90	
	H	1.86026100	-1.65380000	1.15503800	273.26	990.31	1335.27	1510.64	3106.70	
	H	2.37251100	-2.35057800	-0.37576400	330.89	1001.17	1348.56	1515.92	3120.18	
	H	1.09540100	1.55333600	-1.13990200	349.75	1017.77	1369.69	1522.49	3130.03	
	H	3.03786600	1.83919100	0.37079200	403.45	1043.07	1373.38	3004.18	3133.38	
	H	2.25895300	0.85531000	1.60243200	439.11	1064.98	1381.94	3019.96	3142.57	
	H	3.11503300	-0.11317200	-1.16663700	446.11	1074.54	1383.08	3022.17	70.10	
	H	3.91001900	-0.51077900	0.35277900	448.21	1098.65	1388.76	3031.67	85.66	
	H	-0.17235700	0.00135200	1.15219300	534.90	1110.13	1389.49	3036.21	222.07	
	C	-1.37272200	0.50157500	-0.56572800	569.91	1127.21	1409.70	3039.73	260.33	
	H	-1.17961200	0.72173600	-1.62492300	785.69	1151.93	1415.19	3044.72		
	C	-1.99745500	1.75345800	0.06417400	795.18	1173.41	1419.39	3054.49		
	H	-1.44874100	2.65882500	-0.19804500	799.31	1199.57	1481.46	3060.64		
	H	-3.02741300	1.88419400	-0.27760200	833.47	1222.42	1487.08	3061.63		
	H	-2.01345900	1.68070600	1.15586500	865.49	1254.21	1488.50	3091.02		
	C	-2.37058800	-0.67046600	-0.53395800	899.72	1292.68	1493.95	3092.43		
	H	-3.30306700	-0.32994800	-0.99580300						
	H	-2.00526500	-1.48466400	-1.16546600						
	C	-2.67273400	-1.20906600	0.86483600						
	H	-3.43561500	-1.98902700	0.82261300						
H	-1.78345600	-1.64261900	1.32917200							
H	-3.04294600	-0.42132500	1.52543800							
	Rotational constants (GHZ):									
	2.18933	0.82948	0.67448							
TS ₅ γ	C	1.98049100	-1.42482300	-0.03775400	1378.31	836.15	1187.10	1461.19	3055.38	
	C	0.62933100	-1.05226900	-0.65017600	137.15	865.84	1195.94	1481.10	3085.50	
	C	-0.00146500	0.16819300	0.03433800	247.41	900.17	1218.57	1487.29	3092.75	
	C	0.98761600	1.34308000	0.00442800	247.84	909.79	1242.70	1488.10	3094.19	
	C	2.34474900	0.97298700	0.60832000	278.56	941.03	1271.68	1493.04	3097.84	
	C	2.95304800	-0.24709800	-0.08166700	331.05	944.86	1292.89	1494.55	3106.00	
	H	0.76153800	-0.82439800	-1.71735400	346.86	983.55	1301.14	1502.52	3111.45	
	H	-0.03843100	-1.91422600	-0.58937000	395.50	996.77	1312.86	1508.93	3114.23	
	H	1.82316400	-1.72748800	1.00548200	409.38	1010.61	1336.41	1519.70	3121.13	
	H	2.40149900	-2.28963300	-0.55780200	443.17	1023.32	1348.87	1697.04	3143.45	
	H	1.12565400	1.66067100	-1.03882500	445.34	1065.21	1369.57	3010.55	3192.57	
	H	0.57727300	2.19898500	0.54502200	449.78	1075.47	1375.51	3017.83	66.51	
	H	3.02523200	1.82686200	0.54762200	530.63	1095.39	1379.31	3020.66	94.20	
	H	2.21036600	0.75033900	1.67401400	543.31	1107.93	1380.62	3024.68	221.16	
	H	3.17126400	0.00095800	-1.12780900						
H	3.90364300	-0.51638200	0.38672600							

	H	-0.17212700	-0.08793600	1.09083100	604.33	1122.87	1388.84	3033.62	175.81
	C	-1.36002400	0.54092600	-0.59078700	793.48	1133.69	1389.30	3037.30	
	H	-1.17760400	0.76637800	-1.65033300	797.96	1160.52	1411.71	3039.44	
	C	-1.96724300	1.79338900	0.05438700	816.52	1173.13	1416.72	3044.83	
	H	-1.41532000	2.69433000	-0.21568100					
	H	-3.00195900	1.93236400	-0.26929700					
	H	-1.96351900	1.72074900	1.14622200					
	C	-2.37185800	-0.61962100	-0.55759900					
	H	-3.30071600	-0.26805300	-1.02784000					
	H	-2.02762700	-1.44691600	-1.18474400					
	C	-2.70400300	-1.13715800	0.82076900					
	H	-2.82660400	-0.39097600	1.60451900					
	H	-3.47480600	-1.90494500	0.85601600					
	H	-1.62691500	-1.86090200	1.29706500					
	H	-0.91786200	-2.34542300	1.59998100					
	Rotational constants (GHZ):								
		2.10737	0.82058	0.67161					
	C	1.94909100	-1.45349400	0.11263400					
	C	0.57838200	-1.11052500	-0.47416300					
	C	0.00719800	0.19723000	0.09199200					
	C	1.02742300	1.33136400	-0.09184500					
	C	2.40033100	0.98313800	0.48854000					
	C	2.94574900	-0.31577200	-0.10198600					
	H	0.66419200	-1.00932800	-1.56490900	1313.29 <i>i</i>	839.93	1209.22	1480.05	3056.18
	H	-0.11049800	-1.93965900	-0.29895800	135.92	865.34	1222.73	1486.19	3093.72
	H	1.84314600	-1.63857400	1.18904500	200.92	900.36	1255.06	1488.11	3095.65
	H	2.32200500	-2.38028400	-0.33152400	237.85	909.35	1263.57	1492.13	3098.79
	H	1.12879100	1.53996100	-1.16613800	266.12	938.97	1292.74	1494.23	3099.58
	H	0.66500700	2.24877000	0.37692700	278.47	946.21	1301.56	1497.82	3107.31
	H	3.09705200	1.80753200	0.31357900	332.09	987.66	1310.72	1501.26	3109.40
	H	2.31000200	0.87095500	1.57613000	343.14	1003.46	1327.92	1508.96	3113.89
	H	3.11411400	-0.18160700	-1.17757700	371.26	1029.30	1342.88	1517.31	3125.51
TS ₅ β	H	3.91300100	-0.56255600	0.34405900	418.81	1043.79	1356.96	1573.68	3140.80
(S)	H	-0.14404700	0.06561800	1.17427500	436.74	1064.92	1369.66	3004.51	3144.79
	C	-1.35418900	0.54698600	-0.54102500	442.56	1075.57	1381.68	3019.23	68.61
	H	-1.18872500	0.67799900	-1.61986200	496.55	1092.36	1382.62	3024.55	92.44
	C	-1.92263600	1.86885800	0.00585400	530.50	1101.90	1388.87	3032.41	181.89
	H	-1.31710700	2.72473500	-0.29487300	573.21	1123.75	1390.25	3037.48	227.26
	H	-2.93584700	2.03609700	-0.36616000	794.89	1140.21	1407.77	3039.62	
	H	-1.96274900	1.85130900	1.09938800	798.38	1148.80	1410.94	3040.72	
	C	-2.40502400	-0.54266700	-0.37593900	826.21	1190.37	1415.54	3045.56	
	H	-3.35535800	-0.24819300	-0.82690900					
	H	-2.10051900	-1.54076200	-1.21447600					
	C	-2.58043900	-1.17990200	0.98247000					
	H	-3.37796000	-1.92465700	0.96138800					
	H	-1.66725800	-1.67261500	1.32364400					
	H	-2.84893500	-0.42939700	1.73530200					
	H	-1.92361700	-2.24663600	-1.81153900					
	Rotational constants (GHZ):								

	2.06620	0.82929	0.66883							
TS ₅ β (P)	C	2.01773300	-1.43286500	0.14400100						
	C	0.64728300	-1.16799300	-0.48371400						
	C	0.00758300	0.12710200	0.03375600						
	C	0.97783600	1.30354700	-0.14245900						
	C	2.34632900	1.02995500	0.48495900						
	C	2.96539100	-0.25316600	-0.06739200						
	H	0.75502400	-1.09496800	-1.57515900						
	H	-0.00899100	-2.01990700	-0.28793500	1373.87i	835.49	1181.65	1464.94	3062.58	
	H	1.89115500	-1.60123000	1.22061400	123.25	866.75	1204.11	1482.52	3093.13	
	H	2.44632100	-2.34935000	-0.27063900	236.73	902.65	1219.96	1486.45	3093.93	
	H	1.10294400	1.49893900	-1.21692500	254.74	911.27	1238.98	1489.84	3095.41	
	H	0.55511900	2.20888500	0.29999200	259.68	941.04	1288.85	1494.05	3098.74	
	H	3.01107500	1.88131300	0.31527800	319.08	943.80	1293.78	1503.08	3102.04	
	H	2.22747600	0.93205100	1.57097700	340.45	974.21	1305.21	1506.85	3105.67	
	H	3.15560600	-0.13019700	-1.14080300	349.54	997.38	1313.61	1509.77	3113.39	
	H	3.93086700	-0.44811700	0.40715200	425.19	1012.39	1327.46	1517.76	3131.51	
	H	-0.17326300	0.01100800	1.11159400	438.94	1042.11	1345.03	1667.29	3135.00	
	C	-1.34981100	0.40860900	-0.64999400	446.52	1065.45	1364.43	2974.91	3192.64	
	H	-1.13167200	0.54623400	-1.72206800	449.73	1076.38	1369.85	3017.92	83.66	
	C	-1.97936000	1.69644000	-0.15875800	533.13	1099.38	1376.22	3020.65	156.41	
	H	-1.48464000	2.62001400	-0.45141500	557.50	1101.82	1384.87	3034.57	210.85	
	H	-3.06277400	1.75960000	-0.25569900	601.38	1128.29	1389.42	3038.10	69.05	
	H	-1.80914500	1.74442300	1.20550100	788.42	1143.39	1390.78	3041.04		
	C	-2.34652800	-0.75870500	-0.54339600	797.47	1149.88	1407.10	3046.00		
	H	-3.27156300	-0.45642300	-1.04489200	801.94	1176.50	1421.61	3060.63		
	H	-1.96925500	-1.61724100	-1.10460900						
	C	-2.66408400	-1.18090800	0.89081500						
	H	-3.43926600	-1.94950600	0.90509400						
	H	-1.78372900	-1.59006700	1.39242900						
	H	-3.02018500	-0.33618100	1.48599100						
	H	-1.65534000	1.75861700	2.10861600						
		Rotational constants (GHZ):								
		2.11871	0.81692	0.67108						

TS ₅ α	C	-1.99642200	-1.45662800	-0.04839000					
	C	-0.60362100	-1.12702200	0.49254700					
	C	-0.01015200	0.13608000	-0.14870400					
	C	-0.99479400	1.30975500	-0.02010900					
	C	-2.38444900	0.96636800	-0.55986300					
	C	-2.95373200	-0.27799500	0.11927800					
	H	-0.65940400	-0.97162800	1.57849600	1261.88 <i>i</i>	833.63	1213.17	1482.27	3065.06
	H	0.05734900	-1.98179800	0.32814600	118.08	867.63	1233.64	1487.91	3094.56
	H	-1.91789800	-1.70464600	-1.11435700	230.89	901.75	1262.67	1488.82	3095.30
	H	-2.38848800	-2.34490700	0.45415200	242.10	910.86	1276.79	1492.15	3096.17
	H	-1.07195600	1.58391100	1.04059900	264.25	942.29	1294.91	1494.62	3099.65
	H	-0.60863400	2.18447600	-0.54831800	288.76	948.78	1303.01	1497.54	3104.67
	H	-2.31599100	0.78498900	-1.63974500	300.18	997.09	1310.66	1505.91	3106.78
	H	-3.09339500	-0.07483100	1.18800800	339.59	1002.07	1335.30	1509.04	3113.86
	H	-3.93724900	-0.52230500	-0.29099400	350.05	1020.48	1345.07	1510.60	3131.01
	H	0.12044600	-0.06308200	-1.22700300	404.07	1050.06	1350.08	1521.02	3133.58
	C	1.36534100	0.48344300	0.41898200	439.22	1065.40	1368.88	2964.11	3139.65
	H	1.10946600	0.74901200	1.65980700	445.38	1075.28	1375.99	3030.79	75.51
	C	1.96926100	1.76615500	-0.12348200	457.15	1093.78	1388.47	3034.37	78.88
	H	1.40809800	2.64659300	0.19461300	539.96	1101.42	1391.20	3038.35	178.04
	H	2.99899800	1.88572400	0.22026400	562.31	1130.18	1401.93	3038.77	211.20
	H	1.97812300	1.76080400	-1.22030900	785.69	1148.16	1402.40	3040.66	
	C	2.36139900	-0.66336600	0.50842600	790.84	1161.67	1410.17	3046.39	
	H	3.27124000	-0.29091700	0.98908000	798.78	1183.92	1429.02	3058.37	
	H	1.97280800	-1.44956300	1.16090100					
	C	2.71650800	-1.25740100	-0.85922200					
	H	3.47590400	-2.03538100	-0.75930800					
	H	1.84095300	-1.70448200	-1.33656700					
	H	3.10969900	-0.49080700	-1.53158900					
	H	0.88941000	0.94362400	2.60212300					
Rotational constants (GHZ):									
		2.11530	0.81391	0.66688					
TS ₅ α'	C	1.95552900	-1.44654500	0.10150500	1258.20 <i>i</i>	834.85	1204.57	1477.83	3064.96
	C	0.58868400	-1.14242500	-0.51683500	133.60	864.39	1212.90	1489.09	3092.77
	C	0.00946100	0.18369400	-0.05433000	190.23	884.38	1258.25	1491.31	3098.19
	C	1.00358800	1.33270000	-0.13174600	236.47	919.18	1263.20	1495.30	3099.25
	C	2.36650500	0.99197800	0.47583300	274.91	940.49	1286.79	1497.80	3102.53
	C	2.93515300	-0.29555100	-0.11628700	300.56	953.03	1302.91	1501.79	3103.92
	H	0.68563000	-1.10813200	-1.61444500	322.31	988.79	1307.12	1506.41	3106.39
	H	-0.10182400	-1.95939400	-0.29435800	351.24	1002.46	1336.85	1510.64	3127.50
	H	1.82946100	-1.60873100	1.17857500	387.88	1021.27	1354.65	1514.87	3134.48
	H	2.34974500	-2.37623600	-0.31690500	395.23	1048.04	1359.07	1522.42	3136.98
	H	1.13402800	1.60012500	-1.19265800	437.18	1067.88	1369.54	2976.18	3144.43
	H	0.59565100	2.21601200	0.36517300	449.15	1083.94	1378.02	2987.35	73.93
	H	3.05580600	1.82660400	0.32375500	452.07	1101.65	1384.86	2994.38	85.31
	H	2.25088300	0.86593200	1.55871700	535.45	1110.69	1389.54	3035.97	226.19
	H	3.10630300	-0.15988800	-1.19161100					
H	3.90344700	-0.52809600	0.33458100						

	H	-0.14304300	0.04109100	1.25452300	590.86	1128.62	1401.95	3047.57	262.03
	C	-1.37874700	0.52233600	-0.59623700	769.38	1147.72	1415.01	3050.55	
	H	-1.23086000	0.78633600	-1.65650300	791.64	1162.01	1421.83	3059.12	
	C	-1.98568500	1.74762600	0.10236000	794.39	1176.91	1470.18	3062.70	
	H	-1.46278400	2.66755300	-0.16144500					
	H	-3.03208700	1.87059400	-0.18724600					
	H	-1.94595500	1.64050600	1.18979900					
	C	-2.36566200	-0.65848200	-0.58054900					
	H	-3.29749600	-0.31395900	-1.04027600					
	H	-1.99355700	-1.45896600	-1.22583600					
	C	-2.66996600	-1.21836900	0.80911100					
	H	-3.42855600	-2.00151700	0.74979600					
	H	-1.78130300	-1.64822100	1.27649800					
	H	-3.04646200	-0.44155200	1.47881600					
	H	-0.20018400	-0.01183100	2.21409900					
	Rotational constants (GHZ):								
		2.13018	0.82482	0.67450					
	C	-1.98386000	-1.43148200	-0.14157700					
	C	-0.58314700	-1.12268300	0.33792700					
	C	0.03077000	0.18160200	-0.13626900					
	C	-0.97080100	1.33518700	0.03849200					
	C	-2.34521800	1.01609000	-0.55202000					
	C	-2.93028500	-0.24980600	0.07049200					
	H	-0.70344400	-0.96114900	1.66797500	1239.82 <i>i</i>	833.90	1205.68	1476.28	3062.39
	H	0.08624800	-1.98140000	0.28706600	118.53	871.87	1210.34	1486.42	3087.92
	H	-1.94418100	-1.67064900	-1.21495700	187.47	896.43	1218.06	1492.74	3092.64
	H	-2.35987100	-2.32656100	0.36206400	195.22	909.63	1254.73	1499.56	3096.35
	H	-1.07778700	1.54223600	1.11182600	256.36	935.01	1282.82	1500.69	3102.82
	H	-0.57723100	2.24219900	-0.42476100	288.14	944.60	1293.97	1504.83	3111.04
	H	-3.01978800	1.86298200	-0.40062200	302.43	989.54	1304.35	1510.33	3121.71
	H	-2.25042000	0.87576400	-1.63618100	336.42	1001.01	1328.92	1513.94	3128.82
	H	-3.07059500	-0.09114500	1.14604700	352.42	1019.20	1348.23	1522.62	3132.60
	H	-3.91283500	-0.47202200	-0.35343000	400.98	1042.80	1355.15	1556.25	3134.38
	C	1.37650700	0.48729700	0.55656700	447.53	1067.37	1369.67	2962.18	3143.92
	H	1.15252200	0.66701800	1.61637600	457.69	1075.20	1372.52	3004.55	65.39
	C	2.01805200	1.75993000	-0.01015900	491.96	1098.42	1381.16	3030.58	84.98
	H	1.45477700	2.65429300	0.25885000	547.20	1100.02	1385.07	3034.50	259.24
	H	3.03270100	1.88350400	0.37641500	592.54	1130.10	1389.39	3040.44	228.03
	H	2.07776000	1.72152100	-1.10216400	784.62	1144.05	1406.75	3050.14	
	C	2.37011900	-0.68692700	0.50706400	792.42	1163.79	1415.60	3055.36	
	H	3.29474400	-0.36200900	0.99474000	812.37	1188.09	1419.61	3061.02	
	H	1.99329400	-1.51621100	1.11189300					
	C	2.69581500	-1.18653400	-0.90098000					
	H	3.45697900	-1.96846500	-0.86742300					
	H	1.81473700	-1.60575000	-1.39352600					
	H	3.07865200	-0.38106600	-1.53239600					
	H	-0.81785500	-0.80844800	2.59381000					
	Rotational constants (GHZ):								
TS ₅ β'									

	2.12169	0.81749	0.67163						
TS ₅ γ'	C	1.96727800	-1.37083300	-0.11703700					
	C	0.57242200	-1.06713000	-0.61448900					
	C	-0.03297400	0.18463500	0.03949600					
	C	0.95340700	1.35596600	-0.07004400					
	C	2.31815100	1.01913400	0.53346900					
	C	2.93443500	-0.21157000	-0.13262300					
	H	0.60247700	-0.91256600	-1.70545300					
	H	-0.06533900	-1.93823200	-0.44235900	1230.36i	833.07	1201.60	1471.41	3061.72
	H	1.78675600	-1.65603900	1.17545500	125.71	864.76	1220.19	1477.36	3089.49
	H	2.37757600	-2.31106000	-0.48757800	185.96	899.64	1230.66	1490.43	3090.76
	H	1.07434500	1.61943700	-1.13038800	205.10	909.08	1255.91	1498.84	3100.73
	H	0.54855900	2.23730700	0.43175500	250.44	934.57	1275.96	1499.56	3101.89
	H	2.99265000	1.87447600	0.44332200	272.42	945.06	1301.56	1502.74	3109.95
	H	2.19513100	0.82004700	1.60435900	297.07	988.05	1306.12	1511.10	3121.36
	H	3.18237000	0.02929100	-1.17725500	348.89	1001.54	1329.96	1515.33	3121.54
	H	3.87220600	-0.48997600	0.35602800	359.63	1017.05	1347.32	1523.23	3129.45
	H	-0.16690500	-0.02902800	1.10994700	399.04	1041.50	1360.11	1548.99	3134.24
	C	-1.41098500	0.53321700	-0.55663800	442.27	1068.90	1372.05	2988.73	3143.29
	H	-1.24613500	0.80364100	-1.60906000	451.90	1076.90	1373.07	3005.08	68.89
	C	-2.03975800	1.74451800	0.14406300	468.95	1102.59	1382.62	3012.59	83.02
	H	-1.51187300	2.67008800	-0.08877900	559.20	1108.59	1383.56	3019.38	258.74
	H	-3.07910700	1.87311100	-0.16859800	595.39	1129.76	1392.35	3033.07	224.10
	H	-2.02976900	1.62159100	1.23119700	785.49	1146.86	1410.78	3051.39	
	C	-2.38749900	-0.65737600	-0.55248200	795.06	1159.71	1416.34	3055.45	
	H	-3.33661800	-0.31457300	-0.97706700	815.56	1185.80	1420.13	3061.04	
	H	-2.02402800	-1.43669800	-1.22789100					
	C	-2.64547200	-1.26115500	0.82869200					
	H	-3.39159400	-2.05598000	0.76918400					
	H	-1.73721300	-1.69289900	1.25722300					
	H	-3.01905800	-0.51057400	1.52936300					
	H	1.60153400	-1.81780800	2.09215100					
		Rotational constants (GHZ):							
		2.11151	0.82022	0.67165					

TS ₅ δ'	C	-1.91669600	-1.46106600	-0.14646200					
	C	-0.56642500	-1.11712400	0.48923500					
	C	0.04932000	0.16301800	-0.09216000					
	C	-0.95155800	1.32001500	0.04343100					
	C	-2.30540800	1.00559200	-0.59915700					
	C	-2.87581500	-0.29673600	-0.09189200					
	H	-0.70049200	-0.98020900	1.57061200	1253.98 <i>i</i>	832.95	1206.41	1472.03	3062.21
	H	0.11122100	-1.96369000	0.35767600	119.19	866.92	1218.89	1481.81	3088.41
	H	-1.75605800	-1.73581800	-1.19998800	187.95	895.44	1230.71	1485.09	3089.55
	H	-2.35189000	-2.33826500	0.34044300	211.68	920.09	1238.05	1498.03	3093.13
	H	-1.10012900	1.52887500	1.11121100	224.18	939.64	1287.73	1499.31	3110.67
	H	-0.54847000	2.22886800	-0.40753800	280.62	946.14	1303.49	1502.02	3113.32
	H	-3.00772800	1.82512900	-0.42293700	288.81	986.25	1308.19	1510.22	3121.15
	H	-2.17651300	0.93285200	-1.68952200	335.78	1000.52	1322.46	1515.86	3123.49
	H	-3.08698700	-0.09046600	1.21474600	359.14	1015.69	1347.83	1522.68	3129.54
	H	-3.88460100	-0.52013300	-0.44102100	403.01	1040.58	1359.74	1556.50	3133.78
	C	1.40059900	0.50821900	0.56704400	443.42	1063.53	1373.04	3001.49	3143.99
	H	1.19156400	0.73692700	1.62118800	452.77	1084.84	1378.15	3002.66	66.90
	C	2.03515900	1.75441600	-0.06462300	468.25	1096.31	1381.30	3005.62	81.28
	H	1.48526000	2.66306100	0.18311700	564.66	1105.04	1386.88	3024.54	252.49
	H	3.06047000	1.88634300	0.29005900	593.87	1129.49	1388.29	3035.36	260.62
	H	2.06618800	1.67276500	-1.15535900	786.21	1143.42	1410.99	3041.74	
	C	2.39844800	-0.66431200	0.55864400	789.95	1162.19	1415.59	3055.22	
	H	3.32548800	-0.31860300	1.02725100	805.27	1186.36	1419.29	3061.23	
	H	2.02694600	-1.47181000	1.19504300					
	C	2.71628500	-1.21715800	-0.83109200					
	H	3.47930700	-1.99584200	-0.77240700					
	H	1.83270200	-1.65662900	-1.30092100					
	H	3.09300800	-0.43598900	-1.49579200					
	H	-3.18805700	0.06304700	2.14292600					
	Rotational constants (GHZ):								
	2.12570	0.81330	0.66746						
	Cartesian coordinates and rotational constants				Visual				
<i>i</i> BCH	C	-2.08247800	1.41283300	-0.18783400	132.41	922.00	1292.09	1493.47	3092.87
	C	-0.68484500	0.94396600	-0.60057800	174.81	935.01	1305.02	1494.73	3093.94
	C	-0.22263100	-0.26831200	0.21592600	233.81	942.06	1312.58	1498.23	3095.27
	C	-1.26268900	-1.39151900	0.12360800	294.01	963.92	1334.91	1508.05	3099.26
	C	-2.65641500	-0.92533200	0.54727900	312.87	979.17	1353.63	1509.78	3113.48
	C	-3.10396900	0.27862600	-0.28330900	338.61	1001.86	1366.95	1516.27	3119.23
	H	-0.69054600	0.66743700	-1.66427100	405.10	1054.30	1372.13	3016.10	3127.84
	H	0.02594400	1.76861000	-0.49376400	430.21	1061.14	1381.78	3017.25	3130.35
	H	-2.04574300	1.77466900	0.84725200	444.97	1079.50	1386.28	3024.03	238.97
	H	-2.39313800	2.25901100	-0.80675600	457.44	1100.35	1388.47	3032.37	264.48
	H	-1.30282800	-1.74667400	-0.91505700	481.92	1119.31	1400.25	3036.34	71.85
	H	-0.94172100	-2.24132000	0.73459100	577.87	1132.62	1404.86	3040.49	81.56
	H	-3.37480900	-1.74397900	0.45086300	791.89	1154.25	1411.77	3043.22	
	H	-2.63605200	-0.64366800	1.60718900					
H	-3.20486800	-0.02692500	-1.33207300						

	H	-4.08852200	0.62424500	0.04331000	798.80	1187.41	1421.88	3044.93	
	H	-0.16395200	0.03762900	1.26996200	829.54	1202.08	1477.33	3045.50	
	C	1.15142100	-0.78238300	-0.22318900	850.35	1222.70	1481.85	3049.80	
	H	1.43102700	-1.62559900	0.42320800	865.25	1248.05	1488.66	3064.20	
	H	1.06074500	-1.19119600	-1.23832000	908.44	1289.23	1489.22	3083.93	
	C	2.29888300	0.23522800	-0.20689600					
	H	2.08563100	1.01158000	-0.95069900					
	C	2.44841600	0.90519100	1.15934100					
	H	2.58554200	0.14941800	1.94023400					
	H	3.31915300	1.56532200	1.17607200					
	H	1.57188200	1.50215300	1.42121700					
	C	3.60512000	-0.45039100	-0.60937500					
	H	3.51351000	-0.93779600	-1.58334600					
	H	4.42848500	0.26595200	-0.66408900					
	H	3.87537900	-1.21631000	0.12463800					
	Rotational constants (GHZ):								
		2.75978	0.65169	0.59779					
TS _{6,7}	C	2.16463300	-1.39602800	-0.11065500					
	C	0.76317700	-0.97922100	-0.56454400					
	C	0.26180900	0.25817900	0.18890100					
	C	1.27734700	1.40014600	0.05797600					
	C	2.67458900	0.98633600	0.52247900					
	C	3.16182700	-0.24410700	-0.24450600					
	H	0.77878200	-0.75162000	-1.63969200	1389.64 <i>i</i>	851.49	1190.67	1459.65	3053.62
	H	0.07071700	-1.81556100	-0.42969900	128.60	865.41	1191.89	1479.08	3068.33
	H	2.11999500	-1.71002900	0.93959900	175.85	908.68	1219.19	1483.11	3085.81
	H	2.50331500	-2.26266700	-0.68485800	236.57	920.22	1248.31	1488.73	3089.85
	H	1.32508000	1.70685700	-0.99568600	269.29	932.70	1283.24	1489.26	3094.82
	H	0.92808000	2.26971600	0.62370900	298.52	942.55	1292.89	1494.85	3095.87
	H	3.37538800	1.81625800	0.39778200	324.94	957.67	1300.81	1502.48	3099.93
	H	2.64471200	0.75400600	1.59403200	338.00	978.00	1305.47	1508.18	3103.66
	H	3.27224300	0.01463600	-1.30482700	410.29	999.26	1331.28	1509.16	3123.37
	H	4.14854900	-0.55156500	0.11218200	444.27	1047.00	1342.65	1666.59	3135.89
	H	0.19503100	0.00035500	1.25515900	448.42	1060.02	1360.72	2999.23	3188.46
	C	-1.11619000	0.72185500	-0.29040400	467.13	1080.00	1368.59	3016.96	67.57
	H	-1.42491000	1.58652200	0.31119900	492.04	1101.34	1381.96	3023.60	81.37
	H	-1.02351800	1.08067600	-1.32394600	561.54	1111.41	1386.28	3024.23	163.40
	C	-2.23880200	-0.32416000	-0.23583900	586.37	1124.04	1389.05	3034.09	258.30
	H	-1.99080400	-1.13263700	-0.93964900	792.96	1141.70	1399.48	3037.10	
	C	-2.39438300	-0.93854200	1.15720100	799.49	1164.72	1410.45	3040.77	
	H	-2.55569900	-0.15300000	1.90190200	829.99	1167.02	1413.40	3045.59	
	H	-3.25154700	-1.61531600	1.19005500					
	H	-1.50815800	-1.50577400	1.44875700					
	C	-3.53941000	0.28575900	-0.70005000					
	H	-4.41811900	-0.35512900	-0.63815900					
	H	-3.82606800	1.25687500	0.23418900					
	H	-3.49506300	0.86216500	-1.62356500					
	H	-3.95559200	1.88392100	0.88815300					
		Rotational constants (GHZ):							

	2.68134	0.63891	0.58471						
TS ₆ β	C	-2.08521400	1.42025600	-0.10085300					
	C	-0.69411300	0.95541000	-0.53876900					
	C	-0.25295000	-0.30690700	0.21113000					
	C	-1.30699500	-1.40936300	0.04892100					
	C	-2.69596700	-0.94833300	0.49338300					
	C	-3.12325000	0.30932200	-0.26532800					
	H	-0.70135600	0.73715800	-1.61566700	1292.54	845.58	1212.10	1467.41	3045.38
	H	0.02966500	1.76211400	-0.39500100	131.92	864.86	1225.79	1478.26	3050.58
	H	-2.04634700	1.72051800	0.95380400	178.79	910.04	1265.83	1486.38	3083.67
	H	-2.38032800	2.30581900	-0.66996000	238.26	923.38	1286.41	1486.88	3094.88
	H	-1.00229000	-2.29783300	0.61135500	258.41	942.64	1293.21	1487.92	3095.61
	H	-3.42471800	-1.74996600	0.34585300	292.29	947.27	1301.11	1489.60	3099.24
	H	-2.67647000	-0.73072800	1.56833100	309.77	970.44	1311.35	1494.45	3102.17
	H	-3.22571700	0.06826900	-1.33053000	338.03	991.30	1322.70	1500.78	3105.60
	H	-4.10357200	0.64893000	0.07969300	369.44	1006.78	1343.54	1508.92	3107.23
	H	-0.19439500	-0.06437600	1.28166800	398.40	1050.63	1368.63	1516.69	3133.50
	C	1.11424000	-0.81699600	-0.25116600	418.93	1059.32	1381.53	2995.16	3137.85
	H	1.35110100	-1.73475600	0.30986500	446.52	1078.15	1385.29	3016.29	76.17
	H	1.04140600	-1.12029800	-1.30423100	454.75	1102.06	1388.45	3025.83	87.59
	C	2.29415400	0.12802500	-0.10132500	487.77	1119.06	1394.62	3030.54	202.41
	H	2.12957700	1.04866200	-1.00315900	579.19	1126.06	1400.74	3032.33	222.46
	C	2.38107500	0.87506900	1.21154600	792.51	1147.83	1412.49	3036.86	
	H	2.48846000	0.16612600	2.04275200	799.65	1165.31	1415.01	3037.41	
	H	3.25023300	1.53657500	1.22373000	814.67	1182.19	1445.59	3040.02	
	H	1.49167100	1.47841100	1.40396600					
	C	3.60427100	-0.50313400	-0.52407000					
	H	3.51935500	-0.96593200	-1.51030300					
	H	4.40677600	0.23731200	-0.56017200					
	H	3.89746500	-1.28277100	0.18934800					
	H	2.08430700	1.71928000	-1.71329100					
		Rotational constants (GHZ):							
		2.66157	0.64712	0.59041					

TS ₆ α	C	-2.64295500	0.98297300	0.49385800					
	C	-1.24842600	1.38452000	0.01120300					
	C	-0.23938500	0.23993000	0.16289600					
	C	-0.74795000	-1.01422400	-0.56984000					
	C	-2.14496700	-1.41680200	-0.09072800					
	C	-3.13929200	-0.26398700	-0.24053000					
	H	-1.30017700	1.66607000	-1.04907300	1280.27 <i>i</i>	860.59	1201.16	1482.51	3054.66
	H	-0.89005900	2.26300800	0.55648800	124.13	864.56	1213.01	1486.74	3083.14
	H	-2.60597900	0.77653100	1.57036200	167.00	907.68	1222.02	1489.64	3090.37
	H	-3.34283000	1.81118800	0.35453600	241.02	921.49	1255.53	1492.41	3092.52
	H	-0.77571200	-0.80255900	-1.64714700	242.64	933.54	1291.16	1494.47	3095.53
	H	-0.04902900	-1.84380200	-0.42742700	290.96	941.42	1297.81	1497.07	3097.03
	H	-2.49187500	-2.29431300	-0.64318100	311.80	962.71	1304.13	1507.85	3101.23
	H	-2.08945900	-1.70807300	0.96538700	332.37	979.96	1329.00	1509.54	3122.92
	H	-3.25930300	-0.02944300	-1.30538600	363.48	1007.06	1336.41	1515.52	3126.30
	H	-4.12332900	-0.56047200	0.13229900	406.88	1055.97	1346.04	1545.90	3132.19
	C	1.12891300	0.66125300	-0.32485100	439.55	1066.30	1364.54	2996.73	3134.38
	H	1.09358000	1.19146500	-1.28200800	446.33	1081.23	1374.75	3016.17	75.67
	C	2.29113300	-0.30897600	-0.23329600	482.36	1099.15	1382.41	3028.25	83.03
	H	2.10922600	-1.11793800	-0.95680600	518.09	1116.52	1385.54	3035.03	233.40
	C	3.59541800	0.38594400	-0.63003300	579.53	1137.73	1388.66	3038.38	274.62
	H	3.83037100	1.18471600	0.07947200	797.86	1142.59	1403.20	3042.34	
	H	4.42923700	-0.31962800	-0.63411300	802.70	1169.18	1411.83	3046.90	
	H	3.52008900	0.83007100	-1.62558800	831.13	1189.19	1423.87	3052.08	
	C	2.41255000	-0.93287700	1.15861000					
	H	1.53473900	-1.52861300	1.41849200					
	H	3.28750100	-1.58463300	1.21196500					
H	2.52675800	-0.15001000	1.91496600						
H	1.70374100	2.27119900	1.19018300						
Rotational constants (GHZ):									
	2.65690	0.64737	0.58955						
TS ₆ α'	C	-2.06037600	1.41222700	-0.22834200	1244.01 <i>i</i>	851.13	1206.18	1470.96	3051.72
	C	-0.66521400	0.93599700	-0.64318600	134.06	864.56	1218.89	1480.44	3056.85
	C	-0.23141200	-0.30568200	0.11231700	171.14	907.19	1254.11	1481.37	3078.32
	C	-1.27653300	-1.40812800	0.11258400	224.23	916.06	1258.00	1489.08	3097.07
	C	-2.66316700	-0.90810800	0.52266500	263.39	935.38	1280.93	1490.59	3099.14
	C	-3.08902000	0.28611900	-0.33180100	296.17	941.39	1300.32	1493.92	3100.58
	H	-0.66570600	0.69768600	-1.71945900	311.21	963.58	1314.22	1497.59	3104.17
	H	0.06028600	1.74236600	-0.50653800	331.66	980.32	1330.34	1506.67	3115.91
	H	-2.02017500	1.76541100	0.80880800	388.23	1001.57	1358.84	1509.58	3120.86
	H	-2.35920800	2.26440400	-0.84412400	405.38	1051.93	1368.43	1514.65	3129.04
	H	-1.32939800	-1.83050600	-0.90287500	423.63	1072.65	1369.51	2988.06	3135.70
	H	-0.95013900	-2.21957700	0.77143700	447.74	1086.93	1383.27	2996.34	76.00
	H	-3.39116200	-1.71933700	0.44139500	454.01	1100.59	1387.14	3002.42	96.29
	H	-2.63653200	-0.60492100	1.57566000	486.74	1123.42	1396.17	3035.85	234.53
	H	-3.17827000	-0.02931500	-1.37898100					
	H	-4.07453600	0.64335900	-0.02181100					

	H	-0.21854300	0.05067100	1.37722200	591.25	1138.33	1402.97	3036.68	275.40
	C	1.16490700	-0.82109600	-0.18197100	777.39	1151.44	1407.54	3047.65	
	H	1.42367600	-1.57576300	0.57354800	792.83	1159.47	1424.94	3048.86	
	H	1.12679800	-1.35821500	-1.14234000	830.78	1201.01	1465.17	3049.96	
	C	2.29601700	0.21191700	-0.24814500					
	H	2.07480800	0.91696800	-1.05792200					
	C	2.43304200	0.99615200	1.05720600					
	H	2.59315900	0.31138800	1.89657000					
	H	3.28628300	1.67747000	1.01049900					
	H	1.54202000	1.58551700	1.28294000					
	C	3.61236200	-0.48957000	-0.58635300					
	H	3.53786200	-1.04745700	-1.52319300					
	H	4.42835400	0.23035600	-0.68370600					
	H	3.88196700	-1.19598000	0.20517500					
	H	-0.25517600	0.23650400	2.32785500					
	Rotational constants (GHZ):								
		2.65931	0.65126	0.59601					
	C	-2.06334100	1.42935200	-0.27555400					
	C	-0.66310400	0.92850600	-0.63697200					
	C	-0.19987900	-0.19789400	0.29634000					
	C	-1.24956800	-1.28883500	0.36779400					
	C	-2.66467400	-0.83692400	0.64663300					
	C	-3.08325400	0.29057000	-0.30098500					
	H	-0.66420900	0.54878800	-1.66744700	1288.44 <i>i</i>	852.41	1204.47	1476.08	3052.10
	H	0.04811900	1.75839500	-0.60430400	131.85	869.53	1211.83	1480.94	3070.66
	H	-2.03954700	1.87110200	0.72872800	167.75	906.27	1222.60	1487.71	3090.14
	H	-2.36546500	2.22386400	-0.96295100	211.66	919.24	1251.15	1490.89	3097.63
	H	-1.30075500	-1.78125700	-0.88381300	287.92	934.48	1272.55	1493.72	3099.14
	H	-0.93310100	-2.16884200	0.93163300	293.88	939.14	1293.01	1498.89	3104.56
	H	-3.35336800	-1.68279800	0.56888500	314.41	964.82	1310.46	1503.24	3110.02
	H	-2.72537700	-0.47633200	1.68430600	321.83	980.20	1331.81	1509.29	3114.36
	H	-3.15135000	-0.10769900	-1.31991300	341.13	999.95	1343.03	1516.79	3120.28
	H	-4.07680900	0.65850700	-0.03274500	408.24	1054.40	1359.75	1557.48	3127.94
	H	-0.11141200	0.22556100	1.31093000	433.26	1064.61	1366.55	2973.89	3129.73
	C	1.15726500	-0.78467500	-0.10737000	457.08	1077.29	1373.84	3006.55	70.69
	H	1.43765400	-1.55209400	0.62684900	482.65	1097.48	1381.70	3022.66	82.65
	H	1.03684300	-1.30370900	-1.06660800	517.43	1116.25	1388.99	3032.52	235.30
	C	2.31583300	0.21245000	-0.22793500	593.57	1128.93	1399.56	3039.52	257.72
	H	2.09200400	0.90754200	-1.04532600	791.79	1154.04	1404.00	3044.18	
	C	2.51063600	1.02189100	1.05466200	806.66	1166.55	1409.36	3046.44	
	H	2.66012900	0.35179400	1.90813600	830.84	1202.31	1422.47	3051.58	
	H	3.38978600	1.66632700	0.97793300					
	H	1.65009200	1.65805800	1.27453100					
	C	3.60206300	-0.53241700	-0.58759800					
	H	3.47834200	-1.11859000	-1.50158100					
	H	4.43231900	0.16166900	-0.73868600					
	H	3.88201100	-1.22012300	0.21683000					
	H	-1.35777300	-2.07230700	-1.77948200					
	Rotational constants (GHZ):								
TS ₆ β'									

	2.65289	0.64493	0.59235						
TS ₆ γ'	C	-2.04012400	1.42175400	-0.22702600					
	C	-0.65022900	0.94233600	-0.65141200					
	C	-0.19380400	-0.26908200	0.16843700					
	C	-1.22613700	-1.39959300	0.05775200					
	C	-2.62777400	-0.93925700	0.38499800					
	C	-3.07899600	0.30412400	-0.34635200					
	H	-0.66210300	0.66586100	-1.71527600	1289.59i	849.81	1201.84	1469.39	3050.44
	H	0.06643800	1.76177800	-0.54673400	130.73	864.20	1219.64	1476.31	3064.70
	H	-1.99771400	1.75691000	0.81590300	168.35	906.44	1230.25	1480.69	3079.64
	H	-2.34449200	2.28325800	-0.82677300	199.34	923.01	1249.58	1489.99	3090.46
	H	-1.21200100	-1.78694100	-0.97360800	254.25	931.40	1273.16	1493.31	3096.81
	H	-0.93797900	-2.23328700	0.70618100	285.42	936.56	1299.04	1497.92	3102.32
	H	-3.36825400	-1.73920900	0.42070800	300.45	966.10	1305.70	1499.80	3114.41
	H	-2.57408000	-0.57501200	1.67194100	312.73	979.55	1330.76	1509.34	3119.87
	H	-3.22165400	0.05697400	-1.40899500	355.89	999.05	1349.71	1516.04	3122.75
	H	-4.04976400	0.63721900	0.03095700	410.04	1053.63	1361.06	1549.39	3128.31
	C	1.18820700	-0.77906800	-0.24842500	427.08	1063.31	1367.23	2992.12	3130.68
	H	1.45506100	-1.62823900	0.39552500	454.06	1078.89	1372.79	3005.55	68.37
	H	1.11930300	-1.17772900	-1.26935500	460.66	1101.41	1380.62	3017.58	78.86
	C	2.33365300	0.23981100	-0.19764300	506.24	1120.52	1390.07	3020.07	236.81
	H	2.13724700	1.02115800	-0.94090300	613.23	1131.52	1401.12	3035.08	254.25
	C	2.45063500	0.89993900	1.17657200	790.25	1153.37	1404.84	3043.66	
	H	2.56823800	0.13879000	1.95531200	811.44	1158.65	1412.04	3046.05	
	H	3.32140600	1.55882000	1.21839200	829.74	1197.40	1422.56	3049.80	
	C	3.64940300	-0.44206300	-0.57498100					
	H	3.58055300	-0.92369400	-1.55370500					
	H	4.47250400	0.27585500	-0.60695900					
	H	3.90437100	-1.21176200	0.16048900					
	H	-2.49817600	-0.28367100	2.56942900					
	Rotational constants (GHZ):								
	2.65311	0.64137	0.59305						

	C	2.03196600	1.43323900	0.16452300					
	C	0.65348300	0.92736600	0.60108900					
	C	0.18304700	-0.25887000	-0.24729100					
	C	1.22579200	-1.38131700	-0.19263400					
	C	2.60822000	-0.91078100	-0.65070900					
	C	3.04923200	0.31728600	0.11161500					
	H	0.69871000	0.60982900	1.65135900	1307.47 <i>i</i>	852.94	1206.39	1471.80	3050.17
	H	-0.06678400	1.74822200	0.54755000	130.73	865.06	1217.99	1478.37	3065.76
	H	1.94716400	1.88017900	-0.83748300	160.08	913.39	1229.60	1481.93	3089.67
	H	2.37514200	2.22897200	0.83153200	220.94	920.63	1230.48	1484.94	3090.20
	H	1.29628600	-1.74295600	0.84120500	260.50	933.96	1281.44	1493.97	3091.45
	H	0.89448100	-2.22656000	-0.80354000	279.97	944.01	1298.30	1498.34	3100.06
	H	3.34330200	-1.71257100	-0.53828200	298.84	962.59	1309.11	1500.35	3113.94
	H	2.57039000	-0.66752600	-1.72299900	314.23	978.35	1328.38	1509.23	3119.47
	H	4.06838900	0.64265700	-0.10013800	351.46	998.44	1348.47	1516.91	3123.97
	H	0.11007600	0.07617200	-1.29182100	408.21	1052.44	1357.55	1552.39	3127.98
	C	-1.18365400	-0.78932900	0.19564500	430.73	1061.39	1370.60	3002.55	3129.76
	H	-1.47014000	-1.61284200	-0.47257400	452.47	1086.52	1375.45	3007.17	69.11
	H	-1.07716000	-1.22880900	1.19615200	460.79	1095.48	1383.77	3016.35	78.24
	C	-2.33347100	0.22522300	0.22623400	521.07	1120.23	1387.11	3019.16	236.30
	H	-2.11408800	0.97688600	0.99319900	609.88	1128.94	1401.64	3035.60	266.97
	C	-2.50056900	0.93970700	-1.11519200	788.95	1155.04	1405.36	3041.25	
	H	-2.64436400	0.21001500	-1.91933000	797.10	1159.06	1412.23	3043.98	
	H	-3.37349700	1.59688600	-1.09998300	833.74	1201.78	1422.27	3045.68	
	H	-1.62925800	1.54860500	-1.36729000					
	C	-3.63297100	-0.47753300	0.62082400					
	H	-3.52850400	-0.99669700	1.57686700					
	H	-4.45733100	0.23422500	0.70908200					
	H	-3.90991400	-1.21934900	-0.13510000					
	H	3.16351900	-0.09623700	1.38112300					
	H	3.19712700	-0.39904400	2.27584900					
	Rotational constants (GHZ):								
		2.65892	0.64096	0.59140					

TS₆δ'

Table S4. The optimized Cartesian coordinate, frequencies and rotational constants for products (alkyl cyclohexyl radicals).

	Cartesian coordinates and rotational constants			frequencies		
MP1	C	-1.13542700	1.26149700	0.21574600		
	C	0.34047100	1.26036600	-0.18647400	122.57	1100.68 1507.89
	C	1.06275600	0.00000000	0.31228900	161.21	1100.98 2938.99
	C	0.34047000	-1.26036800	-0.18646000	239.44	1138.82 3034.13
	C	-1.13542900	-1.26149400	0.21575800	317.91	1164.70 3037.00
	C	-1.84360500	0.00000000	-0.28352800	331.94	1230.74 3038.96
	H	0.42342400	1.29611900	-1.28019800	408.61	1247.32 3041.82
	H	0.84450300	2.15139300	0.20039800	421.27	1288.94 3046.73
	H	-1.21045600	1.30702300	1.30916600	450.31	1295.26 3087.85
	H	-1.63097700	2.15506200	-0.17303000	490.39	1316.65 3089.88
	H	0.42342300	-1.29613300	-1.28018300	559.65	1330.47 3096.56
	H	0.84449900	-2.15139200	0.20042400	794.51	1363.86 3097.29
	H	-1.63097900	-2.15506100	-0.17301100	796.34	1371.41 3101.54
	H	-1.21046000	-1.30701000	1.30917800	862.09	1385.72 3156.50
	H	-1.84464700	-0.00000500	-1.38041100	882.79	1386.26 3261.01
	H	-2.88943000	0.00000200	0.03510800	892.45	1396.87
	H	0.98794000	0.00001100	1.41534000	916.54	1463.89
	C	2.50126600	0.00000000	-0.07239100	977.74	1482.22
	H	3.05510400	0.92859100	-0.13606700	990.63	1486.85
	H	3.05503800	-0.92861100	-0.13635000	1054.31	1488.95
	Rotational constants (GHZ):			1076.82	1493.96	
	4.26114	2.29808	1.63838			
MP2	C	1.16058500	1.25825300	-0.26316400		
	C	-0.29812500	1.27604500	0.21035600	95.57	1106.09 1503.76
	C	-1.01704200	-0.00005600	-0.10371700	134.89	1118.93 2940.27
	C	-0.29807200	-1.27611100	0.21035400	214.42	1175.51 2943.83
	C	1.16064000	-1.25820300	-0.26317600	271.49	1194.50 2979.06
	C	1.87954500	0.00003600	0.22517000	335.75	1263.13 3036.15
	H	-0.30624200	1.43528500	1.30451900	367.61	1283.43 3049.59
	H	-0.83237400	2.12748900	-0.22250300	416.47	1302.02 3051.34
	H	1.17986300	1.27780200	-1.35859200	447.08	1314.49 3076.74
	H	1.67776600	2.15615200	0.08530000	547.79	1359.77 3077.14
	H	-0.30619300	-1.43535700	1.30451600	747.92	1367.74 3079.87
	H	-0.83224700	-2.12759600	-0.22251300	788.79	1378.32 3097.48
	H	1.67787300	-2.15608400	0.08525600	851.46	1387.03 3099.07
	H	1.17990800	-1.27771700	-1.35860500	861.41	1406.40 3102.76
	H	1.90460300	0.00002900	1.32236100	902.89	1412.52 3123.71
	H	2.91789500	0.00006100	-0.11692600	926.78	1466.34
	C	-2.50917100	0.00000900	-0.10551500	970.41	1474.89
	H	-2.91068000	0.00002000	0.92102700	1000.44	1483.01
	H	-2.91011200	0.88704900	-0.60284100	1002.31	1487.00
	H	-2.91021200	-0.88697400	-0.60286000	1051.76	1491.03
	Rotational constants (GHZ):			1094.52	1491.28	
	4.25331	2.22686	1.59261			

MP3	C	-1.20204800	1.28908900	0.14732100			
	C	0.27370200	1.24667700	-0.07742200	127.42	1095.56	1503.85
	C	1.03407300	0.02721800	0.33795900	192.22	1117.27	2939.91
	C	0.31148300	-1.24064200	-0.14938900	239.20	1142.34	2962.28
	C	-1.16983300	-1.23276100	0.23124600	307.53	1176.14	3034.58
	C	-1.87707300	-0.00256800	-0.33973400	325.17	1231.93	3039.45
	H	0.81674600	2.16167300	-0.28821100	341.46	1264.59	3051.65
	H	-1.40821500	1.39452200	1.22639500	415.48	1279.84	3052.35
	H	-1.64420100	2.16282400	-0.33698300	448.60	1317.46	3088.04
	H	0.40418200	-1.29344700	-1.24160100	504.10	1326.01	3096.03
	H	0.80995900	-2.12484400	0.25998000	598.06	1355.61	3098.35
	H	-1.65432900	-2.14618300	-0.12399800	785.67	1359.15	3102.95
	H	-1.26267200	-1.22836200	1.32461600	822.14	1373.61	3123.91
	H	-1.83070300	-0.03824600	-1.43381800	871.21	1386.33	3130.24
	H	-2.93369000	-0.00199800	-0.05919600	885.21	1409.05	3188.48
	H	1.03784800	-0.01642000	1.44250300	909.29	1418.26	
	C	2.48265800	0.06431200	-0.14308700	975.51	1473.38	
	H	2.51541200	0.10249800	-1.23573200	987.32	1484.83	
	H	3.00356400	0.94439600	0.24163400	1001.13	1490.38	
	H	3.02832400	-0.82437000	0.18304300	1069.55	1498.77	
	Rotational constants (GHZ):				1091.95	1502.12	
	4.36080	2.21178	1.60920				
MP4	C	1.14384400	1.29353800	-0.16715700			
	C	-0.32267300	1.28772000	0.11215900	147.56	1112.10	1502.78
	C	-0.99362200	-0.02003100	-0.34464700	174.17	1117.89	2945.62
	C	-0.21856000	-1.22219900	0.20304100	236.82	1127.98	2960.27
	C	1.24827600	-1.20201700	-0.22971400	281.89	1167.59	3021.02
	C	1.93809600	0.09259200	0.22829300	311.25	1237.31	3035.20
	H	-0.49584700	1.38335200	1.19979500	364.76	1268.27	3048.50
	H	-0.81459500	2.14655500	-0.35300600	417.36	1287.85	3051.43
	H	1.64619300	2.22254000	-0.40611200	435.29	1314.47	3084.07
	H	-0.27595300	-1.20710800	1.30040800	474.13	1333.40	3088.10
	H	-0.69763500	-2.14999800	-0.12531300	616.70	1358.74	3099.82
	H	1.77695400	-2.07066600	0.17174300	783.52	1366.52	3101.13
	H	1.30071500	-1.26680100	-1.32208700	851.50	1369.97	3118.00
	H	2.03259500	0.05720800	1.32745900	854.80	1398.17	3126.75
	H	2.95499800	0.14904800	-0.16682900	876.64	1402.31	3204.95
	H	-0.93703600	-0.05606100	-1.44036200	899.05	1410.94	
	C	-2.45979700	-0.06149100	0.07396500	966.70	1468.39	
	H	-2.54662800	-0.04222200	1.16491600	985.07	1474.23	
	H	-3.00961900	0.79662900	-0.32110500	992.99	1488.53	
	H	-2.94752800	-0.97114500	-0.28513800	1063.78	1497.35	
	Rotational constants (GHZ):				1104.13	1501.70	
	4.39315	2.22126	1.61101				

MP5	C	-1.22822200	1.28012000	0.15710200			
	C	0.26303000	1.25487000	-0.21040900	136.42	1102.12	1503.91
	C	0.95960200	0.00000100	0.32471900	214.74	1123.10	2959.32
	C	0.26303800	-1.25487400	-0.21040700	238.84	1137.60	2961.70
	C	-1.22821300	-1.28012000	0.15710100	244.39	1172.51	3013.29
	C	-1.90080600	0.00000000	-0.21507100	314.61	1241.02	3036.83
	H	0.36560900	1.27147400	-1.30267400	358.95	1256.92	3041.74
	H	0.75975200	2.15134400	0.17371800	427.82	1293.34	3049.39
	H	-1.30811200	1.43633200	1.24685400	454.48	1318.91	3087.07
	H	-1.72518600	2.13271800	-0.31168600	459.73	1330.43	3089.95
	H	0.36562000	-1.27148600	-1.30267200	637.24	1343.40	3097.27
	H	0.75976200	-2.15134400	0.17372700	783.87	1371.99	3097.27
	H	-1.72518200	-2.13271700	-0.31168300	793.87	1381.70	3118.44
	H	-1.30809700	-1.43632900	1.24685400	879.65	1400.45	3126.83
	H	-2.94773500	-0.00002600	-0.49223500	900.49	1404.89	3205.01
	H	0.86055800	0.00000200	1.41980800	932.35	1413.08	
	C	2.44393400	0.00000500	-0.02981700	962.78	1470.63	
	H	2.57543300	0.00000500	-1.11642800	974.87	1478.99	
	H	2.94670000	0.88484400	0.36855100	1005.08	1482.53	
	H	2.94670500	-0.88483000	0.36855100	1040.95	1497.21	
	Rotational constants (GHZ):				1100.63	1503.00	
	4.25718	2.27083	1.61428				
EPI	C	-2.27443000	0.29797800	0.21967400			
	C	-1.30626200	1.41530500	-0.17453900	101.97	1084.60	1494.97
	C	0.11641100	1.10426100	0.29474900	129.36	1094.53	1508.77
	C	0.60971300	-0.24632100	-0.23495400	149.32	1118.69	2976.32
	C	-0.37014200	-1.35705600	0.15453400	218.05	1130.69	3005.95
	C	-1.79463300	-1.05300900	-0.31476800	236.89	1174.60	3024.18
	H	0.80415100	1.89817600	-0.01136700	327.43	1193.67	3030.51
	H	-1.30867400	1.52383100	-1.26613900	368.12	1239.71	3036.88
	H	-1.63926200	2.37128000	0.23858000	423.19	1276.72	3041.41
	H	-2.33913900	0.24869800	1.31362800	444.97	1291.13	3045.50
	H	-3.28037200	0.51713400	-0.14847700	449.38	1298.88	3063.15
	H	0.63917500	-0.18967900	-1.33339200	485.95	1312.36	3083.41
	H	-0.03009900	-2.31334200	-0.25568800	545.67	1337.13	3091.23
	H	-0.36412800	-1.46139300	1.24811700	789.62	1366.97	3094.86
	H	-1.81421700	-1.03269800	-1.41131300	800.13	1373.87	3095.37
	H	-2.47385500	-1.85031400	-0.00104600	813.71	1383.82	3099.74
	H	0.13822800	1.07425300	1.39302400	860.75	1387.54	3167.19
	C	2.02836100	-0.56038000	0.25976700	885.39	1388.89	3272.97
	H	2.28488800	-1.58272500	-0.06231200	907.62	1405.99	
	H	2.02754900	-0.58474300	1.35584300	939.31	1464.02	
	C	3.05702100	0.39836900	-0.23156600	963.95	1473.50	
H	3.04607000	0.71729200	-1.26692000	997.97	1483.32		
H	3.91343900	0.66935000	0.37007400	1056.54	1487.34		
Rotational constants (GHZ):				1072.73	1489.97		
	3.86861	1.34882	1.08615				

EP2	C	2.30195600	0.29495200	-0.20731300			
	C	1.32926100	1.41052400	0.18017800	56.12	1087.55	1494.76
	C	-0.08756700	1.10173000	-0.30853300	115.51	1104.29	1508.56
	C	-0.58828300	-0.26071100	0.22073200	139.52	1118.85	2979.28
	C	0.40144700	-1.36628800	-0.16382000	208.92	1162.31	2998.41
	C	1.81989400	-1.05837600	0.31922200	237.55	1170.87	3030.55
	H	-0.77775700	1.89333000	-0.00204700	304.49	1214.65	3035.62
	H	1.31738600	1.51415700	1.27216700	364.41	1253.16	3037.51
	H	1.66670100	2.36845700	-0.22506200	387.57	1287.12	3041.90
	H	2.37711300	0.24869800	-1.30069500	434.42	1294.29	3045.80
	H	3.30384800	0.51541900	0.17090200	459.03	1308.41	3071.76
	H	-0.60579000	-0.18413400	1.32048700	478.76	1325.24	3090.48
	H	0.05642600	-2.32281000	0.23962000	544.79	1352.27	3092.40
	H	0.40382200	-1.46405100	-1.25761200	793.10	1368.81	3094.33
	H	1.83032000	-1.04154800	1.41595300	800.30	1379.07	3095.68
	H	2.50414500	-1.85281400	0.00923500	857.36	1384.72	3100.07
	H	-0.10092000	1.07200100	-1.40580100	891.36	1386.65	3122.31
	C	-1.97325700	-0.56013900	-0.24966600	901.49	1406.32	3179.51
	H	-2.09640400	-1.21610700	-1.10590300	932.41	1430.10	
	C	-3.13008000	0.26784300	0.19607600	937.32	1477.98	
	H	-3.22569900	1.19468300	-0.38857600	986.37	1483.44	
	H	-4.07529400	-0.26931200	0.09290100	1012.59	1486.62	
	H	-3.01812500	0.56682600	1.24318300	1050.34	1489.60	
	Rotational constants (GHZ):				1065.32	1493.93	
		3.93325	1.30545	1.05887			
	EP3	C	2.25729900	0.00019300	0.40971700	47.68	1096.81
C		1.61721000	-1.25993700	-0.17490500	75.29	1101.21	1509.13
C		0.10352400	-1.27389000	0.07904300	203.97	1105.92	2945.39
C		-0.55112300	-0.00017600	-0.36201000	211.27	1173.34	2948.53
C		0.10324000	1.27374700	0.07886600	229.01	1196.10	3035.57
C		1.61692900	1.26010000	-0.17507600	318.83	1249.91	3042.59
H		-0.36278500	-2.13170200	-0.41600700	363.15	1263.37	3048.26
H		1.79701300	-1.28451800	-1.25551200	379.91	1287.01	3049.89
H		2.07705800	-2.15589900	0.25066000	444.23	1311.90	3057.49
H		2.12472700	0.00025200	1.49916400	468.62	1328.35	3074.44
H		3.33412500	0.00030000	0.22064100	584.31	1337.31	3077.04
H		-0.36326300	2.13138400	-0.41630600	739.67	1359.75	3083.84
H		-0.06029900	1.41722900	1.16233800	784.56	1375.90	3095.37
H		1.79673000	1.28457500	-1.25568500	792.78	1375.99	3097.60
H		2.07657600	2.15622300	0.25036900	855.93	1386.97	3101.33
C		-2.01261700	-0.00031500	-0.67760900	856.69	1398.00	3132.38
H		-2.26136700	-0.88140700	-1.27876200	914.27	1409.54	3133.30
H		-2.26136900	0.88031600	-1.27944200	928.41	1468.60	
C		-2.88747500	0.00019800	0.59139000	942.09	1475.84	
H		-2.68460800	0.88426700	1.20051700	997.19	1486.16	
H		-3.94982200	0.00013500	0.33778400	1046.48	1487.35	
H		-2.68466700	-0.88341000	1.20120500	1050.67	1491.51	
Rotational constants (GHZ):				1051.20	1502.52		
		3.73654	1.33911	1.11238			

EP4	C	2.32121200	0.32523700	-0.23304700			
	C	1.33580400	1.44683800	0.15435100	50.42	1089.97	1503.39
	C	-0.05537500	1.07382000	-0.23696500	105.47	1101.79	1508.33
	C	-0.57681400	-0.25025100	0.22279200	151.32	1141.76	2958.09
	C	0.42958200	-1.35479900	-0.16475600	202.05	1152.34	2997.78
	C	1.84475700	-1.02205900	0.31387700	239.39	1164.23	3034.63
	H	-0.58477000	1.63157100	-1.00098000	273.04	1218.30	3039.16
	H	1.38999600	1.57829700	1.24576300	333.17	1256.59	3043.61
	H	1.63510800	2.39486300	-0.29669200	364.63	1264.23	3049.47
	H	2.38523500	0.26973500	-1.32544600	445.10	1297.10	3059.03
	H	3.32235300	0.55812500	0.14052400	457.61	1305.22	3079.75
	H	-0.61978800	-0.24048300	1.32625400	486.79	1326.18	3086.56
	H	0.09994100	-2.31200700	0.25229100	573.65	1343.31	3094.84
	H	0.42785400	-1.45876000	-1.25717700	773.47	1354.93	3099.68
	H	1.85348600	-0.98773600	1.41050400	803.15	1368.46	3110.07
	H	2.53700200	-1.81481000	0.01735400	842.02	1378.42	3128.02
	C	-1.97965500	-0.55186900	-0.30511600	865.44	1385.06	3135.54
	H	-2.24961600	-1.57668200	-0.02958800	899.20	1415.33	3192.86
	H	-1.95419400	-0.52020300	-1.40087100	933.84	1423.62	
	C	-3.03874200	0.41443700	0.22123600	941.88	1479.79	
	H	-2.81162300	1.44484700	-0.06139300	992.42	1483.35	
	H	-4.02917700	0.16987100	-0.16758500	1029.33	1489.50	
	H	-3.08642300	0.37524700	1.31282200	1038.64	1494.16	
Rotational constants (GHZ):				1074.69	1501.33		
		3.92949	1.31175	1.06223			
EP5	C	-2.3604910	0.3814510	0.1622120	90.98	1103.38	1504.58
	C	-1.3337040	1.4239150	-0.1321000	130.53	1120.99	1514.85
	C	0.0910730	1.1398570	0.2134070	165.91	1126.62	2938.33
	C	0.5360500	-0.2597430	-0.2500680	214.70	1132.81	2960.53
	C	-0.4888560	-1.3081180	0.1951130	248.51	1162.53	3016.12
	C	-1.8944050	-0.9996210	-0.3216640	288.68	1228.32	3026.69
	H	0.7427790	1.9093870	-0.2066600	360.77	1253.33	3040.33
	H	-1.6404830	2.4387700	-0.3527260	373.79	1276.64	3051.82
	H	-2.5274720	0.3216690	1.2516320	428.75	1305.43	3058.89
	H	-3.3227220	0.6443540	-0.2833150	461.20	1317.90	3076.73
	H	0.5568710	-0.2539130	-1.3491720	467.60	1326.71	3085.87
	H	-0.1694170	-2.2986570	-0.1440110	613.21	1358.81	3099.33
	H	-0.5050320	-1.3396740	1.2934700	764.87	1363.89	3100.95
	H	-1.8856550	-1.0105200	-1.4171210	797.07	1375.54	3101.97
	H	-2.5985440	-1.7697730	0.0044720	852.72	1379.75	3128.20
	C	1.9357510	-0.6169130	0.2553010	861.88	1402.84	3137.96
	H	2.1810030	-1.6265160	-0.0913190	894.97	1406.36	3205.53
	H	1.9130660	-0.6641520	1.3510360	925.39	1416.06	
	C	3.0294010	0.3509080	-0.1940320	937.82	1468.65	
	H	2.9034300	1.3382990	0.2546060	981.83	1473.26	
	H	4.0178460	-0.0148310	0.0906230	1030.32	1485.38	
	H	3.0175360	0.4730820	-1.2808970	1057.01	1493.00	
	Rotational constants (GHZ):				1072.44	1498.84	
		3.99211	1.31444	1.06133			

EP6	C	2.3288430	0.3295220	-0.1319140			
	C	1.3761940	1.4482410	0.1291310	80.05	1097.65	1504.58
	C	-0.0481750	1.0993390	-0.3309200	119.09	1106.63	1515.28
	C	-0.5077770	-0.2569990	0.2148650	197.80	1126.35	2957.64
	C	0.4808870	-1.3504660	-0.2039400	211.61	1148.60	2960.58
	C	1.9113430	-1.0473420	0.2652610	237.73	1170.09	2999.45
	H	-0.7327200	1.8916550	-0.0175410	266.97	1231.21	3035.89
	H	1.3404160	1.6563220	1.2126720	353.74	1243.17	3037.17
	H	1.7161620	2.3704490	-0.3480400	372.86	1293.02	3043.85
	H	3.3706990	0.5421780	-0.3374900	443.55	1293.64	3059.50
	H	-0.5039830	-0.1981850	1.3143850	449.43	1309.25	3076.62
	H	0.1542660	-2.3178690	0.1904160	471.36	1335.65	3088.74
	H	0.4715120	-1.4282510	-1.2982950	630.31	1345.20	3096.68
	H	1.9368930	-1.1392440	1.3649160	762.63	1365.97	3097.32
	H	2.6085330	-1.7945070	-0.1212800	783.03	1377.56	3103.25
	H	-0.0754100	1.0605110	-1.4275460	822.68	1391.88	3128.16
	C	-1.9266720	-0.6161690	-0.2361580	881.81	1401.38	3139.76
	H	-2.1650670	-1.6168830	0.1399030	914.01	1408.30	3202.90
	H	-1.9395420	-0.6878610	-1.3306040	933.23	1416.91	
	C	-3.0032890	0.3637550	0.2282080	946.70	1469.33	
H	-2.8941410	1.3410310	-0.2455900	993.99	1477.48		
H	-4.0008030	-0.0078390	-0.0143020	1021.37	1481.80		
H	-2.9549330	0.5092120	1.3111930	1046.37	1490.63		
Rotational constants (GHZ):				1064.08	1497.96		
		3.84866	1.33812	1.06690			
nP1	C	2.22087000	-0.89135100	0.53864300	61.41	1080.15	1493.24
	C	0.89798100	-1.38460900	-0.04938300	96.14	1088.86	1495.36
	C	-0.22282000	-0.34922500	0.09608900	145.47	1102.25	1508.67
	C	0.20551900	0.98761300	-0.51924300	176.45	1127.12	2987.02
	C	1.53414700	1.48209300	0.05845500	228.87	1139.29	3012.90
	C	2.63826000	0.43546800	-0.09814600	236.84	1172.90	3021.58
	H	1.03882500	-1.60090100	-1.11722700	310.63	1189.73	3029.26
	H	0.59600600	-2.32417300	0.42473100	336.03	1237.76	3036.30
	H	2.10493300	-0.75025800	1.62019300	398.45	1241.45	3037.63
	H	3.00120700	-1.64445700	0.39896300	437.07	1291.12	3041.13
	H	0.30276300	0.86132300	-1.60688600	444.78	1292.30	3044.98
	H	-0.56891800	1.74188500	-0.35185900	465.46	1304.52	3069.37
	H	1.82648900	2.41991900	-0.42179500	503.92	1322.93	3080.57
	H	1.39785200	1.70139400	1.12455100	547.15	1342.34	3087.13
	H	2.83401800	0.27523400	-1.16565100	764.41	1365.89	3093.48
	H	3.57037400	0.79606600	0.34531500	797.99	1373.69	3094.20
	H	-0.38840100	-0.17925200	1.16965400	830.93	1380.90	3095.08
	C	-1.52255600	-0.88587300	-0.51166600	856.49	1385.98	3099.13
	H	-1.78840300	-1.81858900	0.00028200	865.81	1388.37	3163.68
	H	-1.34111100	-1.14818800	-1.56081900	907.93	1398.17	3268.21
C	-2.71586900	0.07612600	-0.43745900	911.61	1410.91		
H	-3.58836600	-0.42999000	-0.87891500	924.11	1465.56		
H	-2.53814400	0.94987500	-1.07157300	944.74	1478.28		
C	-3.03208600	0.51134700	0.95168800	991.66	1480.74		

	H	-3.52487100	1.45432400	1.14638400	1038.60	1487.35	
	H	-2.95493300	-0.19375200	1.77078000	1059.38	1489.91	
	Rotational constants (GHZ):						
		3.09905	0.93669	0.82091			
<i>n</i> P2	C	1.75800600	1.45415400	-0.16781800			
	C	0.33295100	1.07399300	0.23894200	47.26	1075.09	1491.42
	C	-0.06390400	-0.30773000	-0.29269300	82.97	1093.31	1494.54
	C	0.95379100	-1.35902000	0.16031300	104.06	1118.02	1508.57
	C	2.38104900	-0.98620300	-0.24631700	157.23	1130.90	2958.70
	C	2.76364500	0.39530800	0.28881600	189.92	1147.96	2992.71
	H	0.26087300	1.05584600	1.33536400	237.50	1173.16	3004.88
	H	-0.37986800	1.82708800	-0.10946400	307.82	1198.46	3023.09
	H	1.80680300	1.54816100	-1.25968200	326.73	1228.92	3024.94
	H	2.02022100	2.43189800	0.24542200	355.82	1275.43	3033.67
	H	0.90104500	-1.44862000	1.25394600	428.73	1290.30	3037.01
	H	0.68453200	-2.33756900	-0.24994900	447.80	1296.37	3040.66
	H	3.08560300	-1.74215800	0.11098500	455.97	1299.79	3045.25
	H	2.45167100	-0.97892800	-1.34095200	471.25	1336.13	3068.89
	H	2.77833300	0.36393800	1.38527700	568.57	1346.46	3083.37
	H	3.77322200	0.66275800	-0.03485200	790.73	1368.91	3091.22
	H	-0.04127000	-0.26757400	-1.39204700	799.39	1383.45	3094.45
	C	-1.48409700	-0.68748600	0.13695800	840.29	1387.19	3095.14
	H	-1.53771100	-0.69217800	1.23518000	861.29	1388.56	3099.41
	H	-1.67786000	-1.73032800	-0.16865300	903.15	1401.40	3129.65
	C	-2.54504700	0.20647300	-0.41104600	916.40	1409.85	3176.21
	H	-2.40386100	0.61084500	-1.40857300	924.27	1429.78	
	C	-3.91072600	0.21993100	0.18458500	946.94	1468.37	
	H	-4.51790400	1.03843500	-0.20533500	987.76	1481.60	
	H	-4.45390900	-0.71484400	-0.02136300	993.11	1482.76	
	H	-3.86392500	0.31671300	1.27425600	1056.37	1487.92	
	Rotational constants (GHZ):				1070.71	1489.44	
		3.70566	0.79851	0.69837			
<i>n</i> P3	C	-1.59056400	1.47438300	0.29467000	48.19	1067.39	1500.66
	C	-0.18552400	1.01275700	-0.09804700	73.11	1090.52	1507.28
	C	0.06917500	-0.45250200	0.32002800	129.18	1115.62	1509.97
	C	-1.01326900	-1.36027800	-0.27380200	193.12	1123.98	2970.53
	C	-2.42048100	-0.89939100	0.11011400	240.08	1159.46	3028.74
	C	-2.65843900	0.55507100	-0.30158100	251.46	1170.99	3030.90
	H	-0.06266400	1.08670900	-1.18635800	275.86	1214.40	3035.58
	H	0.57013700	1.66327900	0.35318000	307.96	1243.37	3037.74
	H	-1.67877900	1.46691400	1.38803400	364.86	1280.74	3041.80
	H	-1.75177200	2.50623800	-0.02918900	429.79	1289.63	3046.09
	H	-0.91258300	-1.34910900	-1.36720100	440.89	1293.99	3056.43
	H	-0.84490400	-2.39154700	0.05041200	461.77	1304.11	3075.88
	H	-3.16860700	-1.55169800	-0.34838000	499.33	1325.17	3089.45
	H	-2.54437600	-0.98999700	1.19621600	547.05	1334.21	3091.36
	H	-2.62417700	0.62872600	-1.39550400	769.74	1354.35	3095.37
	H	-3.65571700	0.87959500	0.00749300	795.93	1368.06	3096.05

	H	-0.02438700	-0.48462400	1.41880100	808.54	1384.05	3100.56
	C	1.44466300	-0.90148300	-0.04822200	857.58	1385.58	3130.54
	H	1.56712700	-1.60149700	-0.87020600	894.21	1390.05	3134.13
	C	2.66635800	-0.28227800	0.54659800	901.12	1402.07	3169.41
	H	3.34212800	-1.06375400	0.91560200	912.28	1436.26	
	H	2.38428600	0.31921300	1.41739500	939.51	1480.98	
	C	3.43942100	0.59431800	-0.45320800	982.40	1485.77	
	H	4.33621300	1.01936600	0.00387200	1030.76	1488.18	
	H	3.74653100	0.00479500	-1.32011900	1050.32	1489.53	
	H	2.81348900	1.41380500	-0.81334800	1055.00	1494.47	
	Rotational constants (GHZ):						
		3.35262	0.86601	0.74413			
<i>n</i> P4	C	1.66151600	-1.35878500	0.11122900			
	C	0.57140500	-1.05573800	-0.92685200	33.45	1081.82	1502.64
	C	-0.17315000	0.20278200	-0.60857100	44.91	1096.71	1504.82
	C	0.64014400	1.40213800	-0.23220900	107.32	1103.34	1508.40
	C	1.72570700	1.06499200	0.79889500	179.77	1109.65	2945.05
	C	2.55354400	-0.13830400	0.34450500	216.67	1173.37	2948.17
	H	1.05605200	-0.95969900	-1.91533200	254.67	1192.86	3014.03
	H	-0.12413900	-1.89672300	-1.00777900	295.17	1226.15	3035.23
	H	1.18362700	-1.63773800	1.05749000	359.94	1255.75	3046.16
	H	2.25981600	-2.21449100	-0.21315000	375.07	1282.60	3048.29
	H	1.13407500	1.80504900	-1.13480400	406.07	1285.31	3050.22
	H	-0.00862100	2.20096300	0.14100200	441.94	1307.90	3052.72
	H	2.36977900	1.93281300	0.96481600	467.50	1317.77	3068.90
	H	1.24575200	0.82852200	1.75561600	545.66	1355.12	3076.74
	H	3.07347300	0.11311700	-0.58869900	727.14	1359.60	3080.61
	H	3.32390400	-0.36941900	1.08504600	790.72	1363.89	3090.12
	C	-1.60861100	0.38147300	-0.99188300	796.07	1375.45	3095.90
	H	-1.93618000	-0.45081100	-1.62545400	851.76	1380.20	3096.93
	H	-1.72530500	1.29819700	-1.58593600	854.21	1387.15	3100.41
	C	-2.54396700	0.46735400	0.22986400	865.26	1409.34	3122.22
	H	-3.55651200	0.70701100	-0.10919100	890.37	1415.43	3132.56
	H	-2.22077500	1.29710700	0.86749500	923.97	1466.29	
	C	-2.55898600	-0.82739000	1.03859700	930.64	1474.55	
	H	-3.23068100	-0.75609700	1.89636200	985.56	1484.51	
	H	-2.89153200	-1.66625400	0.42018200	1038.18	1486.37	
	H	-1.55833200	-1.06268100	1.41088200	1051.83	1490.98	
	Rotational constants (GHZ):				1061.99	1491.18	
		2.60265	1.00892	0.92565			

nP5	C	-1.85712600	1.45077500	0.14020200			
	C	-0.45504000	1.07412300	-0.20629600	58.58	1075.36	1501.15
	C	0.04540100	-0.25304600	0.26834200	77.29	1099.97	1504.63
	C	-0.95073000	-1.35287100	-0.15899300	92.79	1108.46	1511.98
	C	-2.38068400	-1.01674100	0.27077600	147.32	1143.32	2962.27
	C	-2.83276900	0.33470200	-0.28663700	192.89	1152.79	2999.79
	H	0.09162200	1.61828800	-0.96821900	246.23	1162.98	3027.65
	H	-1.94749600	1.57622500	1.22974100	274.81	1215.37	3035.33
	H	-2.13769800	2.40224700	-0.31560500	299.34	1243.82	3039.20
	H	-0.91081800	-1.45263500	-1.25105400	328.17	1261.63	3049.50
	H	-0.63923600	-2.31278500	0.26565200	356.19	1287.07	3051.16
	H	-3.06488900	-1.80563200	-0.05344700	450.39	1294.57	3055.63
	H	-2.42805100	-0.98703800	1.36654500	466.68	1313.98	3064.18
	H	-2.85857200	0.28419100	-1.38086400	511.65	1330.93	3085.41
	H	-3.84553000	0.56997600	0.05257200	588.26	1340.59	3091.19
	H	0.04741300	-0.24679300	1.37240100	741.86	1346.42	3094.74
	C	1.46443700	-0.55794900	-0.21001100	801.99	1354.63	3099.67
	H	1.48347100	-0.51578700	-1.30705400	837.93	1367.96	3110.21
	H	1.72311900	-1.58751100	0.06487000	857.72	1384.48	3124.76
	C	2.51989100	0.39017100	0.35658900	874.80	1402.66	3132.83
	H	2.49255300	0.33909500	1.45063500	904.60	1413.61	3189.87
	H	2.26637500	1.42158700	0.09231700	921.83	1424.36	
	C	3.92514800	0.06076900	-0.14097200	945.13	1479.60	
	H	4.66928400	0.74221700	0.27597100	973.30	1482.44	
	H	4.20896400	-0.95746200	0.13809800	1038.74	1488.94	
H	3.97832500	0.13221700	-1.23055300	1048.35	1490.88		
Rotational constants (GHZ):				1065.71	1496.97		
		3.81907	0.78000	0.68544			
nP6	C	1.89307800	1.40541300	-0.11634600	74.58	1091.11	1498.93
	C	0.45374100	1.15697100	0.19447300	83.38	1104.77	1504.83
	C	-0.01543900	-0.23085100	-0.28100600	131.15	1125.42	1512.13
	C	0.97281800	-1.30475300	0.18648900	165.50	1128.51	2937.93
	C	2.39708400	-1.03109700	-0.29718800	176.46	1133.76	2960.52
	C	2.88629000	0.33720300	0.19996600	248.00	1162.32	3016.96
	H	0.29163100	1.20202000	1.28788000	284.65	1223.52	3022.30
	H	-0.16829700	1.94284600	-0.24012800	298.16	1245.02	3030.82
	H	2.23027700	2.41268800	-0.32719500	351.66	1270.78	3049.23
	H	0.96281200	-1.33727700	1.28487500	369.04	1294.63	3051.79
	H	0.63675400	-2.28681000	-0.16103900	432.09	1300.22	3056.10
	H	3.07399900	-1.81906200	0.04371000	460.92	1322.60	3061.41
	H	2.41341700	-1.04034700	-1.39258600	506.02	1335.28	3084.13
	H	3.02607900	0.27184800	1.29290500	628.12	1340.04	3091.32
	H	3.86503100	0.57652400	-0.22229200	742.53	1362.45	3098.68
	H	-0.01015000	-0.22423800	-1.38015400	794.92	1367.09	3100.95
	C	-1.43386100	-0.55472600	0.19168500	843.15	1376.89	3103.80
	H	-1.44126400	-0.60415000	1.28893300	853.62	1396.08	3126.42
	H	-1.69848200	-1.55894300	-0.16175500	864.96	1403.50	3132.80
	C	-2.50657400	0.42923200	-0.27421400	908.91	1412.32	3205.84
H	-2.42600200	0.56307000	-1.35903600	920.08	1414.29		

	H	-2.33035100	1.41141900	0.17397600	938.75	1468.79	
	C	-3.91412800	-0.04198200	0.08475100	973.23	1474.08	
	H	-4.67263500	0.67461800	-0.23632300	1029.63	1482.98	
	H	-4.13635500	-1.00178900	-0.38872300	1059.64	1491.20	
	H	-4.01451500	-0.17486900	1.16528900	1068.69	1497.04	
	Rotational constants (GHZ):						
		3.89196	0.78133	0.68465			
<i>nP7</i>	C	2.40748300	-1.08088000	0.24891200			
	C	0.96316000	-1.34727300	-0.19911300	66.80	1079.97	1499.43
	C	0.00837900	-0.22942500	0.23457000	74.25	1106.29	1504.95
	C	0.49440600	1.11583400	-0.31641800	125.62	1111.19	1512.27
	C	1.93474500	1.42722300	0.12055700	161.12	1129.14	2957.00
	C	2.85388100	0.28455300	-0.15610400	211.60	1149.00	2960.26
	H	0.93587600	-1.42378000	-1.29323900	242.19	1166.82	3000.39
	H	0.61789100	-2.30639500	0.19948100	252.22	1229.65	3024.31
	H	2.44680200	-1.17238900	1.34819400	296.50	1235.90	3035.84
	H	3.07960200	-1.84592300	-0.14691600	351.61	1276.42	3041.59
	H	0.44771800	1.08007800	-1.41250000	358.54	1286.96	3049.20
	H	-0.16434100	1.92472100	0.00968200	446.76	1303.58	3055.83
	H	2.29042800	2.34084500	-0.36163300	449.14	1317.93	3061.10
	H	1.92178700	1.63521500	1.20464800	517.05	1330.09	3087.60
	H	3.89690000	0.47025900	-0.38091900	637.63	1342.90	3092.85
	H	0.02948300	-0.17263400	1.33385500	741.50	1350.57	3096.86
	C	-1.42413900	-0.55391300	-0.19731400	781.74	1372.60	3097.64
	H	-1.68505700	-1.54938900	0.18274400	808.38	1380.78	3105.68
	H	-1.45704800	-0.62673000	-1.29266000	864.06	1400.79	3126.45
	C	-2.48379300	0.44191800	0.27362800	897.73	1403.51	3132.64
	H	-2.32067900	1.41396000	-0.20013000	907.81	1411.99	3203.68
	H	-2.37592400	0.59926800	1.35291900	919.96	1414.18	
	C	-3.90002500	-0.03702900	-0.03844900	954.72	1469.47	
	H	-4.65026600	0.68689600	0.28563700	979.75	1477.60	
	H	-4.02791800	-0.19418200	-1.11280200	1029.70	1480.59	
	H	-4.10984100	-0.98586800	0.46202800	1043.81	1487.74	
		Rotational constants (GHZ):				1062.66	1495.16
		3.76253	0.79108	0.68781			

<i>iP1</i>	C	-2.04346600	-1.01896200	-0.49146700			
	C	-0.56900400	-1.30746000	-0.20104400	43.55	1058.66	1498.82
	C	0.30802400	-0.07495800	-0.44528100	75.70	1075.00	1509.75
	C	-0.19743400	1.10182300	0.39684200	120.11	1095.23	1511.53
	C	-1.67414700	1.39692400	0.11827300	208.50	1118.23	3004.96
	C	-2.54294400	0.15900200	0.34722700	234.47	1149.29	3014.60
	H	-0.46754800	-1.61518600	0.84715300	254.28	1164.82	3033.84
	H	-0.21478300	-2.14241600	-0.81505200	275.81	1195.55	3036.97
	H	-2.16262500	-0.77985600	-1.55533000	315.71	1216.14	3039.64
	H	-2.64813000	-1.90898600	-0.29699600	366.98	1252.82	3041.66
	H	-0.07003700	0.85644300	1.45915400	416.48	1292.79	3045.44
	H	0.39947700	1.99687200	0.20148200	438.89	1299.71	3057.87
	H	-2.01664400	2.22356100	0.74679900	446.43	1303.50	3082.64
	H	-1.78422200	1.72435600	-0.92295700	469.49	1321.35	3093.31
	H	-2.50412200	-0.11527800	1.40859300	511.45	1342.55	3095.05
	H	-3.58821800	0.37860200	0.11338400	616.40	1368.01	3097.66
	H	0.20191300	0.20182100	-1.50489000	785.24	1371.47	3100.77
	C	1.81365700	-0.38898800	-0.22479700	800.30	1386.55	3130.16
	H	2.02936300	-1.24374700	-0.88114600	852.21	1387.90	3134.76
	C	2.70562700	0.77695700	-0.66212000	872.10	1395.36	3165.33
	H	3.75496500	0.47520100	-0.67110000	901.67	1407.03	3270.17
	H	2.43947300	1.12246200	-1.66438200	906.59	1410.32	
	H	2.61187700	1.62225800	0.02418100	926.65	1469.74	
	C	2.12759200	-0.79732700	1.17780900	938.56	1484.07	
	H	2.57097300	-0.09429100	1.87192700	970.55	1488.23	
	H	1.88085900	-1.78388000	1.54652400	1026.40	1490.74	
Rotational constants (GHZ):				1044.89	1495.40		
		2.88853	1.04768	0.91853			
<i>iP2</i>	C	1.77822000	1.34086900	0.22487500	57.18	1051.05	1497.35
	C	0.29115200	1.10858900	0.50259800	101.87	1070.95	1497.95
	C	-0.29902100	0.02431600	-0.42867500	136.71	1093.96	1509.59
	C	0.51084700	-1.27017900	-0.28559800	153.31	1117.89	2980.95
	C	1.99374800	-1.03815200	-0.58256500	170.17	1147.02	2984.77
	C	2.57433800	0.03921600	0.33601400	242.18	1197.79	2996.40
	H	0.15810900	0.78607200	1.54354400	259.66	1231.41	3032.81
	H	-0.26611700	2.04243300	0.38272800	309.60	1282.92	3036.87
	H	1.89199800	1.74542600	-0.78836200	365.56	1288.54	3039.79
	H	2.17778100	2.09186600	0.91211900	395.82	1293.03	3041.80
	H	0.41200300	-1.64564400	0.74047800	437.13	1317.27	3045.55
	H	0.09939300	-2.03835600	-0.94790600	451.74	1325.65	3071.11
	H	2.55090400	-1.97233700	-0.47128800	494.69	1343.96	3082.39
	H	2.10851800	-0.72246900	-1.62671500	543.97	1358.67	3089.11
	H	2.53682700	-0.31698700	1.37289500	773.81	1367.71	3091.17
	H	3.62693800	0.21621500	0.09904100	798.31	1384.43	3093.76
	H	-0.16359800	0.38796900	-1.45902700	836.93	1385.35	3095.05
	C	-1.77341700	-0.15164200	-0.19955400	864.27	1401.86	3100.05
	C	-2.67883700	0.96450500	-0.61348100	900.00	1410.60	3118.86
	H	-3.67853800	0.59497900	-0.86083500	906.95	1414.73	3127.44
H	-2.81029000	1.70502800	0.19138100	934.30	1476.13		

	H	-2.28571600	1.49927500	-1.48217200	938.73	1477.98	
	C	-2.26041700	-1.08254000	0.86590800	980.25	1482.53	
	H	-1.85202000	-2.09035700	0.75407900	989.67	1487.08	
	H	-1.97575300	-0.73625700	1.87254400	1046.81	1488.41	
	H	-3.35011600	-1.15674700	0.85037900	1048.94	1495.00	
	Rotational constants (GHZ):						
		2.86439	1.03766	0.88568			
<i>iP3</i>	C	-2.03392400	-1.03509800	-0.57378700			
	C	-0.58450900	-1.33741000	-0.17122300	28.96	1089.87	1503.76
	C	0.27514700	-0.10863200	-0.18186200	68.70	1095.14	1509.37
	C	-0.28474500	1.08649000	0.53084800	186.96	1100.89	1515.67
	C	-1.74049800	1.36393300	0.12815000	212.47	1121.96	2944.52
	C	-2.60246000	0.10895300	0.26623100	227.54	1153.75	2949.71
	H	-0.59678800	-1.76854900	0.84622000	269.06	1174.06	3029.75
	H	-0.15564200	-2.10541400	-0.82301000	274.89	1215.43	3036.13
	H	-2.05841100	-0.75038100	-1.63163000	296.22	1260.34	3048.59
	H	-2.64803600	-1.93316300	-0.46544200	354.62	1271.49	3048.81
	H	-0.25828700	0.90827000	1.62133300	405.96	1290.72	3050.62
	H	0.32610500	1.97428500	0.35103500	441.47	1318.54	3055.01
	H	-2.14639600	2.17650200	0.73677400	446.94	1328.19	3075.82
	H	-1.76091100	1.69891000	-0.91507300	492.17	1353.54	3095.59
	H	-2.63009000	-0.19621900	1.32001500	585.33	1360.47	3097.57
	H	-3.63295300	0.32243700	-0.03025900	731.10	1372.49	3101.59
	C	1.75995000	-0.28648200	-0.34367400	790.44	1384.03	3103.13
	H	1.90980000	-1.04401700	-1.12339000	849.25	1388.36	3119.18
	C	2.48540000	0.98792800	-0.78353900	856.61	1397.43	3128.02
	H	3.52185800	0.76285800	-1.04571800	886.75	1410.39	3130.05
	H	2.00097600	1.43796400	-1.65351100	918.14	1415.28	3130.94
	H	2.50552500	1.73046400	0.01841700	926.35	1468.28	
	C	2.38864700	-0.83274400	0.95359200	931.41	1475.79	
	H	1.93168100	-1.77990300	1.24908900	965.59	1487.40	
	H	3.46196500	-0.99752900	0.82610600	978.35	1490.27	
	H	2.25156000	-0.11814500	1.77062600	1048.05	1490.91	
		Rotational constants (GHZ):				1062.70	1496.35
		2.85141	1.03141	0.88965			

iP4	C	-2.06950500	-1.08535000	-0.44525400			
	C	-0.58594900	-1.24243400	-0.37264700	58.19	1065.00	1501.88
	C	0.28684900	-0.03330800	-0.50833500	98.70	1083.67	1510.04
	C	-0.25189000	1.11729000	0.36124600	192.72	1107.97	1516.21
	C	-1.74516900	1.34874800	0.11799900	213.04	1127.04	2923.06
	C	-2.55301900	0.08646700	0.42016900	235.18	1143.41	2958.27
	H	-0.14721900	-2.22030500	-0.54549900	258.25	1178.43	3032.02
	H	-2.36683300	-0.88425200	-1.48919700	274.91	1213.39	3036.87
	H	-2.57132200	-2.01274500	-0.15819200	315.93	1227.26	3050.04
	H	-0.10296300	0.87176700	1.41878300	340.01	1261.51	3051.54
	H	0.30742900	2.03421700	0.15665000	401.69	1272.01	3052.06
	H	-2.09936300	2.18054500	0.73283100	419.38	1310.31	3058.55
	H	-1.90223300	1.63753700	-0.92894700	459.24	1320.83	3092.59
	H	-2.42766800	-0.17407600	1.47709000	480.97	1348.70	3095.47
	H	-3.61907800	0.26173100	0.25312400	571.22	1362.09	3100.25
	H	0.21329600	0.31474600	-1.55670000	609.24	1364.18	3103.97
	C	1.77225300	-0.36721800	-0.26149900	776.63	1375.54	3123.83
	H	2.00817300	-1.20293300	-0.93255800	829.88	1382.92	3125.31
	C	2.69263200	0.79699100	-0.63028300	853.74	1387.08	3127.69
	H	3.74052800	0.49207900	-0.57611000	887.28	1403.61	3130.80
	H	2.49644900	1.15522500	-1.64447700	909.35	1414.25	3173.21
	H	2.56114600	1.63696600	0.05717400	932.19	1422.09	
	C	2.04496900	-0.83031100	1.17177400	934.04	1472.22	
	H	1.35983600	-1.62603900	1.47428800	968.95	1485.78	
	H	3.06700300	-1.20593100	1.26366100	972.34	1488.43	
	H	1.93578700	-0.00377800	1.87905700	1035.01	1491.27	
Rotational constants (GHZ):				1046.12	1500.74		
2.89612				1.03601	0.91524		
iP5	C	1.91310900	1.27621300	-0.19724800	54.71	1087.66	1505.65
	C	0.46409000	1.30196200	0.16035100	109.10	1108.89	1508.14
	C	-0.27378000	0.00115500	-0.21990600	159.46	1111.11	1526.93
	C	0.53731600	-1.21161700	0.25746800	183.00	1138.08	2936.40
	C	1.97152200	-1.20597800	-0.27403500	230.00	1145.34	2960.64
	C	2.71364700	0.06747600	0.15072100	263.31	1168.13	3004.17
	H	0.35039500	1.43701400	1.25262400	273.13	1195.03	3020.08
	H	-0.01598900	2.16421300	-0.30588900	340.04	1233.68	3029.00
	H	2.41183200	2.19859000	-0.46803200	361.10	1255.38	3049.10
	H	0.55579400	-1.21083300	1.35671400	386.49	1277.04	3051.34
	H	0.04767500	-2.13758100	-0.05081100	411.46	1307.82	3053.21
	H	2.50716800	-2.09128600	0.07927600	445.91	1331.02	3098.55
	H	1.94816600	-1.25666700	-1.36827100	472.02	1348.51	3099.41
	H	2.87051400	0.02429100	1.24241500	497.75	1354.61	3107.69
	H	3.70638200	0.11020400	-0.30328100	611.12	1365.53	3109.83
	H	-0.32847900	-0.04111300	-1.31832100	785.85	1369.38	3116.33
	C	-1.71669400	-0.01464700	0.32135100	853.37	1373.41	3122.83
	H	-1.65473100	-0.00875400	1.41847800	860.21	1402.01	3144.02
	C	-2.50474800	1.22346700	-0.11738500	876.76	1403.95	3145.95
	H	-3.54796100	1.14480700	0.19708300	906.19	1407.14	3200.70
H	-2.10252400	2.14444000	0.30649600	929.99	1421.78		

	H	-2.49146500	1.31739300	-1.20866000	935.08	1469.71		
	C	-2.47500800	-1.27442200	-0.10790300	964.07	1474.44		
	H	-2.04708300	-2.18458200	0.31352500	977.40	1487.71		
	H	-3.51730400	-1.22217500	0.21517800	994.05	1490.65		
	H	-2.46912500	-1.36960900	-1.19900500	1067.54	1497.12		
	Rotational constants (GHZ):							
		2.95084	1.05996	0.82880				
<i>iP6</i>	C	1.74824000	1.40279200	0.16843100				
	C	0.27519600	1.08031400	0.46614900	40.52	1055.02	1504.08	
	C	-0.22168900	-0.08192900	-0.40262900	113.37	1086.34	1512.82	
	C	0.63556800	-1.32384700	-0.12991300	200.76	1110.27	1515.39	
	C	2.11739000	-1.05881800	-0.43769900	213.19	1129.20	2958.26	
	C	2.60058900	0.17922700	0.24306400	235.55	1140.89	2960.70	
	H	0.18288400	0.80470400	1.52262600	239.72	1174.38	2998.21	
	H	-0.33468200	1.97410200	0.30762500	255.85	1212.54	3031.80	
	H	1.80462400	1.83277100	-0.84661200	295.55	1232.62	3046.49	
	H	2.11646900	2.17460800	0.84868800	340.27	1245.87	3051.71	
	H	0.54188000	-1.60837400	0.92387400	375.93	1294.42	3053.38	
	H	0.27451500	-2.16668000	-0.72811500	431.93	1310.15	3060.25	
	H	2.72854200	-1.92036100	-0.15794200	452.15	1320.58	3091.49	
	H	2.22404600	-0.94586600	-1.53050500	473.70	1344.55	3095.68	
	H	3.64081200	0.26398900	0.53285400	549.02	1351.66	3096.11	
	H	-0.05456300	0.19963500	-1.45383000	638.36	1360.37	3101.71	
	C	-1.73034000	-0.36824300	-0.26028900	786.85	1378.35	3123.60	
	H	-1.92587500	-1.27660900	-0.84431100	799.33	1395.68	3126.64	
	C	-2.16555300	-0.63941900	1.18233400	853.44	1401.63	3127.58	
	H	-3.21558200	-0.94054600	1.21071200	897.75	1403.90	3136.08	
	H	-1.57964100	-1.43449200	1.64822800	914.91	1411.11	3200.55	
	H	-2.06641700	0.26003700	1.79623300	927.18	1424.46		
	C	-2.58064200	0.75345200	-0.86128800	948.11	1470.87		
	H	-2.28811000	0.96471500	-1.89312300	966.34	1478.32		
	H	-3.63850400	0.47923700	-0.85956800	971.41	1484.02		
	H	-2.48294800	1.67795700	-0.28579500	1035.10	1490.36		
	H	-2.48294800	1.67795700	-0.28579500	1041.12	1497.77		
		Rotational constants (GHZ):						
			2.86046	1.03724	0.91995			

sBP1	C	1.96548500	-1.41426800	0.10324500			
	C	0.57898700	-1.13362600	-0.48084700	-67.87	1065.70	1501.67
	C	-0.05013800	0.14880700	0.08303300	58.33	1072.40	1502.40
	C	0.92173400	1.32584900	-0.08995900	90.99	1097.30	1508.33
	C	2.30583300	1.03754300	0.49564700	125.53	1100.10	1517.52
	C	2.90953700	-0.23128400	-0.10387200	199.69	1124.71	3003.03
	H	0.65713700	-1.03588700	-1.57292400	226.18	1139.07	3021.00
	H	-0.07001100	-1.99112800	-0.28604800	234.46	1161.63	3021.58
	H	1.86699200	-1.60863500	1.17845200	260.46	1189.28	3031.63
	H	2.38151200	-2.32097700	-0.34454100	326.31	1216.77	3036.27
	H	1.02135500	1.54229200	-1.16291800	345.24	1238.27	3040.55
	H	0.51442600	2.22477300	0.37779700	398.92	1286.83	3044.96
	H	2.96632800	1.89299600	0.32938200	415.67	1289.83	3050.81
	H	2.21641300	0.91249100	1.58179600	441.20	1294.80	3055.44
	H	3.07176100	-0.08171300	-1.17848200	442.48	1302.78	3092.57
	H	3.88682000	-0.43871700	0.34040400	466.53	1318.63	3093.74
	H	-0.20799000	-0.00128400	1.16205400	537.27	1340.04	3095.11
	C	-1.42160800	0.45269200	-0.55108900	609.58	1359.04	3098.09
	H	-1.25319900	0.66005300	-1.61688200	780.74	1369.25	3107.27
	C	-2.08325100	1.68217400	0.07886200	794.53	1378.73	3108.20
	H	-1.53679200	2.60002200	-0.14036200	798.00	1381.79	3120.36
	H	-3.10098700	1.80903300	-0.29905900	844.13	1388.59	3146.03
	H	-2.13995400	1.57448100	1.16656000	868.01	1390.07	3169.78
	C	-2.39399300	-0.75709900	-0.48556800	902.80	1408.82	3270.91
	H	-3.33745400	-0.43671800	-0.94124500	910.07	1413.78	
	H	-2.00551100	-1.56420100	-1.11103500	942.35	1466.04	
	C	-2.64940800	-1.26009600	0.89411300	957.36	1481.50	
	H	-3.35753700	-0.76557800	1.54562500	994.63	1487.39	
	H	-2.07238400	-2.07545800	1.31003900	1001.95	1488.49	
	Rotational constants (GHZ):				1036.26	1494.14	
2.23370				0.84515	0.68607		
sBP2	C	2.07723900	-1.46898000	0.23990000	38.76	1062.03	1494.78
	C	0.63264400	-1.22317600	-0.19793400	66.65	1075.88	1498.07
	C	0.10748800	0.14715600	0.25313300	108.54	1094.45	1508.05
	C	1.05202100	1.25299500	-0.23446000	124.68	1110.32	1516.18
	C	2.50092400	1.00579200	0.19465800	182.17	1130.31	2991.54
	C	3.00051700	-0.36213100	-0.26932000	232.65	1136.70	2996.33
	H	0.57625400	-1.26819200	-1.29449000	240.16	1173.49	3003.07
	H	-0.01932300	-2.01520600	0.18029100	278.57	1189.59	3021.03
	H	2.12214500	-1.49854800	1.33560900	319.40	1224.40	3028.59
	H	2.41653900	-2.44535300	-0.11679200	322.11	1243.72	3036.67
	H	0.99942100	1.30129000	-1.33134800	371.55	1289.39	3039.70
	H	0.72703000	2.22562600	0.14209600	394.88	1293.69	3044.96
	H	3.14507800	1.80024000	-0.19212500	441.87	1298.40	3052.43
	H	2.56083300	1.05497200	1.28899200	456.35	1314.28	3075.21
	H	3.02030500	-0.38632900	-1.36586800	480.32	1337.02	3092.46
	H	4.02581300	-0.52976800	0.07162800	527.68	1353.09	3093.94
	H	0.10744700	0.16793500	1.35465200	569.78	1367.57	3096.01
	C	-1.34661000	0.35290600	-0.21136400	797.36	1380.15	3098.39

	H	-1.36485500	0.23970200	-1.30650700	803.87	1386.54	3103.80
	C	-1.87942500	1.76359700	0.11165900	848.63	1387.89	3123.22
	H	-1.35404100	2.53651800	-0.45237300	870.71	1393.32	3126.22
	H	-2.94055200	1.83720800	-0.13595400	896.70	1403.87	3136.25
	H	-1.76574900	1.97653900	1.17921800	906.79	1408.75	3166.88
	C	-2.25698200	-0.68095900	0.37741700	938.37	1423.17	
	H	-2.06037000	-1.00651200	1.39535700	948.56	1478.23	
	C	-3.60289900	-0.94598200	-0.20664900	974.41	1482.09	
	H	-4.34871500	-0.20289900	0.11265300	998.27	1487.47	
	H	-3.57022200	-0.91072100	-1.29985800	1023.93	1489.17	
	H	-3.98654300	-1.92381500	0.09258300	1050.94	1493.42	
	Rotational constants (GHZ):						
		2.50839	0.74216	0.60658			
	<hr/>						
sBP3	C	1.90934400	-1.45324900	0.11084700			
	C	0.53996400	-1.11629200	-0.48550700	79.99	1061.49	1502.01
	C	-0.02747400	0.19187900	0.07896300	95.51	1069.77	1505.33
	C	0.99094900	1.32435000	-0.11853600	142.88	1082.18	1508.36
	C	2.35572300	0.99102500	0.48586900	152.19	1098.05	1515.33
	C	2.90707200	-0.31285500	-0.09129900	200.08	1125.86	2994.89
	H	0.63093100	-1.01684000	-1.57626700	237.98	1135.62	3008.89
	H	-0.14794300	-1.94540100	-0.30125700	252.15	1157.01	3023.19
	H	1.79275000	-1.63985300	1.18573000	263.24	1192.38	3031.29
	H	2.29120500	-2.37820100	-0.32984800	326.78	1222.00	3036.77
	H	1.10690500	1.49860900	-1.19719700	335.29	1248.36	3040.11
	H	0.60528100	2.25480300	0.30697900	402.00	1278.38	3045.39
	H	3.05502000	1.81309200	0.31046600	419.98	1290.73	3059.13
	H	2.25327400	0.88815000	1.57321000	440.93	1295.43	3062.39
	H	3.09124400	-0.18112200	-1.16464100	449.93	1302.40	3093.14
	H	3.86766500	-0.56048600	0.36851600	474.88	1318.04	3093.86
	H	-0.17443000	0.05881000	1.16157900	537.24	1339.25	3094.91
	C	-1.38489600	0.57218300	-0.54288500	596.96	1367.30	3096.85
	H	-1.19842400	0.81716200	-1.59975800	789.81	1369.18	3099.38
	C	-1.96600900	1.78030400	0.11933200	796.42	1379.42	3103.97
	H	-1.69457600	2.04955000	1.13258600	802.54	1383.58	3128.96
	H	-2.78598800	2.31632800	-0.34213500	849.30	1386.29	3132.90
	C	-2.41636300	-0.58425300	-0.54829100	874.75	1389.07	3159.92
	H	-3.34012900	-0.20529900	-0.99628200	891.07	1411.29	3263.14
	H	-2.06282300	-1.38289600	-1.20674500	909.69	1417.03	
	C	-2.72184500	-1.14581200	0.83910800	937.12	1465.81	
	H	-3.50016400	-1.90966800	0.78723200	945.85	1481.86	
	H	-1.83855000	-1.60355200	1.29159000	992.40	1487.11	
	H	-3.07003400	-0.35686900	1.51063700	1012.11	1488.65	
	Rotational constants (GHZ):				1043.99	1494.22	
		2.25206	0.83912	0.68432			

	C	-2.38989600	-0.71971800	-0.87229000			
	C	-1.00512600	-1.25144300	-0.49542500	51.30	1055.71	1495.99
	C	0.00898900	-0.10973100	-0.28937400	65.28	1068.81	1502.83
	C	-0.53151300	0.88012300	0.76248900	110.82	1076.11	1506.81
	C	-1.91377800	1.41422800	0.38100300	127.46	1092.03	1510.30
	C	-2.90742900	0.26980300	0.17338800	164.32	1116.25	2984.23
	H	-1.08121300	-1.83162600	0.43269000	227.93	1144.69	3009.81
	H	-0.63169800	-1.93276000	-1.26535100	239.22	1201.88	3035.84
	H	-2.32765300	-0.21447700	-1.84400500	255.98	1222.78	3036.16
	H	-3.09201900	-1.54945500	-0.99197900	283.00	1253.77	3036.42
	H	-0.59961900	0.36592300	1.72947100	312.18	1283.81	3041.80
	H	0.17726400	1.70408800	0.89228300	370.62	1290.65	3041.94
	H	-2.27822600	2.10022100	1.15074600	435.86	1297.61	3045.72
	H	-1.83258100	1.99308200	-0.54728800	441.24	1327.26	3053.98
	H	-3.05179800	-0.25632100	1.12514000	481.87	1330.82	3075.16
sBP4	H	-3.88374100	0.66205300	-0.12399600	518.87	1354.67	3081.19
	H	0.08085400	0.43386700	-1.24296300	536.61	1360.90	3088.45
	C	1.37940800	-0.62430300	0.05299300	773.55	1365.61	3092.75
	C	1.63959400	-1.18480500	1.41551800	786.22	1372.24	3094.12
	H	0.76548100	-1.70024100	1.82181200	796.53	1385.89	3094.68
	H	2.47213700	-1.89380500	1.39687300	828.11	1386.55	3099.71
	H	1.90792500	-0.39941000	2.13971600	864.06	1397.47	3121.39
	C	2.54487300	-0.18150900	-0.77581300	900.77	1405.96	3128.27
	H	3.40905800	-0.82372400	-0.57772000	903.51	1415.83	3130.00
	H	2.30471100	-0.28943700	-1.84016600	935.70	1477.41	
	C	2.93594100	1.28472800	-0.50854900	943.86	1481.43	
	H	3.79801400	1.58084800	-1.11082500	991.34	1485.78	
	H	2.10758000	1.95481800	-0.75236900	998.04	1487.93	
	H	3.18914800	1.43212900	0.54428900	1022.59	1489.78	
	Rotational constants (GHZ):				1052.52	1493.03	
		2.24019	0.76628	0.71028			
	C	-2.25964000	-0.39989300	-1.07367900	40.47	1077.16	1502.10
	C	-0.95085900	-1.15416100	-0.80109800	57.16	1090.79	1503.75
	C	0.04765400	-0.30257600	-0.07734200	128.68	1095.07	1504.01
	C	-0.46402900	0.41554700	1.13616100	188.26	1100.17	1508.59
	C	-1.77877700	1.15515800	0.84837700	193.28	1116.82	2946.36
	C	-2.80818700	0.22093100	0.21163700	223.92	1154.32	2952.63
	H	-1.19048300	-2.04352200	-0.19041800	229.59	1173.48	3023.14
	H	-0.52254900	-1.53019100	-1.73543700	247.73	1213.53	3035.77
	H	-2.06581800	0.39544900	-1.80225000	282.40	1253.97	3046.71
sBP5	H	-2.99605300	-1.07484600	-1.51821200	318.71	1264.99	3048.16
	H	-0.65111000	-0.31541200	1.94299100	381.85	1288.51	3049.24
	H	0.28183000	1.11406300	1.52526000	427.87	1298.02	3053.22
	H	-2.17347000	1.58789000	1.77160900	439.76	1311.87	3056.74
	H	-1.57574200	1.98551300	0.16211700	478.56	1319.79	3078.76
	H	-3.05676200	-0.57864900	0.92099500	491.12	1353.36	3083.69
	H	-3.73522500	0.76278100	0.00571400	583.60	1359.84	3095.41
	C	1.51062000	-0.62175300	-0.21558600	724.06	1365.26	3097.29
	H	1.67427200	-0.95342200	-1.24982200	791.38	1376.56	3097.81

	C	1.90373500	-1.78482900	0.71519300	802.80	1386.25	3100.97
	H	1.30012900	-2.67330500	0.51565600	842.99	1396.99	3120.20
	H	2.95614200	-2.05096500	0.58410300	856.71	1400.18	3125.14
	H	1.75522900	-1.50079900	1.76114300	872.01	1410.39	3128.77
	C	2.42865400	0.58529000	0.02541000	917.61	1415.33	3133.50
	H	2.40523000	0.86033300	1.08558500	930.71	1468.64	
	H	3.45821700	0.27508200	-0.18072500	957.33	1476.72	
	C	2.07176400	1.79310800	-0.83716700	979.67	1486.37	
	H	2.79152000	2.60353000	-0.70502700	1007.87	1490.35	
	H	2.06044900	1.51994300	-1.89610900	1028.83	1495.09	
	H	1.07859500	2.17560000	-0.58861100	1048.58	1499.52	
	Rotational constants (GHZ):						
		1.93973	0.86298	0.76144			
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	C	1.98305200	-1.40939300	0.11962800			
	C	0.60196200	-1.12733900	-0.47916100	69.89	1054.83	1501.52
	C	-0.00545400	0.17995000	0.08095000	95.57	1073.92	1505.64
	C	0.99738500	1.28140300	-0.07972900	126.88	1088.86	1515.81
	C	2.36795500	1.05693100	0.46625100	187.91	1117.76	1516.71
	C	2.95477500	-0.25023700	-0.10505900	194.49	1144.77	2970.45
	H	0.68373200	-1.03446300	-1.57005500	220.53	1146.97	3008.69
	H	-0.06250200	-1.97194600	-0.27627500	252.46	1171.89	3022.56
	H	1.87426900	-1.58033900	1.19813300	273.71	1197.26	3032.77
	H	2.39041100	-2.33097500	-0.30518600	312.78	1217.48	3038.86
	H	0.83429500	2.04088100	-0.83727800	330.94	1250.33	3049.13
	H	3.02559800	1.90147800	0.25122700	340.04	1264.82	3055.54
	H	2.31871000	0.95388500	1.55997700	414.70	1295.33	3059.80
	H	3.12709200	-0.12368600	-1.17973000	440.24	1308.42	3063.36
	H	3.92246200	-0.46506600	0.35719000	450.90	1315.99	3089.94
sBP6	H	-0.15868800	0.01757700	1.16167800	496.12	1337.32	3093.94
	C	-1.36188000	0.54431800	-0.54826200	549.84	1347.49	3097.97
	H	-1.16352500	0.80868300	-1.59617900	594.34	1352.39	3099.78
	C	-1.96059100	1.77335400	0.14296200	784.23	1367.31	3108.00
	H	-1.30929500	2.64366300	0.04464600	799.03	1371.86	3122.58
	H	-2.93391200	2.02731200	-0.28492900	831.74	1382.59	3130.31
	H	-2.09853600	1.59139300	1.21247600	844.39	1387.32	3135.61
	C	-2.36423700	-0.62177600	-0.56666100	875.61	1414.15	3138.05
	H	-3.29005200	-0.26306400	-1.02844300	909.00	1418.66	3184.35
	H	-1.99025100	-1.41423900	-1.22113100	938.18	1421.52	
	C	-2.68731000	-1.21068000	0.80731000	952.19	1480.83	
	H	-3.42371900	-2.01199500	0.71907900	978.15	1485.18	
	H	-1.79866500	-1.63128400	1.28477000	1000.81	1488.99	
	H	-3.10136500	-0.45700600	1.48065900	1013.76	1493.47	
	Rotational constants (GHZ):				1038.58	1499.79	
		2.24681	0.83312	0.67722			

sBP7	C	-2.00813700	-1.41026100	-0.11592100			
	C	-0.65476600	-1.08121900	0.51638700	72.82	1069.42	1501.22
	C	-0.01051000	0.17106100	-0.09309700	83.26	1088.41	1510.35
	C	-0.98572000	1.36304900	0.00962100	121.95	1109.77	1514.79
	C	-2.36366400	1.02592900	-0.45433300	168.93	1111.64	1522.48
	C	-2.98787500	-0.23868300	0.02990700	196.35	1127.73	2936.96
	H	-0.78390800	-0.92147300	1.59646900	227.81	1148.42	2961.17
	H	0.01048600	-1.94073000	0.40262000	257.81	1165.48	3014.03
	H	-1.86275000	-1.62236200	-1.18113700	269.90	1184.60	3019.40
	H	-2.42725400	-2.31194500	0.33889400	285.46	1232.83	3033.00
	H	-1.01455400	1.67491600	1.07057800	349.81	1244.97	3049.58
	H	-0.60368500	2.21818200	-0.55107600	368.83	1276.52	3055.00
	H	-2.97371600	1.79022700	-0.91956000	396.63	1300.43	3060.94
	H	-3.24845700	-0.14179700	1.09805800	432.90	1306.89	3062.15
	H	-3.92134800	-0.44363600	-0.49928100	450.84	1331.73	3091.45
	H	0.15360300	-0.02066200	-1.16293500	473.02	1342.86	3097.88
	C	1.34830900	0.50493100	0.55324100	559.95	1359.29	3099.62
	H	1.15034700	0.74474400	1.60727100	617.37	1363.85	3105.89
	C	1.98953000	1.73990800	-0.09258800	782.32	1370.86	3108.58
	H	1.43942500	2.65246100	0.14134100	790.30	1373.92	3121.31
	H	3.01388800	1.87417000	0.26400500	834.68	1382.10	3130.57
	H	2.02323200	1.64372200	-1.18202300	853.30	1403.80	3133.84
	C	2.33178200	-0.67950100	0.54692400	867.58	1408.57	3141.59
	H	3.26884100	-0.33928500	0.99957500	904.47	1415.38	3206.11
	H	1.95792500	-1.47410900	1.19817800	935.87	1419.20	
	C	2.62524400	-1.25540500	-0.83883400	942.95	1467.86	
	H	3.38470000	-2.03754000	-0.77938300	979.25	1474.18	
	H	1.73206000	-1.69678600	-1.28798700	1000.54	1487.65	
H	2.99600400	-0.48694500	-1.52144300	1011.69	1495.75		
Rotational constants (GHZ):				1034.21	1499.16		
2.22177				0.84186	0.68004		
sBP8	C	1.99667500	-1.46995900	0.04149300	67.45	1041.73	1502.22
	C	0.62535300	-1.11989100	-0.55685300	83.55	1086.43	1510.90
	C	0.03576700	0.16314500	0.04465600	122.98	1091.32	1516.33
	C	1.03130900	1.31971900	-0.12889000	188.53	1118.77	1523.48
	C	2.40730300	1.00436500	0.47717400	207.35	1131.71	2953.90
	C	2.92917000	-0.30760900	-0.00134300	221.15	1147.00	2958.83
	H	0.72770700	-0.98215500	-1.64107700	244.33	1174.21	3002.63
	H	-0.05170500	-1.96337100	-0.40254400	261.56	1186.49	3022.93
	H	1.83911600	-1.77696900	1.09044800	285.91	1232.66	3036.44
	H	2.42352500	-2.33615700	-0.46965900	349.93	1240.01	3043.29
	H	1.14773500	1.52090800	-1.20159600	368.64	1287.54	3054.82
	H	0.64295900	2.23068200	0.33128900	402.51	1298.33	3061.49
	H	3.11144300	1.81096800	0.25947000	443.27	1309.38	3062.24
	H	2.29644000	0.97855900	1.57528700	448.59	1313.18	3093.38
	H	3.99563200	-0.46722000	-0.10143500	471.26	1345.46	3096.55
	H	-0.09922200	0.00222400	1.12541300	566.86	1350.07	3096.88
	C	-1.33989500	0.50962600	-0.56263500	626.05	1365.51	3109.02
	H	-1.17132700	0.73786300	-1.62416100	783.09	1374.58	3111.35

	C	-1.94945200	1.75644000	0.09218200	787.70	1380.07	3120.61
	H	-1.40977500	2.66495300	-0.17741500	814.29	1385.63	3130.20
	H	-2.98793000	1.88777200	-0.22230200	835.65	1402.79	3134.06
	H	-1.93779500	1.67571100	1.18334700	893.63	1410.10	3143.29
	C	-2.33838900	-0.66158300	-0.51591700	918.59	1415.72	3204.42
	H	-3.28251400	-0.31444800	-0.94806100	938.41	1419.71	
	H	-1.99290400	-1.46948100	-1.16627300	955.51	1469.53	
	C	-2.60266000	-1.21430100	0.88501900	985.46	1478.04	
	H	-3.36835900	-1.99207100	0.85600900	998.65	1483.32	
	H	-1.70187500	-1.65470300	1.31995900	1016.67	1496.34	
	H	-2.95224400	-0.43277800	1.56398600	1041.34	1499.88	
	Rotational constants (GHZ):						
		2.18278	0.85233	0.68674			
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	C	-2.02085400	1.42023400	-0.19927900			
	C	-0.62917000	0.93369600	-0.61252600	73.10	1029.65	1489.03
	C	-0.17545100	-0.27426300	0.21516700	81.07	1058.69	1489.41
	C	-1.22698900	-1.38840200	0.13981400	134.04	1078.15	1494.74
	C	-2.61424300	-0.90380500	0.56404000	136.39	1096.37	1501.27
	C	-3.05360700	0.29505500	-0.27818000	174.45	1109.05	1508.11
	H	-0.64140800	0.64660100	-1.67331700	234.62	1122.37	1509.15
	H	0.08860300	1.75371300	-0.51666000	258.64	1139.20	2971.88
	H	-1.97637100	1.79308600	0.83156900	295.49	1174.49	3016.83
	H	-2.32550000	2.26253000	-0.82636100	314.18	1189.99	3024.08
	H	-1.27504200	-1.75463500	-0.89463700	338.20	1212.24	3024.51
	H	-0.91154900	-2.23424500	0.75897400	401.52	1246.17	3034.01
	H	-3.34065800	-1.71663100	0.47958200	414.48	1274.95	3036.81
	H	-2.58674800	-0.61077300	1.62068300	444.59	1291.84	3040.89
	H	-3.16210100	-0.02101600	-1.32304100	451.47	1297.88	3045.26
iBP1	H	-4.03325700	0.65396100	0.04878900	478.28	1304.42	3052.56
	H	-0.10840200	0.04200600	1.26561600	504.72	1329.85	3067.67
	C	1.18958400	-0.81158400	-0.22334500	581.89	1339.45	3084.87
	H	1.46634300	-1.64844000	0.43052500	792.36	1355.50	3091.53
	H	1.09279200	-1.22766100	-1.23469100	799.09	1368.26	3094.44
	C	2.34996700	0.19741900	-0.22198200	834.02	1380.56	3095.29
	H	2.11775800	0.97918500	-0.96364100	857.28	1385.88	3099.49
	C	2.51952500	0.88334000	1.13736200	866.48	1387.84	3123.35
	H	2.65788900	0.13503600	1.92364800	909.32	1396.22	3134.42
	H	3.39540500	1.53622000	1.13438800	918.19	1407.76	3160.52
	H	1.64923700	1.49137800	1.39350300	939.99	1410.83	3265.26
	C	3.61475700	-0.47492100	-0.64129900	942.58	1464.87	
	H	3.59490500	-1.28310900	-1.36205600	980.01	1478.72	
	H	4.57698400	-0.05782100	-0.37151600	997.86	1482.90	
	Rotational constants (GHZ):						
		2.78799	0.66629	0.61038			

	C	-1.75035400	1.47214000	0.43261800			
	C	-0.41905100	0.99905700	-0.15612800	54.38	1056.26	1490.13
	C	-0.17673400	-0.49126500	0.10166400	68.65	1074.76	1494.32
	C	-1.35925700	-1.32102400	-0.40734400	109.51	1087.07	1502.14
	C	-2.68836400	-0.85274900	0.18851900	120.07	1098.38	1508.73
	C	-2.91868000	0.63402200	-0.08955600	151.33	1124.60	2977.23
	H	-0.41600700	1.17212400	-1.24160200	163.93	1131.73	2981.39
	H	0.40429000	1.58857800	0.25875400	235.82	1194.17	3006.28
	H	-1.70850200	1.38517200	1.52541300	255.89	1212.44	3011.90
	H	-1.90827700	2.53002800	0.20581500	309.23	1275.93	3021.97
	H	-1.40376000	-1.23063400	-1.50125300	330.33	1286.14	3030.18
	H	-1.19185500	-2.37975100	-0.18499800	385.66	1294.14	3036.90
	H	-3.51316400	-1.44823300	-0.21241100	408.94	1297.48	3040.15
	H	-2.67535700	-1.01760900	1.27286700	439.09	1319.14	3045.15
	H	-3.01486000	0.78586900	-1.17174300	446.80	1324.53	3062.98
<i>i</i> BP2	H	-3.85729300	0.96574900	0.36255600	486.83	1340.47	3068.16
	H	-0.10428300	-0.63723300	1.18938000	556.50	1367.49	3069.03
	C	1.14287100	-0.97491900	-0.53488300	781.51	1373.14	3084.36
	H	1.25086900	-2.04355000	-0.29944700	793.95	1385.20	3089.99
	H	1.04857800	-0.89886300	-1.62464700	800.88	1387.69	3093.64
	C	2.35952400	-0.23556200	-0.07375800	849.77	1390.80	3095.22
	C	2.98734900	0.82234700	-0.92085900	865.08	1402.47	3099.38
	H	2.60130000	1.82637000	-0.68267200	910.37	1406.54	3115.68
	H	4.07055600	0.86434600	-0.76456700	931.89	1417.77	3122.58
	H	2.80150000	0.65085200	-1.98347900	943.87	1472.56	
	C	2.69889400	-0.26889500	1.38091300	949.14	1474.14	
	H	2.43039100	-1.22764400	1.83389100	974.35	1478.26	
	H	3.76634400	-0.09627300	1.54675300	987.85	1484.18	
	H	2.16233600	0.51179800	1.94427600	1019.08	1487.51	
	Rotational constants (GHZ):				1038.58	1488.71	
		2.49608	0.71113	0.65373			
	C	-2.52690900	-1.08901900	-0.56388900	41.81	1061.13	1494.57
	C	-1.12812700	-1.38074500	-0.01660500	51.50	1091.61	1505.99
	C	-0.20461600	-0.15204700	-0.10955300	92.73	1109.80	1507.70
	C	-0.86406900	1.04572600	0.60454700	209.35	1115.15	1515.05
	C	-2.26174400	1.33907900	0.05481700	234.94	1116.76	2994.28
	C	-3.16218700	0.10606900	0.14916600	238.07	1152.10	3009.82
	H	-1.20211500	-1.67722300	1.03787100	247.97	1187.76	3032.10
	H	-0.67281800	-2.22034300	-0.54968500	264.91	1200.86	3035.97
<i>i</i> BP3	H	-2.45420700	-0.87022600	-1.63634700	287.17	1203.18	3039.39
	H	-3.16150200	-1.97390400	-0.46423100	314.37	1243.89	3041.35
	H	-0.93330800	0.81172800	1.67478600	362.77	1288.69	3045.78
	H	-0.22100300	1.92611600	0.51534300	394.70	1291.59	3046.68
	H	-2.70825600	2.17969300	0.59307300	437.74	1298.60	3052.37
	H	-2.17794100	1.64370000	-0.99573800	461.02	1321.75	3091.59
	H	-3.31529700	-0.14612000	1.20567900	484.06	1325.77	3093.59
	H	-4.14790200	0.32104000	-0.27223200	522.60	1345.17	3094.28
	H	-0.10168800	0.10930100	-1.17331400	568.87	1357.89	3095.24
	C	1.15220900	-0.44715700	0.43967900	795.60	1371.20	3099.94

	H	1.22416700	-0.76837600	1.47635100	807.47	1383.81	3119.17
	C	2.40612800	-0.17680900	-0.32947800	840.55	1384.77	3123.62
	H	2.30957800	-0.65520600	-1.31588000	864.11	1386.68	3127.68
	C	2.59299100	1.33128300	-0.57785800	899.07	1396.48	3134.35
	H	2.71102000	1.85677200	0.37436000	907.31	1414.69	3157.83
	H	3.48214500	1.51695300	-1.18669800	928.22	1439.93	
	H	1.73115500	1.75856300	-1.09609700	936.45	1480.83	
	C	3.63169200	-0.75990800	0.37296600	954.92	1485.68	
	H	3.52266600	-1.83599900	0.52503300	972.84	1488.49	
	H	4.54016900	-0.58462900	-0.20784600	1007.39	1490.96	
	H	3.76292600	-0.29066700	1.35281100	1052.52	1492.73	
	Rotational constants (GHZ):						
		2.80855	0.64608	0.57094			
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	C	-1.90176000	-1.26096600	-0.50487100			
	C	-0.89509500	-1.27445400	0.65426900	56.07	1072.03	1500.35
	C	-0.11186500	0.00000700	0.73119700	63.45	1078.61	1502.90
	C	-0.89507700	1.27447600	0.65423000	95.48	1096.64	1512.15
	C	-1.90179200	1.26096400	-0.50487200	182.91	1108.10	1515.17
	C	-2.76684500	-0.00001200	-0.46345800	221.95	1112.97	2948.19
	H	-1.45712300	-1.41509400	1.59511700	265.93	1172.23	2950.85
	H	-0.22220100	-2.13261900	0.56874300	287.26	1187.87	3018.94
	H	-1.35240300	-1.28706800	-1.45344400	290.78	1209.95	3035.47
	H	-2.52805100	-2.15648600	-0.46902000	304.82	1231.56	3043.63
	H	-1.45706400	1.41516200	1.59509500	367.94	1256.27	3045.05
	H	-0.22216800	2.13262300	0.56864400	392.88	1285.04	3045.99
	H	-2.52810200	2.15646800	-0.46897400	407.83	1296.79	3046.64
	H	-1.35247300	1.28710500	-1.45346400	410.49	1317.36	3049.75
	H	-3.35969700	-0.00002300	0.46001400	446.16	1321.27	3064.53
iBP4	H	-3.47558900	-0.00002000	-1.29590300	531.03	1356.74	3087.16
	C	1.30209500	0.00000800	1.22156300	571.51	1363.59	3088.59
	H	1.47709100	0.88171800	1.85104600	750.71	1365.78	3096.55
	H	1.47708400	-0.88168800	1.85106600	792.44	1376.92	3096.64
	C	2.36332800	-0.00001200	0.09386300	805.98	1378.10	3099.92
	H	3.34466000	-0.00002200	0.58288300	852.52	1385.99	3115.98
	C	2.25948900	-1.25603900	-0.77091400	859.10	1406.01	3120.37
	H	1.29858800	-1.28177300	-1.29456400	877.44	1410.31	3123.46
	H	3.05126700	-1.27680900	-1.52386100	925.53	1421.37	3126.01
	H	2.34209100	-2.16442100	-0.16777500	928.92	1467.42	
	C	2.25952400	1.25602300	-0.77091000	943.23	1475.12	
	H	2.34209700	2.16440200	-0.16775900	964.74	1482.84	
	H	3.05133200	1.27680100	-1.52382400	978.66	1486.28	
	H	1.29864500	1.28176300	-1.29460000	994.46	1490.73	
	Rotational constants (GHZ):				1043.76	1490.82	
		2.07204	0.86140	0.76590			

	C	2.66535200	-0.88178800	0.53597500			
	C	1.28478000	-1.39282500	0.11673300	55.81	1068.37	1498.25
	C	0.21945600	-0.27703200	0.20337800	89.81	1076.29	1502.00
	C	0.69496900	0.91281400	-0.56738100	106.99	1103.43	1507.96
	C	2.04695600	1.44759000	-0.22697000	166.40	1116.19	1518.01
	C	3.09926600	0.32097000	-0.30524500	203.07	1145.84	2987.29
	H	1.32771900	-1.75628200	-0.91763100	237.49	1161.70	3008.55
	H	0.98147300	-2.23739800	0.74428900	264.52	1167.02	3022.65
	H	2.63343700	-0.58840400	1.59262100	291.57	1203.44	3035.96
	H	3.40364700	-1.68410500	0.45326600	312.83	1218.62	3039.97
	H	0.24225000	1.14769400	-1.52484800	316.75	1245.79	3043.00
	H	2.32402100	2.27806000	-0.87918000	340.80	1266.15	3045.32
	H	2.04220500	1.83212500	0.80338000	407.32	1291.68	3048.50
	H	3.20982000	0.01026300	-1.35018000	437.29	1304.74	3050.29
	H	4.07259200	0.69161000	0.02851000	452.35	1316.59	3067.34
<i>iBP5</i>	H	0.16189700	0.00361000	1.26728500	475.62	1341.81	3085.18
	C	-1.15179900	-0.78061500	-0.24754200	532.07	1343.40	3094.34
	H	-1.06304200	-1.16184600	-1.27316600	596.12	1351.90	3099.11
	H	-1.43655000	-1.63683600	0.37830000	802.30	1368.32	3110.16
	C	-2.28206400	0.25536500	-0.20023000	821.92	1371.50	3113.39
	H	-2.04488600	1.05504800	-0.91147900	846.41	1384.67	3118.72
	C	-3.59866300	-0.39110000	-0.63158000	856.19	1395.49	3127.81
	H	-3.88846600	-1.17459800	0.07608500	879.15	1403.95	3131.18
	H	-4.40743000	0.34278200	-0.66709600	928.97	1420.37	3187.88
	H	-3.51164700	-0.84873700	-1.62039700	934.25	1427.32	
	C	-2.42153000	0.88555800	1.18573600	937.66	1477.45	
	H	-1.53923900	1.47192300	1.45201000	964.27	1482.37	
	H	-3.28768400	1.55077800	1.22343000	978.28	1487.33	
	H	-2.56045600	0.11069900	1.94756200	985.69	1490.35	
	Rotational constants (GHZ):				1042.86	1493.51	
		2.80424	0.65547	0.60381			
	C	-2.12288200	1.38792700	-0.16482600	67.98	1062.08	1496.84
	C	-0.74340000	0.89905700	-0.61187800	81.67	1087.11	1498.27
	C	-0.24914800	-0.27719900	0.23685300	130.94	1107.34	1509.01
	C	-1.27790800	-1.42344900	0.19264600	163.78	1126.60	1516.55
	C	-2.66079100	-0.95463600	0.49992500	186.50	1136.02	2947.29
	C	-3.15977800	0.25578000	-0.21663100	237.32	1141.02	2961.05
	H	-0.78760500	0.58098200	-1.66329600	263.61	1172.81	3017.13
	H	-0.02993200	1.72670400	-0.56270000	284.34	1201.80	3019.70
<i>iBP6</i>	H	-2.05297100	1.75887000	0.86387100	295.92	1223.25	3036.22
	H	-2.44911800	2.22472700	-0.78832900	313.03	1247.53	3044.20
	H	-1.25025400	-1.85249200	-0.82557700	366.26	1272.76	3045.56
	H	-0.97423100	-2.22523800	0.87154600	409.36	1302.67	3049.52
	H	-3.35251100	-1.60513000	1.02023400	423.38	1303.56	3050.52
	H	-3.34244700	0.00959000	-1.27695900	453.69	1327.05	3065.29
	H	-4.11626700	0.58864500	0.19282300	458.79	1349.21	3089.07
	H	-0.18738500	0.06165600	1.27913700	510.89	1357.51	3094.00
	C	1.12542600	-0.78832600	-0.20197800	632.22	1365.06	3098.81
	H	1.41761200	-1.61445500	0.46089600	788.72	1366.68	3100.07

	H	1.03215500	-1.22023900	-1.20719500	821.09	1372.17	3113.77
	C	2.26309200	0.24045600	-0.21565500	848.90	1399.65	3119.20
	H	2.04030200	0.99478700	-0.97908300	853.04	1401.83	3127.65
	C	2.41112300	0.94793400	1.13177400	871.71	1403.88	3130.12
	H	2.55408200	0.21457100	1.93269400	925.47	1410.08	3207.51
	H	3.27816300	1.61308100	1.12852800	931.36	1421.96	
	H	1.53190400	1.54701800	1.37942400	937.40	1467.11	
	C	3.57424900	-0.44368900	-0.60481500	963.46	1473.62	
	H	3.48344200	-0.95862400	-1.56459700	977.78	1479.93	
	H	4.39030700	0.27878700	-0.68282000	989.78	1488.27	
	H	3.85485400	-1.18637600	0.14891300	1052.48	1493.63	
	Rotational constants (GHZ):						
		2.81191	0.66028	0.60252			
	<hr/>						
	C	-2.11102300	1.43272100	-0.23104800			
	C	-0.71829300	0.93665600	-0.65064600	68.54	1042.23	1483.21
	C	-0.27186000	-0.27233500	0.17826900	80.61	1056.66	1493.22
	C	-1.30648100	-1.39743800	0.06036600	130.68	1085.18	1497.78
	C	-2.70428600	-0.94316200	0.50417400	154.10	1103.25	1498.63
	C	-3.10369600	0.31925300	-0.18513500	215.98	1117.94	1509.17
	H	-0.73834600	0.64628800	-1.70900600	231.20	1135.61	1515.97
	H	0.00065300	1.75523300	-0.55512700	247.21	1152.96	2954.44
	H	-2.01981400	1.88593600	0.77166500	267.68	1173.09	2960.53
	H	-2.44905400	2.23038300	-0.89681400	294.56	1201.81	3014.99
	H	-1.35151000	-1.72276800	-0.98634200	312.76	1231.32	3018.56
	H	-0.98604300	-2.26046900	0.65254700	360.29	1232.98	3036.27
	H	-3.43858400	-1.73313800	0.32946400	407.86	1283.26	3041.86
	H	-2.68044700	-0.77802900	1.59525500	430.97	1291.13	3043.56
	H	-4.14831000	0.51711400	-0.39160000	449.35	1306.83	3045.53
<i>iBP7</i>	H	-0.23528700	0.03364200	1.23374700	459.79	1321.41	3049.95
	C	1.11166600	-0.78518400	-0.23310700	527.22	1342.84	3065.04
	H	1.37910200	-1.62623300	0.42104700	640.06	1351.03	3089.05
	H	1.04139800	-1.19682500	-1.24863000	782.06	1369.95	3096.80
	C	2.25765000	0.23372500	-0.19590300	798.12	1370.47	3097.01
	H	2.06242000	1.00503200	-0.94978400	838.02	1379.34	3098.60
	C	2.37400600	0.91251900	1.16924800	863.36	1399.58	3113.62
	H	2.49214200	0.16188400	1.95816400	904.71	1400.67	3119.41
	H	3.24417400	1.57273900	1.20271500	918.69	1404.92	3127.88
	H	1.49152300	1.51128300	1.40616500	933.21	1411.27	3129.63
	C	3.57343200	-0.45384100	-0.56261800	950.48	1421.88	3202.93
	H	3.50487700	-0.94871700	-1.53470300	963.60	1469.12	
	H	4.39715500	0.26296900	-0.60372200	977.45	1476.96	
	H	3.82725400	-1.21379700	0.18335400	992.90	1478.99	
	Rotational constants (GHZ):						
		2.76789	0.66650	0.60695			

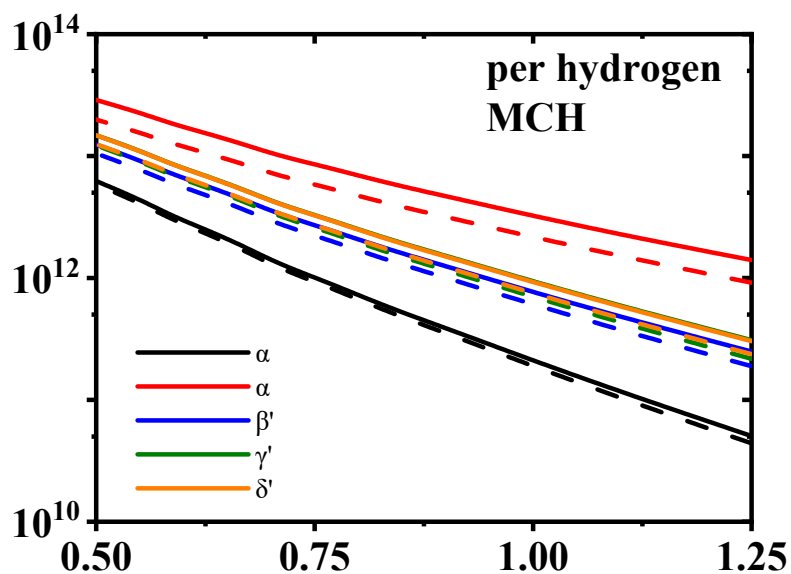


Figure S 1 Comparison of rate constants for H-atom abstractions (on a per hydrogen atom basis) by $\dot{\text{H}}$ atom from methyl cyclohexane (MCH) at different positions (α , α' , β' , γ' , and δ'). The solid lines shows calculations from this work at the QCISD(T)/MP2/CBS//M06-2X/6-311++G(d,p) level. The dashed lines show the results which calculate the geometry and frequencies of Wang et al.¹with MESS program .

References

1. Z. Wang, L. Ye, W. Yuan, L. Zhang, Y. Wang, Z. Cheng, F. Zhang and F. Qi, *Combustion and flame*, 2014, **161**, 84-100.