

Treating dispersion effects in extended systems by hybrid MP2:DFT calculations – Protonation of isobutene in zeolite ferrierite

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Supporting information

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1. Sets of fitted parameters C_6 and E_{add}
2. Vibrational frequencies

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Sets of fitted parameters (C_6 in $\text{nm}^6\text{Jmol}^{-1}$, E_{add} in kJmol^{-1})

structure	$C_6(\text{C}), C_6(\text{H}_a), C_6(\text{O}), C_6(\text{H}_z), E_{\text{add}}$					
	MP2/TZVP			MP2/aug(O)-TZVPP		
2	88.8298,	-0.14071,	2.65186,	-2.07543,	-9.75561	20.2749, 0.72182, 0.88655, -0.24531, -8.18019
3	-1.18961,	1.03438,	19.1003,	-0.15988,	-6.12368	1.10804, 0.27246, 3.09719, -0.19587, -35.5511
4	2.37034,	0.42948,	6.69415,	-0.09658,	82.2181	2.29528, 0.26973, 7.88467, -1.26700, 59.7517
5	1.90801,	1.45225,	0.70989,	-0.22511,	-15.4637	7.17935, 0.66008, 0.92385, -0.25628, -17.0187

Vibrational frequencies (in cm^{-1})

- isobutene (30 vibrational modes)

3124, 3039, 3027, 3026, 2975, 2973, 2926, 2921, 1657, 1443, 1430, 1424, 1411, 1386, 1353, 1351, 1259, 1059, 1042, 979, 956, 926, 871, 806, 678, 425, 422, 368, 204, 169

- unloaded H-FER 1 (648 vibrational modes)

3680, 1244, 1226, 1223, 1221, 1219, 1218, 1217, 1216, 1215, 1213, 1212, 1212, 1211, 1210, 1207, 1205, 1204, 1203, 1203, 1202, 1201, 1200, 1200, 1199, 1198, 1197, 1197, 1196, 1195, 1194, 1193, 1192, 1190, 1190, 1188, 1188, 1186, 1185, 1185, 1183, 1181, 1180, 1178, 1177, 1176, 1175, 1173, 1172, 1171, 1170, 1167, 1166, 1166, 1164, 1161, 1160, 1158, 1157, 1156, 1154, 1153, 1152, 1152, 1150, 1149, 1147, 1147, 1145, 1143, 1138, 1136, 1115, 1107, 1093, 1092, 1091, 1090, 1090, 1089, 1088, 1087, 1086, 1086, 1085, 1085, 1084, 1083, 1083, 1081, 1081, 1080, 1079, 1079, 1078, 1077, 1077, 1076, 1075, 1075, 1074, 1074, 1073, 1073, 1072, 1072, 1071, 1070, 1070, 1069, 1068, 1067, 1067, 1065, 1065, 1064, 1064, 1063, 1062, 1062, 1062, 1061, 1060, 1059, 1059, 1058, 1058, 1058, 1057, 1057, 1056, 1056, 1055, 1055, 1054, 1054, 1054, 1053, 1053, 1051, 1050, 1045, 1041, 1040, 801, 799, 797, 793, 791, 790, 789, 788, 788, 786, 785, 785, 785, 783, 783, 783, 782, 781, 780, 779, 778, 778, 777, 777, 776, 776, 775, 775, 774, 773, 773, 772, 771, 771, 770, 770, 770, 769, 768, 768, 767, 767, 766, 766, 765, 763, 761, 761, 761, 760, 759, 759, 758, 757, 757, 756, 756, 755, 754, 753, 752, 751, 751, 750, 750, 749, 748, 747, 745, 743, 743, 738, 727, 723, 722, 721, 718, 715, 709, 707, 707, 705, 704, 697, 692, 690, 682, 676, 674, 673, 667, 664, 660, 654, 645, 644, 642, 635, 615, 599, 592, 588, 585, 581, 578, 577, 572, 571, 569, 568, 563, 560, 559, 557, 555, 553, 552, 550, 548, 547, 545, 544, 543, 541, 539, 537, 535, 533, 528, 523, 521, 518, 514, 509, 506, 499, 496, 493, 491, 490, 486, 481, 477, 443, 439, 438, 437, 436, 435, 435, 434, 433, 432, 431, 431, 430, 430, 429, 428, 428, 427, 426, 426, 424, 423, 422, 422, 421, 420, 419, 419, 418, 418, 417, 417, 416, 415, 414, 413, 412, 411, 410, 409, 407, 407, 407, 405, 404, 404, 404, 403, 403, 403, 402, 402, 401, 401, 400, 399, 399, 398, 397, 397, 396, 395, 395, 394, 393, 392, 391, 390, 390, 389, 388, 388, 386, 386, 385, 384, 384, 383, 382, 380, 379, 379, 379, 378, 377, 377, 376, 375, 375, 373, 373, 372, 371, 370, 369, 369, 366, 366, 364, 362, 361, 361, 359, 358, 358, 357, 356, 354, 354, 353, 351, 350, 349, 349, 346, 346, 344, 343, 343, 343, 341, 340, 340, 338, 337, 337, 334, 334, 333, 333, 332, 330, 329, 328, 327, 327, 326, 324, 324, 322, 320, 319, 318, 317, 316, 315, 314, 313, 312, 311, 311, 310, 309, 309, 307, 306, 305, 303, 303, 302, 301, 300, 299, 298, 297, 296, 294, 293, 292, 290, 290, 289, 287, 286, 285, 283, 281, 280, 277, 275, 274, 272, 272, 271, 267, 266, 266, 265, 264, 263, 262, 262, 260, 260, 259, 258, 255, 254, 251, 251, 250, 249, 248, 246, 245, 243, 242, 240, 239, 238, 237, 236, 234, 234, 234, 233, 232, 231, 230, 227, 226, 226, 225, 225, 224, 222, 219, 218, 216, 215, 214, 213, 210, 209, 206, 205, 203, 202, 202, 200, 196, 195, 193, 191, 190, 188, 188, 186, 185, 185, 183, 183, 181, 181, 180, 179, 177, 174, 168, 167, 166, 165, 163, 161, 161, 159, 159, 157, 156, 155, 154, 153, 151, 149, 147, 146, 144, 143, 142, 142, 140, 140, 136, 135, 134, 133, 131, 129, 129, 128, 127, 126, 125, 124, 123, 122, 121, 120, 118, 117, 116, 113, 110, 110, 108, 107, 106, 106, 105, 104, 102, 101, 100, 97, 97, 96, 93, 92, 91, 89, 89, 87, 86, 85, 81, 80, 78, 76, 73, 72, 71, 70, 69, 67, 63, 62, 62, 61, 60, 60, 58, 55, 55, 53, 52, 51, 50, 49, 48, 48, 47, 46, 44, 43, 42, 41, 41, 38, 37, 32, 28

- π -complex 2 (684 vibrational modes)

3125, 3053, 3044, 3032, 3001, 2996, 2945, 2939, 2837, 1623, 1445, 1435, 1421, 1412, 1378, 1356, 1355, 1272, 1243, 1227, 1225, 1222, 1221, 1220, 1219, 1218, 1217, 1216, 1214, 1213, 1212, 1209, 1208, 1207, 1206, 1205, 1204, 1202, 1202, 1201, 1200, 1199, 1197, 1197, 1196, 1195, 1194, 1194, 1191, 1191, 1190, 1188, 1186, 1185, 1184, 1184, 1183, 1182, 1181, 1179, 1178, 1176, 1175, 1174, 1172, 1171, 1171, 1169, 1168, 1167, 1166, 1164, 1163, 1161, 1159, 1157, 1156, 1156, 1154, 1153, 1152, 1151, 1149, 1148, 1147, 1145, 1144, 1141, 1139, 1131, 1109, 1095, 1094, 1093, 1093, 1091, 1091, 1090, 1089, 1089, 1088, 1086, 1084, 1083, 1082, 1081, 1081, 1081, 1080, 1079, 1079, 1078, 1077, 1077, 1076, 1075, 1074, 1074, 1073, 1073, 1072, 1072, 1072, 1071, 1070, 1069, 1069, 1068, 1068, 1067, 1066, 1065, 1063, 1062, 1062, 1061, 1061, 1060, 1060, 1060, 1060, 1059, 1059, 1058, 1058, 1057, 1056, 1056, 1056, 1056, 1055, 1054, 1054, 1054, 1053, 1051, 1051, 1050, 1049, 1049, 1048, 1048, 1047, 1035, 982, 954, 929, 894, 830, 815, 801, 797, 793, 791, 790, 789, 787, 787, 787, 786, 785, 785, 783, 783, 782, 781, 780, 780, 778, 778, 778, 777, 776, 776, 775, 775, 774, 774, 773, 773, 772, 772, 772, 770, 769, 769, 769, 768, 768, 767, 767, 766, 765, 764, 763, 763, 762, 761, 761, 759, 759, 759, 758, 756, 756, 756, 755, 754, 753, 753, 752, 752, 751, 751, 750, 749, 748, 746, 744, 743, 740, 736, 727, 723, 722, 721, 716, 714, 708, 707, 707, 706, 702, 697, 692, 691, 687, 681, 675, 672, 672, 667, 664, 659, 654, 646, 643, 643, 635, 615, 601, 592, 587, 585, 582, 578, 577, 572, 570, 569, 566, 563, 559, 558, 557, 555, 553, 551, 549, 548, 547, 545, 544, 542, 541, 539, 537, 535, 533, 530, 523, 521, 520, 515, 513, 506, 499, 496, 492, 491, 490, 486, 481, 478, 456, 444, 439, 438, 436, 436, 435, 434, 434, 434, 433, 432, 432, 430, 430, 429, 429, 427, 427, 425, 424, 424, 423, 423, 422, 422, 420, 420, 420, 418, 418, 417, 417, 416, 415, 415, 414, 413, 412, 412, 410, 409, 409, 408, 407, 407, 406, 405, 404, 404, 403, 403, 403, 402, 401, 401, 399, 399, 398, 398, 397, 397, 396, 396, 395, 394, 393, 392, 392, 390, 389, 388, 388, 387, 387, 386, 385, 384, 384, 382, 382, 381, 381, 379, 379, 378, 378, 377, 376, 376, 375, 375, 374, 372, 372, 372, 370, 370, 369, 368, 367, 364, 363, 362, 361, 359, 359, 358, 358, 356, 355, 353, 353, 351, 350, 350, 349, 348, 347, 345, 344, 343, 342, 341, 340, 339, 338, 337, 336, 335, 333, 332, 331, 330, 329, 329, 327, 326, 326, 325, 324, 324, 322, 320, 319, 318, 316, 315, 315, 314, 313, 312, 311, 310, 309, 309, 307, 307, 305, 305, 304, 303, 302, 301, 299, 298, 297, 296, 296, 295, 294, 292, 290, 289, 289, 287, 285, 283, 283, 281, 279, 277, 276, 274, 273, 271, 270, 269, 267, 266, 265, 264, 263, 262, 261, 261, 259, 257, 256, 255, 254, 253, 252, 250, 249, 247, 245, 244, 243, 241, 241, 239, 237, 237, 235, 234, 233, 232, 231, 230, 230, 229, 227, 227, 226, 225, 223, 222, 220, 218, 217, 215, 214, 213, 211, 209, 207, 204, 204, 202, 201, 197, 196, 195, 194, 192, 191, 190, 189, 188, 187, 186, 185, 185, 184, 183, 182, 181, 180, 177, 175, 171, 168, 166, 165, 165, 162, 161, 160, 160, 158, 157, 157, 154, 154, 153, 151, 149, 148, 145, 144, 143, 142, 142, 141, 138, 137, 136, 136, 134, 134, 131, 130, 128, 127, 126, 126, 124, 124, 121, 120, 119, 117, 117, 115, 114, 112, 110, 108, 108, 106, 104, 104, 103, 103, 101, 100, 99, 98, 97, 96, 96, 94, 92, 92, 91, 89, 89, 87, 85, 84, 83, 82, 79, 78, 77, 75, 72, 72, 70, 69, 67, 66, 65, 63, 62, 61, 60, 59, 56, 55, 55, 55, 53, 52, 51, 50, 49, 48, 46, 46, 44, 43, 42, 39, 38, 36, 33, 30, 28

- *tert*-butoxide **3** (684 vibrational modes)

3099, 3096, 3094, 3048, 3043, 3033, 2979, 2971, 2966, 1472, 1456, 1445, 1436, 1429, 1413, 1380, 1356, 1352, 1247, 1242, 1236, 1228, 1227, 1225, 1224, 1222, 1220, 1217, 1217, 1216, 1214, 1212, 1211, 1208, 1207, 1206, 1205, 1204, 1202, 1202, 1200, 1198, 1197, 1197, 1195, 1194, 1193, 1191, 1190, 1189, 1188, 1186, 1185, 1184, 1183, 1183, 1182, 1181, 1180, 1179, 1178, 1176, 1175, 1174, 1173, 1172, 1171, 1170, 1169, 1168, 1167, 1165, 1163, 1163, 1161, 1159, 1159, 1157, 1156, 1154, 1153, 1152, 1150, 1148, 1147, 1147, 1144, 1141, 1141, 1140, 1130, 1108, 1102, 1094, 1093, 1092, 1091, 1089, 1089, 1088, 1087, 1086, 1085, 1083, 1081, 1080, 1080, 1080, 1079, 1079, 1078, 1077, 1077, 1076, 1076, 1075, 1075, 1074, 1074, 1073, 1072, 1071, 1071, 1071, 1070, 1069, 1069, 1068, 1068, 1067, 1067, 1066, 1066, 1064, 1063, 1063, 1062, 1061, 1060, 1060, 1059, 1058, 1058, 1057, 1057, 1056, 1055, 1055, 1054, 1054, 1052, 1052, 1051, 1050, 1049, 1048, 1048, 1047, 1047, 1046, 1045, 1045, 1039, 1034, 1020, 1014, 936, 909, 890, 831, 801, 797, 792, 791, 790, 789, 788, 787, 786, 785, 785, 784, 783, 782, 781, 781, 779, 779, 778, 778, 777, 776, 775, 775, 774, 773, 773, 773, 773, 772, 772, 771, 771, 770, 769, 769, 768, 767, 767, 766, 766, 765, 764, 764, 763, 762, 762, 761, 760, 759, 759, 759, 758, 757, 756, 755, 754, 754, 753, 752, 752, 751, 751, 750, 749, 748, 747, 746, 742, 741, 738, 729, 727, 723, 723, 720, 717, 714, 707, 706, 706, 703, 698, 697, 691, 689, 678, 674, 673, 669, 669, 663, 660, 655, 647, 645, 642, 632, 616, 602, 593, 589, 585, 584, 579, 578, 573, 569, 568, 566, 562, 560, 560, 559, 557, 555, 552, 552, 550, 547, 546, 545, 541, 540, 539, 538, 536, 535, 530, 527, 525, 522, 519, 513, 510, 505, 497, 494, 492, 490, 488, 484, 480, 479, 455, 446, 442, 438, 438, 437, 436, 435, 434, 434, 434, 433, 432, 431, 430, 429, 428, 426, 426, 425, 425, 424, 423, 422, 421, 421, 420, 420, 419, 419, 418, 417, 417, 417, 416, 415, 414, 413, 412, 412, 410, 410, 409, 408, 408, 407, 406, 406, 404, 404, 403, 403, 402, 401, 401, 400, 400, 398, 398, 398, 397, 396, 396, 396, 395, 394, 393, 393, 393, 391, 391, 390, 389, 389, 388, 388, 387, 385, 384, 384, 383, 382, 381, 380, 379, 379, 379, 378, 377, 376, 375, 375, 374, 374, 374, 371, 370, 369, 369, 367, 367, 366, 365, 363, 362, 361, 360, 359, 359, 357, 356, 355, 354, 352, 352, 351, 349, 349, 347, 347, 345, 342, 341, 340, 339, 338, 337, 336, 335, 334, 334, 333, 332, 331, 330, 329, 328, 328, 326, 326, 325, 325, 324, 322, 321, 321, 320, 319, 317, 316, 314, 312, 312, 311, 310, 309, 307, 307, 306, 305, 304, 302, 302, 301, 300, 300, 299, 297, 296, 296, 293, 292, 292, 291, 289, 288, 287, 285, 285, 283, 282, 282, 280, 279, 277, 275, 273, 272, 270, 269, 269, 267, 266, 265, 265, 262, 261, 260, 260, 259, 258, 256, 255, 253, 253, 251, 250, 248, 248, 246, 244, 243, 242, 241, 238, 237, 236, 234, 234, 233, 232, 230, 230, 229, 228, 228, 226, 224, 222, 221, 218, 218, 215, 215, 214, 212, 210, 209, 205, 205, 204, 203, 202, 200, 200, 198, 197, 196, 195, 193, 191, 190, 189, 188, 187, 187, 186, 185, 182, 181, 180, 178, 176, 175, 172, 171, 169, 167, 165, 165, 162, 162, 161, 157, 157, 155, 154, 154, 152, 151, 151, 150, 148, 145, 144, 143, 142, 141, 138, 138, 137, 135, 135, 134, 133, 130, 130, 128, 128, 126, 124, 124, 122, 122, 119, 119, 117, 115, 113, 112, 111, 110, 108, 106, 105, 104, 103, 102, 102, 101, 100, 99, 97, 95, 94, 90, 90, 89, 89, 85, 85, 83, 81, 80, 79, 77, 76, 75, 74, 73, 72, 71, 69, 67, 65, 64, 64, 62, 61, 60, 59, 58, 57, 56, 55, 54, 53, 52, 52, 49, 49, 48, 47, 46, 44, 41, 39, 37, 31, 29

- *tert*-butyl carbenium ion **4** (684 vibrational modes)

3078, 3069, 3067, 2994, 2976, 2932, 2890, 2862, 2402, 1482, 1449, 1441, 1387, 1371, 1337, 1327, 1299, 1296, 1277, 1245, 1230, 1229, 1226, 1222, 1220, 1219, 1218, 1216, 1215, 1213, 1211, 1210, 1210, 1207, 1205, 1205, 1203, 1203, 1202, 1202, 1200, 1199, 1198, 1198, 1197, 1195, 1194, 1194, 1193, 1192, 1189, 1188, 1186, 1185, 1184, 1183, 1183, 1182, 1181, 1179, 1178, 1176, 1175, 1174, 1172, 1171, 1170, 1169, 1167, 1166, 1165, 1164, 1163, 1162, 1159, 1158, 1156, 1155, 1154, 1153, 1152, 1150, 1148, 1147, 1147, 1145, 1143, 1142, 1140, 1136, 1135, 1115, 1106, 1097, 1093, 1091, 1091, 1090, 1090, 1089, 1087, 1086, 1086, 1083, 1083, 1082, 1081, 1081, 1080, 1080, 1079, 1078, 1078, 1077, 1076, 1074, 1074, 1073, 1073, 1072, 1071, 1071, 1071, 1070, 1070, 1070, 1069, 1067, 1066, 1066, 1064, 1063, 1062, 1062, 1061, 1061, 1061, 1060, 1060, 1059, 1059, 1058, 1058, 1057, 1057, 1056, 1056, 1055, 1055, 1054, 1054, 1054, 1053, 1051, 1051, 1050, 1049, 1047, 1046, 1045, 1039, 1036, 1035, 1033, 1017, 1000, 960, 953, 844, 802, 799, 795, 792, 790, 789, 787, 786, 786, 785, 785, 784, 783, 782, 782, 781, 780, 780, 778, 777, 777, 776, 776, 775, 775, 774, 773, 772, 772, 771, 771, 771, 770, 770, 769, 768, 768, 767, 767, 766, 766, 765, 763, 763, 761, 761, 760, 760, 759, 759, 758, 757, 756, 756, 755, 754, 753, 752, 752, 751, 750, 749, 749, 748, 748, 747, 745, 745, 743, 740, 738, 734, 729, 725, 722, 721, 720, 714, 711, 708, 706, 705, 700, 698, 694, 690, 688, 682, 675, 672, 671, 669, 663, 657, 653, 647, 645, 641, 633, 631, 613, 592, 586, 586, 583, 577, 576, 572, 570, 569, 567, 565, 559, 559, 557, 555, 554, 551, 550, 548, 547, 546, 544, 543, 541, 538, 538, 535, 534, 532, 523, 521, 520, 516, 514, 506, 499, 496, 491, 489, 489, 486, 480, 478, 461, 443, 438, 437, 436, 435, 435, 434, 433, 433, 432, 432, 430, 429, 429, 428, 427, 427, 426, 425, 425, 423, 423, 422, 421, 421, 420, 420, 419, 418, 417, 416, 416, 415, 414, 413, 413, 412, 411, 410, 410, 408, 408, 407, 406, 405, 404, 404, 404, 403, 403, 402, 402, 401, 401, 400, 399, 399, 399, 398, 397, 397, 396, 395, 395, 394, 393, 392, 392, 391, 390, 390, 388, 388, 387, 387, 385, 385, 384, 383, 383, 382, 381, 379, 378, 378, 377, 377, 376, 376, 375, 375, 374, 373, 372, 371, 370, 369, 369, 368, 368, 366, 362, 362, 360, 360, 359, 358, 357, 356, 355, 354, 353, 352, 351, 349, 349, 348, 346, 345, 344, 344, 342, 341, 341, 340, 339, 338, 336, 336, 332, 332, 331, 330, 329, 328, 327, 327, 326, 325, 324, 323, 322, 322, 319, 318, 316, 315, 314, 313, 312, 312, 310, 310, 309, 308, 307, 306, 305, 304, 303, 303, 302, 300, 300, 298, 297, 296, 294, 294, 294, 293, 290, 289, 288, 288, 286, 284, 283, 282, 281, 279, 274, 274, 273, 271, 270, 268, 266, 265, 265, 264, 263, 262, 261, 260, 259, 258, 257, 255, 254, 252, 251, 251, 250, 248, 245, 244, 243, 241, 240, 239, 238, 237, 235, 234, 234, 232, 231, 230, 229, 227, 225, 225, 225, 224, 223, 220, 218, 217, 215, 214, 213, 211, 209, 207, 207, 202, 201, 200, 200, 195, 194, 193, 191, 190, 189, 188, 187, 186, 185, 185, 183, 183, 181, 180, 180, 179, 178, 175, 172, 166, 163, 163, 162, 161, 160, 158, 157, 156, 155, 155, 153, 152, 151, 151, 149, 146, 145, 142, 141, 140, 139, 139, 138, 135, 135, 132, 132, 131, 130, 128, 128, 124, 124, 123, 122, 121, 119, 118, 116, 116, 115, 114, 114, 111, 110, 107, 106, 104, 104, 103, 101, 99, 98, 97, 97, 95, 95, 92, 92, 91, 90, 88, 88, 86, 85, 83, 83, 80, 77, 76, 72, 72, 71, 69, 68, 67, 65, 64, 63, 59, 58, 56, 56, 54, 53, 51, 50, 49, 47, 46, 45, 44, 43, 42, 40, 39, 39, 37, 35, 35, 34, 32, 31, 30, 28, 25, 20, 15, 7

- isobutoxide **5** (684 vibrational modes)

3057, 3047, 3044, 3030, 3013, 2993, 2971, 2961, 2941, 1463, 1452, 1446, 1437, 1432, 1383, 1358, 1349, 1336, 1286, 1273, 1244, 1226, 1223, 1219, 1219, 1218, 1217, 1216, 1215, 1214, 1213, 1210, 1209, 1209, 1207, 1206, 1205, 1203, 1202, 1201, 1200, 1200, 1199, 1198, 1197, 1196, 1196, 1194, 1191, 1191, 1190, 1189, 1188, 1187, 1186, 1185, 1184, 1183, 1181, 1180, 1180, 1178, 1178, 1178, 1176, 1175, 1172, 1171, 1170, 1168, 1167, 1166, 1165, 1164, 1162, 1161, 1159, 1157, 1156, 1155, 1155, 1152, 1151, 1150, 1149, 1149, 1147, 1146, 1144, 1142, 1141, 1138, 1122, 1108, 1098, 1094, 1093, 1092, 1091, 1090, 1089, 1088, 1088, 1087, 1087, 1086, 1085, 1084, 1082, 1082, 1081, 1081, 1081, 1078, 1078, 1078, 1077, 1077, 1075, 1074, 1074, 1073, 1073, 1073, 1072, 1072, 1071, 1070, 1069, 1069, 1069, 1068, 1068, 1066, 1065, 1064, 1063, 1063, 1062, 1061, 1061, 1060, 1060, 1059, 1059, 1059, 1057, 1057, 1056, 1056, 1055, 1055, 1054, 1054, 1054, 1053, 1053, 1052, 1051, 1051, 1050, 1049, 1047, 1046, 1043, 1038, 950, 937, 910, 896, 853, 803, 799, 796, 796, 793, 791, 790, 789, 788, 787, 787, 786, 785, 784, 784, 782, 781, 781, 780, 779, 779, 778, 777, 777, 777, 776, 775, 775, 774, 774, 773, 773, 772, 772, 771, 771, 770, 769, 768, 768, 768, 767, 767, 766, 765, 764, 763, 763, 762, 761, 760, 760, 759, 759, 758, 757, 756, 755, 754, 754, 753, 752, 751, 750, 750, 750, 749, 748, 747, 747, 744, 742, 738, 735, 727, 723, 721, 721, 716, 713, 708, 706, 706, 703, 701, 696, 692, 689, 681, 674, 673, 672, 666, 663, 659, 653, 647, 645, 640, 634, 615, 599, 592, 587, 585, 582, 577, 575, 571, 570, 569, 565, 562, 560, 558, 558, 554, 553, 551, 550, 548, 547, 546, 544, 541, 540, 539, 536, 534, 531, 526, 524, 521, 519, 516, 509, 506, 499, 495, 493, 490, 488, 485, 481, 477, 466, 442, 438, 437, 436, 435, 434, 433, 433, 432, 431, 431, 431, 430, 429, 429, 427, 425, 424, 424, 424, 423, 422, 421, 421, 420, 419, 418, 418, 417, 417, 416, 415, 414, 413, 413, 412, 412, 411, 410, 409, 409, 408, 406, 406, 405, 404, 404, 403, 402, 402, 402, 401, 400, 400, 400, 398, 398, 397, 397, 397, 396, 395, 395, 394, 393, 393, 391, 390, 389, 389, 387, 387, 386, 385, 384, 383, 383, 382, 381, 381, 380, 378, 377, 377, 377, 376, 375, 375, 375, 375, 374, 373, 371, 370, 370, 369, 368, 368, 367, 365, 363, 361, 360, 360, 359, 357, 357, 357, 356, 354, 354, 352, 351, 350, 348, 347, 346, 345, 344, 343, 342, 341, 340, 339, 339, 337, 336, 336, 333, 332, 331, 331, 330, 329, 328, 327, 325, 325, 325, 324, 322, 322, 319, 318, 317, 316, 314, 314, 313, 312, 311, 310, 309, 308, 307, 307, 306, 304, 303, 302, 302, 300, 299, 298, 296, 296, 296, 295, 294, 293, 290, 289, 288, 287, 286, 284, 284, 282, 281, 280, 278, 276, 273, 273, 272, 271, 270, 269, 266, 265, 265, 262, 261, 261, 259, 259, 258, 257, 257, 256, 254, 251, 251, 249, 248, 247, 246, 245, 243, 241, 239, 239, 238, 238, 237, 234, 233, 232, 231, 230, 229, 227, 227, 226, 225, 224, 223, 221, 219, 217, 216, 215, 214, 213, 212, 210, 207, 206, 203, 201, 201, 199, 198, 195, 195, 192, 191, 189, 188, 187, 186, 185, 184, 183, 182, 180, 180, 179, 178, 177, 176, 173, 168, 165, 163, 161, 161, 159, 158, 157, 156, 155, 154, 154, 153, 152, 149, 148, 147, 145, 143, 141, 141, 139, 139, 138, 135, 134, 133, 132, 131, 129, 127, 125, 124, 122, 122, 121, 120, 119, 118, 117, 116, 115, 114, 112, 110, 108, 107, 104, 103, 102, 102, 101, 99, 97, 97, 95, 94, 93, 92, 92, 90, 89, 87, 85, 84, 83, 82, 81, 81, 77, 75, 73, 71, 71, 69, 68, 67, 63, 62, 58, 56, 54, 54, 52, 51, 49, 48, 47, 46, 46, 44, 43, 41, 40, 39, 37, 36, 34, 34, 32, 30, 29, 28, 22, 19, 14, 9