

Supporting Information for: **Reactions of *o*-benzyne with propargyl and benzyl radicals: potential sources of polycyclic aromatic hydrocarbons in combustion**

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Table S1. Geometries, rotational constants, vibrational frequencies, and hindered-rotor parameters of the reactant, products, intermediates and the transition states.^a

species	rotational constants (GHz)	geometries (Å)	frequencies (cm ⁻¹) ^b	parameters for hindered rotations ^c
<i>o</i> -C ₆ H ₄	7.04	C, 0.000000, 1.458281, -0.133835	394, 427, 450	
	5.73	C, 0.000000, 0.702289, 1.056543	603, 626, 750	
	3.16	C, 0.000000, -0.702289, 1.056543	847, 869, 922	
		C, 0.000000, -1.458281, -0.133835	971, 998, 1074	
		C, 0.000000, -0.621928, -1.234452	1108, 1161, 1271	
		C, 0.000000, 0.621928, -1.234452	1305, 1424, 1467	
		H, 0.000000, 2.540578, -0.135723	1482, 2012, 3159	
		H, 0.000000, 1.227778, 2.006190	3174, 3195, 3199	
		H, 0.000000, -1.227778, 2.006190		
		H, 0.000000, -2.540578, -0.135723		
C ₃ H ₃	290.12	C, 0.000000, 0.000000, -1.251200	352, 403, 467	
	9.58	C, 0.000000, 0.000000, 0.115722	637, 682, 1031	
	9.27	C, 0.000000, 0.000000, 1.337847	1089, 1455, 2011	
		H, 0.000000, 0.929631, -1.807109	3139, 3229, 3468	
		H, 0.000000, -0.929631, -1.807109		
		H, 0.000000, 0.000000, 2.400002		
C ₇ H ₅	8.49	C, 0.000000, 0.000000, 0.327054	146, 160, 403	
	1.97	C, 0.000000, 1.174114, -0.525971	513, 523, 561	
	1.60	C, 0.000000, -1.174114, -0.525971	601, 626, 642	
		C, 0.000000, 0.737701, -1.816295	656, 716, 750	
		C, 0.000000, -0.737701, -1.816295	894, 909, 910	
		C, 0.000000, 0.000000, 1.718072	992, 1036, 1087	
		C, 0.000000, 0.000000, 2.931522	1118, 1282, 1300	
		H, 0.000000, 2.192574, -0.169449	1405, 1499, 1525	
		H, 0.000000, -2.192574, -0.169449	2092, 3206, 3218	
		H, 0.000000, 1.355038, -2.703959	3240, 3244, 3469	
		H, 0.000000, -1.355038, -2.703959		
		H, 0.000000, 0.000000, 3.994118		
C ₂ H ₂	0.00	C, 0.000000, 0.000000, 0.599075	642, 642, 772	
	35.64	C, 0.000000, 0.000000, -0.599075	772, 2069, 3420	
	35.64	H, 0.000000, 0.000000, 1.661926	3523	
		H, 0.000000, 0.000000, -1.661926		

Table S1. (Continued.)

species	rotational constants (GHz)	geometries (Å)	frequencies (cm ⁻¹) ^b	parameters for hindered rotations ^c
C ₇ H ₇	5.55	C, 0.000000, 0.000000, 0.993561	198, 359, 389	
	2.71	C, 0.000000, 1.216272, 0.251256	478, 501, 534	
	1.82	C, 0.000000, 1.209621, -1.131383	628, 684, 707	
		C, 0.000000, 0.000000, -1.835778	773, 828, 831	
		C, 0.000000, -1.209621, -1.131383	898, 969, 971	
		C, 0.000000, -1.216272, 0.251256	989, 995, 1036	
		C, 0.000000, 0.000000, 2.397549	1116, 1174, 1184	
		H, 0.000000, 2.157325, 0.790857	1288, 1328, 1352	
		H, 0.000000, 2.148839, -1.673557	1474, 1489, 1502	
		H, 0.000000, 0.000000, -2.919421	1577, 1599, 3144	
		H, 0.000000, -2.148839, -1.673557	3158, 3161, 3173	
		H, 0.000000, -2.157325, 0.790857	3178, 3191, 3241	
		H, 0.000000, 0.926921, 2.957176		
		H, 0.000000, -0.926921, 2.957176		
C ₁₃ H ₁₀	2.19	C, 0.000000, 1.650276, -1.501671	97, 136, 216	
	0.59	C, 0.000000, 3.012606, -1.208713	242, 275, 420	
	0.46	C, 0.000000, 3.456327, 0.115321	422, 437, 480	
		C, 0.000000, 2.541298, 1.170318	498, 553, 576	
		C, 0.000000, 1.183237, 0.884396	637, 645, 711	
		C, 0.000000, 0.734274, -0.450065	741, 754, 756	
		H, 0.000000, 1.313248, -2.532470	796, 814, 854	
		H, 0.000000, 3.736114, -2.016263	870, 879, 930	
		H, 0.000000, 4.519945, 0.325339	947, 973, 987	
		H, 0.000000, 2.892779, 2.196990	989, 1025, 1046	
		C, 0.000000, -1.183237, 0.884396	1052, 1117, 1131	
		C, 0.000000, -2.541298, 1.170318	1163, 1176, 1180	
		C, 0.000000, -3.456327, 0.115321	1192, 1208, 1221	
		C, 0.000000, -3.012606, -1.208713	1253, 1320, 1330	
		C, 0.000000, -1.650276, -1.501671	1345, 1375, 1451	
		C, 0.000000, -0.734274, -0.450065	1479, 1485, 1510	
		C, 0.000000, 0.000000, 1.828428	1511, 1620, 1624	
		H, 0.000000, -2.892779, 2.196990	1650, 1651, 3020	
		H, 0.000000, -4.519945, 0.325339	3044, 3157, 3158	
		H, 0.000000, -3.736114, -2.016263	3163, 3165, 3174	
		H, 0.000000, -1.313248, -2.532470	3176, 3187, 3188	
		H, 0.879085, 0.000000, 2.483600		
		H, -0.879085, 0.000000, 2.483600		

Table S1. (Continued.)

species	rotational constants (GHz)	geometries (Å)	frequencies (cm ⁻¹) ^b	parameters for hindered rotations ^c
A1	4.67	C, 0.006583, -0.933857, 0.000000	(14) ^d , 128, 186	$n = 1$
	1.03	C, 1.209513, -1.642060, 0.000000	305, 321, 416	$V_r = 345$
	0.85	C, 2.432576, -0.976536, 0.000000	423, 479, 607	$I = 29.1$
		C, 2.458733, 0.426456, 0.000000	632, 661, 679	
		C, 1.244546, 1.063098, 0.000000	687, 741, 796	
		C, 0.000000, 0.468014, 0.000000	846, 921, 961	
		H, -0.940455, -1.462506, 0.000000	971, 989, 991	
		H, 1.187156, -2.725892, 0.000000	1043, 1119, 1173	
		H, 3.363176, -1.533908, 0.000000	1195, 1238, 1262	
		H, 3.397203, 0.969892, 0.000000	1316, 1339, 1448	
		C, -1.271405, 1.310332, 0.000000	1461, 1475, 1577	
		C, -2.523237, 0.560509, 0.000000	1634, 2225, 3020	
		C, -3.560339, -0.045460, 0.000000	3042, 3158, 3169	
		H, -4.481398, -0.574777, 0.000000	3176, 3187, 3477	
		H, -1.253752, 1.972106, 0.873500		
		H, -1.253752, 1.972106, -0.873500		
A2	4.99	C, -0.143293, -0.976106, 0.000000	(56) ^d , 116, 199	$n = 2$
	0.98	C, -1.402284, -1.565321, 0.000000	319, 325, 412	$V_r = 1743$
	0.82	C, -2.561710, -0.786381, 0.000000	434, 459, 606	$I = 23.6$
		C, -2.457147, 0.610535, 0.000000	627, 642, 710	
		C, -1.188887, 1.134539, 0.000000	751, 824, 854	
		C, 0.000000, 0.427547, 0.000000	881, 910, 943	
		H, 0.749536, -1.593111, 0.000000	985, 989, 1012	
		H, -1.483297, -2.646403, 0.000000	1042, 1093, 1122	
		H, -3.539470, -1.255849, 0.000000	1171, 1207, 1273	
		H, -3.340829, 1.239109, 0.000000	1319, 1355, 1441	
		C, 1.303930, 1.113211, 0.000000	1467, 1492, 1570	
		C, 2.477455, 0.529670, 0.000000	1631, 2035, 3104	
		C, 3.644352, -0.046334, 0.000000	3135, 3157, 3163	
		H, 1.269268, 2.199924, 0.000000	3173, 3174, 3186	
		H, 4.155148, -0.295914, 0.926378		
		H, 4.155148, -0.295914, -0.926378		
A3	4.70	C, 0.132013, -0.994046, 0.000000	86, 124, 216	
	1.03	C, -0.987858, -1.809049, 0.000000	329, 399, 427	
	0.84	C, -2.271184, -1.253476, 0.000000	435, 478, 517	
		C, -2.422130, 0.135597, 0.000000	628, 639, 665	
		C, -1.307710, 0.959047, 0.000000	685, 704, 781	
		C, 0.000000, 0.415891, 0.000000	835, 842, 916	
		H, 1.124959, -1.427966, 0.000000	978, 997, 1002	
		H, -0.866914, -2.886688, 0.000000	1040, 1069, 1111	
		H, -3.143544, -1.896695, 0.000000	1178, 1185, 1230	
		H, -3.414525, 0.572452, 0.000000	1321, 1351, 1406	
		C, 1.132082, 1.291327, 0.000000	1486, 1507, 1592	
		C, 2.457531, 0.881207, 0.000000	1610, 2075, 3150	
		C, 3.623960, 0.539418, 0.000000	3160, 3166, 3176	
		H, 4.644600, 0.245220, 0.000000	3185, 3192, 3469	
		H, 0.944473, 2.361002, 0.000000		
		H, -1.429282, 2.037182, 0.000000		

Table S1. (Continued.)

species	rotational constants (GHz)	geometries (Å)	frequencies (cm ⁻¹) ^b	parameters for hindered rotations ^c
A4	5.57	C, 0.000000, 1.215130, -0.673015	88, 93, 242	
	0.87	C, 0.000000, 1.207882, -2.059719	256, 309, 410	
	0.75	C, 0.000000, 0.000000, -2.760417	412, 437, 528	
		C, 0.000000, -1.207882, -2.059719	528, 634, 696	
		C, 0.000000, -1.215130, -0.673015	719, 731, 769	
		C, 0.000000, 0.000000, 0.051016	844, 923, 979	
		H, 0.000000, 2.150580, -0.126955	999, 1002, 1029	
		H, 0.000000, 2.147594, -2.600500	1040, 1066, 1101	
		H, 0.000000, 0.000000, -3.844274	1180, 1197, 1306	
		H, 0.000000, -2.147594, -2.600500	1350, 1363, 1469	
		C, 0.000000, 0.000000, 1.456620	1471, 1526, 1592	
		C, 0.000000, 0.000000, 2.690009	1618, 2075, 3133	
		C, 0.000000, 0.000000, 4.043694	3165, 3173, 3185	
		H, 0.000000, -0.928115, 4.603227	3192, 3197, 3218	
		H, 0.000000, -2.150580, -0.126955		
		H, 0.000000, 0.928115, 4.603227		
A5	3.61	C, 0.375721, -0.722528, 0.347465	175, 189, 365	
	1.70	C, 2.425562, 0.078056, -0.223014	403, 500, 531	
	1.19	C, 0.312807, 0.775415, 0.122635	540, 569, 655	
		C, 1.568095, 1.235771, -0.157081	700, 704, 777	
		C, -0.856696, -1.449761, -0.095491	802, 835, 852	
		C, -2.017825, -0.774303, -0.192626	865, 969, 974	
		H, -2.933770, -1.306627, -0.426370	988, 1015, 1033	
		C, -2.089308, 0.667920, -0.014448	1080, 1107, 1164	
		H, -3.061967, 1.144659, -0.061615	1173, 1189, 1240	
		C, -0.968810, 1.422879, 0.124000	1262, 1341, 1389	
		H, -0.817248, -2.525179, -0.230662	1438, 1523, 1563	
		H, -1.025834, 2.506115, 0.143271	1580, 1670, 2879	
		C, 1.809674, -1.090701, -0.011433	3155, 3163, 3176	
		H, 1.866911, 2.262484, -0.314381	3185, 3217, 3226	
		H, 2.221725, -2.087735, 0.037508		
		H, 0.394866, -0.850207, 1.452214		
A6	3.76	C, 0.000000, 0.743175, 0.000000	192, 210, 350	
	1.66	C, 2.317424, 0.817191, 0.000000	388, 424, 540	
	1.16	C, 0.531945, -0.564944, 0.000000	547, 595, 724	
		C, 2.008883, -0.477346, 0.000000	737, 756, 823	
		C, -1.369392, 0.949996, 0.000000	834, 859, 868	
		C, -2.219168, -0.162200, 0.000000	927, 952, 962	
		H, -3.293527, -0.017090, 0.000000	987, 1041, 1106	
		C, -1.695781, -1.455070, 0.000000	1132, 1162, 1175	
		H, -2.369567, -2.304782, 0.000000	1189, 1213, 1248	
		C, -0.315809, -1.669936, 0.000000	1315, 1357, 1438	
		H, -1.782562, 1.953347, 0.000000	1481, 1487, 1600	
		H, 0.084017, -2.678016, 0.000000	1628, 1642, 3032	
		C, 1.145217, 1.748342, 0.000000	3061, 3158, 3165	
		H, 2.680975, -1.324802, 0.000000	3176, 3187, 3208	
		H, 1.130378, 2.398045, 0.881876		
		H, 1.130378, 2.398045, -0.881876		

Table S1. (Continued.)

species	rotational constants (GHz)	geometries (Å)	frequencies (cm ⁻¹) ^b	parameters for hindered rotations ^c
A7	3.94	C, 0.000000, 0.713901, 0.257841	199, 239, 391	
	1.62	C, 0.000000, 0.000000, 2.457468	414, 534, 549	
	1.15	C, 0.000000, -0.713901, 0.257841	559, 579, 712	
		C, 0.000000, -1.140032, 1.645311	743, 754, 759	
		C, 0.000000, 1.414721, -0.939020	804, 864, 875	
		C, 0.000000, 0.695902, -2.145652	887, 902, 943	
		H, 0.000000, 1.232282, -3.087625	979, 1013, 1034	
		C, 0.000000, -0.695902, -2.145652	1081, 1092, 1181	
		H, 0.000000, -1.232282, -3.087625	1185, 1213, 1219	
		C, 0.000000, -1.414721, -0.939020	1329, 1372, 1384	
		H, 0.000000, 2.499577, -0.950471	1464, 1488, 1490	
		H, 0.000000, -2.499577, -0.950471	1618, 1625, 3160	
		C, 0.000000, 1.140032, 1.645311	3166, 3176, 3189	
		H, 0.000000, -2.166838, 1.985769	3203, 3210, 3229	
		H, 0.000000, 0.000000, 3.538069		
		H, 0.000000, 2.166838, 1.985769		
A8	4.43	C, -0.059009, -0.001686, 0.000000	110, 122, 203	
	1.33	C, 0.761092, 2.213823, 0.000000	441, 464, 515	
	1.31	C, -1.158841, 1.030538, 0.000000	529, 610, 720	
		C, -0.722935, 2.287839, 0.000000	749, 753, 787	
		C, -0.076740, -0.956614, 1.182696	816, 819, 825	
		C, -0.076740, -2.222338, 0.736326	864, 941, 955	
		H, -0.078530, -3.113394, 1.350908	955, 965, 991	
		C, -0.076740, -2.222338, -0.736326	1036, 1062, 1079	
		H, -0.078530, -3.113394, -1.350908	1110, 1140, 1190	
		C, -0.076740, -0.956614, -1.182696	1221, 1297, 1321	
		H, -0.078171, -0.613103, 2.207118	1385, 1546, 1569	
		H, -0.078171, -0.613103, -2.207118	1630, 1638, 3184	
		C, 1.159624, 0.931092, 0.000000	3191, 3202, 3214	
		H, -1.305080, 3.198827, 0.000000	3222, 3227, 3232	
		H, 1.409247, 3.081942, 0.000000		
		H, 2.171416, 0.550025, 0.000000		
A9	3.86	C, 0.221421, 0.729382, 0.150787	163, 199, 352	
	1.61	C, 0.329366, -0.779442, 0.367000	411, 486, 532	
	1.17	C, 1.467001, 1.199813, -0.131844	547, 571, 673	
		C, 1.757953, -1.084088, 0.002922	707, 729, 805	
		C, 2.400019, 0.085829, -0.212275	821, 850, 852	
		C, -1.078687, 1.345148, 0.142197	871, 951, 961	
		C, -2.185394, 0.580928, -0.037660	967, 998, 1018	
		H, 1.729887, 2.238062, -0.291031	1064, 1112, 1149	
		H, 2.190608, -2.073572, 0.039817	1157, 1196, 1237	
		H, 3.458196, 0.193324, -0.413787	1285, 1296, 1376	
		C, -0.893319, -1.448428, -0.116475	1400, 1533, 1553	
		C, -2.084289, -0.871379, -0.234347	1618, 1668, 2890	
		H, 0.320875, -0.934922, 1.467371	3151, 3161, 3180	
		H, -2.978670, -1.432750, -0.485585	3190, 3203, 3227	
		H, -3.168001, 1.037165, -0.089362		
		H, -1.157330, 2.426123, 0.190747		

Table S1. (Continued.)

species	rotational constants (GHz)	geometries (Å)	frequencies (cm ⁻¹) ^b	parameters for hindered rotations ^c
A10	3.85	C, -0.274756, -0.816700, 0.153087	155, 187, 353	
	1.61	C, -0.270837, 0.691354, 0.389273	437, 463, 536	
	1.17	C, -1.544358, -1.205214, -0.153615	543, 565, 659	
		C, -1.677871, 1.087967, 0.032586	686, 714, 803	
		C, -2.398311, -0.030088, -0.213541	821, 840, 852	
		C, 0.992582, -1.435553, 0.155476	870, 951, 966	
		C, 2.156753, -0.797247, -0.011940	968, 1006, 1017	
		H, -1.869341, -2.221798, -0.329303	1068, 1107, 1139	
		H, -2.048722, 2.103305, 0.073740	1155, 1191, 1240	
		H, -3.459254, -0.060783, -0.426199	1264, 1323, 1378	
		C, 0.981796, 1.362483, -0.110043	1392, 1516, 1553	
		C, 2.117919, 0.654786, -0.244458	1609, 1668, 2884	
		H, 0.973120, 2.436555, -0.261014	3152, 3165, 3178	
		H, -0.248537, 0.828534, 1.492365	3192, 3210, 3219	
		H, 3.041351, 1.151100, -0.525288		
		H, 3.113881, -1.307635, -0.005248		
A11	6.62	C, 0.702944, -0.000292, 0.165671	(74) ^d , 77, 154	$n = 2$
	0.72	C, 1.576870, 1.181767, 0.026683	210, 231, 339	$V_r = 1820$
	0.68	C, 1.577529, -1.181822, 0.026433	477, 534, 561	$I = 12.7$
		C, 2.836976, 0.734844, -0.174874	622, 670, 674	
		C, 2.837378, -0.734154, -0.175081	720, 778, 818	
		C, -0.597221, -0.000602, 0.374706	829, 849, 891	
		C, -1.889760, -0.000200, 0.573180	900, 925, 938	
		H, 1.230691, 2.202701, 0.082131	1000, 1051, 1096	
		H, 1.231937, -2.202967, 0.081669	1101, 1168, 1219	
		H, 3.715882, 1.349531, -0.315460	1260, 1306, 1364	
		H, 3.716625, -1.348319, -0.315817	1438, 1523, 1607	
		C, -4.192974, 0.000273, -0.322536	1629, 2003, 3111	
		C, -2.892110, -0.000015, -0.510853	3124, 3200, 3212	
		H, -4.897422, 0.000450, 0.495977	3237, 3240, 3241	
		H, -2.261735, -0.000235, 1.596002		
		H, -2.493766, 0.000052, -1.524482		
A12	2.63	C, -0.132792, -0.049264, -0.000038	(96) ^d , 118, 156	$n = 4$
	1.51	C, 0.824194, 0.046270, 1.184324	166, 305, 352	$V_r = 1287$
	1.25	C, 0.824288, 0.046025, -1.184345	456, 491, 521	$I = 11.7$
		C, 2.086523, 0.121021, 0.735380	595, 613, 666	
		C, 2.086579, 0.120913, -0.735314	679, 697, 753	
		C, -1.119940, 1.030306, -0.000171	758, 807, 842	
		C, -1.934035, 1.913895, -0.000035	857, 876, 957	
		H, 0.476398, 0.028618, 2.206931	961, 978, 1013	
		H, 0.476580, 0.028166, -2.206978	1076, 1090, 1141	
		H, 2.977194, 0.176942, 1.347938	1156, 1274, 1297	
		H, 2.977298, 0.176736, -1.347811	1386, 1560, 1641	
		H, -2.642501, 2.705432, -0.000045	1648, 2217, 3116	
		C, -0.779894, -1.457915, 0.000079	3192, 3204, 3231	
		C, -2.058848, -1.716231, 0.000079	3235, 3257, 3477	
		H, -2.998111, -1.186181, -0.000011		
		H, -0.043316, -2.259830, 0.000220		

Table S1. (Continued.)

species	rotational constants (GHz)	geometries (Å)	frequencies (cm ⁻¹) ^b	parameters for hindered rotations ^c
A13	2.01	C, -0.379423, -0.708940, -0.056942	(73) ^d , 107, 148	$n = 3$
	1.79	C, 0.499650, 0.487706, -0.413213	172, 293, 344	$V_r = 1095$
	1.00	C, 0.423818, -1.765053, 0.230203	428, 523, 531	$I = 14.2$
		C, 1.891979, -0.081276, -0.285882	570, 608, 623	
		C, 1.822450, -1.372583, 0.089523	681, 700, 731	
		C, -1.789311, -0.665605, -0.055696	806, 818, 878	
		C, -2.993529, -0.598843, -0.066374	903, 927, 962	
		H, 0.080602, -2.751572, 0.511986	990, 1023, 1040	
		H, 2.784075, 0.502934, -0.463389	1121, 1169, 1206	
		H, 2.661160, -2.034901, 0.260534	1238, 1272, 1280	
		C, 0.275665, 1.683906, 0.512502	1376, 1543, 1631	
		C, -0.068815, 2.881249, 0.118975	1655, 2195, 3034	
		H, 0.427895, 1.473802, 1.570982	3105, 3196, 3213	
		H, -0.295212, 3.398709, -0.801775	3226, 3236, 3477	
		H, -4.054324, -0.546798, -0.069928		
		H, 0.300905, 0.794459, -1.446986		
A14	4.85	C, 1.134396, 0.024028, -0.080776	(77) ^d , 89, 161	$n = 3$
	0.93	C, 0.078198, -0.756971, -0.411322	184, 295, 339	$V_r = 1088$
	0.82	C, 0.654550, 1.410689, 0.118668	444, 496, 530	$I = 13.2$
		C, -1.177552, 0.076702, -0.444730	573, 631, 650	
		C, -0.669752, 1.455904, -0.090120	684, 696, 732	
		C, 2.489128, -0.377691, 0.056281	778, 839, 864	
		C, 3.646468, -0.688598, 0.177176	883, 923, 946	
		H, 0.101161, -1.818097, -0.613547	956, 1021, 1036	
		H, 1.302143, 2.234612, 0.386913	1100, 1180, 1212	
		H, -1.313410, 2.321267, -0.015236	1236, 1257, 1279	
		C, -3.447808, -0.798349, 0.217516	1364, 1562, 1639	
		C, -2.236976, -0.427893, 0.540937	1651, 2208, 3018	
		H, -4.061238, -0.884960, -0.667473	3104, 3203, 3226	
		H, -1.908182, -0.461981, 1.579440	3228, 3234, 3476	
		H, 4.664484, -0.973192, 0.282392		
		H, -1.608865, 0.075421, -1.454268		
A15	2.82	C, -0.413075, -0.001124, 0.242523	125, 154, 245	
	1.67	C, 0.624271, 0.543803, -0.850306	263, 406, 484	
	1.33	C, 0.306026, -1.192745, 0.829802	500, 527, 571	
		C, 1.770448, -0.418545, -0.772508	656, 662, 671	
		C, 1.539310, -1.366165, 0.217231	691, 698, 738	
		C, -1.784668, -0.256154, -0.166347	803, 868, 925	
		C, -2.925205, -0.466103, -0.485435	948, 953, 980	
		H, -0.107196, -1.800772, 1.622771	1009, 1051, 1074	
		H, 2.246479, -2.139764, 0.493941	1093, 1109, 1144	
		C, -0.147472, 1.342206, 0.952667	1194, 1265, 1273	
		C, 0.716384, 1.786069, 0.040063	1323, 1396, 1461	
		H, -0.534415, 1.726347, 1.888715	1630, 2209, 3050	
		H, 1.324413, 2.678945, -0.042779	3174, 3177, 3203	
		H, -3.930076, -0.651726, -0.775348	3206, 3217, 3476	
		H, 0.221326, 0.708112, -1.853649		
		H, 2.663362, -0.348594, -1.379795		

Table S1. (Continued.)

species	rotational constants (GHz)	geometries (Å)	frequencies (cm ⁻¹) ^b	parameters for hindered rotations ^c
A16	3.55	C, -0.802838, 0.274063, 0.094496	100, 150, 252	
	1.39	C, 0.283919, -0.623825, 0.645224	262, 403, 456	
	1.09	C, -0.220088, 1.500019, -0.317197	502, 522, 558	
		C, 1.598531, 0.244461, 0.531034	610, 663, 716	
		C, 1.129044, 1.533773, -0.077712	729, 766, 856	
		C, -2.143282, -0.082817, -0.004872	865, 894, 908	
		C, -3.308968, -0.415249, -0.075898	949, 954, 982	
		H, -0.787791, 2.296348, -0.783380	1014, 1075, 1088	
		H, 1.782954, 2.361717, -0.320419	1172, 1189, 1213	
		C, 0.964140, -1.566969, -0.349241	1234, 1268, 1281	
		C, 2.079690, -0.839589, -0.442414	1297, 1408, 1470	
		H, 0.618066, -2.479588, -0.819818	1626, 2091, 3033	
		H, 2.993268, -0.934782, -1.017836	3051, 3170, 3184	
		H, -4.329824, -0.700638, -0.141536	3202, 3205, 3472	
		H, 2.197620, 0.365419, 1.439553		
		H, 0.044822, -1.051685, 1.622918		
TS(A1-A3)	4.34	C, -0.626457, 1.289600, 0.280761	2224i, 86, 102	
	1.00	C, -1.963781, 1.170455, -0.114127	226, 357, 387	
	0.89	C, -2.541929, -0.075938, -0.380751	403, 436, 509	
		C, -1.809216, -1.267738, -0.268494	620, 622, 634	
		C, -0.495754, -1.113001, 0.137322	666, 715, 749	
		C, 0.089081, 0.105629, 0.402426	803, 869, 901	
		H, -0.184550, 2.261281, 0.470420	947, 990, 992	
		H, -2.569702, 2.063300, -0.221388	1017, 1027, 1122	
		H, -3.582885, -0.121984, -0.684161	1145, 1174, 1202	
		H, -2.259663, -2.228505, -0.485285	1266, 1302, 1343	
		C, 1.482032, -0.353425, 0.762483	1456, 1481, 1585	
		C, 2.597553, -0.030687, -0.052264	1635, 1759, 2156	
		C, 3.543076, 0.210268, -0.764004	3091, 3156, 3171	
		H, 4.373313, 0.431048, -1.388750	3184, 3191, 3474	
		H, 1.692073, -0.438196, 1.829485		
		H, 0.883788, -1.577927, 0.459566		
TS(A1-A6)	3.77	C, 0.207202, -0.615856, 0.000001	416i, 115, 192	
	1.40	C, 2.509259, -0.065962, -0.000017	316, 325, 416	
	1.03	C, 0.118303, 0.765427, 0.000002	476, 488, 595	
		C, 2.427799, 1.161182, 0.000006	634, 666, 695	
		C, -0.989397, -1.337201, 0.000000	731, 743, 797	
		C, -2.210139, -0.659992, -0.000001	853, 926, 963	
		H, -3.135769, -1.224451, -0.000002	964, 985, 986	
		C, -2.251312, 0.734222, -0.000001	1038, 1120, 1171	
		H, -3.205911, 1.250064, -0.000002	1191, 1196, 1238	
		C, -1.061066, 1.475194, 0.000000	1303, 1327, 1452	
		H, -0.972008, -2.423474, -0.000001	1466, 1476, 1586	
		H, -1.083137, 2.559558, -0.000001	1629, 1983, 3030	
		C, 1.608085, -1.228197, 0.000005	3055, 3146, 3157	
		H, 2.710750, 2.189118, 0.000002	3171, 3183, 3423	
		H, 1.766831, -1.861874, -0.879073		
		H, 1.766840, -1.861840, 0.879106		

Table S1. (Continued.)

species	rotational constants (GHz)	geometries (Å)	frequencies (cm ⁻¹) ^b	parameters for hindered rotations ^c
TS(A2-A3)	4.00	C, 0.054397, 0.817581, -0.046484	1453i, 124, 191	
	1.32	C, -1.155444, 1.471448, -0.036777	216, 369, 418	
	1.00	C, -2.316789, 0.688508, 0.005627	443, 484, 525	
		C, -2.217528, -0.706182, 0.042643	607, 622, 685	
		C, -0.977693, -1.330014, 0.047026	699, 747, 790	
		C, 0.213907, -0.568839, 0.034041	843, 865, 917	
		H, 1.592454, 1.353998, -0.473721	945, 980, 986	
		H, -1.221341, 2.552504, -0.095874	1039, 1122, 1151	
		H, -3.290599, 1.166156, -0.007305	1171, 1203, 1250	
		H, -3.119146, -1.307234, 0.074583	1305, 1351, 1368	
		C, 1.539901, -1.177187, -0.073005	1447, 1460, 1559	
		C, 2.579681, -0.316773, 0.054693	1601, 1730, 1857	
		C, 2.635062, 0.977728, 0.014067	3153, 3160, 3169	
		H, 3.191231, 1.710815, 0.580760	3172, 3186, 3223	
		H, 1.623883, -2.201075, -0.419813		
		H, -0.909441, -2.412790, 0.090380		
TS(A2-A4)	5.49	C, 0.709270, 1.303498, -0.000007	2283i, 79, 117	
	0.89	C, 2.100770, 1.174598, 0.000004	236, 341, 374	
	0.77	C, 2.726033, -0.078315, 0.000010	375, 420, 429	
		C, 1.986823, -1.273328, 0.000006	543, 602, 645	
		C, 0.616275, -1.116963, -0.000005	702, 753, 760	
		C, -0.024703, 0.118712, -0.000011	848, 869, 943	
		H, 0.236601, 2.278508, -0.000011	968, 989, 991	
		H, 2.717317, 2.066564, 0.000008	1019, 1021, 1083	
		H, 3.810009, -0.127977, 0.000018	1133, 1181, 1255	
		H, 2.477787, -2.238649, 0.000011	1307, 1362, 1452	
		C, -1.402680, -0.329915, -0.000019	1469, 1501, 1585	
		C, -2.652030, -0.059199, -0.000008	1624, 1795, 2006	
		C, -3.959014, 0.124274, 0.000018	3110, 3158, 3174	
		H, -0.809301, -1.581624, -0.000010	3185, 3189, 3192	
		H, -4.518414, 0.211508, 0.926883		
		H, -4.518456, 0.211495, -0.926823		
TS(A2-A6)	3.84	C, 0.000000, 0.681313, 0.000000	396i, 128, 199	
	1.39	C, -2.290924, 0.955965, 0.000000	338, 342, 403	
	1.03	C, -0.312658, -0.677218, 0.000000	491, 514, 600	
		C, -2.673858, -0.331654, 0.000000	630, 661, 710	
		C, 1.357492, 1.018377, 0.000000	758, 826, 844	
		C, 2.325948, 0.010300, 0.000000	861, 885, 932	
		H, 3.376036, 0.280239, 0.000000	964, 981, 1004	
		C, 1.961749, -1.333505, 0.000000	1034, 1096, 1116	
		H, 2.723272, -2.106002, 0.000000	1174, 1208, 1234	
		C, 0.601543, -1.696751, 0.000000	1312, 1340, 1443	
		H, 1.657107, 2.062003, 0.000000	1464, 1473, 1577	
		H, 0.307422, -2.740739, 0.000000	1621, 1805, 3099	
		C, -1.150306, 1.616163, 0.000000	3151, 3159, 3170	
		H, -1.021705, 2.691180, 0.000000	3172, 3184, 3191	
		H, -2.978029, -0.822314, 0.922093		
		H, -2.978029, -0.822314, -0.922093		

Table S1. (Continued.)

species	rotational constants (GHz)	geometries (Å)	frequencies (cm ⁻¹) ^b	parameters for hindered rotations ^c
TS(A3-A5)	3.63	C, 0.258572, -0.750340, 0.407450	746i, 169, 201	
	1.57	C, 2.464812, 0.179662, -0.222335	348, 426, 466	
	1.13	C, 0.265567, 0.706667, 0.232241	496, 541, 570	
		C, 1.535743, 1.229565, 0.003182	587, 668, 684	
		C, -0.946099, -1.451668, 0.087633	729, 736, 821	
		C, -2.089959, -0.751793, -0.207055	840, 857, 945	
		H, -3.008387, -1.287377, -0.421009	952, 981, 996	
		C, -2.116832, 0.674135, -0.158552	1011, 1094, 1110	
		H, -3.047998, 1.191134, -0.360317	1172, 1184, 1240	
		C, -0.974545, 1.392080, 0.088317	1290, 1337, 1386	
		H, -0.972169, -2.533424, 0.161998	1455, 1462, 1531	
		H, -0.981992, 2.476204, 0.048283	1599, 1653, 3032	
		C, 2.102599, -1.052020, -0.293844	3159, 3165, 3176	
		H, 1.768150, 2.285835, -0.030752	3188, 3201, 3314	
		H, 2.452121, -2.067546, -0.308990		
		H, 0.791130, -1.122554, 1.288572		
TS(A5-A6)	3.75	C, 0.320839, -0.711713, 0.089786	1121i, 212, 238	
	1.68	C, 2.457521, 0.073671, -0.103789	390, 433, 538	
	1.17	C, 0.315043, 0.746447, 0.032281	543, 559, 587	
		C, 1.647604, 1.198756, -0.062708	724, 727, 741	
		C, -0.915577, -1.432492, -0.053377	798, 820, 843	
		C, -2.082567, -0.719585, -0.067576	867, 872, 953	
		H, -3.026967, -1.247174, -0.143411	983, 1014, 1073	
		C, -2.094341, 0.705306, 0.003510	1101, 1135, 1169	
		H, -3.047739, 1.220976, -0.002642	1174, 1192, 1269	
		C, -0.926772, 1.427278, 0.045537	1313, 1365, 1394	
		H, -0.916615, -2.515214, -0.107986	1433, 1473, 1504	
		H, -0.946823, 2.511764, 0.050267	1555, 1645, 2142	
		C, 1.769881, -1.124690, -0.018212	3160, 3167, 3179	
		H, 1.970157, 2.230167, -0.046115	3189, 3216, 3248	
		H, 2.115900, -2.144642, -0.071730		
		H, 0.902306, -1.033750, 1.128906		
TS(A6-A7)	3.76	C, -0.298065, -0.713830, -0.048186	1438i, 206, 234	
	1.68	C, -2.441484, 0.066876, -0.012708	397, 419, 470	
	1.17	C, -0.304132, 0.729096, -0.042312	551, 568, 589	
		C, -1.640059, 1.206424, -0.040862	630, 721, 747	
		C, 0.921056, -1.426336, -0.000217	778, 785, 845	
		C, 2.100969, -0.720251, 0.014043	857, 891, 955	
		H, 3.047535, -1.248634, 0.022979	988, 1012, 1022	
		C, 2.102546, 0.701402, 0.020652	1080, 1135, 1158	
		H, 3.053514, 1.222736, 0.040768	1177, 1230, 1234	
		C, 0.933274, 1.422801, 0.008369	1331, 1334, 1362	
		H, 0.921988, -2.510951, 0.005423	1379, 1483, 1517	
		H, 0.949745, 2.506888, 0.026061	1566, 1648, 2068	
		C, -1.649493, -1.165046, -0.056231	3158, 3166, 3177	
		H, -1.965132, 2.234199, -0.004055	3187, 3238, 3244	
		H, -2.312776, -0.649397, 1.037019		
		H, -2.042552, -2.161654, -0.183483		

Table S1. (Continued.)

species	rotational constants (GHz)	geometries (Å)	frequencies (cm ⁻¹) ^b	parameters for hindered rotations ^c
TS(A7-A8)	4.38	C, -0.009071, 0.392480, 0.064320	422i, 169, 233	
	1.51	C, -2.323021, 0.304387, 0.214907	331, 478, 479	
	1.33	C, -0.561651, -0.744252, -0.803039	553, 568, 709	
		C, -1.905839, -0.827850, -0.594960	717, 752, 766	
		C, 0.614650, -0.873747, 0.668285	797, 823, 829	
		C, 1.971098, -0.832940, 0.404769	870, 891, 907	
		H, 2.678328, -1.604434, 0.677841	946, 956, 1016	
		C, 2.290956, 0.379702, -0.290016	1038, 1077, 1090	
		H, 3.277195, 0.640260, -0.651027	1111, 1150, 1185	
		C, 1.162509, 1.121763, -0.466456	1251, 1294, 1368	
		H, 0.098053, -1.549673, 1.331598	1374, 1421, 1438	
		H, 1.084559, 2.062707, -0.992471	1555, 1570, 3178	
		C, -1.237234, 1.015046, 0.620619	3198, 3199, 3211	
		H, -2.559251, -1.618773, -0.939939	3213, 3227, 3245	
		H, -3.352094, 0.530042, 0.470008		
		H, -1.241168, 1.932339, 1.193427		
TS(A7-A9)	3.92	C, 0.256366, 0.743981, 0.010637	1232i, 185, 219	
	1.62	C, 0.268979, -0.739360, 0.056734	284, 397, 415	
	1.15	C, 1.600009, 1.163530, -0.036844	547, 567, 573	
		C, 1.670278, -1.139468, 0.005241	637, 704, 740	
		C, 2.430877, 0.013889, -0.066945	755, 784, 820	
		C, -0.973579, 1.387977, 0.038589	861, 906, 931	
		C, -2.159906, 0.634798, 0.020300	956, 980, 1005	
		H, 1.945416, 2.186736, 0.025126	1046, 1053, 1085	
		H, 2.018252, -2.161298, -0.029159	1147, 1202, 1241	
		H, 3.510932, 0.039315, -0.122068	1245, 1300, 1339	
		C, -0.951257, -1.506438, -0.041095	1381, 1424, 1470	
		C, -2.145553, -0.754575, -0.110453	1500, 1598, 2203	
		H, -0.231853, -1.241246, 1.081560	3146, 3159, 3174	
		H, -3.081548, -1.277641, -0.280763	3200, 3214, 3234	
		H, -3.111261, 1.156359, 0.049895		
		H, -1.027218, 2.471769, 0.018421		
TS(A8-A11)	3.95	C, -0.522127, -0.020121, 0.000000	440i, 91, 119	
	1.24	C, 1.426091, 1.993053, 0.000000	155, 350, 433	
	1.22	C, -0.789193, 1.319977, 0.000000	524, 551, 580	
		C, -0.015494, 2.386764, 0.000000	629, 643, 665	
		C, -0.545402, -0.914201, 1.181570	726, 753, 795	
		C, -0.545402, -2.189900, 0.735003	806, 811, 872	
		H, -0.536429, -3.080404, 1.349288	896, 928, 937	
		C, -0.545402, -2.189900, -0.735003	960, 998, 1088	
		H, -0.536429, -3.080404, -1.349288	1099, 1149, 1183	
		C, -0.545402, -0.914201, -1.181570	1216, 1301, 1341	
		H, -0.552022, -0.562828, 2.202083	1409, 1522, 1603	
		H, -0.552022, -0.562828, -2.202083	1607, 1759, 3106	
		C, 1.709889, 0.708053, 0.000000	3198, 3198, 3210	
		H, -0.328124, 3.422671, 0.000000	3238, 3242, 3283	
		H, 2.198287, 2.762315, 0.000000		
		H, 2.541396, 0.024326, 0.000000		

Table S1. (Continued.)

species	rotational constants (GHz)	geometries (Å)	frequencies (cm ⁻¹) ^b	parameters for hindered rotations ^c
TS(A8-A12)	3.68	C, -0.043332, 0.021950, 0.000000	486i, 123, 128	
	1.34	C, 1.117067, 2.191040, 0.000000	180, 375, 425	
	1.28	C, -1.119621, 1.034042, 0.000000	485, 503, 524	
		C, -1.220836, 2.260986, 0.000000	592, 666, 671	
		C, -0.076051, -0.934551, 1.183005	675, 728, 751	
		C, -0.076051, -2.199995, 0.736161	752, 811, 837	
		H, -0.079184, -3.092512, 1.348681	863, 873, 959	
		C, -0.076051, -2.199995, -0.736161	961, 988, 1032	
		H, -0.079184, -3.092512, -1.348681	1084, 1091, 1146	
		C, -0.076051, -0.934551, -1.183005	1161, 1224, 1300	
		H, -0.077717, -0.588282, 2.206500	1388, 1563, 1629	
		H, -0.077717, -0.588282, -2.206500	1642, 1967, 3125	
		C, 1.237947, 0.883323, 0.000000	3191, 3202, 3228	
		H, -1.666979, 3.229626, 0.000000	3232, 3234, 3420	
		H, 1.786659, 3.038793, 0.000000		
		H, 2.192005, 0.359695, 0.000000		
TS(A9-A10)	3.97	C, 0.255136, 0.729071, 0.082312	1110i, 202, 223	
	1.60	C, 0.311748, -0.812804, 0.088037	388, 453, 485	
	1.15	C, 1.595690, 1.156377, -0.033060	546, 575, 613	
		C, 1.679330, -1.155365, -0.035340	692, 715, 720	
		C, 2.421884, 0.027016, -0.097214	748, 784, 821	
		C, -1.045519, 1.361054, -0.000811	846, 869, 937	
		C, -2.180825, 0.617628, -0.048961	962, 981, 1057	
		H, 1.917831, 2.187576, -0.028161	1072, 1115, 1140	
		H, 2.064040, -2.163602, -0.032439	1163, 1218, 1225	
		H, 3.502835, 0.064977, -0.133964	1288, 1339, 1407	
		C, -0.955417, -1.449316, -0.013122	1453, 1490, 1512	
		C, -2.146532, -0.839537, -0.056078	1549, 1660, 2060	
		H, 0.218996, -0.051549, 1.135599	3161, 3171, 3186	
		H, -3.077992, -1.392573, -0.108103	3199, 3222, 3237	
		H, -3.147165, 1.107301, -0.096873		
		H, -1.091513, 2.443118, -0.050634		
TS(A10-A11)	3.63	C, -0.335161, -0.757006, 0.300804	413i, 131, 158	
	1.41	C, -0.616924, 0.584965, 0.871902	222, 296, 436	
	1.17	C, -1.462948, -1.106936, -0.534687	502, 551, 593	
		C, -1.852147, 0.970878, 0.378518	623, 644, 657	
		C, -2.355476, -0.064365, -0.484479	726, 751, 798	
		C, 0.913259, -1.221106, 0.357020	815, 818, 846	
		C, 2.148003, -0.799084, 0.222856	872, 900, 929	
		H, -1.536351, -2.005496, -1.128406	963, 1029, 1070	
		H, -2.359889, 1.899597, 0.599920	1083, 1161, 1188	
		H, -3.289120, -0.011671, -1.028725	1220, 1301, 1338	
		C, 1.270053, 1.389570, -0.489988	1367, 1456, 1512	
		C, 2.268420, 0.531500, -0.461105	1594, 1864, 3078	
		H, 1.126683, 2.395154, -0.852790	3178, 3200, 3214	
		H, -0.075388, 1.029816, 1.691885	3237, 3243, 3254	
		H, 3.239919, 0.788398, -0.887890		
		H, 3.031678, -1.266298, 0.640955		

Table S1. (Continued.)

species	rotational constants (GHz)	geometries (Å)	frequencies (cm ⁻¹) ^b	parameters for hindered rotations ^c
TS(A10-A13)	3.16	C, -0.202509, -0.814273, 0.149449	404i, 110, 144	
	1.61	C, -0.317159, 0.662478, 0.498138	224, 304, 423	
	1.12	C, -1.411934, -1.269694, -0.262395	458, 494, 541	
		C, -1.751529, 0.966127, 0.148292	585, 607, 619	
		C, -2.366452, -0.165335, -0.250778	659, 707, 736	
		C, 1.086534, -1.374695, 0.156819	817, 821, 863	
		C, 2.297287, -1.194981, 0.069741	873, 889, 957	
		H, -1.632120, -2.281256, -0.575928	998, 1030, 1060	
		H, -2.205001, 1.940712, 0.271955	1114, 1167, 1203	
		H, -3.409184, -0.259767, -0.524916	1211, 1259, 1280	
		C, 0.779027, 1.530737, -0.117581	1378, 1545, 1634	
		C, 2.014790, 1.153377, -0.350975	1645, 2023, 2958	
		H, 0.483113, 2.561266, -0.335070	3042, 3192, 3209	
		H, -0.226030, 0.759614, 1.593786	3212, 3219, 3435	
		H, 2.871033, 1.673159, -0.759113		
		H, 3.349860, -1.356167, 0.085025		
TS(A12-A15)	2.48	C, -0.354001, 0.063227, 0.169195	562i, 122, 153	
	1.70	C, 0.604297, 0.173543, -1.041559	212, 261, 352	
	1.33	C, 0.374718, -0.940187, 1.050181	467, 492, 540	
		C, 1.658673, -0.685503, -0.841263	577, 645, 665	
		C, 1.518728, -1.332774, 0.445159	676, 680, 744	
		C, -1.726388, -0.322346, -0.146788	748, 806, 818	
		C, -2.865017, -0.621313, -0.389178	845, 890, 896	
		H, 0.007222, -1.238026, 2.021894	954, 1011, 1067	
		H, 2.240726, -2.023828, 0.862051	1076, 1091, 1137	
		C, -0.184641, 1.477039, 0.720475	1153, 1203, 1296	
		C, 0.699155, 2.104582, -0.024858	1383, 1427, 1571	
		H, -0.700281, 1.824497, 1.614778	1634, 2214, 3106	
		H, 1.192382, 3.068730, -0.029885	3190, 3199, 3207	
		H, -3.868343, -0.890445, -0.610973	3226, 3231, 3477	
		H, 0.290770, 0.599669, -1.982873		
		H, 2.484393, -0.838205, -1.523186		
TS(A13-A15)	2.77	C, -0.387544, -0.348791, 0.056681	622i, 135, 153	
	1.63	C, 0.579842, 0.505144, -0.808416	215, 255, 361	
	1.24	C, 0.366804, -1.374046, 0.632918	443, 506, 536	
		C, 1.904392, -0.181112, -0.587834	550, 611, 656	
		C, 1.743771, -1.234852, 0.254009	667, 681, 723	
		C, -1.790184, -0.410772, -0.165043	799, 811, 827	
		C, -2.974198, -0.484145, -0.375822	876, 900, 953	
		H, -0.035408, -2.152387, 1.266228	983, 1007, 1042	
		H, 2.537323, -1.883305, 0.603832	1105, 1138, 1191	
		C, -0.263584, 1.563699, 1.019927	1231, 1247, 1254	
		C, 0.488698, 1.802478, -0.033899	1384, 1400, 1551	
		H, -0.633657, 2.084546, 1.893871	1639, 2198, 3030	
		H, 1.015952, 2.717843, -0.300261	3103, 3190, 3205	
		H, -4.019133, -0.540820, -0.556285	3213, 3222, 3478	
		H, 0.288875, 0.570807, -1.863206		
		H, 2.838065, 0.177694, -0.999302		

Table S1. (Continued.)

species	rotational constants (GHz)	geometries (Å)	frequencies (cm ⁻¹) ^b	parameters for hindered rotations ^c
TS(A13-A16)	2.98	C, -0.745229, 0.386109, 0.081228	586i, 109, 151	
	1.47	C, 0.362267, -0.417873, 0.749600	214, 253, 349	
	1.09	C, -0.205400, 1.545582, -0.413967	463, 526, 542	
		C, 1.589896, 0.471049, 0.540945	586, 601, 666	
		C, 1.196233, 1.614578, -0.124810	677, 689, 744	
		C, -2.074691, -0.056958, -0.018042	813, 834, 866	
		C, -3.209493, -0.467917, -0.077631	888, 905, 930	
		H, -0.764232, 2.299520, -0.953355	952, 1008, 1038	
		H, 1.840984, 2.436943, -0.404133	1097, 1166, 1213	
		C, 1.930923, -1.341084, -0.644621	1231, 1255, 1277	
		C, 0.776486, -1.617058, -0.072372	1380, 1400, 1553	
		H, 2.612940, -1.823580, -1.334622	1638, 2167, 3025	
		H, 0.160288, -2.507901, -0.193182	3099, 3192, 3198	
		H, -4.210091, -0.818697, -0.138486	3210, 3225, 3475	
		H, 0.129395, -0.637114, 1.798684		
		H, 2.504759, 0.352251, 1.103112		
TS(A14-A16)	4.44	C, 0.995173, 0.005606, -0.161412	602i, 99, 154	
	1.08	C, 0.163105, -1.040894, -0.437900	245, 248, 366	
	1.01	C, 0.259809, 1.258060, -0.265679	444, 530, 541	
		C, -1.221772, -0.528541, -0.728136	611, 648, 667	
		C, -1.058586, 0.988662, -0.561381	668, 683, 743	
		C, 2.370621, -0.086647, 0.186883	794, 817, 842	
		C, 3.537579, -0.141114, 0.478507	884, 890, 911	
		H, 0.700070, 2.232250, -0.105885	932, 995, 1020	
		C, -2.345636, 0.365464, 1.044786	1090, 1173, 1196	
		C, -2.180448, -0.782620, 0.418393	1225, 1245, 1269	
		H, -2.874025, 0.724226, 1.920359	1345, 1422, 1571	
		H, -2.584384, -1.761301, 0.676669	1635, 2209, 3010	
		H, 4.566319, -0.197237, 0.737023	3098, 3190, 3206	
		H, -1.592591, -0.841797, -1.712980	3220, 3224, 3477	
		H, 0.432443, -2.087108, -0.403471		
		H, -1.766899, 1.703114, -0.956073		
TS(A11-C ₇ H ₅ +H)	4.50	C, 0.695726, -0.109240, 0.303127	660i, (36) ^d , 71	<i>n</i> = 1
	0.76	C, 1.412935, 1.163062, 0.291346	75, 165, 188	<i>V_r</i> = 959
	0.73	C, 1.614358, -1.127495, -0.199643	278, 467, 539	<i>I</i> = 15.1
		C, 2.662032, 0.922494, -0.187603	540, 556, 575	
		C, 2.787980, -0.507935, -0.494242	639, 644, 676	
		C, -0.577653, -0.310587, 0.720421	715, 760, 761	
		C, -1.788922, -0.476378, 0.977634	780, 785, 900	
		H, 0.992385, 2.105043, 0.608910	904, 910, 917	
		H, 1.371916, -2.174397, -0.302551	1003, 1089, 1092	
		H, 3.445219, 1.654979, -0.327985	1148, 1294, 1323	
		H, 3.677776, -0.978437, -0.889883	1419, 1501, 1557	
		C, -3.785094, 0.678818, -0.626511	1814, 1967, 3202	
		C, -3.025306, -0.287274, -0.668755	3213, 3235, 3240	
		H, -4.293877, 1.570319, -0.341619	3341, 3349, 3444	
		H, -2.491397, -0.698437, 1.753801		
		H, -2.678362, -1.151857, -1.195317		

Table S1. (Continued.)

species	rotational constants (GHz)	geometries (Å)	frequencies (cm ⁻¹) ^b	parameters for hindered rotations ^c
TS(A12-C ₇ H ₅ +H)	2.49	C, -0.074622, -0.294826, 0.000000	602i, (69) ^d , 131	$n = 1$
	1.47	C, 0.819156, -0.265146, -1.177124	147, 166, 243	$V_r = 1034$
	1.18	C, 0.819156, -0.265146, 1.177124	282, 440, 511	$I = 11.9$
		C, 2.094465, -0.147100, -0.731981	516, 541, 582	
		C, 2.094465, -0.147100, 0.731981	640, 644, 647	
		C, -1.286028, -1.039380, 0.000000	669, 735, 755	
		C, -2.317922, -1.661685, 0.000000	762, 797, 884	
		H, 0.468053, -0.307165, -2.196996	921, 934, 951	
		H, 0.468053, -0.307164, 2.196996	1004, 1090, 1098	
		H, 2.979371, -0.067006, -1.349012	1147, 1263, 1297	
		H, 2.979371, -0.067005, 1.349012	1398, 1508, 1581	
		H, -3.213919, -2.232263, 0.000000	1770, 2187, 3200	
		C, -0.577663, 1.672516, 0.000000	3212, 3238, 3242	
		C, -1.780328, 1.987168, 0.000000	3293, 3416, 3475	
		H, -2.839653, 1.861514, 0.000000		
		H, 0.414645, 2.083278, -0.000001		
TS(A13-C ₇ H ₅ +H)	1.93	C, 0.578318, -0.596821, 0.092122	574i, (54) ^d , 113	$n = 1$
	1.68	C, -0.505788, 0.140883, 0.771765	139, 167, 227	$V_r = 1169$
	1.00	C, 0.002197, -1.682032, -0.522147	257, 432, 524	$I = 14.6$
		C, -1.717177, -0.632530, 0.587282	534, 556, 573	
		C, -1.416885, -1.700284, -0.213100	593, 628, 642	
		C, 1.935972, -0.210310, 0.087787	683, 735, 757	
		C, 3.092560, 0.132530, 0.101418	787, 848, 881	
		H, 0.522691, -2.409622, -1.128734	910, 923, 946	
		H, -2.683806, -0.369815, 0.990510	1001, 1023, 1114	
		H, -2.111414, -2.453083, -0.560965	1197, 1245, 1287	
		C, -0.825421, 1.640144, -0.649655	1382, 1473, 1572	
		C, -0.788117, 2.802513, -0.239853	1823, 2193, 3204	
		H, -0.950114, 0.979477, -1.484566	3220, 3224, 3237	
		H, -0.703228, 3.677625, 0.361566	3318, 3440, 3477	
		H, 4.112310, 0.428664, 0.107550		
		H, -0.320392, 0.782195, 1.620919		
TS(A14-C ₇ H ₅ +H)	3.85	C, -1.099671, 0.083049, 0.140393	618i, (61) ^d , 87	$n = 1$
	0.96	C, -0.096517, -0.508732, 0.875027	164, 173, 232	$V_r = 1248$
	0.86	C, -0.592475, 1.364955, -0.385908	263, 440, 501	$I = 13.2$
		C, 1.075456, 0.332604, 0.787965	531, 551, 576	
		C, 0.688264, 1.527215, 0.027782	615, 641, 647	
		C, -2.402402, -0.413313, -0.084015	677, 727, 765	
		C, -3.522106, -0.815036, -0.287583	821, 841, 885	
		H, -0.156318, -1.452003, 1.396047	910, 928, 965	
		H, -1.176263, 2.040450, -0.995108	990, 1017, 1095	
		H, 1.344063, 2.357835, -0.187801	1208, 1253, 1314	
		C, 3.308192, -0.979783, -0.400193	1355, 1499, 1565	
		C, 2.147370, -0.647187, -0.671975	1800, 2180, 3209	
		H, 4.224513, -1.129642, 0.123375	3216, 3235, 3240	
		H, 1.386178, -0.647205, -1.428103	3305, 3429, 3476	
		H, -4.505918, -1.175463, -0.461782		
		H, 1.847081, 0.343394, 1.544424		

Table S1. (Continued.)

species	rotational constants (GHz)	geometries (Å)	frequencies (cm ⁻¹) ^b	parameters for hindered rotations ^c
B1	2.08	C, 3.410404, 0.938169, 0.337686	(10) ^d , (17) ^d , 61	$n = 2$
	0.42	C, 3.689847, 0.183232, -0.807775	186, 226, 281	$V_r = 154$
	0.41	C, 2.777828, -0.781542, -1.239154	339, 414, 416	$I = 64.0$
		C, 1.591938, -1.003449, -0.544363	461, 485, 554	$n = 2$
		C, 1.280556, -0.265076, 0.612771	614, 631, 637	$V_r = 229$
		C, 2.223778, 0.668879, 0.978072	699, 716, 743	$I = 61.4$
		H, 4.101619, 1.694100, 0.693770	750, 820, 830	
		H, 4.611574, 0.350980, -1.354711	857, 857, 910	
		H, 2.994169, -1.365984, -2.126322	939, 946, 978	
		H, 0.888724, -1.751909, -0.897871	985, 991, 1001	
		C, -1.267678, -0.160536, 0.618700	1018, 1043, 1051	
		C, -2.249713, -1.128336, 0.395083	1098, 1120, 1170	
		C, -3.418160, -0.816497, -0.300096	1181, 1187, 1203	
		C, -3.619750, 0.473037, -0.782156	1206, 1217, 1273	
		C, -2.645773, 1.447922, -0.565374	1315, 1329, 1343	
		C, -1.481399, 1.132803, 0.127111	1363, 1448, 1477	
		C, -0.003292, -0.495322, 1.392276	1482, 1489, 1527	
		H, -2.101696, -2.135621, 0.771687	1574, 1625, 1634	
		H, -4.168527, -1.582352, -0.463138	1646, 3033, 3070	
		H, -4.526842, 0.718695, -1.322815	3150, 3153, 3158	
		H, -2.794772, 2.455660, -0.937451	3160, 3168, 3172	
		H, -0.725075, 1.894614, 0.284993	3176, 3184, 3187	
		H, 0.035543, 0.104224, 2.306228		
		H, -0.046232, -1.542112, 1.708952		
B2	2.58	C, -0.357347, 2.868011, -1.404434	55, 59, 111	
	0.40	C, 0.009970, 3.942752, -0.592459	204, 238, 298	
	0.35	C, 0.350563, 3.705735, 0.741815	316, 411, 423	
		C, 0.337045, 2.416644, 1.247595	486, 494, 578	
		C, 0.000000, 1.301952, 0.435970	627, 629, 652	
		C, -0.366128, 1.572923, -0.907199	694, 703, 718	
		H, -0.653038, 3.045351, -2.432780	762, 799, 817	
		H, 0.016955, 4.951399, -0.988962	840, 848, 890	
		H, 0.624183, 4.533418, 1.386911	915, 921, 976	
		H, 0.602806, 2.242914, 2.285150	981, 994, 997	
		C, 0.000000, -1.301952, 0.435970	1002, 1007, 1044	
		C, -0.337045, -2.416644, 1.247595	1046, 1098, 1119	
		C, -0.350563, -3.705735, 0.741815	1179, 1179, 1190	
		C, -0.009970, -3.942752, -0.592459	1203, 1227, 1232	
		C, 0.357347, -2.868011, -1.404434	1328, 1332, 1349	
		C, 0.366128, -1.572923, -0.907199	1362, 1429, 1477	
		C, 0.000000, 0.000000, 1.034967	1497, 1506, 1515	
		H, -0.602806, -2.242914, 2.285150	1589, 1591, 1608	
		H, -0.624183, -4.533418, 1.386911	1621, 3138, 3157	
		H, -0.016955, -4.951399, -0.988962	3158, 3164, 3165	
		H, 0.653038, -3.045351, -2.432780	3174, 3175, 3188	
		H, 0.704549, -0.767062, -1.543840	3189, 3201, 3215	
		H, -0.704549, 0.767062, -1.543840		
		H, 0.000000, 0.000000, 2.121786		

Table S1. (Continued.)

species	rotational constants (GHz)	geometries (Å)	frequencies (cm ⁻¹) ^b	parameters for hindered rotations ^c
B3	1.98	C, -1.626138, -1.489223, 0.119312	67, 113, 189	
	0.60	C, -2.957266, -1.214821, -0.201792	234, 261, 375	
	0.48	C, -3.386315, 0.101279, -0.371830	414, 435, 459	
		C, -2.489518, 1.161753, -0.226947	499, 523, 531	
		C, -1.161973, 0.889181, 0.082879	599, 619, 659	
		C, -0.733570, -0.433414, 0.256456	694, 726, 747	
		H, -1.299587, -2.515305, 0.251751	760, 787, 828	
		H, -3.661511, -2.030612, -0.321780	838, 881, 898	
		H, -4.421812, 0.301906, -0.623471	936, 952, 962	
		H, -2.827221, 2.183959, -0.364508	978, 989, 1001	
		C, 1.186383, 0.943745, 0.260459	1036, 1047, 1103	
		C, 2.444768, 1.190837, -0.196463	1119, 1152, 1155	
		C, 3.352899, 0.124523, -0.419578	1175, 1180, 1196	
		C, 2.907255, -1.218915, -0.314182	1218, 1220, 1239	
		C, 1.652736, -1.528363, 0.122974	1278, 1313, 1343	
		C, 0.742962, -0.453696, 0.642185	1345, 1387, 1428	
		C, -0.011589, 1.862639, 0.281946	1468, 1491, 1505	
		H, 2.738675, 2.202222, -0.462849	1539, 1609, 1626	
		H, 4.356799, 0.333317, -0.768212	1647, 2802, 2966	
		H, 3.578261, -2.016234, -0.617752	3054, 3147, 3152	
		H, 1.324898, -2.560666, 0.181206	3155, 3161, 3171	
		H, 0.037499, 2.637733, -0.488416	3173, 3185, 3191	
		H, -0.113032, 2.379968, 1.248606		
		H, 0.763227, -0.529435, 1.752913		
B4	2.14	C, 0.017105, 1.754881, -1.502600	95, 100, 202	
	0.58	C, 0.000000, 3.050131, -1.116550	224, 250, 378	
	0.46	C, -0.243546, 3.433002, 0.255133	408, 456, 463	
		C, -0.317031, 2.488445, 1.253880	493, 510, 546	
		C, -0.237287, 1.120983, 0.923255	589, 616, 668	
		C, -0.368540, 0.683166, -0.528260	673, 701, 706	
		H, 0.217163, 1.484516, -2.534720	790, 792, 811	
		H, 0.198862, 3.834070, -1.840099	845, 880, 902	
		H, -0.274263, 4.487580, 0.503832	940, 942, 945	
		H, -0.347264, 2.792890, 2.295484	978, 979, 981	
		C, 0.237287, -1.120983, 0.923255	983, 1043, 1061	
		C, 0.317031, -2.488445, 1.253880	1078, 1118, 1156	
		C, 0.243546, -3.433002, 0.255133	1164, 1175, 1184	
		C, 0.000000, -3.050131, -1.116550	1207, 1236, 1269	
		C, -0.017105, -1.754881, -1.502600	1288, 1304, 1339	
		C, 0.368540, -0.683166, -0.528260	1353, 1356, 1395	
		C, 0.000000, 0.000000, 1.720883	1429, 1452, 1483	
		H, 0.347264, -2.792890, 2.295484	1535, 1535, 1631	
		H, 0.274263, -4.487580, 0.503832	1639, 2862, 2870	
		H, -0.198862, -3.834070, -1.840099	3148, 3149, 3155	
		H, -0.217163, -1.484516, -2.534720	3155, 3167, 3168	
		H, 0.000000, 0.000000, 2.804778	3183, 3184, 3185	
		H, 1.439831, -0.452769, -0.698688		
		H, -1.439831, 0.452769, -0.698688		

Table S1. (Continued.)

species	rotational constants (GHz)	geometries (Å)	frequencies (cm ⁻¹) ^b	parameters for hindered rotations ^c
B5	2.16	C, 1.718342, -1.468976, -0.231299	72, 100, 187	
	0.57	C, 3.085072, -1.097610, -0.183063	209, 245, 368	
	0.47	C, 3.439828, 0.273057, -0.058679	385, 432, 476	
		C, 2.505545, 1.234336, 0.192709	493, 520, 545	
		C, 1.097676, 0.832645, 0.534355	593, 607, 657	
		C, 0.743887, -0.552531, 0.035788	673, 690, 727	
		H, 1.454207, -2.464633, -0.577869	760, 776, 791	
		H, 3.853732, -1.836752, -0.373094	850, 862, 884	
		H, 4.477128, 0.558046, -0.203459	909, 948, 960	
		H, 2.782131, 2.281145, 0.261314	964, 977, 986	
		C, -1.119278, 0.875859, -0.280695	996, 1023, 1045	
		C, -2.530371, 1.185782, -0.439887	1066, 1118, 1153	
		C, -3.431056, 0.230674, -0.117652	1161, 1171, 1187	
		C, -3.005305, -1.069687, 0.403435	1201, 1224, 1237	
		C, -1.721882, -1.461866, 0.357374	1273, 1280, 1318	
		C, -0.716495, -0.589023, -0.364711	1335, 1382, 1389	
		C, -0.100881, 1.659805, 0.105291	1421, 1434, 1532	
		H, -2.844916, 2.188802, -0.708292	1586, 1597, 1652	
		H, -4.493367, 0.444593, -0.162901	1688, 2775, 2898	
		H, -3.758839, -1.714680, 0.843381	3142, 3151, 3152	
		H, -1.406971, -2.427020, 0.739639	3161, 3170, 3174	
		H, -0.765392, -0.903977, -1.424125	3177, 3183, 3189	
		H, -0.154056, 2.734710, 0.238283		
		H, 1.065846, 0.824970, 1.649335		
B6	2.10	C, 1.696993, 1.497972, 0.101718	90, 102, 210	
	0.58	C, 3.046127, 1.178177, -0.006435	215, 263, 384	
	0.46	C, 3.456864, -0.153277, -0.127743	406, 448, 451	
		C, 2.516098, -1.186662, -0.148332	511, 524, 545	
		C, 1.167727, -0.878217, -0.037670	613, 618, 662	
		C, 0.749203, 0.465627, 0.093833	691, 728, 740	
		H, 1.386576, 2.531806, 0.206412	767, 782, 813	
		H, 3.788975, 1.968004, 0.010031	854, 874, 914	
		H, 4.513223, -0.384385, -0.206353	941, 967, 979	
		H, 2.841100, -2.216781, -0.252862	986, 994, 1003	
		C, -1.178013, -0.905312, 0.454946	1044, 1054, 1072	
		C, -2.588697, -1.141219, 0.010710	1114, 1125, 1160	
		C, -3.420835, -0.086574, -0.207060	1177, 1181, 1196	
		C, -2.955697, 1.261770, -0.156622	1223, 1247, 1275	
		C, -1.585469, 1.536604, -0.019615	1309, 1326, 1327	
		C, -0.694964, 0.506327, 0.185969	1353, 1392, 1425	
		C, -0.031731, -1.803094, -0.091383	1478, 1491, 1494	
		H, -2.956845, -2.160678, -0.044781	1536, 1594, 1608	
		H, -4.462438, -0.266304, -0.453496	1635, 2842, 3011	
		H, -3.654310, 2.072149, -0.326518	3075, 3150, 3154	
		H, -1.227331, 2.552141, -0.158093	3157, 3164, 3168	
		H, -0.241106, -2.089815, -1.129547	3175, 3187, 3189	
		H, 0.103684, -2.721747, 0.484449		
		H, -1.157162, -1.037119, 1.556870		

Table S1. (Continued.)

species	rotational constants (GHz)	geometries (Å)	frequencies (cm ⁻¹) ^b	parameters for hindered rotations ^c
B7	2.03	C, 0.201419, 1.627203, -1.530275	73, 109, 188	
	0.60	C, 0.000000, 2.934826, -1.233362	193, 216, 298	
	0.47	C, -0.312873, 3.368957, 0.126705	374, 386, 447	
		C, -0.196090, 2.538641, 1.175899	494, 496, 513	
		C, 0.402733, 1.164993, 0.955544	520, 595, 599	
		C, 0.154940, 0.660609, -0.460403	670, 676, 725	
		H, 0.300630, 1.303451, -2.560993	730, 766, 784	
		H, -0.019426, 3.674628, -2.026183	813, 862, 867	
		H, -0.668171, 4.384419, 0.268765	956, 963, 967	
		H, -0.441102, 2.857283, 2.183666	969, 974, 985	
		C, -0.402733, -1.164993, 0.955544	986, 1024, 1047	
		C, 0.196090, -2.538641, 1.175899	1062, 1063, 1158	
		C, 0.312873, -3.368957, 0.126705	1165, 1178, 1179	
		C, 0.000000, -2.934826, -1.233362	1210, 1215, 1245	
		C, -0.201419, -1.627203, -1.530275	1262, 1287, 1316	
		C, -0.154940, -0.660609, -0.460403	1345, 1377, 1405	
		C, 0.000000, 0.000000, 1.809508	1432, 1456, 1564	
		H, 0.441102, -2.857283, 2.183666	1581, 1631, 1669	
		H, 0.668171, -4.384419, 0.268765	1677, 2806, 2808	
		H, 0.019426, -3.674628, -2.026183	3150, 3151, 3158	
		H, -0.300630, -1.303451, -2.560993	3161, 3172, 3173	
		H, 1.500477, 1.322747, 1.055720	3181, 3183, 3199	
		H, -1.500477, -1.322747, 1.055720		
		H, 0.000000, 0.000000, 2.891716		
TS(B1-B2)	2.37	C, -3.150866, -0.550796, -1.176483	2170i, 52, 62	
	0.40	C, -3.830754, 0.389906, -0.387705	74, 210, 216	
	0.38	C, -3.254533, 0.931815, 0.766715	289, 392, 410	
		C, -1.973727, 0.558589, 1.189886	426, 465, 503	
		C, -1.306386, -0.379254, 0.409022	580, 614, 635	
		C, -1.889685, -0.902632, -0.726440	638, 704, 715	
		H, -3.601680, -0.963517, -2.070971	749, 754, 802	
		H, -4.827843, 0.704578, -0.679158	851, 873, 882	
		H, -3.817585, 1.657100, 1.343853	905, 940, 948	
		H, -1.535903, 0.990481, 2.083256	980, 991, 991	
		C, 1.295301, -0.448024, 0.161841	1001, 1012, 1023	
		C, 1.376073, 0.877827, -0.299642	1047, 1104, 1120	
		C, 2.609553, 1.474299, -0.534008	1153, 1173, 1180	
		C, 3.789833, 0.763060, -0.318656	1191, 1202, 1215	
		C, 3.726135, -0.555333, 0.134525	1264, 1306, 1328	
		C, 2.495401, -1.153891, 0.369434	1350, 1377, 1454	
		C, 0.006091, -1.113045, 0.391853	1481, 1484, 1520	
		H, 0.463230, 1.435713, -0.472377	1586, 1609, 1630	
		H, 2.651615, 2.499138, -0.886049	1632, 1760, 3089	
		H, 4.750350, 1.231038, -0.501700	3153, 3156, 3164	
		H, 4.639023, -1.114742, 0.306624	3167, 3174, 3181	
		H, 2.451805, -2.179252, 0.722371	3184, 3187, 3191	
		H, -0.580379, -1.625366, -0.766633		
		H, 0.052746, -1.990296, 1.038736		

Table S1. (Continued.)

species	rotational constants (GHz)	geometries (Å)	frequencies (cm ⁻¹) ^b	parameters for hindered rotations ^c
TS(B1-B3)	1.89	C, -1.764309, -1.582986, -0.121187	387i, 61, 106	
	0.55	C, -3.080109, -1.204397, -0.421985	179, 228, 309	
	0.47	C, -3.444394, 0.142033, -0.398643	330, 398, 415	
		C, -2.509833, 1.129747, -0.080409	481, 497, 534	
		C, -1.192682, 0.769140, 0.214259	584, 615, 621	
		C, -0.871467, -0.577953, 0.178156	702, 720, 737	
		H, -1.471590, -2.627875, -0.135300	745, 805, 806	
		H, -3.815119, -1.961331, -0.675953	836, 860, 874	
		H, -4.464453, 0.425517, -0.632988	921, 937, 968	
		H, -2.807136, 2.174625, -0.067688	978, 985, 994	
		C, 1.193985, 0.890784, 0.365303	1020, 1037, 1039	
		C, 2.179143, 1.188617, -0.556589	1083, 1121, 1161	
		C, 3.149724, 0.237183, -0.904435	1172, 1175, 1183	
		C, 3.112745, -1.040050, -0.338707	1193, 1207, 1244	
		C, 2.139985, -1.362466, 0.596089	1299, 1329, 1331	
		C, 1.142232, -0.418177, 0.945082	1351, 1449, 1462	
		C, -0.051450, 1.717279, 0.568027	1473, 1483, 1512	
		H, 2.182305, 2.160474, -1.040073	1574, 1589, 1608	
		H, 3.919060, 0.490519, -1.624699	1630, 2997, 3070	
		H, 3.864343, -1.772750, -0.611472	3134, 3144, 3152	
		H, 2.145231, -2.334794, 1.075786	3155, 3163, 3165	
		H, -0.054228, 2.611667, -0.060187	3177, 3180, 3188	
		H, -0.150825, 2.052838, 1.609244		
		H, 0.630992, -0.551415, 1.893553		
TS(B2-B4)	2.10	C, 1.780282, -1.507886, -0.338705	896i, 93, 105	
	0.56	C, 3.054404, -1.166491, -0.005824	161, 251, 279	
	0.46	C, 3.444874, 0.220717, 0.102052	394, 407, 417	
		C, 2.537041, 1.228032, 0.001220	478, 514, 554	
		C, 1.140120, 0.906491, -0.136999	576, 601, 620	
		C, 0.761778, -0.491677, -0.506151	668, 695, 710	
		H, 1.524900, -2.544003, -0.539232	732, 783, 802	
		H, 3.813913, -1.931365, 0.112112	813, 850, 852	
		H, 4.488625, 0.451993, 0.285728	870, 914, 961	
		H, 2.835844, 2.263596, 0.126341	967, 970, 981	
		C, -1.149916, 0.905269, 0.256498	988, 993, 1023	
		C, -2.413011, 1.251489, -0.178551	1044, 1097, 1111	
		C, -3.417585, 0.272363, -0.316605	1160, 1167, 1174	
		C, -3.122715, -1.071834, -0.045017	1188, 1191, 1233	
		C, -1.876159, -1.464925, 0.409432	1288, 1314, 1334	
		C, -0.829048, -0.492782, 0.594673	1368, 1399, 1428	
		C, 0.068883, 1.691530, 0.191554	1458, 1484, 1505	
		H, -2.614616, 2.276819, -0.471476	1533, 1565, 1596	
		H, -4.407660, 0.554268, -0.653305	1639, 3065, 3091	
		H, -3.906262, -1.815807, -0.149020	3150, 3153, 3158	
		H, -1.700974, -2.495881, 0.695803	3159, 3171, 3174	
		H, 0.120351, 2.759479, 0.367769	3183, 3184, 3191	
		H, -0.224471, -0.619828, 1.492897		
		H, 0.196671, -0.581035, -1.433084		

Table S1. (Continued.)

species	rotational constants (GHz)	geometries (Å)	frequencies (cm ⁻¹) ^b	parameters for hindered rotations ^c
TS(B3-B5)	2.14	C, -1.696431, -1.474627, 0.134085	1543i, 98, 103	
	0.58	C, -3.058019, -1.156480, -0.027601	193, 245, 269	
	0.46	C, -3.458165, 0.185217, -0.133151	396, 411, 449	
		C, -2.543660, 1.222180, -0.131727	467, 514, 527	
		C, -1.145709, 0.902248, -0.098139	559, 600, 627	
		C, -0.750136, -0.477842, 0.123447	668, 694, 711	
		H, -1.402774, -2.506474, 0.301055	731, 768, 790	
		H, -3.801611, -1.943768, -0.029228	798, 837, 856	
		H, -4.515628, 0.418108, -0.199857	860, 931, 932	
		H, -2.868172, 2.253749, -0.205806	955, 964, 973	
		C, 1.188058, 0.928498, 0.235557	978, 1019, 1034	
		C, 2.570421, 1.199925, 0.116560	1054, 1117, 1158	
		C, 3.447338, 0.163566, -0.090007	1159, 1166, 1172	
		C, 2.960358, -1.179962, -0.325623	1185, 1203, 1215	
		C, 1.666065, -1.517123, -0.144662	1259, 1297, 1313	
		C, 0.727139, -0.508697, 0.466630	1342, 1379, 1425	
		C, 0.082275, 1.749235, 0.032805	1445, 1464, 1483	
		H, 2.923378, 2.226665, 0.113417	1531, 1549, 1621	
		H, 4.507406, 0.361158, -0.197037	1637, 1786, 2770	
		H, 3.662581, -1.919627, -0.696976	3151, 3154, 3155	
		H, 1.305994, -2.518912, -0.351087	3161, 3175, 3179	
		H, 0.776450, -0.681309, 1.566926	3186, 3192, 3210	
		H, 0.074208, 2.825621, -0.074974		
		H, -0.599028, 1.267973, -1.175475		
TS(B3-B6)	2.10	C, -1.692543, -1.507343, 0.055272	2543i, 79, 125	
	0.58	C, -3.046238, -1.197522, -0.041818	204, 217, 242	
	0.46	C, -3.476635, 0.130076, -0.107372	378, 392, 417	
		C, -2.542413, 1.172637, -0.085244	435, 486, 524	
		C, -1.191122, 0.878834, -0.004906	539, 609, 621	
		C, -0.754343, -0.466896, 0.075370	653, 698, 712	
		H, -1.372613, -2.541977, 0.113586	730, 759, 781	
		H, -3.776832, -1.998916, -0.063267	798, 832, 858	
		H, -4.534751, 0.353316, -0.179000	921, 936, 947	
		H, -2.878561, 2.203281, -0.143450	966, 972, 975	
		C, 1.187903, 0.941388, 0.171599	982, 1044, 1083	
		C, 2.571439, 1.176525, -0.031960	1096, 1139, 1146	
		C, 3.461291, 0.136096, -0.123123	1169, 1176, 1182	
		C, 2.989319, -1.241169, -0.124196	1195, 1213, 1227	
		C, 1.673269, -1.552254, -0.008370	1297, 1308, 1343	
		C, 0.689780, -0.507997, 0.194746	1360, 1399, 1469	
		C, -0.017020, 1.849922, 0.010187	1476, 1481, 1492	
		H, 2.920691, 2.201331, -0.115986	1509, 1597, 1612	
		H, 4.519357, 0.331212, -0.241370	1632, 2129, 2961	
		H, 3.714237, -2.035302, -0.263008	2999, 3154, 3155	
		H, 1.339358, -2.581007, -0.086880	3160, 3162, 3173	
		H, 0.046430, 2.411661, -0.933369	3181, 3187, 3197	
		H, -0.107856, 2.598544, 0.807151		
		H, 1.014414, 0.184083, 1.224484		

Table S1. (Continued.)

species	rotational constants (GHz)	geometries (Å)	frequencies (cm ⁻¹) ^b	parameters for hindered rotations ^c
TS(B4-B5)	2.13	C, -1.680281, -1.513708, -0.138190	1848i, 96, 105	
	0.58	C, -2.972789, -1.164361, -0.321395	191, 237, 258	
	0.46	C, -3.446006, 0.182610, -0.092674	393, 405, 444	
		C, -2.559861, 1.214354, 0.110474	467, 500, 521	
		C, -1.176063, 0.940387, 0.220955	546, 594, 617	
		C, -0.738365, -0.508803, 0.474622	667, 677, 691	
		H, -1.328000, -2.519878, -0.337213	708, 748, 776	
		H, -3.680931, -1.899555, -0.690877	784, 815, 839	
		H, -4.503984, 0.389465, -0.203556	859, 916, 934	
		H, -2.904307, 2.243805, 0.106382	949, 962, 979	
		C, 1.112585, 0.945388, -0.089372	981, 985, 1044	
		C, 2.539154, 1.246119, -0.162808	1094, 1124, 1146	
		C, 3.443363, 0.228521, -0.141936	1153, 1164, 1172	
		C, 3.059036, -1.148316, -0.003263	1180, 1222, 1232	
		C, 1.725018, -1.487145, 0.148598	1269, 1303, 1312	
		C, 0.727595, -0.501891, 0.107461	1336, 1384, 1420	
		C, -0.070092, 1.750029, 0.030204	1430, 1452, 1479	
		H, 2.859386, 2.279677, -0.219073	1501, 1534, 1628	
		H, 4.500182, 0.463989, -0.210220	1635, 2179, 2745	
		H, 3.822000, -1.915563, 0.009148	3148, 3154, 3162	
		H, 1.439362, -2.520390, 0.317539	3165, 3171, 3184	
		H, -0.092190, 2.817134, -0.146257	3187, 3200, 3203	
		H, 0.874954, 0.217851, -1.062253		
		H, -0.766234, -0.655630, 1.580331		
TS(B5-B7)	2.08	C, -1.667569, 1.524024, 0.117304	1426i, 93, 116	
	0.58	C, -2.997635, 1.211128, -0.076352	196, 233, 247	
	0.46	C, -3.397740, -0.154203, -0.313416	392, 399, 439	
		C, -2.544934, -1.192976, -0.159221	476, 495, 518	
		C, -1.185049, -0.942433, 0.438501	528, 539, 603	
		C, -0.720671, 0.495171, 0.235810	609, 672, 688	
		H, -1.348918, 2.562291, 0.108814	717, 731, 736	
		H, -3.733178, 2.000358, -0.175633	763, 828, 840	
		H, -4.405645, -0.336534, -0.673587	851, 918, 949	
		H, -2.846113, -2.211823, -0.377080	967, 970, 975	
		C, 1.135519, -0.960227, -0.039997	978, 984, 1013	
		C, 2.570525, -1.208497, -0.101826	1054, 1059, 1109	
		C, 3.444832, -0.169257, -0.135979	1145, 1159, 1166	
		C, 3.007249, 1.202982, -0.068830	1186, 1200, 1203	
		C, 1.687590, 1.525885, 0.042764	1233, 1256, 1313	
		C, 0.682063, 0.499938, 0.073848	1356, 1390, 1413	
		C, 0.013704, -1.791863, 0.109100	1426, 1478, 1482	
		H, 2.921391, -2.234022, -0.098506	1527, 1538, 1624	
		H, 4.508867, -0.370336, -0.188322	1641, 2024, 2615	
		H, 3.752791, 1.988868, -0.086996	3146, 3149, 3166	
		H, 1.378871, 2.559792, 0.148738	3172, 3173, 3185	
		H, -1.335540, -1.060886, 1.548695	3185, 3194, 3227	
		H, 0.908389, -0.264558, -1.054950		
		H, 0.031789, -2.871181, 0.118589		

Table S1. (Continued.)

species	rotational constants (GHz)	geometries (Å)	frequencies (cm ⁻¹) ^b	parameters for hindered rotations ^c
TS(B6-B7)	2.06	C, 1.644035, 1.520796, -0.023683	1553i, 91, 115	
	0.59	C, 2.981908, 1.222834, -0.112972	195, 223, 249	
	0.47	C, 3.446134, -0.130681, -0.098867	389, 404, 440	
		C, 2.581182, -1.186529, -0.040632	485, 489, 522	
		C, 1.152223, -0.925816, -0.083349	524, 537, 605	
		C, 0.688244, 0.476220, 0.070421	609, 681, 693	
		H, 1.317014, 2.553891, 0.023515	729, 739, 760	
		H, 3.710017, 2.024192, -0.163069	781, 823, 845	
		H, 4.514339, -0.316714, -0.115745	860, 935, 938	
		H, 2.942594, -2.208563, -0.020352	966, 972, 975	
		C, -1.199881, -0.946256, 0.459073	980, 1004, 1041	
		C, -2.549893, -1.175429, -0.178495	1055, 1061, 1129	
		C, -3.378344, -0.124831, -0.341116	1155, 1166, 1174	
		C, -2.957577, 1.235118, -0.061086	1178, 1204, 1208	
		C, -1.639589, 1.529884, 0.170574	1245, 1277, 1325	
		C, -0.689511, 0.480541, 0.255022	1360, 1374, 1411	
		C, -0.019426, -1.806930, 0.130870	1427, 1461, 1480	
		H, -2.857479, -2.187582, -0.418001	1515, 1543, 1624	
		H, -4.378395, -0.279458, -0.733768	1642, 2363, 2655	
		H, -3.684116, 2.033914, -0.154588	3150, 3155, 3159	
		H, -1.311727, 2.563970, 0.207828	3166, 3172, 3178	
		H, 0.753187, -1.248524, -1.147757	3184, 3188, 3230	
		H, -1.373321, -1.063492, 1.562839		
		H, 0.010859, -2.885172, 0.084533		
TS(B3-C ₁₃ H ₁₀ +H)	2.13	C, -1.659402, -1.497270, 0.031567	951i, 98, 132	
	0.58	C, -3.018431, -1.205138, -0.074209	210, 240, 264	
	0.46	C, -3.459153, 0.118729, -0.129498	399, 408, 425	
		C, -2.545043, 1.173217, -0.082749	457, 490, 514	
		C, -1.189533, 0.886987, 0.014584	522, 559, 579	
		C, -0.748356, -0.445407, 0.073279	638, 640, 708	
		H, -1.324073, -2.527303, 0.082326	736, 746, 761	
		H, -3.740520, -2.013038, -0.112434	800, 815, 850	
		H, -4.519638, 0.328822, -0.211466	865, 879, 931	
		H, -2.893593, 2.199877, -0.127805	948, 973, 984	
		C, 1.176690, 0.900398, 0.059783	989, 1021, 1042	
		C, 2.523959, 1.183523, -0.063290	1050, 1114, 1129	
		C, 3.441297, 0.128668, -0.137824	1163, 1173, 1179	
		C, 3.000894, -1.201327, -0.135218	1189, 1205, 1220	
		C, 1.653840, -1.504044, -0.013800	1246, 1313, 1323	
		C, 0.730491, -0.449718, 0.183754	1343, 1363, 1448	
		C, -0.010243, 1.835602, 0.077266	1469, 1478, 1501	
		H, 2.870364, 2.209835, -0.129402	1510, 1588, 1623	
		H, 4.499247, 0.342520, -0.237412	1630, 1650, 3005	
		H, 3.723131, -2.002534, -0.245233	3048, 3158, 3159	
		H, 1.316137, -2.534006, -0.020726	3165, 3167, 3176	
		H, 0.006516, 2.541486, -0.759897	3179, 3188, 3189	
		H, -0.032737, 2.435296, 0.997169		
		H, 0.713113, -0.526270, 1.943023		

Table S1. (Continued.)

species	rotational constants (GHz)	geometries (Å)	frequencies (cm ⁻¹) ^b	parameters for hindered rotations ^c
TS(B6-C ₁₃ H ₁₀ +H)	2.13	C, -1.670811, -1.506685, 0.024002	793i, 97, 133	
	0.58	C, -3.030841, -1.207511, 0.002773	215, 239, 277	
	0.46	C, -3.467783, 0.119239, -0.032599	390, 416, 433	
		C, -2.548107, 1.169923, -0.050716	463, 492, 502	
		C, -1.191022, 0.878305, -0.032699	518, 568, 575	
		C, -0.748741, -0.458599, 0.008477	634, 648, 714	
		H, -1.338769, -2.538569, 0.057330	744, 751, 754	
		H, -3.758631, -2.011054, 0.017791	793, 813, 851	
		H, -4.530427, 0.334012, -0.045260	871, 880, 933	
		H, -2.894642, 2.197790, -0.079306	949, 972, 987	
		C, 1.174524, 0.876134, 0.102304	990, 1021, 1043	
		C, 2.546013, 1.149940, -0.041355	1050, 1118, 1130	
		C, 3.444099, 0.091474, -0.084847	1165, 1173, 1179	
		C, 2.989295, -1.233581, -0.050733	1191, 1206, 1219	
		C, 1.625434, -1.520785, -0.010112	1247, 1322, 1328	
		C, 0.714099, -0.469813, 0.031780	1340, 1366, 1453	
		C, -0.007394, 1.820683, -0.068854	1467, 1483, 1503	
		H, 2.899799, 2.174773, -0.071238	1507, 1595, 1619	
		H, 4.507601, 0.290072, -0.154332	1630, 1648, 3019	
		H, 3.707371, -2.045115, -0.085292	3076, 3158, 3161	
		H, 1.284792, -2.550127, -0.033736	3165, 3168, 3175	
		H, 0.057779, 2.326005, -1.040580	3178, 3188, 3189	
		H, -0.058099, 2.597460, 0.697516		
		H, 1.150637, 0.972412, 1.952583		

^a Computed at the B3LYP/6-311G(d,p) level. ^b Unscaled harmonic frequencies. ^c Symmetry numbers (*n*), barrier heights (*V_r* / cm⁻¹) and reduced moments of inertia (*I* / amu Å²) for intramolecular hindered rotors. ^d Treated as hindered internal rotations.