Ab initio study of hydrogen migration across n-alkyl radicals

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Supporting Information.

MP2/6-31G(d) frequencies and rotational constants for the reactants, products, and transition state species used in this study (**Table S1).** G4 frequencies and rotational constants for the reactants, products, and transition state species used in this study (**Table S2).**
MP2/6-31G(d) Arrhenius pre-exponential A-factors for the forward and reverse H-migration using (**Table S3).** G4 Arrhenius pre-exponential A-factors for the forward and reverse H-migration (**Table S4)** Skodje and Trular tunneling transmission coefficient determined using MP2/6-31G(d) frequencies and G2 energy values (**Table S5).** Skodje and Trular tunneling transmission coefficient determined using G4 frequencies and energy values (**Table S6).** Skodje and Trular tunneling transmission coefficient determined using MP2/6-31G(d) frequencies and CBS-Q energy values (**Table S7).** Wigner tunneling transmission coefficient determined using MP2/6-31G(d) frequencies (**Table S8)**. C-C bond distances in Å for G2 ground state alkyl radicals. **Bold values** are bonds that contain a radical center Atom Labeling is given in figure S3. (**Table S9.A**). Bond angles for the carbon chain in G2 ground state alkyl radicals. **Bold values** are C-C$^{\bullet}$-C bond angles. *Italicized values* are C$^{\bullet}$-C-C bond angles. Atom Labeling is given in figure S3. (**Table S9.B**). Dihedral angles for the carbon chain in G2 ground state alkyl radicals. **Bold values** are C-C$^{\bullet}$-C-C dihedral angles. *Italicized values* are C$^{\bullet}$-C-C-C dihedral angles. Atom Labeling is given in figure S3. (**Table S9.C**). Selected bond lengths for the G2 Hydrogen migration transition states for alkyl radicals. E=Equatorial R group, A=Axial R group, RMS=Root mean square deviation from corresponding cycloalkane for B_1-B_7 RMS*= Root mean square deviation from corresponding methylcycloalkane for B_1-B_7. **Bold values** are bonds that contain a radical center. Atom Labeling is given in figure S4. (**Table S10.A**). Selected bond angles for the G2 Hydrogen migration transition states for alkyl radicals. E=Equatorial R group, A=Axial R group, RMS=Root mean square deviation of A_1-A_6 from corresponding cycloalkane, RMS*= Root mean square deviation of A_1-A_7 from corresponding methylcycloalkane. **Bold values** are C-C$^{\bullet}$-C bond angles. *Italicized values* are C$^{\bullet}$-C-C bond angles. Atom Labeling is given in figure S4. (**Table S10.B**). Selected dihedral angles for the G2 Hydrogen migration transition states for alkyl radicals. E=Equatorial R group, A=Axial R group, RMS=Root mean square deviation of D_1-D_5 from corresponding cycloalkane, RMS*= Root mean square deviation from corresponding methylcycloalkane. **Bold values** are C-C$^{\bullet}$-C-C dihedral angles. *Italicized values* are C$^{\bullet}$-C-C-C dihedral angles. Atom Labeling is given in figure S4. (**Table S10.C**). Cartesian coordinates of G2 reactants and products (**Table

S11). Cartesian coordinates of G2 transition state species (**Table S12**). Schematic diagram of the ΔH_{rxn} for the G4 data set for C_nH_{n+1} and the other unique isomers at 0 K (**Figure S1**). Schematic diagram of the ΔH_{rxn} for the CBS-Q data set for C_nH_{n+1} and the other unique isomers at 0 K (**Figure S2**). Angle between the bridge head carbons and the migrating hydrogen in the transition state, A_β in figure S4 (**Figure S5**). Arrhenius pre-exponential A-factors for the reverse direction of the alkyl Nsp reactions (**Figure S6**). Graph of distance between bridge head carbons and migrating hydrogen. For labeling see figure S4. Dashed line is from Dybala-Defratyka (2004) (**Figure S7**).

Table S1

Species	Rxn Type	Vibrational Frequencies (cm^{-1})	Rotational Constants (GHz)		
			A	B	C
$^{\bullet}CH_2CH_3$		162, 464, 840, 1030, 1108, 1248, 1469, 1538, 1552, 1558, 3067, 3152, 3197, 3243, 3351	103.529	22.698	21.071
$^{\bullet}CH_2CH_3$	3pp	-2232, 580, 761, 806, 822, 1184, 1236, 1354, 1474, 1501, 2414, 3236, 3240, 3348, 3366	107.731	24.119	21.747
$^{\bullet}CH_2CH_2CH_3$		153, 265, 377, 477, 785, 922, 954, 1099, 1131, 1223, 1321, 1413, 1470, 1530, 1546, 1564, 1571, 3044, 3107, 3126, 3195, 3201, 3230, 3338	32.683	9.010	7.822
$CH_3{}^{\bullet}CH_2CH_3$		137, 164, 368, 454, 920, 970, 981, 1087, 1197, 1227, 1425, 1478, 1479, 1539, 1549, 1552, 1562, 3051, 3053, 3136, 3136, 3190, 3191, 3253	37.131	8.374	7.481
$^{\bullet}CH_2CH_2CH_3$	4pp	-2517, 201, 535, 697, 797, 913, 986, 1014, 1035, 1103, 1228, 1279, 1293, 1439, 1471, 1491, 1562, 1900, 3150, 3175, 3180, 3209, 3290, 3290	24.888	11.376	9.227
$^{\bullet}CH_2CH_2CH_3$	$3s_{\alpha}p$	-2227, 220, 373, 385, 738, 754, 938, 957, 1086, 1207, 1237, 1346, 1418, 1480, 1486, 1550, 1562, 2399, 3073, 3149, 3191, 3228, 3248, 3349	37.551	8.656	7.654
$^{\bullet}CH_2(CH_2)_2CH_3$		124, 153, 255, 270, 430, 475, 754, 854, 902, 996, 1080, 1118, 1141, 1217, 1299, 1354, 1365, 1444, 1472, 1528, 1543, 1558, 1564, 1572, 3030, 3099, 3101, 3115, 3151, 3189, 3192, 3230, 3338	25.164	3.827	3.559
$CH_3{}^{\bullet}CHCH_2CH_3$		75, 141, 250, 270, 437, 455, 798, 880, 1011, 1020, 1073, 1121, 1180, 1227, 1318, 1361, 1460, 1470, 1480, 1543, 1544, 1557, 1563, 1570, 3027, 3052, 3103, 3106, 3136, 3189, 3193, 3200, 3234	26.414	3.655	3.439
$^{\bullet}CH_2(CH_2)_2CH_3$	5pp	-2259, 237, 340, 578, 587, 678, 875, 882, 922, 968, 997, 1033, 1084, 1139, 1231, 1261, 1290, 1362, 1382, 1468, 1513, 1520, 1552, 1567, 1718, 3108, 3110, 3155, 3163, 3168, 3172, 3259, 3260	11.595	6.746	4.988
$^{\bullet}CH_2(CH_2)_2CH_3$	$4s_{\alpha}p$	-2503, 104, 235, 362, 394, 659, 782, 879, 908, 978, 1000, 1057, 1110, 1167, 1219, 1268, 1289, 1383, 1439, 1468, 1484, 1549, 1557, 1560, 1896, 3080, 3136, 3156, 3177, 3182, 3193, 3202, 3288	16.366	4.648	4.387
$^{\bullet}CH_2(CH_2)_2CH_3$	$3s_{\alpha}p$	-2215, 114, 244, 267, 384, 452, 731, 755, 822, 883, 1001, 1081, 1127, 1209, 1223, 1314, 1352, 1363, 1457, 1470, 1484, 1550, 1562, 1569, 2396, 3053, 3105, 3113, 3191, 3198, 3227, 3233, 3348	25.811	3.756	3.538
$^{\bullet}CH_2(CH_2)_3CH_3$		110, 119, 155, 187, 261, 399, 413, 472, 748, 800, 896, 945, 982, 1066, 1108, 1131, 1143, 1212, 1282, 1320, 1351, 1369, 1408, 1454, 1471, 1528, 1542, 1553, 1561, 1565, 1574, 3030, 3084, 3093, 3101, 3114, 3129, 3150, 3190, 3191, 3229, 3338	18.136	2.022	1.910
$CH_3{}^{\bullet}CH(CH_2)_2CH_3$		67, 107, 146, 197, 256, 399, 412, 455, 760, 888, 909, 969, 1021, 1080, 1107, 1140, 1183, 1219, 1298, 1324, 1361, 1415, 1464, 1471, 1480, 1540, 1543, 1557, 1558, 1564, 1572, 3013, 3052,	19.195	1.949	1.858

		3090, 3099, 3101, 3136, 3149, 3188, 3189, 3191, 3234			
$CH_3CH_2{}^{\bullet}CHCH_2CH_3$		61, 71, 186, 255, 256, 405, 416, 457, 782, 814, 908, 983, 1059, 1084, 1093, 1134, 1184, 1216, 1308, 1326, 1327, 1411, 1467, 1471, 1480, 1540, 1549, 1563, 1563, 1569, 1570, 3026, 3028, 3102, 3105, 3106, 3106, 3193, 3193, 3199, 3200, 3215	16.723	1.990	1.875
${}^{\bullet}CH_2(CH_2)_3CH_3$	6pp	-2064, 153, 310, 363, 434, 476, 605, 691, 838, 857, 886, 917, 952, 1034, 1045, 1102, 1137, 1141, 1234, 1254, 1296, 1327, 1393, 1405, 1415, 1488, 1514, 1515, 1545, 1550, 1560, 1583, 3078, 3079, 3090, 3130, 3132, 3151, 3154, 3155, 3241, 3243	6.670	4.399	3.028
${}^{\bullet}CH_2(CH_2)_3CH_3$	$5s_\alpha{}^Ep$	-2232, 141, 205, 230, 350, 494, 562, 585, 835, 889, 903, 933, 959, 1012, 1040, 1079, 1141, 1174, 1225, 1262, 1284, 1339, 1375, 1417, 1465, 1491, 1517, 1548, 1552, 1558, 1563, 1722, 3077, 3094, 3107, 3142, 3152, 3156, 3161, 3168, 3189, 3259	9.127	3.125	2.629
${}^{\bullet}CH_2(CH_2)_3CH_3$	$5s_\alpha{}^Ap$	-2224, 145, 204, 215, 366, 494, 599, 628, 827, 868, 885, 948, 950, 1031, 1036, 1067, 1128, 1168, 1209, 1261, 1278, 1357, 1375, 1398, 1461, 1481, 1516, 1546, 1553, 1560, 1567, 1719, 3083, 3099, 3112, 3148, 3160, 3164, 3169, 3178, 3193, 3260	7.650	3.516	3.064
${}^{\bullet}CH_2(CH_2)_3CH_3$	$4s_\beta p$	-2489, 98, 105, 248, 255, 382, 449, 664, 765, 817, 890, 922, 997, 1016, 1036, 1081, 1132, 1156, 1224, 1264, 1287, 1324, 1345, 1423, 1445, 1469, 1484, 1548, 1556, 1562, 1568, 1893, 3062, 3104, 3114, 3136, 3170, 3176, 3191, 3196, 3198, 3287	11.852	2.433	2.284
${}^{\bullet}CH_2(CH_2)_3CH_3$	$3s_\alpha p$	-2214, 102, 114, 191, 256, 370, 404, 434, 729, 755, 772, 898, 915, 975, 1066, 1107, 1147, 1207, 1220, 1296, 1325, 1348, 1363, 1411, 1463, 1471, 1484, 1546, 1557, 1564, 1572, 2395, 3040, 3096, 3100, 3101, 3148, 3189, 3191, 3227, 3233, 3348	19.081	1.984	1.895
${}^{\bullet}CH_2(CH_2)_4CH_3$		79, 102, 137, 147, 162, 260, 307, 379, 448, 495, 746, 770, 853, 927, 934, 1003, 1071, 1083, 1117, 1130, 1151, 1209, 1272, 1299, 1332, 1366, 1370, 1376, 1432, 1456, 1471, 1528, 1542, 1550, 1555, 1565, 1565, 1575, 3030, 3076, 3086, 3094, 3101, 3114, 3118, 3139, 3151, 3189, 3190, 3229, 3337	15.303	1.177	1.133
$CH_3{}^{\bullet}CH(CH_2)_3CH_3$		54, 98, 124, 130, 164, 260, 307, 376, 448, 478, 751, 811, 929, 941, 951, 1027, 1068, 1099, 1116, 1148, 1183, 1216, 1281, 1302, 1349, 1368, 1379, 1440, 1464, 1471, 1479, 1540, 1543, 1553, 1556, 1561, 1565, 1574, 3014, 3052, 3083, 3090, 3094, 3101, 3128, 3136, 3149, 3188, 3189, 3191, 3235	15.814	1.147	1.110
$CH_3(CH_2)_2{}^{\bullet}CHCH_2CH_3$		51, 57, 114, 161, 251, 258, 303, 382, 453, 479, 757, 800, 891, 931, 942, 1067, 1074, 1099, 1115, 1145, 1183, 1211, 1294, 1304, 1320, 1361, 1376, 1435, 1469, 1471, 1480, 1538, 1547, 1558, 1563, 1564, 1570, 1572, 3013, 3027, 3091, 3099, 3101, 3104, 3106, 3149, 3189, 3191, 3193, 3199, 3215	14.646	1.154	1.114
${}^{\bullet}CH_2(CH_2)_4CH_3$	7pp	-2012, 126, 173, 316, 345, 384, 430, 535, 564, 631, 797, 847, 848, 902, 963, 971, 994, 1054, 1095, 1105, 1158, 1195, 1230, 1279, 1296, 1332, 1335, 1410, 1423, 1431, 1432, 1499, 1505, 1513, 1513, 1543, 1547, 1552, 1558, 3069, 3069, 3079, 3079, 3118, 3120, 3130, 3135, 3144, 3144, 3230, 3231	4.268	3.058	2.018

$^{\bullet}CH_2(CH_2)_4CH_3$	$6s_{\alpha}{}^{E}p$	-2036, 108, 170, 211, 303, 346, 419, 468, 508, 617, 834, 851, 862, 910, 953, 964, 1014, 1051, 1097, 1121, 1151, 1180, 1227, 1254, 1281, 1327, 1364, 1397, 1412, 1428, 1466, 1506, 1514, 1541, 1549, 1552, 1557, 1561, 1591, 3065, 3076, 3077, 3089, 3115, 3130, 3143, 3149, 3154, 3155, 3188, 3243	5.209	2.382	1.841
$^{\bullet}CH_2(CH_2)_4CH_3$	$6s_{\alpha}{}^{A}p$	-2023, 126, 159, 201, 286, 379, 432, 486, 570, 602, 831, 842, 863, 891, 956, 963, 993, 1058, 1085, 1105, 1147, 1180, 1214, 1250, 1279, 1327, 1379, 1399, 1405, 1416, 1463, 1495, 1514, 1539, 1547, 1555, 1559, 1562, 1591, 3065, 3075, 3082, 3095, 3124, 3129, 3151, 3154, 3158, 3164, 3189, 3243	4.864	2.594	2.051
$^{\bullet}CH_2(CH_2)_4CH_3$	$5s_{\beta}{}^{E}p$	-2213, 85, 125, 175, 258, 286, 420, 491, 563, 586, 799, 848, 893, 928, 939, 965, 1009, 1045, 1075, 1090, 1158, 1164, 1227, 1257, 1275, 1322, 1336, 1369, 1384, 1439, 1469, 1489, 1516, 1546, 1551, 1562, 1563, 1568, 1719, 3058, 3094, 3102, 3106, 3116, 3136, 3150, 3160, 3167, 3191, 3193, 3259	6.893	1.792	1.554
$^{\bullet}CH_2(CH_2)_4CH_3$	$5s_{\beta}{}^{A}p$	-2203, 83, 131, 182, 260, 284, 411, 498, 613, 625, 789, 846, 881, 890, 946, 964, 1016, 1062, 1075, 1084, 1127, 1166, 1215, 1260, 1276, 1322, 1352, 1359, 1379, 1430, 1469, 1479, 1516, 1545, 1551, 1563, 1565, 1568, 1718, 3065, 3098, 3102, 3111, 3122, 3147, 3163, 3166, 3171, 3190, 3193, 3259	6.021	2.005	1.752
$^{\bullet}CH_2(CH_2)_4CH_3$	$4s_{\beta}p$	-2488, 71, 92, 139, 177, 257, 358, 398, 437, 673, 755, 790, 865, 919, 943, 972, 1000, 1045, 1081, 1106, 1129, 1170, 1220, 1261, 1287, 1303, 1316, 1362, 1392, 1433, 1451, 1471, 1484, 1544, 1556, 1557, 1564, 1572, 1892, 3048, 3096, 3100, 3101, 3136, 3146, 3170, 3176, 3189, 3191, 3198, 3287	10.006	1.354	1.321
$^{\bullet}CH_2(CH_2)_4CH_3$	$3s_{\alpha}p$	-2214, 74, 101, 135, 152, 260, 309, 356, 407, 477, 729, 754, 757, 824, 933, 937, 971, 1072, 1085, 1116, 1154, 1204, 1220, 1282, 1301, 1340, 1358, 1367, 1377, 1437, 1463, 1471, 1483, 1545, 1552, 1561, 1565, 1574, 2395, 3040, 3082, 3092, 3099, 3101, 3127, 3148, 3189, 3190, 3227, 3233, 3347	15.482	1.164	1.128
$^{\bullet}CH_2(CH_2)_5CH_3$		66, 77, 103, 139, 147, 163, 253, 260, 314, 418, 465, 503, 745, 757, 808, 890, 926, 952, 1025, 1050, 1091, 1098, 1119, 1130, 1158, 1207, 1266, 1285, 1317, 1347, 1356, 1369, 1375, 1406, 1444, 1457, 1471, 1528, 1542, 1549, 1551, 1558, 1565, 1567, 1575, 3030, 3074, 3078, 3088, 3093, 3101, 3114, 3115, 3127, 3143, 3152, 3189, 3190, 3229, 3337	12.614	0.749	0.727
$CH_3{}^{\bullet}CH(CH_2)_4CH_3$		51, 70, 100, 117, 136, 164, 254, 260, 314, 418, 456, 493, 748, 776, 866, 920, 954, 986, 1031, 1047, 1095, 1109, 1120, 1154, 1182, 1214, 1273, 1287, 1330, 1351, 1365, 1371, 1411, 1451, 1463, 1471, 1479, 1539, 1543, 1550, 1554, 1557, 1565, 1565, 1575, 3014, 3052, 3075, 3085, 3091, 3094, 3101, 3118, 3136, 3137, 3150, 3188, 3189, 3190, 3235	13.059	0.733	0.714
$CH_3CH_2{}^{\bullet}CH(CH_2)_3CH_3$		46, 49, 93, 126, 137, 246, 258, 261, 317, 425, 453, 495, 750, 791, 819, 919, 948, 963, 1047, 1078, 1088, 1113, 1120, 1153, 1183, 1209, 1280, 1288, 1318, 1349, 1351, 1368, 1408, 1449, 1469, 1471, 1479, 1537, 1547, 1552, 1561, 1563, 1565, 1570, 1574, 3014, 3027, 3083, 3090, 3094, 3101, 3103, 3106, 3128, 3149, 3189, 3191, 3193, 3199, 3215	11.434	0.741	0.719

$CH_3(CH_2)_2{}^{\bullet}CH(CH_2)_2CH_3$		42, 48, 91, 123, 157, 251, 255, 257, 312, 426, 454, 496, 753, 767, 879, 905, 918, 948, 1043, 1086, 1095, 1114, 1126, 1152, 1183, 1208, 1286, 1295, 1303, 1349, 1359, 1363, 1410, 1445, 1471, 1471, 1479, 1536, 1545, 1557, 1558, 1564, 1564, 1572, 1572, 3012, 3015, 3089, 3092, 3099, 3100, 3101, 3101, 3149, 3149, 3189, 3189, 3191, 3191, 3215	12.516	0.732	0.714
${}^{\bullet}CH_2(CH_2)_5CH_3$	8pp	-2069, 104, 184, 224, 245, 314, 364, 426, 470, 507, 595, 648, 763, 799, 878, 887, 938, 941, 980, 1005, 1051, 1098, 1127, 1157, 1160, 1173, 1207, 1264, 1281, 1301, 1325, 1354, 1388, 1415, 1417, 1433, 1441, 1497, 1515, 1517, 1531, 1547, 1552, 1555, 1567, 1569, 3063, 3074, 3084, 3092, 3097, 3115, 3124, 3132, 3139, 3142, 3145, 3148, 3223, 3227	3.157	2.161	1.480
${}^{\bullet}CH_2(CH_2)_5CH_3$	$7s_{\alpha}^{E}p$	-1965, 94, 151, 189, 218, 271, 328, 346, 404, 495, 554, 571, 798, 828, 853, 901, 918, 938, 987, 1000, 1062, 1075, 1124, 1134, 1158, 1195, 1226, 1269, 1296, 1321, 1330, 1369, 1414, 1428, 1431, 1435, 1464, 1512, 1513, 1519, 1541, 1545, 1551, 1554, 1556, 1560, 3055, 3066, 3078, 3078, 3079, 3105, 3117, 3129, 3133, 3137, 3144, 3157, 3186, 3231	3.474	1.837	1.321
${}^{\bullet}CH_2(CH_2)_5CH_3$	$7s_{\alpha}^{A}p$	-1970, 95, 122, 181, 245, 291, 353, 361, 432, 496, 546, 599, 779, 798, 866, 876, 926, 941, 979, 1004, 1037, 1077, 1113, 1131, 1171, 1204, 1210, 1264, 1295, 1325, 1333, 1390, 1410, 1422, 1431, 1435, 1464, 1504, 1511, 1517, 1538, 1545, 1548, 1555, 1560, 1565, 3055, 3065, 3078, 3080, 3088, 3114, 3117, 3129, 3139, 3144, 3146, 3162, 3191, 3231	3.105	2.057	1.544
${}^{\bullet}CH_2(CH_2)_5CH_3$	$6s_{\beta}^{E}p$	-2014, 79, 102, 134, 237, 273, 319, 389, 447, 469, 502, 616, 800, 838, 854, 881, 911, 964, 986, 1008, 1050, 1083, 1105, 1129, 1161, 1170, 1227, 1252, 1274, 1313, 1338, 1344, 1393, 1404, 1412, 1440, 1469, 1505, 1514, 1541, 1547, 1551, 1560, 1563, 1568, 1590, 3056, 3067, 3076, 3089, 3101, 3113, 3115, 3129, 3134, 3149, 3153, 3190, 3192, 3241	4.273	1.447	1.180
${}^{\bullet}CH_2(CH_2)_5CH_3$	$6s_{\beta}^{A}p$	-2004, 88, 118, 128, 245, 272, 315, 382, 455, 510, 569, 602, 798, 826, 850, 879, 904, 956, 976, 989, 1059, 1088, 1097, 1115, 1148, 1172, 1220, 1249, 1278, 1320, 1326, 1356, 1391, 1402, 1414, 1429, 1469, 1494, 1513, 1539, 1547, 1551, 1559, 1563, 1568, 1590, 3062, 3065, 3075, 3094, 3101, 3120, 3123, 3128, 3147, 3151, 3153, 3190, 3192, 3241	3.956	1.599	1.302
${}^{\bullet}CH_2(CH_2)_5CH_3$	$5s_{\beta}^{E}p$	-2212, 71, 76, 138, 165, 248, 258, 357, 392, 518, 573, 588, 762, 848, 879, 899, 929, 943, 957, 1003, 1050, 1068, 1095, 1110, 1157, 1170, 1226, 1254, 1271, 1309, 1313, 1352, 1364, 1376, 1412, 1447, 1470, 1489, 1516, 1543, 1550, 1557, 1562, 1564, 1572, 1719, 3044, 3094, 3095, 3100, 3103, 3106, 3135, 3145, 3150, 3160, 3167, 3189, 3191, 3259	6.333	1.029	0.949
${}^{\bullet}CH_2(CH_2)_5CH_3$	$5s_{\beta}^{A}p$	-2202, 73, 77, 140, 175, 234, 257, 385, 396, 506, 610, 626, 762, 838, 871, 882, 922, 939, 972, 999, 1039, 1090, 1092, 1101, 1136, 1174, 1211, 1259, 1273, 1301, 1321, 1357, 1363, 1378, 1402, 1443, 1470, 1477, 1516, 1543, 1549, 1557, 1564, 1565, 1571, 1718, 3051, 3094, 3098, 3100, 3106, 3113, 3144, 3147, 3163, 3166, 3171, 3188, 3190, 3258	5.211	1.153	1.075
${}^{\bullet}CH_2(CH_2)_5CH_3$	$4s_{\beta}p$	-2488, 62, 67, 122, 132, 151, 260, 300, 339, 418, 475, 672, 750, 776, 821, 896, 928, 949, 993, 999, 1043, 1070, 1097, 1115, 1132, 1173, 1220, 1260, 1284, 1288, 1299, 1351, 1363, 1369, 1418, 1438, 1454, 1471, 1484, 1543, 1552, 1556, 1561, 1565, 1573, 1893, 3048, 3081, 3092, 3100, 3101, 3127, 3136, 3148, 3170, 3176, 3189, 3191, 3198, 3287	8.449	0.842	0.822

$^{\bullet}CH_2(CH_2)_5CH_3$	$3s_{\alpha}p$	-2214, 62, 76, 106, 134, 152, 252, 260, 313, 386, 424, 499, 729, 750, 756, 785, 876, 922, 954, 1003, 1051, 1093, 1100, 1118, 1161, 1202, 1221, 1273, 1286, 1326, 1348, 1355, 1364, 1372, 1408, 1450, 1462, 1471, 1483, 1544, 1550, 1555, 1565, 1565, 1574, 2395, 3040, 3075, 3084, 3093, 3100, 3101, 3117, 3136, 3150, 3189, 3190, 3227, 3233, 3347	12.931	0.741	0.723
$^{\bullet}CH_2(CH_2)_6CH_3$		50, 70, 81, 116, 134, 156, 168, 202, 260, 284, 346, 451, 483, 497, 745, 752, 781, 846, 913, 934, 963, 1034, 1053, 1071, 1099, 1111, 1119, 1131, 1162, 1205, 1263, 1275, 1305, 1328, 1346, 1361, 1373, 1376, 1382, 1425, 1450, 1457, 1471, 1528, 1542, 1548, 1550, 1554, 1561, 1565, 1569, 1575, 3030, 3074, 3075, 3081, 3089, 3093, 3100, 3113, 3114, 3120, 3133, 3146, 3152, 3189, 3190, 3229, 3337	11.117	0.503	0.492
$CH_3{}^{\bullet}CH(CH_2)_5CH_3$		42, 65, 80, 88, 129, 153, 157, 208, 260, 284, 344, 447, 481, 484, 746, 761, 815, 910, 926, 945, 1006, 1039, 1051, 1067, 1107, 1116, 1122, 1158, 1183, 1212, 1267, 1277, 1316, 1331, 1354, 1368, 1375, 1385, 1430, 1455, 1463, 1471, 1479, 1539, 1543, 1549, 1551, 1556, 1558, 1565, 1568, 1575, 3014, 3052, 3074, 3078, 3086, 3092, 3093, 3100, 3114, 3126, 3136, 3142, 3151, 3188, 3189, 3190, 3234	11.386	0.495	0.486
$CH_3CH_2{}^{\bullet}CH(CH_2)_4CH_3$		39, 45, 71, 103, 115, 154, 204, 254, 260, 289, 344, 453, 481, 484, 747, 772, 801, 868, 926, 947, 996, 1047, 1066, 1082, 1101, 1116, 1126, 1159, 1183, 1207, 1272, 1277, 1316, 1331, 1333, 1365, 1371, 1384, 1427, 1454, 1469, 1471, 1478, 1537, 1547, 1550, 1555, 1563, 1565, 1565, 1570, 1575, 3014, 3027, 3075, 3085, 3092, 3094, 3101, 3103, 3106, 3118, 3137, 3150, 3189, 3190, 3193, 3199, 3215	10.391	0.498	0.488
$CH_3(CH_2)_2{}^{\bullet}CH(CH_2)_3CH_3$		33, 44, 74, 111, 126, 149, 202, 256, 260, 286, 346, 450, 482, 484, 749, 761, 811, 892, 923, 940, 958, 1045, 1067, 1091, 1106, 1115, 1137, 1157, 1183, 1207, 1277, 1281, 1299, 1330, 1349, 1361, 1368, 1384, 1429, 1452, 1471, 1471, 1479, 1536, 1544, 1552, 1558, 1561, 1564, 1565, 1572, 1574, 3012, 3015, 3083, 3089, 3091, 3095, 3099, 3101, 3101, 3128, 3149, 3149, 3189, 3189, 3190, 3191, 3215	10.303	0.496	0.487
$^{\bullet}CH_2(CH_2)_6CH_3$	9pp	-2123, 69, 114, 217, 241, 284, 327, 337, 366, 432, 459, 470, 539, 742, 761, 793, 846, 857, 889, 927, 938, 1009, 1020, 1052, 1067, 1121, 1127, 1141, 1165, 1197, 1204, 1254, 1278, 1288, 1325, 1338, 1365, 1380, 1416, 1417, 1429, 1434, 1446, 1510, 1513, 1520, 1529, 1543, 1546, 1554, 1556, 1570, 1577, 3055, 3066, 3081, 3083, 3095, 3106, 3108, 3122, 3132, 3132, 3134, 3136, 3147, 3177, 3214, 3218	2.447	1.541	1.093
$^{\bullet}CH_2(CH_2)_6CH_3$	$8s_{\alpha}{}^{E}p$	-2033, 71, 165, 180, 209, 224, 253, 272, 354, 371, 471, 485, 519, 626, 758, 792, 869, 875, 920, 932, 969, 999, 1006, 1033, 1084, 1113, 1135, 1155, 1171, 1190, 1207, 1255, 1274, 1291, 1323, 1353, 1367, 1387, 1416, 1426, 1432, 1442, 1463, 1509, 1516, 1542, 1547, 1549, 1554, 1555, 1562, 1566, 1569, 3050, 3071, 3079, 3083, 3091, 3097, 3108, 3112, 3126, 3131, 3140, 3144, 3147, 3157, 3185, 3226	2.392	1.608	1.154
$^{\bullet}CH_2(CH_2)_6CH_3$	$8s_{\alpha}{}^{A}p$	-2043, 84, 147, 199, 214, 227, 262, 295, 365, 405, 479, 502, 527, 624, 749, 793, 850, 875, 886, 939, 961, 998, 1008, 1030, 1067, 1106, 1141, 1157, 1172, 1190, 1198, 1252, 1265, 1288, 1324, 1352, 1377, 1397, 1410, 1418, 1432, 1440, 1463, 1509, 1518, 1519, 1546, 1546, 1554, 1557,	2.547	1.441	1.036

		1559, 1567, 1571, 3052, 3070, 3082, 3084, 3096, 3100, 3117, 3122, 3133, 3141, 3144, 3147, 3149, 3162, 3188, 3225			
$^{\bullet}CH_2(CH_2)_6CH_3$	$7s_{\beta}{}^{E}p$	-1950, 76, 89, 131, 183, 205, 269, 315, 344, 395, 415, 486, 552, 573, 789, 807, 844, 852, 912, 929, 950, 991, 1013, 1046, 1082, 1090, 1124, 1150, 1162, 1184, 1228, 1262, 1289, 1311, 1324, 1346, 1347, 1406, 1419, 1428, 1431, 1437, 1469, 1511, 1514, 1519, 1540, 1544, 1549, 1552, 1556, 1564, 1569, 3055, 3059, 3066, 3077, 3079, 3102, 3104, 3112, 3117, 3126, 3129, 3134, 3142, 3190, 3193, 3229	2.972	1.170	0.908
$^{\bullet}CH_2(CH_2)_6CH_3$	$7s_{\beta}{}^{A}p$	-1958, 77, 89, 107, 212, 240, 269, 332, 350, 367, 458, 495, 558, 600, 772, 801, 812, 870, 891, 925, 957, 969, 1013, 1037, 1079, 1098, 1120, 1134, 1171, 1201, 1212, 1264, 1290, 1319, 1326, 1338, 1355, 1409, 1420, 1425, 1432, 1438, 1469, 1503, 1511, 1516, 1539, 1544, 1550, 1552, 1558, 1563, 1569, 3054, 3059, 3064, 3077, 3087, 3102, 3112, 3116, 3123, 3129, 3133, 3141, 3143, 3190, 3194, 3229	2.606	1.338	1.051
$^{\bullet}CH_2(CH_2)_6CH_3$	$6s_{\beta}{}^{E}p$	-2012, 62, 76, 102, 147, 214, 256, 307, 339, 380, 462, 470, 525, 617, 763, 832, 853, 884, 888, 926, 936, 990, 1016, 1048, 1087, 1093, 1123, 1127, 1157, 1174, 1226, 1252, 1269, 1302, 1317, 1331, 1365, 1375, 1396, 1412, 1421, 1448, 1470, 1504, 1514, 1540, 1545, 1550, 1557, 1560, 1564, 1572, 1589, 3042, 3067, 3076, 3089, 3094, 3100, 3101, 3114, 3129, 3133, 3144, 3148, 3153, 3188, 3190, 3241	3.989	0.857	0.757
$^{\bullet}CH_2(CH_2)_6CH_3$	$6s_{\beta}{}^{A}p$	-2003, 70, 80, 107, 154, 204, 257, 294, 369, 403, 458, 502, 571, 602, 763, 836, 847, 867, 886, 926, 939, 976, 1002, 1036, 1082, 1102, 1115, 1120, 1151, 1179, 1216, 1248, 1276, 1301, 1313, 1333, 1364, 1385, 1399, 1405, 1415, 1444, 1470, 1492, 1513, 1539, 1545, 1550, 1557, 1559, 1564, 1571, 1589, 3049, 3064, 3074, 3094, 3094, 3100, 3108, 3123, 3128, 3143, 3148, 3151, 3153, 3188, 3190, 3241	3.518	0.951	0.848
$^{\bullet}CH_2(CH_2)_6CH_3$	$5s_{\beta}{}^{E}p$	-2211, 52, 67, 103, 135, 161, 223, 261, 303, 333, 461, 519, 573, 588, 752, 809, 853, 896, 917, 932, 941, 975, 1011, 1049, 1065, 1078, 1108, 1116, 1160, 1172, 1226, 1252, 1267, 1294, 1299, 1339, 1355, 1368, 1372, 1388, 1430, 1452, 1471, 1488, 1516, 1542, 1549, 1552, 1561, 1563, 1565, 1573, 1719, 3044, 3080, 3092, 3094, 3101, 3103, 3106, 3125, 3135, 3147, 3150, 3160, 3167, 3189, 3190, 3259	5.388	0.664	0.622
$^{\bullet}CH_2(CH_2)_6CH_3$	$5s_{\beta}{}^{A}p$	-2201, 50, 70, 112, 133, 167, 208, 261, 307, 362, 462, 504, 612, 625, 752, 800, 866, 877, 886, 934, 945, 993, 1004, 1029, 1069, 1093, 1103, 1119, 1136, 1176, 1210, 1258, 1270, 1286, 1300, 1350, 1357, 1367, 1372, 1381, 1423, 1451, 1471, 1476, 1516, 1542, 1549, 1552, 1561, 1565, 1565, 1573, 1718, 3051, 3079, 3092, 3098, 3101, 3105, 3113, 3126, 3146, 3147, 3163, 3166, 3171, 3189, 3190, 3258	4.654	0.727	0.688
$^{\bullet}CH_2(CH_2)_6CH_3$	$4s_{\beta}p$	-2488, 48, 59, 99, 102, 139, 156, 242, 260, 299, 395, 423, 494, 673, 747, 765, 795, 856, 914, 929, 960, 999, 1011, 1040, 1060, 1093, 1105, 1120, 1132, 1175, 1219, 1258, 1275, 1285, 1289, 1332, 1343, 1365, 1372, 1394, 1429, 1444, 1456, 1471, 1484, 1543, 1550, 1555, 1556, 1565, 1565, 1574, 1893, 3048, 3075, 3084, 3093, 3100, 3101, 3117, 3136, 3136, 3149, 3170, 3176, 3189, 3190, 3198, 3287	7.573	0.553	0.546

${}^{\bullet}CH_2(CH_2)_6CH_3$	$3s_{\alpha}p$	-2214, 49, 67, 84, 107, 142, 158, 205, 260, 283, 345, 386, 479, 489, 729, 747, 755, 767, 825, 915, 929, 951, 1023, 1051, 1073, 1101, 1111, 1120, 1165, 1201, 1221, 1268, 1275, 1314, 1331, 1347, 1357, 1369, 1375, 1384, 1428, 1454, 1462, 1471, 1483, 1544, 1549, 1551, 1558, 1565, 1567, 1575, 2395, 3040, 3074, 3078, 3086, 3093, 3099, 3100, 3114, 3126, 3141, 3150, 3189, 3190, 3227, 3233, 3347	11.182	0.500	0.491

Table S2

Species	Rxn Type	Vibrational Frequencies (cm^{-1})	Rotational Constants (GHz) A	B	C
$^{\bullet}CH_2CH_3$		120, 465, 807, 979, 1066, 1194, 1398, 1466, 1480, 1483, 2955, 3047, 3092, 3154, 3255	103.618	22.705	21.047
$^{\bullet}CH_2CH_3$	3pp	-1932, 538, 735, 749, 783, 1138, 1195, 1289, 1418, 1439, 2249, 3152, 3157, 3257, 3280	107.314	23.903	21.583
$^{\bullet}CH_2CH_2CH_3$		111, 247, 365, 466, 754, 882, 921, 1050, 1087, 1173, 1268, 1360, 1408, 1463, 1466, 1498, 1505, 2928, 3016, 3034, 3101, 3108, 3145, 3248	32.874	8.941	7.752
$CH_3{}^{\bullet}CH_2CH_3$		113, 123, 360, 414, 883, 936, 942, 1035, 1151, 1178, 1368, 1406, 1413, 1469, 1480, 1480, 1491, 2943, 2948, 3030, 3032, 3091, 3092, 3171	37.575	8.288	7.419
$^{\bullet}CH_2CH_2CH_3$	4pp	-2099, 163, 502, 658, 758, 878, 922, 955, 977, 1037, 1185, 1242, 1254, 1344, 1415, 1434, 1493, 1778, 3070, 3097, 3103, 3115, 3204, 3206	25.092	11.096	9.067
$^{\bullet}CH_2CH_2CH_3$	$3s_{\alpha}p$	-1934, 206, 360, 365, 698, 716, 897, 921, 1039, 1162, 1192, 1283, 1364, 1415, 1429, 1483, 1494, 2223, 2975, 3051, 3096, 3149, 3166, 3266	37.803	8.529	7.565
$^{\bullet}CH_2(CH_2)_2CH_3$		100, 133, 238, 260, 423, 469, 728, 821, 864, 962, 1034, 1073, 1092, 1168, 1247, 1311, 1321, 1387, 1412, 1462, 1466, 1491, 1499, 1509, 2917, 3009, 3022, 3028, 3055, 3094, 3102, 3146, 3248	25.181	3.796	3.527
$CH_3{}^{\bullet}CHCH_2CH_3$		63, 112, 233, 260, 409, 427, 767, 846, 973, 986, 1027, 1072, 1136, 1181, 1270, 1314, 1402, 1408, 1414, 1469, 1475, 1486, 1497, 1505, 2917, 2946, 2999, 3032, 3033, 3091, 3099, 3107, 3157	26.464	3.626	3.413
$^{\bullet}CH_2(CH_2)_2CH_3$	5pp	-1845, 210, 326, 558, 562, 641, 835, 845, 882, 931, 961, 985, 1036, 1083, 1186, 1221, 1250, 1322, 1337, 1391, 1453, 1458, 1486, 1501, 1632, 3030, 3033, 3062, 3076, 3090, 3091, 3174, 3175	11.567	6.623	4.902
$^{\bullet}CH_2(CH_2)_2CH_3$	$4s_{\alpha}p$	-2097, 94, 219, 351, 365, 616, 739, 840, 863, 935, 946, 1001, 1059, 1120, 1175, 1230, 1255, 1331, 1350, 1406, 1429, 1484, 1490, 1493, 1766, 2993, 3057, 3060, 3095, 3101, 3102, 3118, 3205	16.809	4.487	4.257
$^{\bullet}CH_2(CH_2)_2CH_3$	$3s_{\alpha}p$	-1931, 107, 233, 256, 365, 436, 696, 718, 791, 845, 967, 1032, 1083, 1166, 1180, 1265, 1298, 1317, 1403, 1409, 1428, 1479, 1496, 1506, 2219, 2950, 3023, 3032, 3098, 3105, 3148, 3154, 3265	25.904	3.711	3.496
$^{\bullet}CH_2(CH_2)_3CH_3$		95, 110, 131, 179, 243, 390, 401, 468, 726, 771, 861, 911, 942, 1025, 1063, 1087, 1096, 1164, 1233, 1285, 1305, 1328, 1364, 1397, 1413, 1462, 1466, 1485, 1497, 1499, 1512, 2917, 3006, 3009, 3018, 3029, 3033, 3058, 3095, 3101, 3145, 3248	18.203	2.002	1.892

$CH_3{}^{\bullet}CH(CH_2)_2CH_3$		57, 99, 128, 188, 240, 386, 401, 417, 736, 855, 875, 933, 981, 1038, 1060, 1093, 1140, 1173, 1249, 1285, 1318, 1368, 1405, 1411, 1417, 1467, 1475, 1486, 1491, 1499, 1509, 2907, 2946, 2990, 3020, 3028, 3033, 3053, 3090, 3094, 3101, 3156	19.303	1.930	1.842
$CH_3CH_2{}^{\bullet}CHCH_2CH_3$		50, 59, 181, 237, 241, 390, 403, 412, 753, 781, 874, 947, 1023, 1041, 1046, 1086, 1143, 1172, 1261, 1276, 1281, 1365, 1406, 1411, 1421, 1464, 1475, 1497, 1498, 1505, 1505, 2915, 2920, 2999, 3004, 3033, 3034, 3100, 3100, 3107, 3107, 3141	16.589	1.977	1.863
${}^{\bullet}CH_2(CH_2)_3CH_3$	6pp	-1683, 145, 292, 346, 426, 458, 573, 659, 808, 820, 851, 885, 915, 999, 1003, 1057, 1080, 1086, 1191, 1202, 1256, 1282, 1353, 1357, 1365, 1409, 1455, 1455, 1479, 1484, 1495, 1507, 2996, 2998, 3013, 3039, 3045, 3069, 3079, 3081, 3158, 3160	6.633	4.326	2.982
${}^{\bullet}CH_2(CH_2)_3CH_3$	$5s_{\alpha}{}^{E}p$	-1839, 139, 190, 216, 334, 473, 534, 566, 800, 852, 868, 895, 917, 979, 998, 1028, 1091, 1125, 1181, 1221, 1243, 1304, 1332, 1366, 1403, 1415, 1456, 1484, 1486, 1492, 1499, 1635, 2993, 3019, 3030, 3054, 3058, 3066, 3076, 3091, 3098, 3176	9.101	3.067	2.584
${}^{\bullet}CH_2(CH_2)_3CH_3$	$5s_{\alpha}{}^{A}p$	-1832, 135, 181, 200, 349, 467, 577, 590, 790, 834, 849, 908, 909, 994, 995, 1023, 1081, 1117, 1167, 1221, 1239, 1321, 1329, 1347, 1397, 1410, 1455, 1482, 1488, 1493, 1500, 1629, 3001, 3026, 3035, 3058, 3064, 3076, 3091, 3092, 3108, 3175	7.711	3.403	2.964
${}^{\bullet}CH_2(CH_2)_3CH_3$	$4s_{\beta}p$	-2092, 89, 99, 236, 238, 361, 428, 620, 729, 784, 854, 878, 931, 981, 992, 1026, 1089, 1108, 1180, 1226, 1254, 1280, 1307, 1341, 1384, 1410, 1429, 1478, 1490, 1497, 1505, 1762, 2967, 3023, 3033, 3059, 3092, 3099, 3102, 3106, 3111, 3205	12.096	2.357	2.217
${}^{\bullet}CH_2(CH_2)_3CH_3$	$3s_{\alpha}p$	-1930, 96, 111, 184, 245, 355, 391, 417, 697, 718, 747, 866, 880, 937, 1024, 1061, 1104, 1163, 1178, 1250, 1286, 1293, 1321, 1367, 1406, 1414, 1427, 1476, 1491, 1500, 1509, 2219, 2940, 3011, 3020, 3029, 3053, 3095, 3101, 3148, 3154, 3265	19.169	1.960	1.872
${}^{\bullet}CH_2(CH_2)_4CH_3$		71, 87, 112, 134, 149, 241, 301, 367, 456, 496, 726, 746, 822, 890, 900, 965, 1023, 1043, 1067, 1085, 1107, 1162, 1223, 1265, 1286, 1323, 1329, 1338, 1386, 1404, 1418, 1468, 1473, 1491, 1495, 1503, 1505, 1515, 2926, 3004, 3012, 3019, 3025, 3028, 3030, 3049, 3066, 3096, 3101, 3149, 3252	15.325	1.166	1.122
$CH_3{}^{\bullet}CH(CH_2)_3CH_3$		49, 92, 114, 123, 141, 246, 298, 361, 385, 467, 731, 783, 894, 910, 918, 985, 1020, 1059, 1068, 1100, 1136, 1169, 1231, 1267, 1303, 1326, 1337, 1393, 1409, 1417, 1423, 1470, 1478, 1489, 1492, 1501, 1504, 1514, 2913, 2949, 2991, 3010, 3018, 3029, 3030, 3037, 3061, 3096, 3099, 3101, 3165	15.826	1.136	1.100
$CH_3(CH_2)_2{}^{\bullet}CHCH_2CH_3$		42, 53, 114, 150, 237, 249, 296, 372, 393, 469, 733, 772, 861, 895, 911, 1021, 1038, 1054, 1074, 1098, 1138, 1167, 1246, 1263, 1271, 1318, 1338, 1389, 1415, 1417, 1428, 1467, 1478, 1497, 1503, 1505, 1508, 1511, 2912, 2923, 2993, 3002, 3024, 3030, 3035, 3058, 3096, 3101, 3102, 3107, 3147	14.543	1.146	1.106
${}^{\bullet}CH_2(CH_2)_4CH_3$	7pp	-1623, 117, 174, 306, 332, 375, 416, 518, 528, 613, 761, 816, 822, 863, 932, 936, 950, 1021, 1050, 1055, 1104, 1142, 1183, 1234, 1246, 1286, 1294, 1366, 1376, 1383, 1385, 1427, 1445, 1457, 1458, 1482, 1485, 1493, 1498, 2992, 2992, 3007, 3009, 3033, 3035, 3053, 3055, 3071,	4.243	2.998	1.982

		3072, 3148, 3150			
$^{\bullet}CH_2(CH_2)_4CH_3$	$6s_{\alpha}{}^{E}p$	-1673, 103, 161, 193, 286, 333, 410, 449, 493, 585, 803, 816, 831, 872, 917, 931, 972, 1020, 1054, 1068, 1097, 1127, 1182, 1206, 1240, 1281, 1323, 1354, 1365, 1379, 1412, 1430, 1459, 1481, 1488, 1489, 1495, 1500, 1514, 2989, 2996, 3000, 3015, 3030, 3046, 3058, 3068, 3071, 3083, 3099, 3163	5.184	2.338	1.808
$^{\bullet}CH_2(CH_2)_4CH_3$	$6s_{\alpha}{}^{A}p$	-1661, 112, 151, 189, 268, 366, 417, 468, 539, 573, 794, 811, 832, 855, 923, 929, 953, 1025, 1039, 1062, 1095, 1126, 1170, 1203, 1238, 1282, 1336, 1354, 1359, 1369, 1408, 1429, 1458, 1479, 1487, 1491, 1497, 1501, 1510, 2989, 2998, 3003, 3023, 3042, 3048, 3066, 3073, 3083, 3086, 3102, 3163	4.851	2.528	2.002
$^{\bullet}CH_2(CH_2)_4CH_3$	$5s_{\beta}{}^{E}p$	-1828, 84, 125, 164, 242, 268, 406, 467, 534, 567, 773, 815, 855, 891, 901, 927, 967, 1008, 1026, 1042, 1111, 1115, 1180, 1216, 1233, 1284, 1292, 1327, 1344, 1384, 1414, 1419, 1460, 1483, 1491, 1502, 1505, 1508, 1618, 2970, 3023, 3030, 3033, 3035, 3057, 3068, 3079, 3093, 3099, 3105, 3178	6.892	1.753	1.524
$^{\bullet}CH_2(CH_2)_4CH_3$	$5s_{\beta}{}^{A}p$	-1819, 82, 123, 160, 239, 269, 397, 473, 584, 596, 759, 810, 843, 859, 911, 925, 971, 1020, 1036, 1041, 1079, 1118, 1171, 1218, 1236, 1277, 1311, 1322, 1336, 1375, 1412, 1417, 1460, 1483, 1492, 1502, 1506, 1508, 1614, 2979, 3029, 3032, 3032, 3042, 3063, 3080, 3093, 3096, 3100, 3104, 3178	6.082	1.931	1.692
$^{\bullet}CH_2(CH_2)_4CH_3$	$4s_{\beta}p$	-2075, 69, 87, 134, 170, 242, 342, 390, 419, 624, 730, 758, 833, 887, 904, 928, 942, 999, 1036, 1055, 1083, 1125, 1175, 1222, 1253, 1258, 1283, 1321, 1336, 1357, 1399, 1417, 1433, 1480, 1497, 1497, 1504, 1512, 1744, 2963, 3015, 3024, 3029, 3058, 3063, 3095, 3097, 3102, 3104, 3115, 3207	10.265	1.316	1.285
$^{\bullet}CH_2(CH_2)_4CH_3$	$3s_{\alpha}p$	-1903, 69, 98, 130, 143, 249, 302, 348, 394, 468, 704, 737, 743, 798, 896, 905, 936, 1023, 1048, 1065, 1114, 1161, 1175, 1235, 1269, 1280, 1311, 1328, 1339, 1393, 1411, 1419, 1437, 1481, 1492, 1501, 1505, 1514, 2194, 2943, 3010, 3016, 3022, 3030, 3038, 3062, 3096, 3101, 3154, 3161, 3269	15.543	1.151	1.115
$^{\bullet}CH_2(CH_2)_5CH_3$		60, 68, 99, 100, 139, 147, 242, 246, 304, 412, 473, 498, 726, 736, 780, 857, 890, 917, 985, 1004, 1049, 1051, 1068, 1085, 1114, 1160, 1217, 1252, 1270, 1307, 1318, 1327, 1332, 1366, 1396, 1404, 1418, 1467, 1472, 1491, 1491, 1499, 1504, 1508, 1516, 2925, 3003, 3006, 3015, 3019, 3024, 3025, 3029, 3037, 3055, 3067, 3095, 3100, 3149, 3251	12.649	0.741	0.719
$CH_3{}^{\bullet}CH(CH_2)_4CH_3$		45, 66, 94, 109, 116, 149, 244, 246, 305, 380, 419, 482, 730, 751, 836, 885, 923, 953, 990, 1001, 1047, 1064, 1079, 1106, 1137, 1167, 1224, 1256, 1284, 1314, 1325, 1329, 1370, 1403, 1410, 1419, 1422, 1470, 1478, 1489, 1491, 1494, 1504, 1505, 1515, 2915, 2949, 2989, 3004, 3013, 3020, 3028, 3029, 3030, 3047, 3064, 3095, 3098, 3100, 3164	13.103	0.726	0.708
$CH_3CH_2{}^{\bullet}CH(CH_2)_3CH_3$		40, 43, 91, 117, 124, 237, 243, 246, 307, 383, 417, 485, 729, 764, 790, 885, 916, 930, 1001, 1039, 1044, 1065, 1081, 1106, 1137, 1164, 1231, 1251, 1270, 1302, 1314, 1326, 1367, 1400, 1416, 1417, 1428, 1467, 1478, 1493, 1501, 1503, 1504, 1508, 1514, 2914, 2924, 2992, 3000,	11.347	0.736	0.713

		3011, 3019, 3030, 3035, 3037, 3061, 3096, 3101, 3102, 3107, 3148,			
$CH_3(CH_2)_2{}^{\bullet}CH(CH_2)_2CH_3$		33, 41, 88, 118, 142, 235, 243, 245, 301, 394, 421, 484, 729, 744, 849, 873, 882, 915, 1001, 1044, 1051, 1066, 1087, 1105, 1137, 1163, 1241, 1250, 1253, 1313, 1317, 1320, 1367, 1397, 1416, 1417, 1427, 1466, 1477, 1497, 1497, 1503, 1504, 1511, 1511, 2911, 2915, 2992, 2997, 3024, 3025, 3029, 3030, 3058, 3058, 3095, 3096, 3101, 3102, 3147	12.307	0.727	0.711
${}^{\bullet}CH_2(CH_2)_5CH_3$	8pp	-1666, 97, 175, 198, 229, 298, 352, 413, 455, 483, 567, 619, 731, 760, 839, 851, 902, 904, 946, 968, 1008, 1057, 1083, 1104, 1115, 1121, 1163, 1222, 1236, 1262, 1279, 1313, 1353, 1369, 1374, 1387, 1396, 1433, 1443, 1462, 1464, 1484, 1488, 1494, 1504, 1506, 2983, 2997, 3014, 3022, 3026, 3030, 3039, 3049, 3063, 3068, 3070, 3073, 3144, 3147	3.098	2.126	1.447
${}^{\bullet}CH_2(CH_2)_5CH_3$	$7s_{\alpha}{}^{E}p$	-1609, 89, 150, 182, 202, 264, 321, 333, 391, 482, 520, 551, 763, 801, 825, 864, 887, 902, 953, 962, 1020, 1037, 1076, 1083, 1105, 1143, 1180, 1225, 1247, 1279, 1287, 1327, 1370, 1382, 1384, 1386, 1410, 1438, 1453, 1459, 1481, 1484, 1492, 1492, 1497, 1498, 2980, 2988, 3000, 3007, 3008, 3022, 3032, 3052, 3053, 3057, 3065, 3073, 3098, 3151	3.438	1.803	1.297
${}^{\bullet}CH_2(CH_2)_5CH_3$	$7s_{\alpha}{}^{A}p$	-1614, 84, 122, 167, 226, 285, 337, 351, 420, 473, 518, 575, 749, 770, 828, 850, 888, 907, 949, 965, 994, 1043, 1068, 1084, 1118, 1153, 1164, 1221, 1248, 1280, 1291, 1345, 1367, 1376, 1383, 1389, 1411, 1434, 1449, 1459, 1478, 1484, 1489, 1497, 1498, 1502, 2979, 2987, 3002, 3008, 3019, 3033, 3037, 3053, 3058, 3069, 3073, 3075, 3104, 3151	3.115	1.987	1.494
${}^{\bullet}CH_2(CH_2)_5CH_3$	$6s_{\beta}{}^{E}p$	-1672, 70, 96, 129, 226, 254, 300, 377, 435, 451, 487, 583, 774, 806, 820, 851, 874, 932, 943, 970, 1010, 1044, 1059, 1074, 1110, 1122, 1181, 1205, 1233, 1269, 1297, 1301, 1353, 1360, 1366, 1389, 1415, 1428, 1459, 1480, 1485, 1490, 1499, 1502, 1507, 1509, 2969, 2992, 2999, 3015, 3026, 3030, 3032, 3045, 3060, 3071, 3082, 3098, 3104, 3162	4.269	1.409	1.153
${}^{\bullet}CH_2(CH_2)_5CH_3$	$6s_{\beta}{}^{A}p$	-1660, 80, 103, 125, 234, 258, 301, 370, 439, 490, 539, 573, 772, 795, 814, 844, 872, 919, 946, 952, 1015, 1048, 1055, 1068, 1097, 1122, 1175, 1203, 1237, 1275, 1285, 1315, 1352, 1357, 1368, 1380, 1417, 1430, 1458, 1481, 1485, 1490, 1497, 1503, 1505, 1511, 2976, 2990, 2998, 3021, 3032, 3034, 3043, 3048, 3071, 3079, 3082, 3099, 3104, 3163	3.963	1.543	1.263
${}^{\bullet}CH_2(CH_2)_5CH_3$	$5s_{\beta}{}^{E}p$	-1828, 68, 78, 131, 160, 231, 250, 342, 380, 497, 542, 573, 743, 816, 843, 865, 887, 906, 924, 960, 1007, 1027, 1045, 1066, 1109, 1125, 1180, 1213, 1229, 1265, 1276, 1317, 1324, 1334, 1368, 1394, 1416, 1419, 1459, 1480, 1491, 1498, 1504, 1505, 1512, 1619, 2959, 3017, 3023, 3025, 3029, 3034, 3055, 3058, 3068, 3079, 3093, 3096, 3101, 3178	6.341	1.008	0.931
${}^{\bullet}CH_2(CH_2)_5CH_3$	$5s_{\beta}{}^{A}p$	-1819, 70, 74, 136, 159, 216, 244, 370, 384, 483, 585, 594, 740, 805, 837, 846, 884, 905, 936, 959, 996, 1043, 1051, 1055, 1090, 1128, 1168, 1218, 1233, 1255, 1285, 1320, 1323, 1336, 1356, 1390, 1413, 1418, 1460, 1480, 1491, 1497, 1504, 1507, 1511, 1614, 2968, 3018, 3024, 3029, 3030, 3041, 3056, 3063, 3081, 3093, 3096, 3098, 3101, 3178	5.291	1.111	1.038
${}^{\bullet}CH_2(CH_2)_5CH_3$	$4s_{\beta}p$	-2075, 59, 67, 119, 125, 146, 245, 292, 323, 404, 463, 623, 729, 745, 791, 859, 890, 917, 939, 954, 997, 1017, 1054, 1065, 1086, 1130, 1174, 1220, 1239, 1255, 1269, 1307, 1325, 1329, 1340, 1383, 1404, 1418, 1433, 1480, 1492, 1497, 1501, 1504, 1514, 1746, 2964, 3010, 3015, 3020,	8.652	0.821	0.802

		3030, 3037, 3061, 3063, 3096, 3097, 3101, 3104, 3114, 3207			
$^{\bullet}CH_2(CH_2)_5CH_3$	$3s_{\alpha}p$	-1903, 60, 73, 104, 128, 147, 246, 249, 304, 377, 417, 487, 703, 734, 742, 764, 848, 885, 920, 970, 1005, 1049, 1057, 1070, 1121, 1159, 1176, 1227, 1257, 1274, 1297, 1317, 1327, 1332, 1369, 1403, 1413, 1419, 1437, 1481, 1491, 1495, 1505, 1505, 1515, 2194, 2944, 3004, 3011, 3017, 3022, 3029, 3030, 3048, 3065, 3096, 3101, 3154, 3161, 3269	12.976	0.733	0.715
$^{\bullet}CH_2(CH_2)_6CH_3$		46, 61, 80, 96, 111, 140, 158, 198, 242, 275, 339, 460, 471, 497, 726, 732, 756, 816, 878, 900, 926, 993, 1014, 1025, 1056, 1065, 1070, 1085, 1120, 1159, 1214, 1244, 1260, 1293, 1304, 1321, 1330, 1334, 1347, 1383, 1403, 1405, 1418, 1468, 1473, 1489, 1491, 1495, 1502, 1503, 1510, 1517, 2925, 3002, 3004, 3009, 3015, 3020, 3024, 3025, 3029, 3030, 3044, 3058, 3068, 3095, 3100, 3149, 3252	11.132	0.498	0.487
$CH_3{}^{\bullet}CH(CH_2)_5CH_3$		39, 62, 77, 81, 109, 141, 147, 198, 247, 275, 336, 384, 470, 472, 729, 739, 787, 878, 893, 912, 971, 999, 1008, 1020, 1058, 1067, 1085, 1111, 1138, 1165, 1218, 1247, 1269, 1297, 1312, 1327, 1334, 1348, 1389, 1405, 1410, 1418, 1422, 1470, 1478, 1489, 1491, 1491, 1499, 1504, 1508, 1516, 2915, 2949, 2989, 3003, 3006, 3016, 3020, 3025, 3029, 3030, 3036, 3053, 3066, 3095, 3098, 3100, 3164	11.391	0.491	0.481
$CH_3CH_2{}^{\bullet}CH(CH_2)_4CH_3$		35, 40, 68, 95, 106, 144, 196, 239, 241, 280, 337, 385, 471, 473, 728, 747, 774, 837, 892, 913, 962, 1003, 1020, 1045, 1054, 1067, 1088, 1113, 1137, 1162, 1223, 1244, 1268, 1284, 1296, 1324, 1329, 1347, 1385, 1404, 1416, 1417, 1426, 1467, 1478, 1491, 1495, 1503, 1503, 1505, 1508, 1515, 2914, 2923, 2992, 3001, 3004, 3013, 3021, 3028, 3029, 3035, 3047, 3064, 3095, 3100, 3101, 3107, 3148	10.296	0.494	0.484
$CH_3(CH_2)_2{}^{\bullet}CH(CH_2)_3CH_3$		29, 34, 73, 107, 123, 133, 196, 234, 251, 276, 337, 391, 472, 473, 728, 739, 785, 860, 889, 906, 925, 1005, 1020, 1055, 1060, 1066, 1097, 1110, 1137, 1161, 1231, 1240, 1249, 1297, 1305, 1318, 1328, 1346, 1384, 1403, 1416, 1418, 1427, 1466, 1477, 1492, 1497, 1501, 1503, 1505, 1511, 1514, 2911, 2915, 2991, 2996, 3011, 3019, 3024, 3029, 3030, 3037, 3058, 3061, 3095, 3096, 3100, 3101, 3148	10.019	0.494	0.484
$^{\bullet}CH_2(CH_2)_6CH_3$	9pp	-1714, 85, 108, 209, 230, 263, 316, 331, 359, 416, 439, 451, 517, 705, 732, 760, 811, 825, 854, 894, 903, 970, 983, 1016, 1023, 1080, 1087, 1092, 1116, 1150, 1156, 1210, 1237, 1242, 1283, 1297, 1324, 1347, 1374, 1377, 1382, 1389, 1401, 1434, 1447, 1459, 1464, 1480, 1484, 1491, 1496, 1511, 1516, 2977, 2987, 3009, 3014, 3022, 3026, 3033, 3040, 3051, 3054, 3063, 3064, 3067, 3092, 3135, 3139	2.379	1.531	1.075
$^{\bullet}CH_2(CH_2)_6CH_3$	$8s_{\alpha}{}^{E}p$	-1663, 70, 158, 171, 198, 203, 240, 256, 343, 355, 456, 469, 497, 594, 728, 755, 831, 841, 887, 900, 930, 966, 969, 992, 1038, 1074, 1088, 1109, 1118, 1141, 1163, 1217, 1228, 1253, 1280, 1313, 1326, 1353, 1375, 1380, 1387, 1397, 1413, 1447, 1455, 1463, 1484, 1485, 1493, 1494, 1499, 1503, 1506, 2972, 2994, 3001, 3012, 3018, 3022, 3029, 3030, 3048, 3052, 3062, 3064, 3069, 3075, 3098, 3149	2.513	1.408	1.011
$^{\bullet}CH_2(CH_2)_6CH_3$	$8s_{\alpha}{}^{A}p$	-1670, 78, 136, 191, 202, 206, 239, 284, 353, 390, 466, 474, 511, 594, 719, 755, 812, 847, 850,	2.349	1.570	1.127

		901, 926, 956, 976, 994, 1024, 1066, 1097, 1114, 1120, 1138, 1154, 1214, 1222, 1249, 1281, 1312, 1339, 1355, 1368, 1376, 1386, 1395, 1413, 1443, 1449, 1463, 1484, 1485, 1493, 1497, 1500, 1504, 1507, 2974, 2992, 3006, 3015, 3026, 3028, 3034, 3042, 3051, 3064, 3069, 3070, 3074, 3076, 3103, 3148			
$^{\bullet}CH_2(CH_2)_6CH_3$	$7s_{\beta}{}^{E}p$	-1612, 73, 85, 133, 179, 199, 258, 307, 331, 383, 405, 472, 518, 555, 764, 773, 816, 824, 882, 890, 917, 955, 979, 1004, 1040, 1048, 1077, 1098, 1114, 1137, 1181, 1218, 1241, 1271, 1281, 1301, 1309, 1365, 1375, 1382, 1385, 1390, 1416, 1438, 1455, 1463, 1480, 1483, 1488, 1492, 1498, 1504, 1509, 2973, 2982, 2988, 3007, 3008, 3023, 3025, 3032, 3033, 3050, 3053, 3056, 3072, 3099, 3104, 3151	2.949	1.141	0.888
$^{\bullet}CH_2(CH_2)_6CH_3$	$7s_{\beta}{}^{A}p$	-1618, 65, 78, 103, 198, 232, 257, 323, 336, 358, 447, 468, 532, 577, 749, 769, 783, 837, 860, 891, 919, 940, 979, 996, 1031, 1065, 1073, 1088, 1117, 1151, 1167, 1221, 1243, 1273, 1286, 1294, 1314, 1368, 1374, 1379, 1384, 1391, 1416, 1436, 1452, 1460, 1479, 1483, 1488, 1494, 1498, 1504, 1509, 2972, 2981, 2986, 3008, 3018, 3032, 3032, 3036, 3040, 3053, 3058, 3066, 3072, 3099, 3104, 3150	2.618	1.282	1.012
$^{\bullet}CH_2(CH_2)_6CH_3$	$6s_{\beta}{}^{E}p$	-1672, 58, 67, 95, 145, 203, 239, 290, 325, 368, 449, 455, 509, 585, 743, 803, 819, 852, 855, 893, 900, 949, 981, 1007, 1041, 1054, 1072, 1078, 1106, 1129, 1179, 1205, 1228, 1257, 1282, 1287, 1323, 1338, 1354, 1365, 1378, 1398, 1417, 1429, 1459, 1479, 1483, 1489, 1497, 1500, 1504, 1509, 1511, 2958, 2992, 2999, 3014, 3016, 3022, 3029, 3031, 3045, 3054, 3062, 3071, 3082, 3095, 3100, 3162	3.991	0.837	0.740
$^{\bullet}CH_2(CH_2)_6CH_3$	$6s_{\beta}{}^{A}p$	-1661, 62, 74, 96, 147, 196, 245, 276, 353, 392, 446, 482, 540, 573, 743, 809, 810, 837, 850, 894, 903, 945, 964, 997, 1038, 1056, 1070, 1075, 1102, 1130, 1172, 1202, 1233, 1256, 1275, 1293, 1322, 1346, 1357, 1361, 1370, 1394, 1417, 1429, 1458, 1481, 1484, 1489, 1497, 1498, 1504, 1506, 1512, 2966, 2990, 2998, 3017, 3021, 3026, 3029, 3043, 3047, 3056, 3071, 3080, 3082, 3095, 3100, 3162	3.541	0.918	0.821
$^{\bullet}CH_2(CH_2)_6CH_3$	$5s_{\beta}{}^{E}p$	-1828, 52, 69, 100, 131, 158, 208, 244, 290, 320, 447, 499, 542, 572, 735, 784, 821, 857, 884, 893, 904, 941, 970, 1004, 1020, 1035, 1063, 1070, 1111, 1130, 1180, 1212, 1225, 1251, 1265, 1304, 1315, 1329, 1330, 1350, 1383, 1400, 1416, 1419, 1459, 1480, 1491, 1493, 1501, 1504, 1505, 1514, 1619, 2960, 3009, 3016, 3021, 3024, 3030, 3034, 3037, 3056, 3060, 3068, 3079, 3093, 3096, 3100, 3178	5.408	0.651	0.611
$^{\bullet}CH_2(CH_2)_6CH_3$	$5s_{\beta}{}^{A}p$	-1819, 51, 63, 108, 128, 155, 189, 240, 296, 347, 451, 480, 584, 596, 733, 773, 828, 841, 856, 899, 905, 960, 965, 986, 1021, 1049, 1057, 1071, 1094, 1132, 1166, 1216, 1230, 1240, 1269, 1307, 1321, 1329, 1332, 1340, 1375, 1401, 1413, 1418, 1460, 1480, 1491, 1492, 1501, 1503, 1508, 1513, 1614, 2969, 3009, 3017, 3023, 3029, 3029, 3037, 3041, 3060, 3063, 3081, 3093, 3096, 3098, 3100, 3178	4.731	0.702	0.665
$^{\bullet}CH_2(CH_2)_6CH_3$	$4s_{\beta}p$	-2075, 47, 59, 95, 99, 135, 149, 234, 245, 288, 378, 415, 480, 624, 729, 738, 766, 825, 878, 892, 924, 941, 973, 999, 1006, 1043, 1061, 1072, 1088, 1133, 1174, 1219, 1230, 1252, 1261, 1289, 1309, 1325, 1329, 1339, 1361, 1396, 1406, 1418, 1433, 1480, 1491, 1495, 1497, 1504, 1505,	7.783	0.540	0.534

		1515, 1746, 2964, 3004, 3011, 3017, 3021, 3028, 3029, 3048, 3062, 3064, 3095, 3096, 3100, 3104, 3114, 3207			
$^{\bullet}CH_2(CH_2)_6CH_3$	$3s_{\alpha}p$	-1903, 44, 65, 81, 102, 138, 149, 200, 250, 274, 339, 376, 470, 477, 703, 732, 741, 748, 799, 886, 894, 913, 988, 1010, 1025, 1057, 1066, 1073, 1125, 1158, 1176, 1220, 1247, 1267, 1287, 1300, 1316, 1331, 1336, 1348, 1388, 1405, 1414, 1417, 1437, 1481, 1490, 1491, 1499, 1505, 1508, 1516, 2194, 2944, 3004, 3006, 3014, 3018, 3022, 3026, 3029, 3037, 3054, 3067, 3095, 3100, 3154, 3161, 3269	11.216	0.494	0.485

Table S3

	rxn. type	Direction	Temperature 200	300	400	500	600	700	800	900	1000	1500	2000	2500
C_2H_5	3pp	Forward	2.65E+12	3.14E+12	3.53E+12	3.91E+12	4.27E+12	4.62E+12	4.95E+12	5.27E+12	5.57E+12	6.81E+12	7.72E+12	8.40E+12
		Reverse	2.65E+12	3.14E+12	3.53E+12	3.91E+12	4.27E+12	4.62E+12	4.95E+12	5.27E+12	5.57E+12	6.81E+12	7.72E+12	8.40E+12
C_3H_7	$3s_{\alpha}p$	Forward	2.91E+12	3.72E+12	4.39E+12	4.99E+12	5.53E+12	6.03E+12	6.49E+12	6.92E+12	7.32E+12	8.93E+12	1.01E+13	1.10E+13
		Reverse	2.21E+12	2.60E+12	2.96E+12	3.32E+12	3.68E+12	4.02E+12	4.35E+12	4.66E+12	4.95E+12	6.17E+12	7.07E+12	7.73E+12
	4pp	Forward	2.98E+12	3.81E+12	4.50E+12	5.11E+12	5.67E+12	6.18E+12	6.66E+12	7.09E+12	7.50E+12	9.16E+12	1.04E+13	1.12E+13
		Reverse	2.98E+12	3.81E+12	4.50E+12	5.11E+12	5.67E+12	6.18E+12	6.66E+12	7.09E+12	7.50E+12	9.16E+12	1.04E+13	1.12E+13
C_4H_9	$3s_{\beta}p$	Forward	3.09E+12	3.87E+12	4.51E+12	5.09E+12	5.62E+12	6.11E+12	6.56E+12	6.98E+12	7.36E+12	8.95E+12	1.01E+13	1.09E+13
		Reverse	2.03E+12	2.41E+12	2.77E+12	3.13E+12	3.48E+12	3.81E+12	4.14E+12	4.45E+12	4.74E+12	5.95E+12	6.84E+12	7.50E+12
	$4s_{\alpha}$ p	Forward	2.98E+12	3.35E+12	3.54E+12	3.70E+12	3.85E+12	4.01E+12	4.16E+12	4.32E+12	4.47E+12	5.17E+12	5.74E+12	6.18E+12
		Reverse	1.96E+12	2.09E+12	2.17E+12	2.27E+12	2.38E+12	2.50E+12	2.63E+12	2.75E+12	2.88E+12	3.44E+12	3.88E+12	4.23E+12
	5pp	Forward	1.42E+12	1.18E+12	1.02E+12	9.16E+11	8.57E+11	8.23E+11	8.05E+11	7.96E+11	7.93E+11	8.18E+11	8.57E+11	8.93E+11
		Reverse	1.42E+12	1.18E+12	1.02E+12	9.16E+11	8.57E+11	8.23E+11	8.05E+11	7.96E+11	7.93E+11	8.18E+11	8.57E+11	8.93E+11
C_5H_{11}	$3s_{\beta}p$	Forward	3.09E+12	3.87E+12	4.52E+12	5.10E+12	5.64E+12	6.13E+12	6.59E+12	7.01E+12	7.40E+12	9.01E+12	1.02E+13	1.10E+13
		Reverse	1.97E+12	2.35E+12	2.70E+12	3.05E+12	3.40E+12	3.73E+12	4.05E+12	4.36E+12	4.65E+12	5.84E+12	6.72E+12	7.38E+12
	$4s_{\beta}$ p	Forward	2.95E+12	3.26E+12	3.42E+12	3.56E+12	3.69E+12	3.83E+12	3.98E+12	4.12E+12	4.26E+12	4.92E+12	5.45E+12	5.87E+12
		Reverse	1.55E+12	1.69E+12	1.79E+12	1.89E+12	1.99E+12	2.10E+12	2.22E+12	2.33E+12	2.44E+12	2.95E+12	3.35E+12	3.66E+12
	$5s_{\alpha}^{E}p$	Forward	1.34E+12	1.17E+12	1.06E+12	9.84E+11	9.43E+11	9.20E+11	9.10E+11	9.08E+11	9.11E+11	9.56E+11	1.01E+12	1.06E+12
		Reverse	8.52E+11	7.12E+11	6.31E+11	5.89E+11	5.68E+11	5.61E+11	5.60E+11	5.64E+11	5.71E+11	6.20E+11	6.68E+11	7.07E+11
	$5s_{\alpha}^{A}p$	Forward	1.27E+12	1.10E+12	9.84E+11	9.10E+11	8.68E+11	8.44E+11	8.33E+11	8.30E+11	8.31E+11	8.70E+11	9.17E+11	9.59E+11
		Reverse	8.11E+11	6.70E+11	5.88E+11	5.45E+11	5.23E+11	5.14E+11	5.13E+11	5.16E+11	5.22E+11	5.64E+11	6.06E+11	6.40E+11
	6pp	Forward	8.44E+11	6.05E+11	4.76E+11	4.04E+11	3.63E+11	3.38E+11	3.23E+11	3.14E+11	3.08E+11	3.05E+11	3.15E+11	3.25E+11
		Reverse	8.44E+11	6.05E+11	4.76E+11	4.04E+11	3.63E+11	3.38E+11	3.23E+11	3.14E+11	3.08E+11	3.05E+11	3.15E+11	3.25E+11
C_6H_{13}	$3s_{\beta}p$	Forward	3.11E+12	3.88E+12	4.52E+12	5.10E+12	5.63E+12	6.12E+12	6.57E+12	6.99E+12	7.38E+12	8.97E+12	1.01E+13	1.10E+13
		Reverse	1.96E+12	2.34E+12	2.69E+12	3.04E+12	3.38E+12	3.71E+12	4.03E+12	4.33E+12	4.62E+12	5.81E+12	6.68E+12	7.33E+12

	$4s_{\beta}\ p$	Forward	3.00E+12	3.30E+12	3.45E+12	3.58E+12	3.71E+12	3.84E+12	3.99E+12	4.13E+12	4.27E+12	4.93E+12	5.45E+12	5.87E+12
		Reverse	1.51E+12	1.65E+12	1.74E+12	1.83E+12	1.94E+12	2.05E+12	2.16E+12	2.27E+12	2.38E+12	2.87E+12	3.25E+12	3.56E+12
	$5s_{\beta}^{E}p$	Forward	1.39E+12	1.20E+12	1.07E+12	9.96E+11	9.51E+11	9.26E+11	9.14E+11	9.11E+11	9.13E+11	9.56E+11	1.01E+12	1.05E+12
		Reverse	7.02E+11	6.02E+11	5.42E+11	5.11E+11	4.97E+11	4.93E+11	4.95E+11	5.00E+11	5.08E+11	5.56E+11	6.02E+11	6.39E+11
	$5s_{\beta}^{A}p$	Forward	1.27E+12	1.08E+12	9.47E+11	8.69E+11	8.24E+11	7.98E+11	7.85E+11	7.80E+11	7.80E+11	8.11E+11	8.52E+11	8.89E+11
		Reverse	6.42E+11	5.38E+11	4.78E+11	4.46E+11	4.30E+11	4.25E+11	4.25E+11	4.28E+11	4.34E+11	4.72E+11	5.09E+11	5.39E+11
	$6s_{\alpha}^{E}p$	Forward	7.58E+11	5.75E+11	4.74E+11	4.17E+11	3.83E+11	3.62E+11	3.50E+11	3.43E+11	3.39E+11	3.42E+11	3.55E+11	3.68E+11
		Reverse	4.79E+11	3.46E+11	2.82E+11	2.48E+11	2.30E+11	2.20E+11	2.15E+11	2.13E+11	2.12E+11	2.21E+11	2.34E+11	2.46E+11
	$6s_{\alpha}^{A}p$	Forward	6.75E+11	5.00E+11	4.05E+11	3.53E+11	3.22E+11	3.04E+11	2.93E+11	2.86E+11	2.83E+11	2.84E+11	2.94E+11	3.05E+11
		Reverse	4.27E+11	3.01E+11	2.41E+11	2.10E+11	1.93E+11	1.84E+11	1.80E+11	1.77E+11	1.77E+11	1.84E+11	1.94E+11	2.03E+11
	7pp	Forward	5.12E+11	3.32E+11	2.47E+11	2.02E+11	1.77E+11	1.62E+11	1.52E+11	1.46E+11	1.42E+11	1.37E+11	1.39E+11	1.42E+11
		Reverse	5.12E+11	3.32E+11	2.47E+11	2.02E+11	1.77E+11	1.62E+11	1.52E+11	1.46E+11	1.42E+11	1.37E+11	1.39E+11	1.42E+11
C_7H_{15}	$3s_{\beta}p$	Forward	3.10E+12	3.87E+12	4.52E+12	5.09E+12	5.62E+12	6.10E+12	6.55E+12	6.97E+12	7.36E+12	8.95E+12	1.01E+13	1.10E+13
		Reverse	1.96E+12	2.33E+12	2.68E+12	3.03E+12	3.37E+12	3.70E+12	4.02E+12	4.32E+12	4.60E+12	5.79E+12	6.66E+12	7.31E+12
	$4s_{\beta}\ p$	Forward	3.02E+12	3.31E+12	3.46E+12	3.58E+12	3.71E+12	3.85E+12	3.98E+12	4.13E+12	4.27E+12	4.91E+12	5.44E+12	5.85E+12
		Reverse	1.50E+12	1.63E+12	1.73E+12	1.82E+12	1.92E+12	2.03E+12	2.14E+12	2.25E+12	2.36E+12	2.85E+12	3.23E+12	3.53E+12
	$5s_{\beta}^{E}p$	Forward	1.41E+12	1.22E+12	1.08E+12	1.01E+12	9.59E+11	9.34E+11	9.22E+11	9.19E+11	9.20E+11	9.64E+11	1.02E+12	1.06E+12
		Reverse	6.76E+11	5.82E+11	5.26E+11	4.97E+11	4.83E+11	4.80E+11	4.82E+11	4.87E+11	4.95E+11	5.43E+11	5.88E+11	6.25E+11
	$5s_{\beta}^{A}p$	Forward	1.28E+12	1.08E+12	9.49E+11	8.69E+11	8.23E+11	7.97E+11	7.83E+11	7.77E+11	7.77E+11	8.06E+11	8.47E+11	8.83E+11
		Reverse	6.18E+11	5.18E+11	4.60E+11	4.29E+11	4.15E+11	4.09E+11	4.09E+11	4.12E+11	4.18E+11	4.54E+11	4.90E+11	5.19E+11
	$6s_{\beta}^{E}p$	Forward	7.50E+11	5.62E+11	4.59E+11	4.02E+11	3.68E+11	3.48E+11	3.35E+11	3.28E+11	3.24E+11	3.25E+11	3.37E+11	3.49E+11
		Reverse	3.73E+11	2.77E+11	2.29E+11	2.04E+11	1.91E+11	1.84E+11	1.80E+11	1.79E+11	1.79E+11	1.88E+11	2.00E+11	2.11E+11
	$6s_{\beta}^{A}p$	Forward	5.94E+11	4.26E+11	3.39E+11	2.92E+11	2.64E+11	2.47E+11	2.37E+11	2.31E+11	2.28E+11	2.27E+11	2.34E+11	2.42E+11
		Reverse	2.95E+11	2.10E+11	1.69E+11	1.48E+11	1.37E+11	1.31E+11	1.28E+11	1.26E+11	1.26E+11	1.31E+11	1.39E+11	1.46E+11
	$7s_{\alpha}^{E}p$	Forward	4.24E+11	2.95E+11	2.32E+11	1.98E+11	1.78E+11	1.66E+11	1.58E+11	1.54E+11	1.51E+11	1.49E+11	1.53E+11	1.57E+11
		Reverse	2.68E+11	1.77E+11	1.38E+11	1.18E+11	1.07E+11	1.01E+11	9.71E+10	9.52E+10	9.43E+10	9.61E+10	1.01E+11	1.05E+11
	$7s_{\alpha}^{A}p$	Forward	4.05E+11	2.74E+11	2.12E+11	1.78E+11	1.59E+11	1.47E+11	1.40E+11	1.35E+11	1.32E+11	1.29E+11	1.32E+11	1.36E+11
		Reverse	2.56E+11	1.65E+11	1.26E+11	1.06E+11	9.54E+10	8.93E+10	8.58E+10	8.39E+10	8.28E+10	8.37E+10	8.73E+10	9.08E+10
	8pp	Forward	2.52E+11	1.44E+11	9.87E+10	7.68E+10	6.47E+10	5.75E+10	5.28E+10	4.98E+10	4.77E+10	4.36E+10	4.31E+10	4.34E+10
		Reverse	2.52E+11	1.44E+11	9.87E+10	7.68E+10	6.47E+10	5.75E+10	5.28E+10	4.98E+10	4.77E+10	4.36E+10	4.31E+10	4.34E+10

C_8H_{17}	$3s_\beta p$	forward	3.11E+12	3.88E+12	4.52E+12	5.09E+12	5.62E+12	6.10E+12	6.55E+12	6.97E+12	7.36E+12	8.95E+12	1.01E+13	1.10E+13
		reverse	1.96E+12	2.33E+12	2.68E+12	3.03E+12	3.37E+12	3.70E+12	4.02E+12	4.32E+12	4.60E+12	5.79E+12	6.66E+12	7.31E+12
	$4s_\beta$ p	Forward	3.03E+12	3.32E+12	3.46E+12	3.58E+12	3.71E+12	3.84E+12	3.98E+12	4.12E+12	4.26E+12	4.91E+12	5.43E+12	5.84E+12
		Reverse	1.50E+12	1.63E+12	1.72E+12	1.82E+12	1.92E+12	2.03E+12	2.14E+12	2.25E+12	2.35E+12	2.84E+12	3.22E+12	3.52E+12
	$5s_\beta{}^E p$	Forward	1.42E+12	1.23E+12	1.09E+12	1.01E+12	9.63E+11	9.37E+11	9.25E+11	9.21E+11	9.22E+11	9.65E+11	1.02E+12	1.06E+12
		Reverse	6.71E+11	5.78E+11	5.22E+11	4.93E+11	4.80E+11	4.77E+11	4.79E+11	4.84E+11	4.92E+11	5.40E+11	5.85E+11	6.22E+11
	$5s_\beta{}^A p$	Forward	1.30E+12	1.09E+12	9.54E+11	8.72E+11	8.25E+11	7.98E+11	7.84E+11	7.78E+11	7.77E+11	8.06E+11	8.46E+11	8.82E+11
		Reverse	6.13E+11	5.14E+11	4.56E+11	4.26E+11	4.11E+11	4.06E+11	4.06E+11	4.09E+11	4.15E+11	4.51E+11	4.86E+11	5.15E+11
	$6s_\beta{}^E p$	Forward	7.56E+11	5.65E+11	4.61E+11	4.04E+11	3.70E+11	3.49E+11	3.37E+11	3.29E+11	3.25E+11	3.27E+11	3.39E+11	3.51E+11
		Reverse	3.56E+11	2.66E+11	2.21E+11	1.97E+11	1.84E+11	1.78E+11	1.74E+11	1.73E+11	1.74E+11	1.83E+11	1.95E+11	2.05E+11
	$6s_\beta{}^A p$	Forward	5.92E+11	4.23E+11	3.36E+11	2.89E+11	2.61E+11	2.45E+11	2.35E+11	2.28E+11	2.25E+11	2.24E+11	2.31E+11	2.38E+11
		Reverse	2.79E+11	1.99E+11	1.61E+11	1.41E+11	1.30E+11	1.24E+11	1.21E+11	1.20E+11	1.20E+11	1.25E+11	1.33E+11	1.39E+11
	$7s_\beta{}^E p$	Forward	3.91E+11	2.68E+11	2.09E+11	1.77E+11	1.59E+11	1.47E+11	1.40E+11	1.36E+11	1.33E+11	1.30E+11	1.34E+11	1.38E+11
		Reverse	1.94E+11	1.32E+11	1.04E+11	8.97E+10	8.20E+10	7.76E+10	7.52E+10	7.39E+10	7.34E+10	7.54E+10	7.93E+10	8.30E+10
	$7s_\beta{}^A p$	Forward	3.52E+11	2.31E+11	1.75E+11	1.46E+11	1.29E+11	1.19E+11	1.12E+11	1.08E+11	1.06E+11	1.02E+11	1.04E+11	1.07E+11
		Reverse	1.74E+11	1.14E+11	8.71E+10	7.39E+10	6.67E+10	6.26E+10	6.03E+10	5.90E+10	5.84E+10	5.92E+10	6.19E+10	6.45E+10
	$8s_\alpha{}^E p$	Forward	1.90E+11	1.16E+11	8.40E+10	6.79E+10	5.88E+10	5.32E+10	4.96E+10	4.73E+10	4.57E+10	4.28E+10	4.28E+10	4.33E+10
		Reverse	1.20E+11	6.96E+10	4.99E+10	4.04E+10	3.53E+10	3.23E+10	3.04E+10	2.93E+10	2.85E+10	2.77E+10	2.82E+10	2.89E+10
	$8s_\alpha{}^A p$	Forward	1.70E+11	9.76E+10	6.84E+10	5.41E+10	4.61E+10	4.14E+10	3.83E+10	3.63E+10	3.49E+10	3.24E+10	3.21E+10	3.25E+10
		Reverse	1.07E+11	5.87E+10	4.06E+10	3.21E+10	2.77E+10	2.51E+10	2.35E+10	2.25E+10	2.18E+10	2.09E+10	2.12E+10	2.16E+10
	9pp	Forward	1.68E+11	8.75E+10	5.72E+10	4.30E+10	3.54E+10	3.08E+10	2.79E+10	2.60E+10	2.47E+10	2.19E+10	2.13E+10	2.12E+10
		Reverse	1.68E+11	8.75E+10	5.72E+10	4.30E+10	3.54E+10	3.08E+10	2.79E+10	2.60E+10	2.47E+10	2.19E+10	2.13E+10	2.12E+10

Table S4

	rxn. type	Direction	Temperature											
			200	300	400	500	600	700	800	900	1000	1500	2000	2500
C_2H_5	3pp	Forward	2.4E+12	2.7E+12	3.0E+12	3.4E+12	3.7E+12	4.0E+12	4.3E+12	4.5E+12	4.8E+12	5.8E+12	6.6E+12	7.2E+12
		Reverse	2.4E+12	2.7E+12	3.0E+12	3.4E+12	3.7E+12	4.0E+12	4.3E+12	4.5E+12	4.8E+12	5.8E+12	6.6E+12	7.2E+12
C_3H_7	$3s_\alpha p$	Forward	2.4E+12	3.0E+12	3.5E+12	3.9E+12	4.4E+12	4.7E+12	5.1E+12	5.4E+12	5.7E+12	7.0E+12	7.9E+12	8.5E+12
		Reverse	1.8E+12	2.0E+12	2.3E+12	2.5E+12	2.8E+12	3.0E+12	3.2E+12	3.4E+12	3.6E+12	4.5E+12	5.1E+12	5.5E+12
	4pp	Forward	2.9E+12	3.2E+12	3.4E+12	3.6E+12	3.8E+12	3.9E+12	4.1E+12	4.3E+12	4.5E+12	5.3E+12	6.0E+12	6.5E+12
		Reverse	2.9E+12	3.2E+12	3.4E+12	3.6E+12	3.8E+12	3.9E+12	4.1E+12	4.3E+12	4.5E+12	5.3E+12	6.0E+12	6.5E+12
C_4H_9	$3s_\beta p$	Forward	2.6E+12	3.1E+12	3.6E+12	4.1E+12	4.5E+12	4.9E+12	5.2E+12	5.6E+12	5.9E+12	7.1E+12	8.0E+12	8.7E+12
		Reverse	1.6E+12	1.9E+12	2.1E+12	2.4E+12	2.6E+12	2.8E+12	3.0E+12	3.3E+12	3.5E+12	4.3E+12	4.9E+12	5.3E+12
	$4s_\alpha$ p	Forward	3.1E+12	3.5E+12	3.7E+12	3.9E+12	4.1E+12	4.3E+12	4.5E+12	4.7E+12	4.9E+12	5.8E+12	6.5E+12	7.0E+12
		Reverse	2.0E+12	2.1E+12	2.2E+12	2.2E+12	2.4E+12	2.5E+12	2.6E+12	2.8E+12	2.9E+12	3.5E+12	3.9E+12	4.3E+12
	5pp	Forward	1.8E+12	1.5E+12	1.3E+12	1.2E+12	1.1E+12	1.1E+12	1.0E+12	1.0E+12	1.0E+12	1.1E+12	1.1E+12	1.2E+12
		Reverse	1.8E+12	1.5E+12	1.3E+12	1.2E+12	1.1E+12	1.1E+12	1.0E+12	1.0E+12	1.0E+12	1.1E+12	1.1E+12	1.2E+12
C_5H_{11}	$3s_\beta p$	Forward	2.5E+12	3.1E+12	3.5E+12	4.0E+12	4.4E+12	4.7E+12	5.1E+12	5.4E+12	5.7E+12	6.9E+12	7.8E+12	8.4E+12
		Reverse	1.6E+12	1.9E+12	2.1E+12	2.4E+12	2.6E+12	2.9E+12	3.1E+12	3.3E+12	3.5E+12	4.4E+12	5.0E+12	5.4E+12
	$4s_\beta$ p	Forward	3.1E+12	3.4E+12	3.6E+12	3.8E+12	3.9E+12	4.1E+12	4.3E+12	4.5E+12	4.7E+12	5.5E+12	6.2E+12	6.7E+12
		Reverse	1.5E+12	1.6E+12	1.7E+12	1.8E+12	1.9E+12	2.0E+12	2.1E+12	2.2E+12	2.3E+12	2.8E+12	3.2E+12	3.5E+12
	$5s_\alpha^E p$	Forward	1.6E+12	1.4E+12	1.2E+12	1.1E+12	1.1E+12	1.1E+12	1.1E+12	1.1E+12	1.1E+12	1.1E+12	1.2E+12	1.3E+12
		Reverse	1.0E+12	8.4E+11	7.4E+11	6.9E+11	6.6E+11	6.6E+11	6.6E+11	6.6E+11	6.7E+11	7.3E+11	7.8E+11	8.2E+11
	$5s_\alpha^A p$	Forward	1.8E+12	1.6E+12	1.4E+12	1.3E+12	1.3E+12	1.3E+12	1.2E+12	1.3E+12	1.3E+12	1.3E+12	1.4E+12	1.5E+12
		Reverse	1.2E+12	9.7E+11	8.6E+11	8.0E+11	7.7E+11	7.6E+11	7.6E+11	7.7E+11	7.8E+11	8.5E+11	9.1E+11	9.6E+11
	6pp	Forward	1.3E+12	8.8E+11	6.9E+11	5.9E+11	5.3E+11	4.9E+11	4.7E+11	4.6E+11	4.6E+11	4.6E+11	4.7E+11	4.9E+11
		Reverse	1.3E+12	8.8E+11	6.9E+11	5.9E+11	5.3E+11	4.9E+11	4.7E+11	4.6E+11	4.6E+11	4.6E+11	4.7E+11	4.9E+11
C_6H_{13}	$3s_\beta p$	Forward	2.3E+12	2.8E+12	3.2E+12	3.6E+12	3.9E+12	4.2E+12	4.5E+12	4.8E+12	5.0E+12	6.0E+12	6.8E+12	7.3E+12
		Reverse	1.6E+12	1.8E+12	2.0E+12	2.3E+12	2.5E+12	2.7E+12	2.9E+12	3.1E+12	3.2E+12	4.0E+12	4.5E+12	4.9E+12
	$4s_\beta$ p	Forward	2.3E+12	2.4E+12	2.5E+12	2.6E+12	2.7E+12	2.9E+12	3.0E+12	3.1E+12	3.2E+12	3.8E+12	4.3E+12	4.6E+12

		Reverse	1.3E+12	1.4E+12	1.4E+12	1.5E+12	1.6E+12	1.7E+12	1.8E+12	1.9E+12	2.0E+12	2.5E+12	2.8E+12	3.1E+12
	$5s_{\beta}^{E}p$	Forward	1.0E+12	8.5E+11	7.5E+11	7.0E+11	6.7E+11	6.6E+11	6.5E+11	6.5E+11	6.6E+11	7.0E+11	7.4E+11	7.8E+11
		Reverse	5.7E+11	4.8E+11	4.3E+11	4.1E+11	4.0E+11	3.9E+11	4.0E+11	4.0E+11	4.1E+11	4.5E+11	4.9E+11	5.2E+11
	$5s_{\beta}^{A}p$	Forward	1.0E+12	8.4E+11	7.4E+11	6.9E+11	6.6E+11	6.4E+11	6.4E+11	6.4E+11	6.4E+11	6.8E+11	7.2E+11	7.6E+11
		Reverse	5.6E+11	4.7E+11	4.2E+11	4.0E+11	3.9E+11	3.9E+11	3.9E+11	3.9E+11	4.0E+11	4.4E+11	4.7E+11	5.0E+11
	$6s_{\alpha}^{E}p$	Forward	5.7E+11	4.2E+11	3.5E+11	3.1E+11	2.8E+11	2.7E+11	2.6E+11	2.6E+11	2.6E+11	2.6E+11	2.8E+11	2.9E+11
		Reverse	3.9E+11	2.8E+11	2.2E+11	1.9E+11	1.8E+11	1.7E+11	1.7E+11	1.7E+11	1.7E+11	1.7E+11	1.8E+11	1.9E+11
	$6s_{\alpha}^{A}p$	Forward	5.2E+11	3.8E+11	3.1E+11	2.7E+11	2.5E+11	2.4E+11	2.3E+11	2.3E+11	2.3E+11	2.3E+11	2.4E+11	2.5E+11
		Reverse	3.6E+11	2.5E+11	2.0E+11	1.7E+11	1.6E+11	1.5E+11	1.5E+11	1.5E+11	1.5E+11	1.5E+11	1.6E+11	1.7E+11
	7pp	Forward	3.6E+11	2.2E+11	1.7E+11	1.4E+11	1.2E+11	1.1E+11	1.0E+11	9.9E+10	9.7E+10	9.4E+10	9.6E+10	9.8E+10
		Reverse	3.6E+11	2.2E+11	1.7E+11	1.4E+11	1.2E+11	1.1E+11	1.0E+11	9.9E+10	9.7E+10	9.4E+10	9.6E+10	9.8E+10
C_7H_{15}	$3s_{\beta}p$	Forward	2.1E+12	2.5E+12	2.9E+12	3.2E+12	3.4E+12	3.7E+12	3.9E+12	4.2E+12	4.4E+12	5.3E+12	5.9E+12	6.4E+12
		Reverse	1.5E+12	1.6E+12	1.8E+12	2.0E+12	2.2E+12	2.4E+12	2.5E+12	2.7E+12	2.8E+12	3.5E+12	3.9E+12	4.3E+12
	$4s_{\beta}$ p	Forward	2.1E+12	2.2E+12	2.3E+12	2.4E+12	2.5E+12	2.6E+12	2.7E+12	2.8E+12	2.9E+12	3.3E+12	3.7E+12	4.0E+12
		Reverse	1.2E+12	1.2E+12	1.3E+12	1.3E+12	1.4E+12	1.5E+12	1.5E+12	1.6E+12	1.7E+12	2.1E+12	2.3E+12	2.5E+12
	$5s_{\beta}^{E}p$	Forward	9.3E+11	7.8E+11	6.8E+11	6.3E+11	6.0E+11	5.9E+11	5.8E+11	5.8E+11	5.9E+11	6.2E+11	6.6E+11	6.9E+11
		Reverse	4.6E+11	3.8E+11	3.4E+11	3.2E+11	3.1E+11	3.0E+11	3.1E+11	3.1E+11	3.1E+11	3.4E+11	3.7E+11	3.9E+11
	$5s_{\beta}^{A}p$	Forward	9.4E+11	7.7E+11	6.8E+11	6.2E+11	5.9E+11	5.8E+11	5.7E+11	5.7E+11	5.7E+11	6.0E+11	6.4E+11	6.6E+11
		Reverse	4.6E+11	3.8E+11	3.3E+11	3.1E+11	3.0E+11	3.0E+11	3.0E+11	3.0E+11	3.0E+11	3.3E+11	3.6E+11	3.8E+11
	$6s_{\beta}^{E}p$	Forward	5.6E+11	4.1E+11	3.3E+11	2.9E+11	2.7E+11	2.6E+11	2.5E+11	2.5E+11	2.4E+11	2.5E+11	2.6E+11	2.7E+11
		Reverse	3.1E+11	2.3E+11	1.9E+11	1.6E+11	1.5E+11	1.5E+11	1.5E+11	1.5E+11	1.5E+11	1.5E+11	1.6E+11	1.7E+11
	$6s_{\beta}^{A}p$	Forward	4.5E+11	3.1E+11	2.5E+11	2.2E+11	2.0E+11	1.9E+11	1.8E+11	1.8E+11	1.7E+11	1.8E+11	1.8E+11	1.9E+11
		Reverse	2.5E+11	1.7E+11	1.4E+11	1.2E+11	1.1E+11	1.1E+11	1.0E+11	1.0E+11	1.0E+11	1.1E+11	1.1E+11	1.2E+11
	$7s_{\alpha}^{E}p$	Forward	2.8E+11	1.9E+11	1.5E+11	1.3E+11	1.1E+11	1.1E+11	1.0E+11	9.9E+10	9.8E+10	9.7E+10	1.0E+11	1.0E+11
		Reverse	2.0E+11	1.2E+11	9.4E+10	8.0E+10	7.2E+10	6.8E+10	6.5E+10	6.4E+10	6.3E+10	6.4E+10	6.7E+10	6.9E+10
	$7s_{\alpha}^{A}p$	Forward	2.9E+11	1.9E+11	1.5E+11	1.3E+11	1.1E+11	1.1E+11	1.0E+11	9.7E+10	9.6E+10	9.5E+10	9.7E+10	1.0E+11
		Reverse	2.0E+11	1.3E+11	9.5E+10	8.0E+10	7.2E+10	6.7E+10	6.4E+10	6.3E+10	6.2E+10	6.3E+10	6.5E+10	6.7E+10
	8pp	Forward	1.8E+11	1.0E+11	7.1E+10	5.6E+10	4.8E+10	4.3E+10	4.0E+10	3.8E+10	3.6E+10	3.4E+10	3.4E+10	3.4E+10
		Reverse	1.8E+11	1.0E+11	7.1E+10	5.6E+10	4.8E+10	4.3E+10	4.0E+10	3.8E+10	3.6E+10	3.4E+10	3.4E+10	3.4E+10
C_8H_{17}	$3s_{\beta}p$	forward	2.3E+12	2.7E+12	3.1E+12	3.4E+12	3.7E+12	4.0E+12	4.3E+12	4.5E+12	4.7E+12	5.7E+12	6.4E+12	6.9E+12

	reverse	1.6E+12	1.8E+12	2.0E+12	2.2E+12	2.4E+12	2.6E+12	2.8E+12	2.9E+12	3.1E+12	3.8E+12	4.3E+12	4.7E+12
$4s_{\beta}$ p	Forward	2.1E+12	2.2E+12	2.3E+12	2.3E+12	2.4E+12	2.5E+12	2.6E+12	2.7E+12	2.9E+12	3.3E+12	3.7E+12	4.0E+12
	Reverse	1.1E+12	1.1E+12	1.2E+12	1.2E+12	1.3E+12	1.4E+12	1.5E+12	1.5E+12	1.6E+12	1.9E+12	2.2E+12	2.4E+12
$5s_{\beta}^{E}$p	Forward	9.1E+11	7.6E+11	6.7E+11	6.2E+11	5.9E+11	5.8E+11	5.7E+11	5.7E+11	5.8E+11	6.1E+11	6.5E+11	6.8E+11
	Reverse	4.4E+11	3.6E+11	3.2E+11	3.0E+11	3.0E+11	2.9E+11	2.9E+11	3.0E+11	3.0E+11	3.3E+11	3.5E+11	3.8E+11
$5s_{\beta}^{A}$p	Forward	9.8E+11	8.2E+11	7.2E+11	6.6E+11	6.3E+11	6.2E+11	6.1E+11	6.1E+11	6.1E+11	6.5E+11	6.9E+11	7.2E+11
	Reverse	4.7E+11	3.9E+11	3.5E+11	3.3E+11	3.2E+11	3.1E+11	3.1E+11	3.2E+11	3.2E+11	3.5E+11	3.8E+11	4.0E+11
$6s_{\beta}^{E}$p	Forward	5.9E+11	4.3E+11	3.5E+11	3.1E+11	2.9E+11	2.7E+11	2.7E+11	2.6E+11	2.6E+11	2.7E+11	2.8E+11	2.9E+11
	Reverse	2.8E+11	2.1E+11	1.7E+11	1.5E+11	1.4E+11	1.4E+11	1.4E+11	1.4E+11	1.4E+11	1.4E+11	1.5E+11	1.6E+11
$6s_{\beta}^{A}$p	Forward	4.7E+11	3.4E+11	2.7E+11	2.3E+11	2.1E+11	2.0E+11	1.9E+11	1.9E+11	1.9E+11	1.9E+11	2.0E+11	2.1E+11
	Reverse	2.3E+11	1.6E+11	1.3E+11	1.1E+11	1.1E+11	1.0E+11	1.0E+11	9.9E+10	9.9E+10	1.0E+11	1.1E+11	1.1E+11
$7s_{\beta}^{E}$p	Forward	2.6E+11	1.7E+11	1.3E+11	1.1E+11	9.8E+10	9.2E+10	8.8E+10	8.5E+10	8.3E+10	8.2E+10	8.5E+10	8.7E+10
	Reverse	1.4E+11	8.9E+10	6.8E+10	5.8E+10	5.3E+10	5.0E+10	4.8E+10	4.7E+10	4.7E+10	4.7E+10	4.9E+10	5.1E+10
$7s_{\beta}^{A}$p	Forward	2.9E+11	1.9E+11	1.4E+11	1.2E+11	1.1E+11	9.9E+10	9.5E+10	9.2E+10	9.0E+10	8.9E+10	9.1E+10	9.4E+10
	Reverse	1.5E+11	9.8E+10	7.5E+10	6.4E+10	5.7E+10	5.4E+10	5.2E+10	5.1E+10	5.0E+10	5.1E+10	5.3E+10	5.5E+10
$8s_{\alpha}^{E}$p	Forward	1.4E+11	8.7E+10	6.4E+10	5.2E+10	4.6E+10	4.2E+10	3.9E+10	3.8E+10	3.7E+10	3.5E+10	3.6E+10	3.6E+10
	Reverse	1.0E+11	5.8E+10	4.1E+10	3.4E+10	2.9E+10	2.7E+10	2.6E+10	2.5E+10	2.4E+10	2.4E+10	2.4E+10	2.5E+10
$8s_{\alpha}^{A}$p	Forward	1.2E+11	6.8E+10	4.8E+10	3.9E+10	3.4E+10	3.0E+10	2.9E+10	2.7E+10	2.6E+10	2.5E+10	2.5E+10	2.6E+10
	Reverse	8.2E+10	4.5E+10	3.1E+10	2.5E+10	2.2E+10	2.0E+10	1.9E+10	1.8E+10	1.7E+10	1.7E+10	1.7E+10	1.7E+10
9pp	Forward	9.5E+10	4.7E+10	3.1E+10	2.3E+10	1.9E+10	1.7E+10	1.5E+10	1.4E+10	1.4E+10	1.2E+10	1.2E+10	1.2E+10
	Reverse	9.5E+10	4.7E+10	3.1E+10	2.3E+10	1.9E+10	1.7E+10	1.5E+10	1.4E+10	1.4E+10	1.2E+10	1.2E+10	1.2E+10

Table S5

	rxn. type	Direction	Temperature											
			200	300	400	500	600	700	800	900	1000	1500	2000	2500
C_2H_5	3pp	Forward	1.2E+27	3.5E+12	2.9E+05	6.5E+01	5.9E+00	3.1E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	1.2E+27	3.5E+12	2.9E+05	6.5E+01	5.9E+00	3.1E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
C_3H_7	$3s_\alpha p$	Forward	6.1E+25	8.5E+11	1.6E+05	5.8E+01	5.9E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	6.1E+25	8.5E+11	1.6E+05	5.8E+01	5.9E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	4pp	Forward	1.7E+29	3.4E+14	2.1E+07	1.7E+03	1.8E+01	4.9E+00	2.9E+00	2.2E+00	1.9E+00	1.3E+00	1.2E+00	1.1E+00
		Reverse	1.7E+29	3.4E+14	2.1E+07	1.7E+03	1.8E+01	4.9E+00	2.9E+00	2.2E+00	1.9E+00	1.3E+00	1.2E+00	1.1E+00
C_4H_9	$3s_\beta p$	Forward	5.8E+25	7.6E+11	1.4E+05	5.2E+01	5.7E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	5.8E+25	7.6E+11	1.4E+05	5.2E+01	5.7E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	$4s_\alpha$ p	Forward	1.0E+28	7.9E+13	9.5E+06	1.2E+03	1.7E+01	4.8E+00	2.9E+00	2.2E+00	1.8E+00	1.3E+00	1.1E+00	1.1E+00
		Reverse	1.0E+28	7.9E+13	9.5E+06	1.2E+03	1.7E+01	4.8E+00	2.9E+00	2.2E+00	1.8E+00	1.3E+00	1.1E+00	1.1E+00
	5pp	Forward	1.7E+17	1.4E+08	6.2E+03	4.0E+01	6.3E+00	3.2E+00	2.3E+00	1.9E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	1.7E+17	1.4E+08	6.2E+03	4.0E+01	6.3E+00	3.2E+00	2.3E+00	1.9E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
C_5H_{11}	$3s_\beta p$	Forward	4.9E+25	6.9E+11	1.3E+05	5.1E+01	5.7E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	4.9E+25	6.9E+11	1.3E+05	5.1E+01	5.7E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	$4s_\beta$ p	Forward	5.1E+27	5.2E+13	7.1E+06	9.8E+02	1.6E+01	4.6E+00	2.9E+00	2.2E+00	1.8E+00	1.3E+00	1.1E+00	1.1E+00
		Reverse	5.1E+27	5.2E+13	7.1E+06	9.8E+02	1.6E+01	4.6E+00	2.9E+00	2.2E+00	1.8E+00	1.3E+00	1.1E+00	1.1E+00
	$5s_\alpha^E p$	Forward	5.2E+15	2.5E+07	2.7E+03	3.1E+01	5.8E+00	3.1E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	5.2E+15	2.5E+07	2.7E+03	3.1E+01	5.8E+00	3.1E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	$5s_\alpha^A p$	Forward	5.5E+15	2.5E+07	2.6E+03	2.9E+01	5.7E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	5.5E+15	2.5E+07	2.6E+03	2.9E+01	5.7E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	6pp	Forward	3.9E+12	4.5E+05	2.8E+02	1.2E+01	4.0E+00	2.5E+00	1.9E+00	1.7E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	3.9E+12	4.5E+05	2.8E+02	1.2E+01	4.0E+00	2.5E+00	1.9E+00	1.7E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
C_6H_{13}	$3s_\beta p$	Forward	4.9E+25	6.9E+11	1.3E+05	5.1E+01	5.7E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	4.9E+25	6.9E+11	1.3E+05	5.1E+01	5.7E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	$4s_\beta$ p	Forward	5.0E+27	5.1E+13	6.9E+06	9.7E+02	1.6E+01	4.6E+00	2.8E+00	2.2E+00	1.8E+00	1.3E+00	1.1E+00	1.1E+00
		Reverse	5.0E+27	5.1E+13	6.9E+06	9.7E+02	1.6E+01	4.6E+00	2.8E+00	2.2E+00	1.8E+00	1.3E+00	1.1E+00	1.1E+00

	$5s_{\beta}^{E}p$	Forward	3.2E+15	1.8E+07	2.2E+03	2.7E+01	5.5E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	3.2E+15	1.8E+07	2.2E+03	2.7E+01	5.5E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	$5s_{\beta}^{A}p$	Forward	2.8E+15	1.6E+07	2.0E+03	2.6E+01	5.4E+00	2.9E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	2.8E+15	1.6E+07	2.0E+03	2.6E+01	5.4E+00	2.9E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	$6s_{\alpha}^{E}p$	Forward	4.6E+10	6.1E+04	1.3E+02	9.8E+00	3.7E+00	2.4E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	4.6E+10	6.1E+04	1.3E+02	9.8E+00	3.7E+00	2.4E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
	$6s_{\alpha}^{A}p$	Forward	4.1E+10	5.5E+04	1.2E+02	9.4E+00	3.6E+00	2.4E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	4.1E+10	5.5E+04	1.2E+02	9.4E+00	3.6E+00	2.4E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
	7pp	Forward	3.7E+11	1.3E+05	1.5E+02	9.4E+00	3.6E+00	2.4E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	3.7E+11	1.3E+05	1.5E+02	9.4E+00	3.6E+00	2.4E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
C_7H_{15}	$3s_{\beta}p$	Forward	4.9E+25	6.9E+11	1.3E+05	5.1E+01	5.7E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	4.9E+25	6.9E+11	1.3E+05	5.1E+01	5.7E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	$4s_{\beta}$ p	Forward	5.0E+27	5.1E+13	6.9E+06	9.6E+02	1.6E+01	4.6E+00	2.8E+00	2.2E+00	1.8E+00	1.3E+00	1.1E+00	1.1E+00
		Reverse	5.0E+27	5.1E+13	6.9E+06	9.6E+02	1.6E+01	4.6E+00	2.8E+00	2.2E+00	1.8E+00	1.3E+00	1.1E+00	1.1E+00
	$5s_{\beta}^{E}p$	Forward	3.1E+15	1.8E+07	2.1E+03	2.7E+01	5.5E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	3.1E+15	1.8E+07	2.1E+03	2.7E+01	5.5E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	$5s_{\beta}^{A}p$	Forward	2.4E+15	1.5E+07	1.9E+03	2.6E+01	5.4E+00	2.9E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	2.4E+15	1.5E+07	1.9E+03	2.6E+01	5.4E+00	2.9E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	$6s_{\beta}^{E}p$	Forward	2.9E+10	4.5E+04	1.1E+02	9.1E+00	3.6E+00	2.4E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	2.9E+10	4.5E+04	1.1E+02	9.1E+00	3.6E+00	2.4E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
	$6s_{\beta}^{A}p$	Forward	2.0E+10	3.7E+04	1.0E+02	8.7E+00	3.5E+00	2.3E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	2.0E+10	3.7E+04	1.0E+02	8.7E+00	3.5E+00	2.3E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
	$7s_{\alpha}^{E}p$	Forward	8.1E+09	2.2E+04	7.4E+01	7.6E+00	3.3E+00	2.2E+00	1.8E+00	1.6E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	8.1E+09	2.2E+04	7.4E+01	7.6E+00	3.3E+00	2.2E+00	1.8E+00	1.6E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
	$7s_{\alpha}^{A}p$	Forward	2.2E+10	3.3E+04	8.5E+01	7.9E+00	3.3E+00	2.2E+00	1.8E+00	1.6E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	2.2E+10	3.3E+04	8.5E+01	7.9E+00	3.3E+00	2.2E+00	1.8E+00	1.6E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
	8pp	Forward	5.6E+13	1.4E+06	4.2E+02	1.3E+01	4.0E+00	2.5E+00	1.9E+00	1.7E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	5.6E+13	1.4E+06	4.2E+02	1.3E+01	4.0E+00	2.5E+00	1.9E+00	1.7E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
C_8H_{17}	$3s_{\beta}p$	forward	4.9E+25	6.9E+11	1.3E+05	5.1E+01	5.7E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		reverse	4.9E+25	6.9E+11	1.3E+05	5.1E+01	5.7E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00

$4s_{\beta}p$	Forward	5.0E+27	5.1E+13	6.9E+06	9.6E+02	1.6E+01	4.6E+00	2.8E+00	2.2E+00	1.8E+00	1.3E+00	1.1E+00	1.1E+00
	Reverse	5.0E+27	5.1E+13	6.9E+06	9.6E+02	1.6E+01	4.6E+00	2.8E+00	2.2E+00	1.8E+00	1.3E+00	1.1E+00	1.1E+00
$5s_{\beta}^{E}p$	Forward	3.1E+15	1.8E+07	2.1E+03	2.7E+01	5.5E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	Reverse	3.1E+15	1.8E+07	2.1E+03	2.7E+01	5.5E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
$5s_{\beta}^{A}p$	Forward	2.4E+15	1.5E+07	1.9E+03	2.5E+01	5.3E+00	2.9E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	Reverse	2.4E+15	1.5E+07	1.9E+03	2.5E+01	5.3E+00	2.9E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
$6s_{\beta}^{E}p$	Forward	2.5E+10	4.2E+04	1.1E+02	9.0E+00	3.6E+00	2.3E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
	Reverse	2.5E+10	4.2E+04	1.1E+02	9.0E+00	3.6E+00	2.3E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
$6s_{\beta}^{A}p$	Forward	1.7E+10	3.5E+04	9.8E+01	8.7E+00	3.5E+00	2.3E+00	1.8E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
	Reverse	1.7E+10	3.5E+04	9.8E+01	8.7E+00	3.5E+00	2.3E+00	1.8E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
$7s_{\beta}^{E}p$	Forward	5.4E+09	1.7E+04	6.6E+01	7.3E+00	3.2E+00	2.2E+00	1.8E+00	1.6E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
	Reverse	5.4E+09	1.7E+04	6.6E+01	7.3E+00	3.2E+00	2.2E+00	1.8E+00	1.6E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
$7s_{\beta}^{A}p$	Forward	1.3E+10	2.6E+04	7.5E+01	7.5E+00	3.3E+00	2.2E+00	1.8E+00	1.6E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
	Reverse	1.3E+10	2.6E+04	7.5E+01	7.5E+00	3.3E+00	2.2E+00	1.8E+00	1.6E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
$8s_{\alpha}^{E}p$	Forward	1.4E+12	2.5E+05	2.0E+02	1.0E+01	3.7E+00	2.4E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
	Reverse	1.4E+12	2.5E+05	2.0E+02	1.0E+01	3.7E+00	2.4E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
$8s_{\alpha}^{A}p$	Forward	2.4E+12	3.3E+05	2.3E+02	1.1E+01	3.8E+00	2.4E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
	Reverse	2.4E+12	3.3E+05	2.3E+02	1.1E+01	3.8E+00	2.4E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
9pp	Forward	2.8E+14	3.8E+06	7.7E+02	1.7E+01	4.5E+00	2.7E+00	2.0E+00	1.7E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
	Reverse	2.8E+14	3.8E+06	7.7E+02	1.7E+01	4.5E+00	2.7E+00	2.0E+00	1.7E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00

Table S6

	rxn. type	Direction	Temperature 200	300	400	500	600	700	800	900	1000	1500	2000	2500
C_2H_5	3pp	Forward	1.6E+24	5.4E+09	8.6E+02	7.1E+00	3.0E+00	2.1E+00	1.7E+00	1.5E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	1.6E+24	5.4E+09	8.6E+02	7.1E+00	3.0E+00	2.1E+00	1.7E+00	1.5E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
C_3H_7	$3s_{\alpha}p$	Forward	1.1E+23	1.8E+09	6.6E+02	7.0E+00	3.0E+00	2.1E+00	1.7E+00	1.5E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	1.1E+23	1.8E+09	6.6E+02	7.0E+00	3.0E+00	2.1E+00	1.7E+00	1.5E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
	4pp	Forward	1.0E+26	2.3E+11	2.1E+04	1.7E+01	4.1E+00	2.5E+00	2.0E+00	1.7E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	1.0E+26	2.3E+11	2.1E+04	1.7E+01	4.1E+00	2.5E+00	2.0E+00	1.7E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
C_4H_9	$3s_{\beta}p$	Forward	1.2E+23	1.8E+09	6.3E+02	6.9E+00	3.0E+00	2.1E+00	1.7E+00	1.5E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	1.2E+23	1.8E+09	6.3E+02	6.9E+00	3.0E+00	2.1E+00	1.7E+00	1.5E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
	$4s_{\alpha}$ p	Forward	1.0E+25	9.2E+10	1.6E+04	1.7E+01	4.1E+00	2.5E+00	2.0E+00	1.7E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	1.0E+25	9.2E+10	1.6E+04	1.7E+01	4.1E+00	2.5E+00	2.0E+00	1.7E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
	5pp	Forward	6.9E+14	7.1E+05	7.7E+01	5.5E+00	2.7E+00	2.0E+00	1.7E+00	1.5E+00	1.4E+00	1.1E+00	1.1E+00	1.0E+00
		Reverse	6.9E+14	7.1E+05	7.7E+01	5.5E+00	2.7E+00	2.0E+00	1.7E+00	1.5E+00	1.4E+00	1.1E+00	1.1E+00	1.0E+00
C_5H_{11}	$3s_{\beta}p$	Forward	1.1E+23	1.8E+09	6.4E+02	6.9E+00	3.0E+00	2.1E+00	1.7E+00	1.5E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	1.1E+23	1.8E+09	6.4E+02	6.9E+00	3.0E+00	2.1E+00	1.7E+00	1.5E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
	$4s_{\beta}$ p	Forward	6.1E+24	7.1E+10	1.4E+04	1.7E+01	4.1E+00	2.5E+00	1.9E+00	1.7E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	6.1E+24	7.1E+10	1.4E+04	1.7E+01	4.1E+00	2.5E+00	1.9E+00	1.7E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
	$5s_{\alpha}^{E}p$	Forward	4.0E+13	2.4E+05	6.3E+01	5.4E+00	2.7E+00	2.0E+00	1.7E+00	1.5E+00	1.4E+00	1.1E+00	1.1E+00	1.0E+00
		Reverse	4.0E+13	2.4E+05	6.3E+01	5.4E+00	2.7E+00	2.0E+00	1.7E+00	1.5E+00	1.4E+00	1.1E+00	1.1E+00	1.0E+00
	$5s_{\alpha}^{A}p$	Forward	4.1E+13	2.3E+05	5.9E+01	5.3E+00	2.7E+00	2.0E+00	1.6E+00	1.5E+00	1.4E+00	1.1E+00	1.1E+00	1.0E+00
		Reverse	4.1E+13	2.3E+05	5.9E+01	5.3E+00	2.7E+00	2.0E+00	1.6E+00	1.5E+00	1.4E+00	1.1E+00	1.1E+00	1.0E+00
	6pp	Forward	4.0E+10	6.3E+03	1.6E+01	3.6E+00	2.2E+00	1.7E+00	1.5E+00	1.4E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
		Reverse	4.0E+10	6.3E+03	1.6E+01	3.6E+00	2.2E+00	1.7E+00	1.5E+00	1.4E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
C_6H_{13}	$3s_{\beta}p$	Forward	1.1E+23	1.8E+09	6.4E+02	7.0E+00	3.0E+00	2.1E+00	1.7E+00	1.5E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	1.1E+23	1.8E+09	6.4E+02	7.0E+00	3.0E+00	2.1E+00	1.7E+00	1.5E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
	$4s_{\beta}$ p	Forward	6.2E+24	7.2E+10	1.4E+04	1.7E+01	4.1E+00	2.5E+00	2.0E+00	1.7E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	6.2E+24	7.2E+10	1.4E+04	1.7E+01	4.1E+00	2.5E+00	2.0E+00	1.7E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00

	$5s_{\beta}{}^{E}p$	Forward	2.9E+13	2.1E+05	5.9E+01	5.3E+00	2.7E+00	2.0E+00	1.6E+00	1.5E+00	1.4E+00	1.1E+00	1.1E+00	1.0E+00
		Reverse	2.9E+13	2.1E+05	5.9E+01	5.3E+00	2.7E+00	2.0E+00	1.6E+00	1.5E+00	1.4E+00	1.1E+00	1.1E+00	1.0E+00
	$5s_{\beta}{}^{A}p$	Forward	2.5E+13	1.8E+05	5.4E+01	5.2E+00	2.7E+00	2.0E+00	1.6E+00	1.5E+00	1.4E+00	1.1E+00	1.1E+00	1.0E+00
		Reverse	2.5E+13	1.8E+05	5.4E+01	5.2E+00	2.7E+00	2.0E+00	1.6E+00	1.5E+00	1.4E+00	1.1E+00	1.1E+00	1.0E+00
	$6s_{\alpha}{}^{E}p$	Forward	1.1E+09	2.0E+03	1.4E+01	3.6E+00	2.2E+00	1.7E+00	1.5E+00	1.4E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
		Reverse	1.1E+09	2.0E+03	1.4E+01	3.6E+00	2.2E+00	1.7E+00	1.5E+00	1.4E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
	$6s_{\alpha}{}^{A}p$	Forward	9.5E+08	1.8E+03	1.3E+01	3.5E+00	2.2E+00	1.7E+00	1.5E+00	1.4E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
		Reverse	9.5E+08	1.8E+03	1.3E+01	3.5E+00	2.2E+00	1.7E+00	1.5E+00	1.4E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
	7pp	Forward	3.7E+09	1.9E+03	1.1E+01	3.2E+00	2.1E+00	1.7E+00	1.5E+00	1.3E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
		Reverse	3.7E+09	1.9E+03	1.1E+01	3.2E+00	2.1E+00	1.7E+00	1.5E+00	1.3E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
C_7H_{15}	$3s_{\beta}p$	Forward	1.1E+23	1.8E+09	6.4E+02	7.0E+00	3.0E+00	2.1E+00	1.7E+00	1.5E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	1.1E+23	1.8E+09	6.4E+02	7.0E+00	3.0E+00	2.1E+00	1.7E+00	1.5E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
	$4s_{\beta}$ p	Forward	6.2E+24	7.2E+10	1.4E+04	1.7E+01	4.1E+00	2.5E+00	2.0E+00	1.7E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	6.2E+24	7.2E+10	1.4E+04	1.7E+01	4.1E+00	2.5E+00	2.0E+00	1.7E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
	$5s_{\beta}{}^{E}p$	Forward	2.9E+13	2.1E+05	5.9E+01	5.3E+00	2.7E+00	2.0E+00	1.6E+00	1.5E+00	1.4E+00	1.1E+00	1.1E+00	1.0E+00
		Reverse	2.9E+13	2.1E+05	5.9E+01	5.3E+00	2.7E+00	2.0E+00	1.6E+00	1.5E+00	1.4E+00	1.1E+00	1.1E+00	1.0E+00
	$5s_{\beta}{}^{A}p$	Forward	2.2E+13	1.7E+05	5.4E+01	5.2E+00	2.7E+00	2.0E+00	1.6E+00	1.5E+00	1.4E+00	1.1E+00	1.1E+00	1.0E+00
		Reverse	2.2E+13	1.7E+05	5.4E+01	5.2E+00	2.7E+00	2.0E+00	1.6E+00	1.5E+00	1.4E+00	1.1E+00	1.1E+00	1.0E+00
	$6s_{\beta}{}^{E}p$	Forward	8.6E+08	1.8E+03	1.4E+01	3.6E+00	2.2E+00	1.7E+00	1.5E+00	1.4E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
		Reverse	8.6E+08	1.8E+03	1.4E+01	3.6E+00	2.2E+00	1.7E+00	1.5E+00	1.4E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
	$6s_{\beta}{}^{A}p$	Forward	5.8E+08	1.5E+03	1.3E+01	3.5E+00	2.2E+00	1.7E+00	1.5E+00	1.4E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
		Reverse	5.8E+08	1.5E+03	1.3E+01	3.5E+00	2.2E+00	1.7E+00	1.5E+00	1.4E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
	$7s_{\alpha}{}^{E}p$	Forward	1.9E+08	7.6E+02	9.7E+00	3.1E+00	2.1E+00	1.7E+00	1.5E+00	1.3E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
		Reverse	1.9E+08	7.6E+02	9.7E+00	3.1E+00	2.1E+00	1.7E+00	1.5E+00	1.3E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
	$7s_{\alpha}{}^{A}p$	Forward	4.6E+08	1.0E+03	1.0E+01	3.2E+00	2.1E+00	1.7E+00	1.5E+00	1.3E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
		Reverse	4.6E+08	1.0E+03	1.0E+01	3.2E+00	2.1E+00	1.7E+00	1.5E+00	1.3E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
	8pp	Forward	2.8E+11	1.0E+04	1.5E+01	3.5E+00	2.2E+00	1.7E+00	1.5E+00	1.4E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
		Reverse	2.8E+11	1.0E+04	1.5E+01	3.5E+00	2.2E+00	1.7E+00	1.5E+00	1.4E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
C_8H_{17}	$3s_{\beta}p$	forward	1.1E+23	1.8E+09	6.4E+02	7.0E+00	3.0E+00	2.1E+00	1.7E+00	1.5E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
		reverse	1.1E+23	1.8E+09	6.4E+02	7.0E+00	3.0E+00	2.1E+00	1.7E+00	1.5E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00

$4s_{\beta}$ p	Forward	6.2E+24	7.2E+10	1.4E+04	1.7E+01	4.1E+00	2.5E+00	2.0E+00	1.7E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
	Reverse	6.2E+24	7.2E+10	1.4E+04	1.7E+01	4.1E+00	2.5E+00	2.0E+00	1.7E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
$5s_{\beta}^{E}p$	Forward	2.9E+13	2.1E+05	5.9E+01	5.3E+00	2.7E+00	2.0E+00	1.6E+00	1.5E+00	1.4E+00	1.1E+00	1.1E+00	1.0E+00
	Reverse	2.9E+13	2.1E+05	5.9E+01	5.3E+00	2.7E+00	2.0E+00	1.6E+00	1.5E+00	1.4E+00	1.1E+00	1.1E+00	1.0E+00
$5s_{\beta}^{A}p$	Forward	2.2E+13	1.7E+05	5.4E+01	5.2E+00	2.7E+00	2.0E+00	1.6E+00	1.5E+00	1.4E+00	1.1E+00	1.1E+00	1.0E+00
	Reverse	2.2E+13	1.7E+05	5.4E+01	5.2E+00	2.7E+00	2.0E+00	1.6E+00	1.5E+00	1.4E+00	1.1E+00	1.1E+00	1.0E+00
$6s_{\beta}^{E}p$	Forward	7.6E+08	1.8E+03	1.4E+01	3.6E+00	2.2E+00	1.7E+00	1.5E+00	1.4E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
	Reverse	7.6E+08	1.8E+03	1.4E+01	3.6E+00	2.2E+00	1.7E+00	1.5E+00	1.4E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
$6s_{\beta}^{A}p$	Forward	5.2E+08	1.5E+03	1.3E+01	3.5E+00	2.2E+00	1.7E+00	1.5E+00	1.4E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
	Reverse	5.2E+08	1.5E+03	1.3E+01	3.5E+00	2.2E+00	1.7E+00	1.5E+00	1.4E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
$7s_{\beta}^{E}p$	Forward	1.6E+08	7.3E+02	9.8E+00	3.2E+00	2.1E+00	1.7E+00	1.5E+00	1.3E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
	Reverse	1.6E+08	7.3E+02	9.8E+00	3.2E+00	2.1E+00	1.7E+00	1.5E+00	1.3E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
$7s_{\beta}^{A}p$	Forward	3.4E+08	9.5E+02	1.0E+01	3.2E+00	2.1E+00	1.7E+00	1.5E+00	1.3E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
	Reverse	3.4E+08	9.5E+02	1.0E+01	3.2E+00	2.1E+00	1.7E+00	1.5E+00	1.3E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
$8s_{\alpha}^{E}p$	Forward	1.7E+10	4.2E+03	1.4E+01	3.5E+00	2.2E+00	1.7E+00	1.5E+00	1.4E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
	Reverse	1.7E+10	4.2E+03	1.4E+01	3.5E+00	2.2E+00	1.7E+00	1.5E+00	1.4E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
$8s_{\alpha}^{A}p$	Forward	2.7E+10	5.1E+03	1.5E+01	3.6E+00	2.2E+00	1.7E+00	1.5E+00	1.4E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
	Reverse	2.7E+10	5.1E+03	1.5E+01	3.6E+00	2.2E+00	1.7E+00	1.5E+00	1.4E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
9pp	Forward	1.4E+12	2.7E+04	2.2E+01	3.9E+00	2.3E+00	1.8E+00	1.5E+00	1.4E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00
	Reverse	1.4E+12	2.7E+04	2.2E+01	3.9E+00	2.3E+00	1.8E+00	1.5E+00	1.4E+00	1.3E+00	1.1E+00	1.1E+00	1.0E+00

Table S7

	rxn. type	Direction	Temperature											
			200	300	400	500	600	700	800	900	1000	1500	2000	2500
C_2H_5	3pp	Forward	9.0E+26	3.0E+12	2.7E+05	6.5E+01	5.9E+00	3.1E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	9.0E+26	3.0E+12	2.7E+05	6.5E+01	5.9E+00	3.1E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
C_3H_7	$3s_\alpha p$	Forward	3.3E+25	6.5E+11	1.4E+05	5.7E+01	5.9E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	3.3E+25	6.5E+11	1.4E+05	5.7E+01	5.9E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	4pp	Forward	8.7E+28	2.5E+14	1.8E+07	1.6E+03	1.8E+01	4.9E+00	2.9E+00	2.2E+00	1.9E+00	1.3E+00	1.2E+00	1.1E+00
		Reverse	8.7E+28	2.5E+14	1.8E+07	1.6E+03	1.8E+01	4.9E+00	2.9E+00	2.2E+00	1.9E+00	1.3E+00	1.2E+00	1.1E+00
C_4H_9	$3s_\beta p$	Forward	3.7E+25	6.1E+11	1.3E+05	5.1E+01	5.7E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	3.7E+25	6.1E+11	1.3E+05	5.1E+01	5.7E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	$4s_\alpha$ p	Forward	5.3E+27	5.8E+13	8.1E+06	1.1E+03	1.7E+01	4.8E+00	2.9E+00	2.2E+00	1.8E+00	1.3E+00	1.1E+00	1.1E+00
		Reverse	5.3E+27	5.8E+13	8.1E+06	1.1E+03	1.7E+01	4.8E+00	2.9E+00	2.2E+00	1.8E+00	1.3E+00	1.1E+00	1.1E+00
	5pp	Forward	6.9E+16	9.3E+07	5.2E+03	3.9E+01	6.2E+00	3.2E+00	2.3E+00	1.9E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	6.9E+16	9.3E+07	5.2E+03	3.9E+01	6.2E+00	3.2E+00	2.3E+00	1.9E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
C_5H_{11}	$3s_\beta p$	Forward	3.6E+25	6.0E+11	1.2E+05	5.1E+01	5.7E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	3.6E+25	6.0E+11	1.2E+05	5.1E+01	5.7E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	$4s_\beta$ p	Forward	4.4E+27	4.8E+13	6.8E+06	9.7E+02	1.6E+01	4.6E+00	2.9E+00	2.2E+00	1.8E+00	1.3E+00	1.1E+00	1.1E+00
		Reverse	4.4E+27	4.8E+13	6.8E+06	9.7E+02	1.6E+01	4.6E+00	2.9E+00	2.2E+00	1.8E+00	1.3E+00	1.1E+00	1.1E+00
	$5s_\alpha^E p$	Forward	2.1E+15	1.6E+07	2.3E+03	3.0E+01	5.8E+00	3.1E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	2.1E+15	1.6E+07	2.3E+03	3.0E+01	5.8E+00	3.1E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	$5s_\alpha^A p$	Forward	4.1E+15	2.1E+07	2.4E+03	2.9E+01	5.7E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	4.1E+15	2.1E+07	2.4E+03	2.9E+01	5.7E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	6pp	Forward	3.8E+11	1.7E+05	2.0E+02	1.1E+01	3.9E+00	2.5E+00	1.9E+00	1.7E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	3.8E+11	1.7E+05	2.0E+02	1.1E+01	3.9E+00	2.5E+00	1.9E+00	1.7E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
C_6H_{13}	$3s_\beta p$	Forward	5.7E+25	7.4E+11	1.3E+05	5.1E+01	5.7E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	5.7E+25	7.4E+11	1.3E+05	5.1E+01	5.7E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	$4s_\beta$ p	Forward	2.6E+27	3.7E+13	6.0E+06	9.2E+02	1.6E+01	4.6E+00	2.8E+00	2.2E+00	1.8E+00	1.3E+00	1.1E+00	1.1E+00
		Reverse	2.6E+27	3.7E+13	6.0E+06	9.2E+02	1.6E+01	4.6E+00	2.8E+00	2.2E+00	1.8E+00	1.3E+00	1.1E+00	1.1E+00

	$5s_{\beta}{}^{E}p$	Forward	1.7E+15	1.4E+07	1.9E+03	2.7E+01	5.5E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	1.7E+15	1.4E+07	1.9E+03	2.7E+01	5.5E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	$5s_{\beta}{}^{A}p$	Forward	3.3E+15	1.7E+07	2.0E+03	2.6E+01	5.4E+00	2.9E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	3.3E+15	1.7E+07	2.0E+03	2.6E+01	5.4E+00	2.9E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	$6s_{\alpha}{}^{E}p$	Forward	2.2E+10	4.5E+04	1.2E+02	9.7E+00	3.7E+00	2.4E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	2.2E+10	4.5E+04	1.2E+02	9.7E+00	3.7E+00	2.4E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
	$6s_{\alpha}{}^{A}p$	Forward	2.7E+10	4.6E+04	1.2E+02	9.3E+00	3.6E+00	2.4E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	2.7E+10	4.6E+04	1.2E+02	9.3E+00	3.6E+00	2.4E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
	7pp	Forward	3.7E+11	1.3E+05	1.5E+02	9.4E+00	3.6E+00	2.4E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	3.7E+11	1.3E+05	1.5E+02	9.4E+00	3.6E+00	2.4E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
C_7H_{15}	$3s_{\beta}p$	Forward	4.2E+25	6.4E+11	1.3E+05	5.1E+01	5.7E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	4.2E+25	6.4E+11	1.3E+05	5.1E+01	5.7E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	$4s_{\beta}$ p	Forward	7.1E+26	2.0E+13	4.4E+06	8.3E+02	1.5E+01	4.6E+00	2.8E+00	2.2E+00	1.8E+00	1.3E+00	1.1E+00	1.1E+00
		Reverse	7.1E+26	2.0E+13	4.4E+06	8.3E+02	1.5E+01	4.6E+00	2.8E+00	2.2E+00	1.8E+00	1.3E+00	1.1E+00	1.1E+00
	$5s_{\beta}{}^{E}p$	Forward	6.9E+13	3.2E+06	1.1E+03	2.4E+01	5.4E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	6.9E+13	3.2E+06	1.1E+03	2.4E+01	5.4E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	$5s_{\beta}{}^{A}p$	Forward	2.9E+14	5.8E+06	1.3E+03	2.4E+01	5.3E+00	2.9E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	2.9E+14	5.8E+06	1.3E+03	2.4E+01	5.3E+00	2.9E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	$6s_{\beta}{}^{E}p$	Forward	3.4E+09	1.9E+04	8.5E+01	8.7E+00	3.6E+00	2.4E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	3.4E+09	1.9E+04	8.5E+01	8.7E+00	3.6E+00	2.4E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
	$6s_{\beta}{}^{A}p$	Forward	4.8E+09	2.1E+04	8.4E+01	8.5E+00	3.5E+00	2.3E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	4.8E+09	2.1E+04	8.4E+01	8.5E+00	3.5E+00	2.3E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
	$7s_{\alpha}{}^{E}p$	Forward	2.0E+09	1.2E+04	6.3E+01	7.4E+00	3.3E+00	2.2E+00	1.8E+00	1.6E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	2.0E+09	1.2E+04	6.3E+01	7.4E+00	3.3E+00	2.2E+00	1.8E+00	1.6E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
	$7s_{\alpha}{}^{A}p$	Forward	6.4E+09	2.0E+04	7.4E+01	7.7E+00	3.3E+00	2.2E+00	1.8E+00	1.6E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	6.4E+09	2.0E+04	7.4E+01	7.7E+00	3.3E+00	2.2E+00	1.8E+00	1.6E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
	8pp	Forward	3.2E+13	1.1E+06	3.9E+02	1.3E+01	4.0E+00	2.5E+00	1.9E+00	1.7E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
		Reverse	3.2E+13	1.1E+06	3.9E+02	1.3E+01	4.0E+00	2.5E+00	1.9E+00	1.7E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
C_8H_{17}	$3s_{\beta}p$	forward	2.7E+25	5.2E+11	1.2E+05	5.0E+01	5.7E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
		reverse	2.7E+25	5.2E+11	1.2E+05	5.0E+01	5.7E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00

$4s_{\beta}$ p	Forward	7.1E+26	1.9E+13	4.4E+06	8.3E+02	1.5E+01	4.6E+00	2.8E+00	2.2E+00	1.8E+00	1.3E+00	1.1E+00	1.1E+00
	Reverse	7.1E+26	1.9E+13	4.4E+06	8.3E+02	1.5E+01	4.6E+00	2.8E+00	2.2E+00	1.8E+00	1.3E+00	1.1E+00	1.1E+00
$5s_{\beta}^{E}p$	Forward	1.7E+13	1.7E+06	8.6E+02	2.2E+01	5.4E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	Reverse	1.7E+13	1.7E+06	8.6E+02	2.2E+01	5.4E+00	3.0E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
$5s_{\beta}^{A}p$	Forward	3.4E+13	2.2E+06	9.1E+02	2.2E+01	5.3E+00	2.9E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
	Reverse	3.4E+13	2.2E+06	9.1E+02	2.2E+01	5.3E+00	2.9E+00	2.2E+00	1.8E+00	1.6E+00	1.2E+00	1.1E+00	1.1E+00
$6s_{\beta}^{E}p$	Forward	1.7E+08	5.4E+03	5.7E+01	8.0E+00	3.5E+00	2.3E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
	Reverse	1.7E+08	5.4E+03	5.7E+01	8.0E+00	3.5E+00	2.3E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
$6s_{\beta}^{A}p$	Forward	1.4E+08	4.8E+03	5.3E+01	7.7E+00	3.4E+00	2.3E+00	1.8E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
	Reverse	1.4E+08	4.8E+03	5.3E+01	7.7E+00	3.4E+00	2.3E+00	1.8E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
$7s_{\beta}^{E}p$	Forward	1.4E+08	4.1E+03	4.4E+01	6.8E+00	3.2E+00	2.2E+00	1.8E+00	1.6E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
	Reverse	1.4E+08	4.1E+03	4.4E+01	6.8E+00	3.2E+00	2.2E+00	1.8E+00	1.6E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
$7s_{\beta}^{A}p$	Forward	1.4E+09	1.1E+04	5.9E+01	7.3E+00	3.2E+00	2.2E+00	1.8E+00	1.6E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
	Reverse	1.4E+09	1.1E+04	5.9E+01	7.3E+00	3.2E+00	2.2E+00	1.8E+00	1.6E+00	1.4E+00	1.2E+00	1.1E+00	1.1E+00
$8s_{\alpha}^{E}p$	Forward	1.6E+11	1.0E+05	1.5E+02	1.0E+01	3.7E+00	2.4E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
	Reverse	1.6E+11	1.0E+05	1.5E+02	1.0E+01	3.7E+00	2.4E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
$8s_{\alpha}^{A}p$	Forward	4.3E+11	1.6E+05	1.8E+02	1.1E+01	3.8E+00	2.4E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
	Reverse	4.3E+11	1.6E+05	1.8E+02	1.1E+01	3.8E+00	2.4E+00	1.9E+00	1.6E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
9pp	Forward	8.5E+13	2.3E+06	6.5E+02	1.6E+01	4.5E+00	2.7E+00	2.0E+00	1.7E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00
	Reverse	8.5E+13	2.3E+06	6.5E+02	1.6E+01	4.5E+00	2.7E+00	2.0E+00	1.7E+00	1.5E+00	1.2E+00	1.1E+00	1.1E+00

Table S8

	rxn. type	Direction	Temperature 200	300	400	500	600	700	800	900	1000	1500	2000	2500
C_2H_5	3pp	Forward	11.7	5.8	3.7	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
		Reverse	11.7	5.8	3.7	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
C_3H_7	$3s_\alpha p$	Forward	11.7	5.8	3.7	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
		Reverse	11.7	5.8	3.7	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
	4pp	Forward	14.7	7.1	4.4	3.2	2.5	2.1	1.9	1.7	1.5	1.2	1.1	1.1
		Reverse	14.7	7.1	4.4	3.2	2.5	2.1	1.9	1.7	1.5	1.2	1.1	1.1
C_4H_9	$3s_\beta p$	Forward	11.6	5.7	3.6	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
		Reverse	11.6	5.7	3.6	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
	$4s_\alpha$ p	Forward	14.5	7.0	4.4	3.2	2.5	2.1	1.8	1.7	1.5	1.2	1.1	1.1
		Reverse	14.5	7.0	4.4	3.2	2.5	2.1	1.8	1.7	1.5	1.2	1.1	1.1
	5pp	Forward	12.0	5.9	3.8	2.8	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
		Reverse	12.0	5.9	3.8	2.8	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
C_5H_{11}	$3s_\beta p$	Forward	11.6	5.7	3.6	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
		Reverse	11.6	5.7	3.6	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
	$4s_\beta$ p	Forward	14.4	6.9	4.3	3.1	2.5	2.1	1.8	1.7	1.5	1.2	1.1	1.1
		Reverse	14.4	6.9	4.3	3.1	2.5	2.1	1.8	1.7	1.5	1.2	1.1	1.1
	$5s_\alpha^E p$	Forward	11.7	5.8	3.7	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
		Reverse	11.7	5.8	3.7	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
	$5s_\alpha^A p$	Forward	11.7	5.7	3.7	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
		Reverse	11.7	5.7	3.7	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
	6pp	Forward	10.2	5.1	3.3	2.5	2.0	1.7	1.6	1.5	1.4	1.2	1.1	1.1
		Reverse	10.2	5.1	3.3	2.5	2.0	1.7	1.6	1.5	1.4	1.2	1.1	1.1
C_6H_{13}	$3s_\beta p$	Forward	11.6	5.7	3.6	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
		Reverse	11.6	5.7	3.6	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
	$4s_\beta$ p	Forward	14.3	6.9	4.3	3.1	2.5	2.1	1.8	1.7	1.5	1.2	1.1	1.1
		Reverse	14.3	6.9	4.3	3.1	2.5	2.1	1.8	1.7	1.5	1.2	1.1	1.1

	$5s_{\beta}{}^{E}p$	Forward	11.6	5.7	3.6	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
		Reverse	11.6	5.7	3.6	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
	$5s_{\beta}{}^{A}p$	Forward	11.5	5.7	3.6	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
		Reverse	11.5	5.7	3.6	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
	$6s_{\alpha}{}^{E}p$	Forward	9.9	5.0	3.2	2.4	2.0	1.7	1.6	1.4	1.4	1.2	1.1	1.1
		Reverse	9.9	5.0	3.2	2.4	2.0	1.7	1.6	1.4	1.4	1.2	1.1	1.1
	$6s_{\alpha}{}^{A}p$	Forward	9.8	4.9	3.2	2.4	2.0	1.7	1.6	1.4	1.4	1.2	1.1	1.1
		Reverse	9.8	4.9	3.2	2.4	2.0	1.7	1.6	1.4	1.4	1.2	1.1	1.1
	7pp	Forward	9.7	4.9	3.2	2.4	2.0	1.7	1.5	1.4	1.3	1.2	1.1	1.1
		Reverse	9.7	4.9	3.2	2.4	2.0	1.7	1.5	1.4	1.3	1.2	1.1	1.1
C_7H_{15}	$3s_{\beta}p$	Forward	11.6	5.7	3.6	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
		Reverse	11.6	5.7	3.6	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
	$4s_{\beta}$ p	Forward	14.3	6.9	4.3	3.1	2.5	2.1	1.8	1.7	1.5	1.2	1.1	1.1
		Reverse	14.3	6.9	4.3	3.1	2.5	2.1	1.8	1.7	1.5	1.2	1.1	1.1
	$5s_{\beta}{}^{E}p$	Forward	11.5	5.7	3.6	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
		Reverse	11.5	5.7	3.6	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
	$5s_{\beta}{}^{A}p$	Forward	11.5	5.6	3.6	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
		Reverse	11.5	5.6	3.6	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
	$6s_{\beta}{}^{E}p$	Forward	9.7	4.9	3.2	2.4	2.0	1.7	1.5	1.4	1.3	1.2	1.1	1.1
		Reverse	9.7	4.9	3.2	2.4	2.0	1.7	1.5	1.4	1.3	1.2	1.1	1.1
	$6s_{\beta}{}^{A}p$	Forward	9.7	4.8	3.2	2.4	2.0	1.7	1.5	1.4	1.3	1.2	1.1	1.1
		Reverse	9.7	4.8	3.2	2.4	2.0	1.7	1.5	1.4	1.3	1.2	1.1	1.1
	$7s_{\alpha}{}^{E}p$	Forward	9.3	4.7	3.1	2.3	1.9	1.7	1.5	1.4	1.3	1.1	1.1	1.1
		Reverse	9.3	4.7	3.1	2.3	1.9	1.7	1.5	1.4	1.3	1.1	1.1	1.1
	$7s_{\alpha}{}^{A}p$	Forward	9.4	4.7	3.1	2.3	1.9	1.7	1.5	1.4	1.3	1.1	1.1	1.1
		Reverse	9.4	4.7	3.1	2.3	1.9	1.7	1.5	1.4	1.3	1.1	1.1	1.1
	8pp	Forward	10.2	5.1	3.3	2.5	2.0	1.8	1.6	1.5	1.4	1.2	1.1	1.1
		Reverse	10.2	5.1	3.3	2.5	2.0	1.8	1.6	1.5	1.4	1.2	1.1	1.1
C_8H_{17}	$3s_{\beta}p$	forward	11.6	5.7	3.6	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
		reverse	11.6	5.7	3.6	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1

$4s_{\beta}$ p	Forward	14.3	6.9	4.3	3.1	2.5	2.1	1.8	1.7	1.5	1.2	1.1	1.1
	Reverse	14.3	6.9	4.3	3.1	2.5	2.1	1.8	1.7	1.5	1.2	1.1	1.1
$5s_{\beta}{}^{E}p$	Forward	11.5	5.7	3.6	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
	Reverse	11.5	5.7	3.6	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
$5s_{\beta}{}^{A}p$	Forward	11.4	5.6	3.6	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
	Reverse	11.4	5.6	3.6	2.7	2.2	1.9	1.7	1.5	1.4	1.2	1.1	1.1
$6s_{\beta}{}^{E}p$	Forward	9.7	4.9	3.2	2.4	2.0	1.7	1.5	1.4	1.3	1.2	1.1	1.1
	Reverse	9.7	4.9	3.2	2.4	2.0	1.7	1.5	1.4	1.3	1.2	1.1	1.1
$6s_{\beta}{}^{A}p$	Forward	9.6	4.8	3.2	2.4	2.0	1.7	1.5	1.4	1.3	1.2	1.1	1.1
	Reverse	9.6	4.8	3.2	2.4	2.0	1.7	1.5	1.4	1.3	1.2	1.1	1.1
$7s_{\beta}{}^{E}p$	Forward	9.2	4.6	3.0	2.3	1.9	1.7	1.5	1.4	1.3	1.1	1.1	1.1
	Reverse	9.2	4.6	3.0	2.3	1.9	1.7	1.5	1.4	1.3	1.1	1.1	1.1
$7s_{\beta}{}^{A}p$	Forward	9.3	4.7	3.1	2.3	1.9	1.7	1.5	1.4	1.3	1.1	1.1	1.1
	Reverse	9.3	4.7	3.1	2.3	1.9	1.7	1.5	1.4	1.3	1.1	1.1	1.1
$8s_{\alpha}{}^{E}p$	Forward	9.9	5.0	3.2	2.4	2.0	1.7	1.6	1.4	1.4	1.2	1.1	1.1
	Reverse	9.9	5.0	3.2	2.4	2.0	1.7	1.6	1.4	1.4	1.2	1.1	1.1
$8s_{\alpha}{}^{A}p$	Forward	10.0	5.0	3.3	2.4	2.0	1.7	1.6	1.4	1.4	1.2	1.1	1.1
	Reverse	10.0	5.0	3.3	2.4	2.0	1.7	1.6	1.4	1.4	1.2	1.1	1.1
9pp	Forward	10.7	5.3	3.4	2.6	2.1	1.8	1.6	1.5	1.4	1.2	1.1	1.1
	Reverse	10.7	5.3	3.4	2.6	2.1	1.8	1.6	1.5	1.4	1.2	1.1	1.1

Table S9.A.

Alkyl Radical	Radical Sites	Location Type	Bond Distance						
			B_1	B_2	B_3	B_4	B_5	B_6	B_7
Ethyl	1 or 2	Primary	**1.489**	-	-	-	-	-	-
Propyl	1 or 3	Primary	**1.491**	1.527	-	-	-	-	-
Butyl	1 or 4	Primary	**1.490**	1.529	1.524	-	-	-	-
Pentyl	1 or 5	Primary	**1.490**	1.529	1.525	1.525	-	-	-
Hexyl	1 or 6	Primary	**1.490**	1.529	1.525	1.525	1.525	-	-
Heptyl	1 or 7	Primary	**1.490**	1.529	1.525	1.525	1.525	1.525	-
Octyl	1 or 8	Primary	**1.490**	1.529	1.525	1.526	1.525	1.525	1.525
Propyl	2	α-Secondary	**1.490**	**1.490**	-	-	-	-	-
Butyl	2 or 3	α-Secondary	**1.491**	**1.492**	1.527	-	-	-	-
Pentyl	2 or 4	α-Secondary	**1.491**	**1.492**	1.527	1.524	-	-	-
Hexyl	2 or 5	α-Secondary	**1.491**	**1.492**	1.527	1.525	1.525	-	-
Heptyl	2 or 6	α-Secondary	**1.490**	**1.492**	1.528	1.525	1.525	1.525	-
Octyl	2 or 7	α-Secondary	**1.491**	**1.492**	1.528	1.525	1.525	1.525	1.525
Pentyl	3	β-Secondary	1.527	**1.492**	**1.492**	1.527	-	-	-
Hexyl	3 or 4	β-Secondary	1.527	**1.492**	**1.492**	1.528	1.524	-	-
Heptyl	3 or 5	β-Secondary	1.527	**1.492**	**1.492**	1.528	1.525	1.525	-
Octyl	3 or 6	β-Secondary	1.527	**1.492**	**1.492**	1.528	1.525	1.525	1.525
Heptyl	4	γ-Secondary	1.524	1.528	**1.492**	**1.492**	1.528	1.524	-
Octyl	4 or 5	γ-Secondary	1.524	1.528	**1.492**	**1.492**	1.528	1.525	1.525

Table S9.B.

Alkyl Radical	Radical Sites	Location Type	Bond Angle					
			A_1	A_2	A_3	A_4	A_5	A_6
Ethyl	1 or 2	Primary	-	-	-	-	-	-
Propyl	1 or 3	Primary	*112.8*	-	-	-	-	-
Butyl	1 or 4	Primary	*113.2*	112.6	-	-	-	-
Pentyl	1 or 5	Primary	*113.2*	113.1	112.7	-	-	-
Hexyl	1 or 6	Primary	*113.1*	113.1	113.2	112.8	-	-
Heptyl	1 or 7	Primary	*113.1*	113.0	113.2	113.3	112.8	-
Octyl	1 or 8	Primary	*113.1*	113.0	113.2	113.2	113.3	112.8
Propyl	2	α-Secondary	**120.1**	-	-	-	-	-
Butyl	2 or 3	α-Secondary	**120.6**	*113.2*	-	-	-	-
Pentyl	2 or 4	α-Secondary	**120.7**	*113.7*	112.7	-	-	-
Hexyl	2 or 5	α-Secondary	**120.6**	*113.6*	113.2	112.8	-	-
Heptyl	2 or 6	α-Secondary	**120.6**	*113.6*	113.1	113.3	112.8	-
Octyl	2 or 7	α-Secondary	**120.6**	*113.6*	113.1	113.2	113.3	112.8
Pentyl	3	β-Secondary	*113.2*	**121.2**	*113.2*	-	-	-
Hexyl	3 or 4	β-Secondary	*113.2*	**121.2**	*113.6*	112.7	-	-
Heptyl	3 or 5	β-Secondary	*113.2*	**121.2**	*113.5*	113.2	112.8	-
Octyl	3 or 6	β-Secondary	*113.2*	**121.2**	*113.5*	113.1	113.3	112.8
Heptyl	4	γ-Secondary	112.7	*113.6*	**121.3**	*113.6*	112.7	-
Octyl	4 or 5	γ-Secondary	112.7	*113.6*	**121.3**	*113.5*	113.2	112.8

Table S9.C.

Alkyl Radical	Radical Sites	Location type	Dihedral Angle				
			D_1	D_2	D_3	D_4	D_5
Ethyl	1 or 2	Primary	-	-	-	-	-
Propyl	1 or 3	Primary	-	-	-	-	-
Butyl	1 or 4	Primary	*-178.8*	-	-	-	-
Pentyl	1 or 5	Primary	*-178.8*	180.0	-	-	-
Hexyl	1 or 6	Primary	*-178.8*	180.0	180.0	-	-
Heptyl	1 or 7	Primary	*-178.8*	180.0	180.0	180.0	-
Octyl	1 or 8	Primary	*-178.8*	180.0	180.0	180.0	180.0
Propyl	2	α-Secondary	-	-	-	-	-
Butyl	2 or 3	α-Secondary	**167.9**	-	-	-	-
Pentyl	2 or 4	α-Secondary	**167.2**	*179.4*	-	-	-
Hexyl	2 or 5	α-Secondary	**167.2**	*179.4*	-180.0	-	-
Heptyl	2 or 6	α-Secondary	**167.1**	*179.4*	-180.0	-180.0	-
Octyl	2 or 7	α-Secondary	**167.1**	*179.4*	-180.0	-180.0	-180.0
Pentyl	3	β-Secondary	**-167.5**	**167.5**	-	-	-
Hexyl	3 or 4	β-Secondary	**-167.5**	**166.5**	*179.4*	-	-
Heptyl	3 or 5	β-Secondary	**-167.6**	**166.5**	*179.4*	-180.0	-
Octyl	3 or 6	β-Secondary	**-167.6**	**166.4**	*179.3*	-180.0	-180.0
Heptyl	4	γ-Secondary	*179.4*	**166.5**	**-166.5**	*-179.4*	-
Octyl	4 or 5	γ-Secondary	*179.4*	**166.6**	**-166.5**	*-179.4*	180.0

Table S10.A.

Alkyl Radical / Cycloalkane	Migration Type	Bond Length										
		B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_{α}	B_{β}	RMS	RMS*
Cyclopropane		1.501	-	-	-	-	-	-	1.501	1.501	-	-
Methylcyclopropane		1.502	1.507	-	-	-	-	-	1.505	1.502	0.001	-
Ethyl	3pp	**1.485**	-	-	-	-	-	-	1.280	1.280	0.016	-
Propyl	$3s_{\alpha}p$	**1.486**	**1.497**	-	-	-	-	-	1.284	1.281	0.015	0.013
Butyl	$3s_{\alpha}p$	**1.486**	**1.498**	1.525	-	-	-	-	1.284	1.282	0.015	0.013
Pentyl	$3s_{\alpha}p$	**1.486**	**1.497**	1.526	1.524	-	-	-	1.284	1.282	0.015	0.013
Hexyl	$3s_{\alpha}p$	**1.486**	**1.497**	1.526	1.525	1.525	-	-	1.284	1.282	0.015	0.013
Heptyl	$3s_{\alpha}p$	**1.486**	**1.497**	1.527	1.525	1.525	1.525	-	1.284	1.282	0.015	0.013
Octyl	$3s_{\alpha}p$	**1.486**	**1.497**	1.527	1.525	1.525	1.525	1.525	1.284	1.282	0.015	0.013
Cyclobutane		1.543	1.543	-	-	-	-	-	1.543	1.543	-	-
Methylcyclobutane		1.543	1.545	1.514	-	-	-	-	1.543	1.545	0.001	-
Propyl	4pp	**1.525**	**1.525**	-	-	-	-	-	1.381	1.381	0.018	-
Butyl	$4s_{\alpha}p$	**1.524**	**1.529**	**1.504**	-	-	-	-	1.387	1.378	0.017	0.015
Pentyl	$4s_{\beta}p$	**1.525**	**1.529**	**1.505**	1.525	-	-	-	1.387	1.380	0.016	0.015
Hexyl	$4s_{\beta}p$	**1.524**	**1.529**	**1.505**	1.525	1.525	-	-	1.387	1.380	0.017	0.015
Heptyl	$4s_{\beta}p$	**1.524**	**1.529**	**1.505**	1.525	1.525	1.525	-	1.387	1.380	0.017	0.015
Octyl	$4s_{\beta}p$	**1.524**	**1.529**	**1.505**	1.526	1.525	1.525	1.525	1.387	1.380	0.017	0.015
Cyclopentane		1.532	1.527	1.532	-	-	-	-	1.547	1.547	-	-
Methylcyclopentane^{E}		1.552	1.537	1.529	1.520	-	-	-	1.537	1.529	0.013	-
Methylcyclopentane^{A}		1.550	1.540	1.532	1.526	-	-	-	1.540	1.532	0.013	-
Butyl	5pp	**1.518**	1.541	**1.518**	-	-	-	-	1.356	1.356	0.014	-
Pentyl^{E}	$5s_{\alpha}^{E}p$	**1.517**	1.541	**1.519**	**1.505**	-	-	-	1.369	1.347	0.014	0.020
Hexyl^{E}	$5s_{\beta}^{E}p$	**1.517**	1.541	**1.519**	**1.505**	1.526	-	-	1.368	1.349	0.014	0.020
Heptyl^{E}	$5s_{\gamma}^{E}p$	**1.517**	1.541	**1.519**	**1.505**	1.526	1.525	-	1.368	1.348	0.014	0.020
Octyl^{E}	$5s_{\gamma}^{E}p$	**1.517**	1.541	**1.519**	**1.505**	1.526	1.525	1.525	1.368	1.348	0.014	0.020
Pentyl^{A}	$5s_{\alpha}^{A}p$	**1.517**	1.544	**1.521**	**1.509**	-	-	-	1.369	1.344	0.015	0.019
Hexyl^{A}	$5s_{\beta}^{A}p$	**1.517**	1.544	**1.521**	**1.509**	1.525	-	-	1.368	1.345	0.015	0.019
Heptyl^{A}	$5s_{\gamma}^{A}p$	**1.517**	1.544	**1.521**	**1.509**	1.526	1.525	-	1.368	1.345	0.015	0.019
Octyl^{A}	$5s_{\gamma}^{A}p$	**1.517**	1.544	**1.521**	**1.509**	1.526	1.525	1.525	1.368	1.344	0.015	0.019
Cyclohexane		1.528	1.528	1.528	1.528	-	-	-	1.528	1.528	-	-
Methylcyclohexane^{E}		1.527	1.527	1.527	1.529	1.524	-	-	1.527	1.529	0.001	-
Methylcyclohexane^{A}		1.527	1.527	1.529	1.533	1.528	-	-	1.529	1.533	0.003	-
Pentyl	6pp	**1.513**	1.533	1.533	**1.513**	-	-	-	1.337	1.337	0.011	-
Hexyl^{E}	$6s_{\alpha}^{E}p$	**1.513**	1.534	1.532	**1.515**	**1.509**	-	-	1.352	1.325	0.011	0.012
Heptyl^{E}	$6s_{\beta}^{E}p$	**1.513**	1.534	1.532	**1.515**	**1.509**	1.525	-	1.351	1.326	0.011	0.012
Octyl^{E}	$6s_{\gamma}^{E}p$	**1.513**	1.534	1.532	**1.515**	**1.509**	1.526	1.525	1.351	1.326	0.011	0.012
Hexyl^{A}	$6s_{\alpha}^{A}p$	**1.512**	1.533	1.534	**1.517**	**1.511**	-	-	1.353	1.323	0.010	0.013
Heptyl^{A}	$6s_{\beta}^{A}p$	**1.512**	1.532	1.535	**1.517**	**1.511**	1.525	-	1.353	1.324	0.011	0.013
Octyl^{A}	$6s_{\gamma}^{A}p$	**1.512**	1.532	1.534	**1.517**	**1.511**	1.526	1.525	1.353	1.324	0.010	0.013
Cycloheptane		1.532	1.530	1.527	1.530	1.532	-	-	1.532	1.532	-	-
Methylcycloheptane^{E}		1.532	1.530	1.527	1.530	1.534	1.528	-	1.532	1.534	0.001	-
Methylcycloheptane^{A}		1.539	1.529	1.530	1.527	1.532	1.527	-	1.533	1.534	0.004	-
Hexyl	7pp	**1.510**	1.532	1.533	1.532	**1.510**	-	-	1.327	1.327	0.014	-
Heptyl^{E}	$7s_{\alpha}^{E}p$	**1.510**	1.532	1.533	1.532	**1.511**	**1.509**	-	1.345	1.311	0.014	0.015
Octyl^{E}	$7s_{\beta}^{E}p$	**1.510**	1.532	1.533	1.532	**1.511**	**1.510**	1.525	1.345	1.313	0.014	0.015
Heptyl^{A}	$7s_{\alpha}^{A}p$	**1.510**	1.532	1.533	1.533	**1.515**	**1.511**	-	1.346	1.312	0.013	0.015
Octyl^{A}	$7s_{\beta}^{A}p$	**1.510**	1.532	1.533	1.533	**1.515**	**1.512**	1.526	1.347	1.314	0.013	0.015
Cyclooctane		1.526	1.526	1.534	1.538	1.532	1.532	-	1.534	1.538	-	-
Methylcyclooctane^{E}		1.526	1.526	1.534	1.537	1.533	1.535	1.530	1.533	1.541	0.001	-
Methylcyclooctane^{A}		1.528	1.525	1.534	1.540	1.532	1.538	1.529	1.535	1.542	0.003	-
Heptyl	8pp	**1.510**	1.530	1.530	1.541	1.533	**1.511**	-	1.331	1.343	0.011	-
Octyl^{E}	$8s_{\alpha}^{E}p$	**1.510**	1.530	1.530	1.541	1.532	**1.512**	**1.510**	1.347	1.327	0.011	0.013
Octyl^{A}	$8s_{\alpha}^{A}p$	**1.510**	1.530	1.530	1.541	1.534	**1.517**	**1.513**	1.351	1.329	0.009	0.012
Cyclononane		1.547	1.534	1.531	1.541	1.528	1.528	1.541	1.534	1.531	-	-
Octyl	9pp	**1.513**	1.531	1.531	1.537	1.528	1.531	**1.511**	1.342	1.341	0.017	-

Table S10.B.

Alkyl Radical / Cycloalkane	Migration Type	Bond Angles										
		A_1	A_2	A_3	A_4	A_5	A_6	A_α	A_β	A_γ	RMS	RMS*
Cyclopropane		-	-	-	-	-	-	60.0	60.0	60.0	-	-
Methylcyclopropane		120.0	-	-	-	-	-	59.9	59.9	60.2	-	-
Ethyl	3pp	-	-	-	-	-	-	54.5	70.9	54.5	-	-
Propyl	$3s_\alpha p$	**119.7**	-	-	-	-	-	54.5	70.8	54.7	-	0.3
Butyl	$3s_\alpha p$	**120.3**	*113.2*	-	-	-	-	54.6	70.8	54.7	-	0.3
Pentyl	$3s_\alpha p$	**120.3**	*113.7*	112.7	-	-	-	54.6	70.8	54.7	-	0.3
Hexyl	$3s_\alpha p$	**120.3**	*113.6*	113.2	112.8	-	-	54.5	70.8	54.7	-	0.3
Heptyl	$3s_\alpha p$	**120.3**	*113.6*	113.1	113.3	112.8	-	54.6	70.8	54.7	-	0.3
Octyl	$3s_\alpha p$	**120.3**	*113.6*	113.1	113.2	113.3	112.8	54.5	70.8	54.7	-	0.3
Cyclobutane		87.9	-	-	-	-	-	87.9	87.9	87.9	-	-
Methylcyclobutane		88.1	119.4	-	-	-	-	88.1	88.1	87.6	0.2	-
Propyl	4pp	*91.0*	-	-	-	-	-	82.6	103.9	82.6	3.1	-
Butyl	$4s_\alpha p$	*91.3*	**118.3**	-	-	-	-	82.1	104.3	82.3	3.4	2.4
Pentyl	$4s_\beta p$	*91.3*	**118.7**	*113.0*	-	-	-	82.2	104.2	82.3	3.4	2.3
Hexyl	$4s_\beta p$	*91.3*	**118.6**	*113.4*	112.7	-	-	82.2	104.2	82.3	3.4	2.3
Heptyl	$4s_\beta p$	*91.3*	**118.6**	*113.4*	113.2	112.7	-	82.2	104.2	82.3	3.4	2.3
Octyl	$4s_\beta p$	*91.3*	**118.6**	*113.4*	113.1	113.2	112.8	82.2	104.2	82.3	3.4	2.3
Cyclopentane		102.8	102.8	-	-	-	-	105.0	105.9	105.0	-	-
Methylcyclopentane^E		105.5	104.4	114.6	-	-	-	105.5	104.4	101.7	2.2	-
Methylcyclopentane^A		105.6	104.6	112.0	-	-	-	105.6	104.6	101.7	2.4	-
Butyl	5pp	*104.1*	*104.1*	-	-	-	-	93.1	132.0	93.1	1.3	-
Pentyl^E	$5s_\alpha^E p$	*104.1*	*104.4*	**118.7**	-	-	-	92.5	132.6	92.7	1.5	2.5
Hexyl^E	$5s_\beta^E p$	*104.2*	*104.4*	**119.3**	*112.8*	-	-	92.5	132.5	92.8	1.5	2.8
Heptyl^E	$5s_\gamma^E p$	*104.2*	*104.4*	**119.3**	*113.3*	112.7	-	92.5	132.5	92.8	1.5	2.8
Octyl^E	$5s_\gamma^E p$	*104.2*	*104.4*	**119.3**	*113.2*	113.2	112.8	92.5	132.5	92.8	1.5	2.8
Pentyl^A	$5s_\alpha^A p$	*104.3*	*104.7*	**116.2**	-	-	-	93.0	132.8	92.7	1.7	2.5
Hexyl^A	$5s_\beta^A p$	*104.4*	*104.8*	**116.8**	*112.8*	-	-	93.1	132.7	92.9	1.8	2.9
Heptyl^A	$5s_\gamma^A p$	*104.4*	*104.7*	**116.7**	*113.2*	112.8	-	93.1	132.7	92.9	1.8	2.8
Octyl^A	$5s_\gamma^A p$	*104.4*	*104.7*	**116.7**	*113.2*	113.3	112.8	93.1	132.7	92.9	1.8	2.8
Cyclohexane		111.1	111.1	111.1				111.1	111.1	111.1	-	-
Methylcyclohexane^E		110.9	111.1	112.0	111.5			111.1	112.0	110.1	0.5	-
Methylcyclohexane^A		111.1	110.9	112.6	112.1			110.9	112.6	109.9	0.9	-
Pentyl	6pp	111.0	110.6	111.0				101.0	152.3	101.0	0.3	-
Hexyl^E	$6s_\alpha^E p$	110.9	110.5	111.3	116.8			100.7	153.4	100.3	0.4	2.7
Heptyl^E	$6s_\beta^E p$	110.9	110.5	111.3	117.3	112.8		100.6	153.5	100.5	0.4	2.9
Octyl^E	$6s_\gamma^E p$	110.9	110.5	111.3	117.3	113.2	112.8	100.6	153.5	100.5	0.4	2.9
Hexyl^A	$6s_\alpha^A p$	110.8	110.5	111.8	115.8			100.4	153.2	100.4	0.6	1.9
Heptyl^A	$6s_\beta^A p$	110.8	110.6	111.8	116.3	112.6		100.2	153.0	100.7	0.5	2.1
Octyl^A	$6s_\gamma^A p$	110.8	110.6	111.8	116.3	113.1	112.8	100.2	153.0	100.7	0.5	2.1
Cycloheptane		113.1	116.0	116.0	113.1			115.6	115.9	115.6	-	-
Methylcycloheptane^E		112.9	115.9	116.1	113.6	111.1		115.7	116.8	113.9	0.3	-
Methylcycloheptane^A		116.5	113.6	115.7	117.4	113.2		117.7	117.7	112.4	3.0	-
Hexyl	7pp	113.7	116.0	116.0	113.7			104.6	164.9	104.6	0.4	-
Heptyl^E	$7s_\alpha^E p$	113.7	116.0	115.9	114.2	115.8		104.0	166.4	103.6	0.6	2.2
Octyl^E	$7s_\beta^E p$	113.7	116.0	115.9	114.1	116.3	112.8	103.9	166.1	103.8	0.6	2.4
Heptyl^A	$7s_\alpha^A p$	113.7	115.9	115.9	115.3	116.5		104.8	166.9	104.1	1.1	2.4
Octyl^A	$7s_\beta^A p$	113.7	116.0	115.9	115.4	116.9	112.5	104.8	166.4	104.3	1.2	2.5
Cyclooctane		117.0	117.0	115.0	115.5	118.8		117.0	115.0	115.5	-	-
Methylcyclooctane^E		116.9	116.9	115.0	116.0	119.6	108.6	117.1	115.3	113.6	0.4	-
Methylcyclooctane^A		117.5	116.4	115.4	114.3	120.5	113.0	119.7	118.9	115.2	1.0	-
Heptyl	8pp	113.3	114.9	115.7	113.0	113.8		104.5	165.9	110.6	3.2	-
Octyl^E	$8s_\alpha^E p$	113.3	114.9	115.7	112.9	114.2	115.8	103.8	166.9	109.4	3.0	4.2
Octyl^A	$8s_\alpha^A p$	113.3	114.6	115.4	112.6	114.4	115.1	105.4	168.8	109.2	3.1	3.3
Cyclononane		116.8	116.6	116.3	113.6	114.2	113.6	116.8	116.6	116.3	-	-
Octyl	9pp	116.5	114.4	114.3	113.9	113.8	113.5	112.7	170.9	110.9	1.2	-

Table S10.C.

Alkyl Radical / Cycloalkane	Migration Type	Dihedral Angle										
		D_1	D_2	D_3	D_4	D_5	D_α	D_β	D_γ	D_δ	RMS	RMS*
Cyclopropane		-	-	-	-	-	-	-	-	-	-	-
Methylcyclopropane		-	-	-	-	-	-	-	-	-	-	-
Ethyl	3pp	-	-	-	-	-	-	-	-	-	-	-
Propyl	$3s_{\alpha}p$	-	-	-	-	-	-	-	-	-	-	-
Butyl	$3s_{\alpha}p$	**-158.4**	-	-	-	-	-	-	-	-	-	-
Pentyl	$3s_{\alpha}p$	**-157.6**	*-178.2*	-	-	-	-	-	-	-	-	-
Hexyl	$3s_{\alpha}p$	**-157.7**	*-178.1*	-179.9	-	-	-	-	-	-	-	-
Heptyl	$3s_{\alpha}p$	**-157.6**	*-178.1*	-179.9	180.0	-	-	-	-	-	-	-
Octyl	$3s_{\alpha}p$	**-157.6**	*-178.1*	-179.9	180.0	180.0	-	-	-	-	-	-
Cyclobutane		-	-	-	-	-	21.6	-21.6	21.6	-21.6	-	-
Methylcyclobutane		-144.4	-	-	-	-	21.6	-21.6	21.6	-21.6	-	-
Propyl	4pp	-	-	-	-	-	0.0	0.0	0.0	0.0	-	-
Butyl	$4s_{\alpha}p$	**-111.4**	-	-	-	-	-0.2	0.2	-0.2	0.2	-	33.0
Pentyl	$4s_{\beta}p$	**-110.4**	**166.8**	-	-	-	-0.5	0.6	-0.6	0.5	-	34.0
Hexyl	$4s_{\beta}p$	**-110.3**	**166.5**	*179.2*	-	-	-0.6	0.7	-0.7	0.7	-	34.1
Heptyl	$4s_{\beta}p$	**-110.2**	**166.5**	*179.1*	179.8	-	-0.7	0.7	-0.7	0.7	-	34.2
Octyl	$4s_{\beta}p$	**-110.2**	**166.5**	*179.1*	179.8	-180.0	-0.7	0.7	-0.8	0.7	-	34.2
Cyclopentane		43.5	-	-	-	-	-35.1	13.4	13.3	-35.0	-	-
Methylcyclopentane^{E}		25.6	-165.5	-	-	-	0.0	-25.6	41.3	-41.3	17.9	-
Methylcyclopentane^{A}		25.3	79.1	-	-	-	0.0	-25.3	40.7	-40.7	18.2	-
Butyl	5pp	*38.4*	-	-	-	-	-28.1	11.5	11.5	-28.1	5.1	-
Pentyl^{E}	$5s_{\alpha}^{E}p$	*38.6*	**-146.6**	-	-	-	-28.2	11.8	11.1	-28.1	4.9	16.2
Hexyl^{E}	$5s_{\beta}^{E}p$	*38.4*	**-145.4**	**172.7**	-	-	-28.4	12.5	10.3	-27.6	5.1	16.9
Heptyl^{E}	$5s_{\gamma}^{E}p$	*38.4*	**-145.4**	**172.4**	*179.7*		-28.4	12.5	10.4	-27.6	5.1	16.9
Octyl^{E}	$5s_{\gamma}^{E}p$	*38.4*	**-145.4**	**172.3**	*179.7*	179.9	-28.4	12.5	10.3	-27.6	5.1	16.9
Pentyl^{A}	$5s_{\alpha}^{A}p$	*36.8*	**82.9**	**-**	-	-	-26.2	9.4	12.5	-27.6	6.7	8.6
Hexyl^{A}	$5s_{\beta}^{A}p$	*36.4*	**82.8**	**-169.8**	-	-	-25.9	9.4	12.3	-27.2	7.1	8.3
Heptyl^{A}	$5s_{\gamma}^{A}p$	*36.4*	**82.7**	**-169.4**	*-178.8*	-	-25.9	9.3	12.4	-27.3	7.1	8.3
Octyl^{A}	$5s_{\gamma}^{A}p$	*36.4*	**82.6**	**-169.3**	*-178.8*	-179.8	-25.9	9.3	12.4	-27.3	7.1	8.2
Cyclohexane		-55.7	55.7				55.7	-55.7	55.7	-55.7	-	-
Methylcyclohexane^{E}		-55.5	55.9	-179.4			55.5	-55.9	55.2	-55.2	0.2	-
Methylcyclohexane^{A}		-55.7	55.5	71.4			55.7	-55.5	54.0	-54.0	0.1	-
Pentyl	6pp	-59.7	59.7				35.5	-26.2	26.2	-35.5	4.0	-
Hexyl^{E}	$6s_{\alpha}^{E}p$	-59.5	60.2	-154.6			34.6	-24.3	24.6	-34.5	4.2	14.7
Heptyl^{E}	$6s_{\beta}^{E}p$	-59.9	59.8	-153.1	176.7		34.8	-23.2	22.9	-34.6	4.2	15.6
Octyl^{E}	$6s_{\gamma}^{E}p$	-59.9	59.8	-153.1	176.5	179.7	34.8	-23.2	23.0	-34.6	4.2	15.6
Hexyl^{A}	$6s_{\alpha}^{A}p$	-59.9	58.5	79.9			36.7	-28.2	26.6	-34.1	3.6	5.7
Heptyl^{A}	$6s_{\beta}^{A}p$	-60.3	57.9	80.2	-173.9		37.4	-28.4	26.1	-33.4	3.6	5.9
Octyl^{A}	$6s_{\gamma}^{A}p$	-60.2	58.0	80.0	-173.7	-179.1	37.4	-28.7	26.5	-33.5	3.6	5.8
Cycloheptane		-70.4	52.6	-70.4			87.2	-39.2	-39.2	87.2	-	-
Methylcycloheptane^{E}		-69.9	52.1	-71.2	-148.8		86.9	-38.9	-39.2	87.3	0.6	-
Methylcycloheptane^{A}		-80.0	76.5	-57.3	-63.8		25.6	49.0	-83.5	65.4	16.7	-
Hexyl	7pp	-71.3	70.4	-71.3			55.9	-25.2	-25.2	55.9	10.3	-
Heptyl^{E}	$7s_{\alpha}^{E}p$	-70.9	70.4	-71.9	172.7		55.9	-30.7	-19.4	55.1	10.3	21.3
Octyl^{E}	$7s_{\beta}^{E}p$	-70.9	70.4	-71.9	172.3	-178.1	56.1	-32.5	-17.6	55.0	10.3	21.5
Heptyl^{A}	$7s_{\alpha}^{A}p$	-72.3	71.7	-69.4	-64.7		53.6	-18.1	-28.7	52.6	11.1	7.6
Octyl^{A}	$7s_{\beta}^{A}p$	-72.2	71.4	-69.4	-64.5	-178.3	54.1	-20.6	-26.4	52.7	10.9	7.6
Cyclooctane		-65.0	-44.3	100.7	-65.1		65.0	44.3	-100.7	65.1	-	-
Methylcyclooctane^{E}		-64.8	-43.7	100.5	-65.6	-173.1	64.5	46.3	-100.9	64.3	0.4	-
Methylcyclooctane^{A}		-65.1	-39.6	105.4	-69.5	-74.8	58.0	51.1	-92.8	57.5	4.0	-
Heptyl	8pp	-47.6	-57.9	114.3	-71.8		76.2	46.7	-107.0	44.6	13.4	-
Octyl^{E}	$8s_{\alpha}^{E}p$	-47.5	-57.8	114.1	-72.2	164.8	76.4	54.4	-112.4	44.4	13.4	15.6
Octyl^{A}	$8s_{\alpha}^{A}p$	-47.0	-57.0	117.3	-72.1	-78.4	74.2	64.3	-116.0	39.0	14.2	12.6
Cyclononane		-82.8	70.4	-117.8	65.5	65.5	120.1	-82.8	70.4	-117.8		-
Octyl	9pp	-67.3	81.6	-140.7	62.4	53.5	70.0	154.3	-172.6	-67.9	14.4	-

Table S11.

Radical site on carbon 1

Ethyl

C	0.797896	0.000000	-0.033210
C	-0.698024	0.000001	0.001495
H	-1.110731	-0.887366	-0.492986
H	1.353164	0.926868	0.070834
H	1.353158	-0.926872	0.070832
H	-1.084093	-0.000083	1.034451
H	-1.110728	0.887445	-0.492847

Butyl

C	-1.885886	-0.130798	0.019938
H	-2.008736	-0.656766	0.975791
H	-2.025965	-0.864586	-0.784566
H	-2.689700	0.611769	-0.060317
C	-0.505486	0.524681	-0.071327
H	-0.411092	1.069275	-1.021471
H	-0.396453	1.273485	0.727385
C	0.637209	-0.494256	0.038392
H	0.538294	-1.244639	-0.760942
H	0.516563	-1.055858	0.984469
C	1.994479	0.134730	-0.019358
H	2.167009	1.102856	0.444470
H	2.868179	-0.441678	-0.310693

Hexyl

C	-0.593537	-0.366574	0.020336
H	-0.629489	-0.960831	0.947516
H	-0.639319	-1.089727	-0.809692
C	0.732586	0.396234	-0.043266
H	0.773961	0.989135	-0.969343
H	0.780386	1.116993	0.788227
C	1.957828	-0.526703	0.019626
H	1.919789	-1.246204	-0.812497
H	1.890612	-1.137917	0.939763
C	3.256285	0.217992	-0.011490
H	3.348423	1.174716	0.496781
H	4.174278	-0.268146	-0.330240
C	-1.818930	0.550274	-0.040525
H	-1.772727	1.272069	0.788885

Propyl

C	1.223649	-0.247188	-0.041544
H	1.286574	-0.766764	-1.005181
H	1.273738	-1.004069	0.751724
C	-0.076911	0.560128	0.058600
H	-0.099061	1.331451	-0.724910
H	-0.081502	1.113740	1.015448
C	-1.300186	-0.297331	-0.043048
H	-1.302221	-1.297247	0.384044
H	-2.260366	0.128480	-0.321003
H	2.103527	0.400750	0.055831

Pentyl

C	1.204096	0.524165	0.042317
H	1.186671	1.105089	0.976912
H	1.198489	1.258900	-0.776999
C	-0.060523	-0.334842	-0.041768
H	-0.049612	-0.916689	-0.975802
H	-0.058552	-1.068697	0.779712
C	-1.352652	0.491238	0.023419
H	-1.363765	1.222875	-0.798894
H	-1.338647	1.093233	0.951976
C	-2.590506	-0.349373	-0.027759
H	-2.612631	-1.317930	0.465748
H	-3.540904	0.070525	-0.345627
C	2.487490	-0.308836	-0.022575
H	3.382168	0.323714	0.038654
H	2.529070	-1.030040	0.804082
H	2.540277	-0.875090	-0.961558

Heptyl

C	-0.000041	-0.000012	0.000040
H	-0.000080	-0.000004	1.097888
H	1.046135	-0.000032	-0.332828
H	-0.458936	-0.938771	-0.335521
C	-0.747994	1.219351	-0.546893
H	-0.760751	1.182861	-1.646718
H	-1.799915	1.182835	-0.225616
C	-0.128259	2.544691	-0.093592

H	-1.781933	1.143149	-0.966835
C	-3.139035	-0.223459	0.023256
H	-4.004047	0.450440	-0.021616
H	-3.220219	-0.929940	-0.813138
H	-3.210895	-0.800315	0.954572

Octyl

C	-3.108736	0.538588	-0.026561
H	-3.088184	1.149754	-0.941515
H	-3.082487	1.245664	0.816326
C	-1.858352	-0.344947	0.017569
H	-1.878070	-0.957391	0.933263
H	-1.883824	-1.053369	-0.825902
C	-0.552537	0.454374	-0.030397
H	-0.527487	1.162622	0.813081
H	-0.533140	1.066396	-0.946162
C	0.696972	-0.430814	0.013965
H	0.671677	-1.139039	-0.829559
H	0.677981	-1.042891	0.929859
C	2.001663	0.369530	-0.034683
H	2.029482	1.075663	0.810154
H	2.026599	0.980551	-0.949493
C	3.251880	-0.520321	0.011594
H	3.233708	-1.224924	-0.833851
H	3.201529	-1.150275	0.920114
C	4.529319	0.260331	-0.004888
H	4.595127	1.209305	0.521692
H	5.460305	-0.194033	-0.332734
C	-4.407067	-0.272233	0.021896
H	-4.462916	-0.868353	0.942126
H	-5.290483	0.378142	-0.010705
H	-4.468671	-0.964871	-0.827664

H	0.925063	2.582119	-0.414569
H	-0.115023	2.582182	1.007409
C	-0.867411	3.772514	-0.634239
H	-1.920562	3.734337	-0.312987
H	-0.880372	3.734920	-1.735288
C	-0.246025	5.096041	-0.178956
H	0.806023	5.136757	-0.502488
H	-0.233444	5.139608	0.920489
C	-0.988173	6.324589	-0.723828
H	-2.039435	6.293582	-0.399083
H	-1.019621	6.255204	-1.827902
C	-0.365190	7.620215	-0.305760
H	0.716090	7.706079	-0.230752
H	-0.940921	8.541660	-0.294357

Radical site on carbon 2

Propyl

C	1.296702	-0.201220	0.006581
H	1.292689	-1.074703	-0.660386
H	1.488007	-0.583519	1.025127
H	2.148687	0.432784	-0.266933
C	0.000000	0.543230	-0.072897
H	0.000000	1.606127	0.162790

Butyl

C	-1.983967	-0.046986	-0.070416
H	-2.070407	-0.827391	-0.839243
H	-2.685888	0.757654	-0.321003
H	-2.329776	-0.497663	0.876916
C	-0.576819	0.454664	0.033589
H	-0.413839	1.466175	0.406869

C	-1.296702	-0.201220	0.006581
H	-1.488007	-0.583518	1.025127
H	-2.148687	0.432784	-0.266933
H	-1.292689	-1.074704	-0.660386

Pentyl

C	-2.610898	-0.230205	-0.073186
H	-2.583800	-1.009763	-0.847258
H	-3.420209	0.467691	-0.320195
H	-2.890138	-0.732140	0.870345
C	-1.289984	0.466609	0.037446
H	-1.274359	1.490191	0.412981
C	-0.017050	-0.320680	0.106519
H	-0.041851	-1.126277	-0.646220
H	0.057659	-0.839760	1.082967
C	1.242478	0.530643	-0.096500
H	1.261411	1.331123	0.658068
H	1.185021	1.028586	-1.074914
C	2.529542	-0.293364	-0.005874
H	3.419021	0.332069	-0.153618
H	2.618195	-0.776751	0.975901
H	2.544524	-1.082992	-0.768493

Heptyl

C	-0.000037	0.000009	0.000012
H	-0.000101	0.000035	1.098942
H	1.058601	-0.000008	-0.315390
H	-0.439241	0.945445	-0.341101
C	-0.741131	-1.184164	-0.539626
H	-1.190943	-1.106321	-1.529871
C	-0.480126	-2.556934	0.001453
H	0.521535	-2.907836	-0.317563
H	-0.433251	-2.514688	1.102370
C	-1.526604	-3.593143	-0.427950
H	-1.568331	-3.631511	-1.527913
H	-2.521036	-3.262342	-0.092048
C	-1.240329	-4.994786	0.118055
H	-1.196607	-4.956366	1.218342
H	-0.242820	-5.321163	-0.217438
C	-2.282332	-6.032477	-0.310029
H	-2.325123	-6.070710	-1.409032
H	-3.278073	-5.705460	0.025440
C	-1.986061	-7.429746	0.242499

C	0.570260	-0.507102	0.102896
H	0.432046	-1.294010	-0.655542
H	0.560750	-1.036929	1.074857
C	1.934000	0.166783	-0.088335
H	2.102282	0.931574	0.680695
H	1.991636	0.657404	-1.067478
H	2.752355	-0.560969	-0.022471

Hexyl

C	3.270744	-0.098222	0.120018
H	3.282243	-0.833535	0.936618
H	4.020244	0.670924	0.343082
H	3.609047	-0.629355	-0.787525
C	1.905217	0.490634	-0.056752
H	1.823371	1.487865	-0.490090
C	0.695885	-0.392744	-0.107212
H	0.762073	-1.151319	0.690423
H	0.684414	-0.968669	-1.054021
C	-0.626988	0.372785	0.021548
H	-0.688349	1.128256	-0.777725
H	-0.632579	0.927597	0.972085
C	-1.856272	-0.537429	-0.047179
H	-1.792898	-1.293085	0.750401
H	-1.844571	-1.091732	-0.997893
C	-3.171180	0.236995	0.081289
H	-3.270186	0.977705	-0.722964
H	-4.039791	-0.431825	0.030260
H	-3.217452	0.775063	1.037069

Octyl

C	4.554531	-0.129724	0.149377
H	4.539308	-0.842846	0.985362
H	4.888992	-0.693216	-0.739898
H	5.320513	0.626567	0.360120
C	3.205896	0.487408	-0.058081
H	3.153307	1.474223	-0.518965
C	1.975586	-0.367062	-0.098165
H	1.958840	-0.966952	-1.029880
H	2.015177	-1.106017	0.719385
C	0.670818	0.434021	-0.002719
H	0.636421	1.169481	-0.821873
H	0.670420	1.013121	0.933104
C	-0.579229	-0.448757	-0.060671

H	-1.967924	-7.421559	1.340178
H	-2.743123	-8.158060	-0.075117
H	-1.008288	-7.789238	-0.103962

H	-0.543663	-1.185574	0.757645
H	-0.573125	-1.029138	-0.997159
C	-1.883301	0.349244	0.032744
H	-1.919719	1.086118	-0.785576
H	-1.889484	0.929984	0.968980
C	-3.135169	-0.531446	-0.024115
H	-3.098034	-1.266866	0.793743
H	-3.128097	-1.111086	-0.959583
C	-4.431791	0.278081	0.070066
H	-5.316308	-0.370243	0.027650
H	-4.474130	0.842501	1.010772
H	-4.504462	0.999347	-0.754435

Radical site on carbon 3

Pentyl

C	-2.505206	-0.414714	0.098472
H	-2.401890	-1.069757	0.971964
H	-2.585070	-1.052039	-0.791500
H	-3.445485	0.141813	0.198261
C	-1.304901	0.532599	-0.015995
H	-1.462914	1.214898	-0.873279
H	-1.259198	1.186852	0.868943
C	0.000000	-0.188404	-0.168751
H	0.000000	-1.127731	-0.725987
C	1.304901	0.532599	-0.015995
H	1.259198	1.186852	0.868943
H	1.462914	1.214898	-0.873279
C	2.505206	-0.414714	0.098472
H	2.585070	-1.052039	-0.791500
H	3.445485	0.141813	0.198261
H	2.401890	-1.069757	0.971964

Heptyl

C	-0.000661	-0.005878	0.014607
H	-0.007927	-0.020276	1.112292
H	1.047612	-0.010793	-0.311544
H	-0.449140	0.941152	-0.311613
C	-0.755722	-1.211220	-0.553092
H	-0.760921	-1.160486	-1.652476
C	-0.150299	-2.546752	-0.112364
H	0.903766	-2.590840	-0.429114

Hexyl

C	-0.000008	-0.000007	0.000016
H	-0.000006	0.000005	1.097568
H	1.044587	-0.000018	-0.335655
H	-0.466391	-0.934188	-0.335482
C	-0.761568	1.214351	-0.544622
H	-0.237737	2.138881	-0.234284
H	-0.723352	1.216801	-1.645440
C	-2.191125	1.260428	-0.097063
H	-2.424818	0.877989	0.898900
C	-3.172676	2.197193	-0.732983
H	-3.040582	2.182110	-1.827597
H	-2.956554	3.241021	-0.429502
C	-4.633392	1.877998	-0.389750
H	-4.758268	1.895195	0.703223
H	-4.861376	0.851805	-0.711427
C	-5.616394	2.857519	-1.036301
H	-5.527754	2.837698	-2.130410
H	-6.655036	2.613363	-0.779753
H	-5.421405	3.885882	-0.704868

Octyl

C	-3.117750	0.582999	0.042310
H	-3.027416	1.249794	0.913052
H	-3.111033	1.233467	-0.845345
C	-1.903472	-0.349207	-0.006741
H	-1.992770	-1.017339	-0.878361

H	-0.145157	-2.603687	0.986766
C	-0.898620	-3.761487	-0.676330
H	-0.921873	-3.683732	-1.781586
H	-1.954703	-3.722111	-0.361996
C	-0.302513	-5.073026	-0.263648
H	0.783129	-5.127474	-0.157835
C	-1.050854	-6.357865	-0.451502
H	-1.112138	-6.606347	-1.528531
H	-2.094712	-6.223277	-0.126646
C	-0.419731	-7.536357	0.299576
H	-0.393395	-7.340855	1.378397
H	-0.982912	-8.463351	0.134108
H	0.611401	-7.705417	-0.036292
H	-1.809376	-1.169257	-0.238100

C	-0.570582	0.401315	-0.076325
H	-0.563683	1.051335	-0.965445
H	-0.476269	1.067493	0.794557
C	0.643454	-0.535633	-0.126858
H	0.529013	-1.220247	-0.990760
H	0.641800	-1.188905	0.761303
C	1.952315	0.189179	-0.212329
H	1.982643	1.118363	-0.785473
C	3.248940	-0.520052	0.036442
H	3.463836	-1.218923	-0.794750
H	3.151485	-1.156203	0.930356
C	4.434815	0.437244	0.205502
H	4.273826	1.109399	1.057002
H	5.369940	-0.111039	0.375197
H	4.566665	1.056621	-0.690938
H	-1.909787	-1.001130	0.881499
C	-4.444581	-0.178604	0.112427
H	-5.301533	0.506166	0.146725
H	-4.569827	-0.829468	-0.762779
H	-4.485721	-0.812840	1.007598

Radical site on carbon 4

Heptyl			
C	0.005192	-0.003281	-0.015693
H	0.001014	0.002671	1.082192
H	1.052474	-0.019596	-0.344734
H	-0.439052	0.939877	-0.358225
C	-0.758311	-1.213605	-0.559741
H	-1.809834	-1.162481	-0.240086
H	-0.767023	-1.187622	-1.658739
C	-0.156905	-2.546321	-0.095398
H	0.897666	-2.603971	-0.412285
H	-0.127251	-2.555579	1.012507
C	-0.898585	-3.745509	-0.602691
H	-1.982647	-3.665613	-0.708632
C	-0.305163	-5.118916	-0.518476
H	-0.295047	-5.467184	0.533677
H	0.754888	-5.081476	-0.819725
C	-1.043231	-6.157575	-1.372805
H	-1.034575	-5.830233	-2.422244
H	-2.099575	-6.190100	-1.066908

Octyl			
C	4.479158	0.080351	0.229513
H	4.715354	0.721652	-0.629753
H	4.486243	0.711282	1.127954
H	5.286427	-0.656049	0.330767
C	3.119145	-0.598921	0.048500
H	3.143604	-1.245569	-0.841291
H	2.912666	-1.257315	0.904314
C	1.971974	0.409428	-0.095377
H	1.941926	1.061307	0.793443
H	2.198518	1.086206	-0.943358
C	0.632519	-0.233469	-0.290509
H	0.592650	-1.161290	-0.865237
C	-0.635021	0.552998	-0.146535
H	-0.752382	1.248024	-1.001725
H	-0.567583	1.199846	0.743790
C	-1.889711	-0.324454	-0.048899
H	-1.791900	-1.000292	0.814256
H	-1.952279	-0.968516	-0.940300

C	-0.430048	-7.555636	-1.257722
H	-0.455063	-7.911234	-0.219296
H	-0.970632	-8.284163	-1.875172
H	0.618360	-7.552399	-1.583547

C	-3.181333	0.487607	0.080349
H	-3.272959	1.163321	-0.783508
H	-3.116747	1.132362	0.969888
C	-4.427151	-0.397842	0.176117
H	-5.341848	0.201504	0.268478
H	-4.528537	-1.029757	-0.715887
H	-4.370630	-1.060905	1.049225

Table S12

1,2 H-migrations

Ethyl

C	-0.746188	0.000000	-0.024417
C	0.746188	0.000000	-0.024417
H	0.000000	0.000000	1.022307
H	-1.274729	0.934440	-0.182325
H	-1.274729	-0.934440	-0.182325
H	1.274729	-0.934440	-0.182325
H	1.274729	0.934440	-0.182325

Butyl

C	0.611770	-0.433220	-0.119339
C	1.994174	0.091410	0.093321
H	1.281865	-0.519340	0.977124
C	-0.557980	0.510455	-0.175061
H	0.532629	-1.400344	-0.616272
H	2.848875	-0.484346	-0.248976
H	2.123649	1.148186	0.308535
C	-1.895450	-0.170993	0.132168
H	-0.390250	1.334084	0.535995
H	-0.601474	0.984056	-1.172100
H	-1.893377	-0.591591	1.145176
H	-2.731516	0.535633	0.054853
H	-2.085486	-0.992251	-0.570866

Hexyl

C	1.931244	-0.456961	-0.146711
C	3.266178	0.129235	0.180180
H	2.554246	-0.597049	0.971846
C	0.706719	0.415334	-0.181940
H	1.937615	-1.380236	-0.726379

Propyl

C	-0.042458	0.524753	0.030129
C	-1.312604	-0.258365	-0.036808
H	-0.825485	0.290334	1.023469
C	1.277581	-0.192311	-0.026264
H	-0.100581	1.564197	-0.288556
H	-2.222479	0.217485	-0.389806
H	-1.258680	-1.343095	-0.018447
H	2.099333	0.433467	0.341829
H	1.252651	-1.104747	0.585068
H	1.520123	-0.502098	-1.055900

Pentyl

C	1.317937	0.437655	0.117543
C	2.611353	-0.278530	-0.098370
H	1.985835	0.418720	-0.983525
C	0.026781	-0.330052	0.186721
H	1.379858	1.410220	0.606192
H	3.540728	0.174499	0.233744
H	2.589229	-1.345126	-0.302634
C	-1.208432	0.518201	-0.136174
H	0.073805	-1.183541	-0.509129
H	-0.087059	-0.774896	1.192862
C	-2.512863	-0.274384	-0.015527
H	-1.238254	1.384696	0.541352
H	-1.107145	0.924526	-1.152805
H	-2.643732	-0.663356	1.002698
H	-3.385233	0.347997	-0.251650
H	-2.516687	-1.131077	-0.702262

H	4.170571	-0.362920	-0.165037
H	3.317701	1.169770	0.487582
C	-0.601479	-0.359398	0.013308
H	0.790981	1.190503	0.596985
H	0.669564	0.963189	-1.141858
C	-1.844186	0.531556	-0.068434
H	-0.671915	-1.152104	-0.748449
H	-0.575520	-0.870404	0.987956
C	-3.145154	-0.251951	0.128725
H	-1.772052	1.325200	0.690732
H	-1.862827	1.040063	-1.044189
H	-3.161535	-0.744282	1.109813
H	-4.023727	0.402809	0.067029
H	-3.253028	-1.031435	-0.636799

Octyl

C	3.226381	-0.452642	-0.143796
C	4.542753	0.145556	0.232884
H	3.831102	-0.626670	0.979987
C	1.985060	0.395993	-0.166817
H	3.262386	-1.350905	-0.760508
H	5.463295	-0.314013	-0.114578
H	4.567230	1.173312	0.583581
C	0.689622	-0.411932	-0.027413
H	2.039350	1.140397	0.644109
H	1.953768	0.981527	-1.104423
C	-0.568725	0.458336	-0.097218
H	0.649820	-1.174293	-0.821513
H	0.708990	-0.960961	0.926362
C	-1.864414	-0.346706	0.041669
H	-0.528216	1.222742	0.695303
H	-0.581022	1.006824	-1.052559
H	-1.852578	-0.895502	0.996942
H	-1.905638	-1.111123	-0.750735
C	-3.124636	0.521126	-0.027202
H	-3.082639	1.284133	0.764735
H	-3.135522	1.068741	-0.981712
C	-4.412647	-0.295529	0.112557
H	-4.436998	-0.828111	1.072272
H	-5.303349	0.343566	0.060781
H	-4.490337	-1.044871	-0.686028

Heptyl

C	2.601229	0.405668	0.138739
C	3.895049	-0.269285	-0.183055
H	3.228541	0.490600	-0.983799
C	1.323560	-0.385927	0.188994
H	2.668470	1.334516	0.705597
H	4.830219	0.168488	0.153444
H	3.878821	-1.315119	-0.476175
C	0.066960	0.467857	-0.016797
H	1.356304	-1.176880	-0.577887
H	1.253550	-0.915427	1.157382
C	-1.229163	-0.341815	0.081258
H	0.049745	1.275266	0.732403
H	0.123785	0.960319	-0.999588
C	-2.486967	0.507769	-0.123857
H	-1.211846	-1.151473	-0.666089
H	-1.279506	-0.834132	1.065674
H	-2.435874	0.998953	-1.107337
H	-2.503730	1.315823	0.623101
C	-3.776507	-0.312358	-0.024180
H	-4.665476	0.313700	-0.173656
H	-3.794882	-1.107550	-0.780958
H	-3.863096	-0.788542	0.961273

1,3 H-migrations

Propyl

C	-1.091947	-0.338367	0.000000
C	0.000000	0.737699	0.000001
C	1.091947	-0.338367	0.000000
H	0.000000	-1.186577	-0.000004
H	-1.660027	-0.482580	0.921088
H	-1.660031	-0.482573	-0.921088
H	0.000000	1.375547	-0.889629
H	0.000000	1.375546	0.889631
H	1.660031	-0.482573	-0.921088
H	1.660027	-0.482580	0.921088

Pentyl

C	-0.118152	-0.193967	0.499839
C	-1.491087	-0.676913	0.007667
C	-1.972964	0.767882	-0.161493
H	-0.695013	1.045629	0.304152
H	0.054195	-0.299605	1.577500
C	1.088591	-0.409228	-0.384969
H	-1.441982	-1.244421	-0.929272
H	-2.057901	-1.259973	0.741653
H	-2.084879	1.148226	-1.179033
H	-2.708159	1.143417	0.553069
C	2.310631	0.393299	0.070583
H	1.337329	-1.484478	-0.410909
H	0.827307	-0.136341	-1.419391
H	2.596989	0.122109	1.094957
H	3.175583	0.210212	-0.579526
H	2.094416	1.468786	0.057034

Heptyl

C	-1.411573	-0.171551	0.575492
C	-2.781124	-0.551490	-0.008724
C	-3.087027	0.915968	-0.326587
H	-1.832519	1.099975	0.238957
H	-1.345765	-0.207689	1.669322
C	-0.163461	-0.577124	-0.174886
H	-2.712866	-1.196236	-0.892983
H	-3.469202	-1.011601	0.708862
H	-3.066129	1.221604	-1.374799
H	-3.837917	1.420796	0.284549

Butyl

C	-0.452007	0.117760	0.545352
C	0.719544	0.725661	-0.241546
C	1.552549	-0.544929	-0.042524
H	0.413805	-0.951858	0.639202
H	-0.577038	0.509534	1.560206
C	-1.721725	-0.219255	-0.202335
H	0.474935	0.939015	-1.288902
H	1.151906	1.626161	0.208018
H	1.712099	-1.187640	-0.910785
H	2.392369	-0.496000	0.653416
H	-1.495109	-0.782471	-1.117952
H	-2.402969	-0.824906	0.407615
H	-2.260158	0.692738	-0.504504

Hexyl

C	-0.797119	-0.261248	0.543254
C	-2.110050	-0.648289	-0.155084
C	-2.543276	0.819992	-0.221968
H	-1.326060	1.008389	0.418647
H	-0.756136	-0.486893	1.615407
C	0.501923	-0.415509	-0.214143
H	-1.959749	-1.115735	-1.135468
H	-2.770195	-1.287702	0.441080
H	-2.524389	1.309146	-1.198162
H	-3.353103	1.139769	0.436882
C	1.681130	0.299762	0.452376
H	0.740125	-1.489023	-0.325680
H	0.370645	-0.029775	-1.238621
C	2.991913	0.115293	-0.317410
H	1.445385	1.370304	0.540462
H	1.798517	-0.076700	1.479632
H	2.905532	0.508064	-1.339006
H	3.823355	0.637250	0.172999
H	3.258941	-0.947105	-0.390317

Octyl

C	-2.066170	-0.166488	0.563094
C	-3.399451	-0.560318	-0.091597
C	-3.695583	0.902151	-0.440213
H	-2.475105	1.099197	0.191550

C	1.099545	0.131537	0.324244
H	-0.025482	-1.670998	-0.098673
H	-0.303433	-0.366500	-1.247940
C	2.364757	-0.297519	-0.424423
H	0.963958	1.219731	0.225788
H	1.227937	-0.067243	1.400172
H	2.233723	-0.101621	-1.499452
H	2.495187	-1.385604	-0.323397
C	3.619892	0.420474	0.080026
H	3.787231	0.215431	1.145488
H	4.515324	0.100595	-0.467972
H	3.523901	1.507591	-0.038772

H	-2.060260	-0.191920	1.659194
C	-0.776545	-0.571395	-0.113847
H	-3.279120	-1.213053	-0.964371
H	-4.123331	-1.017746	0.591665
H	-3.618787	1.197896	-1.488659
H	-4.481770	1.408166	0.123735
C	0.453225	0.150152	0.446609
H	-0.636553	-1.663566	-0.019306
H	-0.858711	-0.372012	-1.194986
C	1.759251	-0.279250	-0.228317
H	0.316375	1.236270	0.329731
H	0.523053	-0.037600	1.529791
H	1.688080	-0.094694	-1.312275
H	1.892087	-1.366629	-0.110128
C	2.990026	0.443588	0.327279
H	3.060411	0.258793	1.409856
H	2.856367	1.529404	0.208556
C	4.289633	0.006938	-0.355183
H	5.158840	0.535580	0.056479
H	4.458716	-1.069891	-0.224213
H	4.253402	0.209537	-1.433574

1,4 H-migrations

Butyl			
C	-1.232866	0.679666	-0.135602
C	-0.740243	-0.717249	0.225359
C	0.740243	-0.717249	-0.225359
C	1.232866	0.679666	0.135602
H	0.000000	1.230448	0.000000
H	1.473734	0.828453	1.193136
H	1.952057	1.162770	-0.530062
H	1.325847	-1.524397	0.235906
H	0.790123	-0.856552	-1.314462
H	-0.790123	-0.856552	1.314462
H	-1.325847	-1.524397	-0.235906
H	-1.473735	0.828453	-1.193136
H	-1.952057	1.162770	0.530062

Pentyl	Axial		
C	0.841164	0.040652	0.637610
C	-0.149651	1.110225	0.179995

Pentyl	Equatorial		
C	0.792399	0.025155	0.463553
C	-0.128036	-1.000708	-0.191082

C	-1.252619	0.323467	-0.573193	C	-1.550927	-0.449218	0.062102
C	-1.397598	-0.967396	0.224198	C	-1.398084	1.056087	-0.119010
H	-0.109673	-0.910387	0.688628	H	-0.084631	1.031193	0.269358
H	-2.003590	-0.889179	1.132405	H	-1.362230	1.398262	-1.158452
H	-1.578713	-1.896206	-0.321995	H	-1.986924	1.717352	0.520997
H	-2.188288	0.893537	-0.657546	H	-2.303791	-0.899770	-0.599698
H	-0.920252	0.097510	-1.595352	H	-1.850531	-0.669851	1.096347
H	-0.591477	1.606024	1.056187	H	0.067574	-1.023040	-1.274222
H	0.314435	1.891650	-0.440185	H	0.011931	-2.023394	0.187886
C	1.862733	-0.407858	-0.388908	H	0.812715	-0.060916	1.558224
H	2.572401	0.401979	-0.619322	C	2.147911	0.283487	-0.155084
H	2.443407	-1.267437	-0.031075	H	2.050750	0.531871	-1.220339
H	1.381120	-0.698395	-1.332023	H	2.667836	1.112887	0.341315
H	1.256456	0.176368	1.642067	H	2.797723	-0.603407	-0.084293

Hexyl	Axial			Hexyl	Equatorial		
C	-0.262878	-0.446101	0.614014	C	0.262394	-0.286459	0.377227
C	1.052293	-1.104275	0.199947	C	-0.957410	-1.072277	-0.094750
C	1.827025	0.009310	-0.551104	C	-2.146714	-0.116169	0.161637
C	1.480491	1.284256	0.209145	C	-1.601599	1.257638	-0.209083
H	0.285661	0.783094	0.653567	H	-0.318880	0.903750	0.115584
H	2.049009	1.448087	1.130131	H	-1.556835	1.466018	-1.283105
H	1.335045	2.204096	-0.362542	H	-1.933198	2.120671	0.373072
H	2.906294	-0.192490	-0.597676	H	-3.047452	-0.400548	-0.400266
H	1.468166	0.081460	-1.586604	H	-2.407594	-0.135339	1.229201
H	1.617404	-1.401052	1.095150	H	-0.869048	-1.264438	-1.175053
H	0.908934	-2.007730	-0.411483	H	-1.073961	-2.045947	0.402493
C	-1.359015	-0.394297	-0.431864	H	0.362766	-0.267561	1.472062
H	-0.944471	-0.030410	-1.384343	C	1.579565	-0.459369	-0.345565
H	-1.721211	-1.417707	-0.631254	C	2.649732	0.527630	0.132233
C	-2.533453	0.494525	-0.010835	H	1.945642	-1.492404	-0.210226
H	-2.201040	1.528569	0.146172	H	1.415977	-0.337971	-1.427336
H	-3.324251	0.503824	-0.771784	H	2.844756	0.403698	1.205328
H	-2.975295	0.138752	0.929015	H	3.597872	0.381301	-0.400687
H	-0.631020	-0.698987	1.615834	H	2.324144	1.562809	-0.031257

Heptyl	Axial			Heptyl	Equatorial		
C	0.416444	-0.587846	0.667219	C	-0.368760	-0.334048	0.440043
C	1.701005	-1.070029	-0.005214	C	-1.578484	-1.051807	-0.151694
C	2.276051	0.192016	-0.698507	C	-2.746862	-0.058626	0.054972
C	1.954914	1.327675	0.266224	C	-2.124141	1.304727	-0.219622
H	0.876765	0.670612	0.797653	H	-0.883585	0.887253	0.183939
H	2.639131	1.427194	1.114893	H	-1.991048	1.550622	-1.278299

H	1.662112	2.294114	-0.151354
H	3.348402	0.094862	-0.918469
H	1.764759	0.358265	-1.656219
H	2.410352	-1.421689	0.757753
H	1.535108	-1.901331	-0.706636
C	-0.819738	-0.504406	-0.205970
H	-0.574475	0.005384	-1.151611
H	-1.140750	-1.523677	-0.487492
C	-1.985851	0.223950	0.470372
H	-2.222186	-0.277475	1.420990
H	-1.668138	1.244664	0.729950
C	-3.237652	0.277641	-0.409952
H	-3.588105	-0.733205	-0.656365
H	-4.059709	0.805156	0.090358
H	-3.030940	0.797965	-1.354401
H	0.216640	-0.994843	1.665918

H	-2.465650	2.158435	0.370517
H	-3.613162	-0.285295	-0.582322
H	-3.087345	-0.106796	1.098954
H	-1.416610	-1.206981	-1.229399
H	-1.768362	-2.037848	0.296172
H	-0.351485	-0.359856	1.539157
C	0.991516	-0.533884	-0.189693
C	2.066454	0.391202	0.391542
H	1.312812	-1.584343	-0.064357
H	0.916325	-0.371301	-1.277099
C	3.440265	0.173476	-0.248839
H	1.751954	1.436374	0.254265
H	2.133911	0.228804	1.477745
H	3.402370	0.357019	-1.330598
H	3.784931	-0.857900	-0.097822
H	4.195028	0.845570	0.178889

Octyl	Axial		
C	-1.025304	-0.580376	-0.690746
C	-2.374256	-0.965464	-0.085113
C	-2.837856	0.304489	0.674116
C	-2.369160	1.457961	-0.205324
H	-1.348178	0.725167	-0.750561
H	-3.011210	1.682136	-1.063125
H	-1.991490	2.360022	0.282293
H	-3.921158	0.307531	0.859113
H	-2.343860	0.355658	1.653724
H	-3.090761	-1.192047	-0.887782
H	-2.318420	-1.851782	0.564435
C	0.183520	-0.681775	0.218338
H	-0.039743	-0.209615	1.188538
H	0.388402	-1.744740	0.439986
C	1.438866	-0.037411	-0.379016
H	1.655455	-0.499028	-1.355651
H	1.237719	1.026831	-0.578941
C	2.668800	-0.163083	0.524796
H	2.449327	0.295154	1.501087
H	2.866810	-1.227549	0.721981
C	3.915003	0.488979	-0.081117
H	3.749921	1.559658	-0.258942
H	4.785003	0.388748	0.580346
H	4.170245	0.027108	-1.043819
H	-0.835737	-0.943172	-1.708285

Octyl	Equatorial		
C	-0.972481	-0.361680	0.443237
C	-2.268953	-0.984031	-0.067309
C	-3.320560	0.138244	0.102752
C	-2.569156	1.407859	-0.278546
H	-1.366034	0.888249	0.119784
H	-2.446090	1.570198	-1.354413
H	-2.800784	2.328796	0.261773
H	-4.226212	-0.035839	-0.495170
H	-3.629665	0.193042	1.156132
H	-2.159603	-1.223994	-1.136053
H	-2.545244	-1.913841	0.450428
H	-0.921410	-0.319169	1.540772
C	0.338328	-0.743110	-0.207550
C	1.520282	0.100870	0.282340
H	0.553538	-1.811158	-0.020068
H	0.243388	-0.643603	-1.300907
C	2.849865	-0.289133	-0.369975
H	1.311718	1.163872	0.083513
H	1.608695	0.003426	1.376104
H	2.759282	-0.193531	-1.462597
H	3.054131	-1.351867	-0.169859
C	4.022059	0.562779	0.125541
H	4.965035	0.268941	-0.352920
H	3.852860	1.625749	-0.090493
H	4.150084	0.459937	1.211038

1,5 H-migrations

Pentyl			
C	1.300213	1.003952	0.061201
C	1.264336	-0.484901	-0.242555
C	0.000000	-1.134808	0.347493
C	-1.264336	-0.484901	-0.242555
C	-1.300213	1.003952	0.061201
H	0.000000	1.316317	-0.017364
H	-1.841426	1.631267	-0.653330
H	-1.560464	1.248335	1.096627
H	-1.264474	-0.643217	-1.331430
H	-2.162456	-0.990569	0.147278
H	0.000000	-2.216051	0.148065
H	0.000000	-1.011657	1.442299
H	1.264474	-0.643217	-1.331430
H	2.162456	-0.990569	0.147279
H	1.560464	1.248335	1.096627
H	1.841426	1.631267	-0.653330

Hexyl	Axial		
C	1.084808	1.409531	0.103793
C	-1.123488	0.123286	0.620267
C	-0.354841	-1.179507	0.434762
C	0.826528	-1.010151	-0.539274
C	1.793667	0.072546	-0.028496
H	0.869501	1.907260	-0.847959
H	0.042395	-1.518808	1.403566
H	-1.027260	-1.976890	0.074208
H	1.354919	-1.967169	-0.657787
H	0.456174	-0.729867	-1.537417
H	2.185106	-0.239232	0.951674
H	2.662568	0.146893	-0.702757
H	-0.134455	1.001657	0.533191
H	1.489011	2.103569	0.846486
H	-1.547632	0.248530	1.623901
C	-2.103629	0.473586	-0.484370
H	-2.927469	-0.255632	-0.531110
H	-2.546117	1.465918	-0.328462
H	-1.615010	0.478027	-1.467631

Hexyl	Equatorial		
C	-1.063825	1.456396	0.154142
C	1.100945	0.029723	0.446637
C	0.335720	-1.156396	-0.120259
C	-1.163447	-1.060731	0.209403
C	-1.763765	0.223209	-0.392499
H	-1.344524	1.720946	1.179185
H	0.455366	-1.177764	-1.215666
H	0.750550	-2.106466	0.256529
H	-1.695543	-1.943921	-0.172648
H	-1.300479	-1.053898	1.302513
H	-1.649036	0.183349	-1.486168
H	-2.847168	0.258803	-0.193285
H	1.194611	-0.021773	1.539955
H	0.201815	0.993310	0.287472
H	-1.038875	2.332056	-0.501243
C	2.397338	0.398212	-0.247095
H	2.857288	1.288299	0.200813
H	3.132243	-0.420526	-0.187367
H	2.225960	0.605104	-1.312066

Heptyl	Axial		
C	0.934625	1.595159	0.157755

Heptyl	Equatorial		
C	-1.058672	1.598436	0.088979

C	-0.584669	-0.463443	0.658528	C	0.585042	-0.409038	0.374778
C	0.614690	-1.363451	0.387185	C	-0.532624	-1.330917	-0.089097
C	1.609079	-0.710310	-0.591728	C	-1.912802	-0.763863	0.285402
C	2.099197	0.640399	-0.041250	C	-2.122584	0.614283	-0.368390
H	0.515064	1.999936	-0.769911	H	-1.198083	1.977119	1.107169
H	1.144105	-1.572963	1.329223	H	-0.483091	-1.443001	-1.184301
H	0.283716	-2.338464	-0.010108	H	-0.408370	-2.342078	0.333345
H	2.461605	-1.383273	-0.763724	H	-2.707268	-1.457226	-0.026586
H	1.128758	-0.554589	-1.569995	H	-1.986064	-0.666517	1.380328
H	2.605611	0.466498	0.920299	H	-2.074356	0.494050	-1.461173
H	2.854917	1.069466	-0.719461	H	-3.134362	0.986778	-0.139577
H	-0.016205	0.733471	0.594166	H	0.732817	-0.445226	1.464096
H	1.063839	2.368726	0.920442	H	0.011290	0.777275	0.205510
H	-0.988192	-0.551062	1.676185	H	-0.802562	2.398113	-0.612579
C	-1.672696	-0.456446	-0.399758	C	1.888734	-0.453725	-0.397330
H	-2.125860	-1.460695	-0.468157	H	2.323731	-1.467182	-0.337628
H	-1.228508	-0.258637	-1.387168	H	1.681742	-0.278002	-1.464336
C	-2.762748	0.580756	-0.112267	C	2.909151	0.571181	0.107829
H	-2.339406	1.592988	-0.085095	H	3.846892	0.519420	-0.460095
H	-3.549094	0.562287	-0.877721	H	2.513388	1.590901	0.017437
H	-3.235222	0.390323	0.860244	H	3.146825	0.397435	1.165371

Octyl	Axial			Octyl	Equatorial		
C	1.343899	1.611995	0.250539	C	-1.518351	1.623361	0.125589
C	0.065588	-0.596260	0.783561	C	-0.020259	-0.487867	0.457750
C	1.277030	-1.371308	0.279414	C	-1.150948	-1.324958	-0.121521
C	2.070723	-0.570236	-0.770238	C	-2.520393	-0.687920	0.170827
C	2.534488	0.774862	-0.184292	C	-2.599632	0.720891	-0.445382
H	0.766504	2.044263	-0.574218	H	-1.712591	1.976476	1.143986
H	1.949270	-1.600194	1.120518	H	-1.024900	-1.404124	-1.213434
H	0.965465	-2.340769	-0.146087	H	-1.117768	-2.354993	0.271273
H	2.936820	-1.155658	-1.111487	H	-3.327730	-1.321422	-0.224378
H	1.445211	-0.387250	-1.657498	H	-2.670738	-0.621941	1.260216
H	3.185312	0.576950	0.680895	H	-2.475354	0.633455	-1.535282
H	3.151330	1.312597	-0.922918	H	-3.602611	1.146391	-0.278586
H	0.531215	0.644939	0.741896	H	0.041178	-0.568815	1.552884
H	1.524436	2.338125	1.048632	H	-0.509913	0.735402	0.290628
H	-0.182754	-0.790617	1.835479	H	-1.163431	2.428357	-0.525009
C	-1.157241	-0.603784	-0.115266	C	1.333340	-0.586175	-0.217181
H	-1.546567	-1.634351	-0.203891	H	1.708434	-1.624874	-0.160162
H	-0.872791	-0.301461	-1.136009	H	1.220389	-0.366928	-1.291524
C	-2.274813	0.316095	0.387218	C	2.377444	0.358432	0.387504
H	-1.888984	1.343883	0.458629	H	2.008956	1.392667	0.316629

H	-2.553129	0.019352	1.409757	H	2.482325	0.140877	1.461078
C	-3.512680	0.287849	-0.513721	C	3.742415	0.245511	-0.297314
H	-3.930302	-0.725653	-0.575383	H	4.475074	0.930073	0.148812
H	-4.300404	0.953092	-0.137681	H	4.140763	-0.774089	-0.212883
H	-3.262586	0.607478	-1.533922	H	3.666212	0.485840	-1.365876

1,6 H-migrations

Hexyl			
C	-1.291168	1.267601	0.263437
C	-1.617383	-0.096948	-0.313995
C	-0.732432	-1.228428	0.235931
C	0.732423	-1.228431	-0.235932
C	1.617380	-0.096957	0.313997
C	1.291179	1.267594	-0.263438
H	-1.356599	1.318963	1.356376
H	-1.808116	2.108918	-0.210118
H	-1.522005	-0.067038	-1.410825
H	-2.672356	-0.343740	-0.108172
H	-1.181079	-2.189852	-0.057497
H	-0.757642	-1.204443	1.337776
H	0.757632	-1.204443	-1.337777
H	1.181065	-2.189858	0.057493
H	1.521999	-0.067046	1.410826
H	2.672352	-0.343758	0.108178
H	1.808127	2.108908	0.210123
H	1.356622	1.318956	-1.356376
H	0.000005	1.447846	-0.000006

Heptyl	Axial			Heptyl	Equatorial		
C	0.926441	-1.586046	0.536655	C	0.000130	0.000125	-0.000067
C	1.664689	-0.703678	-0.451463	C	0.000084	0.000158	1.516473
C	1.609362	0.793656	-0.102106	C	1.408824	0.000058	2.133777
C	0.252307	1.485650	-0.320999	C	2.207999	-1.307171	1.988599
C	-0.863461	1.105440	0.668722	C	2.690576	-1.644791	0.567965
C	-1.392857	-0.314998	0.538274	C	1.584749	-2.079263	-0.376549
H	1.296621	-1.513754	1.565695	H	0.545281	0.837275	-0.451140
H	0.794546	-2.628240	0.227378	H	-0.978896	-0.144663	-0.468720
H	1.255970	-0.852226	-1.463297	H	-0.554007	-0.876947	1.886467
H	2.722423	-1.012689	-0.505775	H	-0.546692	0.882767	1.889310
H	2.358050	1.318514	-0.715221	H	1.314112	0.220388	3.208199
H	1.922540	0.932180	0.945874	H	1.992472	0.830204	1.703050

H	-0.081708	1.307498	-1.354748
H	0.411733	2.572171	-0.243189
H	-0.488407	1.259680	1.693020
H	-1.700649	1.814619	0.541240
H	-0.317716	-1.068939	0.602203
H	-1.978478	-0.619556	1.415637
C	-2.090199	-0.657813	-0.766082
H	-2.444831	-1.696520	-0.763379
H	-2.963941	-0.008038	-0.933784
H	-1.423844	-0.537964	-1.629667

H	1.605331	-2.145129	2.375588
H	3.088924	-1.238373	2.645171
H	3.206736	-0.767516	0.143504
H	3.451806	-2.442398	0.628713
H	1.010981	-2.928546	0.020332
H	0.725134	-1.086972	-0.330175
C	1.992679	-2.262776	-1.825613
H	2.752258	-3.053323	-1.932370
H	1.136282	-2.537839	-2.454634
H	2.424960	-1.337155	-2.229540

Octyl	Axial		
C	-0.592782	1.687149	0.696866
C	-1.532713	1.321180	-0.435656
C	-2.203111	-0.052469	-0.261354
C	-1.293652	-1.276528	-0.467097
C	-0.244497	-1.526627	0.631021
C	0.883985	-0.508282	0.699155
H	-1.067855	1.708625	1.684439
H	0.020610	2.578396	0.526533
H	-0.988911	1.337711	-1.393323
H	-2.321413	2.087656	-0.524261
H	-3.033183	-0.124674	-0.980889
H	-2.662220	-0.105806	0.739622
H	-0.802560	-1.201369	-1.449430
H	-1.937154	-2.168119	-0.523286
H	-0.759842	-1.562237	1.604214
H	0.187419	-2.531833	0.479367
H	0.272660	0.655040	0.779481
C	1.805631	-0.424749	-0.504973
H	2.241682	-1.419724	-0.704346
H	1.229139	-0.163798	-1.404600
C	2.930308	0.597389	-0.309437
H	2.520434	1.601610	-0.142837
H	3.545595	0.338983	0.562266
H	3.589928	0.642528	-1.185478
H	1.446660	-0.575373	1.641382

Octyl	Equatorial		
C	-0.535864	1.706909	0.320659
C	-1.868653	1.288697	-0.270184
C	-2.356290	-0.086304	0.216709
C	-1.576638	-1.303656	-0.311034
C	-0.148835	-1.473990	0.234715
C	0.844495	-0.458912	-0.300717
H	-0.515064	1.728040	1.416482
H	-0.098168	2.613811	-0.109877
H	-1.798130	1.276142	-1.369324
H	-2.637354	2.040970	-0.024861
H	-3.409165	-0.203929	-0.082553
H	-2.349456	-0.102914	1.318988
H	-1.541525	-1.262158	-1.412008
H	-2.152480	-2.207588	-0.059463
H	-0.173669	-1.413512	1.335495
H	0.205864	-2.492026	-0.003850
H	0.883543	-0.453721	-1.400533
H	0.299963	0.702817	-0.010567
C	2.222452	-0.471046	0.333243
H	2.119061	-0.339300	1.421674
H	2.688159	-1.462225	0.191741
C	3.143524	0.613916	-0.233960
H	4.135317	0.585704	0.235180
H	3.279396	0.484255	-1.315579
H	2.718565	1.611947	-0.067529

1,7 H-migrations

Heptyl			
C	-0.000026	-0.000200	-0.000091

C	-0.000107	-0.000180	1.517998
C	1.407573	-0.000001	2.139597
C	2.145336	-1.349893	1.969189
C	3.390017	-1.320033	1.068894
C	3.139205	-0.832449	-0.365789
C	1.942945	-1.495529	-1.022816
H	1.839964	-2.569506	-0.830008
H	1.830599	-1.271141	-2.089329
H	4.051597	-1.005061	-0.960039
H	2.986659	0.258209	-0.371483
H	4.163233	-0.689508	1.534625
H	3.807722	-2.338334	1.026785
H	1.440223	-2.097790	1.577643
H	2.454330	-1.726734	2.955205
H	1.314305	0.234498	3.209688
H	1.997446	0.821164	1.703526
H	-0.554380	0.884052	1.877550
H	-0.549637	-0.875972	1.894251
H	0.382545	0.931022	-0.435239
H	-0.951154	-0.283922	-0.463491
H	0.886357	-0.893760	-0.476830

Octyl	Axial		
C	-1.622571	-0.227413	0.540811
C	-1.334649	1.256890	0.353597
C	-0.061593	1.561920	-0.457900
C	1.235045	1.244155	0.325499
C	2.120147	0.143959	-0.279228
C	1.414739	-1.206609	-0.475530
C	0.626624	-1.652553	0.741163
H	1.130310	-1.502102	1.702916
H	0.208373	-2.662504	0.665462
H	2.171977	-1.963058	-0.742312
H	0.737587	-1.155269	-1.341612
H	2.523984	0.484722	-1.245214
H	2.988071	-0.002838	0.382841
H	0.972161	0.959699	1.354760
H	1.843164	2.155900	0.419204
H	-0.073791	2.625565	-0.736073
H	-0.084513	1.008029	-1.408082
H	-2.203639	1.725610	-0.142551
H	-1.242344	1.747913	1.334009
H	-0.478628	-0.872325	0.761965

Octyl	Equatorial		
C	1.533296	0.171420	-0.354967
C	1.196387	-1.281598	-0.070596
C	-0.263709	-1.662106	-0.370066
C	-1.265153	-1.068519	0.650070
C	-2.237298	-0.015831	0.095500
C	-1.568131	1.207412	-0.548848
C	-0.462841	1.801633	0.302932
H	-0.670829	1.846749	1.377956
H	-0.064648	2.753030	-0.067052
H	-2.344463	1.961402	-0.760359
H	-1.150099	0.933514	-1.530440
H	-2.908796	-0.488513	-0.638042
H	-2.878469	0.328168	0.922421
H	-0.704927	-0.629429	1.488672
H	-1.864800	-1.878666	1.090444
H	-0.344781	-2.758610	-0.367816
H	-0.519961	-1.345679	-1.393106
H	1.872683	-1.924300	-0.662695
H	1.411705	-1.510322	0.985581
H	1.448176	0.400114	-1.427494

C	-2.230599	-0.921709	-0.666666
H	-2.311314	-2.005293	-0.508762
H	-3.242469	-0.538956	-0.871941
H	-1.631603	-0.759741	-1.572127
H	-2.190183	-0.437184	1.457047
H	0.571616	0.953347	0.127307
C	2.835966	0.673268	0.239701
H	3.700822	0.122383	-0.162411
H	2.992389	1.738408	0.024282
H	2.843282	0.544333	1.330404

1,8 H-migrations

Octyl			
C	1.916288	-0.875728	0.176646
C	1.961924	0.412194	-0.660757
C	-1.924679	-0.884464	-0.059108
C	1.389591	1.620450	0.058402
C	-2.071501	0.612426	-0.377784
C	-1.255980	1.568877	0.477822
H	2.615871	-0.771195	1.020948
H	1.431611	0.269696	-1.613543
H	1.765409	1.752991	1.080620
H	-2.175979	-1.065398	0.998407
H	-3.137767	0.880621	-0.275210
H	2.286167	-1.717381	-0.429808
H	3.011449	0.610628	-0.938349
H	-2.679731	-1.425550	-0.649649
H	1.468769	2.555696	-0.507521
H	-1.828741	0.772941	-1.440641
H	-1.334835	1.383447	1.555826
H	-1.459883	2.623369	0.256651
C	0.521435	-1.204806	0.725093
H	0.195720	-0.385018	1.376109
H	0.590867	-2.088260	1.377379
C	-0.535450	-1.464270	-0.369765
H	-0.202082	-1.049374	-1.332235
H	-0.619791	-2.548962	-0.532240
H	0.063180	1.493672	0.229953

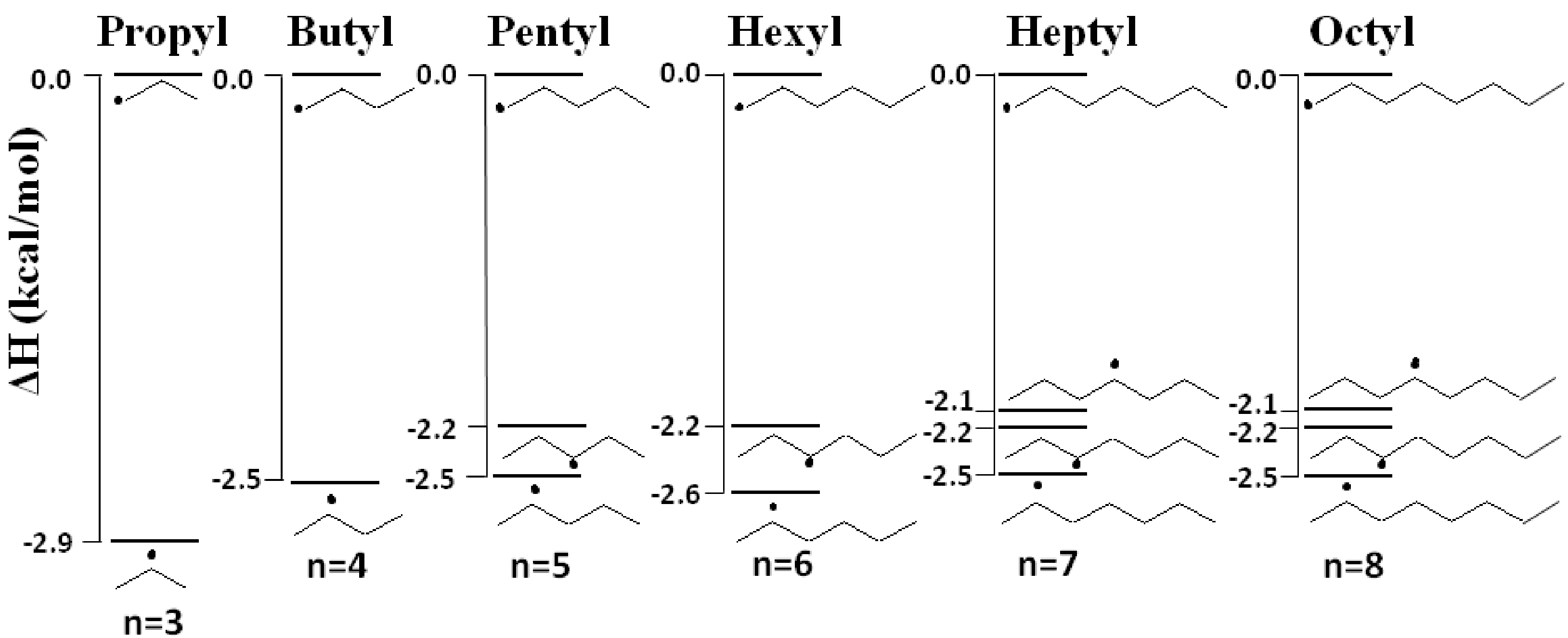

Propyl
Butyl
Pentyl
Hexyl
Heptyl
Octyl
ΔH (kcal/mol)
0.0
-2.9
n=3
0.0
-2.5
n=4
0.0
-2.2
-2.5
n=5
0.0
-2.2
-2.6
n=6
0.0
-2.1
-2.2
-2.5
n=7
0.0
-2.1
-2.2
-2.5
n=8

Figure S1

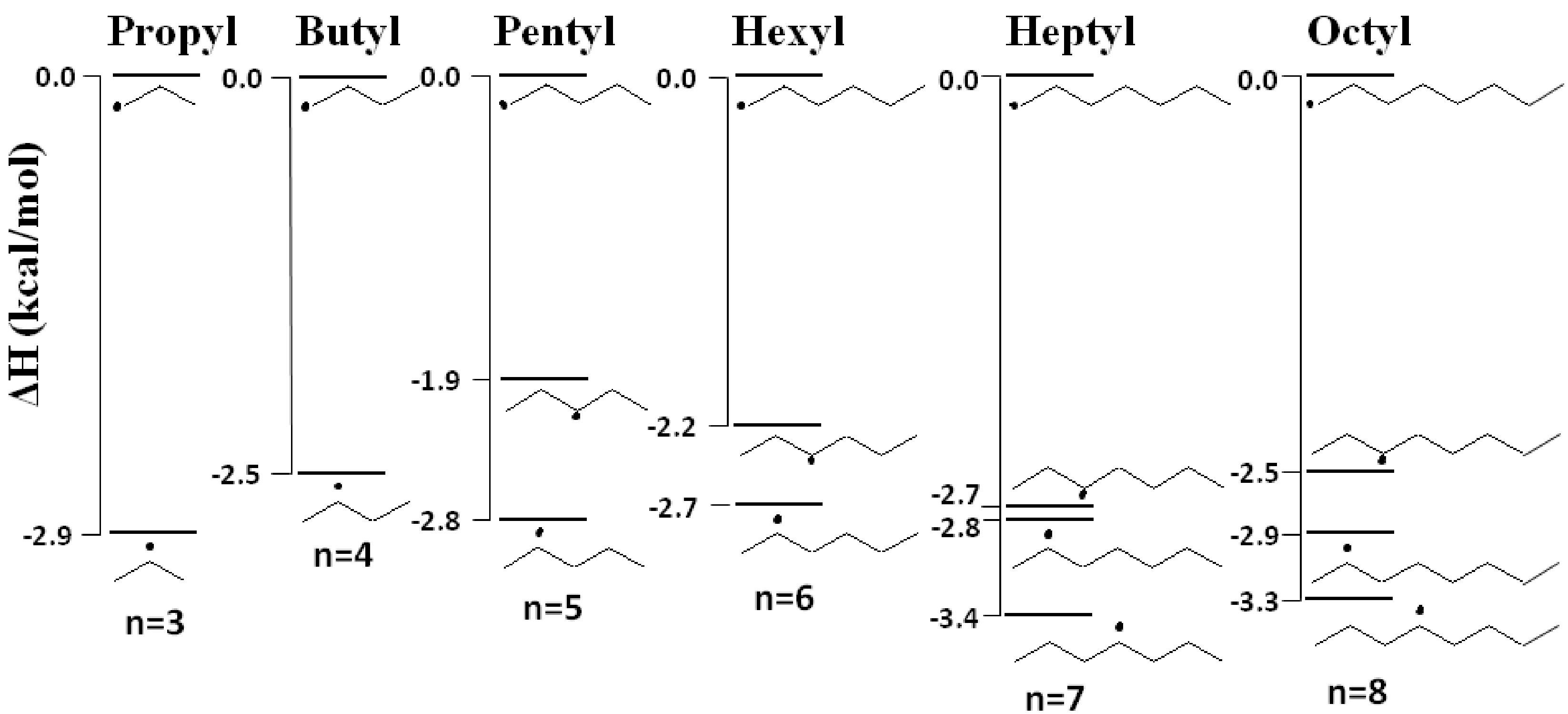

Propyl
Butyl
Pentyl
Hexyl
Heptyl
Octyl
ΔH (kcal/mol)
0.0
-2.9
n=3
0.0
-2.5
n=4
0.0
-1.9
-2.8
n=5
0.0
-2.2
-2.7
n=6
0.0
-2.7
-2.8
-3.4
n=7
0.0
-2.5
-2.9
-3.3
n=8

Figure S2

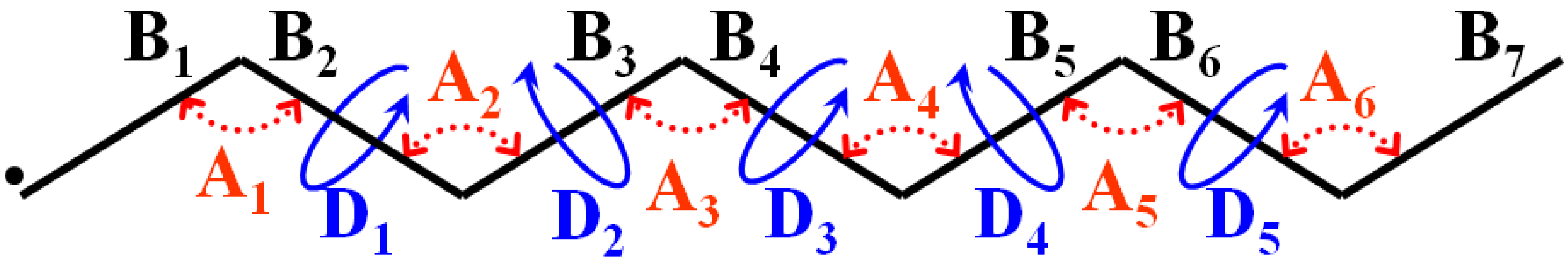
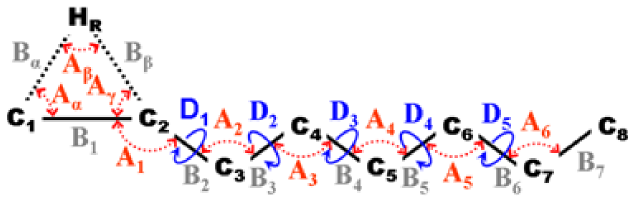
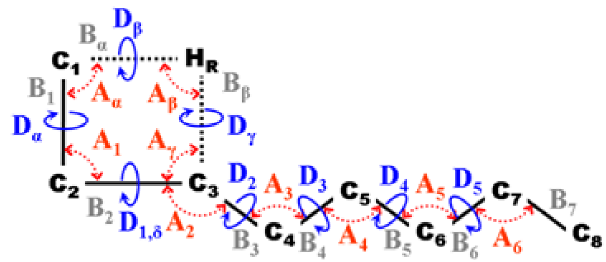


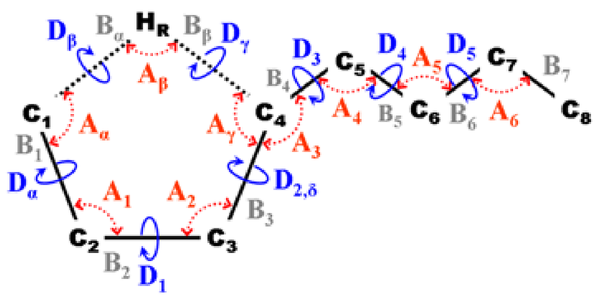
Figure S3



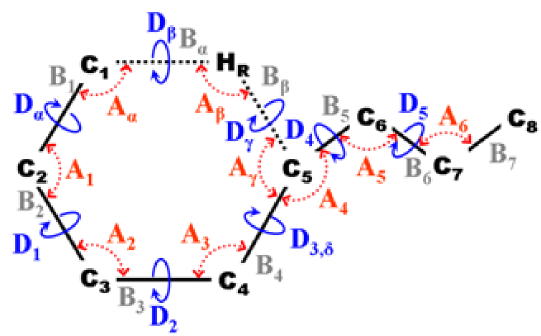
1,2 H-Migration



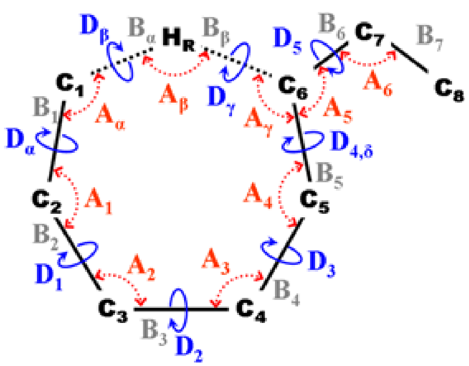
1,3 H-Migration



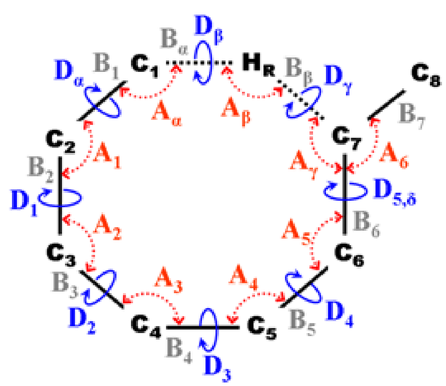
1,4 H-Migration



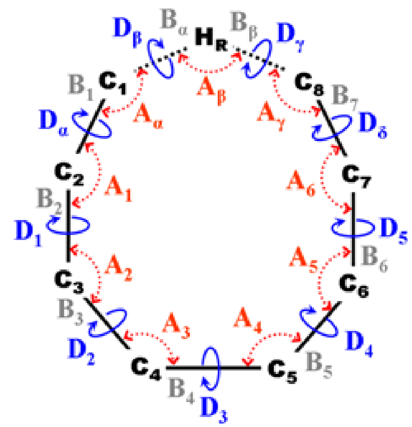
1,5 H-Migration



1,6 H-Migration



1,7 H-Migration



1,8 H-Migration

Figure S4

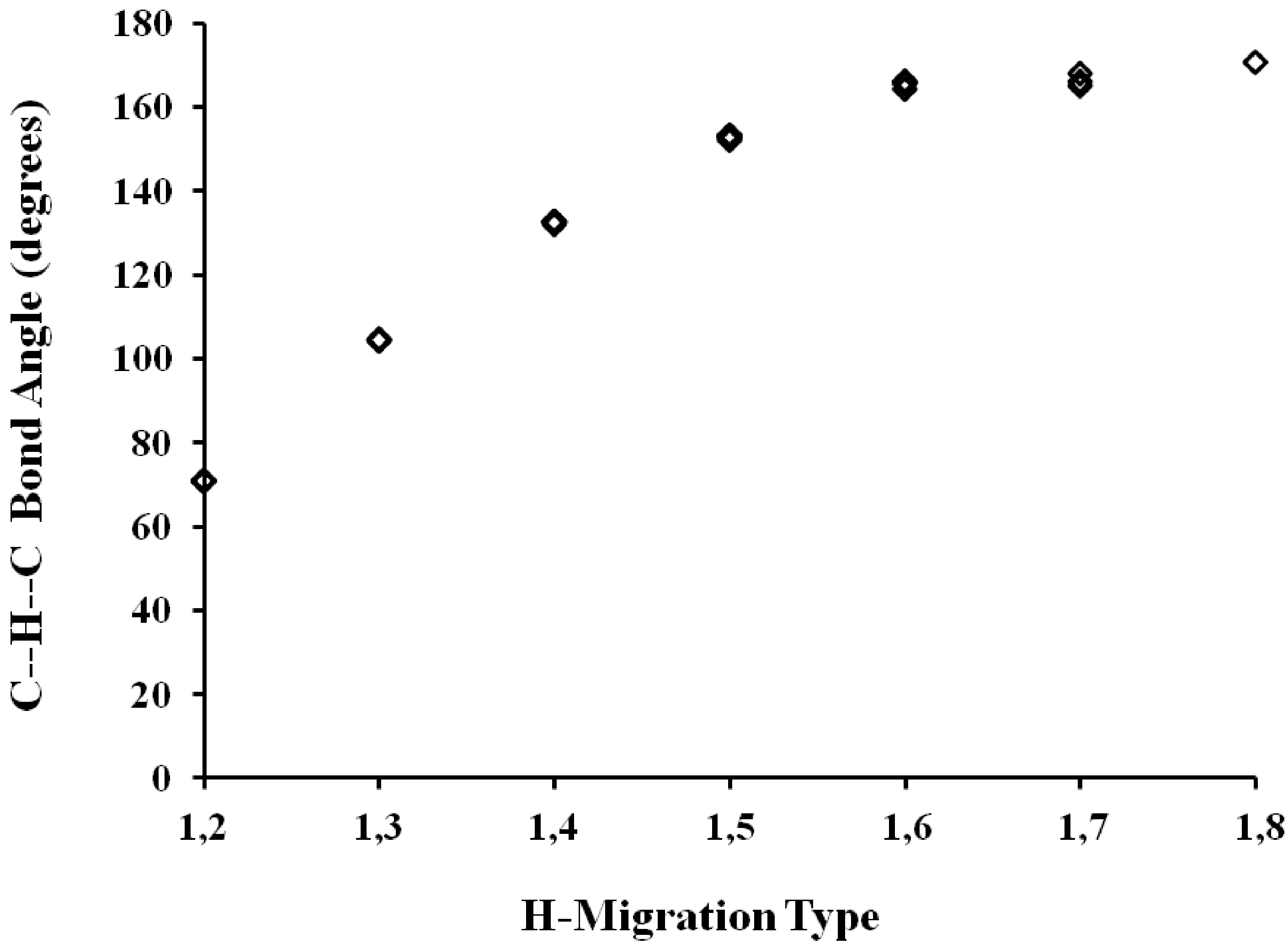
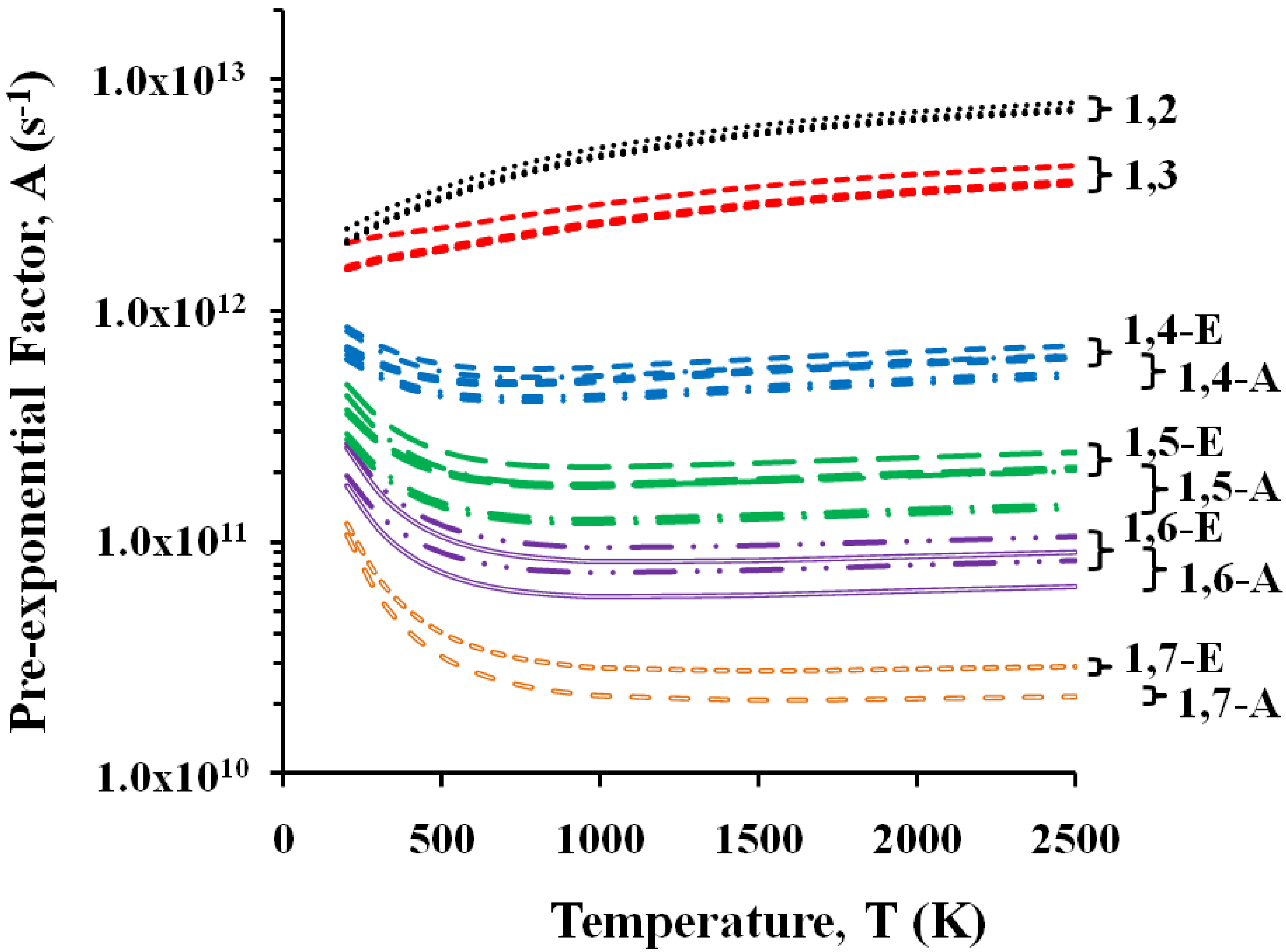

180
160
140
120
100
80
60
40
20
0
C--H--C Bond Angle (degrees)
1,2
1,3
1,4
1,5
1,6
1,7
1,8
H-Migration Type

Figure S5



Pre-exponential Factor, A (s-1)
1.0x10^13
1.0x10^12
1.0x10^11
1.0x10^10
0
500
1000
1500
2000
2500
Temperature, T (K)
1,2
1,3
1,4-E
1,4-A
1,5-E
1,5-A
1,6-E
1,6-A
1,7-E
1,7-A

Figure S6

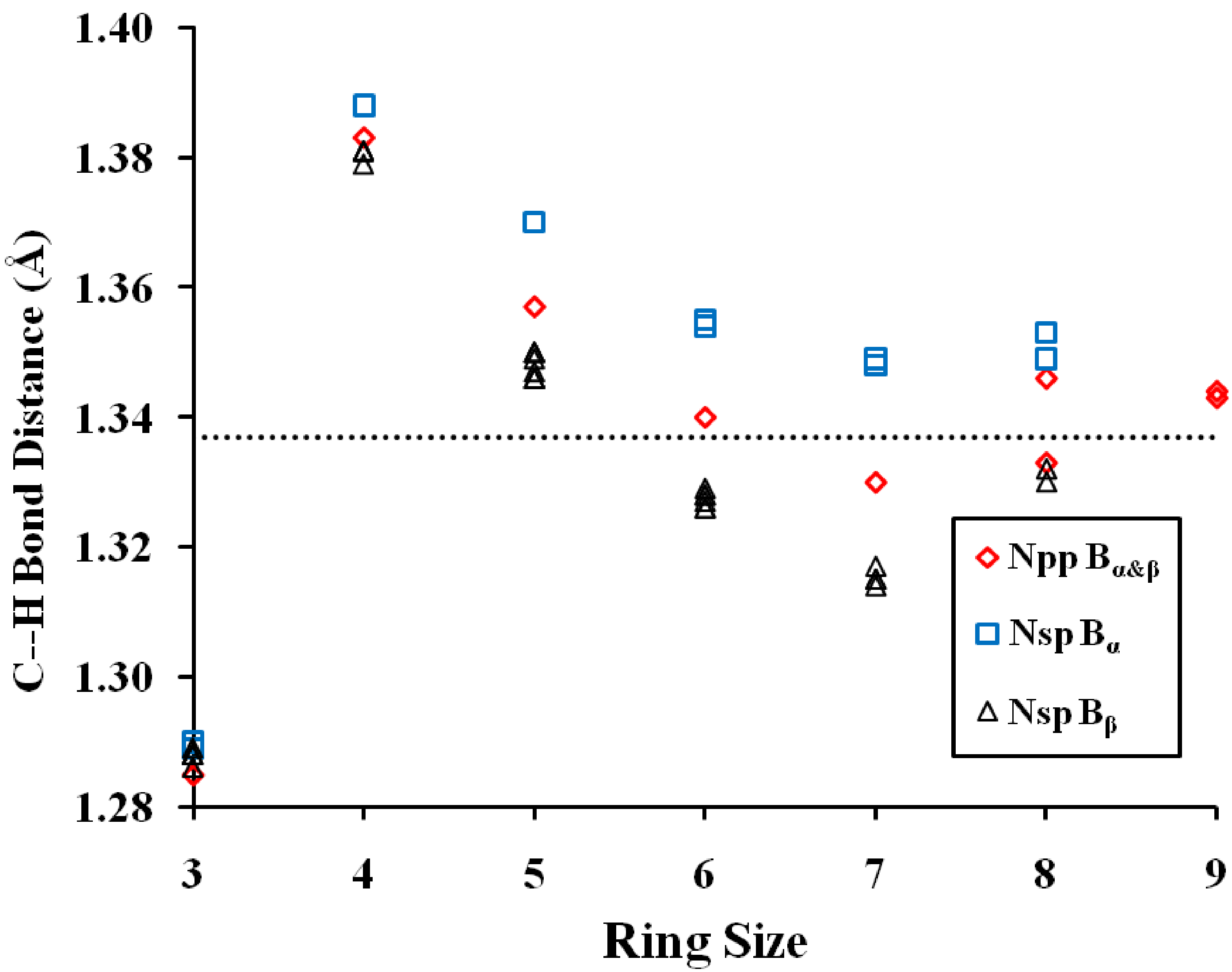

1.40
1.38
1.36
1.34
1.32
1.30
1.28
C--H Bond Distance (Å)
3
4
5
6
7
8
9
Ring Size
Npp $B_{\alpha\&\beta}$
Nsp B_{α}
Nsp B_{β}

Figure S7