Ab Initio Study of Chain Branching Reactions Involving Second Generation Products in Hydrocarbon Combustion Mechanisms

Alexander C. Davis and Joseph S. Francisco

Department of Chemistry and Department of Earth and Atmospheric Science
Purdue University, West Lafayette, Indiana 47907-1393

Supporting Information.

G4 frequencies and rotational constants for the reactants, products, and transition state species of s-alkyl radicals H-migrations (**Table S.1**)

G4 heat capacities for s-alkyl radicals and transition states. Units are cal mol^{-1} K^{-1} for S, cal mol^{-1} K^{-1} for Cp and kcal mol^{-1} for ddH. (**Table S.2**)

G4 Arrhenius pre-exponential A-factors for the forward and reverse s-alkyl radical H-migrations. (**Table S.3**)

Skodje and Truhlar tunneling transmission coefficient for s-alkyl radical H-migrations, determined using G4 frequencies and energy values. (**Table S.4**)

Wigner tunneling transmission coefficient for s-alkyl radical H-migrations, determined using G4 frequencies and energy values. (**Table S.5**)

G4 cartesian coordinates for s-alkyl radical H-migration reactants and products. (**Table S.6**)

G4 cartesian coordinates for s-alkyl radical H-migration transition states. (**Table S.7**)

Evans Polanyi plot of activation energy versus reaction enthalpy for s-alkyl radical H-migrations (**Figure S.1**).

Table S.1: G4 frequencies and rotational constants for the reactants, products, and transition state species of s-alkyl radicals H-migrations.

Methylalkyl radical	rxn type	Frequencies (cm^{-1})	Rotational Constants (GHz) A	B	C
2-Butyl		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
2-Butyl	$3s_{\alpha}s_{\alpha}$	-1944, 159, 182, 211, 265, 402, 621, 738, 849, 970, 1039, 1043, 1054, 1150, 1213, 1260, 1317, 1403, 1413, 1419, 1482, 1484, 1492, 1497, 2199, 2970, 2974, 3048, 3048, 3094, 3094, 3155, 3167	27.025	3.580	3.421
2-Pentyl		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
3-Pentyl		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
2-Pentyl	$3s_{\beta}s_{\alpha}$	-1940, 91, 137, 181, 207, 253, 380, 395, 625, 731, 791, 872, 949, 1014, 1047, 1071, 1086, 1163, 1195, 1246, 1293, 1297, 1365, 1408, 1412, 1422, 1480, 1483, 1494, 1496, 1505, 2196, 2947, 2972, 3022, 3032, 3048, 3094, 3098, 3105, 3146, 3163	19.174	1.914	1.845
2-Pentyl	$4^{c}s_{\alpha}s_{\alpha}$	-2104, 65, 184, 201, 258, 346, 364, 533, 698, 843, 863, 882, 898, 972, 1047, 1071, 1104, 1138, 1168, 1212, 1253, 1331, 1341, 1374, 1403, 1410, 1483, 1484, 1488, 1492, 1494, 1773, 2987, 2988, 3047, 3055, 3058, 3088, 3094, 3097, 3110, 3119	9.529	2.621	2.381
2-Pentyl	$4^{t}s_{\alpha}s_{\alpha}$	-2096, 54, 160, 204, 225, 289, 397, 592, 712, 817, 843, 889, 890, 974, 1045, 1071, 1100, 1128, 1164, 1218, 1253, 1318, 1355, 1355, 1407, 1407, 1480, 1485, 1489, 1491, 1491, 1770, 2989, 2989, 3049, 3054, 3055, 3089, 3095, 3095, 3113, 3118	13.044	2.324	2.263
2-Hexyl		48, 86, 110, 124, 143, 246, 298, 361, 411, 463, 730, 781, 894, 907, 916, 986, 1021, 1058, 1068, 1103, 1140, 1170, 1234, 1267, 1303, 1326, 1337, 1391, 1404, 1411, 1416, 1466, 1474, 1485, 1486, 1497, 1499, 1512, 2906, 2946, 2991, 3006, 3016, 3029, 3032, 3032, 3057, 3090, 3095, 3100, 3157	15.826	1.136	1.100
3-Hexyl		43, 48, 111, 154, 239, 249, 293, 371, 415, 464, 732, 770, 857, 895, 908, 1021, 1036, 1054, 1073, 1099, 1143, 1168, 1247, 1263, 1272, 1318, 1338, 1386, 1408, 1411, 1423, 1463, 1474, 1491, 1498, 1500, 1505, 1509, 2906, 2918, 2993, 3002, 3021, 3028, 3034, 3054, 3095, 3100, 3101, 3106, 3141	14.543	1.146	1.106
2-Hexyl	$3s_{\beta}s_{\alpha}$	-1939, 76, 98, 119, 193, 204, 244, 296, 364, 447, 625, 730, 754, 871, 896, 908, 1021, 1037, 1057, 1073, 1107, 1159, 1193, 1237, 1271, 1287, 1321, 1335, 1388, 1410, 1414, 1421, 1477, 1483, 1492, 1494, 1499, 1510, 2197, 2937, 2972, 3010, 3020, 3028, 3048, 3053, 3094, 3094, 3101, 3146, 3163	16.087	1.125	1.097
2-Hexyl	$4^{c}s_{\beta}s_{\alpha}$	-2099, 56, 93, 176, 222, 239, 273, 358, 414, 550, 693, 782, 840, 869, 888, 922, 988, 1018, 1057, 1095, 1099, 1130, 1171, 1208, 1252, 1281, 1309, 1337, 1354, 1391, 1408, 1412, 1478, 1483, 1490, 1492, 1497, 1505, 1767, 2962, 2987, 3022, 3032, 3047, 3056, 3086, 3094, 3098, 3102, 3105, 3116	6.720	1.573	1.440
2-Hexyl	$4^{t}s_{\beta}s_{\alpha}$	-2090, 56, 96, 137, 213, 229, 256, 334, 434, 599, 710, 782, 825, 840, 894, 916, 989, 1019, 1056, 1090, 1098, 1125, 1170, 1214, 1253, 1277, 1304, 1332, 1356, 1388, 1407, 1413, 1478, 1481, 1488, 1491, 1498, 1505, 1766, 2963, 2989, 3019, 3032, 3049, 3054, 3087, 3095, 3097, 3103, 3105, 3116	8.396	1.445	1.352
2-Hexyl	$5s_{\alpha}^{A}s_{\alpha}^{A}$	-1835, 100, 144, 183, 198, 205, 352, 357, 574, 597, 782, 801, 809, 878, 927, 930, 944, 1021, 1056, 1056, 1114, 1120, 1161, 1212, 1229, 1318, 1324, 1337, 1361, 1400, 1406, 1422, 1480, 1486, 1489, 1491, 1495, 1500, 1627, 2998, 2998, 3024, 3033, 3056, 3060, 3062, 3076, 3090, 3091, 3108, 3109	5.634	2.064	1.880

2-Hexyl	$5s_{\alpha}^{A}s_{\alpha}^{E}$	-1848, 88, 152, 181, 189, 260, 341, 371, 493, 576, 761, 807, 845, 877, 925, 940, 954, 1014, 1052, 1083, 1115, 1128, 1165, 1224, 1227, 1303, 1327, 1345, 1371, 1403, 1405, 1421, 1480, 1485, 1487, 1489, 1495, 1498, 1633, 2988, 2996, 3020, 3027, 3050, 3055, 3060, 3066, 3075, 3090, 3096, 3108	4.869	2.248	1.804
2-Hexyl	$5s_{\alpha}^{E}s_{\alpha}^{E}$	-1850, 115, 145, 179, 185, 207, 353, 381, 510, 534, 743, 833, 840, 884, 926, 937, 967, 1002, 1062, 1084, 1127, 1128, 1176, 1225, 1229, 1297, 1318, 1366, 1370, 1402, 1408, 1430, 1483, 1485, 1486, 1490, 1493, 1498, 1643, 2988, 2989, 3017, 3020, 3050, 3054, 3055, 3058, 3069, 3075, 3095, 3096	5.655	1.950	1.597
3-Hexyl	$3s_{\beta}s_{\beta}$	-1935, 62, 104, 126, 163, 242, 247, 312, 356, 455, 634, 727, 789, 792, 902, 902, 1023, 1036, 1073, 1089, 1096, 1168, 1185, 1234, 1282, 1282, 1301, 1339, 1385, 1408, 1408, 1425, 1478, 1480, 1496, 1496, 1505, 1506, 2193, 2945, 2948, 3021, 3021, 3031, 3032, 3098, 3098, 3105, 3105, 3143, 3154	15.315	1.123	1.103
2-Heptyl		45, 71, 96, 110, 122, 153, 245, 247, 305, 402, 422, 479, 729, 750, 833, 885, 921, 950, 989, 1002, 1048, 1065, 1076, 1110, 1140, 1168, 1226, 1256, 1285, 1315, 1325, 1330, 1370, 1399, 1405, 1414, 1415, 1467, 1475, 1484, 1486, 1489, 1500, 1502, 1514, 2908, 2946, 2991, 3000, 3009, 3017, 3023, 3028, 3033, 3043, 3060, 3090, 3094, 3100, 3156	13.103	0.726	0.708
3-Heptyl		38, 40, 87, 118, 129, 234, 243, 247, 308, 406, 414, 481, 728, 762, 787, 884, 913, 929, 1001, 1038, 1042, 1066, 1078, 1108, 1142, 1165, 1233, 1251, 1270, 1302, 1314, 1326, 1366, 1396, 1408, 1412, 1421, 1463, 1474, 1485, 1497, 1498, 1499, 1505, 1512, 2907, 2918, 2992, 3001, 3007, 3016, 3028, 3032, 3034, 3057, 3094, 3100, 3100, 3107, 3141	11.347	0.736	0.713
4-Heptyl		34, 44, 87, 119, 152, 239, 243, 244, 302, 416, 422, 480, 729, 742, 847, 870, 882, 914, 998, 1046, 1048, 1066, 1086, 1106, 1142, 1165, 1242, 1251, 1255, 1314, 1317, 1320, 1367, 1393, 1410, 1412, 1422, 1463, 1473, 1491, 1492, 1499, 1500, 1509, 1509, 2905, 2909, 2992, 2998, 3020, 3021, 3028, 3028, 3053, 3054, 3094, 3094, 3101, 3101, 3140	12.307	0.727	0.711
2-Heptyl	$3s_{\beta}s_{\alpha}$	-1940, 58, 84, 95, 133, 182, 199, 243, 254, 301, 412, 462, 625, 730, 742, 797, 884, 920, 932, 1006, 1028, 1059, 1064, 1075, 1116, 1159, 1191, 1230, 1256, 1278, 1313, 1315, 1328, 1368, 1399, 1410, 1414, 1421, 1477, 1483, 1486, 1494, 1498, 1499, 1512, 2196, 2937, 2972, 3005, 3010, 3017, 3028, 3032, 3047, 3057, 3094, 3094, 3100, 3146, 3163	13.070	0.721	0.706
2-Heptyl	$4^{c}s_{\beta}s_{\alpha}$	-2099, 44, 79, 108, 158, 200, 242, 249, 353, 375, 391, 565, 696, 746, 835, 863, 871, 903, 929, 946, 1033, 1051, 1061, 1092, 1114, 1134, 1169, 1205, 1251, 1258, 1286, 1321, 1335, 1345, 1370, 1396, 1408, 1413, 1475, 1483, 1490, 1491, 1492, 1499, 1510, 1766, 2951, 2987, 3010, 3020, 3028, 3047, 3052, 3056, 3086, 3094, 3095, 3100, 3102, 3116	5.443	0.972	0.904
2-Heptyl	$4^{t}s_{\beta}s_{\alpha}$	-2091, 43, 82, 100, 138, 188, 214, 249, 314, 385, 418, 607, 710, 748, 815, 850, 866, 904, 926, 944, 1035, 1052, 1056, 1089, 1112, 1130, 1168, 1210, 1252, 1257, 1282, 1320, 1328, 1355, 1361, 1397, 1406, 1413, 1475, 1481, 1488, 1491, 1492, 1500, 1509, 1766, 2952, 2988, 3008, 3020, 3028, 3049, 3052, 3054, 3087, 3094, 3095, 3100, 3103, 3116	7.374	0.880	0.847
2-Heptyl	$5s_{\beta}^{A}s_{\alpha}^{A}$	-1830, 78, 94, 121, 169, 205, 240, 282, 357, 400, 574, 611, 754, 788, 803, 849, 878, 918, 942, 963, 1008, 1045, 1059, 1075, 1107, 1123, 1167, 1211, 1228, 1277, 1311, 1320, 1329, 1349, 1382, 1404, 1409, 1423, 1477, 1483, 1488, 1494, 1497, 1499, 1504, 1624, 2972, 2998, 3024, 3025, 3030, 3034, 3056, 3062, 3075, 3091, 3091, 3098, 3103, 3108	3.952	1.391	1.200
2-Heptyl	$5s_{\beta}^{A}s_{\alpha}^{E}$	-1844, 64, 88, 138, 181, 212, 245, 288, 367, 403, 491, 589, 736, 798, 823, 850, 888, 921, 945, 967, 1012, 1040, 1071, 1079, 1112, 1130, 1171, 1223, 1225, 1276, 1302, 1316, 1331, 1365, 1383, 1405, 1410, 1422, 1477, 1484, 1486, 1492, 1496, 1498, 1505, 1630, 2969, 2988, 3019, 3024, 3029, 3030, 3050, 3055, 3065, 3075, 3091, 3095, 3098, 3103	3.231	1.599	1.201

2-Heptyl	$5s_{\beta}^{E}s_{\alpha}^{E}$	-1846, 77, 110, 135, 153, 191, 249, 283, 372, 413, 511, 534, 740, 785, 839, 856, 898, 932, 951, 962, 997, 1038, 1069, 1106, 1121, 1130, 1178, 1221, 1223, 1284, 1293, 1309, 1344, 1368, 1387, 1405, 1412, 1429, 1479, 1484, 1486, 1492, 1498, 1500, 1506, 1637, 2962, 2988, 3018, 3019, 3025, 3031, 3049, 3054, 3056, 3067, 3074, 3095, 3098, 3103	3.730	1.349	1.066
2-Heptyl	$6s_{\alpha}^{A}s_{\alpha}^{A}$	-1697, 92, 109, 171, 187, 234, 239, 334, 385, 457, 496, 542, 763, 800, 808, 865, 866, 925, 958, 968, 990, 1037, 1078, 1079, 1127, 1130, 1160, 1205, 1214, 1283, 1334, 1338, 1356, 1357, 1374, 1403, 1408, 1424, 1474, 1478, 1485, 1485, 1490, 1495, 1497, 1514, 2985, 2987, 2995, 2996, 3021, 3039, 3045, 3059, 3063, 3069, 3082, 3083, 3098, 3102	2.973	2.063	1.462
2-Heptyl	$6s_{\alpha}^{A}s_{\alpha}^{E}$	-1699, 95, 117, 167, 185, 197, 260, 342, 370, 431, 468, 565, 789, 803, 831, 844, 884, 898, 959, 963, 1009, 1035, 1071, 1097, 1125, 1133, 1169, 1204, 1223, 1283, 1322, 1344, 1355, 1370, 1381, 1403, 1407, 1430, 1475, 1480, 1485, 1489, 1491, 1494, 1495, 1519, 2984, 2987, 2991, 2998, 3014, 3027, 3043, 3054, 3060, 3064, 3068, 3083, 3096, 3100	3.178	1.787	1.341
2-Heptyl	$6s_{\alpha}^{E}s_{\alpha}^{E}$	-1713, 92, 95, 186, 192, 247, 270, 331, 374, 404, 436, 521, 764, 808, 844, 866, 881, 936, 957, 962, 1020, 1045, 1078, 1100, 1122, 1138, 1181, 1208, 1228, 1281, 1323, 1330, 1365, 1379, 1381, 1404, 1408, 1426, 1476, 1484, 1486, 1486, 1492, 1493, 1496, 1522, 2984, 2986, 2989, 2991, 3010, 3021, 3032, 3053, 3055, 3063, 3064, 3068, 3095, 3096	2.887	1.913	1.273
3-Heptyl	$3s_{\beta}s_{\beta}$	-1935, 55, 76, 96, 137, 162, 234, 248, 277, 300, 404, 470, 634, 726, 750, 793, 870, 886, 919, 1000, 1043, 1056, 1080, 1093, 1108, 1165, 1184, 1228, 1263, 1276, 1297, 1317, 1322, 1365, 1395, 1408, 1411, 1424, 1475, 1480, 1491, 1496, 1500, 1506, 1509, 2193, 2936, 2947, 3010, 3020, 3021, 3028, 3032, 3053, 3094, 3098, 3100, 3105, 3143, 3154	12.929	0.717	0.706
3-Heptyl	$4^{c}s_{\beta}s_{\beta}$	-2094, 44, 88, 95, 182, 222, 240, 261, 281, 390, 441, 560, 689, 770, 792, 844, 882, 886, 953, 987, 1016, 1027, 1089, 1095, 1099, 1118, 1175, 1204, 1250, 1280, 1280, 1305, 1314, 1347, 1372, 1400, 1412, 1412, 1476, 1480, 1488, 1497, 1498, 1505, 1506, 1762, 2962, 2962, 3020, 3023, 3032, 3032, 3048, 3085, 3094, 3098, 3099, 3105, 3105, 3109	4.244	1.105	0.965
3-Heptyl	$4^{t}s_{\beta}s_{\beta}$	-2087, 45, 82, 115, 125, 210, 241, 261, 284, 408, 438, 608, 730, 772, 798, 820, 851, 905, 949, 955, 997, 1028, 1057, 1090, 1101, 1134, 1173, 1211, 1253, 1273, 1287, 1305, 1328, 1349, 1369, 1389, 1405, 1413, 1476, 1478, 1488, 1497, 1498, 1505, 1505, 1767, 2963, 3013, 3020, 3027, 3032, 3049, 3051, 3085, 3095, 3097, 3099, 3102, 3105, 3109	7.910	0.912	0.874
2-Octyl		38, 65, 79, 82, 116, 142, 150, 200, 248, 275, 335, 411, 468, 469, 729, 738, 785, 876, 892, 910, 969, 998, 1009, 1021, 1060, 1070, 1081, 1115, 1140, 1166, 1221, 1247, 1271, 1299, 1312, 1327, 1334, 1349, 1388, 1401, 1405, 1413, 1414, 1466, 1475, 1483, 1484, 1486, 1494, 1500, 1506, 1515, 2908, 2946, 2990, 2999, 3002, 3012, 3017, 3020, 3028, 3032, 3033, 3049, 3062, 3090, 3094, 3100, 3156	11.391	0.491	0.481
3-Octyl		32, 37, 64, 97, 109, 146, 196, 238, 243, 281, 333, 411, 466, 470, 727, 746, 771, 834, 891, 912, 960, 1002, 1020, 1043, 1054, 1070, 1085, 1116, 1142, 1163, 1226, 1243, 1269, 1285, 1297, 1324, 1330, 1347, 1384, 1400, 1408, 1413, 1421, 1463, 1474, 1484, 1489, 1497, 1499, 1502, 1505, 1514, 2907, 2918, 2992, 3000, 3002, 3009, 3018, 3023, 3028, 3033, 3043, 3061, 3094, 3099, 3100, 3106, 3141	10.296	0.494	0.484
4-Octyl		26, 40, 72, 106, 125, 141, 196, 240, 247, 277, 335, 421, 467, 470, 728, 738, 782, 858, 888, 906, 923, 1002, 1020, 1054, 1059, 1067, 1096, 1112, 1142, 1163, 1233, 1241, 1251, 1298, 1306, 1318, 1328, 1347, 1383, 1398, 1410, 1412, 1421, 1462, 1473, 1485, 1491, 1497, 1499, 1500, 1509, 1512, 2905, 2909, 2993, 2998, 3007, 3016, 3021, 3028, 3028, 3033, 3053, 3057, 3094, 3095, 3100, 3101, 3140	10.019	0.494	0.484
2-Octyl	$3s_{\beta}s_{\alpha}$	-1940, 48, 72, 75, 117, 141, 173, 197, 216, 249, 277, 336, 450, 466, 625, 729, 736, 764, 845, 891, 914, 966, 1004, 1031, 1033, 1065, 1072, 1074, 1123, 1159, 1190,	11.517	0.487	0.480

		1224, 1247, 1268, 1297, 1302, 1325, 1332, 1347, 1385, 1402, 1412, 1414, 1420, 1477, 1483, 1484, 1490, 1494, 1500, 1503, 1514, 2196, 2938, 2972, 3000, 3006, 3013, 3018, 3023, 3028, 3043, 3047, 3060, 3094, 3095, 3100, 3146, 3163			
2-Octyl	$4^{c}s_{\beta}s_{\alpha}$	-2100, 39, 59, 94, 118, 140, 190, 237, 250, 292, 340, 361, 459, 562, 696, 736, 786, 853, 868, 889, 897, 949, 955, 1015, 1046, 1061, 1068, 1094, 1117, 1135, 1169, 1204, 1242, 1250, 1271, 1307, 1326, 1329, 1339, 1355, 1387, 1398, 1407, 1414, 1475, 1483, 1486, 1490, 1491, 1498, 1499, 1512, 1764, 2951, 2987, 3005, 3010, 3017, 3028, 3032, 3047, 3056, 3057, 3086, 3094, 3094, 3100, 3101, 3116	4.658	0.632	0.599
2-Octyl	$4^{t}s_{\beta}s_{\alpha}$	-2091, 44, 60, 92, 108, 142, 171, 213, 250, 260, 346, 376, 463, 606, 710, 737, 787, 832, 854, 890, 898, 947, 955, 1014, 1050, 1057, 1069, 1090, 1115, 1133, 1168, 1208, 1240, 1254, 1267, 1307, 1323, 1329, 1339, 1356, 1384, 1400, 1406, 1416, 1475, 1481, 1485, 1488, 1490, 1498, 1501, 1512, 1765, 2953, 2988, 3005, 3009, 3017, 3029, 3032, 3049, 3054, 3057, 3087, 3094, 3095, 3100, 3103, 3116	5.863	0.588	0.565
2-Octyl	$5s_{\beta}^{A}s_{\alpha}^{A}$	-1830, 62, 69, 105, 127, 177, 205, 212, 246, 357, 375, 399, 575, 609, 737, 791, 804, 815, 877, 897, 907, 946, 956, 991, 1042, 1054, 1073, 1081, 1114, 1129, 1165, 1207, 1227, 1255, 1285, 1318, 1321, 1329, 1345, 1364, 1391, 1405, 1412, 1422, 1475, 1483, 1488, 1491, 1494, 1499, 1500, 1509, 1624, 2961, 2998, 3012, 3019, 3024, 3028, 3034, 3051, 3057, 3062, 3076, 3091, 3092, 3095, 3100, 3108	3.532	0.851	0.776
2-Octyl	$5s_{\beta}^{A}s_{\alpha}^{E}$	-1844, 51, 71, 107, 134, 187, 192, 244, 256, 353, 377, 404, 495, 588, 729, 776, 813, 857, 877, 896, 905, 941, 970, 994, 1045, 1052, 1076, 1092, 1122, 1131, 1168, 1221, 1223, 1255, 1284, 1306, 1320, 1332, 1355, 1371, 1392, 1406, 1412, 1422, 1474, 1484, 1486, 1491, 1492, 1498, 1500, 1509, 1630, 2959, 2988, 3011, 3018, 3021, 3028, 3029, 3050, 3052, 3055, 3065, 3075, 3092, 3094, 3096, 3100	2.771	0.980	0.802
2-Octyl	$5s_{\beta}^{E}s_{\alpha}^{E}$	-1847, 63, 72, 112, 138, 159, 195, 228, 243, 336, 389, 402, 515, 557, 734, 756, 833, 852, 885, 896, 906, 957, 971, 984, 1041, 1061, 1077, 1107, 1127, 1130, 1177, 1217, 1221, 1265, 1280, 1305, 1324, 1331, 1367, 1372, 1395, 1405, 1412, 1429, 1476, 1484, 1486, 1491, 1493, 1498, 1499, 1510, 1636, 2951, 2988, 3012, 3018, 3019, 3021, 3028, 3049, 3051, 3054, 3057, 3067, 3074, 3094, 3096, 3100	3.350	0.820	0.699
2-Octyl	$6s_{\beta}^{A}s_{\alpha}^{A}$	-1700, 72, 84, 99, 165, 195, 212, 251, 297, 357, 406, 458, 512, 542, 746, 791, 808, 810, 869, 887, 933, 941, 985, 992, 1031, 1058, 1079, 1091, 1121, 1131, 1164, 1206, 1214, 1274, 1284, 1317, 1336, 1353, 1357, 1367, 1384, 1406, 1410, 1423, 1475, 1477, 1480, 1484, 1492, 1493, 1497, 1503, 1510, 2966, 2986, 2988, 2996, 3019, 3027, 3030, 3039, 3045, 3061, 3068, 3076, 3082, 3096, 3099, 3102	2.328	1.439	1.020
2-Octyl	$6s_{\beta}^{A}s_{\alpha}^{E}$	-1698, 76, 79, 106, 151, 190, 231, 252, 300, 335, 379, 461, 477, 568, 756, 796, 831, 834, 843, 894, 914, 940, 975, 1010, 1035, 1057, 1084, 1096, 1119, 1135, 1173, 1204, 1223, 1277, 1282, 1317, 1326, 1357, 1366, 1380, 1383, 1406, 1409, 1430, 1475, 1479, 1484, 1485, 1492, 1493, 1497, 1504, 1515, 2970, 2984, 2987, 2992, 3013, 3024, 3028, 3030, 3042, 3054, 3063, 3067, 3077, 3095, 3096, 3102	2.217	1.354	0.954
2-Octyl	$6s_{\beta}^{E}s_{\alpha}^{E}$	-1711, 62, 84, 98, 175, 196, 233, 272, 312, 361, 379, 431, 436, 515, 753, 793, 818, 844, 883, 887, 940, 959, 980, 1001, 1047, 1052, 1086, 1112, 1117, 1137, 1182, 1207, 1221, 1268, 1299, 1302, 1328, 1360, 1366, 1380, 1390, 1407, 1412, 1424, 1475, 1480, 1485, 1487, 1492, 1496, 1499, 1506, 1520, 2961, 2984, 2987, 2991, 3010, 3021, 3021, 3031, 3031, 3054, 3056, 3064, 3068, 3094, 3097, 3102	2.238	1.327	0.908
2-Octyl	$7s_{\alpha}^{A}s_{\alpha}^{A}$	-1646, 67, 90, 163, 175, 184, 207, 277, 308, 345, 393, 443, 511, 538, 748, 777, 807, 860, 861, 877, 918, 926, 986, 990, 1022, 1051, 1091, 1100, 1134, 1157, 1159, 1199, 1244, 1280, 1284, 1338, 1351, 1368, 1376, 1385, 1388, 1404, 1409, 1430, 1438, 1471, 1474, 1480, 1488, 1493, 1494, 1496, 1498, 2973, 2973, 2997, 2998, 3014, 3015, 3031, 3034, 3051, 3057, 3063, 3065, 3072, 3074, 3099, 3100	2.197	1.512	1.165
2-Octyl	$7s_{\alpha}^{A}s_{\alpha}^{E}$	-1654, 69, 95, 170, 180, 192, 219, 275, 323, 332, 358, 441, 482, 517, 752, 772, 821, 834, 884, 900, 919, 932, 980, 997, 1046, 1054, 1093, 1101, 1126, 1151, 1165, 1215, 1244, 1277, 1285, 1329, 1345, 1373, 1382, 1385, 1389, 1403, 1410, 1425, 1442, 1473, 1478, 1482, 1489, 1489, 1492, 1496, 1497, 2972, 2974, 2994,	2.091	1.620	1.071

		2995, 3003, 3015, 3018, 3032, 3049, 3052, 3055, 3060, 3064, 3072, 3095, 3099			
2-Octyl	$7s_{\alpha}{}^{E}s_{\alpha}{}^{E}$	-1650, 71, 134, 146, 169, 192, 223, 257, 291, 331, 333, 435, 489, 508, 772, 786, 812, 831, 892, 896, 932, 935, 972, 1012, 1049, 1071, 1090, 1102, 1114, 1143, 1178, 1221, 1248, 1273, 1283, 1324, 1334, 1380, 1383, 1385, 1388, 1403, 1408, 1431, 1448, 1476, 1479, 1484, 1487, 1489, 1491, 1495, 1495, 2973, 2973, 2993, 2994, 3003, 3003, 3017, 3017, 3049, 3050, 3052, 3053, 3060, 3062, 3095, 3095	1.932	1.660	0.968
3-Octyl	$3s_{\beta}s_{\beta}$	-1935, 41, 68, 79, 112, 133, 159, 207, 245, 253, 273, 343, 455, 460, 634, 726, 738, 790, 797, 888, 910, 934, 1001, 1023, 1055, 1067, 1079, 1096, 1117, 1164, 1185, 1224, 1248, 1270, 1294, 1301, 1313, 1328, 1347, 1382, 1400, 1408, 1411, 1424, 1475, 1480, 1484, 1496, 1497, 1499, 1506, 1511, 2193, 2937, 2947, 3004, 3010, 3017, 3021, 3028, 3032, 3032, 3057, 3095, 3098, 3100, 3105, 3143, 3154	10.964	0.486	0.480
3-Octyl	$4^{c}s_{\beta}s_{\beta}$	-2094, 33, 75, 90, 106, 160, 209, 238, 247, 272, 360, 387, 433, 574, 691, 744, 782, 835, 868, 885, 904, 933, 971, 1014, 1039, 1055, 1087, 1098, 1104, 1128, 1173, 1201, 1250, 1257, 1279, 1287, 1308, 1321, 1343, 1356, 1383, 1402, 1412, 1412, 1474, 1479, 1488, 1492, 1497, 1499, 1505, 1510, 1761, 2951, 2962, 3009, 3020, 3022, 3028, 3032, 3048, 3053, 3085, 3094, 3095, 3099, 3100, 3105, 3109	3.277	0.743	0.656
3-Octyl	$4^{t}s_{\beta}s_{\beta}$	-2088, 36, 71, 80, 119, 134, 183, 222, 248, 279, 372, 406, 430, 615, 727, 758, 772, 824, 858, 877, 907, 937, 957, 971, 1041, 1054, 1059, 1088, 1118, 1136, 1171, 1207, 1252, 1256, 1279, 1287, 1321, 1327, 1348, 1356, 1374, 1397, 1405, 1413, 1475, 1477, 1488, 1492, 1497, 1500, 1505, 1509, 1767, 2953, 3008, 3013, 3020, 3027, 3028, 3049, 3051, 3053, 3085, 3094, 3095, 3098, 3101, 3102, 3109	6.911	0.596	0.582
3-Octyl	$5s_{\beta}{}^{A}s_{\beta}{}^{A}$	-1824, 64, 87, 89, 93, 159, 240, 246, 256, 300, 388, 416, 572, 621, 743, 770, 794, 821, 871, 873, 922, 935, 989, 1008, 1018, 1060, 1069, 1083, 1100, 1125, 1172, 1209, 1226, 1276, 1277, 1309, 1313, 1323, 1337, 1368, 1392, 1408, 1410, 1423, 1477, 1478, 1487, 1496, 1497, 1498, 1504, 1505, 1617, 2972, 2972, 3024, 3025, 3026, 3030, 3031, 3034, 3057, 3075, 3090, 3091, 3097, 3098, 3103, 3103	2.504	1.095	0.861
3-Octyl	$5s_{\beta}{}^{A}s_{\beta}{}^{E}$	-1838, 52, 75, 93, 131, 170, 231, 246, 253, 338, 399, 410, 488, 590, 735, 770, 806, 840, 868, 882, 932, 951, 974, 1016, 1018, 1050, 1074, 1095, 1121, 1124, 1175, 1217, 1220, 1276, 1284, 1291, 1316, 1328, 1342, 1379, 1390, 1409, 1410, 1423, 1476, 1479, 1486, 1495, 1496, 1498, 1504, 1506, 1624, 2961, 2970, 3019, 3023, 3025, 3030, 3031, 3031, 3049, 3061, 3073, 3092, 3097, 3098, 3102, 3103	2.150	1.247	0.878
3-Octyl	$5s_{\beta}{}^{E}s_{\beta}{}^{E}$	-1841, 58, 85, 103, 119, 145, 228, 245, 254, 338, 399, 419, 510, 535, 736, 780, 792, 843, 875, 915, 939, 940, 973, 992, 1024, 1045, 1088, 1115, 1121, 1122, 1180, 1216, 1218, 1281, 1283, 1289, 1301, 1339, 1348, 1380, 1392, 1409, 1413, 1428, 1477, 1478, 1488, 1498, 1498, 1500, 1504, 1506, 1630, 2961, 2962, 3018, 3019, 3024, 3025, 3031, 3031, 3048, 3054, 3064, 3073, 3097, 3098, 3103, 3103	2.288	1.098	0.790
4-Octyl	$3s_{\beta}s_{\beta}$	-1933, 46, 63, 70, 127, 128, 148, 234, 241, 243, 275, 335, 451, 464, 634, 726, 744, 758, 872, 874, 889, 907, 996, 1030, 1058, 1060, 1081, 1108, 1109, 1163, 1183, 1224, 1257, 1260, 1289, 1301, 1320, 1321, 1343, 1381, 1399, 1410, 1412, 1425, 1476, 1477, 1491, 1492, 1499, 1499, 1509, 1509, 2194, 2935, 2938, 3010, 3010, 3020, 3020, 3028, 3028, 3052, 3053, 3094, 3094, 3101, 3101, 3143, 3154	11.481	0.483	0.478

Table S.2: G4 heat capacities for s-alkyl radicals and transition states. Units are cal mol^{-1} K^{-1} for S, cal mol^{-1} K^{-1} for Cp and kJ mol^{-1} for ddH.

Alkyl radical	Rxn Type	ddH	S	Cp 100	200	298	300	400	500	600	700	800	900	1000	1500
2-Butyl		4.6	77.8	13.3	17.7	22.5	22.6	28.2	33.6	38.3	42.4	45.9	49.0	51.7	60.8
2-Butyl	$3s_\alpha s_\alpha$	4.3	74.8	12.3	16.9	21.8	21.9	27.5	32.8	37.5	41.5	44.9	47.9	50.5	59.3
2-Pentyl		5.4	85.3	15.6	21.2	27.3	27.5	34.7	41.5	47.5	52.7	57.1	61.0	64.4	75.7
3-Pentyl		5.3	85.7	15.1	21.0	27.3	27.4	34.7	41.5	47.5	52.7	57.1	61.0	64.4	75.6
2-Pentyl	$3s_\beta s_\alpha$	5.1	82.4	14.5	20.4	26.7	26.8	34.0	40.8	46.7	51.8	56.1	59.9	63.2	74.2
2-Pentyl	$4^c s_\alpha s_\alpha$	4.9	81.0	13.4	19.2	25.8	26.0	33.6	40.6	46.7	51.9	56.3	60.1	63.4	74.3
2-Pentyl	$4^t s_\alpha s_\alpha$	4.9	81.8	13.9	19.3	25.9	26.0	33.6	40.7	46.8	52.0	56.4	60.2	63.5	74.4
2-Hexyl		6.2	93.2	18.1	24.8	32.2	32.4	41.2	49.5	56.8	63.0	68.4	73.0	77.1	90.5
3-Hexyl		6.1	93.2	17.4	24.5	32.1	32.3	41.1	49.5	56.7	63.0	68.4	73.0	77.0	90.5
2-Hexyl	$3s_\beta s_\alpha$	5.9	90.0	16.9	23.9	31.5	31.7	40.5	48.7	55.9	62.1	67.4	71.9	75.9	89.1
2-Hexyl	$4^c s_\beta s_\alpha$	5.7	88.5	15.6	22.7	30.7	30.9	40.1	48.6	56.0	62.2	67.6	72.2	76.1	89.2
2-Hexyl	$4^t s_\beta s_\alpha$	5.7	89.1	16.1	22.8	30.7	30.9	40.1	48.7	56.0	62.3	67.6	72.2	76.1	89.2
2-Hexyl	$5s_\alpha^A s_\alpha^A$	5.4	85.6	14.9	21.8	30.0	30.1	39.6	48.3	55.8	62.1	67.5	72.1	76.1	89.2
2-Hexyl	$5s_\alpha^A s_\alpha^E$	5.4	85.7	14.8	21.8	30.0	30.2	39.6	48.3	55.8	62.1	67.5	72.1	76.1	89.2
2-Hexyl	$5s_\alpha^E s_\alpha^E$	5.4	85.7	15.0	21.9	30.1	30.2	39.6	48.2	55.7	62.1	67.5	72.1	76.1	89.2
3-Hexyl	$3s_\beta s_\beta$	5.9	90.1	16.7	23.8	31.5	31.7	40.5	48.8	55.9	62.1	67.4	71.9	75.9	89.1
2-Heptyl		7.0	100.5	20.4	28.3	37.1	37.3	47.6	57.4	66.0	73.3	79.6	85.0	89.7	105.4
3-Heptyl		7.0	101.3	20.0	28.1	37.0	37.2	47.6	57.5	66.0	73.3	79.6	85.0	89.7	105.4
4-Heptyl		7.0	100.9	19.8	28.0	37.0	37.2	47.6	57.4	66.0	73.3	79.6	85.0	89.7	105.4
2-Heptyl	$3s_\beta s_\alpha$	6.8	97.6	19.3	27.5	36.4	36.6	47.0	56.7	65.2	72.4	78.6	83.9	88.6	104.0
2-Heptyl	$4^c s_\beta s_\alpha$	6.5	96.2	18.1	26.2	35.6	35.8	46.5	56.6	65.2	72.6	78.8	84.2	88.8	104.1
2-Heptyl	$4^t s_\beta s_\alpha$	6.6	96.8	18.5	26.3	35.6	35.8	46.6	56.6	65.3	72.6	78.8	84.2	88.8	104.1
2-Heptyl	$5s_\beta^A s_\alpha^A$	6.2	93.1	17.2	25.2	34.8	35.0	46.0	56.2	65.0	72.4	78.7	84.1	88.7	104.1
2-Heptyl	$5s_\beta^A s_\alpha^E$	6.3	93.3	17.1	25.3	34.9	35.1	46.0	56.2	65.0	72.4	78.7	84.1	88.7	104.1
2-Heptyl	$5s_\beta^E s_\alpha^E$	6.3	93.1	17.2	25.4	34.9	35.1	46.0	56.2	64.9	72.4	78.7	84.1	88.7	104.1
2-Heptyl	$6s_\alpha^A s_\alpha^A$	6.1	90.7	16.2	24.8	34.6	34.8	45.9	56.2	65.0	72.5	78.8	84.2	88.8	104.2
2-Heptyl	$6s_\alpha^A s_\alpha^E$	6.1	91.0	16.3	24.9	34.6	34.8	45.9	56.2	65.0	72.4	78.7	84.1	88.8	104.2
2-Heptyl	$6s_\alpha^E s_\alpha^E$	6.1	91.1	16.1	25.0	34.6	34.8	45.9	56.1	64.9	72.4	78.7	84.1	88.8	104.2
3-Heptyl	$3s_\beta s_\beta$	6.8	97.6	19.1	27.3	36.4	36.6	47.0	56.7	65.2	72.4	78.6	83.9	88.6	103.9
3-Heptyl	$4^c s_\beta s_\beta$	6.5	95.9	17.9	26.1	35.5	35.7	46.5	56.6	65.2	72.6	78.8	84.2	88.8	104.1
3-Heptyl	$4^t s_\beta s_\beta$	6.5	96.0	18.2	26.1	35.5	35.7	46.5	56.6	65.2	72.6	78.8	84.2	88.8	104.1
2-Octyl		7.9	108.1	22.9	31.8	42.0	42.2	54.1	65.4	75.2	83.6	90.8	97.0	102.4	120.3
3-Octyl		7.9	109.0	22.5	31.7	41.9	42.1	54.1	65.4	75.2	83.6	90.8	97.0	102.4	120.3
4-Octyl		7.8	108.6	22.3	31.6	41.9	42.1	54.1	65.4	75.2	83.6	90.8	97.0	102.4	120.3
2-Octyl	$3s_\beta s_\alpha$	7.6	105.0	21.7	31.0	41.3	41.5	53.4	64.6	74.4	82.7	89.8	95.9	101.2	118.8
2-Octyl	$4^c s_\beta s_\alpha$	7.4	103.9	20.5	29.8	40.5	40.7	53.0	64.5	74.5	82.9	90.0	96.2	101.5	119.0
2-Octyl	$4^t s_\beta s_\alpha$	7.4	104.1	20.9	29.9	40.5	40.7	53.0	64.6	74.5	82.9	90.0	96.2	101.5	119.0
2-Octyl	$5s_\beta^A s_\alpha^A$	7.1	100.6	19.6	28.7	39.7	39.9	52.5	64.2	74.2	82.7	89.9	96.1	101.4	119.0
2-Octyl	$5s_\beta^A s_\alpha^E$	7.1	100.7	19.4	28.8	39.7	39.9	52.5	64.2	74.2	82.7	89.9	96.1	101.4	119.0
2-Octyl	$5s_\beta^E s_\alpha^E$	7.1	100.7	19.6	28.9	39.8	40.0	52.5	64.1	74.2	82.7	89.9	96.1	101.4	119.0
2-Octyl	$6s_\beta^A s_\alpha^A$	6.9	98.2	18.5	28.3	39.5	39.7	52.4	64.2	74.2	82.8	90.0	96.2	101.5	119.1
2-Octyl	$6s_\beta^A s_\alpha^E$	6.9	98.5	18.6	28.4	39.5	39.7	52.4	64.1	74.2	82.7	89.9	96.1	101.5	119.1
2-Octyl	$6s_\beta^E s_\alpha^E$	6.9	98.6	18.4	28.4	39.5	39.7	52.3	64.0	74.1	82.7	89.9	96.1	101.5	119.1
2-Octyl	$7s_\alpha^A s_\alpha^A$	6.8	97.0	18.1	28.2	39.4	39.6	52.3	64.1	74.2	82.7	89.9	96.1	101.5	119.1
2-Octyl	$7s_\alpha^A s_\alpha^E$	6.8	96.9	18.0	28.3	39.4	39.7	52.3	64.1	74.2	82.7	89.9	96.1	101.5	119.1
2-Octyl	$7s_\alpha^E s_\alpha^E$	6.9	97.1	18.2	28.5	39.5	39.7	52.3	64.0	74.1	82.7	89.9	96.1	101.5	119.1
3-Octyl	$3s_\beta s_\beta$	7.6	105.4	21.6	30.9	41.3	41.5	53.4	64.7	74.4	82.7	89.8	95.9	101.2	118.8
3-Octyl	$4^c s_\beta s_\beta$	7.3	103.7	20.3	29.7	40.4	40.7	53.0	64.6	74.5	82.9	90.0	96.2	101.5	119.0

3-Octyl	$4^{t}s_{\beta}s_{\beta}$	7.4	103.7	20.6	29.6	40.4	40.6	53.0	64.6	74.5	82.9	90.0	96.2	101.4	119.0
3-Octyl	$5s_{\beta}^{A}s_{\beta}^{A}$	7.1	100.7	19.6	28.7	39.7	39.9	52.5	64.2	74.2	82.7	89.9	96.1	101.4	119.0
3-Octyl	$5s_{\beta}^{A}s_{\beta}^{E}$	7.1	100.6	19.3	28.7	39.7	39.9	52.5	64.2	74.2	82.7	89.9	96.1	101.4	119.0
3-Octyl	$5s_{\beta}^{E}s_{\beta}^{E}$	7.1	100.7	19.5	28.8	39.7	39.9	52.5	64.2	74.2	82.7	89.9	96.1	101.4	119.0
4-Octyl	$3s_{\beta}s_{\beta}$	7.6	105.4	21.6	30.9	41.3	41.5	53.5	64.7	74.4	82.7	89.8	96.0	101.2	118.8

Table S.3: G4 Arrhenius pre-exponential A-factors for the forward and reverse s-alkyl radical H-migrations.

Alkyl Radical	rxn type		Temperature (K) 200	300	400	500	600	700	800	900	1000	1500	2000	2500
2-Butyl	$3s_{\alpha}s_{\alpha}$	Forward	1.7E+12	2.1E+12	2.5E+12	2.8E+12	3.1E+12	3.4E+12	3.7E+12	4.0E+12	4.2E+12	5.2E+12	5.9E+12	6.5E+12
		Reverse	1.7E+12	2.1E+12	2.5E+12	2.8E+12	3.1E+12	3.4E+12	3.7E+12	4.0E+12	4.2E+12	5.2E+12	5.9E+12	6.5E+12
2-Pentyl	$3s_{\beta}s_{\alpha}$	Forward	1.8E+12	2.2E+12	2.6E+12	3.0E+12	3.4E+12	3.7E+12	4.0E+12	4.3E+12	4.6E+12	5.6E+12	6.4E+12	7.0E+12
		Reverse	1.4E+12	1.8E+12	2.1E+12	2.4E+12	2.7E+12	3.0E+12	3.3E+12	3.5E+12	3.8E+12	4.7E+12	5.4E+12	5.9E+12
2-Pentyl	$4^{c}s_{\alpha}s_{\alpha}$	Forward	1.6E+12	1.7E+12	1.8E+12	1.9E+12	2.0E+12	2.1E+12	2.2E+12	2.3E+12	2.4E+12	2.8E+12	3.2E+12	3.5E+12
		Reverse	1.6E+12	1.7E+12	1.8E+12	1.9E+12	2.0E+12	2.1E+12	2.2E+12	2.3E+12	2.4E+12	2.8E+12	3.2E+12	3.5E+12
2-Pentyl	$4^{t}s_{\alpha}s_{\alpha}$	Forward	2.0E+12	2.2E+12	2.4E+12	2.6E+12	2.8E+12	2.9E+12	3.1E+12	3.3E+12	3.4E+12	4.2E+12	4.7E+12	5.2E+12
		Reverse	2.0E+12	2.2E+12	2.4E+12	2.6E+12	2.8E+12	2.9E+12	3.1E+12	3.3E+12	3.4E+12	4.2E+12	4.7E+12	5.2E+12
2-Hexyl	$3s_{\beta}s_{\alpha}$	Forward	1.6E+12	2.0E+12	2.3E+12	2.6E+12	2.9E+12	3.1E+12	3.4E+12	3.6E+12	3.8E+12	4.7E+12	5.4E+12	5.8E+12
		Reverse	1.3E+12	1.7E+12	2.0E+12	2.4E+12	2.7E+12	3.0E+12	3.2E+12	3.5E+12	3.7E+12	4.6E+12	5.3E+12	5.8E+12
2-Hexyl	$4^{c}s_{\beta}s_{\alpha}$	Forward	1.5E+12	1.5E+12	1.5E+12	1.6E+12	1.7E+12	1.7E+12	1.8E+12	1.9E+12	2.0E+12	2.3E+12	2.6E+12	2.8E+12
		Reverse	1.2E+12	1.3E+12	1.4E+12	1.4E+12	1.5E+12	1.6E+12	1.7E+12	1.8E+12	1.9E+12	2.3E+12	2.6E+12	2.8E+12
2-Hexyl	$4^{t}s_{\beta}s_{\alpha}$	Forward	1.7E+12	1.8E+12	1.9E+12	2.0E+12	2.1E+12	2.2E+12	2.3E+12	2.5E+12	2.6E+12	3.1E+12	3.5E+12	3.8E+12
		Reverse	1.4E+12	1.6E+12	1.7E+12	1.8E+12	2.0E+12	2.1E+12	2.2E+12	2.3E+12	2.5E+12	3.0E+12	3.4E+12	3.7E+12
2-Hexyl	$5s_{\alpha}^{A}s_{\alpha}^{A}$	Forward	5.9E+11	5.1E+11	4.6E+11	4.4E+11	4.4E+11	4.4E+11	4.4E+11	4.5E+11	4.5E+11	5.0E+11	5.4E+11	5.7E+11
		Reverse	5.9E+11	5.1E+11	4.6E+11	4.4E+11	4.4E+11	4.4E+11	4.4E+11	4.5E+11	4.5E+11	5.0E+11	5.4E+11	5.7E+11
2-Hexyl	$5s_{\alpha}^{A}s_{\alpha}^{E}$	Forward	6.3E+11	5.4E+11	4.9E+11	4.7E+11	4.6E+11	4.7E+11	4.7E+11	4.8E+11	4.9E+11	5.3E+11	5.8E+11	6.1E+11
		Reverse	6.3E+11	5.4E+11	4.9E+11	4.7E+11	4.6E+11	4.7E+11	4.7E+11	4.8E+11	4.9E+11	5.3E+11	5.8E+11	6.1E+11
2-Hexyl	$5s_{\alpha}^{E}s_{\alpha}^{E}$	Forward	6.2E+11	5.4E+11	5.0E+11	4.8E+11	4.7E+11	4.8E+11	4.8E+11	4.9E+11	5.0E+11	5.5E+11	5.9E+11	6.3E+11
		Reverse	6.2E+11	5.4E+11	5.0E+11	4.8E+11	4.7E+11	4.8E+11	4.8E+11	4.9E+11	5.0E+11	5.5E+11	5.9E+11	6.3E+11
3-Hexyl	$3s_{\beta}s_{\beta}$	Forward	1.4E+12	1.8E+12	2.2E+12	2.6E+12	2.9E+12	3.2E+12	3.5E+12	3.7E+12	4.0E+12	5.0E+12	5.7E+12	6.2E+12
		Reverse	1.4E+12	1.8E+12	2.2E+12	2.6E+12	2.9E+12	3.2E+12	3.5E+12	3.7E+12	4.0E+12	5.0E+12	5.7E+12	6.2E+12
2-Heptyl	$3s_{\beta}s_{\alpha}$	Forward	1.8E+12	2.3E+12	2.7E+12	3.0E+12	3.4E+12	3.7E+12	4.0E+12	4.3E+12	4.6E+12	5.7E+12	6.5E+12	7.1E+12
		Reverse	1.1E+12	1.5E+12	1.7E+12	2.0E+12	2.2E+12	2.5E+12	2.7E+12	2.9E+12	3.0E+12	3.8E+12	4.3E+12	4.7E+12
2-Heptyl	$4^{c}s_{\beta}s_{\alpha}$	Forward	1.7E+12	1.8E+12	1.8E+12	1.9E+12	2.0E+12	2.1E+12	2.2E+12	2.3E+12	2.4E+12	2.9E+12	3.2E+12	3.5E+12
		Reverse	1.2E+12	1.3E+12	1.4E+12	1.5E+12	1.6E+12	1.7E+12	1.8E+12	1.9E+12	2.0E+12	2.4E+12	2.7E+12	2.9E+12
2-Heptyl	$4^{t}s_{\beta}s_{\alpha}$	Forward	2.0E+12	2.1E+12	2.3E+12	2.4E+12	2.5E+12	2.7E+12	2.8E+12	3.0E+12	3.1E+12	3.8E+12	4.3E+12	4.6E+12
		Reverse	1.4E+12	1.6E+12	1.7E+12	1.9E+12	2.0E+12	2.2E+12	2.3E+12	2.4E+12	2.5E+12	3.1E+12	3.5E+12	3.9E+12
2-Heptyl	$5s_{\beta}^{A}s_{\alpha}^{A}$	Forward	6.6E+11	5.7E+11	5.2E+11	5.0E+11	4.9E+11	4.9E+11	4.9E+11	5.0E+11	5.1E+11	5.6E+11	6.0E+11	6.4E+11
		Reverse	4.1E+11	3.6E+11	3.4E+11	3.2E+11	3.2E+11	3.2E+11	3.3E+11	3.3E+11	3.4E+11	3.7E+11	4.0E+11	4.3E+11
2-Heptyl	$5s_{\beta}^{A}s_{\alpha}^{E}$	Forward	7.2E+11	6.2E+11	5.7E+11	5.4E+11	5.4E+11	5.4E+11	5.4E+11	5.5E+11	5.6E+11	6.2E+11	6.7E+11	7.1E+11
		Reverse	4.5E+11	4.0E+11	3.7E+11	3.6E+11	3.5E+11	3.5E+11	3.6E+11	3.6E+11	3.7E+11	4.1E+11	4.5E+11	4.7E+11

2-Heptyl	$5s_{\beta}^{E}s_{\alpha}^{E}$	Forward	6.6E+11	5.7E+11	5.3E+11	5.1E+11	5.0E+11	5.0E+11	5.0E+11	5.1E+11	5.2E+11	5.7E+11	6.2E+11	6.6E+11
		Reverse	4.2E+11	3.7E+11	3.4E+11	3.3E+11	3.3E+11	3.3E+11	3.3E+11	3.4E+11	3.5E+11	3.8E+11	4.1E+11	4.4E+11
2-Heptyl	$6s_{\alpha}^{A}s_{\alpha}^{A}$	Forward	3.1E+11	2.4E+11	2.0E+11	1.8E+11	1.7E+11	1.7E+11	1.7E+11	1.7E+11	1.7E+11	1.8E+11	2.0E+11	2.1E+11
		Reverse	3.1E+11	2.4E+11	2.0E+11	1.8E+11	1.7E+11	1.7E+11	1.7E+11	1.7E+11	1.7E+11	1.8E+11	2.0E+11	2.1E+11
2-Heptyl	$6s_{\alpha}^{A}s_{\alpha}^{E}$	Forward	3.4E+11	2.6E+11	2.2E+11	2.0E+11	2.0E+11	1.9E+11	1.9E+11	1.9E+11	1.9E+11	2.1E+11	2.2E+11	2.3E+11
		Reverse	3.4E+11	2.6E+11	2.2E+11	2.0E+11	2.0E+11	1.9E+11	1.9E+11	1.9E+11	1.9E+11	2.1E+11	2.2E+11	2.3E+11
2-Heptyl	$6s_{\alpha}^{E}s_{\alpha}^{E}$	Forward	3.6E+11	2.8E+11	2.4E+11	2.2E+11	2.1E+11	2.0E+11	2.0E+11	2.0E+11	2.0E+11	2.1E+11	2.3E+11	2.4E+11
		Reverse	3.6E+11	2.8E+11	2.4E+11	2.2E+11	2.1E+11	2.0E+11	2.0E+11	2.0E+11	2.0E+11	2.1E+11	2.3E+11	2.4E+11
3-Heptyl	$3s_{\beta}s_{\beta}$	Forward	1.2E+12	1.5E+12	1.8E+12	2.1E+12	2.3E+12	2.5E+12	2.7E+12	2.9E+12	3.1E+12	3.9E+12	4.4E+12	4.8E+12
		Reverse	1.4E+12	1.8E+12	2.1E+12	2.5E+12	2.8E+12	3.1E+12	3.3E+12	3.6E+12	3.8E+12	4.8E+12	5.5E+12	6.0E+12
3-Heptyl	$4^{c}s_{\beta}s_{\beta}$	Forward	1.0E+12	1.0E+12	1.1E+12	1.1E+12	1.2E+12	1.2E+12	1.3E+12	1.4E+12	1.4E+12	1.7E+12	1.9E+12	2.0E+12
		Reverse	1.0E+12	1.0E+12	1.1E+12	1.1E+12	1.2E+12	1.2E+12	1.3E+12	1.4E+12	1.4E+12	1.7E+12	1.9E+12	2.0E+12
3-Heptyl	$4^{t}s_{\beta}s_{\beta}$	Forward	9.7E+11	1.0E+12	1.1E+12	1.1E+12	1.2E+12	1.2E+12	1.3E+12	1.4E+12	1.4E+12	1.7E+12	1.9E+12	2.1E+12
		Reverse	9.7E+11	1.0E+12	1.1E+12	1.1E+12	1.2E+12	1.2E+12	1.3E+12	1.4E+12	1.4E+12	1.7E+12	1.9E+12	2.1E+12
2-Octyl	$3s_{\beta}s_{\alpha}$	Forward	1.7E+12	2.0E+12	2.4E+12	2.7E+12	3.0E+12	3.3E+12	3.6E+12	3.8E+12	4.1E+12	5.0E+12	5.7E+12	6.2E+12
		Reverse	9.9E+11	1.2E+12	1.5E+12	1.7E+12	1.9E+12	2.1E+12	2.3E+12	2.4E+12	2.6E+12	3.2E+12	3.6E+12	4.0E+12
2-Octyl	$4^{c}s_{\beta}s_{\alpha}$	Forward	1.8E+12	1.8E+12	1.9E+12	2.0E+12	2.0E+12	2.1E+12	2.3E+12	2.4E+12	2.5E+12	2.9E+12	3.3E+12	3.6E+12
		Reverse	1.1E+12	1.2E+12	1.3E+12	1.4E+12	1.5E+12	1.6E+12	1.7E+12	1.8E+12	1.9E+12	2.2E+12	2.5E+12	2.8E+12
2-Octyl	$4^{t}s_{\beta}s_{\alpha}$	Forward	1.8E+12	1.9E+12	2.0E+12	2.1E+12	2.2E+12	2.3E+12	2.5E+12	2.6E+12	2.7E+12	3.3E+12	3.7E+12	4.0E+12
		Reverse	1.2E+12	1.3E+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
2-Octyl	$5s_{\beta}^{A}s_{\alpha}^{A}$	Forward	6.4E+11	5.5E+11	5.0E+11	4.8E+11	4.7E+11	4.7E+11	4.7E+11	4.8E+11	4.8E+11	5.3E+11	5.7E+11	6.1E+11
		Reverse	4.2E+11	3.8E+11	3.5E+11	3.4E+11	3.4E+11	3.4E+11	3.5E+11	3.6E+11	3.6E+11	4.0E+11	4.4E+11	4.7E+11
2-Octyl	$5s_{\beta}^{A}s_{\alpha}^{E}$	Forward	6.9E+11	5.9E+11	5.3E+11	5.1E+11	5.0E+11	5.0E+11	5.0E+11	5.1E+11	5.2E+11	5.7E+11	6.1E+11	6.5E+11
		Reverse	4.5E+11	4.1E+11	3.8E+11	3.7E+11	3.7E+11	3.7E+11	3.7E+11	3.8E+11	3.9E+11	4.3E+11	4.7E+11	5.0E+11
2-Octyl	$5s_{\beta}^{E}s_{\alpha}^{E}$	Forward	6.6E+11	5.7E+11	5.2E+11	5.0E+11	4.9E+11	4.9E+11	5.0E+11	5.1E+11	5.1E+11	5.7E+11	6.1E+11	6.5E+11
		Reverse	4.3E+11	3.9E+11	3.7E+11	3.6E+11	3.6E+11	3.7E+11	3.7E+11	3.8E+11	3.9E+11	4.3E+11	4.7E+11	5.0E+11
2-Octyl	$6s_{\beta}^{A}s_{\alpha}^{A}$	Forward	3.0E+11	2.2E+11	1.9E+11	1.7E+11	1.6E+11	1.6E+11	1.5E+11	1.5E+11	1.6E+11	1.7E+11	1.8E+11	1.9E+11
		Reverse	1.8E+11	1.3E+11	1.1E+11	1.0E+11	1.0E+11	9.8E+10	9.7E+10	9.7E+10	9.8E+10	1.1E+11	1.1E+11	1.2E+11
2-Octyl	$6s_{\beta}^{A}s_{\alpha}^{E}$	Forward	3.3E+11	2.5E+11	2.1E+11	1.9E+11	1.8E+11	1.8E+11	1.7E+11	1.7E+11	1.8E+11	1.9E+11	2.0E+11	2.1E+11
		Reverse	2.0E+11	1.5E+11	1.3E+11	1.2E+11	1.1E+11	1.1E+11	1.1E+11	1.1E+11	1.1E+11	1.2E+11	1.3E+11	1.3E+11
2-Octyl	$6s_{\beta}^{E}s_{\alpha}^{E}$	Forward	3.5E+11	2.6E+11	2.2E+11	2.0E+11	1.9E+11	1.9E+11	1.8E+11	1.8E+11	1.8E+11	2.0E+11	2.1E+11	2.2E+11
		Reverse	2.1E+11	1.6E+11	1.4E+11	1.3E+11	1.2E+11	1.2E+11	1.2E+11	1.2E+11	1.2E+11	1.2E+11	1.3E+11	1.4E+11
2-Octyl	$7s_{\alpha}^{A}s_{\alpha}^{A}$	Forward	2.0E+11	1.4E+11	1.2E+11	1.0E+11	9.6E+10	9.2E+10	9.0E+10	9.0E+10	9.0E+10	9.4E+10	1.0E+11	1.0E+11
		Reverse	2.0E+11	1.4E+11	1.2E+11	1.0E+11	9.6E+10	9.2E+10	9.0E+10	9.0E+10	9.0E+10	9.4E+10	1.0E+11	1.0E+11
2-Octyl	$7s_{\alpha}^{A}s_{\alpha}^{E}$	Forward	1.9E+11	1.3E+11	1.1E+11	9.4E+10	8.8E+10	8.4E+10	8.3E+10	8.2E+10	8.2E+10	8.6E+10	9.1E+10	9.6E+10
		Reverse	1.9E+11	1.3E+11	1.1E+11	9.4E+10	8.8E+10	8.4E+10	8.3E+10	8.2E+10	8.2E+10	8.6E+10	9.1E+10	9.6E+10
2-Octyl	$7s_{\alpha}^{E}s_{\alpha}^{E}$	Forward	1.9E+11	1.4E+11	1.1E+11	1.0E+11	9.4E+10	9.1E+10	9.0E+10	8.9E+10	9.0E+10	9.4E+10	1.0E+11	1.1E+11

		Reverse	1.9E+11	1.4E+11	1.1E+11	1.0E+11	9.4E+10	9.1E+10	9.0E+10	8.9E+10	9.0E+10	9.4E+10	1.0E+11	1.1E+11
3-Octyl	$3s_{\beta}s_{\beta}$	Forward	1.2E+12	1.5E+12	1.8E+12	2.0E+12	2.3E+12	2.5E+12	2.7E+12	2.9E+12	3.1E+12	3.9E+12	4.4E+12	4.8E+12
		Reverse	1.3E+12	1.7E+12	2.1E+12	2.4E+12	2.7E+12	3.0E+12	3.2E+12	3.5E+12	3.7E+12	4.6E+12	5.3E+12	5.8E+12
3-Octyl	$4^{c}s_{\beta}s_{\beta}$	Forward	1.0E+12	1.1E+12	1.1E+12	1.2E+12	1.2E+12	1.3E+12	1.3E+12	1.4E+12	1.5E+12	1.7E+12	2.0E+12	2.1E+12
		Reverse	1.1E+12	1.2E+12	1.3E+12	1.3E+12	1.4E+12	1.5E+12	1.6E+12	1.7E+12	1.7E+12	2.1E+12	2.4E+12	2.6E+12
3-Octyl	$4^{t}s_{\beta}s_{\beta}$	Forward	9.7E+11	1.0E+12	1.1E+12	1.1E+12	1.2E+12	1.2E+12	1.3E+12	1.4E+12	1.4E+12	1.7E+12	1.9E+12	2.1E+12
		Reverse	1.1E+12	1.2E+12	1.2E+12	1.3E+12	1.4E+12	1.5E+12	1.5E+12	1.6E+12	1.7E+12	2.0E+12	2.3E+12	2.5E+12
3-Octyl	$5s_{\beta}^{A}s_{\beta}^{A}$	Forward	4.1E+11	3.6E+11	3.3E+11	3.2E+11	3.1E+11	3.1E+11	3.2E+11	3.2E+11	3.3E+11	3.6E+11	3.9E+11	4.2E+11
		Reverse	4.1E+11	3.6E+11	3.3E+11	3.2E+11	3.1E+11	3.1E+11	3.2E+11	3.2E+11	3.3E+11	3.6E+11	3.9E+11	4.2E+11
3-Octyl	$5s_{\beta}^{A}s_{\beta}^{E}$	Forward	4.0E+11	3.5E+11	3.2E+11	3.0E+11	3.0E+11	3.0E+11	3.0E+11	3.1E+11	3.1E+11	3.4E+11	3.7E+11	4.0E+11
		Reverse	4.0E+11	3.5E+11	3.2E+11	3.0E+11	3.0E+11	3.0E+11	3.0E+11	3.1E+11	3.1E+11	3.4E+11	3.7E+11	4.0E+11
3-Octyl	$5s_{\beta}^{E}s_{\beta}^{E}$	Forward	4.0E+11	3.5E+11	3.2E+11	3.1E+11	3.0E+11	3.0E+11	3.1E+11	3.1E+11	3.2E+11	3.5E+11	3.8E+11	4.0E+11
		Reverse	4.0E+11	3.5E+11	3.2E+11	3.1E+11	3.0E+11	3.0E+11	3.1E+11	3.1E+11	3.2E+11	3.5E+11	3.8E+11	4.0E+11
4-Octyl	$3s_{\beta}s_{\beta}$	Forward	1.3E+12	1.7E+12	2.1E+12	2.4E+12	2.7E+12	3.0E+12	3.3E+12	3.6E+12	3.8E+12	4.8E+12	5.5E+12	6.0E+12
		Reverse	1.3E+12	1.7E+12	2.1E+12	2.4E+12	2.7E+12	3.0E+12	3.3E+12	3.6E+12	3.8E+12	4.8E+12	5.5E+12	6.0E+12

Table S.4: Skodje and Truhlar tunneling transmission coefficient for s-alkyl radical H-migrations, determined using G4 frequencies and energy values.

Alkyl radical	rxn type		Temperature (K) 200	300	400	500	600	700	800	900	1000	1500	2000	2500
2-Butyl	$3s_\alpha s_\alpha$	Forward	1.3E+24	8.1E+09	1552	8.2	3.2	2.2	1.8	1.6	1.4	1.2	1.1	1.1
		Reverse	1.3E+24	8.1E+09	1552	8.2	3.2	2.2	1.8	1.6	1.4	1.2	1.1	1.1
2-Pentyl	$3s_\beta s_\alpha$	Forward	4.5E+23	5.0E+09	1307	8.1	3.2	2.2	1.8	1.6	1.4	1.2	1.1	1.1
		Reverse	4.5E+23	5.0E+09	1307	8.1	3.2	2.2	1.8	1.6	1.4	1.2	1.1	1.1
2-Pentyl	$4^c s_\alpha s_\alpha$	Forward	1.5E+26	3.8E+11	34549	20.9	4.4	2.6	2.0	1.7	1.5	1.2	1.1	1.1
		Reverse	1.5E+26	3.8E+11	34549	20.9	4.4	2.6	2.0	1.7	1.5	1.2	1.1	1.1
2-Pentyl	$4^t s_\alpha s_\alpha$	Forward	8.0E+25	2.7E+11	27974	19.7	4.3	2.6	2.0	1.7	1.5	1.2	1.1	1.1
		Reverse	8.0E+25	2.7E+11	27974	19.7	4.3	2.6	2.0	1.7	1.5	1.2	1.1	1.1
2-Hexyl	$3s_\beta s_\alpha$	Forward	3.9E+23	4.7E+09	1281	8.1	3.2	2.2	1.8	1.6	1.4	1.2	1.1	1.1
		Reverse	3.9E+23	4.7E+09	1281	8.1	3.2	2.2	1.8	1.6	1.4	1.2	1.1	1.1
2-Hexyl	$4^c s_\beta s_\alpha$	Forward	3.0E+25	1.8E+11	25433	20.0	4.3	2.6	2.0	1.7	1.5	1.2	1.1	1.1
		Reverse	3.0E+25	1.8E+11	25433	20.0	4.3	2.6	2.0	1.7	1.5	1.2	1.1	1.1
2-Hexyl	$4^t s_\beta s_\alpha$	Forward	1.6E+25	1.3E+11	20359	18.6	4.2	2.6	2.0	1.7	1.5	1.2	1.1	1.1
		Reverse	1.6E+25	1.3E+11	20359	18.6	4.2	2.6	2.0	1.7	1.5	1.2	1.1	1.1
2-Hexyl	$5s_\alpha^A s_\alpha^A$	Forward	2.1E+14	4.5E+05	71	5.4	2.7	2.0	1.7	1.5	1.4	1.1	1.1	1.0
		Reverse	2.1E+14	4.5E+05	71	5.4	2.7	2.0	1.7	1.5	1.4	1.1	1.1	1.0
2-Hexyl	$5s_\alpha^A s_\alpha^E$	Forward	2.3E+14	5.2E+05	80	5.7	2.8	2.0	1.7	1.5	1.4	1.1	1.1	1.0
		Reverse	2.3E+14	5.2E+05	80	5.7	2.8	2.0	1.7	1.5	1.4	1.1	1.1	1.0
2-Hexyl	$5s_\alpha^E s_\alpha^E$	Forward	1.8E+14	4.9E+05	80	5.7	2.8	2.0	1.7	1.5	1.4	1.1	1.1	1.0
		Reverse	1.8E+14	4.9E+05	80	5.7	2.8	2.0	1.7	1.5	1.4	1.1	1.1	1.0
3-Hexyl	$3s_\beta s_\beta$	Forward	6.5E+23	5.4E+09	1249	7.9	3.2	2.2	1.8	1.5	1.4	1.2	1.1	1.1
		Reverse	6.5E+23	5.4E+09	1249	7.9	3.2	2.2	1.8	1.5	1.4	1.2	1.1	1.1
2-Heptyl	$3s_\beta s_\alpha$	Forward	5.1E+23	5.2E+09	1321	8.1	3.2	2.2	1.8	1.6	1.4	1.2	1.1	1.1
		Reverse	5.1E+23	5.2E+09	1321	8.1	3.2	2.2	1.8	1.6	1.4	1.2	1.1	1.1
2-Heptyl	$4^c s_\beta s_\alpha$	Forward	2.8E+25	1.8E+11	25124	19.9	4.3	2.6	2.0	1.7	1.5	1.2	1.1	1.1
		Reverse	2.8E+25	1.8E+11	25124	19.9	4.3	2.6	2.0	1.7	1.5	1.2	1.1	1.1
2-Heptyl	$4^t s_\beta s_\alpha$	Forward	1.6E+25	1.3E+11	20411	18.7	4.2	2.6	2.0	1.7	1.5	1.2	1.1	1.1
		Reverse	1.6E+25	1.3E+11	20411	18.7	4.2	2.6	2.0	1.7	1.5	1.2	1.1	1.1
2-Heptyl	$5s_\beta^A s_\alpha^A$	Forward	5.5E+13	2.6E+05	62	5.3	2.7	2.0	1.6	1.5	1.4	1.1	1.1	1.0
		Reverse	5.5E+13	2.6E+05	62	5.3	2.7	2.0	1.6	1.5	1.4	1.1	1.1	1.0
2-Heptyl	$5s_\beta^A s_\alpha^E$	Forward	6.0E+13	3.1E+05	71	5.6	2.8	2.0	1.7	1.5	1.4	1.1	1.1	1.0
		Reverse	6.0E+13	3.1E+05	71	5.6	2.8	2.0	1.7	1.5	1.4	1.1	1.1	1.0
2-Heptyl	$5s_\beta^E s_\alpha^E$	Forward	5.9E+13	3.1E+05	72	5.6	2.8	2.0	1.7	1.5	1.4	1.1	1.1	1.0
		Reverse	5.9E+13	3.1E+05	72	5.6	2.8	2.0	1.7	1.5	1.4	1.1	1.1	1.0
2-Heptyl	$6s_\alpha^A s_\alpha^A$	Forward	5.4E+09	3.9E+03	16	3.8	2.3	1.8	1.5	1.4	1.3	1.1	1.1	1.0
		Reverse	5.4E+09	3.9E+03	16	3.8	2.3	1.8	1.5	1.4	1.3	1.1	1.1	1.0
2-Heptyl	$6s_\alpha^A s_\alpha^E$	Forward	4.3E+09	3.7E+03	17	3.8	2.3	1.8	1.5	1.4	1.3	1.1	1.1	1.0
		Reverse	4.3E+09	3.7E+03	17	3.8	2.3	1.8	1.5	1.4	1.3	1.1	1.1	1.0
2-Heptyl	$6s_\alpha^E s_\alpha^E$	Forward	5.7E+09	4.4E+03	18	3.9	2.3	1.8	1.5	1.4	1.3	1.1	1.1	1.0
		Reverse	5.7E+09	4.4E+03	18	3.9	2.3	1.8	1.5	1.4	1.3	1.1	1.1	1.0
3-Heptyl	$3s_\beta s_\beta$	Forward	5.6E+23	5.1E+09	1227	7.9	3.2	2.2	1.8	1.5	1.4	1.2	1.1	1.1
		Reverse	5.6E+23	5.1E+09	1227	7.9	3.2	2.2	1.8	1.5	1.4	1.2	1.1	1.1
3-Heptyl	$4^c s_\beta s_\beta$	Forward	3.7E+25	1.9E+11	24120	19.2	4.3	2.6	2.0	1.7	1.5	1.2	1.1	1.1
		Reverse	3.7E+25	1.9E+11	24120	19.2	4.3	2.6	2.0	1.7	1.5	1.2	1.1	1.1
3-Heptyl	$4^t s_\beta s_\beta$	Forward	3.8E+25	1.8E+11	21900	18.3	4.2	2.6	2.0	1.7	1.5	1.2	1.1	1.1

		Reverse	3.8E+25	1.8E+11	21900	18.3	4.2	2.6	2.0	1.7	1.5	1.2	1.1	1.1
2-Octyl	$3s_\beta s_\alpha$	Forward	1.2E+24	7.3E+09	1422	8.1	3.2	2.2	1.8	1.6	1.4	1.2	1.1	1.1
		Reverse	1.2E+24	7.3E+09	1422	8.1	3.2	2.2	1.8	1.6	1.4	1.2	1.1	1.1
2-Octyl	$4^c s_\beta s_\alpha$	Forward	3.3E+25	1.9E+11	25831	20.0	4.3	2.6	2.0	1.7	1.5	1.2	1.1	1.1
		Reverse	3.3E+25	1.9E+11	25831	20.0	4.3	2.6	2.0	1.7	1.5	1.2	1.1	1.1
2-Octyl	$4^t s_\beta s_\alpha$	Forward	2.0E+25	1.4E+11	21301	18.8	4.2	2.6	2.0	1.7	1.5	1.2	1.1	1.1
		Reverse	2.0E+25	1.4E+11	21301	18.8	4.2	2.6	2.0	1.7	1.5	1.2	1.1	1.1
2-Octyl	$5s_\beta^A s_\alpha^A$	Forward	4.0E+13	2.4E+05	62	5.4	2.7	2.0	1.7	1.5	1.4	1.1	1.1	1.0
		Reverse	4.0E+13	2.4E+05	62	5.4	2.7	2.0	1.7	1.5	1.4	1.1	1.1	1.0
2-Octyl	$5s_\beta^A s_\alpha^E$	Forward	4.3E+13	2.7E+05	69	5.6	2.8	2.0	1.7	1.5	1.4	1.1	1.1	1.0
		Reverse	4.3E+13	2.7E+05	69	5.6	2.8	2.0	1.7	1.5	1.4	1.1	1.1	1.0
2-Octyl	$5s_\beta^E s_\alpha^E$	Forward	4.4E+13	2.8E+05	71	5.6	2.8	2.0	1.7	1.5	1.4	1.1	1.1	1.0
		Reverse	4.4E+13	2.8E+05	71	5.6	2.8	2.0	1.7	1.5	1.4	1.1	1.1	1.0
2-Octyl	$6s_\beta^A s_\alpha^A$	Forward	1.5E+09	2.7E+03	16	3.8	2.3	1.8	1.5	1.4	1.3	1.1	1.1	1.0
		Reverse	1.5E+09	2.7E+03	16	3.8	2.3	1.8	1.5	1.4	1.3	1.1	1.1	1.0
2-Octyl	$6s_\beta^A s_\alpha^E$	Forward	1.1E+09	2.4E+03	16	3.8	2.3	1.8	1.5	1.4	1.3	1.1	1.1	1.0
		Reverse	1.1E+09	2.4E+03	16	3.8	2.3	1.8	1.5	1.4	1.3	1.1	1.1	1.0
2-Octyl	$6s_\beta^E s_\alpha^E$	Forward	1.7E+09	3.0E+03	17	3.9	2.3	1.8	1.5	1.4	1.3	1.1	1.1	1.0
		Reverse	1.7E+09	3.0E+03	17	3.9	2.3	1.8	1.5	1.4	1.3	1.1	1.1	1.0
2-Octyl	$7s_\alpha^A s_\alpha^A$	Forward	2.5E+09	2.1E+03	12	3.4	2.1	1.7	1.5	1.4	1.3	1.1	1.1	1.0
		Reverse	2.5E+09	2.1E+03	12	3.4	2.1	1.7	1.5	1.4	1.3	1.1	1.1	1.0
2-Octyl	$7s_\alpha^A s_\alpha^E$	Forward	1.4E+09	1.9E+03	13	3.4	2.2	1.7	1.5	1.4	1.3	1.1	1.1	1.0
		Reverse	1.4E+09	1.9E+03	13	3.4	2.2	1.7	1.5	1.4	1.3	1.1	1.1	1.0
2-Octyl	$7s_\alpha^E s_\alpha^E$	Forward	5.7E+08	1.4E+03	12	3.4	2.2	1.7	1.5	1.4	1.3	1.1	1.1	1.0
		Reverse	5.7E+08	1.4E+03	12	3.4	2.2	1.7	1.5	1.4	1.3	1.1	1.1	1.0
3-Octyl	$3s_\beta s_\beta$	Forward	7.0E+23	5.6E+09	1258	7.9	3.2	2.2	1.8	1.5	1.4	1.2	1.1	1.1
		Reverse	7.0E+23	5.6E+09	1258	7.9	3.2	2.2	1.8	1.5	1.4	1.2	1.1	1.1
3-Octyl	$4^c s_\beta s_\beta$	Forward	2.6E+25	1.6E+11	23171	19.3	4.3	2.6	2.0	1.7	1.5	1.2	1.1	1.1
		Reverse	2.6E+25	1.6E+11	23171	19.3	4.3	2.6	2.0	1.7	1.5	1.2	1.1	1.1
3-Octyl	$4^t s_\beta s_\beta$	Forward	2.9E+25	1.6E+11	21277	18.4	4.2	2.6	2.0	1.7	1.5	1.2	1.1	1.1
		Reverse	2.9E+25	1.6E+11	21277	18.4	4.2	2.6	2.0	1.7	1.5	1.2	1.1	1.1
3-Octyl	$5s_\beta^A s_\beta^A$	Forward	4.2E+13	2.3E+05	58	5.3	2.7	2.0	1.6	1.5	1.4	1.1	1.1	1.0
		Reverse	4.2E+13	2.3E+05	58	5.3	2.7	2.0	1.6	1.5	1.4	1.1	1.1	1.0
3-Octyl	$5s_\beta^A s_\beta^E$	Forward	5.2E+13	2.8E+05	67	5.5	2.7	2.0	1.7	1.5	1.4	1.1	1.1	1.0
		Reverse	5.2E+13	2.8E+05	67	5.5	2.7	2.0	1.7	1.5	1.4	1.1	1.1	1.0
3-Octyl	$5s_\beta^E s_\beta^E$	Forward	5.4E+13	2.9E+05	69	5.5	2.7	2.0	1.7	1.5	1.4	1.1	1.1	1.0
		Reverse	5.4E+13	2.9E+05	69	5.5	2.7	2.0	1.7	1.5	1.4	1.1	1.1	1.0
4-Octyl	$3s_\beta s_\beta$	Forward	5.6E+23	5.0E+09	1199	7.9	3.2	2.2	1.8	1.5	1.4	1.2	1.1	1.1
		Reverse	5.6E+23	5.0E+09	1199	7.9	3.2	2.2	1.8	1.5	1.4	1.2	1.1	1.1

Table S.5: Wigner tunneling transmission coefficient for s-alkyl radical H-migrations, determined using G4 frequencies and energy values

Alkyl radical	rxn type		Temperature (K)											
			200	300	400	500	600	700	800	900	1000	1500	2000	2500
2-Butyl	$3s_\alpha s_\alpha$	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
2-Pentyl	$3s_\beta s_\alpha$	Forward	9.1	4.6	3.0	2.3	1.9	1.7	1.5	1.4	1.3	1.1	1.1	1.1
		Reverse	9.1	4.6	3.0	2.3	1.9	1.7	1.5	1.4	1.3	1.1	1.1	1.1
2-Pentyl	$4^c s_\alpha s_\alpha$	Forward	10.5	5.2	3.4	2.5	2.1	1.8	1.6	1.5	1.4	1.2	1.1	1.1
		Reverse	10.5	5.2	3.4	2.5	2.1	1.8	1.6	1.5	1.4	1.2	1.1	1.1
2-Pentyl	$4^t s_\alpha s_\alpha$	Forward	10.5	5.2	3.4	2.5	2.1	1.8	1.6	1.5	1.4	1.2	1.1	1.1
		Reverse	10.5	5.2	3.4	2.5	2.1	1.8	1.6	1.5	1.4	1.2	1.1	1.1
2-Hexyl	$3s_\beta s_\alpha$	Forward	9.1	4.6	3.0	2.3	1.9	1.7	1.5	1.4	1.3	1.1	1.1	1.1
		Reverse	9.1	4.6	3.0	2.3	1.9	1.7	1.5	1.4	1.3	1.1	1.1	1.1
2-Hexyl	$4^c s_\beta s_\alpha$	Forward	10.5	5.2	3.4	2.5	2.1	1.8	1.6	1.5	1.4	1.2	1.1	1.1
		Reverse	10.5	5.2	3.4	2.5	2.1	1.8	1.6	1.5	1.4	1.2	1.1	1.1
2-Hexyl	$4^t s_\beta s_\alpha$	Forward	10.4	5.2	3.4	2.5	2.0	1.8	1.6	1.5	1.4	1.2	1.1	1.1
		Reverse	10.4	5.2	3.4	2.5	2.0	1.8	1.6	1.5	1.4	1.2	1.1	1.1
2-Hexyl	$5s_\alpha^A s_\alpha^A$	Forward	8.3	4.2	2.8	2.2	1.8	1.6	1.5	1.4	1.3	1.1	1.1	1.0
		Reverse	8.3	4.2	2.8	2.2	1.8	1.6	1.5	1.4	1.3	1.1	1.1	1.0
2-Hexyl	$5s_\alpha^A s_\alpha^E$	Forward	8.4	4.3	2.8	2.2	1.8	1.6	1.5	1.4	1.3	1.1	1.1	1.0
		Reverse	8.4	4.3	2.8	2.2	1.8	1.6	1.5	1.4	1.3	1.1	1.1	1.0
2-Hexyl	$5s_\alpha^E s_\alpha^E$	Forward	8.4	4.3	2.8	2.2	1.8	1.6	1.5	1.4	1.3	1.1	1.1	1.0
		Reverse	8.4	4.3	2.8	2.2	1.8	1.6	1.5	1.4	1.3	1.1	1.1	1.0
3-Hexyl	$3s_\beta s_\beta$	Forward	9.1	4.6	3.0	2.3	1.9	1.7	1.5	1.4	1.3	1.1	1.1	1.1
		Reverse	9.1	4.6	3.0	2.3	1.9	1.7	1.5	1.4	1.3	1.1	1.1	1.1
2-Heptyl	$3s_\beta s_\alpha$	Forward	9.1	4.6	3.0	2.3	1.9	1.7	1.5	1.4	1.3	1.1	1.1	1.1
		Reverse	9.1	4.6	3.0	2.3	1.9	1.7	1.5	1.4	1.3	1.1	1.1	1.1
2-Heptyl	$4^c s_\beta s_\alpha$	Forward	10.5	5.2	3.4	2.5	2.1	1.8	1.6	1.5	1.4	1.2	1.1	1.1
		Reverse	10.5	5.2	3.4	2.5	2.1	1.8	1.6	1.5	1.4	1.2	1.1	1.1
2-Heptyl	$4^t s_\beta s_\alpha$	Forward	10.4	5.2	3.4	2.5	2.0	1.8	1.6	1.5	1.4	1.2	1.1	1.1
		Reverse	10.4	5.2	3.4	2.5	2.0	1.8	1.6	1.5	1.4	1.2	1.1	1.1
2-Heptyl	$5s_\beta^A s_\alpha^A$	Forward	8.2	4.2	2.8	2.2	1.8	1.6	1.5	1.4	1.3	1.1	1.1	1.0
		Reverse	8.2	4.2	2.8	2.2	1.8	1.6	1.5	1.4	1.3	1.1	1.1	1.0
2-Heptyl	$5s_\beta^A s_\alpha^E$	Forward	8.3	4.3	2.8	2.2	1.8	1.6	1.5	1.4	1.3	1.1	1.1	1.0
		Reverse	8.3	4.3	2.8	2.2	1.8	1.6	1.5	1.4	1.3	1.1	1.1	1.0
2-Heptyl	$5s_\beta^E s_\alpha^E$	Forward	8.3	4.3	2.8	2.2	1.8	1.6	1.5	1.4	1.3	1.1	1.1	1.0
		Reverse	8.3	4.3	2.8	2.2	1.8	1.6	1.5	1.4	1.3	1.1	1.1	1.0
2-Heptyl	$6s_\alpha^A s_\alpha^A$	Forward	7.2	3.8	2.6	2.0	1.7	1.5	1.4	1.3	1.2	1.1	1.1	1.0
		Reverse	7.2	3.8	2.6	2.0	1.7	1.5	1.4	1.3	1.2	1.1	1.1	1.0
2-Heptyl	$6s_\alpha^A s_\alpha^E$	Forward	7.2	3.8	2.6	2.0	1.7	1.5	1.4	1.3	1.2	1.1	1.1	1.0
		Reverse	7.2	3.8	2.6	2.0	1.7	1.5	1.4	1.3	1.2	1.1	1.1	1.0
2-Heptyl	$6s_\alpha^E s_\alpha^E$	Forward	7.3	3.8	2.6	2.0	1.7	1.5	1.4	1.3	1.3	1.1	1.1	1.0
		Reverse	7.3	3.8	2.6	2.0	1.7	1.5	1.4	1.3	1.3	1.1	1.1	1.0
3-Heptyl	$3s_\beta s_\beta$	Forward	9.1	4.6	3.0	2.3	1.9	1.7	1.5	1.4	1.3	1.1	1.1	1.1
		Reverse	9.1	4.6	3.0	2.3	1.9	1.7	1.5	1.4	1.3	1.1	1.1	1.1
3-Heptyl	$4^c s_\beta s_\beta$	Forward	10.5	5.2	3.4	2.5	2.1	1.8	1.6	1.5	1.4	1.2	1.1	1.1
		Reverse	10.5	5.2	3.4	2.5	2.1	1.8	1.6	1.5	1.4	1.2	1.1	1.1
3-Heptyl	$4^t s_\beta s_\beta$	Forward	10.4	5.2	3.3	2.5	2.0	1.8	1.6	1.5	1.4	1.2	1.1	1.1

		Reverse	10.4	5.2	3.3	2.5	2.0	1.8	1.6	1.5	1.4	1.2	1.1	1.1
2-Octyl	$3s_{\beta}s_{\alpha}$	Forward	9.1	4.6	3.0	2.3	1.9	1.7	1.5	1.4	1.3	1.1	1.1	1.1
		Reverse	9.1	4.6	3.0	2.3	1.9	1.7	1.5	1.4	1.3	1.1	1.1	1.1
2-Octyl	$4^{c}s_{\beta}s_{\alpha}$	Forward	10.5	5.2	3.4	2.5	2.1	1.8	1.6	1.5	1.4	1.2	1.1	1.1
		Reverse	10.5	5.2	3.4	2.5	2.1	1.8	1.6	1.5	1.4	1.2	1.1	1.1
2-Octyl	$4^{t}s_{\beta}s_{\alpha}$	Forward	10.4	5.2	3.4	2.5	2.0	1.8	1.6	1.5	1.4	1.2	1.1	1.1
		Reverse	10.4	5.2	3.4	2.5	2.0	1.8	1.6	1.5	1.4	1.2	1.1	1.1
2-Octyl	$5s_{\beta}^{A}s_{\alpha}^{A}$	Forward	8.2	4.2	2.8	2.2	1.8	1.6	1.5	1.4	1.3	1.1	1.1	1.0
		Reverse	8.2	4.2	2.8	2.2	1.8	1.6	1.5	1.4	1.3	1.1	1.1	1.0
2-Octyl	$5s_{\beta}^{A}s_{\alpha}^{E}$	Forward	8.3	4.3	2.8	2.2	1.8	1.6	1.5	1.4	1.3	1.1	1.1	1.0
		Reverse	8.3	4.3	2.8	2.2	1.8	1.6	1.5	1.4	1.3	1.1	1.1	1.0
2-Octyl	$5s_{\beta}^{E}s_{\alpha}^{E}$	Forward	8.4	4.3	2.8	2.2	1.8	1.6	1.5	1.4	1.3	1.1	1.1	1.0
		Reverse	8.4	4.3	2.8	2.2	1.8	1.6	1.5	1.4	1.3	1.1	1.1	1.0
2-Octyl	$6s_{\beta}^{A}s_{\alpha}^{A}$	Forward	7.2	3.8	2.6	2.0	1.7	1.5	1.4	1.3	1.2	1.1	1.1	1.0
		Reverse	7.2	3.8	2.6	2.0	1.7	1.5	1.4	1.3	1.2	1.1	1.1	1.0
2-Octyl	$6s_{\beta}^{A}s_{\alpha}^{E}$	Forward	7.2	3.8	2.6	2.0	1.7	1.5	1.4	1.3	1.2	1.1	1.1	1.0
		Reverse	7.2	3.8	2.6	2.0	1.7	1.5	1.4	1.3	1.2	1.1	1.1	1.0
2-Octyl	$6s_{\beta}^{E}s_{\alpha}^{E}$	Forward	7.3	3.8	2.6	2.0	1.7	1.5	1.4	1.3	1.3	1.1	1.1	1.0
		Reverse	7.3	3.8	2.6	2.0	1.7	1.5	1.4	1.3	1.3	1.1	1.1	1.0
2-Octyl	$7s_{\alpha}^{A}s_{\alpha}^{A}$	Forward	6.8	3.6	2.5	1.9	1.6	1.5	1.4	1.3	1.2	1.1	1.1	1.0
		Reverse	6.8	3.6	2.5	1.9	1.6	1.5	1.4	1.3	1.2	1.1	1.1	1.0
2-Octyl	$7s_{\alpha}^{A}s_{\alpha}^{E}$	Forward	6.9	3.6	2.5	1.9	1.7	1.5	1.4	1.3	1.2	1.1	1.1	1.0
		Reverse	6.9	3.6	2.5	1.9	1.7	1.5	1.4	1.3	1.2	1.1	1.1	1.0
2-Octyl	$7s_{\alpha}^{E}s_{\alpha}^{E}$	Forward	6.9	3.6	2.5	1.9	1.7	1.5	1.4	1.3	1.2	1.1	1.1	1.0
		Reverse	6.9	3.6	2.5	1.9	1.7	1.5	1.4	1.3	1.2	1.1	1.1	1.0
3-Octyl	$3s_{\beta}s_{\beta}$	Forward	9.1	4.6	3.0	2.3	1.9	1.7	1.5	1.4	1.3	1.1	1.1	1.1
		Reverse	9.1	4.6	3.0	2.3	1.9	1.7	1.5	1.4	1.3	1.1	1.1	1.1
3-Octyl	$4^{c}s_{\beta}s_{\beta}$	Forward	10.5	5.2	3.4	2.5	2.1	1.8	1.6	1.5	1.4	1.2	1.1	1.1
		Reverse	10.5	5.2	3.4	2.5	2.1	1.8	1.6	1.5	1.4	1.2	1.1	1.1
3-Octyl	$4^{t}s_{\beta}s_{\beta}$	Forward	10.4	5.2	3.3	2.5	2.0	1.8	1.6	1.5	1.4	1.2	1.1	1.1
		Reverse	10.4	5.2	3.3	2.5	2.0	1.8	1.6	1.5	1.4	1.2	1.1	1.1
3-Octyl	$5s_{\beta}^{A}s_{\beta}^{A}$	Forward	8.2	4.2	2.8	2.1	1.8	1.6	1.4	1.4	1.3	1.1	1.1	1.0
		Reverse	8.2	4.2	2.8	2.1	1.8	1.6	1.4	1.4	1.3	1.1	1.1	1.0
3-Octyl	$5s_{\beta}^{A}s_{\beta}^{E}$	Forward	8.3	4.2	2.8	2.2	1.8	1.6	1.5	1.4	1.3	1.1	1.1	1.0
		Reverse	8.3	4.2	2.8	2.2	1.8	1.6	1.5	1.4	1.3	1.1	1.1	1.0
3-Octyl	$5s_{\beta}^{E}s_{\beta}^{E}$	Forward	8.3	4.2	2.8	2.2	1.8	1.6	1.5	1.4	1.3	1.1	1.1	1.0
		Reverse	8.3	4.2	2.8	2.2	1.8	1.6	1.5	1.4	1.3	1.1	1.1	1.0
4-Octyl	$3s_{\beta}s_{\beta}$	Forward	9.1	4.6	3.0	2.3	1.9	1.7	1.5	1.4	1.3	1.1	1.1	1.1
		Reverse	9.1	4.6	3.0	2.3	1.9	1.7	1.5	1.4	1.3	1.1	1.1	1.1

Table S.6: G4 Cartesian coordinates for s-alkyl radical H-migration reactants and products

2-Butyl			
	Cartesian Coordinates (Å)		
C	0.005760	-0.008390	-0.004552
H	0.032628	-0.000834	1.092963
H	1.059352	-0.049145	-0.334382
H	-0.459375	-0.945728	-0.326049
C	-0.708890	1.183134	-0.544081
H	-1.210718	1.097984	-1.505051
C	-0.483515	2.550058	0.011937
H	0.523552	2.914016	-0.267799
H	-0.462533	2.501029	1.111143
C	-1.523722	3.580479	-0.443679
H	-2.530352	3.287589	-0.128615
H	-1.313211	4.570703	-0.028317
H	-1.531802	3.671572	-1.535347

2-Pentyl			
	Cartesian Coordinates (Å)		
C	0.000122	-0.015265	-0.004439
H	0.037772	-0.001716	1.092622
H	1.049811	-0.070410	-0.344448
H	-0.479051	-0.948922	-0.316154
C	-0.706323	1.181126	-0.544144
H	-1.214245	1.096355	-1.501954
C	-0.468892	2.547965	0.005633
H	0.531964	2.915296	-0.295417
H	-0.425092	2.502619	1.105181
C	-1.516447	3.584188	-0.425966
H	-2.509325	3.242011	-0.108660
H	-1.545888	3.625801	-1.522669
C	-1.246783	4.982650	0.133691
H	-0.271869	5.360242	-0.194994
H	-2.007844	5.698148	-0.193126
H	-1.244624	4.977236	1.229527

3-Pentyl			
	Cartesian Coordinates (Å)		
C	0.003530	-0.009024	0.001971
H	0.010539	-0.006706	1.096620
H	1.045602	-0.014661	-0.335853
H	-0.460350	-0.942049	-0.332254
C	-0.743122	1.213785	-0.545508
H	-0.783679	1.139914	-1.648968
H	-1.796157	1.180614	-0.228214
C	-0.138753	2.516704	-0.139237
H	0.933691	2.549318	0.046184
C	-0.864889	3.811029	-0.298269
H	-1.913485	3.686372	0.010901
H	-0.922416	4.086726	-1.368513
C	-0.229688	4.973144	0.475354
H	0.804198	5.138781	0.153403
H	-0.781138	5.905192	0.318451
H	-0.212501	4.765902	1.550098

2-Hexyl			
	Cartesian Coordinates (Å)		
C	0.017290	-0.008274	-0.006350
H	0.000924	-0.030934	1.091126
H	1.062622	0.027663	-0.329491
H	-0.382081	-0.983853	-0.336870
C	-0.771569	1.136455	-0.543888
H	-0.484580	1.560044	-1.503436
C	-2.109354	1.499362	0.009669
H	-2.084602	1.438881	1.108922
H	-2.866188	0.748753	-0.291713
C	-2.601989	2.887811	-0.420942
H	-2.619030	2.937079	-1.518659
H	-1.875171	3.644100	-0.096034
C	-3.989208	3.242958	0.123665
H	-3.971777	3.191709	1.220601
H	-4.711364	2.482240	-0.202055
C	-4.472085	4.627826	-0.315134
H	-4.532860	4.698172	-1.406997
H	-5.464405	4.852730	0.088387
H	-3.787895	5.412282	0.027175

3-Hexyl

	Cartesian Coordinates (Å)		
C	0.006376	-0.012885	0.003289
H	0.012030	-0.016391	1.098726
H	1.046897	-0.023093	-0.335340
H	-0.467465	-0.942335	-0.328233
C	-0.744810	1.210382	-0.537010
H	-0.199304	2.124026	-0.233042
H	-0.703258	1.217732	-1.636474
C	-2.166686	1.287740	-0.089403
H	-2.425996	0.848457	0.872563
C	-3.151399	2.208074	-0.729582
H	-3.015270	2.196977	-1.822194
H	-2.945553	3.256029	-0.435568
C	-4.614773	1.888641	-0.389793
H	-4.738950	1.905404	0.700919
H	-4.839333	0.862185	-0.705045
C	-5.608007	2.858160	-1.034296
H	-5.531788	2.835463	-2.127254
H	-6.640158	2.609293	-0.768409
H	-5.420472	3.889053	-0.713137

2-Heptyl

	Cartesian Coordinates (Å)		
C	-0.003744	0.024295	-0.003632
H	0.041565	0.007121	1.093085
H	1.043296	0.085262	-0.350765
H	-0.489189	0.956902	-0.308789
C	-0.708809	-1.17329	-0.542578
H	-1.22248	-1.087835	-1.497219
C	-0.462523	-2.540803	0.002191
H	0.537848	-2.902718	-0.306442
H	-0.411692	-2.497082	1.101394
C	-1.509481	-3.579167	-0.425348
H	-1.545502	-3.620672	-1.522763
H	-2.502887	-3.240545	-0.102708
C	-1.240639	-4.981733	0.127508
H	-1.202998	-4.93953	1.225319
H	-0.243883	-5.31571	-0.194316
C	-2.283893	-6.01878	-0.302094
H	-2.320482	-6.061477	-1.398869
H	-3.27922	-5.684499	0.019761
C	-2.0097	-7.41813	0.25536
H	-2.001527	-7.413028	1.351137
H	-2.771016	-8.13508	-0.067976
H	-1.035897	-7.793766	-0.078617

3-Heptyl

	Cartesian Coordinates (Å)		
C	0.004707	0.018927	0.004904
H	0.004679	0.024287	1.100666
H	1.05013	0.024622	-0.323634
H	-0.454812	0.953483	-0.332113
C	-0.740148	-1.201745	-0.54209
H	-0.754183	-1.161859	-1.639568
C	-0.127996	-2.532268	-0.09361
H	0.92299	-2.574398	-0.411806
H	-0.113647	-2.579091	1.00335
C	-0.867148	-3.761986	-0.640585
H	-0.905171	-3.685366	-1.744939
H	-1.92176	-3.729724	-0.325784
C	-0.260359	-5.063312	-0.233884
H	0.814641	-5.097498	-0.064592

4-Heptyl

	Cartesian Coordinates (Å)		
C	-0.002143	0.022806	-0.026161
H	-0.022714	0.059994	1.068914
H	1.049263	0.022252	-0.335219
H	-0.457271	0.945747	-0.399017
C	-0.734221	-1.214012	-0.551805
H	-1.790016	-1.171333	-0.253666
H	-0.728646	-1.211314	-1.648783
C	-0.127529	-2.533851	-0.05161
H	0.93141	-2.588629	-0.347182
H	-0.106342	-2.509667	1.055648
C	-0.847835	-3.749691	-0.53066
H	-1.923897	-3.679271	-0.682012
C	-0.231884	-5.108414	-0.497006
H	-0.191915	-5.487941	0.542923

C	-0.991914	-6.357145	-0.371788	H	0.822391	-5.046332	-0.808233
H	-1.076175	-6.635277	-1.439624	C	-0.963745	-6.14493	-1.362599
H	-2.032567	-6.230313	-0.03751	H	-0.985222	-5.791859	-2.40106
C	-0.339711	-7.51833	0.388899	H	-2.011542	-6.203036	-1.040022
H	-0.295639	-7.308416	1.462376	C	-0.329705	-7.536386	-1.301064
H	-0.896458	-8.449797	0.248081	H	-0.323869	-7.924349	-0.276133
H	0.685621	-7.686572	0.041903	H	-0.87425	-8.252261	-1.924729
H	-1.791076	-1.161819	-0.225675	H	0.708885	-7.514293	-1.649954

2-Octyl

Cartesian Coordinates (Å)			
C	-0.000864	0.027101	-0.001769
H	0.044886	0.009111	1.094921
H	1.046114	0.087064	-0.349274
H	-0.485337	0.960489	-0.306073
C	-0.707520	-1.169318	-0.541237
H	-1.221729	-1.082599	-1.495471
C	-0.462048	-2.537488	0.002231
H	0.538053	-2.899730	-0.306930
H	-0.410904	-2.494787	1.101471
C	-1.509673	-3.574954	-0.425934
H	-1.546034	-3.615545	-1.523342
H	-2.502815	-3.236228	-0.102689
C	-1.240917	-4.978200	0.125882
H	-1.203108	-4.935894	1.223593
H	-0.244053	-5.310957	-0.196490
C	-2.284231	-6.014492	-0.304487
H	-2.321821	-6.058743	-1.402172
H	-3.281355	-5.681549	0.016727
C	-2.018162	-7.418580	0.248811
H	-1.980070	-7.373510	1.345410
H	-1.022562	-7.751681	-0.073708
C	-3.066100	-8.447337	-0.184495
H	-2.846705	-9.439449	0.222670
H	-4.067090	-8.161254	0.157597
H	-3.105085	-8.536870	-1.275987

3-Ocytl

Cartesian Coordinates (Å)			
C	-0.001002	0.013211	0.002751
H	0.000886	0.010519	1.100889
H	1.054558	0.012280	-0.300331
C	-0.671645	-1.268263	-0.503781
H	-0.675915	-1.264804	-1.603076
C	0.001496	-2.549581	-0.003252
H	1.056869	-2.549937	-0.309122
H	0.004830	-2.559272	1.094629
C	-0.668095	-3.833593	-0.514700
H	-0.695768	-3.797499	-1.621369
H	-1.726749	-3.844237	-0.212666
C	-0.001609	-5.087274	-0.055153
H	1.072600	-5.062173	0.120801
C	-0.667315	-6.420128	-0.147631
H	-0.719967	-6.747714	-1.203423
H	-1.718168	-6.330388	0.165815
C	0.027936	-7.514358	0.672144
H	0.041859	-7.258271	1.736383
H	-0.479060	-8.477820	0.561854
H	1.066590	-7.644911	0.349304
H	-1.727996	-1.268720	-0.199633
C	-0.677240	1.289855	-0.504309
H	-0.175440	2.186565	-0.127122
H	-0.664054	1.336796	-1.599061
H	-1.724845	1.336236	-0.186168

4-Octyl

Cartesian Coordinates (Å)			
C	-0.000596	0.024986	-0.032630
H	-0.008526	0.062593	1.062595
H	1.047167	0.025203	-0.353824

H	-0.460793	0.947397	-0.400544
C	-0.737614	-1.212678	-0.549297
H	-1.790081	-1.170466	-0.239551
H	-0.744143	-1.210713	-1.646278
C	-0.124634	-2.531724	-0.054985
H	0.931503	-2.585361	-0.360872
H	-0.092369	-2.507568	1.052024
C	-0.848082	-3.748522	-0.526923
H	-1.924480	-3.677522	-0.675328
C	-0.233775	-5.108054	-0.487783
H	-0.200003	-5.484973	0.553226
H	0.821992	-5.046799	-0.793561
C	-0.962527	-6.144713	-1.355358
H	-0.975790	-5.796780	-2.396761
H	-2.014233	-6.200118	-1.041675
C	-0.339824	-7.542681	-1.289800
H	-0.326927	-7.884120	-0.245985
H	0.711813	-7.485454	-1.601101
C	-1.073702	-8.570419	-2.155379
H	-0.608024	-9.558618	-2.086339
H	-2.119964	-8.673209	-1.846208
H	-1.070372	-8.274059	-3.210327

Table S.7: G4 Cartesian coordinates for s-alkyl radical H-migration transition states.

2-Butyl: $3s_{\alpha}s_{\alpha}$

Cartesian Coordinates (Å)			
C	-0.00733	0.004445	-0.014025
C	0.001125	-0.011844	1.486109
C	1.287151	-0.015946	2.251641
C	1.377017	-0.642161	3.611998
H	0.50704	1.014098	2.104688
H	2.191834	0.094506	1.660462
H	-0.867107	-0.394883	2.014838
H	2.247439	-0.284769	4.170779
H	0.485901	-0.419798	4.211345
H	1.448491	-1.740345	3.552366
H	-0.970639	0.334697	-0.414736
H	0.762752	0.678355	-0.408471
H	0.203265	-0.992208	-0.434775

2-Pentyl: $3s_{\beta}s_{\alpha}$

Cartesian Coordinates (Å)			
C	-0.010277	0.002762	-0.017266
C	-0.001415	-0.013677	1.483014
C	1.284277	-0.010912	2.248336
C	1.391053	-0.636152	3.610059
C	2.559927	-0.099415	4.443698
H	0.496129	1.014765	2.103594
H	2.189735	0.110022	1.658190
H	-0.867267	-0.402516	2.011334
H	0.449863	-0.480373	4.154848
H	1.488256	-1.731467	3.510589
H	-0.977406	0.322845	-0.416990
H	0.752342	0.684870	-0.412069
H	0.210519	-0.991551	-0.438295
H	2.616755	-0.597605	5.416626
H	3.514567	-0.261479	3.931044
H	2.456848	0.976804	4.616141

2-Pentyl: $4^{c}s_{\alpha}s_{\alpha}$

Cartesian Coordinates (Å)			
C	-0.057018	-0.091884	-0.032697
C	-0.003321	0.004079	1.470522
C	1.351903	0.036923	2.191149
C	1.091681	1.420721	2.802994
C	2.004134	2.574522	2.474496
H	-0.063512	1.309300	2.001420
H	0.713752	1.396036	3.826360
H	2.192978	0.046735	1.489768
H	1.521608	-0.769744	2.909283
H	2.187942	2.644831	1.396027
H	1.584858	3.529402	2.806312
H	2.986980	2.461176	2.957572
H	-0.783342	-0.540711	2.004852
H	-1.063560	0.104209	-0.414941
H	0.626813	0.623364	-0.504548
H	0.238627	-1.092746	-0.383577

2-Pentyl: $4^{t}s_{\alpha}s_{\alpha}$

Cartesian Coordinates (Å)			
C	-0.004046	0.018106	-0.031971
C	-0.000452	0.005662	1.475005
C	1.338115	-0.006952	2.228437
C	1.119687	-1.427913	2.769585
C	0.908016	-1.635308	4.247162
H	-0.074466	-1.284407	2.036098
H	1.691289	-2.204510	2.259352
H	1.416819	0.751570	3.012843
H	2.208637	0.093282	1.573546
H	-0.790360	0.584924	1.955305
H	0.166893	-0.932383	4.646039
H	0.561443	-2.649401	4.468992
H	1.837283	-1.473312	4.814677
H	-0.999621	-0.187733	-0.437146
H	0.317530	0.993469	-0.428391
H	0.685473	-0.731511	-0.438282

2-Hexyl: $3s_{\beta}s_{\alpha}$

Cartesian Coordinates (Å)

2-Hexyl: $4^{c}s_{\beta}s_{\alpha}$

Cartesian Coordinates (Å)

C	-0.011410	0.010106	-0.021525	C	-0.058029	-0.136943	-0.036498
C	-0.003523	-0.015096	1.478623	C	-0.006580	-0.015447	1.464972
C	1.282368	-0.012377	2.244245	C	1.348744	0.040201	2.184471
C	1.391388	-0.642040	3.603292	C	1.084591	1.437194	2.762115
C	2.549082	-0.098319	4.451253	C	1.981326	2.593537	2.393711
C	2.659224	-0.773101	5.820685	C	1.423326	3.956811	2.813177
H	0.490714	1.011314	2.104953	H	-0.077116	1.299228	1.971639
H	2.187055	0.114138	1.654176	H	0.718508	1.441125	3.791260
H	-0.867984	-0.410648	2.004139	H	2.190803	0.033419	1.484260
H	0.446525	-0.501053	4.147593	H	1.519040	-0.746918	2.923715
H	1.503687	-1.736730	3.501659	H	2.162709	2.584826	1.310236
H	-0.979916	0.327748	-0.419866	H	2.972675	2.447757	2.855344
H	0.747986	0.698424	-0.411783	H	-0.782199	-0.557783	2.008059
H	0.214624	-0.980549	-0.448389	H	-1.065703	0.044541	-0.422917
H	3.489675	-0.229846	3.900199	H	0.620490	0.575945	-0.519508
H	2.421291	0.984117	4.576939	H	0.246303	-1.141032	-0.370267
H	2.817281	-1.852731	5.719466	H	1.263078	4.000453	3.896155
H	3.494025	-0.367712	6.400930	H	2.107830	4.767590	2.544971
H	1.745208	-0.628562	6.407857	H	0.460644	4.151118	2.329159

2-Hexyl: $4^{t}s_{\beta}s_{\alpha}$

Cartesian Coordinates (Å)			
C	0.002562	0.038232	-0.042216
C	0.002150	0.016214	1.464620
C	1.338403	-0.012026	2.221823
C	1.101395	-1.428176	2.765203
C	0.862665	-1.631717	4.240899
C	0.361263	-3.035893	4.591020
H	-0.086144	-1.276269	2.019485
H	1.673498	-2.215634	2.269917
H	1.426765	0.747676	3.004141
H	2.211060	0.073933	1.567866
H	-0.783497	0.599867	1.946691
H	0.144691	-0.881302	4.600060
H	1.795603	-1.429354	4.793578
H	-0.993852	-0.155849	-0.451090
H	0.334068	1.013122	-0.431566
H	0.686189	-0.715112	-0.451564
H	1.077132	-3.800731	4.270008
H	0.214071	-3.149726	5.669547
H	-0.591541	-3.246713	4.094489

2-Hexyl: $5s_{\alpha}^{A}s_{\alpha}^{A}$

Cartesian Coordinates (Å)			
C	-0.011550	-0.030586	-0.000480
C	-0.003947	-0.034588	1.527852
C	1.492837	0.022439	1.943604
C	2.185244	0.879576	0.884364
H	1.218735	0.587480	-0.053254
H	-0.514834	-0.906545	1.954153
H	-0.526554	0.851575	1.904177
H	1.918365	-0.987073	1.940755
H	1.621111	0.414986	2.959757
C	0.116020	-1.365136	-0.700437
H	-0.785783	-1.978383	-0.556209
H	0.259051	-1.245260	-1.779213
H	0.961505	-1.946105	-0.314420
H	-0.739620	0.636443	-0.465103
C	2.181523	2.377795	1.090916
H	2.814437	2.664286	1.943858
H	2.559828	2.909324	0.211766
H	1.174150	2.755590	1.300553
H	3.136810	0.493412	0.515257

2-Hexyl: $5s_{\alpha}^{A}s_{\alpha}^{E}$

	Cartesian Coordinates (Å)		
C	-0.008004	-0.024243	-0.005737
C	0.011711	-0.019339	1.522851
C	1.509961	0.009632	1.922908
C	2.187690	0.890398	0.879270
C	3.600334	0.580740	0.451582
H	1.228096	0.587582	-0.065409
H	-0.516284	-0.875348	1.960587
H	-0.482798	0.884875	1.895805
H	1.929831	-1.003127	1.871884
H	1.659365	0.358386	2.951714
H	2.001411	1.958102	1.032562
H	3.709071	-0.469810	0.158510
H	3.912423	1.200916	-0.395439
H	4.320361	0.761028	1.264777
C	0.091453	-1.364408	-0.699491
H	-0.821767	-1.959508	-0.549608
H	0.232647	-1.252399	-1.779350
H	0.925920	-1.961571	-0.314367
H	-0.730606	0.650843	-0.467229

2-Hexyl: $5s_{\alpha}^{E}s_{\alpha}^{E}$

	Cartesian Coordinates (Å)		
C	0.005734	0.011920	-0.024029
C	0.006233	0.008981	1.483868
C	1.333761	0.004415	2.234124
C	1.070730	-0.823334	3.515395
C	0.156816	-1.961662	3.073889
C	-0.887434	-2.485499	4.027242
H	-0.357844	-1.199815	2.043386
H	-0.733296	0.685136	1.924687
H	1.716622	1.008117	2.453976
H	2.093991	-0.498624	1.622062
H	0.544333	-0.202090	4.251938
H	1.997141	-1.164837	3.992266
H	0.684131	-2.747662	2.523898
H	-1.499414	-1.672178	4.434133
H	-1.558240	-3.200994	3.539895
H	-0.433256	-3.003582	4.885980
H	-1.003438	-0.119221	-0.428725
H	0.395086	0.958151	-0.430421
H	0.636735	-0.789689	-0.425076

3-Hexyl: $3s_{\beta}s_{\beta}$

	Cartesian Coordinates (Å)		
C	-0.012471	0.005664	-0.019053
C	-0.008114	-0.001326	1.513782
C	1.369580	0.003766	2.112734
C	1.617796	-0.467779	3.510407
C	2.746017	0.079225	4.338158
C	3.167377	-0.841960	5.488466
H	1.908780	-1.136748	2.432729
H	0.766483	-0.911776	4.020999
H	2.114490	0.679065	1.698479
H	3.610639	0.275018	3.689320
H	2.463577	1.065195	4.746995
H	-0.558857	-0.879222	1.878268
H	-0.577673	0.869485	1.882979
H	3.970734	-0.394800	6.082286
H	2.325954	-1.038515	6.162149
H	3.518820	-1.807095	5.109563
H	-1.032914	0.028475	-0.414203
H	0.514614	0.883594	-0.408793

2-Heptyl: $3s_{\beta}s_{\alpha}$

	Cartesian Coordinates (Å)		
C	-0.017238	0.008141	-0.024029
C	-0.006324	-0.016211	1.476124
C	1.280912	-0.010306	2.239448
C	1.392961	-0.640492	3.598233
C	2.551931	-0.096998	4.444078
C	2.67076	-0.766929	5.816669
C	3.831456	-0.224018	6.654602
H	0.486669	1.011581	2.101187
H	2.184358	0.118021	1.647916
H	-0.868848	-0.413549	2.003489
H	0.448742	-0.499719	4.143554
H	1.504832	-1.734963	3.494866
H	-0.987323	0.323167	-0.420613
H	0.739676	0.698094	-0.416211
H	0.21036	-0.98221	-0.450781
H	3.493815	-0.228569	3.893171
H	2.426443	0.986521	4.57142
H	2.791001	-1.850156	5.681705

H	0.488368	-0.882930	-0.416766

H	1.728989	-0.634545	6.366132
H	3.719872	0.850836	6.836413
H	3.890397	-0.721303	7.627953
H	4.790475	-0.373374	6.145928

2-Heptyl: $4^{c}s_{\beta}s_{\alpha}$

Cartesian Coordinates (Å)			
C	-0.077629	-0.180853	-0.024702
C	-0.013254	-0.037417	1.474314
C	1.348624	0.03512	2.179787
C	1.086958	1.442856	2.732746
C	1.973367	2.594411	2.327678
C	1.420064	3.969569	2.719892
C	2.342554	5.124926	2.323507
H	-0.084085	1.285031	1.960652
H	0.735728	1.465941	3.766737
H	2.18484	0.01505	1.472972
H	1.526108	-0.736414	2.933621
H	2.143211	2.564309	1.241722
H	2.972398	2.465882	2.780321
H	-0.781383	-0.575158	2.032385
H	-1.089656	-0.010107	-0.404584
H	0.592793	0.528545	-0.523879
H	0.229096	-1.188022	-0.346764
H	1.247998	3.991853	3.804126
H	0.435401	4.103506	2.254674
H	1.919576	6.092084	2.612836
H	3.322982	5.033349	2.804447
H	2.508508	5.145651	1.240447

2-Heptyl: $4^{t}s_{\beta}s_{\alpha}$

Cartesian Coordinates (Å)			
C	0.007556	0.042832	-0.050446
C	0.005045	0.021867	1.45639
C	1.339819	-0.010966	2.215857
C	1.094687	-1.424437	2.763312
C	0.84866	-1.622072	4.238258
C	0.335077	-3.021075	4.598574
C	0.110224	-3.212365	6.100523
H	-0.089319	-1.26961	2.012949
H	1.665939	-2.2154	2.272798
H	1.431831	0.750985	2.995484
H	2.213641	0.067339	1.562476
H	-0.779084	0.608739	1.937024
H	0.133862	-0.866023	4.594916
H	1.780752	-1.425575	4.796602
H	-0.989086	-0.147643	-0.460472
H	0.343377	1.016144	-0.440067
H	0.688763	-0.713458	-0.458398
H	1.050745	-3.770775	4.2359
H	-0.600167	-3.208644	4.056258
H	-0.257198	-4.218701	6.324892
H	1.03874	-3.064111	6.663358
H	-0.625263	-2.496779	6.485193

2-Heptyl: $5s_{\beta}^{A}s_{\alpha}^{A}$

Cartesian Coordinates (Å)			
C	0.010581	-0.029659	-0.008996
C	-0.003236	-0.028864	1.518712
C	1.487353	0.030202	1.957401
C	2.198861	0.876729	0.902347
H	1.245598	0.582756	-0.04835
H	-0.519327	-0.900272	1.939902
H	-0.532786	0.85725	1.885135
H	1.911131	-0.979899	1.97061
H	1.599846	0.431895	2.971863
C	0.141105	-1.364247	-0.711415

2-Heptyl: $5s_{\beta}^{A}s_{\alpha}^{E}$

Cartesian Coordinates (Å)			
C	0.027026	-0.022146	-0.023633
C	0.020896	-0.018513	1.504565
C	1.511775	0.011743	1.932595
C	2.210718	0.887074	0.898539
C	3.630958	0.573326	0.499628
H	1.268519	0.583972	-0.063759
H	-0.5133	-0.876005	1.931772
H	-0.482188	0.883866	1.8702
H	1.931854	-1.00149	1.894641
H	1.641631	0.36545	2.962381

H	-0.762426	-1.964918	-0.516037	H	2.023609	1.955743	1.0438
H	0.970688	-1.935039	-0.272542	H	3.744266	-0.479183	0.215324
H	-0.70765	0.63943	-0.488611	H	3.959983	1.188091	-0.34496
C	2.196838	2.376599	1.096811	H	4.335594	0.757847	1.325229
H	2.816851	2.667907	1.957537	C	0.12804	-1.359884	-0.724772
H	2.590945	2.899812	0.219609	H	-0.786404	-1.942398	-0.524075
H	1.187377	2.759029	1.287097	H	0.947508	-1.948099	-0.290043
H	3.155056	0.484645	0.551787	H	-0.683598	0.657966	-0.499055
C	0.346287	-1.239293	-2.22428	C	0.326665	-1.241631	-2.239143
H	0.41281	-2.221843	-2.701922	H	0.368431	-2.226192	-2.715527
H	-0.484808	-0.697797	-2.689868	H	-0.495385	-0.682797	-2.700268
H	1.266137	-0.690597	-2.452477	H	1.256683	-0.713568	-2.474643

2-Heptyl: $5s_{\beta}^{E}s_{\alpha}^{E}$

Cartesian Coordinates (Å)			
C	0.021135	0.035936	-0.030462
C	0.015346	0.024802	1.477398
C	1.339664	0.005274	2.232671
C	1.065491	-0.825341	3.509946
C	0.14101	-1.952541	3.063061
C	-0.920266	-2.466217	4.005627
C	-1.86673	-3.485544	3.362108
H	-0.361249	-1.184567	2.028416
H	-0.720353	0.704715	1.918891
H	1.730574	1.004671	2.458004
H	2.097632	-0.501955	1.621298
H	0.545138	-0.201542	4.248554
H	1.987768	-1.178661	3.985953
H	0.660674	-2.748382	2.517872
H	-1.498769	-1.619152	4.398915
H	-0.442133	-2.926819	4.886703
H	-0.987476	-0.083493	-0.440167
H	0.4211	0.980674	-0.42991
H	0.646267	-0.769389	-0.433226
H	-2.614805	-3.842795	4.076699
H	-2.396475	-3.046454	2.51013
H	-1.314728	-4.357316	2.99367

2-Heptyl: $6s_{\alpha}^{A}s_{\alpha}^{A}$

Cartesian Coordinates (Å)			
C	-0.0144	-0.019932	-0.000896
C	-0.009556	-0.007278	1.523032
C	1.420683	0.008679	2.100494
C	2.205125	1.240355	1.604399
C	2.303875	1.285683	0.084294
H	1.110029	0.711956	-0.233896
H	1.698707	2.143185	1.968197
H	3.207526	1.244258	2.058737
H	1.38128	0.007176	3.195436
H	1.948524	-0.909175	1.810995
H	-0.539748	0.88199	1.886489
H	-0.555949	-0.876324	1.919735
H	-0.81857	0.572022	-0.444497
C	0.162144	-1.366293	-0.672083
H	-0.703992	-2.01994	-0.489829
H	0.271911	-1.267105	-1.756914
H	1.044508	-1.896643	-0.296798
C	3.40072	0.45897	-0.554294
H	3.317256	0.449253	-1.645951
H	4.396425	0.856413	-0.306611
H	3.380776	-0.581622	-0.21167
H	2.237499	2.293771	-0.331911

2-Heptyl: $6s_{\alpha}^{A}s_{\alpha}^{E}$

Cartesian Coordinates (Å)			
C	-0.009512	-0.024562	-0.000961
C	-0.001413	-0.019316	1.522649

2-Heptyl: $6s_{\alpha}^{E}s_{\alpha}^{E}$

Cartesian Coordinates (Å)			
C	-0.024757	-0.001236	-0.002185
C	-0.009278	-0.01084	1.517595

C	1.429221	0.011011	2.101528	C	1.42581	0.005156	2.07726
C	2.206886	1.238428	1.594284	C	2.193065	1.251625	1.598437
C	2.32336	1.243292	0.079311	C	2.282511	1.312258	0.082562
H	1.108037	0.715581	-0.23804	H	1.072189	0.773037	-0.237284
H	2.996195	0.463147	-0.292025	H	2.960616	0.556118	-0.326777
H	1.685668	2.149476	1.921388	H	1.675558	2.148356	1.968013
H	3.200848	1.271211	2.065597	H	3.194824	1.270235	2.053422
H	1.386296	0.016496	3.196321	H	1.402311	-0.024612	3.17227
H	1.966053	-0.903986	1.817527	H	1.956907	-0.899796	1.751068
H	-0.541304	0.862077	1.890916	H	-0.543535	0.874108	1.891694
H	-0.537183	-0.896082	1.916921	H	-0.553212	-0.882463	1.911459
H	-0.82678	0.551972	-0.440646	C	2.456692	2.672779	-0.553547
C	2.525239	2.577169	-0.602802	H	3.411018	3.137895	-0.262516
H	3.479873	3.041516	-0.311856	H	2.446525	2.613966	-1.646776
H	2.533296	2.478427	-1.693156	H	1.661285	3.362099	-0.246684
H	1.732622	3.285938	-0.33542	C	-1.246845	0.570402	-0.684873
C	0.200783	-1.362916	-0.678506	H	-1.132083	0.58895	-1.77357
H	-0.636012	-2.048859	-0.480245	H	-2.149591	-0.019696	-0.464191
H	0.285487	-1.25697	-1.764965	H	-1.44824	1.595055	-0.350855
H	1.110935	-1.859101	-0.322518	H	0.299959	-0.955406	-0.430169

3-Hexyl: $3s_{\beta}s_{\beta}$

Cartesian Coordinates (Å)			
C	-0.019629	0.00328	-0.021495
C	-0.011276	-0.00371	1.511317
C	1.367816	0.005787	2.107043
C	1.619291	-0.46528	3.504599
C	2.74668	0.08233	4.332303
C	3.183802	-0.842283	5.476331
C	4.302249	-0.248094	6.335935
H	1.910971	-1.132959	2.426341
H	0.769333	-0.911713	4.01523
H	2.109464	0.684061	1.691923
H	3.609884	0.290376	3.683842
H	2.460448	1.063277	4.753111
H	-0.558239	-0.883427	1.877134
H	-0.582806	0.865201	1.881998
H	2.314193	-1.06515	6.108699
H	3.505693	-1.803091	5.055673
H	-1.041186	0.023021	-0.413943
H	0.503795	0.882787	-0.412596
H	0.482814	-0.883815	-0.420528

3-Heptyl: $4^{c}s_{\beta}s_{\beta}$

Cartesian Coordinates (Å)			
C	-0.057904	-0.088567	-0.053901
C	-0.014023	0.029825	1.449842
C	1.334149	0.059845	2.182595
C	1.097582	1.467244	2.747027
C	2.02187	2.59989	2.372838
C	1.493476	3.978916	2.778897
H	-0.063188	1.348958	1.951449
H	0.727241	1.48805	3.774418
H	2.183555	0.026333	1.492099
H	1.476433	-0.724828	2.930192
H	2.20719	2.578147	1.290185
H	3.007859	2.435411	2.839613
H	-0.808413	-0.498312	1.982029
H	0.675132	0.59964	-0.496698
H	0.275232	-1.09765	-0.350321
H	1.330843	4.035368	3.860917
H	0.536957	4.190763	2.290059
C	-1.443942	0.181432	-0.64705
H	-1.439899	0.072873	-1.736094

H	4.59028	-0.927648	7.144153
H	5.197638	-0.045739	5.737202
H	3.991407	0.698575	6.792056

3-Heptyl: $4^{t}s_{\beta}s_{\beta}$

Cartesian Coordinates (Å)			
C	0.01184	0.027005	-0.034587
C	0.008067	0.018543	1.475776
C	1.338987	-0.013979	2.243623
C	1.070023	-1.410663	2.821484
C	0.79752	-1.566829	4.297148
C	0.265753	-2.951794	4.677594
H	-0.101036	-1.263223	2.050845
H	1.640218	-2.220574	2.361441
H	1.442667	0.764581	3.005016
H	2.217042	0.032812	1.59264
H	-0.773517	0.61897	1.94615
H	0.08509	-0.794562	4.619041
H	1.722282	-1.363167	4.862894
H	-0.976761	-0.265837	-0.407947
H	0.717397	-0.730442	-0.402253
H	0.974507	-3.737215	4.392546
H	-0.680942	-3.16132	4.168967
H	0.096245	-3.03181	5.75588
C	0.390314	1.39502	-0.632067
H	1.385779	1.710578	-0.302497
H	0.395721	1.359509	-1.72706
H	-0.321251	2.168501	-0.324028

2-Octyl: $4^{c}s_{\beta}s_{\alpha}$

Cartesian Coordinates (Å)			
C	-0.071060	-0.205137	-0.021699
C	-0.010782	-0.054688	1.476828
C	1.349469	0.028080	2.184427
C	1.081230	1.438610	2.727160
C	1.962348	2.590905	2.312057
C	1.404338	3.966458	2.694948
C	2.315699	5.129265	2.289222
C	1.751993	6.499989	2.673032

H	-2.186877	-0.516429	-0.245248
H	-1.780653	1.195403	-0.407862
H	2.196957	4.771736	2.50614

2-Octyl: $3s_{\beta}s_{\alpha}$

Cartesian Coordinates (Å)			
C	-0.019578	0.016875	-0.027032
C	-0.008511	-0.015019	1.472979
C	1.278828	-0.010072	2.236166
C	1.392405	-0.645786	3.592279
C	2.549607	-0.101840	4.440677
C	2.669063	-0.775647	5.811048
C	3.826304	-0.237609	6.659333
C	3.933967	-0.911497	8.030044
H	0.482398	1.010768	2.102918
H	2.181964	0.122966	1.645195
H	-0.870084	-0.416920	1.998435
H	0.447631	-0.510221	4.137884
H	1.507798	-1.739411	3.484376
H	-0.990492	0.331446	-0.421947
H	0.735538	0.710763	-0.415737
H	0.210532	-0.970699	-0.458836
H	3.491543	-0.229275	3.889082
H	2.420429	0.980840	4.570554
H	2.792590	-1.859410	5.674911
H	1.726721	-0.648038	6.362659
H	3.703934	0.845630	6.792270
H	4.768354	-0.369427	6.110614
H	4.768365	-0.507034	8.611717
H	3.018976	-0.765926	8.615227
H	4.091023	-1.991305	7.929111

2-Octyl: $4^{t}s_{\beta}s_{\alpha}$

Cartesian Coordinates (Å)			
C	0.013021	0.060257	-0.054536
C	0.011450	0.031120	1.452159
C	1.346364	-0.012122	2.210900
C	1.092418	-1.425357	2.754935
C	0.840676	-1.623586	4.229053
C	0.322317	-3.021424	4.585786
C	0.085205	-3.221753	6.086102
C	-0.427539	-4.621934	6.433333

H	-0.088930	1.269862	1.956213	H	-0.089346	-1.262357	2.002894
H	0.730737	1.468123	3.761203	H	1.660920	-2.218624	2.265017
H	2.187396	0.005944	1.479702	H	1.444420	0.747566	2.992013
H	1.527974	-0.737359	2.944203	H	2.220062	0.061455	1.556804
H	2.130143	2.552459	1.226130	H	-0.769399	0.619366	1.936456
H	2.962385	2.468688	2.764005	H	0.126779	-0.865517	4.582974
H	-0.777259	-0.593999	2.035638	H	1.771568	-1.429509	4.789996
H	-1.083197	-0.041922	-0.404574	H	-0.984935	-0.122650	-0.464808
H	0.596352	0.505944	-0.522534	H	0.353768	1.033872	-0.439108
H	0.242291	-1.211900	-0.338604	H	0.689856	-0.697430	-0.467145
H	1.235227	3.999025	3.780418	H	1.038264	-3.774667	4.227924
H	0.416645	4.094791	2.232220	H	-0.611137	-3.209176	4.038407
H	3.302038	4.995324	2.753342	H	1.019690	-3.028440	6.629760
H	2.485815	5.093933	1.204772	H	-0.631883	-2.470114	6.442495
H	1.603127	6.577885	3.755898	H	0.284902	-5.393257	6.119746
H	2.424538	7.309055	2.370917	H	-0.587283	-4.735118	7.510292
H	0.782173	6.677322	2.194639	H	-1.379384	-4.830753	5.932088

2-Octyl: $5s_{\beta}^{A}s_{\alpha}^{A}$				2-Octyl: $5s_{\beta}^{A}s_{\alpha}^{E}$			
Cartesian Coordinates (Å)				Cartesian Coordinates (Å)			
C	0.021626	-0.030886	-0.006316	C	0.052588	-0.031768	-0.029826
C	-0.003115	-0.022640	1.521452	C	0.025282	-0.022500	1.498324
C	1.484119	0.042434	1.970253	C	1.509498	0.028067	1.946844
C	2.200111	0.887499	0.917072	C	2.211273	0.909222	0.919697
H	1.253968	0.586686	-0.038933	C	3.640744	0.612721	0.541102
H	-0.520180	-0.893006	1.943479	H	1.285846	0.591103	-0.054447
H	-0.537230	0.864283	1.879256	H	-0.504296	-0.884685	1.921688
H	1.910734	-0.966361	1.989720	H	-0.493702	0.875276	1.852950
H	1.588433	0.447931	2.984078	H	1.942970	-0.979790	1.918062
C	0.163091	-1.367986	-0.700899	H	1.620533	0.386583	2.977173
H	-0.740538	-1.972842	-0.513343	H	2.008417	1.975806	1.058966
H	0.990554	-1.936245	-0.252351	H	3.771817	-0.439318	0.262734
H	-0.696299	0.632877	-0.493556	H	3.972954	1.228436	-0.301548
C	2.191808	2.388057	1.105870	H	4.331801	0.809782	1.375257
H	2.804884	2.684670	1.969757	C	0.181666	-1.370098	-0.724316
H	2.590247	2.909264	0.229430	H	-0.727963	-1.966242	-0.536707
H	1.179801	2.767824	1.287727	H	1.002865	-1.947966	-0.276622
H	3.159924	0.497302	0.574383	H	-0.660958	0.636970	-0.516699
C	0.383256	-1.258788	-2.214577	C	0.401431	-1.263371	-2.238315
H	-0.440738	-0.682553	-2.656048	H	-0.416009	-0.676896	-2.678473
H	1.294284	-0.676859	-2.403458	H	1.319173	-0.692634	-2.428808
C	0.485998	-2.619376	-2.908620	C	0.486026	-2.624998	-2.932728

H	-0.426941	-3.207896	-2.763240	H	-0.434395	-3.201623	-2.786781
H	0.642081	-2.508841	-3.986362	H	0.642699	-2.516282	-4.010566
H	1.321743	-3.205527	-2.510039	H	1.314329	-3.222226	-2.534999

2-Octyl: $5s_{\beta}^{E}s_{\alpha}^{E}$				2-Octyl: $6s_{\beta}^{A}s_{\alpha}^{A}$			
Cartesian Coordinates (Å)				Cartesian Coordinates (Å)			
C	0.031642	0.050138	-0.034180	C	0.005609	-0.015238	-0.013009
C	0.022792	0.032987	1.473600	C	-0.004131	-0.007134	1.510915
C	1.345594	0.005278	2.231141	C	1.418045	0.010135	2.108015
C	1.065327	-0.828153	3.505062	C	2.208930	1.239575	1.618073
C	0.136863	-1.950401	3.053062	C	2.336160	1.272709	0.099994
C	-0.926938	-2.461359	3.993652	H	1.144663	0.701662	-0.237113
C	-1.880400	-3.481406	3.357522	H	1.693925	2.144088	1.965315
C	-2.947987	-3.994196	4.327153	H	3.202808	1.249360	2.090694
H	-0.359891	-1.177016	2.019827	H	1.362532	0.013187	3.202281
H	-0.710930	0.714238	1.916335	H	1.949831	-0.908904	1.829782
H	1.740346	1.002264	2.460525	H	-0.540731	0.879414	1.871429
H	2.102538	-0.503171	1.619507	H	-0.553534	-0.878549	1.898117
H	0.546137	-0.204503	4.244556	H	-0.786152	0.590909	-0.462768
H	1.984997	-1.187078	3.981925	C	0.158459	-1.361904	-0.693114
H	0.654953	-2.746534	2.506970	H	-0.688614	-2.007986	-0.408149
H	-1.506074	-1.613311	4.386683	H	1.053052	-1.874219	-0.314439
H	-0.452601	-2.923318	4.877431	C	3.446017	0.440449	-0.508369
H	-0.976626	-0.062950	-0.446499	H	3.392992	0.429989	-1.601940
H	0.436847	0.994657	-0.428857	H	4.436264	0.834395	-0.234491
H	0.653961	-0.756367	-0.438936	H	3.413054	-0.599611	-0.165024
H	-2.363125	-3.024868	2.483965	H	2.280227	2.277683	-0.325201
H	-1.296451	-4.327849	2.972635	C	0.226676	-1.271077	-2.220763
H	-3.613004	-4.717243	3.844407	H	0.306320	-2.262567	-2.677590
H	-2.493324	-4.487349	5.193766	H	-0.670525	-0.788795	-2.624852
H	-3.567603	-3.172725	4.704180	H	1.090923	-0.681950	-2.545020

2-Octyl: $6s_{\beta}^{A}s_{\alpha}^{E}$				2-Octyl: $6s_{\beta}^{E}s_{\alpha}^{E}$			
Cartesian Coordinates (Å)				Cartesian Coordinates (Å)			
C	0.052588	-0.031768	-0.029826	C	-0.007010	0.020191	-0.020438
C	0.025282	-0.022500	1.498324	C	-0.005288	0.004075	1.499178
C	1.509498	0.028067	1.946844	C	1.424182	0.001907	2.073625
C	2.211273	0.909222	0.919697	C	2.210855	1.240602	1.606715
C	3.640744	0.612721	0.541102	C	2.318649	1.303022	0.092298
H	1.285846	0.591103	-0.054447	H	1.105031	0.780188	-0.244029
H	-0.504296	-0.884685	1.921688	H	2.991256	0.538683	-0.310788
H	-0.493702	0.875276	1.852950	H	1.699385	2.142455	1.972220

H	1.942970	-0.979790	1.918062	H	3.207455	1.246842	2.073282
H	1.620533	0.386583	2.977173	H	1.388469	-0.030713	3.168226
H	2.008417	1.975806	1.058966	H	1.948081	-0.908197	1.750265
H	3.771817	-0.439318	0.262734	H	-0.533481	0.892854	1.872698
H	3.972954	1.228436	-0.301548	H	-0.561807	-0.863585	1.883808
H	4.331801	0.809782	1.375257	C	2.519172	2.662338	-0.538776
C	0.181666	-1.370098	-0.724316	H	3.477925	3.112139	-0.238531
H	-0.727963	-1.966242	-0.536707	H	2.518075	2.606367	-1.632351
H	1.002865	-1.947966	-0.276622	H	1.731782	3.363092	-0.237154
H	-0.660958	0.636970	-0.516699	C	-1.214345	0.612203	-0.715612
C	0.401431	-1.263371	-2.238315	H	-2.119621	0.053796	-0.422785
H	-0.416009	-0.676896	-2.678473	H	-1.377175	1.637132	-0.354569
H	1.319173	-0.692634	-2.428808	H	0.304700	-0.938029	-0.451817
C	0.486026	-2.624998	-2.932728	C	-1.101738	0.614875	-2.243513
H	-0.434395	-3.201623	-2.786781	H	-1.997449	1.037311	-2.709622
H	0.642699	-2.516282	-4.010566	H	-0.240541	1.204941	-2.574756
H	1.314329	-3.222226	-2.534999	H	-0.972956	-0.402146	-2.630352

2-Octyl: $7s_{\alpha}^{A}s_{\alpha}^{A}$

Cartesian Coordinates (Å)			
C	-0.013517	0.020348	0.017728
C	0.013020	0.051329	1.538274
C	1.413016	0.018058	2.184750
C	2.182160	-1.311179	2.062348
C	2.772441	-1.626235	0.672744
C	1.761900	-1.964277	-0.412175
H	-0.567529	-0.795529	1.927088
H	-0.507690	0.956515	1.890002
H	1.291012	0.240523	3.251989
H	2.031835	0.831316	1.782089
H	1.532989	-2.134612	2.389193
H	3.012751	-1.287829	2.778510
H	3.376303	-0.767738	0.350585
H	3.479910	-2.464106	0.781188
H	0.827017	-0.989553	-0.312164
C	1.028023	-3.283846	-0.281909
H	0.301057	-3.418271	-1.089377
H	1.724268	-4.134690	-0.323132
H	0.484975	-3.362365	0.666415
H	2.161885	-1.809378	-1.418415
H	-0.971999	-0.330292	-0.375935
C	0.488544	1.253563	-0.705659

2-Octyl: $7s_{\alpha}^{A}s_{\alpha}^{E}$

Cartesian Coordinates (Å)			
C	0.022792	-0.035253	-0.025122
C	0.012581	-0.009336	1.487757
C	1.363369	-0.042589	2.175310
C	1.316259	0.200307	3.695322
C	0.991498	1.637893	4.144427
C	-0.466046	2.100454	3.945684
C	-0.900128	2.314053	2.503585
H	-0.691384	-0.728019	1.922112
H	2.028392	0.701297	1.712696
H	1.842474	-1.017726	1.990972
H	2.293745	-0.069653	4.113518
H	0.593546	-0.492587	4.149816
H	1.676971	2.334624	3.643464
H	1.222216	1.715986	5.214068
H	-1.131042	1.364154	4.416035
H	-0.610170	3.036399	4.509080
H	-0.530238	1.165727	1.885422
H	0.459350	-0.968689	-0.411279
H	-0.987858	0.045317	-0.438558
H	0.619405	0.788443	-0.434584
C	-0.256275	3.460812	1.750697
H	-0.613506	3.511155	0.717142

H	0.467146	1.116104	-1.791596	H	-0.485057	4.428232	2.222752
H	-0.130306	2.133396	-0.474858	H	0.835224	3.373750	1.718604
H	1.517357	1.505380	-0.425995	H	-1.988341	2.303992	2.391908

2-Octyl: $7s_{\alpha}^{E}s_{\alpha}^{E}$

Cartesian Coordinates (Å)			
C	0.027107	-0.017859	-0.029974
C	0.017357	-0.011330	1.483014
C	1.370369	-0.015378	2.167513
C	1.318703	0.179834	3.693907
C	0.934593	1.587549	4.189240
C	-0.531563	2.007567	3.979309
C	-0.909457	2.284110	2.537088
C	-2.376862	2.526565	2.259840
H	-0.668420	-0.751159	1.910686
H	2.004099	0.767732	1.725888
H	1.885684	-0.965421	1.952860
H	2.307944	-0.061061	4.102048
H	0.627249	-0.556098	4.128815
H	1.594018	2.328767	3.715404
H	1.152951	1.636154	5.263150
H	-1.191347	1.226640	4.385260
H	-0.730257	2.904821	4.587295
H	-0.255908	3.029535	2.070396
H	-0.540207	1.151230	1.893727
H	-2.745188	3.420391	2.785575
H	-2.569384	2.675514	1.192445
H	-2.991066	1.683186	2.597284
H	0.497451	-0.929542	-0.428080
H	-0.985783	0.031330	-0.442606
H	0.593274	0.832558	-0.428315

3-Octyl: $3s_{\beta}s_{\beta}$

Cartesian Coordinates (Å)			
C	-0.024360	0.005079	-0.023828
C	-0.013888	-0.001088	1.508974
C	1.365952	0.007965	2.103046
C	1.618864	-0.464884	3.499732
C	2.746797	0.081668	4.327814
C	3.183223	-0.845571	5.469561
C	4.300271	-0.260456	6.339822
C	4.727161	-1.190930	7.478145
H	1.909525	-1.131153	2.420302
H	0.769491	-0.912321	4.010419
H	2.107084	0.686768	1.687874
H	3.609317	0.290543	3.678875
H	2.460006	1.061881	4.749669
H	-0.560760	-0.880381	1.875938
H	-0.584544	0.868255	1.879985
H	2.313116	-1.072904	6.101500
H	3.507966	-1.806141	5.047858
H	-1.046463	0.025372	-0.414842
H	0.499196	0.883945	-0.416183
H	0.476825	-0.882646	-0.423048
H	5.169324	-0.031490	5.708334
H	3.969036	0.700241	6.756229
H	5.524173	-0.745950	8.082221
H	3.886521	-1.410510	8.145934
H	5.097298	-2.146729	7.090662

3-Octyl: $4^{c}s_{\beta}s_{\beta}$

Cartesian Coordinates (Å)			
C	-0.078750	-0.130860	-0.051808
C	-0.023165	0.013027	1.449316
C	1.331400	0.065060	2.168956
C	1.094061	1.484031	2.704227
C	2.005498	2.612597	2.289904
C	1.479643	4.003153	2.665155
H	-0.076030	1.341089	1.927093
H	0.738625	1.526152	3.736153

3-Octyl: $4^{t}s_{\beta}s_{\beta}$

Cartesian Coordinates (Å)			
C	0.013735	0.031591	-0.042935
C	0.008843	0.023551	1.467396
C	1.338647	-0.012039	2.236844
C	1.062832	-1.405518	2.819879
C	0.782074	-1.553800	4.294450
C	0.239899	-2.933267	4.686723
H	-0.104502	-1.257297	2.044086
H	1.633330	-2.218717	2.366219

H	2.175362	0.018230	1.472716	H	1.446265	0.769292	2.994764
H	1.482337	-0.701374	2.933573	H	2.217151	0.026959	1.585928
H	2.178432	2.567138	1.204940	H	-0.771647	0.625985	1.937027
H	3.000092	2.468357	2.747527	H	0.071263	-0.776746	4.611733
H	-0.809299	-0.511372	1.997191	H	1.704844	-1.353150	4.866563
H	0.646166	0.554507	-0.512044	H	-0.975600	-0.258001	-0.416891
H	0.258486	-1.142598	-0.334138	H	0.717006	-0.728285	-0.409970
H	1.304524	4.040819	3.748468	H	0.951564	-3.704261	4.362954
H	0.499506	4.152564	2.195107	H	-0.686495	-3.124139	4.130548
C	-1.471323	0.120559	-0.637806	C	0.397228	1.398203	-0.640481
H	-1.475518	-0.005685	-1.724946	H	1.393690	1.710265	-0.310609
H	-2.206413	-0.575343	-0.218554	H	0.402872	1.362532	-1.735472
H	-1.812512	1.136142	-0.412227	H	-0.311706	2.174230	-0.332774
C	2.427487	5.134540	2.259498	C	-0.019310	-3.074009	6.188735
H	2.024150	6.113477	2.536998	H	-0.407258	-4.067122	6.436264
H	3.404226	5.027473	2.744712	H	0.899490	-2.922347	6.766418
H	2.597317	5.140042	1.176847	H	-0.751198	-2.335639	6.535310

3-Octyl: $5s_{\beta}^{A}s_{\beta}^{A}$			
Cartesian Coordinates (Å)			
C	-0.003854	-0.048293	-0.009054
C	-0.002106	-0.041558	1.518629
C	1.492102	0.034562	1.943295
C	2.187925	0.877445	0.875669
H	1.225309	0.574704	-0.064866
H	-0.505080	-0.916652	1.948011
H	-0.537119	0.840457	1.886892
H	1.925050	-0.971449	1.963394
H	1.609260	0.447031	2.952911
C	2.186419	2.380523	1.055538
H	2.787386	2.638720	1.942952
H	1.168567	2.725739	1.282447
C	2.726931	3.141784	-0.158890
H	2.118652	2.946089	-1.048276
H	2.730320	4.222335	0.015397
H	3.754415	2.837975	-0.388411
H	3.142984	0.488783	0.514525
C	0.134398	-1.384298	-0.707363
H	0.975015	-1.943563	-0.274720
H	-0.760138	-1.994331	-0.500059
C	0.322571	-1.263295	-2.222736
H	1.233400	-0.704530	-2.462466

3-Octyl: $5s_{\beta}^{A}s_{\beta}^{E}$			
Cartesian Coordinates (Å)			
C	-0.015096	0.109630	-0.033041
C	-0.010558	0.016541	1.474039
C	1.314399	0.012708	2.227258
C	1.089766	-0.914986	3.450548
C	0.173381	-2.035216	2.959749
H	-0.346683	-1.231831	1.962577
H	-0.775716	0.641308	1.948155
H	1.651278	1.013657	2.521810
H	2.097955	-0.405020	1.582406
H	0.591290	-0.352921	4.248452
H	2.034748	-1.286601	3.865389
H	0.386562	1.088802	-0.344441
H	0.679351	-0.633699	-0.447641
C	-1.404684	-0.078403	-0.651751
H	-1.370982	0.005392	-1.742480
H	-1.815767	-1.062026	-0.401011
H	-2.106640	0.676492	-0.280592
C	0.819945	-3.238570	2.307582
H	1.419458	-3.778335	3.059227
H	1.539212	-2.908763	1.545695
C	-0.186736	-4.206647	1.677733
H	-0.766151	-3.714706	0.889227

H	0.396118	-2.246946	-2.697054
H	-0.519724	-0.733831	-2.682013
H	-0.734643	0.610631	-0.483830

H	0.314421	-5.073495	1.235643
H	-0.896607	-4.577229	2.425581
H	-0.647887	-2.300064	3.629762

3-Octyl: $5s_{\beta}^{E}s_{\beta}^{E}$

Cartesian Coordinates (Å)			
C	0.011842	0.028292	-0.033329
C	-0.001176	0.006332	1.476075
C	1.314795	-0.004209	2.245163
C	1.041926	-0.860659	3.505985
C	0.138606	-1.994161	3.032877
C	-0.922086	-2.539517	3.957966
C	-1.849290	-3.560477	3.289480
H	-0.368682	-1.216293	2.007683
H	-0.752450	0.673218	1.913861
H	1.685817	0.997548	2.492020
H	2.087997	-0.488159	1.634120
H	0.505875	-0.257141	4.250213
H	1.965458	-1.207771	3.984132
H	0.674566	-2.772565	2.478326
H	-1.515417	-1.707728	4.361631
H	-0.444128	-3.009002	4.834453
H	0.455443	0.974258	-0.387231
H	0.679052	-0.762031	-0.403558
H	-2.597508	-3.940882	3.991880
H	-2.379302	-3.113694	2.441574
H	-1.282493	-4.417789	2.909762
C	-1.378951	-0.134611	-0.656291
H	-1.333219	-0.105950	-1.749417
H	-1.830720	-1.087849	-0.362104
H	-2.052954	0.665022	-0.329555

4-Octyl: $3s_{\beta}s_{\beta}$

Cartesian Coordinates (Å)			
C	-0.018676	0.008893	-0.025992
C	-0.009673	-0.005457	1.504447
C	1.405508	-0.003730	2.098385
C	1.437223	-0.055549	3.599048
C	2.623419	0.423722	4.375534
C	2.971063	-0.151142	5.718863
C	3.836187	0.773036	6.586418
C	4.213315	0.153522	7.934232
H	1.499512	1.067855	4.252832
H	3.408532	0.904008	3.796454
H	0.789436	-0.764304	4.109301
H	2.046928	-0.397426	6.261287
H	3.494299	-1.115969	5.589911
H	1.942759	0.891069	1.752516
H	1.970774	-0.857011	1.681620
H	4.748730	1.032364	6.033463
H	3.300616	1.717287	6.745450
H	-0.549148	-0.890597	1.866663
H	-0.559378	0.862197	1.890105
H	4.831733	0.833549	8.528443
H	3.321100	-0.085368	8.524134
H	4.776694	-0.776647	7.799318
H	-1.039456	0.005232	-0.420841
H	0.485725	0.900086	-0.416485
H	0.499322	-0.866574	-0.433544

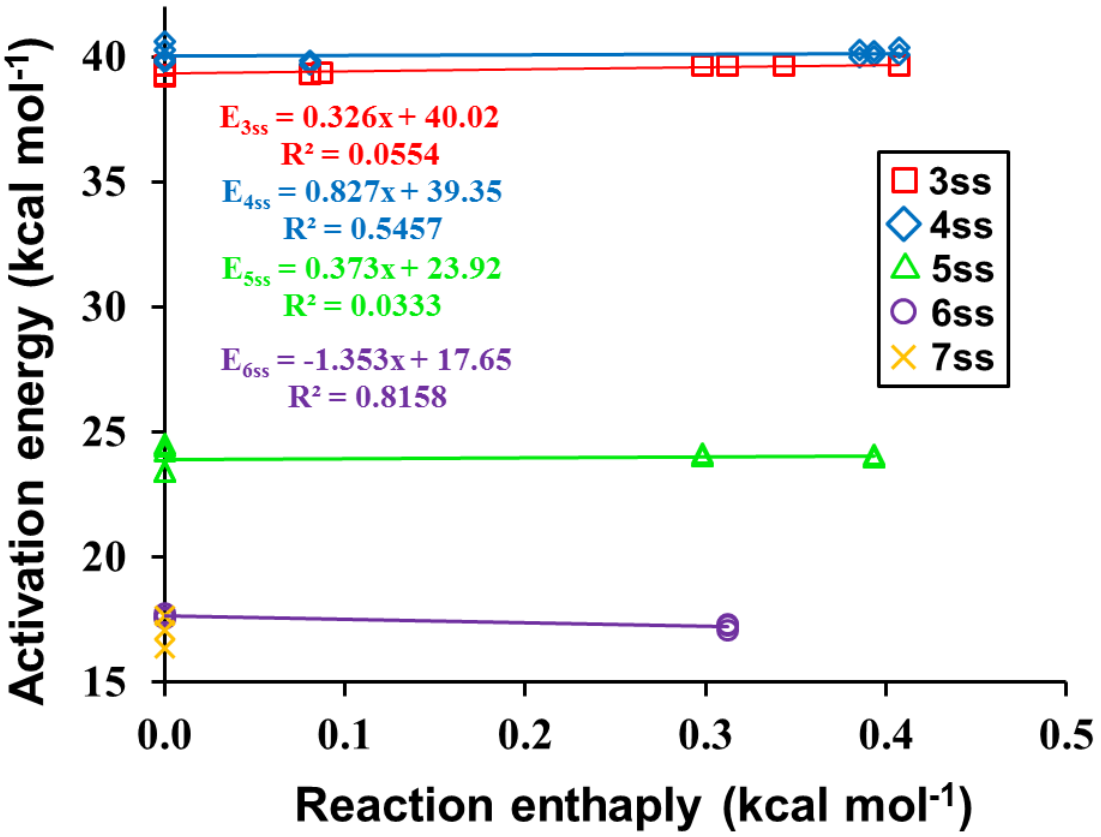

Figure S.1 Evans Polanyi plot of activation energy versus reaction enthalpy for s-alkyl radical H-migrations