

Supporting Information
for
A Combined Crossed Molecular Beam and
Theoretical Investigation of the Reaction of the
Meta-Tolyl Radical with Vinylacetylene - Toward
the Formation of Methylnaphthalenes

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List of Contents:

Table S1. Optimized geometries, and computed vibrational frequencies of the reactants, various intermediates, transition states and products of the reaction of meta-tolyl radical with vinylacetylene calculated at the UM06-2x/cc-pvtz level of theory.....	3
Table S2. Forward and reverse RRKM rate constants (in s^{-1}) as functions of the collision energy E (in $kJ mol^{-1}$) for the reaction steps from the reaction of meta-tolyl radical with vinylacetylene producing the initial adduct i1	51
Table S3. Statistical product branching ratios (%) from the initial adduct i1 as functions of the collision energy E (in $kJ mol^{-1}$).....	52

Table S1. Optimized geometries, and computed vibrational frequencies of the reactants, various intermediates, transition states and products of the reaction of meta-tolyl radical with vinylacetylene calculated at the UM06-2x/cc-pvtz level of theory.

<p>meta-tolyl radical</p> <p>C 0.241480 0.324442 -0.010249 C 1.634851 0.305546 0.016081 C 2.256005 1.526698 0.023504 C 1.626693 2.741765 0.007815 C 0.227676 2.751699 -0.014953 C -0.444108 1.531765 -0.026138 H -0.308383 -0.607784 -0.021975 H 2.184867 -0.625380 0.025880 H 2.180111 3.673079 0.010172 H -1.526565 1.528656 -0.050656 C -0.525640 4.053072 -0.001567 H -1.515420 3.938294 -0.440514 H -0.654685 4.412431 1.020974 H 0.009692 4.823164 -0.555266</p>	<p>98, 211, 352, 426, 491, 522, 628, 691, 780, 804, 886, 917, 1004, 1011, 1014, 1068, 1078, 1112, 1182, 1230, 1307, 1317, 1414, 1454, 1497, 1500, 1513, 1608, 1683, 3055, 3120, 3149, 3174, 3175, 3189, 3202,</p>
<p>vinylacetylene</p> <p>C -3.970166 -0.234909 -0.107709 H -3.495103 -1.206236 -0.107709 H -5.050158 -0.199441 -0.107709 C -3.253014 0.883524 -0.107709 H -3.746733 1.848225 -0.107709 C -1.825648 0.907183 -0.107709 C -0.627469 0.951568 -0.107709 H 0.434193 0.983652 -0.107709</p>	<p>226, 318, 563, 706, 712, 720, 893, 980, 1018, 1112, 1325, 1447, 1705, 2250, 3154, 3164, 3250, 3480,</p>
<p>i1</p> <p>C -1.490273 -0.339969 -0.259228 C -0.191061 -0.167367 -0.734065 C 0.383722 1.093123 -0.673952 C -0.307039 2.188737 -0.156935 C -1.600741 1.994548 0.307574 C -2.189664 0.736512 0.255803 H -1.943536 -1.323446 -0.293187</p>	<p>18, 31, 117, 139, 177, 216, 269, 286, 396, 403, 448, 496, 532, 549, 575, 581, 652, 700, 725, 758, 812, 872, 918, 932, 945, 1016, 1019, 1030, 1039, 1070, 1134, 1145, 1189, 1195, 1203, 1280, 1294, 1336, 1352, 1405, 1414, 1476, 1480, 1496, 1513, 1544, 1672, 1689, 2042, 3043, 3055, 3097, 3116, 3140, 3161, 3169, 3173, 3185, 3201,</p>

<p>H 1.396300 1.231955 -1.038110 H -2.151612 2.832483 0.716210 H -3.197704 0.599194 0.623790 C 0.341707 3.545030 -0.121085 H -0.243374 4.245808 0.471646 H 1.342966 3.488354 0.306287 H 0.439371 3.955486 -1.127424 C 0.571138 -1.351166 -1.291523 H 0.052186 -1.752604 -2.162626 C 0.735283 -2.436839 -0.272974 H 1.231478 -2.193954 0.657541 C 0.255951 -3.715264 -0.454266 C -0.177644 -4.835532 -0.630569 H -0.553267 -5.817787 -0.778727 H 1.554123 -1.010700 -1.629221</p>	<p>3469,</p>
<p>i2</p> <p>C -0.555359 -1.404113 0.644703 C 0.799233 -1.336009 0.335009 C 1.296690 -0.212100 -0.304678 C 0.467341 0.855304 -0.647151 C -0.882915 0.767949 -0.334455 C -1.391514 -0.354444 0.307845 H -0.944673 -2.286945 1.136679 H 2.352082 -0.163005 -0.551212 H -1.544155 1.583329 -0.600252 H -2.446577 -0.408955 0.540701 C 1.032136 2.075385 -1.320662 H 1.465479 2.756954 -0.586316 H 1.819383 1.807317 -2.024378 H 0.258867 2.618896 -1.861018 C 1.729067 -2.473695 0.738498 H 2.704080 -2.274043 0.273084 C 1.891892 -2.519753 2.227135 H 1.997399 -3.463060 2.738465 H 2.056496 -1.595719 2.759662 C 1.260054 -3.763566 0.221117 C 0.870312 -4.820896 -0.182453 H 0.525234 -5.756307 -0.548917</p>	<p>29, 78, 102, 159, 187, 208, 215, 278, 310, 387, 424, 452, 459, 531, 552, 618, 660, 717, 725, 731, 775, 820, 865, 918, 928, 944, 1017, 1017, 1027, 1071, 1083, 1104, 1130, 1187, 1198, 1234, 1284, 1304, 1342, 1348, 1417, 1452, 1477, 1496, 1511, 1542, 1671, 1689, 2262, 2999, 3055, 3115, 3142, 3165, 3169, 3175, 3181, 3201, 3290, 3481,</p>
<p>i3</p>	

<p>C -0.644824 -0.072648 -0.154726 C 0.732072 -0.085862 0.051428 C 1.414277 1.124640 0.145569 C 0.750820 2.341208 0.033775 C -0.627153 2.331370 -0.163633 C -1.319225 1.133697 -0.258574 H -1.177256 -1.012021 -0.220957 H 2.486948 1.115968 0.298282 H -1.159550 3.271370 -0.240971 H -2.390460 1.140186 -0.408857 C 1.513388 3.636176 0.095453 H 2.360346 3.562765 0.776348 H 1.904399 3.900488 -0.888856 H 0.874865 4.453453 0.427277 C 1.464449 -1.381026 0.128278 C 1.245871 -2.310331 -0.780489 H 1.621799 -3.303029 -0.972290 C 2.416322 -1.641395 1.227336 H 3.015621 -2.537801 1.112424 C 2.551735 -0.904388 2.324427 H 1.963301 -0.012234 2.490891 H 3.255680 -1.188288 3.094351</p>	<p>50, 106, 143, 171, 216, 261, 328, 360, 439, 463, 500, 529, 540, 619, 696, 715, 735, 774, 824, 859, 892, 934, 954, 974, 1001, 1019, 1023, 1027, 1035, 1066, 1125, 1143, 1197, 1236, 1312, 1322, 1335, 1352, 1411, 1439, 1462, 1495, 1501, 1542, 1654, 1666, 1685, 1705, 3049, 3111, 3135, 3147, 3160, 3175, 3179, 3190, 3204, 3236, 3239,</p>
<p>i4</p> <p>C -2.187029 -0.364251 -0.370248 C -0.912964 -0.165500 0.158176 C -0.298055 1.081346 0.136949 C -0.988232 2.149166 -0.425760 C -2.259768 1.968567 -0.957462 C -2.858244 0.723428 -0.933307 H -0.390562 -1.006777 0.600579 H -0.528821 3.129734 -0.445810 H -2.784514 2.809681 -1.390668 H -3.849419 0.579652 -1.344589 C 1.089982 1.262818 0.686950 H 1.836826 1.131063 -0.098068 H 1.220832 2.261119 1.102171 H 1.301154 0.535232 1.469252 C -2.792944 -1.698381 -0.321632 H -2.189977 -2.482594 0.142288 C -3.983310 -2.026972 -0.783406</p>	<p>45, 78, 89, 123, 193, 215, 233, 249, 308, 384, 446, 504, 528, 546, 630, 684, 721, 775, 806, 853, 919, 924, 948, 972, 977, 1017, 1017, 1023, 1026, 1073, 1129, 1142, 1197, 1200, 1246, 1299, 1315, 1332, 1352, 1420, 1444, 1474, 1497, 1510, 1544, 1661, 1680, 1689, 1739, 3060, 3070, 3107, 3122, 3144, 3161, 3166, 3168, 3189, 3206, 3255,</p>

<p>C -4.794054 -3.200705 -0.865614 H -4.364215 -4.109626 -0.444994 C -6.008016 -3.238023 -1.412220 H -6.453738 -2.347672 -1.835700 H -6.579142 -4.154513 -1.447233</p>	
<p>i5</p> <p>C -2.211525 -0.911396 -0.006893 C -0.819612 -1.017680 0.003010 C -0.142899 0.180432 -0.005450 C -0.672907 1.443476 -0.023959 C -2.071356 1.500387 -0.037119 C -2.823645 0.337490 -0.027370 H -2.826586 -1.801673 -0.002549 H -2.561576 2.466594 -0.059734 H -3.903307 0.399349 -0.040165 C 0.176685 2.684269 -0.007755 H 0.373421 2.999321 1.018176 H 1.135994 2.506595 -0.489567 H -0.325981 3.504057 -0.518729 C -0.065821 -2.325925 0.019611 H 0.595514 -2.365978 -0.847433 H 0.584491 -2.350606 0.895496 C -0.955399 -3.569887 0.025029 H -1.610419 -3.558997 0.898799 H -1.600000 -3.573822 -0.856482 C -0.162760 -4.795491 0.040124 C 0.510913 -5.785114 0.052285 H 1.102592 -6.667187 0.062601</p>	<p>49, 82, 93, 99, 196, 211, 217, 274, 380, 391, 475, 487, 516, 524, 622, 706, 717, 724, 762, 766, 805, 922, 930, 978, 1000, 1006, 1021, 1052, 1062, 1080, 1125, 1190, 1215, 1256, 1279, 1299, 1325, 1338, 1388, 1413, 1453, 1482, 1491, 1498, 1501, 1507, 1621, 1686, 2264, 3060, 3063, 3076, 3096, 3117, 3126, 3155, 3163, 3195, 3213, 3478,</p>
<p>i6</p> <p>C -2.088685 -0.920844 -0.273208 C -0.725757 -1.001967 -0.131775 C -0.065209 0.221703 0.012276 C -0.746734 1.434032 0.007752 C -2.132118 1.430103 -0.147390 C -2.827112 0.232843 -0.289444 H 1.013730 0.220939 0.132176 H -2.672253 2.369148 -0.156465 H -3.902231 0.223650 -0.410051 C -0.003606 2.728477 0.199675</p>	<p>44, 68, 89, 97, 192, 212, 234, 285, 369, 404, 432, 487, 533, 544, 614, 702, 714, 722, 756, 779, 817, 910, 925, 975, 978, 1006, 1024, 1044, 1070, 1072, 1151, 1184, 1202, 1248, 1270, 1308, 1320, 1328, 1387, 1418, 1438, 1479, 1486, 1496, 1500, 1504, 1638, 1671, 2263, 3057, 3060, 3070, 3093, 3114, 3120, 3148, 3157, 3173, 3196, 3482,</p>

<p>H 0.057274 2.986064 1.258623 H 1.013668 2.659196 -0.182475 H -0.505842 3.549067 -0.310480 C 0.031632 -2.304533 -0.150251 H 0.495164 -2.442629 -1.129661 H 0.846487 -2.262955 0.573623 C -0.859006 -3.512212 0.151260 H -1.338205 -3.380632 1.123527 H -1.662847 -3.569075 -0.586050 C -0.104577 -4.761352 0.143673 C 0.539842 -5.770518 0.132687 H 1.104340 -6.670143 0.124089</p>	
<p>i7</p> <p>C 0.007111 0.008621 -0.003397 C -0.008915 0.007333 1.382506 C 1.179528 0.005494 2.098740 C 2.389812 0.005252 1.424959 C 2.438143 0.003254 0.034518 C 1.235553 0.005528 -0.680925 C -1.273161 0.084544 -0.801253 C -1.193937 -0.709479 -2.114617 C 0.092640 -0.370359 -2.758778 C 1.213202 -0.027789 -2.161225 H -0.957906 0.010935 1.904467 H 1.161626 0.002722 3.180090 H -1.457485 1.134456 -1.051221 H -2.115480 -0.256106 -0.199175 H -1.226605 -1.786797 -1.922751 H -2.045204 -0.468667 -2.751247 H 2.119446 0.186638 -2.713249 C 3.762035 -0.012945 -0.679615 H 3.840890 -0.872514 -1.346683 H 3.897209 0.883273 -1.287977 H 4.582742 -0.060368 0.032999 H 3.317356 0.000652 1.983638</p>	<p>118, 135, 152, 231, 281, 283, 386, 437, 459, 482, 522, 545, 568, 652, 723, 754, 798, 816, 858, 873, 931, 933, 983, 1006, 1012, 1035, 1060, 1065, 1119, 1177, 1192, 1206, 1214, 1265, 1290, 1297, 1334, 1340, 1378, 1411, 1468, 1478, 1479, 1490, 1513, 1524, 1659, 1672, 1716, 3033, 3042, 3044, 3103, 3103, 3106, 3136, 3170, 3182, 3185, 3201,</p>
<p>i8</p> <p>C 0.031648 -0.062340 -0.014208 C -0.000432 0.137458 1.284983 C 1.281324 0.141424 2.019665 C 2.476757 0.240732 1.290306</p>	<p>103, 124, 145, 230, 263, 301, 393, 410, 428, 463, 487, 556, 603, 675, 728, 754, 783, 819, 873, 892, 919, 921,</p>

<p>C 2.406372 0.470265 -0.200294 C 1.230069 -0.273231 -0.856101 H 0.415404 -0.048004 3.965356 H -0.923345 0.248199 1.842526 C 1.337600 0.023306 3.401759 C 3.684534 0.202157 1.964221 H 3.346320 0.189057 -0.675281 H 1.081019 0.088667 -1.873420 C 3.750107 0.072335 3.352209 C 2.558833 -0.009198 4.060711 H 4.607248 0.281104 1.398531 H 2.584899 -0.102257 5.139342 C 5.080112 0.005039 4.049784 H 4.973067 0.183906 5.118314 H 5.537059 -0.977954 3.920436 H 5.774245 0.742516 3.647027 H 1.435789 -1.346423 -0.921951 H 2.264688 1.542284 -0.370841</p>	<p>966, 987, 1012, 1032, 1034, 1074, 1154, 1174, 1187, 1207, 1227, 1258, 1284, 1317, 1331, 1338, 1371, 1420, 1465, 1468, 1478, 1497, 1507, 1545, 1643, 1692, 1718, 3033, 3041, 3060, 3097, 3101, 3122, 3141, 3157, 3159, 3174, 3191,</p>
<p>i9</p> <p>C -5.086707 -1.536317 0.196459 C -3.607775 -1.602558 0.024394 C -2.914771 -0.262692 0.003946 C -3.645281 0.935691 0.140371 C -5.067376 0.875891 0.301086 C -5.743658 -0.353267 0.323852 H -3.172028 -2.220983 0.819976 C -1.536598 -0.216127 -0.152763 C -2.957935 2.173318 0.115400 H -6.819117 -0.353813 0.446912 C -1.584305 2.180000 -0.042904 C -0.867711 0.994694 -0.177078 H 0.206394 1.021645 -0.299906 H -5.629030 1.791428 0.405798 H -0.986129 -1.143925 -0.256150 H -5.633733 -2.469300 0.217226 H -1.060606 3.127584 -0.062267 C -3.708035 3.467452 0.259551 H -4.448778 3.588455 -0.532894 H -4.242081 3.512607 1.210480 H -3.024766 4.312914 0.215587 H -3.369284 -2.145085 -0.899720</p>	<p>77, 137, 206, 224, 276, 292, 433, 463, 477, 499, 517, 547, 559, 671, 694, 728, 792, 795, 810, 871, 917, 957, 959, 992, 995, 999, 1060, 1068, 1103, 1121, 1179, 1190, 1211, 1235, 1251, 1288, 1314, 1357, 1406, 1418, 1441, 1444, 1462, 1492, 1507, 1533, 1589, 1643, 1664, 2995, 3006, 3048, 3105, 3138, 3166, 3175, 3179, 3196, 3204, 3219,</p>
<p>i10</p>	

<p>C -5.049941 -1.521533 0.166559 C -3.652667 -1.504674 0.068331 C -2.938166 -0.265562 0.013689 C -3.639325 0.956412 0.058639 C -5.144171 0.977186 0.166739 C -5.779226 -0.372366 0.214657 H -3.094244 -2.429724 0.033347 C -1.539609 -0.228581 -0.083645 C -2.933227 2.146947 0.005566 H -5.559316 1.549456 -0.673007 H -6.857354 -0.415967 0.291417 C -1.544938 2.183040 -0.090930 C -0.858226 0.970036 -0.134199 H -3.482373 3.083072 0.041518 H 0.222155 0.972981 -0.207993 H -5.433698 1.551998 1.055912 H -0.994822 -1.164115 -0.117727 H -5.561208 -2.474838 0.206117 C -0.817721 3.496842 -0.149518 H -1.087768 4.053879 -1.048129 H -1.070171 4.122151 0.707813 H 0.260718 3.349886 -0.156073</p>	<p>77, 97, 166, 187, 261, 323, 406, 439, 448, 492, 505, 565, 602, 673, 712, 728, 774, 791, 855, 888, 908, 940, 963, 987, 988, 991, 1031, 1069, 1090, 1159, 1177, 1183, 1209, 1240, 1270, 1294, 1317, 1348, 1387, 1418, 1436, 1450, 1476, 1493, 1505, 1530, 1584, 1630, 1678, 3000, 3015, 3056, 3116, 3139, 3151, 3173, 3174, 3190, 3196, 3206,</p>
<p>i11</p> <p>C -1.419277 0.243401 0.722872 C -0.193823 -0.092664 0.158595 C 0.613712 0.921621 -0.350140 C 0.216852 2.252069 -0.315183 C -1.018551 2.565620 0.246708 C -1.828236 1.568194 0.764965 H -2.055546 -0.535009 1.124732 H 1.582441 0.669582 -0.768453 H -1.342237 3.598556 0.279604 H -2.784885 1.821768 1.202019 C 1.119542 3.335241 -0.838623 H 1.771145 3.709223 -0.046748 H 1.755039 2.965121 -1.641761 H 0.542699 4.178383 -1.216294 C 0.216772 -1.521007 0.088216 C 0.780008 -2.095593 -1.202603</p>	<p>31, 98, 128, 147, 215, 235, 311, 332, 393, 428, 461, 535, 552, 593, 691, 723, 732, 765, 809, 817, 893, 915, 916, 938, 957, 1007, 1010, 1024, 1037, 1049, 1071, 1093, 1121, 1147, 1190, 1196, 1262, 1312, 1347, 1384, 1418, 1456, 1477, 1499, 1513, 1543, 1668, 1688, 1818, 3060, 3123, 3128, 3144, 3154, 3155, 3171, 3189, 3201, 3222, 3254,</p>

<p>C 1.646557 -1.896931 -0.020424 H -0.398272 -2.199061 0.667422 H 0.902050 -1.404632 -2.027436 H 0.511072 -3.108324 -1.470608 C 2.795255 -1.943390 0.548294 H 3.801207 -2.247253 0.315516</p>	
<p>i12</p> <p>C -0.849395 -0.718089 -0.498218 C 0.310225 -0.892323 0.291143 C 1.316206 0.055835 0.328833 C 1.176974 1.217643 -0.433753 C 0.046619 1.415641 -1.220089 C -0.953792 0.468508 -1.257254 H 0.417916 -1.790675 0.886810 H 1.956937 1.968270 -0.406795 H -0.048153 2.321268 -1.804384 H -1.834350 0.624406 -1.867381 C 2.551422 -0.156088 1.160096 H 3.403862 -0.408770 0.527416 H 2.810462 0.748021 1.710708 H 2.413391 -0.964439 1.875752 C -1.880580 -1.680456 -0.540302 H -2.746170 -1.496373 -1.160659 C -1.832169 -2.956999 0.240337 H -0.942019 -3.535428 -0.034389 H -1.721525 -2.743089 1.310120 C -3.013848 -3.793337 0.048092 C -3.986494 -4.470013 -0.117368 H -4.847965 -5.073911 -0.261808</p>	<p>37, 91, 121, 124, 193, 201, 246, 332, 346, 396, 446, 501, 524, 532, 614, 616, 691, 701, 702, 766, 799, 875, 905, 923, 964, 978, 1002, 1002, 1035, 1070, 1093, 1128, 1177, 1203, 1215, 1253, 1290, 1323, 1342, 1416, 1433, 1460, 1462, 1492, 1506, 1523, 1620, 1644, 2266, 3017, 3038, 3058, 3120, 3139, 3167, 3172, 3174, 3194, 3202, 3468,</p>
<p>i13</p> <p>C -2.036391 -0.178999 -0.284166 C -0.653762 -0.316990 -0.369661 C 0.167530 0.778741 -0.096487 C -0.370064 2.005967 0.259629 C -1.758058 2.124363 0.340253 C -2.583515 1.043421 0.073673 H -2.664617 -1.033549 -0.499207 H 1.241900 0.660504 -0.172637 H -2.192156 3.078753 0.612717</p>	<p>42, 85, 92, 117, 211, 225, 249, 323, 378, 390, 433, 465, 489, 534, 553, 598, 700, 713, 756, 812, 824, 880, 923, 952, 975, 986, 1020, 1024, 1031, 1046, 1071, 1121, 1128, 1156, 1191, 1193, 1282, 1312, 1346, 1379, 1419, 1465, 1470, 1498, 1509, 1534, 1658, 1684, 1880, 3059, 3096, 3122, 3149, 3157, 3170, 3182, 3193, 3208, 3266, 3275,</p>

<p>H -3.657219 1.156134 0.140067 C 0.516124 3.179648 0.573498 H 0.616571 3.309671 1.652514 H 1.513619 3.042107 0.159959 H 0.101427 4.102741 0.169815 C -0.083857 -1.589323 -0.748805 C -0.483727 -2.990801 -1.160280 C 0.896406 -2.409455 -0.913668 H -0.789462 -3.144389 -2.192404 H 1.940566 -2.655746 -0.848566 C -1.093250 -3.886912 -0.189150 H -1.782305 -4.659150 -0.494652 H -0.844536 -3.794035 0.858214</p>	
<p>i14</p> <p>C -2.327955 -2.476962 0.820771 C -0.996819 -2.483930 0.322363 C -0.467341 -1.265485 -0.191782 C -1.214772 -0.108473 -0.208350 C -2.523541 -0.135484 0.290778 C -3.063995 -1.313751 0.797912 H -2.744582 -3.393692 1.213189 H 0.544974 -1.264728 -0.574494 H -3.115759 0.770614 0.278346 H -4.076844 -1.317902 1.178209 C -0.644225 1.174502 -0.747105 H -0.549118 1.917848 0.045607 H 0.339869 1.017889 -1.184575 H -1.296238 1.596057 -1.512665 C -0.245195 -3.628359 0.333442 C 0.472844 -4.713189 0.370115 H 0.436490 -5.391099 -0.482691 C 1.352104 -5.127577 1.485138 H 1.792441 -6.112860 1.385132 C 1.628042 -4.393800 2.555712 H 1.210086 -3.402059 2.680744 H 2.278438 -4.764999 3.334642</p>	<p>33, 45, 87, 124, 166, 183, 226, 315, 340, 419, 438, 524, 542, 554, 619, 637, 696, 728, 801, 846, 891, 898, 916, 960, 978, 990, 1011, 1022, 1046, 1070, 1078, 1122, 1144, 1185, 1240, 1294, 1338, 1341, 1351, 1418, 1433, 1443, 1493, 1497, 1503, 1595, 1627, 1715, 1886, 3057, 3085, 3117, 3149, 3158, 3186, 3187, 3189, 3204, 3224, 3248,</p>
<p>i15</p> <p>C -0.394418 0.506183 1.298750 C 0.745199 0.336466 0.484498</p>	

<p>C 1.223475 1.463364 -0.224327 C 0.612126 2.697097 -0.135876 C -0.514465 2.830549 0.683497 C -1.006802 1.740499 1.390072 H -0.784187 -0.340827 1.847248 H 2.098991 1.345133 -0.852991 H -1.002369 3.794066 0.764113 H -1.879333 1.859588 2.018800 C 1.134921 3.883676 -0.897684 H 1.397678 4.696031 -0.219042 H 2.020049 3.623621 -1.475169 H 0.380352 4.266259 -1.586100 C 1.404056 -0.911155 0.365479 H 2.283169 -0.955480 -0.270162 C 1.015993 -2.118551 1.098546 H 1.449284 -2.287117 2.082094 C 0.135192 -3.060949 0.611485 H -0.297647 -2.881986 -0.374046 C -0.241914 -4.197842 1.269094 H -0.901225 -5.020138 1.049100</p>	<p>-490, 59, 82, 111, 184, 213, 230, 282, 321, 390, 419, 472, 523, 529, 559, 611, 637, 708, 748, 801, 811, 855, 890, 916, 919, 944, 1001, 1005, 1021, 1066, 1096, 1130, 1169, 1180, 1198, 1248, 1254, 1311, 1328, 1345, 1377, 1417, 1456, 1479, 1489, 1507, 1519, 1615, 1649, 3056, 3101, 3114, 3136, 3148, 3152, 3158, 3171, 3186, 3196, 3266,</p>
<p>i16</p> <p>C -2.493340 -2.614840 -0.021301 C -1.099889 -2.622157 -0.040340 C -0.423984 -1.408809 -0.052483 C -1.101413 -0.191595 -0.045293 C -2.490822 -0.209117 -0.030525 C -3.181722 -1.414074 -0.017411 H -3.030414 -3.555412 -0.014177 H 0.660623 -1.409314 -0.071076 H -3.036181 0.726649 -0.031525 H -4.263614 -1.412947 -0.007645 C -0.344509 1.107791 -0.026637 H -0.170046 1.438316 0.999144 H 0.626755 1.004955 -0.508663 H -0.899300 1.894639 -0.535833 C -0.344763 -3.923298 -0.051776 C -0.761306 -4.982239 0.969607 C -0.798360 -4.986775 -1.052390 H 0.730632 -3.736687 -0.071659 C -1.125074 -5.870967 -0.033066</p>	<p>40, 47, 132, 139, 215, 253, 318, 381, 406, 457, 531, 558, 572, 615, 681, 732, 803, 818, 884, 916, 921, 930, 943, 954, 967, 988, 1019, 1025, 1029, 1071, 1131, 1155, 1183, 1195, 1207, 1208, 1275, 1308, 1310, 1351, 1356, 1417, 1473, 1481, 1498, 1512, 1545, 1669, 1690, 3052, 3073, 3117, 3144, 3159, 3172, 3181, 3196, 3203, 3229, 3244,</p>

<p>H -0.771279 -4.990177 2.047772 H -0.849184 -4.999396 -2.129428 H -1.513077 -6.879463 -0.023465</p>	
<p>i17</p> <p>C -0.312971 -1.079684 -1.162266 C 0.823961 -1.093315 -0.352087 C 1.094199 0.026369 0.435058 C 0.281311 1.154286 0.404786 C -0.827024 1.152982 -0.436034 C -1.124975 0.040193 -1.210098 H -0.546972 -1.948574 -1.764287 H 1.941988 0.003726 1.109060 H -1.467392 2.025557 -0.474395 H -1.996138 0.047287 -1.851425 C 0.573679 2.332092 1.293307 H 0.112702 2.198518 2.273701 H 1.644845 2.454090 1.448048 H 0.180547 3.253533 0.866452 C 1.673396 -2.294294 -0.318822 H 1.140724 -3.238475 -0.357816 C 3.008845 -2.343075 -0.265554 H 3.485942 -3.314307 -0.210551 C 3.918228 -1.201539 -0.331264 H 3.486765 -0.232532 -0.583314 C 5.214698 -1.288965 -0.145892 H 6.050437 -0.609362 -0.167931</p>	<p>54, 83, 103, 154, 190, 220, 259, 344, 357, 443, 458, 519, 534, 556, 692, 717, 733, 753, 795, 830, 846, 904, 936, 951, 962, 1021, 1023, 1027, 1028, 1074, 1104, 1131, 1192, 1200, 1250, 1271, 1279, 1325, 1349, 1418, 1436, 1473, 1496, 1509, 1540, 1649, 1664, 1682, 1715, 3060, 3094, 3123, 3144, 3154, 3179, 3181, 3187, 3196, 3215, 3267,</p>
<p>i18</p> <p>C -0.373947 -0.710455 -1.682448 C 0.798302 -0.945189 -0.964492 C 1.139699 -0.063235 0.062873 C 0.327544 1.007031 0.410690 C -0.846324 1.209795 -0.312083 C -1.189202 0.362538 -1.353261 H -0.624227 -1.348647 -2.519178 H 2.062006 -0.228939 0.608581 H -1.485907 2.048049 -0.063953 H -2.090921 0.546235 -1.922126 C 0.689040 1.919751 1.549573 H 0.113997 1.667244 2.442184</p>	<p>44, 91, 117, 164, 183, 219, 254, 330, 362, 432, 468, 512, 544, 552, 687, 704, 735, 777, 792, 822, 839, 905, 921, 939, 962, 1018, 1022, 1025, 1026, 1072, 1097, 1133, 1191, 1202, 1243, 1264, 1284, 1333, 1350, 1416, 1427, 1471, 1494, 1509, 1543, 1653, 1661, 1686, 1719, 3060, 3092, 3123, 3143, 3156, 3163, 3177, 3179, 3194, 3208, 3257,</p>

<p>H 1.745268 1.839884 1.800341 H 0.471286 2.958630 1.303346 C 1.706879 -2.060050 -1.278394 H 2.764433 -1.823772 -1.227222 C 1.370982 -3.317328 -1.585656 H 2.163050 -4.020093 -1.815309 C 0.020109 -3.872518 -1.584713 H -0.777171 -3.243745 -1.187906 C -0.271869 -5.085425 -1.992434 H -1.162020 -5.689384 -2.053593</p>	
<p>i19</p> <p>C -5.744434 -3.054118 0.308146 C -4.380076 -3.025642 0.208008 C -3.698606 -1.830994 -0.070025 C -4.488230 -0.639046 -0.548654 C -5.944255 -0.668178 -0.141957 C -6.506059 -1.842159 0.202211 H -1.735413 -2.623407 0.241339 H -6.254029 -3.976291 0.549132 H -3.799378 -3.919041 0.404521 C -2.302910 -1.722675 0.038560 C -3.768772 0.660203 -0.324994 H -7.565215 -1.874698 0.427671 C -2.440639 0.696228 -0.131495 C -1.668573 -0.510798 -0.025779 H -1.937932 1.649057 -0.028303 H -0.595901 -0.448446 0.089364 C -6.737639 0.594106 -0.254500 H -6.412416 1.334977 0.479284 H -6.613768 1.050355 -1.241137 H -7.796431 0.400440 -0.095643 H -4.333045 1.579037 -0.402628 H -4.528903 -0.749180 -1.661472</p>	<p>74, 146, 219, 265, 288, 381, 398, 452, 453, 496, 513, 561, 572, 657, 703, 757, 776, 803, 831, 858, 918, 959, 976, 985, 1001, 1009, 1028, 1057, 1065, 1081, 1096, 1162, 1185, 1206, 1218, 1256, 1269, 1346, 1366, 1378, 1417, 1427, 1472, 1484, 1501, 1521, 1559, 1671, 1687, 2759, 3040, 3091, 3140, 3172, 3174, 3177, 3184, 3204, 3207, 3213,</p>
<p>i20</p> <p>C -5.861165 -2.973825 0.234756 C -4.533894 -3.019101 0.035016 C -3.786229 -1.809659 -0.442323 C -4.519727 -0.519784 -0.182625 C -5.914540 -0.556328 -0.055492</p>	<p>83, 119, 149, 236, 270, 352, 380, 438, 450, 486, 505, 584,</p>

<p>C -6.587793 -1.741502 0.105199 H -1.821161 -2.691933 0.098776 H -6.396558 -3.867691 0.527008 H -3.979867 -3.942575 0.149154 C -2.347853 -1.753296 -0.022636 C -3.778213 0.674023 -0.120423 H -6.454267 0.382781 -0.019980 H -7.661260 -1.743978 0.229542 C -2.413224 0.681342 -0.008286 C -1.719027 -0.580678 0.127943 H -4.320619 1.613349 -0.095299 H -0.666674 -0.557738 0.386463 C -1.623808 1.949710 0.083866 H -1.050680 1.984848 1.013305 H -0.903750 2.021542 -0.734682 H -2.270094 2.824556 0.045982 H -3.758342 -1.904330 -1.554855</p>	<p>610, 675, 694, 711, 744, 796, 863, 877, 903, 938, 967, 996, 1001, 1006, 1012, 1056, 1079, 1084, 1104, 1176, 1180, 1190, 1215, 1254, 1272, 1350, 1365, 1398, 1414, 1433, 1458, 1483, 1492, 1518, 1562, 1666, 1689, 2778, 3039, 3089, 3140, 3159, 3169, 3171, 3172, 3191, 3196, 3212,</p>
<p>i21 C -1.560669 0.123090 -0.152807 C -0.201230 0.228188 0.021153 C 0.531092 1.371994 0.232361 C -0.216785 2.547873 0.297779 C -1.600830 2.519805 0.154423 C -2.270942 1.329736 -0.067390 H 0.291354 3.488731 0.473393 H -2.161735 3.441809 0.225831 H -3.347491 1.316088 -0.170317 C 2.028064 1.358662 0.373539 H 2.503979 1.191444 -0.593406 H 2.387980 2.306777 0.769142 H 2.348956 0.559061 1.039526 C -2.201722 -1.192641 -0.340816 H -1.760345 -1.992037 0.243882 C -3.237322 -1.506138 -1.122409 H -3.603769 -2.525634 -1.056570 C -3.945899 -0.660420 -2.093232 H -5.020736 -0.803505 -2.147360 C -3.367287 0.182176 -2.939938 H -3.950850 0.749449 -3.651950 H -2.294343 0.326934 -2.944139</p>	<p>34, 85, 103, 120, 178, 206, 224, 318, 341, 438, 472, 510, 520, 562, 642, 726, 728, 785, 795, 836, 906, 937, 966, 987, 996, 1014, 1021, 1031, 1045, 1067, 1095, 1120, 1188, 1226, 1278, 1302, 1326, 1333, 1417, 1418, 1447, 1470, 1490, 1499, 1508, 1617, 1676, 1721, 1726, 3063, 3125, 3142, 3148, 3150, 3156, 3169, 3173, 3194, 3209, 3240,</p>

<p>i22</p> <p>C -1.285284 0.076426 -0.592853 C -0.033885 0.135140 0.035752 C 0.596728 1.339072 0.333428 C -0.039431 2.530506 0.000116 C -1.284462 2.518056 -0.629717 C -1.846188 1.301334 -0.894311 H 0.455479 -0.796269 0.302315 H 0.437522 3.475495 0.230941 H -1.781739 3.442753 -0.891992 C 1.954738 1.345952 0.982066 H 2.739872 1.198749 0.238437 H 2.145660 2.293813 1.482495 H 2.044593 0.547448 1.717526 C -1.893947 -1.235882 -0.834931 H -1.261721 -2.066728 -0.540673 C -3.113447 -1.546619 -1.287677 H -3.372533 -2.600962 -1.279747 C -4.181369 -0.658853 -1.756767 H -5.173810 -0.882392 -1.376514 C -4.042049 0.322272 -2.640562 H -4.888967 0.919429 -2.950287 H -3.084638 0.542029 -3.094175</p>	<p>36, 110, 123, 132, 181, 202, 231, 314, 380, 427, 442, 513, 537, 578, 645, 713, 733, 803, 816, 824, 901, 920, 965, 975, 993, 1007, 1024, 1029, 1039, 1075, 1095, 1147, 1186, 1239, 1276, 1299, 1331, 1333, 1408, 1418, 1443, 1475, 1495, 1498, 1507, 1635, 1667, 1715, 1717, 3059, 3121, 3139, 3140, 3152, 3155, 3160, 3171, 3174, 3188, 3248,</p>
<p>i23</p> <p>C -5.871252 -3.029120 0.000284 C -4.493691 -3.015946 0.000134 C -3.790775 -1.800745 0.000245 C -4.510806 -0.589838 0.000477 C -5.907133 -0.608726 0.000593 C -6.574443 -1.829115 0.000522 H -1.830397 -2.728903 -0.000082 H -6.406979 -3.968778 0.000218 H -3.934328 -3.943033 -0.000045 C -2.357984 -1.785340 0.000108 C -3.781364 0.729191 0.000630 H -7.657049 -1.838636 0.000654 C -2.293577 0.623011 0.000431 C -1.651380 -0.577339 0.000195 H -4.105205 1.326087 0.864707</p>	<p>112, 143, 185, 250, 265, 278, 441, 466, 480, 499, 517, 553, 569, 682, 697, 727, 779, 793, 827, 861, 926, 948, 972, 991, 993, 1010, 1067, 1068, 1107, 1121, 1177, 1193, 1218, 1221, 1242, 1290, 1313, 1363, 1391, 1420, 1437, 1442, 1484, 1492, 1505, 1527, 1583, 1648, 1659, 2995, 3001, 3053, 3108, 3141, 3175, 3176, 3185, 3195, 3202, 3204,</p>

<p>H -1.726523 1.544114 0.000488 H -0.569200 -0.600858 0.000066 C -6.684145 0.678009 0.000927 H -6.448777 1.284543 0.877910 H -6.449211 1.284720 -0.876046 H -7.754795 0.485407 0.001173 H -4.105413 1.326416 -0.863138</p>	
<p>i24</p> <p>C -5.953698 -3.004106 0.004382 C -4.465571 -3.109740 -0.013859 C -3.747552 -1.784382 -0.009719 C -4.463510 -0.573805 0.010124 C -5.895135 -0.591253 0.027065 C -6.596684 -1.803849 0.023629 H -1.803660 -2.671177 -0.040162 H -6.521915 -3.924528 0.001954 H -4.130243 -3.707768 0.843671 C -2.359472 -1.740507 -0.025106 C -3.751643 0.638297 0.013409 H -6.427794 0.349404 0.042787 H -7.678818 -1.783012 0.036634 C -2.371640 0.676917 -0.001946 C -1.677141 -0.536785 -0.021372 H -4.312954 1.565949 0.028623 H -0.594077 -0.530262 -0.033600 C -1.620179 1.979284 0.002000 H -0.967891 2.048425 0.873556 H -0.989593 2.066363 -0.883765 H -2.300505 2.828621 0.019044 H -4.150125 -3.691850 -0.889634</p>	<p>36, 95, 125, 230, 259, 311, 408, 439, 445, 485, 505, 579, 601, 679, 709, 724, 773, 799, 839, 892, 919, 948, 962, 970, 992, 996, 1020, 1066, 1097, 1163, 1177, 1193, 1211, 1220, 1272, 1290, 1325, 1360, 1377, 1411, 1440, 1450, 1457, 1490, 1499, 1558, 1581, 1631, 1683, 3002, 3013, 3052, 3112, 3137, 3165, 3171, 3176, 3183, 3195, 3204,</p>
<p>i25</p> <p>C 0.067532 -0.156933 -0.128965 C -0.008907 -0.072680 1.260310 C 1.166706 0.019626 1.991904 C 2.416398 0.020625 1.374609 C 2.468405 -0.068391 -0.010145 C 1.300170 -0.157251 -0.757612 H -0.844900 -0.212072 -0.709894 H 1.112866 0.090709 3.073317</p>	<p>20, 63, 110, 134, 211, 245, 257, 312, 386, 434, 456, 527, 551, 609, 659, 718, 732, 762, 816, 862, 870, 919, 937, 946, 984, 1019, 1019, 1028, 1038, 1069, 1132, 1142, 1189, 1198, 1207, 1282, 1308, 1336, 1349, 1393, 1415, 1477, 1482, 1497, 1513, 1542, 1668, 1689, 1797, 3053, 3057, 3100, 3115, 3118, 3147, 3164, 3169, 3184, 3203,</p>

<p>H 3.429435 -0.065489 -0.509272 H 1.355618 -0.222704 -1.836138 C 3.671247 0.096913 2.200064 H 4.532242 0.355229 1.586109 H 3.576448 0.843244 2.988597 H 3.877486 -0.861480 2.679834 C -1.357386 -0.044209 1.940519 H -1.959932 -0.898267 1.627117 C -2.103406 1.225778 1.610229 H -1.563176 2.135553 1.864391 C -3.687796 1.288570 1.697292 C -3.140942 1.287468 0.547710 H -1.216934 -0.115625 3.022108 H -4.446369 1.312468 2.453618</p>	<p>3313,</p>
<p>i26</p> <p>C -0.068817 0.651011 0.256600 C 0.028128 0.420106 1.638553 C 1.289449 0.064540 2.157851 C 2.409881 -0.060920 1.358986 C 2.278763 0.175669 -0.011441 C 1.049520 0.527216 -0.548972 H -1.015612 0.925640 -0.180499 H 1.376872 -0.116979 3.223314 H 3.145756 0.083621 -0.654235 H 0.961934 0.708010 -1.612188 C 3.744400 -0.440765 1.938780 H 4.481351 0.344479 1.765818 H 3.675349 -0.609713 3.011810 H 4.124718 -1.351910 1.475471 C -1.071001 0.522191 2.550385 H -0.835608 0.316237 3.586517 C -2.423854 0.849916 2.300735 H -3.068476 0.860685 3.175168 C -3.041286 1.147920 1.159521 C -3.716173 1.445225 0.092973 H -3.813557 2.470972 -0.248043 H -4.197169 0.676779 -0.503843</p>	<p>24, 91, 121, 132, 199, 210, 270, 321, 323, 411, 445, 515, 536, 553, 565, 703, 716, 767, 793, 813, 899, 903, 911, 927, 940, 989, 1000, 1010, 1012, 1031, 1069, 1135, 1156, 1194, 1214, 1266, 1331, 1350, 1375, 1415, 1419, 1461, 1488, 1490, 1513, 1536, 1635, 1664, 1957, 3054, 3107, 3115, 3136, 3151, 3166, 3170, 3179, 3193, 3201, 3233,</p>
<p>i27</p> <p>C 0.000142 0.228615 -0.066029</p>	

<p>C -0.126669 -0.226845 1.258747 C 1.051582 -0.395879 2.009401 C 2.299462 -0.125595 1.473445 C 2.388279 0.327334 0.156368 C 1.241227 0.501853 -0.605917 H -0.893832 0.366154 -0.661235 H 0.986243 -0.746250 3.028625 H 3.360803 0.541829 -0.269590 H 1.319319 0.853878 -1.625852 C 3.548777 -0.322761 2.287827 H 4.154667 0.583764 2.297685 H 3.311559 -0.585925 3.316901 H 4.163150 -1.120181 1.867174 C -1.441500 -0.490944 1.760322 H -2.246123 -0.329980 1.054745 C -1.849719 -0.931810 3.040399 H -2.920396 -1.067309 3.165965 C -1.131718 -1.207361 4.127204 C -0.508642 -1.491133 5.228372 H -0.148112 -2.494279 5.432926 H -0.316254 -0.732592 5.980525</p>	<p>33, 95, 112, 135, 197, 212, 269, 309, 350, 404, 447, 524, 535, 540, 563, 703, 730, 753, 761, 820, 899, 902, 926, 929, 931, 994, 1004, 1007, 1012, 1043, 1067, 1129, 1152, 1187, 1215, 1274, 1311, 1350, 1376, 1415, 1438, 1471, 1476, 1493, 1512, 1533, 1637, 1661, 1959, 3055, 3109, 3116, 3141, 3148, 3168, 3177, 3182, 3188, 3199, 3224,</p>
<p>ilent</p> <p>C -1.236899 -0.464092 0.007528 C 0.052464 -0.052375 -0.207667 C 0.487204 1.245851 -0.169082 C -0.453304 2.244495 0.107615 C -1.774121 1.866209 0.334011 C -2.166694 0.534393 0.286586 H -1.515391 -1.509954 -0.028287 H 1.525091 1.507404 -0.342744 H -2.508990 2.630676 0.553419 H -3.200534 0.272062 0.471817 C -0.042346 3.691004 0.132950 H 0.006373 4.095820 -0.879530 H -0.753046 4.291772 0.697872 H 0.942888 3.811721 0.582065 C 1.610255 -1.867502 -0.554369 H 2.110227 -1.248657 -1.285546 H 1.870647 -1.728366 0.485319 C 0.862546 -2.915163 -0.944943</p>	<p>-267, 22, 40, 64, 78, 101, 204, 215, 230, 351, 384, 426, 491, 521, 563, 596, 667, 696, 718, 738, 778, 789, 882, 896, 919, 922, 995, 1001, 1009, 1011, 1068, 1075, 1113, 1114, 1182, 1227, 1303, 1309, 1314, 1416, 1432, 1453, 1493, 1500, 1513, 1604, 1615, 1680, 2218, 3054, 3118, 3143, 3155, 3163, 3175, 3184, 3188, 3201, 3252, 3472,</p>

<p>H 0.670452 -3.085174 -1.997139 C 0.241260 -3.807404 -0.030877 C -0.297825 -4.562697 0.732293 H -0.765390 -5.232142 1.411578</p>	
<p>i1-p3</p> <p>C -1.642796 -0.145670 0.245377 C -0.385446 -0.197663 -0.356441 C 0.288717 0.995833 -0.601882 C -0.248910 2.229119 -0.252205 C -1.498221 2.253863 0.357226 C -2.189937 1.074271 0.600510 H -2.202335 -1.054233 0.419691 H 1.269358 0.955156 -1.064990 H -1.935252 3.203453 0.639416 H -3.166365 1.110413 1.064560 C 0.508443 3.496323 -0.538080 H 0.023646 4.356812 -0.081012 H 1.527548 3.435588 -0.156174 H 0.571965 3.675862 -1.612278 C 0.250183 -1.465314 -0.756686 H 1.009467 -1.393366 -1.527539 H 1.804482 -1.242172 0.385208 C -0.169290 -2.697945 -0.395149 H -0.953998 -2.818657 0.341286 C 0.419402 -3.885018 -0.895091 C 0.912120 -4.900481 -1.306047 H 1.347908 -5.796583 -1.674162</p>	<p>-838, 59, 71, 85, 115, 208, 219, 233, 301, 386, 411, 416, 443, 464, 507, 535, 585, 651, 680, 718, 719, 784, 810, 882, 918, 939, 950, 1015, 1017, 1031, 1033, 1050, 1068, 1136, 1195, 1201, 1270, 1309, 1323, 1336, 1352, 1415, 1468, 1496, 1506, 1545, 1644, 1668, 1688, 2226, 3054, 3115, 3142, 3156, 3173, 3175, 3187, 3195, 3205, 3475,</p>
<p>i1-i5</p> <p>C -2.081048 -1.292271 0.084128 C -0.725947 -1.580319 -0.035340 C 0.169207 -0.534860 0.020380 C -0.160766 0.795103 0.184060 C -1.528165 1.054299 0.300503 C -2.468690 0.030000 0.251214 H -2.821286 -2.081848 0.040891 H -1.858872 2.078452 0.427922 H -3.519163 0.272369 0.340671 C 0.868855 1.886888 0.251757</p>	<p>-1830, 42, 99, 116, 187, 195, 229, 241, 396, 409, 437, 500, 506, 543, 568, 595, 669, 706, 715, 754, 790, 852, 917, 934, 970, 1005, 1011, 1029, 1046, 1062, 1087, 1112, 1186, 1190, 1230, 1282, 1297, 1308, 1333, 1357, 1417, 1453, 1485, 1492, 1506, 1513, 1638, 1671, 1679, 2214, 3059, 3072, 3110, 3123, 3127, 3152, 3164, 3171,</p>

<p>H 1.390584 1.861835 1.209389 H 1.616872 1.764670 -0.530429 H 0.406966 2.866478 0.142367 C -0.063930 -2.926360 -0.211709 H -0.139163 -3.513125 0.704199 H -0.523423 -3.508162 -1.011258 C 1.405255 -2.606114 -0.516492 H 1.631490 -2.563568 -1.579758 H 1.358744 -1.363704 -0.199764 C 2.412667 -3.281316 0.238455 C 3.254303 -3.827342 0.899716 H 4.000288 -4.314464 1.477615</p>	<p>3196, 3477,</p>
<p>i1-i6</p> <p>C -1.545589 -1.675146 -0.010560 C -0.203500 -1.451089 0.221825 C 0.262257 -0.145406 0.175081 C -0.615462 0.902954 -0.102759 C -1.961743 0.623472 -0.330414 C -2.452222 -0.681581 -0.285565 H 1.310577 0.069071 0.356574 H -2.641495 1.439498 -0.544551 H -3.500268 -0.883641 -0.461817 C -0.102483 2.316727 -0.156691 H 0.402626 2.583997 0.771990 H 0.618781 2.438443 -0.965878 H -0.912164 3.025737 -0.317832 C 0.577117 -2.717581 0.481977 H 1.233873 -2.942487 -0.358761 H 1.201261 -2.642104 1.372852 C -0.487204 -3.813305 0.629207 H -0.773764 -4.009320 1.660228 H -1.478596 -3.123870 0.197798 C -0.333747 -5.007483 -0.139925 C -0.217470 -5.995184 -0.814117 H -0.115130 -6.872387 -1.403758</p>	<p>-1856, 34, 43, 102, 163, 213, 251, 267, 368, 408, 419, 445, 530, 556, 563, 623, 653, 699, 711, 755, 821, 841, 912, 922, 953, 977, 1012, 1023, 1030, 1069, 1085, 1152, 1174, 1192, 1258, 1265, 1296, 1315, 1330, 1360, 1416, 1448, 1480, 1491, 1500, 1504, 1654, 1662, 1677, 2211, 3053, 3072, 3110, 3111, 3128, 3138, 3165, 3170, 3201, 3467,</p>
<p>i1-i12</p> <p>C -0.014075 0.000170 -0.021312 C 0.021830 -0.003375 1.375968</p>	

<p>C 1.235625 -0.004948 2.042984 C 2.430996 -0.006126 1.341612 C 2.424627 -0.014685 -0.058832 C 1.181334 -0.008870 -0.715273 H 1.253864 0.004060 3.124750 H 1.165639 -0.011796 -1.799363 C 3.630294 -0.033826 -0.852537 H 3.564570 0.179082 -1.910273 C 5.003615 -0.111859 -0.302789 H 4.328085 -1.123213 -0.761740 C 6.131388 0.199808 -1.083064 C 7.091030 0.450060 -1.766756 H 7.939945 0.683272 -2.360636 H 5.125438 -0.257139 0.759662 H 3.364113 0.018132 1.886428 C -1.332905 0.012161 -0.743438 H -1.930824 -0.859006 -0.473052 H -1.911524 0.898227 -0.479530 H -1.193558 0.006831 -1.822795 H -0.905830 0.001061 1.934354</p>	<p>-1712, 63, 75, 117, 124, 212, 225, 248, 297, 403, 410, 452, 499, 532, 559, 598, 632, 708, 729, 742, 763, 793, 822, 901, 922, 946, 1009, 1013, 1016, 1043, 1075, 1129, 1168, 1187, 1201, 1220, 1268, 1319, 1335, 1356, 1421, 1435, 1490, 1494, 1517, 1544, 1641, 1675, 2184, 2192, 3063, 3126, 3142, 3164, 3178, 3193, 3199, 3206, 3222, 3474,</p>
<p>i1a-i17a</p> <p>C -0.017104 0.014240 -0.000855 C 0.031315 0.065827 1.391572 C 1.253209 0.095853 2.049095 C 2.438772 0.070886 1.337780 C 2.424221 0.011015 -0.063052 C 1.176097 -0.008203 -0.704614 H 1.279884 0.147637 3.129495 H 1.150853 -0.047587 -1.787828 C 3.620937 -0.034178 -0.868986 H 3.498251 0.055286 -1.941227 C 4.902596 -0.172424 -0.377945 H 5.079248 -0.380198 0.669940 C 6.089148 -0.121877 -1.185365 C 7.044788 -0.294197 -1.945661 H 7.921562 -0.018743 -2.485365 H 5.795374 0.981492 -0.545916 H 3.377263 0.116839 1.873043 H -0.891040 0.089032 1.958419 C -1.339491 -0.034408 -0.715316</p>	<p>-1766, 69, 87, 98, 122, 213, 225, 252, 300, 403, 415, 448, 489, 526, 534, 580, 626, 647, 713, 784, 787, 799, 829, 908, 931, 955, 1006, 1011, 1017, 1021, 1040, 1075, 1134, 1199, 1205, 1260, 1277, 1319, 1333, 1355, 1421, 1455, 1497, 1505, 1531, 1542, 1610, 1647, 1673, 2025, 3062, 3125, 3142, 3167, 3179, 3182, 3188, 3195, 3205, 3422,</p>

<p>H -2.028879 0.708158 -0.313841 H -1.219771 0.149920 -1.781368 H -1.806960 -1.013065 -0.594317</p>	
<p>i1a-i17b</p> <p>C 0.048904 0.345081 -0.047892 C -0.045280 -0.051290 1.295577 C 1.149860 -0.238918 2.009528 C 2.388527 -0.050537 1.415248 C 2.446890 0.331874 0.076097 C 1.279634 0.531576 -0.647573 H -0.860321 0.499930 -0.615075 H 1.111431 -0.519375 3.051472 H 3.410741 0.477157 -0.396308 H 1.332141 0.833196 -1.685253 C 3.656555 -0.232953 2.203936 H 4.364789 -0.861139 1.663333 H 4.142176 0.728086 2.380950 H 3.458627 -0.692516 3.170403 C -1.359856 -0.235119 1.859023 H -2.185944 0.038906 1.215498 C -1.732722 -0.775115 3.077015 H -2.787788 -0.770043 3.323598 C -0.919284 -1.345210 4.114733 H -1.440688 -2.187595 3.261603 C -0.243397 -1.629918 5.109084 H 0.263650 -2.308014 5.757644</p>	<p>-1734, 30, 101, 113, 141, 194, 215, 305, 343, 388, 409, 451, 499, 516, 534, 571, 648, 714, 726, 753, 765, 799, 838, 907, 915, 941, 985, 1008, 1012, 1016, 1034, 1069, 1134, 1186, 1195, 1247, 1278, 1326, 1357, 1413, 1421, 1469, 1493, 1496, 1519, 1544, 1637, 1653, 1669, 2024, 3054, 3114, 3142, 3172, 3178, 3189, 3193, 3206, 3233, 3395,</p>
<p>i1a-i18</p> <p>C -0.005535 0.377150 0.150280 C 0.078135 0.285154 1.546886 C 1.343575 0.048800 2.114822 C 2.485816 -0.086584 1.347306 C 2.370502 0.016637 -0.040184 C 1.134852 0.243771 -0.624843 H -0.959543 0.533921 -0.327236 H 1.420360 -0.027981 3.193785 H 3.254098 -0.086040 -0.658300 H 1.055763 0.313218 -1.701787 C 3.826487 -0.338999 1.980232</p>	<p>-1729, 24, 90, 121, 135, 197, 215, 297, 325, 375, 411, 451, 494, 511, 544, 569, 650, 708, 716, 764, 788, 804, 824, 900, 911, 938, 975, 1000, 1014, 1018, 1026, 1067, 1135, 1188, 1202, 1243, 1269, 1344, 1352, 1414, 1419,</p>

<p>H 3.744222 -0.418417 3.062708 H 4.264712 -1.264063 1.603832 H 4.522952 0.468489 1.750862 C -1.048146 0.411675 2.438288 H -0.836846 0.240044 3.485968 C -2.352195 0.785222 2.167029 H -3.058372 0.767098 2.988549 C -2.950692 1.185211 0.924123 H -2.538154 2.151257 1.702855 C -3.542940 1.311258 -0.152905 H -3.954917 1.876391 -0.958144</p>	<p>1449, 1489, 1500, 1531, 1540, 1642, 1645, 1674, 2017, 3055, 3116, 3141, 3162, 3168, 3171, 3191, 3198, 3255, 3393,</p>
<p>i2ent</p> <p>C -0.785732 -1.584710 -0.171772 C 0.544562 -1.294148 -0.005069 C 1.090291 -0.039985 -0.077443 C 0.240138 1.037552 -0.344018 C -1.116107 0.780470 -0.527341 C -1.627145 -0.508245 -0.442950 H -1.162501 -2.595867 -0.091281 H 2.152321 0.121700 0.071550 H -1.783954 1.605780 -0.740535 H -2.686408 -0.677881 -0.588802 C 0.779803 2.440224 -0.403060 H 1.781354 2.458181 -0.830982 H 0.137980 3.083173 -1.003287 H 0.841682 2.871748 0.597630 C 2.046858 -2.990129 0.281086 H 2.081996 -3.010389 -0.801351 C 3.081105 -2.452970 0.971714 H 3.134983 -2.533227 2.047617 H 3.852230 -1.894404 0.461561 C 1.114025 -3.891620 0.891650 C 0.334980 -4.658986 1.383130 H -0.346915 -5.342907 1.825556</p>	<p>-469, 16, 75, 92, 94, 131, 211, 222, 239, 355, 393, 428, 490, 514, 539, 561, 649, 695, 698, 721, 785, 788, 881, 890, 893, 923, 955, 1004, 1010, 1011, 1068, 1076, 1104, 1115, 1184, 1229, 1284, 1309, 1319, 1415, 1425, 1454, 1495, 1499, 1513, 1574, 1611, 1681, 2249, 3053, 3114, 3146, 3166, 3167, 3171, 3174, 3188, 3200, 3270, 3475,</p>
<p>i2-p4</p> <p>C 0.077399 -0.547672 -0.039238 C -0.025744 -0.057525 1.255105 C 1.132357 0.286115 1.949999</p>	

<p>C 2.385701 0.171629 1.367888 C 2.468868 -0.304187 0.059311 C 1.326858 -0.663210 -0.634496 H -0.816682 -0.828966 -0.578727 H 1.050191 0.625802 2.976352 H 3.440628 -0.402107 -0.409329 H 1.405616 -1.037520 -1.646277 C 3.633696 0.519253 2.131247 H 3.399690 1.044170 3.055496 H 4.192926 -0.381575 2.388486 H 4.290681 1.152080 1.534580 C -1.365130 0.133762 1.892763 H -0.990228 -1.055481 3.190611 C -1.650237 1.254467 2.603166 H -2.648316 1.434948 2.973011 H -0.874017 1.966897 2.841945 C -2.452223 -0.685156 1.415845 C -3.350581 -1.357418 0.996720 H -4.150195 -1.956237 0.635474</p>	<p>-1125, 46, 115, 124, 154, 208, 221, 293, 349, 394, 424, 456, 479, 511, 525, 539, 634, 653, 673, 696, 721, 734, 735, 828, 862, 908, 921, 951, 958, 1017, 1025, 1028, 1070, 1132, 1142, 1201, 1237, 1311, 1322, 1352, 1417, 1422, 1475, 1495, 1513, 1538, 1591, 1667, 1687, 2255, 3060, 3124, 3143, 3162, 3171, 3184, 3200, 3215, 3265, 3474,</p>
<p>i2-i11</p> <p>C -0.549405 -1.683756 -0.239719 C 0.168996 -0.574528 0.193103 C -0.499420 0.622496 0.421306 C -1.872561 0.733256 0.229023 C -2.573544 -0.388001 -0.206843 C -1.918516 -1.587825 -0.438353 H -0.030603 -2.614760 -0.432204 H 0.073706 1.486458 0.737919 H -3.641690 -0.315616 -0.372978 H -2.475668 -2.449088 -0.782506 C -2.597061 2.018954 0.518169 H -1.904516 2.816038 0.778972 H -3.191106 2.339534 -0.337808 H -3.284558 1.883982 1.355751 C 1.643978 -0.683959 0.415026 C 2.577692 -0.832660 -0.767192 C 2.533113 0.424692 0.026557 H 1.939156 -1.226812 1.306795 H 2.132552 -0.798554 -1.753269 H 3.447984 -1.465974 -0.662519</p>	<p>-150, -21, 119, 176, 257, 270, 401, 411, 439, 454, 478, 554, 595, 696, 732, 762, 800, 837, 849, 881, 910, 924, 957, 992, 1011, 1022, 1045, 1068, 1153, 1183, 1221, 1230, 1261, 1275, 1280, 1290, 1331, 1341, 1371, 1414, 1459, 1472, 1491, 1497, 1505, 1556, 1651, 1691, 1744, 3051, 3059, 3074, 3084, 3110, 3112, 3136, 3155, 3168, 3170, 3185,</p>

C 2.930383 1.627926 0.227104 H 3.623354 2.328635 -0.205583	
i3ent C -0.452995 0.151733 0.723935 C 0.840543 0.236756 0.264427 C 1.424935 1.389299 -0.191815 C 0.678938 2.573483 -0.165854 C -0.631107 2.521077 0.299655 C -1.195529 1.328383 0.737811 H -0.874759 -0.784446 1.067159 H 2.442433 1.390365 -0.566842 H -1.222289 3.428126 0.314109 H -2.219582 1.315255 1.089086 C 1.295069 3.866985 -0.623394 H 0.537846 4.636406 -0.763018 H 2.015473 4.233655 0.109722 H 1.827149 3.734406 -1.565374 C 2.007113 -1.685305 -0.043660 C 2.144993 -1.708576 -1.254014 H 2.159688 -1.544066 -2.304565 C 2.143920 -2.218126 1.289183 H 2.427676 -3.264640 1.302744 C 1.991558 -1.570884 2.438069 H 1.714509 -0.527551 2.475437 H 2.150617 -2.088085 3.373797	-468, 28, 62, 76, 96, 110, 183, 214, 244, 342, 363, 430, 468, 506, 526, 588, 620, 702, 712, 726, 788, 790, 874, 901, 923, 995, 999, 1010, 1011, 1028, 1064, 1070, 1104, 1115, 1182, 1226, 1308, 1319, 1329, 1416, 1444, 1453, 1494, 1501, 1509, 1609, 1678, 1706, 2067, 3058, 3117, 3147, 3165, 3169, 3179, 3183, 3193, 3203, 3266, 3455,
i3-i13 C -2.013204 -0.192353 -0.270132 C -0.631924 -0.314386 -0.357103 C 0.178202 0.788498 -0.083468 C -0.370032 2.008434 0.276889 C -1.760286 2.113369 0.359196 C -2.573478 1.025746 0.089408 H -2.635927 -1.052101 -0.481329 H 1.254090 0.679019 -0.160441 H -2.203478 3.061969 0.637676 H -3.648339 1.126130 0.158410 C 0.499591 3.196852 0.581083 H 0.410070 3.483784 1.629794 H 1.546999 2.981815 0.378364	-710, 45, 90, 99, 132, 202, 224, 306, 330, 399, 443, 461, 515, 532, 549, 589, 644, 689, 716, 732, 802, 823, 880, 923, 952, 971, 992, 1020, 1022, 1029, 1070, 1126, 1132, 1191, 1197, 1259, 1310, 1314, 1348, 1389, 1417, 1471, 1495, 1511, 1515, 1535, 1660, 1687, 1809, 3057, 3119, 3148, 3154, 3170, 3176, 3176, 3192, 3207, 3256, 3297,

<p>H 0.205832 4.058774 -0.018491 C -0.035062 -1.591004 -0.738212 C -0.640545 -2.901058 -1.114978 C 1.097547 -2.185784 -0.891550 H -0.822498 -3.075606 -2.168026 H 2.166696 -2.268750 -0.830327 C -1.095300 -3.814328 -0.196954 H -1.530336 -4.750983 -0.513218 H -0.978760 -3.637236 0.863419</p>	
<p>i4ent</p> <p>C -0.218197 -0.163804 0.039812 C -0.116046 -0.290263 1.399355 C 1.096753 0.057699 2.006100 C 2.135607 0.508910 1.197878 C 1.986909 0.620944 -0.179972 C 0.782330 0.279644 -0.786643 H -0.940821 -0.649387 2.005786 H 3.079770 0.775943 1.655782 H 2.814652 0.972921 -0.782556 H 0.639261 0.358344 -1.857203 C 1.254060 -0.039615 3.498673 H 2.302839 0.004241 3.787273 H 0.735014 0.781316 3.996419 H 0.833161 -0.970689 3.877642 C -2.246824 -0.696871 -1.074852 H -2.659824 -0.954190 -0.128508 C -2.089640 -0.481313 -2.255720 C -1.777625 -0.209914 -3.612141 H -1.483045 -1.061710 -4.214651 C -1.833039 1.006537 -4.157023 H -2.125386 1.868521 -3.573372 H -1.586733 1.158288 -5.198023</p>	<p>-352, 19, 43, 70, 91, 114, 132, 214, 232, 335, 360, 421, 490, 521, 565, 577, 678, 696, 699, 716, 782, 807, 877, 904, 916, 977, 1001, 1005, 1008, 1029, 1070, 1074, 1114, 1116, 1180, 1226, 1309, 1318, 1321, 1417, 1445, 1453, 1494, 1501, 1514, 1611, 1672, 1679, 2130, 3062, 3125, 3144, 3153, 3170, 3170, 3180, 3186, 3193, 3267, 3427,</p>
<p>i4-p5</p> <p>C -2.493699 0.060347 -0.669904 C -1.257391 0.130267 -0.027431 C -0.495492 1.289849 -0.060204 C -0.997122 2.396725 -0.741248 C -2.225816 2.340649 -1.380534 C -2.977558 1.177370 -1.350928</p>	

<p>H -0.896501 -0.738845 0.507974 H -0.418103 3.311791 -0.765113 H -2.603069 3.209750 -1.902277 H -3.936999 1.122362 -1.845608 C 0.850563 1.347116 0.607348 H 1.011322 2.315048 1.080749 H 0.948687 0.572586 1.365742 H 1.648022 1.202071 -0.123495 C -3.273120 -1.150142 -0.662869 H -2.969145 -1.595410 1.177803 C -4.003242 -2.071281 -0.969005 C -4.812664 -3.207963 -1.217856 H -4.289407 -4.119913 -1.482342 C -6.143630 -3.202143 -1.142929 H -6.687158 -2.305538 -0.879260 H -6.711738 -4.098805 -1.345034</p>	<p>-780, 56, 57, 108, 129, 154, 198, 213, 251, 348, 356, 432, 461, 527, 537, 540, 592, 612, 705, 719, 722, 818, 859, 916, 954, 980, 993, 1017, 1023, 1024, 1032, 1075, 1111, 1130, 1194, 1215, 1309, 1310, 1325, 1344, 1420, 1449, 1470, 1498, 1508, 1534, 1656, 1677, 1686, 2258, 3061, 3124, 3148, 3165, 3174, 3181, 3183, 3196, 3209, 3264,</p>
<p>i4-i14</p> <p>C 0.163085 -0.193658 -0.137050 C 0.185184 0.172332 1.221837 C 1.425744 0.238850 1.889225 C 2.607600 -0.044103 1.230628 C 2.563156 -0.407846 -0.118348 C 1.347804 -0.477921 -0.787368 H -0.781681 -0.243194 -0.659983 H 1.444218 0.523593 2.933547 H 3.484408 -0.631911 -0.640662 H 1.325911 -0.753022 -1.833637 C 3.926756 0.028639 1.949257 H 4.634259 0.649166 1.398815 H 3.811489 0.445645 2.947986 H 4.369295 -0.963932 2.045335 C -1.016841 0.420712 1.918391 C -2.087529 0.862809 2.447145 H -1.838364 -0.371056 2.530848 C -3.180888 1.586885 2.953504 H -4.085385 1.536962 2.358502 C -3.183400 2.252661 4.130416 H -2.297871 2.312846 4.746271 H -4.081326 2.737373 4.481465</p>	<p>-1895, 44, 54, 96, 124, 178, 207, 215, 317, 335, 389, 399, 452, 506, 533, 555, 585, 634, 697, 704, 797, 843, 851, 891, 908, 941, 981, 1006, 1008, 1028, 1069, 1094, 1126, 1191, 1212, 1287, 1294, 1306, 1346, 1415, 1426, 1453, 1494, 1506, 1521, 1578, 1620, 1657, 2122, 2361, 3057, 3117, 3147, 3168, 3175, 3182, 3194, 3197, 3211, 3265,</p>
<p>i4-i22</p>	

<p>C -1.829881 -0.228882 -0.269734 C -0.586335 0.182522 0.167709 C -0.220499 1.531682 0.053773 C -1.115459 2.434956 -0.499487 C -2.384826 2.032751 -0.949604 C -2.699099 0.712658 -0.818475 H 0.110726 -0.528361 0.598172 H -0.829763 3.476239 -0.586073 H -3.067788 2.754468 -1.377528 H -3.734422 -0.178548 -1.077520 C 1.132789 1.978445 0.535727 H 1.928183 1.437809 0.021217 H 1.281531 3.042842 0.364724 H 1.247698 1.787592 1.603573 C -2.456769 -1.560448 -0.270386 H -1.968665 -2.450502 0.110183 C -3.681457 -1.525907 -0.791623 C -4.709219 -2.498773 -1.032079 H -4.479030 -3.521237 -0.737774 C -5.890966 -2.221279 -1.579428 H -6.140682 -1.211763 -1.879420 H -6.632535 -2.990866 -1.738680</p>	<p>-1876, 66, 98, 111, 112, 213, 261, 262, 312, 393, 403, 424, 533, 554, 587, 649, 694, 731, 776, 826, 874, 933, 937, 970, 973, 977, 1005, 1017, 1027, 1072, 1082, 1136, 1159, 1184, 1217, 1260, 1299, 1313, 1365, 1417, 1438, 1458, 1492, 1493, 1506, 1652, 1656, 1669, 1711, 1758, 3056, 3118, 3126, 3141, 3166, 3168, 3172, 3181, 3207, 3260,</p>
<p>i5-i7</p> <p>C 0.000133 0.014624 0.001273 C -0.015756 0.029335 1.396799 C 1.170997 0.045564 2.116361 C 2.392520 0.041623 1.458727 C 2.451892 0.021380 0.063284 C 1.243533 0.020899 -0.597897 C -1.277832 0.011907 -0.801379 C -1.331219 -1.124388 -1.847332 C -0.101991 -1.063132 -2.630831 C 1.064838 -0.735845 -2.740805 H -0.965958 0.031408 1.918174 H 1.143123 0.057820 3.197368 H -1.367852 0.959328 -1.336464 H -2.133250 -0.071034 -0.130961 H -1.394033 -2.096482 -1.353884 H -2.218779 -1.015268 -2.470552</p>	<p>-491, 58, 76, 114, 169, 216, 261, 334, 367, 402, 472, 496, 514, 535, 615, 696, 710, 735, 764, 800, 835, 901, 924, 969, 986, 1002, 1003, 1028, 1048, 1061, 1121, 1185, 1188, 1208, 1268, 1286, 1327, 1333, 1370, 1408, 1446, 1471, 1481, 1486, 1500, 1508, 1627, 1677, 2079, 3047, 3058, 3063, 3101, 3109, 3112, 3133, 3162, 3175, 3200, 3430,</p>

<p>H 2.042467 -0.590088 -3.138639 C 3.761571 -0.010648 -0.675818 H 4.599465 0.112298 0.008053 H 3.886260 -0.962795 -1.194966 H 3.808611 0.782512 -1.422277 H 3.314718 0.051686 2.028043</p>	
<p>i6-i8</p> <p>C -5.210692 -1.227347 -0.368243 C -4.763059 -2.335867 -0.436330 C -2.648170 0.263279 0.658975 C -3.619078 1.233804 0.564912 C -5.071519 0.954141 0.843206 C -5.738906 0.130519 -0.273272 H -0.603466 -0.364968 0.487171 H -4.365827 -3.319281 -0.4964i5 C -1.318866 0.441438 0.393787 C -3.175519 2.494644 0.166235 H -5.606856 1.898588 0.942672 H -6.813530 0.078035 -0.090175 C -1.834951 2.750826 -0.119871 C -0.913267 1.716644 -0.001147 H -3.896498 3.302423 0.082702 H 0.131655 1.904544 -0.217144 C -1.404899 4.120888 -0.570361 H -1.895102 4.900261 0.012551 H -0.328320 4.246948 -0.470002 H -1.662771 4.284535 -1.618237 H -5.598499 0.636428 -1.230663 H -5.172271 0.412568 1.784052</p>	<p>-43, 23, 77, 122, 166, 226, 276, 301, 358, 403, 438, 517, 522, 546, 619, 709, 717, 722, 734, 818, 837, 891, 914, 959, 976, 1004, 1008, 1034, 1050, 1070, 1144, 1184, 1189, 1238, 1272, 1300, 1324, 1352, 1372, 1416, 1436, 1476, 1488, 1493, 1496, 1501, 1639, 1669, 2258, 3056, 3060, 3066, 3104, 3118, 3118, 3137, 3156, 3174, 3196, 3473,</p>
<p>i7-i9</p> <p>C -4.865689 -1.458032 -0.432260 C -3.629566 -1.469474 0.140549 C -2.847711 -0.242388 -0.000199 C -3.552173 0.975690 -0.047308 C -5.059143 0.956920 0.133992 C -5.614531 -0.273981 -0.537981 H -3.195739 -2.353627 0.585972 C -1.445869 -0.240871 -0.090390 C -2.863662 2.168128 -0.194357</p>	<p>-1603, 119, 144, 173, 232, 273, 292, 412, 463, 468, 492, 521, 543, 583, 677, 697, 750, 766, 794, 808, 864, 917, 941, 965, 998, 1007, 1053, 1068, 1100, 1114, 1188, 1191, 1207, 1224, 1258, 1286, 1293, 1321, 1346, 1404, 1420, 1453, 1457, 1488, 1493, 1510, 1530, 1643, 1668, 2154, 3022, 3052, 3109, 3109, 3142, 3163, 3174, 3180,</p>

<p>H -5.512764 1.864691 -0.261886 H -6.033963 -1.336915 0.129672 C -1.478358 2.169405 -0.281735 C -0.781393 0.971024 -0.223836 H -3.411768 3.101573 -0.230704 H 0.299335 0.974303 -0.292423 H -6.416168 -0.204421 -1.264640 H -5.283864 0.929265 1.206434 H -0.943947 3.102831 -0.394581 C -0.683899 -1.534973 -0.051059 H -0.802991 -2.033850 0.913094 H -1.044647 -2.224154 -0.815766 H 0.378682 -1.364766 -0.212162</p>	<p>3196, 3202,</p>
<p>i8-i10</p> <p>C -4.767508 -1.536909 0.376274 C -3.693909 -1.407651 -0.452278 C -2.902160 -0.192470 -0.287274 C -3.563379 0.976977 0.139087 C -5.070624 0.938873 0.311165 C -5.464922 -0.413318 0.853386 H -1.016545 -1.023863 -0.866125 H -3.359653 -2.187861 -1.122787 C -1.531994 -0.130512 -0.535902 C -2.843985 2.142948 0.323119 H -5.538115 1.100174 -0.666891 H -6.077186 -0.499286 1.744150 C -1.470387 2.202835 0.083522 C -0.829592 1.050342 -0.358137 H -3.361905 3.039015 0.649563 H 0.234000 1.077699 -0.560144 C -0.713946 3.481773 0.309681 H 0.293358 3.419995 -0.098234 H -1.220523 4.326386 -0.158034 H -0.630861 3.701394 1.375712 H -6.034022 -1.359494 0.125051 H -5.413549 1.742070 0.962351</p>	<p>-1616, 73, 104, 172, 216, 263, 331, 406, 412, 450, 478, 505, 571, 592, 683, 724, 736, 782, 794, 821, 861, 910, 932, 963, 989, 1004, 1022, 1067, 1095, 1146, 1174, 1194, 1220, 1238, 1264, 1283, 1291, 1329, 1341, 1398, 1415, 1454, 1467, 1477, 1495, 1507, 1542, 1636, 1684, 2150, 3032, 3051, 3104, 3112, 3139, 3156, 3161, 3173, 3187, 3190,</p>
<p>i9-p1</p> <p>C 0.050782 0.114108 0.054905 C 0.108462 -0.031095 1.427908</p>	

<p>C 1.367921 -0.025076 2.100991 C 2.559387 0.000331 1.335731 C 2.455326 0.062190 -0.077519 C 1.234055 0.131611 -0.696872 H -0.790833 0.065118 2.023060 C 1.441071 -0.071732 3.508681 C 3.819375 -0.022412 2.002747 H 1.180810 0.207363 -1.774544 C 3.842486 -0.063886 3.372299 C 2.655657 -0.087852 4.132193 H 2.715018 -0.122202 5.211585 H 3.356444 0.075863 -0.674440 H 0.521714 -0.100254 4.079951 H -0.907716 0.176317 -0.441446 H 4.796478 -0.080141 3.884303 C 5.097750 0.001744 1.214406 H 5.958047 -0.022123 1.879659 H 5.164009 -0.854906 0.541538 H 5.167027 0.902076 0.601361 H -0.225431 -1.852952 1.571457</p>	<p>-893, 128, 168, 212, 240, 281, 290, 391, 446, 461, 487, 488, 521, 570, 579, 650, 722, 760, 804, 815, 831, 880, 910, 936, 1000, 1007, 1014, 1034, 1055, 1066, 1086, 1108, 1164, 1188, 1194, 1236, 1270, 1293, 1379, 1407, 1416, 1434, 1470, 1492, 1504, 1511, 1562, 1644, 1663, 1695, 3050, 3107, 3144, 3173, 3175, 3187, 3192, 3206, 3206, 3225,</p>
<p>i10-p2</p> <p>C -4.968240 -1.655513 -0.154871 C -3.598462 -1.645014 -0.188179 C -2.883696 -0.423608 -0.244809 C -3.597054 0.796172 -0.232834 C -5.020867 0.760304 -0.120918 C -5.687792 -0.450266 -0.149612 H -3.041658 -2.573595 -0.193412 C -1.471329 -0.378094 -0.327970 C -2.887567 2.013867 -0.301899 H -5.569716 1.686767 -0.232614 H -6.768628 -0.468099 -0.130524 C -1.520698 2.043990 -0.385823 C -0.814672 0.815759 -0.397301 H -3.448678 2.941455 -0.280892 H 0.266581 0.835918 -0.461735 H -5.116285 1.153610 1.690556 H -0.919423 -1.309811 -0.336850 H -5.502572 -2.595587 -0.139779 C -0.757836 3.335041 -0.464282</p>	<p>-889, 90, 119, 179, 246, 262, 308, 390, 415, 428, 457, 514, 528, 536, 632, 657, 716, 772, 795, 807, 853, 899, 907, 930, 972, 1001, 1013, 1026, 1035, 1058, 1070, 1150, 1164, 1182, 1202, 1238, 1280, 1293, 1389, 1400, 1415, 1423, 1470, 1489, 1501, 1515, 1562, 1635, 1662, 1709, 3051, 3109, 3141, 3172, 3173, 3175, 3183, 3191, 3195, 3207,</p>

<p>H -0.178499 3.386226 -1.387558 H -1.426242 4.193109 -0.433260 H -0.053199 3.419639 0.364355</p>	
<p>i11-i12</p> <p>C -0.516010 -1.814181 0.139103 C 0.226660 -0.689180 -0.234513 C -0.450505 0.524919 -0.407085 C -1.822300 0.624702 -0.232838 C -2.539024 -0.515198 0.130277 C -1.885751 -1.724370 0.315267 H -0.009431 -2.759546 0.286148 H 0.106658 1.419253 -0.659667 H -3.610220 -0.448758 0.274278 H -2.448586 -2.603061 0.601206 C -2.534032 1.932306 -0.446669 H -3.032724 1.945505 -1.417507 H -3.297336 2.090864 0.314503 H -1.839955 2.770414 -0.416480 C 1.661770 -0.811522 -0.408244 C 2.524392 0.228449 -1.049823 C 2.650756 0.397210 0.380738 H 2.100504 -1.790151 -0.277797 H 2.017485 1.022411 -1.587735 H 3.408097 -0.137001 -1.561018 C 2.912997 0.756150 1.539712 H 2.813662 0.677190 2.599942</p>	<p>-740, 43, 56, 85, 185, 210, 222, 323, 349, 398, 427, 456, 534, 542, 561, 584, 708, 720, 738, 803, 831, 905, 908, 929, 934, 1001, 1017, 1018, 1034, 1068, 1088, 1116, 1145, 1160, 1196, 1214, 1272, 1318, 1353, 1411, 1421, 1470, 1475, 1494, 1510, 1543, 1649, 1674, 1929, 3051, 3114, 3115, 3141, 3179, 3187, 3188, 3195, 3214, 3223, 3376,</p>
<p>i12-p3</p> <p>C -0.888147 -0.735345 -0.752458 C 0.284419 -0.956926 -0.021242 C 1.303005 -0.018203 0.017579 C 1.142934 1.171183 -0.694419 C -0.015917 1.415325 -1.413035 C -1.030464 0.472308 -1.437438 H 0.395034 -1.871355 0.548989 H 1.933233 1.911712 -0.674213 H -0.130034 2.344851 -1.954145 H -1.937965 0.661516 -1.996611 C 2.546663 -0.252835 0.829377</p>	<p>-801, 76, 88, 102, 125, 207, 218, 242, 296, 346, 388, 414, 450, 487, 507, 532, 577, 635, 680, 717, 735, 773, 809, 898, 909, 949, 972, 1001, 1017, 1020, 1031, 1034, 1074, 1130, 1192, 1195, 1268, 1308, 1313, 1345, 1352, 1420,</p>

<p>H 2.617875 -1.288932 1.154632 H 3.439577 -0.011565 0.252952 H 2.551153 0.379253 1.718791 C -1.965900 -1.712265 -0.804336 H -2.920677 -1.361917 -1.178987 C -1.876536 -2.995603 -0.387699 H -0.913764 -3.425048 -0.139931 H -1.898910 -2.761432 1.558945 C -2.964133 -3.912787 -0.494351 C -3.866004 -4.698059 -0.582024 H -4.666771 -5.391437 -0.660576</p>	<p>1475, 1493, 1511, 1536, 1638, 1660, 1684, 2248, 3062, 3125, 3143, 3167, 3168, 3179, 3182, 3198, 3200, 3474,</p>
<p>i12-i25</p> <p>C 0.005211 0.475359 -0.078379 C 0.503355 0.662408 1.049929 C 2.313667 -0.138754 0.882151 C 2.769903 0.329660 -0.429457 C 1.952869 0.249974 -1.512221 C 0.480498 -0.066011 -1.370271 H 2.816830 -0.173247 2.993708 H 0.363061 1.018094 2.049348 C 3.123140 0.190265 2.020777 C 4.035382 1.021191 -0.497571 H 2.306128 0.584369 -2.479313 H -0.069395 0.346992 -2.214817 C 4.749235 1.336657 0.607161 C 4.255537 0.923221 1.895003 H 4.380322 1.339238 -1.475001 H 4.840739 1.168009 2.773562 C 6.036791 2.104439 0.542404 H 5.951324 3.052894 1.076316 H 6.847541 1.543798 1.011707 H 6.318564 2.317941 -0.486934 H 1.841331 -1.113855 0.911653 H 0.292381 -1.147037 -1.375110</p>	<p>-952, 91, 101, 133, 202, 268, 286, 355, 378, 425, 442, 483, 552, 563, 653, 678, 680, 738, 788, 798, 828, 893, 910, 931, 949, 975, 1002, 1011, 1035, 1059, 1071, 1115, 1187, 1199, 1209, 1232, 1296, 1326, 1370, 1398, 1417, 1459, 1479, 1487, 1498, 1522, 1590, 1693, 1890, 3013, 3046, 3100, 3101, 3136, 3142, 3173, 3179, 3193, 3199, 3353,</p>
<p>i12-i26</p> <p>C -0.029186 0.504187 -0.141270 C 0.428147 0.814811 0.976887 C 2.264235 0.062498 0.947025 C 2.748096 0.421314 -0.388893</p>	

<p>C 1.970623 0.210461 -1.484964 C 0.506157 -0.142734 -1.359189 H 0.239676 1.265303 1.929832 C 3.007099 0.507418 2.098168 C 3.989199 1.147832 -0.481969 H 2.347307 0.463151 -2.467910 H -0.028658 0.163794 -2.256899 C 4.633933 1.571559 0.627553 C 4.123907 1.265212 1.929575 H 4.363565 1.389650 -1.468680 H 4.674264 1.600040 2.800272 H 1.821204 -0.923391 1.049664 H 0.355331 -1.225293 -1.261511 C 2.516863 0.096975 3.453950 H 1.552077 0.556810 3.682572 H 2.368749 -0.983889 3.500746 H 3.219028 0.384161 4.234067 H 5.546731 2.145057 0.542417</p>	<p>-946, 78, 109, 149, 192, 239, 291, 355, 402, 443, 461, 514, 524, 544, 654, 662, 684, 743, 752, 797, 825, 905, 906, 930, 966, 979, 997, 1017, 1035, 1051, 1080, 1096, 1182, 1190, 1209, 1230, 1300, 1328, 1385, 1390, 1416, 1453, 1464, 1481, 1496, 1545, 1596, 1679, 1897, 3019, 3038, 3092, 3107, 3132, 3141, 3175, 3180, 3182, 3202, 3347,</p>
<p>i13-i14</p> <p>C -1.824496 -0.409919 0.565504 C -0.475214 -0.469106 0.189871 C 0.218817 0.726232 -0.058935 C -0.403461 1.955992 0.073899 C -1.746484 1.993115 0.451697 C -2.445677 0.819413 0.693259 H -2.364758 -1.328538 0.747833 H 1.258111 0.676655 -0.358035 H -2.243210 2.949910 0.554122 H -3.486911 0.863125 0.983673 C 0.350595 3.234766 -0.167116 H 0.538543 3.754418 0.773760 H 1.310359 3.045564 -0.644123 H -0.222306 3.908916 -0.803709 C 0.159472 -1.721679 0.009172 C 0.091704 -3.050777 -1.213175 C 0.812459 -2.820844 0.068183 H 0.590238 -2.755789 -2.128209 H 1.464167 -3.390246 0.715816 C -1.092674 -3.766586 -1.299959</p>	<p>-676, 35, 66, 108, 124, 201, 213, 281, 348, 420, 440, 450, 511, 532, 552, 570, 711, 720, 740, 770, 808, 902, 905, 922, 929, 959, 1012, 1014, 1019, 1067, 1079, 1129, 1144, 1178, 1194, 1246, 1276, 1302, 1346, 1381, 1416, 1456, 1494, 1501, 1508, 1526, 1636, 1665, 1938, 3055, 3118, 3145, 3158, 3161, 3183, 3190, 3195, 3197, 3210, 3264,</p>

<p>H -1.570642 -3.933605 -2.253487 H -1.577609 -4.143773 -0.410387</p>	
<p>i14-p5</p> <p>C -2.185940 -1.532641 1.832243 C -0.971956 -1.772984 1.185043 C -0.580290 -0.944920 0.127786 C -1.377535 0.110251 -0.289643 C -2.583624 0.335186 0.371891 C -2.983891 -0.479009 1.420568 H -2.487853 -2.171639 2.649836 H 0.363736 -1.138834 -0.364947 H -3.213004 1.159852 0.060459 H -3.923309 -0.289730 1.921921 C -0.964358 0.982969 -1.442290 H -1.161273 2.032896 -1.227578 H 0.095413 0.869914 -1.662580 H -1.523411 0.721447 -2.342186 C -0.134429 -2.848978 1.593828 C 0.563014 -3.815382 1.826814 H 0.188276 -4.841918 0.210405 C 1.460866 -4.739228 2.455981 H 1.629761 -4.546699 3.509982 C 2.085107 -5.753800 1.868568 H 1.938705 -5.979737 0.821312 H 2.758331 -6.380920 2.435266</p>	<p>-683, 32, 72, 74, 108, 110, 211, 234, 275, 328, 371, 417, 461, 531, 543, 556, 578, 624, 709, 716, 722, 816, 861, 919, 948, 984, 990, 1017, 1020, 1022, 1030, 1073, 1109, 1136, 1202, 1221, 1306, 1318, 1329, 1355, 1419, 1449, 1468, 1494, 1510, 1545, 1657, 1683, 1714, 2266, 3060, 3124, 3144, 3161, 3170, 3180, 3193, 3198, 3214, 3258,</p>
<p>i14-i17</p> <p>C -0.001432 -0.206346 -0.117821 C -0.101798 -0.017294 1.265960 C 1.069581 0.070065 2.020588 C 2.324191 -0.000160 1.428462 C 2.397763 -0.176060 0.050000 C 1.243253 -0.278532 -0.715748 H -0.903312 -0.307842 -0.706498 H 0.989138 0.197372 3.093921 H 3.367899 -0.245886 -0.426239 H 1.318510 -0.428243 -1.784599 C 3.570813 0.133134 2.258863 H 3.821898 1.184444 2.410506</p>	<p>-1898, 26, 94, 95, 104, 211, 284, 314, 338, 395, 448, 461, 532, 567, 637, 655, 717, 721, 808, 825, 857, 917, 930, 937, 942, 958, 1006, 1014, 1021, 1034, 1070, 1072, 1130, 1179, 1192, 1219, 1273, 1304, 1317, 1345, 1417,</p>

<p>H 3.438654 -0.317915 3.241445 H 4.420211 -0.343969 1.772701 C -1.390862 0.077331 1.908372 H -1.690504 -0.298339 3.200429 C -2.615663 0.462842 1.572688 H -2.895864 0.892782 0.618651 C -3.573600 0.251796 2.690516 H -4.627411 0.490004 2.614480 C -2.981419 -0.254315 3.756869 H -3.316220 -0.568516 4.732612</p>	<p>1461, 1501, 1503, 1529, 1624, 1651, 1676, 1706, 1745, 3056, 3121, 3149, 3168, 3177, 3177, 3182, 3186, 3202, 3249,</p>
<p>i15-i16</p> <p>C -2.617492 -2.300658 0.213595 C -1.226625 -2.414304 0.214761 C -0.457687 -1.250433 0.156151 C -1.039704 0.008911 0.117869 C -2.430015 0.094683 0.143378 C -3.212368 -1.050475 0.189800 H -3.224446 -3.196665 0.215159 H 0.623386 -1.338013 0.149406 H -2.902182 1.069247 0.118613 H -4.290705 -0.964740 0.196868 C -0.194415 1.249290 0.025263 H -0.035485 1.529605 -1.017678 H -0.674953 2.090502 0.522822 H 0.783662 1.095042 0.478349 C -0.576892 -3.725729 0.273162 C -1.180857 -4.884799 0.799702 C -0.314047 -5.333091 -1.120146 H 0.503494 -3.710755 0.219370 C -0.690510 -5.957827 0.014997 H -2.007984 -4.891979 1.498092 H 0.196675 -5.606042 -2.035907 H -0.629297 -7.010320 0.264644</p>	<p>-622, 55, 90, 101, 149, 220, 294, 321, 394, 430, 458, 530, 574, 592, 669, 702, 726, 752, 786, 824, 832, 906, 918, 924, 953, 970, 1020, 1023, 1028, 1066, 1071, 1131, 1170, 1192, 1200, 1258, 1279, 1330, 1348, 1355, 1416, 1443, 1480, 1501, 1503, 1540, 1542, 1663, 1684, 3055, 3121, 3149, 3161, 3167, 3168, 3177, 3180, 3193, 3195, 3214,</p>
<p>i16-i17</p> <p>C -2.617312 -2.272861 -0.122686 C -1.237547 -2.395263 -0.286299 C -0.455921 -1.237303 -0.292466 C -1.018728 0.024103 -0.165835</p>	

<p>C -2.402204 0.118864 -0.021376 C -3.194443 -1.019124 -0.000338 H -3.227528 -3.165172 -0.070388 H 0.618606 -1.332579 -0.405210 H -2.858436 1.095438 0.087806 H -4.264675 -0.927107 0.128235 C -0.168998 1.264253 -0.206121 H 0.877818 1.032499 -0.017948 H -0.235130 1.745314 -1.183549 H -0.499588 1.988775 0.537647 C -0.610600 -3.709541 -0.441660 C -0.220034 -5.353147 0.877138 C -1.278896 -4.850167 -0.929274 H 0.469529 -3.704379 -0.502407 C -0.720094 -5.946486 -0.226810 H 0.380738 -5.652416 1.727679 H -2.174789 -4.832753 -1.536873 H -0.696142 -6.992762 -0.507216</p>	<p>-620, 57, 63, 106, 150, 220, 294, 324, 393, 431, 457, 529, 580, 595, 680, 712, 728, 759, 798, 828, 839, 916, 925, 926, 957, 970, 1019, 1024, 1026, 1069, 1071, 1131, 1174, 1193, 1202, 1257, 1276, 1330, 1348, 1355, 1417, 1444, 1481, 1493, 1505, 1539, 1542, 1659, 1682, 3055, 3117, 3143, 3169, 3176, 3180, 3184, 3197, 3205, 3209, 3219,</p>
<p>i16-i18</p> <p>C -2.601349 -2.254885 -0.001470 C -1.243361 -2.378469 -0.293587 C -0.461687 -1.221991 -0.358655 C -1.006147 0.038764 -0.166826 C -2.370840 0.135185 0.103947 C -3.160899 -1.000919 0.186707 H -3.207085 -3.146443 0.096888 H 0.597077 -1.318198 -0.572734 H -2.812712 1.111797 0.261715 H -4.214616 -0.908183 0.413269 C -0.160385 1.278303 -0.264705 H -0.347068 1.945533 0.576673 H 0.899992 1.033147 -0.278502 H -0.389437 1.831661 -1.176857 C -0.638202 -3.691525 -0.526517 C -0.130662 -5.357142 0.723158 C -1.353490 -4.822917 -0.966779 H 0.431361 -3.687361 -0.689002 C -0.734372 -5.931524 -0.337950 H 0.545543 -5.671062 1.509445</p>	<p>-619, 50, 59, 103, 150, 221, 294, 323, 394, 430, 456, 529, 575, 595, 673, 703, 724, 752, 789, 826, 833, 906, 920, 924, 951, 970, 1016, 1020, 1024, 1068, 1073, 1129, 1171, 1192, 1201, 1259, 1276, 1331, 1348, 1355, 1416, 1443, 1480, 1493, 1503, 1540, 1541, 1661, 1682, 3055, 3114, 3143, 3165, 3167, 3176, 3178, 3182, 3189, 3200, 3203,</p>

<p>H -2.302526 -4.793235 -1.486908 H -0.740027 -6.973010 -0.636567</p>	
<p>i17-i19</p> <p>C -5.699638 -2.945451 0.638551 C -4.348898 -2.910535 0.342886 C -3.798402 -1.802203 -0.297486 C -4.639896 -0.735785 -0.673058 C -6.023605 -0.784610 -0.398170 C -6.525839 -1.877392 0.279412 H -1.790243 -2.542554 -0.767015 H -6.120305 -3.801381 1.148315 H -3.704236 -3.731899 0.629397 C -2.358984 -1.664709 -0.481591 C -3.618037 0.912557 0.448046 H -7.583363 -1.918388 0.509684 C -2.326591 0.647005 0.423708 C -1.707756 -0.524035 -0.202785 H -1.644739 1.302002 0.966116 H -0.631345 -0.498971 -0.314638 C -6.897856 0.351276 -0.839586 H -6.800604 0.524661 -1.912557 H -7.945462 0.157231 -0.617300 H -6.607386 1.277215 -0.338009 H -4.188853 1.699876 0.917743 H -4.290586 -0.054178 -1.440012</p>	<p>-444, 61, 100, 143, 167, 229, 288, 358, 394, 447, 476, 522, 538, 559, 660, 715, 727, 767, 775, 821, 853, 913, 915, 939, 974, 997, 1004, 1017, 1026, 1035, 1066, 1119, 1183, 1186, 1214, 1254, 1277, 1326, 1342, 1413, 1433, 1438, 1487, 1496, 1536, 1603, 1644, 1652, 1684, 3044, 3088, 3100, 3144, 3158, 3175, 3177, 3185, 3195, 3202, 3219,</p>
<p>i17-i27</p> <p>C 0.002728 0.169670 -0.046382 C -0.114823 -0.058615 1.329626 C 1.063053 -0.195756 2.076166 C 2.316252 -0.140719 1.480998 C 2.398069 0.061271 0.105607 C 1.245737 0.223174 -0.650201 H -0.895521 0.291614 -0.638501 H 1.006204 -0.299671 3.150449 H 3.369817 0.104731 -0.370992 H 1.319342 0.391597 -1.716331 C 3.568774 -0.274654 2.303213 H 4.145066 0.651388 2.286246</p>	<p>-1865, 43, 68, 105, 158, 188, 219, 259, 300, 348, 380, 436, 469, 510, 535, 567, 608, 713, 731, 751, 752, 826, 872, 908, 918, 939, 957, 984, 1013, 1020, 1033, 1068, 1132, 1184, 1194, 1235, 1278, 1327, 1352, 1413, 1425, 1471, 1492, 1506, 1530, 1585, 1657, 1679, 1915, 2361,</p>

<p>H 3.337855 -0.509043 3.340861 H 4.210166 -1.064037 1.910313 C -1.443685 -0.147573 1.910216 H -2.248288 0.223755 1.288031 C -1.809037 -0.680750 3.104007 H -2.865637 -0.688264 3.348196 C -1.018866 -1.361169 4.048169 H -0.145530 -2.214842 3.876770 C -0.477746 -1.816602 5.126446 H -0.128931 -1.418774 6.079804</p>	<p>3054, 3088, 3112, 3145, 3166, 3168, 3173, 3183, 3198, 3212,</p>
<p>i18-i19</p> <p>C -5.340947 -3.198074 0.988914 C -4.028917 -3.113823 0.559174 C -3.619966 -2.051515 -0.244350 C -4.566060 -1.086548 -0.643968 C -5.912119 -1.189843 -0.231568 C -6.270665 -2.229155 0.603475 H -1.615436 -2.712852 -0.832877 H -5.650144 -4.016068 1.625071 H -3.303211 -3.856609 0.865981 C -2.216950 -1.846292 -0.582296 C -3.568835 0.732332 0.201617 H -7.296848 -2.308989 0.940507 C -2.269225 0.547756 0.075393 C -1.627173 -0.643871 -0.486669 H -1.589088 1.298770 0.477158 H -0.570129 -0.563717 -0.705904 C -6.903412 -0.170151 -0.707849 H -7.896533 -0.362244 -0.306115 H -6.598989 0.833931 -0.404827 H -6.968966 -0.169276 -1.797342 H -4.150346 1.528055 0.643282 H -4.336287 -0.472291 -1.506982</p>	<p>-445, 60, 99, 144, 166, 227, 293, 358, 394, 449, 475, 521, 537, 559, 662, 715, 726, 766, 774, 823, 855, 915, 922, 936, 973, 997, 1003, 1017, 1027, 1034, 1063, 1117, 1182, 1184, 1212, 1254, 1278, 1323, 1340, 1411, 1430, 1435, 1484, 1497, 1535, 1604, 1642, 1651, 1684, 3044, 3100, 3102, 3138, 3166, 3172, 3174, 3178, 3194, 3205, 3218,</p>
<p>i18-i20</p> <p>C -5.707767 -2.859645 0.658115 C -4.431632 -2.991920 0.353147 C -3.887953 -1.310474 -1.002089 C -4.711453 -0.315239 -0.434092</p>	

<p>C -6.130946 -0.587990 -0.245066 C -6.577596 -1.772373 0.202348 H -1.866862 -1.815310 -1.560963 H -6.160995 -3.562779 1.356764 H -3.677185 -3.701962 0.657896 C -2.500917 -1.081658 -1.081147 C -4.133376 0.860888 0.038972 H -6.834837 0.224622 -0.385211 H -7.639544 -1.899533 0.369613 C -2.762487 1.068265 -0.001031 C -1.954058 0.069214 -0.562586 H -4.775252 1.620296 0.471933 H -0.883480 0.227695 -0.615861 C -2.144776 2.321064 0.551909 H -1.396640 2.722764 -0.132036 H -2.897250 3.088447 0.725290 H -1.644113 2.123003 1.501651 H -4.340285 -2.043145 -1.657303</p>	<p>-458, 80, 109, 148, 205, 227, 292, 345, 404, 431, 449, 514, 539, 572, 660, 698, 735, 775, 794, 817, 865, 907, 922, 926, 966, 990, 999, 1016, 1026, 1039, 1071, 1116, 1178, 1191, 1210, 1258, 1276, 1320, 1343, 1420, 1422, 1471, 1493, 1497, 1522, 1594, 1626, 1663, 1682, 3053, 3101, 3113, 3145, 3161, 3165, 3169, 3175, 3191, 3194, 3215,</p>
<p>i18-i26</p> <p>C -0.118388 0.343141 0.183240 C -0.019160 0.161525 1.567744 C 1.256506 -0.024530 2.116575 C 2.405539 0.000692 1.341754 C 2.276304 0.201779 -0.031776 C 1.023376 0.362646 -0.602250 H -1.087642 0.415030 -0.286939 H 1.343695 -0.184002 3.185882 H 3.161991 0.215230 -0.654752 H 0.932860 0.490748 -1.672874 C 3.761988 -0.158222 1.971314 H 4.161697 0.811206 2.274733 H 3.714110 -0.787147 2.859120 H 4.469715 -0.602058 1.272593 C -1.166541 0.157931 2.459211 H -0.994071 -0.260329 3.442945 C -2.407204 0.659438 2.230128 H -3.131655 0.597389 3.034694 C -2.874933 1.384148 1.120078 H -2.318455 2.271606 0.470511</p>	<p>-1842, -1842, 26, 26, 40, 40, 116, 116, 152, 152, 190, 190, 215, 215, 264, 264, 299, 299, 330, 330, 386, 386, 435, 435, 465, 465, 509, 509, 536, 536, 573, 573, 609, 609, 707, 707, 725, 725, 754, 754, 781, 781, 826, 826, 857, 857, 908, 908, 919, 919, 947, 947, 956, 956, 972, 972, 1016, 1016, 1022, 1022, 1028, 1028, 1069, 1069, 1137, 1137, 1185, 1185, 1200, 1200, 1232, 1232, 1280, 1280, 1338, 1338, 1350, 1350, 1416, 1416, 1423, 1423, 1458, 1458, 1494, 1494, 1500, 1500, 1540, 1540, 1582, 1582, 1654, 1654,</p>

C -3.574038 1.874800 0.153335 H -4.227604 1.493731 -0.632104	
i19-p1 C -5.744514 -3.023357 0.569171 C -4.381149 -2.982831 0.535759 C -3.704792 -1.760301 0.338697 C -4.471485 -0.576393 0.048706 C -5.911548 -0.628257 0.208612 C -6.502171 -1.832948 0.437871 H -1.729376 -2.587481 0.494194 H -6.257077 -3.961984 0.729359 H -3.797895 -3.884057 0.676700 C -2.297036 -1.676451 0.350254 C -3.768037 0.679304 0.036387 H -7.580556 -1.884214 0.521486 C -2.410486 0.717276 0.087518 C -1.658187 -0.476702 0.207884 H -1.895949 1.667691 0.044023 H -0.578249 -0.429262 0.226325 C -6.716905 0.619651 0.022094 H -6.462047 1.378345 0.764254 H -6.528024 1.052939 -0.964339 H -7.780434 0.406895 0.103751 H -4.332095 1.594971 -0.067720 H -4.533430 -0.761263 -1.571346	-1162, 110, 163, 216, 246, 285, 396, 414, 459, 463, 507, 528, 557, 574, 601, 647, 712, 747, 791, 814, 822, 875, 894, 935, 986, 995, 1006, 1017, 1041, 1064, 1084, 1097, 1158, 1191, 1196, 1230, 1268, 1290, 1382, 1399, 1413, 1430, 1470, 1482, 1496, 1508, 1549, 1632, 1679, 1694, 3037, 3093, 3138, 3171, 3173, 3184, 3185, 3203, 3206, 3211,
i19-i26 C -0.219725 0.428912 0.075499 C 0.044141 0.137095 1.421030 C 1.472452 0.034629 1.964699 C 2.333817 0.997282 1.192398 C 2.101555 1.070058 -0.201837 C 0.957923 0.555919 -0.756921 H -0.445831 -0.758122 0.697406 C 1.597300 0.127989 3.457885 C 3.343829 1.702085 1.842014 H 2.840143 1.575595 -0.815615 C 3.475374 1.653658 3.211314 C 2.568134 0.886103 4.007829	-1062, 75, 142, 181, 241, 263, 326, 411, 426, 454, 487, 527, 542, 569, 652, 708, 760, 785, 786, 833, 894, 914, 932, 968, 986, 991, 1029, 1051, 1064, 1091, 1110, 1164, 1189, 1204, 1246, 1252, 1283, 1334, 1361, 1370, 1390, 1415, 1433, 1465, 1482, 1491, 1511, 1551, 1671, 2227, 2884, 3039, 3091, 3138, 3147, 3151, 3180, 3187, 3191, 3215,

<p>H 4.007599 2.321745 1.251317 H 2.671071 0.914648 5.085623 H 1.821748 -0.980034 1.688239 H 0.847337 0.513984 -1.832593 H 4.251194 2.224810 3.701251 C 0.675714 -0.715777 4.279439 H -0.356530 -0.364710 4.220250 H 0.676755 -1.748986 3.921218 H 0.971389 -0.712406 5.326535 H -0.768381 0.216452 2.138576</p>	
<p>i19-i23</p> <p>C 0.007988 -0.022426 -0.025365 C 0.022059 0.048416 1.357249 C 1.217043 0.128880 2.060528 C 2.469724 0.078473 1.343348 C 2.438363 0.086228 -0.098044 C 1.220936 0.012800 -0.727571 H 0.337768 0.211736 4.040308 H -0.926783 -0.077067 -0.563634 H -0.906271 0.057874 1.914986 C 1.271915 0.239396 3.493879 C 3.700679 0.286200 2.103672 H 1.203727 -0.002508 -1.810919 C 3.685613 0.500854 3.463115 C 2.442799 0.434442 4.153446 H 4.612253 0.623667 4.001669 H 2.434464 0.545865 5.229754 C 3.728765 0.087892 -0.853550 H 4.320340 0.983505 -0.648571 H 4.346047 -0.773663 -0.572338 H 3.549576 0.037595 -1.925212 H 4.626473 0.309787 1.546233 H 3.147983 -1.066023 1.721561</p>	<p>-1631, 115, 187, 228, 261, 278, 350, 410, 435, 469, 478, 519, 553, 588, 635, 715, 748, 777, 798, 807, 845, 863, 922, 943, 969, 995, 1011, 1030, 1034, 1068, 1081, 1105, 1170, 1184, 1188, 1251, 1259, 1283, 1354, 1406, 1420, 1433, 1472, 1485, 1494, 1501, 1533, 1588, 1648, 1684, 3021, 3076, 3137, 3170, 3179, 3182, 3198, 3212, 3213, 3227,</p>
<p>i20-p2</p> <p>C -5.894631 -2.963681 0.408211 C -4.536734 -2.981244 0.363719 C -3.799714 -1.762760 0.172946 C -4.512665 -0.517167 0.272842 C -5.921560 -0.548442 0.288752</p>	

<p>C -6.599061 -1.736523 0.329395 H -1.838373 -2.668178 0.412491 H -6.445822 -3.887907 0.515972 H -3.986440 -3.911567 0.420563 C -2.371585 -1.728111 0.351526 C -3.775077 0.687113 0.271373 H -6.461778 0.390123 0.282983 H -7.680155 -1.742381 0.345656 C -2.407246 0.696685 0.301884 C -1.711879 -0.545394 0.386391 H -4.320161 1.624225 0.261381 H -0.633669 -0.529615 0.490564 C -1.619935 1.974083 0.297328 H -0.978859 2.036530 1.178483 H -0.969887 2.023844 -0.577933 H -2.273609 2.843902 0.286146 H -3.775494 -1.789555 -1.452084</p>	<p>-1199, 103, 148, 165, 259, 281, 380, 396, 442, 479, 486, 516, 567, 601, 629, 649, 710, 758, 763, 811, 843, 889, 897, 933, 964, 990, 1007, 1016, 1028, 1043, 1067, 1149, 1162, 1185, 1199, 1223, 1276, 1287, 1386, 1401, 1412, 1422, 1471, 1490, 1498, 1511, 1543, 1624, 1680, 1703, 3053, 3109, 3146, 3169, 3174, 3176, 3182, 3193, 3195, 3206,</p>
<p>i20-i24</p> <p>C 0.020062 -0.114653 -0.010072 C 0.012846 -0.118473 1.375549 C 1.188319 -0.049555 2.110470 C 2.451152 -0.035453 1.406217 C 2.421107 0.072454 -0.025281 C 1.236470 0.007947 -0.712197 H 0.293949 -0.079853 4.085491 H -0.908782 -0.163672 -0.562080 H -0.927152 -0.161220 1.912520 C 1.230912 -0.012253 3.547226 C 3.671642 0.138810 2.184251 C 3.645684 0.279308 3.555316 C 2.395469 0.163939 4.225782 H 4.566384 0.374690 4.108986 H 2.375482 0.218409 5.306327 H 4.596267 0.197375 1.623691 H 3.114060 -1.167415 1.753965 C 1.211193 0.096333 -2.212254 H 2.211258 0.219930 -2.623171 H 0.774134 -0.807271 -2.639692 H 0.598552 0.938058 -2.537421 H 3.357966 0.183007 -0.557600</p>	<p>-1692, 97, 132, 151, 261, 287, 360, 407, 439, 457, 496, 527, 619, 623, 689, 712, 733, 781, 791, 798, 852, 884, 921, 956, 964, 992, 1008, 1028, 1043, 1051, 1063, 1141, 1166, 1185, 1204, 1237, 1266, 1295, 1362, 1385, 1415, 1440, 1453, 1484, 1490, 1500, 1547, 1573, 1647, 1687, 3057, 3116, 3147, 3173, 3175, 3177, 3189, 3196, 3198, 3224,</p>

<p>i20-i25</p> <p>C -0.031212 0.020412 0.113424 C 0.074665 -0.391089 1.383255 C 1.309677 -0.029097 2.182348 C 2.458424 0.431155 1.310941 C 2.374331 0.518468 -0.032738 C 1.061956 0.475323 -0.661655 H 0.186410 0.920829 3.860869 H -0.623515 -1.087264 1.830350 C 1.162928 0.843322 3.399628 C 3.651708 0.822635 2.041441 H 3.251362 0.769507 -0.617273 H 0.877576 1.073351 -1.546265 C 3.557461 1.297137 3.298464 C 2.240310 1.424537 3.928146 H 4.600319 0.846978 1.517043 H 2.168437 2.009007 4.837584 C 4.743816 1.799952 4.061540 H 4.619424 2.856521 4.308494 H 4.847236 1.263293 5.006833 H 5.664875 1.681992 3.494471 H 1.661670 -0.993957 2.600044 H 0.363442 -0.601349 -1.000979</p>	<p>-1841, 93, 111, 162, 231, 293, 331, 389, 414, 434, 474, 541, 550, 604, 658, 691, 712, 746, 790, 832, 845, 891, 922, 930, 1007, 1009, 1024, 1056, 1067, 1094, 1123, 1184, 1190, 1205, 1216, 1260, 1277, 1305, 1352, 1390, 1412, 1417, 1439, 1478, 1493, 1560, 1640, 1651, 1723, 2027, 2890, 3040, 3096, 3135, 3161, 3166, 3173, 3182, 3193, 3198,</p>
<p>i21-i23</p> <p>C 0.005561 -0.009364 -0.004653 C 0.000733 -0.008269 1.343031 C 2.347303 0.004470 1.666792 C 2.822416 0.806888 0.643501 C 1.999057 1.359066 -0.434512 C 0.759164 0.963683 -0.770798 H -0.489424 -0.807806 -0.546831 H 0.253266 0.887110 1.893744 C 3.109390 -0.573136 2.648088 C 4.207565 1.022583 0.641745 H 2.506716 2.063390 -1.083792 H 0.341145 1.321297 -1.705159 C 5.020279 0.456683 1.610553 C 4.489579 -0.343859 2.616806 H 4.642624 1.640351 -0.135408</p>	<p>-1038, 81, 115, 139, 230, 261, 333, 367, 417, 441, 481, 490, 573, 606, 670, 697, 751, 759, 799, 861, 899, 923, 937, 981, 986, 1001, 1012, 1054, 1063, 1080, 1146, 1174, 1180, 1212, 1242, 1252, 1278, 1357, 1369, 1387, 1412, 1416, 1459, 1469, 1477, 1482, 1507, 1563, 1676, 2199, 2871, 3043, 3098, 3121, 3138, 3149, 3165, 3176, 3182, 3186,</p>

<p>H -0.472417 -0.804580 1.902126 H 6.086585 0.640337 1.585810 C 2.494455 -1.445303 3.737624 H 2.723698 -2.481684 3.551267 H 2.891446 -1.168850 4.700079 H 1.424851 -1.322440 3.748298 H 5.123041 -0.765477 3.376426</p>	
<p>i22-i24</p> <p>C -0.205300 -0.272582 -0.029080 C -0.214144 0.487562 1.083493 C 2.040063 0.141777 1.720814 C 2.723611 0.099831 0.517389 C 2.092156 0.117642 -0.803608 C 0.792685 -0.102812 -1.067106 H 2.018528 0.105505 3.864134 H -0.901191 -1.098953 -0.125529 H 0.276925 1.450624 1.095769 C 2.614835 0.061463 2.959716 C 4.114083 -0.040893 0.625737 H 2.778900 0.196216 -1.638853 H 0.494470 -0.248981 -2.099224 C 4.734759 -0.129622 1.861217 C 4.004615 -0.082417 3.046501 H 4.708924 -0.085590 -0.279528 H -0.891162 0.278327 1.900940 H 5.810923 -0.239613 1.908887 C 4.684237 -0.148041 4.385593 H 4.105000 -0.743657 5.090510 H 5.677789 -0.585184 4.300859 H 4.794531 0.850503 4.812759</p>	<p>-408, 82, 110, 130, 196, 222, 304, 342, 399, 425, 426, 489, 565, 593, 644, 706, 731, 789, 804, 841, 857, 893, 925, 969, 988, 991, 1012, 1015, 1028, 1066, 1088, 1165, 1197, 1225, 1236, 1291, 1296, 1316, 1411, 1413, 1435, 1468, 1493, 1499, 1523, 1591, 1615, 1658, 1687, 3057, 3118, 3143, 3143, 3149, 3158, 3172, 3172, 3174, 3192, 3233,</p>
<p>i23-p1</p> <p>C -5.747783 -3.199578 -0.235509 C -4.383110 -3.198498 -0.211254 C -3.671149 -1.977556 -0.261810 C -4.388174 -0.759316 -0.341305 C -5.808859 -0.775977 -0.353196 C -6.456899 -1.984120 -0.303807 H -1.720710 -2.889240 -0.173058 H -6.293529 -4.132609 -0.197156</p>	<p>-870, 142, 173, 216, 259, 291, 298, 409, 443, 464, 484, 490, 521, 572, 578, 647, 721, 770, 800, 805, 838, 880, 909, 940, 1002, 1007, 1019, 1038, 1058, 1072, 1091, 1108, 1168, 1183, 1196, 1236, 1271, 1294, 1384, 1407, 1419, 1434, 1470, 1491, 1503, 1511, 1561, 1648, 1659,</p>

H -3.827390 -4.125713 -0.152322 C -2.254241 -1.949480 -0.240748 C -3.649212 0.464097 -0.370545 H -7.539448 -2.003389 -0.311817 C -2.267510 0.446478 -0.418264 C -1.569800 -0.766687 -0.324505 H -3.976651 0.945507 1.399588 H -1.723533 1.377321 -0.500129 H -0.488408 -0.764522 -0.329572 C -6.577501 0.512743 -0.395266 H -6.309943 1.150445 0.450802 H -6.364758 1.074744 -1.306570 H -7.647997 0.323895 -0.356608 H -4.172164 1.389204 -0.568117	1693, 3046, 3102, 3139, 3176, 3178, 3184, 3190, 3200, 3203, 3209,
i24-p2 C -5.998004 -2.814916 0.377659 C -4.631547 -2.809511 0.588730 C -3.902717 -1.584019 0.521031 C -4.572427 -0.407341 0.115487 C -5.958503 -0.470447 -0.173223 C -6.653087 -1.642981 -0.031960 H -2.009003 -2.418215 1.118799 H -6.555998 -3.733774 0.492131 H -4.143324 -3.677118 1.014129 C -2.524942 -1.514498 0.818163 C -3.841514 0.801084 0.022482 H -6.465526 0.433112 -0.487716 H -7.716017 -1.668004 -0.230171 C -2.505803 0.856970 0.315973 C -1.849774 -0.331729 0.720684 H -4.364849 1.698118 -0.288757 H -0.792198 -0.292067 0.952278 C -1.722039 2.134280 0.215441 H -2.357585 2.967705 -0.077033 H -1.254603 2.378641 1.170411 H -0.922798 2.039368 -0.521312 H -4.054895 -3.521689 -1.024722	-894, 110, 141, 171, 262, 268, 286, 388, 419, 426, 456, 511, 525, 547, 631, 651, 716, 769, 793, 811, 848, 893, 903, 932, 973, 1001, 1009, 1027, 1035, 1056, 1070, 1150, 1161, 1184, 1202, 1235, 1278, 1292, 1392, 1396, 1413, 1421, 1472, 1490, 1503, 1516, 1559, 1636, 1661, 1708, 3051, 3110, 3143, 3171, 3173, 3174, 3179, 3190, 3193, 3207,
1-methylnaphthalene (p1) C -5.001462 -1.547949 0.186087	134, 173, 208, 252, 292, 423, 443, 481, 486, 521, 551, 579, 649, 722, 754, 805, 805, 824, 880, 891, 936, 992, 1000, 1013, 1023, 1054, 1071, 1089, 1107, 1171, 1192,

<p>C -3.644559 -1.515947 0.032190 C -2.943592 -0.287554 0.005803 C -3.666748 0.926051 0.141678 C -5.072699 0.858068 0.300213 C -5.723036 -0.344585 0.321660 H -3.081316 -2.435048 -0.072211 C -1.537080 -0.246277 -0.153916 C -2.963985 2.167922 0.115304 H -6.797318 -0.375723 0.443505 C -1.604013 2.155699 -0.041581 C -0.883489 0.949426 -0.176830 H 0.190708 0.982693 -0.298897 H -5.638202 1.773598 0.405346 H -0.996575 -1.178727 -0.256721 H -5.526140 -2.493441 0.204527 H -1.066216 3.095343 -0.062212 C -3.708171 3.464656 0.259466 H -4.450007 3.586866 -0.531557 H -4.239512 3.512315 1.211651 H -3.021302 4.306945 0.212899</p>	<p>1196, 1238, 1275, 1299, 1387, 1414, 1423, 1440, 1476, 1491, 1510, 1514, 1569, 1660, 1681, 1706, 3050, 3108, 3139, 3172, 3175, 3182, 3188, 3198, 3204, 3209,</p>
<p>2-methylnaphthalene (p2)</p> <p>C -5.005912 -1.538075 0.184481 C -3.644791 -1.519325 0.064410 C -2.939391 -0.294160 0.029582 C -3.661948 0.920736 0.120947 C -5.070691 0.870112 0.245305 C -5.726871 -0.328131 0.276019 H -3.085641 -2.444216 -0.005596 C -1.529297 -0.235738 -0.094903 C -2.953899 2.147168 0.085349 H -6.803969 -0.354259 0.371424 C -1.592530 2.187195 -0.035328 C -0.880866 0.962861 -0.125896 H -3.517318 3.070874 0.155524 H 0.197892 0.992756 -0.221980 H -5.620165 1.800723 0.315509 H -0.974325 -1.163171 -0.165124 H -5.536944 -2.479848 0.210027 C -0.835478 3.483719 -0.076229 H -1.506351 4.336389 0.007981</p>	<p>66, 119, 182, 263, 283, 407, 412, 454, 489, 519, 529, 635, 653, 717, 766, 795, 800, 846, 886, 902, 929, 973, 993, 1009, 1024, 1027, 1054, 1069, 1157, 1167, 1186, 1206, 1239, 1282, 1297, 1394, 1411, 1415, 1430, 1477, 1487, 1503, 1521, 1565, 1652, 1686, 1716, 3047, 3106, 3137, 3168, 3172, 3175, 3179, 3190, 3194, 3207,</p>

H -0.111164 3.536201 0.738108 H -0.279415 3.577648 -1.010393	
1-meta-tolyl-vinylacetylene (p3) C -0.793610 -0.695936 -0.470426 C 0.393772 -1.029638 0.189183 C 1.422222 -0.114520 0.341384 C 1.258742 1.169449 -0.182240 C 0.094314 1.518048 -0.842841 C -0.926617 0.590102 -0.988938 H 0.526346 -2.028519 0.585335 H 2.056297 1.893799 -0.070383 H -0.020823 2.514641 -1.247064 H -1.838350 0.861360 -1.505753 C 2.697193 -0.484435 1.047748 H 3.552864 -0.385471 0.378752 H 2.872378 0.173162 1.899931 H 2.666876 -1.509955 1.410528 C -1.901370 -1.638272 -0.642941 H -2.722018 -1.288677 -1.259918 C -1.995568 -2.861893 -0.112415 H -1.212070 -3.255493 0.523506 C -3.111871 -3.715860 -0.332234 C -4.043990 -4.451987 -0.504009 H -4.871752 -5.099004 -0.659706	54, 57, 69, 106, 187, 213, 246, 339, 377, 410, 460, 518, 532, 598, 605, 707, 716, 719, 820, 860, 915, 955, 985, 989, 1018, 1022, 1026, 1033, 1070, 1110, 1131, 1195, 1217, 1305, 1322, 1328, 1345, 1417, 1450, 1468, 1491, 1507, 1539, 1657, 1679, 1700, 2359, 3055, 3118, 3139, 3165, 3178, 3179, 3180, 3197, 3210, 3262,
2-meta-tolyl-vinylacetylene (p4) C -0.177143 -0.480215 0.092822 C -0.233884 -0.065963 1.422728 C 0.946311 0.301019 2.063155 C 2.175994 0.238107 1.416990 C 2.210880 -0.196063 0.096458 C 1.040525 -0.546616 -0.561659 H -1.087452 -0.728098 -0.435512 H 0.903407 0.635960 3.092479 H 3.160050 -0.251506 -0.422111 H 1.077823 -0.866243 -1.594471 C 3.434193 0.660056 2.124312 H 3.615634 1.726948 1.981570 H 3.363490 0.478005 3.195502 H 4.300740 0.123880 1.740062	43, 116, 149, 214, 240, 291, 343, 421, 428, 456, 519, 541, 626, 669, 694, 716, 722, 732, 753, 825, 879, 928, 951, 954, 964, 1018, 1019, 1026, 1070, 1126, 1148, 1201, 1243, 1313, 1348, 1355, 1416, 1443, 1469, 1491, 1506, 1546, 1663, 1685, 1700, 2249, 3051, 3114, 3136, 3166, 3176, 3187, 3196, 3211, 3260, 3473,

<p>C -1.526315 -0.025510 2.155313 C -2.564347 -0.809203 1.853291 C -1.631733 0.893535 3.253822 H -3.488493 -0.743317 2.408166 H -2.500003 -1.539816 1.059485 C -1.714832 1.666181 4.166660 H -1.796055 2.351624 4.974162</p>	
<p>4-meta-tolyl-vinylacetylene (p5)</p> <p>C 0.006424 0.005539 0.010193 C -0.062058 0.006163 1.406824 C 1.087069 -0.015309 2.182590 C 2.323971 -0.036680 1.539784 C 2.405873 -0.037822 0.156458 C 1.253997 -0.016954 -0.613365 H 3.229934 -0.051810 2.133516 H 3.373381 -0.054831 -0.326779 H 1.307825 -0.017165 -1.692763 C 1.010637 -0.021216 3.684369 H 1.432524 -0.941730 4.089783 H 1.575940 0.810352 4.106096 H -0.018835 0.058475 4.027828 C -1.191856 0.028353 -0.766215 C -2.199934 0.047572 -1.425084 C -3.408035 0.070861 -2.177780 H -4.327983 0.071747 -1.604307 C -3.455991 0.091495 -3.507325 H -4.403493 0.109005 -4.026535 H -2.552552 0.091308 -4.101376 H -1.034538 0.024972 1.881592</p>	<p>54, 57, 69, 106, 187, 213, 246, 339, 377, 410, 460, 518, 532, 598, 605, 707, 716, 719, 820, 860, 915, 955, 985, 989, 1018, 1022, 1026, 1033, 1070, 1110, 1131, 1195, 1217, 1305, 1322, 1328, 1345, 1417, 1450, 1468, 1491, 1507, 1539, 1657, 1679, 1700, 2359, 3055, 3118, 3139, 3165, 3178, 3179, 3180, 3197, 3210, 3262,</p>

Table S2. Forward and reverse RRKM rate constants (in s^{-1}) as functions of the collision energy E (in $kJ\ mol^{-1}$) for the reaction steps from the reaction of meta-tolyl radical with vinylacetylene producing the initial adduct **i1**

Channel	TS	0.0	5.0	10.0	15.0	20.0	25.0	30.0	35.0	40.0	45.0	50.0	55.0	60.0
i1 – i5	1-6	1.5E+0 1	3.0E+0 1	5.7E+0 1	1.0E+0 2	1.7E+0 2	2.9E+0 2	4.7E+0 2	7.4E+0 2	1.1E+0 3	1.7E+0 3	2.4E+0 3	3.5E+0 3	5.1E+03
i5 - i1	1-6	1.9E+0 8	1.4E+0 8	2.1E+0 8	2.9E+0 8	4.0E+0 8	5.3E+0 8	6.9E+0 8	8.9E+0 8	1.1E+0 9	1.4E+0 9	1.7E+0 9	2.1E+0 9	2.5E+09
i1 – i6	1-5	9.1E+0 0	1.7E+0 1	3.1E+0 1	5.5E+0 1	9.2E+0 1	1.5E+0 2	2.4E+0 2	3.7E+0 2	5.6E+0 2	8.0E+0 2	1.2E+0 3	1.7E+0 3	2.4E+03
i6- i1	1-5	2.7E+0 8	2.0E+0 8	2.7E+0 8	3.7E+0 8	4.9E+0 8	6.3E+0 8	8.0E+0 8	1.0E+0 9	1.2E+0 9	1.5E+0 9	1.8E+0 9	2.1E+0 9	2.5E+09
i1 - 1-Meta-tolyl- vinylacetylene	i1-p3	6.7E-03	1.3E-02	4.0E-02	1.1E-01	2.8E-01	6.6E-01	1.4E+0 0	3.0E+0 0	5.8E+0 0	1.0E+0 1	1.9E+0 1	3.3E+0 1	5.7E+01
i6 - i8	6-8	1.1E+1 2	1.1E+1 2	1.1E+1 2	1.1E+1 2	1.1E+1 2	1.1E+1 2	1.1E+1 2	1.1E+1 2	1.1E+1 2	1.1E+1 2	1.1E+1 2	1.1E+1 2	1.1E+12
i8 - i6	6-8	4.3E+0 4	6.2E+0 4	8.8E+0 4	1.2E+0 5	1.7E+0 5	2.3E+0 5	3.1E+0 5	4.1E+0 5	5.3E+0 5	6.8E+0 5	8.7E+0 5	1.1E+0 6	1.4E+06
i8 - i10	8-10	9.9E+0 3	7.1E+0 3	1.0E+0 4	1.4E+0 4	1.9E+0 4	2.6E+0 4	3.5E+0 4	4.6E+0 4	6.1E+0 4	7.7E+0 4	9.9E+0 4	1.3E+0 5	1.6E+05
i10 - i8	8-10	3.6E-02	5.8E-02	9.2E-02	1.4E-01	2.2E-01	3.3E-01	5.0E-01	7.4E-01	1.1E+0 0	1.5E+0 0	2.1E+0 0	3.0E+0 0	4.2E+00
i10 - 2- Methylnaphthalen e	i10- p2	1.6E+0 8	8.9E+0 7	1.0E+0 8	1.1E+0 8	1.3E+0 8	1.5E+0 8	1.6E+0 8	1.8E+0 8	2.1E+0 8	2.3E+0 8	2.6E+0 8	2.8E+0 8	3.2E+08
i5 - i7	5-7	1.5E+1 2	1.5E+1 2	1.5E+1 2	1.5E+1 2	1.5E+1 2	1.5E+1 2	1.5E+1 2	1.5E+1 2	1.5E+1 2	1.5E+1 2	1.5E+1 2	1.5E+1 2	1.5E+12
i7 - i5	5-7	2.8E+0 5	4.1E+0 5	5.8E+0 5	8.1E+0 5	1.1E+0 6	1.5E+0 6	2.1E+0 6	2.8E+0 6	3.7E+0 6	4.7E+0 6	6.1E+0 6	7.8E+0 6	9.9E+06
i7 - i9	7-9	4.8E+0 4	3.4E+0 4	4.8E+0 4	6.6E+0 4	9.0E+0 4	1.2E+0 5	1.6E+0 5	2.1E+0 5	2.8E+0 5	3.5E+0 5	4.6E+0 5	5.8E+0 5	7.3E+05
i9 - i7	7-9	3.6E-02	5.8E-02	9.2E-02	1.4E-01	2.2E-01	3.3E-01	4.9E-01	7.3E-01	1.1E+0 0	1.5E+0 0	2.1E+0 0	3.0E+0 0	4.1E+00
i9 – 1- Methylnaphthalen e	i9-p1	1.1E+0 8	6.2E+0 7	7.1E+0 7	8.0E+0 7	9.1E+0 7	1.0E+0 8	1.2E+0 8	1.3E+0 8	1.5E+0 8	1.6E+0 8	1.8E+0 8	2.0E+0 8	2.2E+08

Table S3. Statistical product branching ratios (%) from the initial adduct **ii** as functions of the collision energy E (in kJ mol⁻¹)

Product	0.0	5.0	10.0	15.0	20.0	25.0	30.0	35.0	40.0	45.0	50.0	55.0	60.0
1-meta-tolyl-vinylacetylene (p3) + H	0.0	0.0	0.0	0.1	0.1	0.1	0.2	0.2	0.3	0.3	0.4	0.5	0.6
1-methylnaphthalaene (p1) + H	63.0	63.7	64.4	64.9	65.4	65.8	66.2	66.2	66.5	66.8	67.0	67.3	67.5
2-methylnaphthalaene (p2) + H	37.0	36.2	35.6	35.0	34.5	34.0	33.6	33.6	33.2	32.8	32.5	32.2	31.9