**Supporting Information for**

**Mechanistical study on the formation of hydroxyacetone (CH3COCH2OH), methyl acetate (CH3COOCH3), and 3-hydroxypropanal (HCOCH2CH2OH) along with their enol tautomers (prop-1-ene-1,2-diol (CH3C(OH)CHOH), prop-2-ene-1,2-diol (CH2C(OH)CH2OH), 1-methoxyethen-1-ol (CH3OC(OH)CH2) and prop-1-ene-1,3-diol (HOCH2CHCHOH)) in interstellar ice analogs**

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**Table S1.** Error analysis of adiabatic ionization energies (IE) and relative energies (Erel) of distinct C3H6O2 isomers; IEs and Erel were computed at the CCSD(T)-F12/CC-pVTZ-F12//ωB97X-D/cc-pVTZ level of theory including the zero-point vibrational energy corrections. Their computed Cartesian coordinates and vibrational frequencies are shown in Table S2.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Name | Isomer | Structure | Erel  (kJ mol-1) | Experimental IE (eV) | Computed IE (eV) | IE difference to lower bound (eV) | IE difference to upper bound (eV) | IE range after error analysis (eV) | Corrected IE with electric field effect (eV) |
| Hydroxyacetone | **1a** |  | 39 |  | 9.60 |  |  | 9.52 – 9.68 | 9.49 – 9.65 |
| **1b** |  | 53 |  | 10.08 |  |  | 10.00 – 10.16 | 9.97 – 10.13 |
| Methyl acetate | **2a** |  | 0 | 10.25 ± 0.05 1 | 10.27 | −0.07 | 0.03 | 10.19 – 10.35 | 10.16 – 10.32 |
| **2b** |  | 31 |  | 9.41 |  |  | 9.33 – 9.49 | 9.30 – 9.46 |
| 3-hydroxypropanal | **3a** |  | 78 |  | 10.03 |  |  | 9.95 – 10.11 | 9.92 – 10.08 |
| **3b** |  | 68 | 9.90 ± 0.05 2 | 9.88 | −0.03 | 0.07 | 9.80 – 9.96 | 9.77 – 9.93 |
| **3c** |  | 82 |  | 10.11 |  |  | 10.03 – 10.19 | 10.00 – 10.16 |
| 2-methoxyacetaldehyde | **4a** |  | 131 |  | 9.47 |  |  | 9.39 – 9.55 | 9.36 – 9.52 |
| **4b** |  | 123 |  | 9.55 |  |  | 9.47 – 9.63 | 9.44 – 9.60 |
| **4c** |  | 127 |  | 9.51 |  |  | 9.43 – 9.59 | 9.40 – 9.56 |
| prop-1-ene-1,2-diol | **5a** |  | 102 |  | 7.81 |  |  | 7.73 – 7.89 | 7.70 – 7.86 |
| **5b** |  | 101 |  | 7.85 |  |  | 7.77 – 7.93 | 7.74 – 7.90 |
| prop-2-ene-1,2-diol | **6a** |  | 106 |  | 8.90 |  |  | 8.82 – 8.98 | 8.79 – 8.95 |
| **6b** |  | 101 |  | 8.86 |  |  | 8.78 – 8.94 | 8.75 – 8.91 |
| 1-methoxyethen-1-ol | **7a** |  | 123 |  | 8.13 |  |  | 8.05 – 8.21 | 8.02 – 8.18 |
| **7b** |  | 116 |  | 8.42 |  |  | 8.34 – 8.50 | 8.31 – 8.47 |
| prop-1-ene-1,3-diol | **8a** |  | 117 |  | 8.78 |  |  | 8.70 – 8.86 | 8.67 – 8.83 |
| **8b** |  | 120 |  | 8.89 |  |  | 8.81 – 8.97 | 8.78 – 8.94 |
| **8c** |  | 120 |  | 8.57 |  |  | 8.49 – 8.65 | 8.46 – 8.62 |
| 2-methoxyethen-1-ol | **9a** |  | 163 |  | 7.88 |  |  | 7.80 – 7.96 | 7.77 – 7.93 |
| **9b** |  | 165 |  | 8.01 |  |  | 7.93 – 8.09 | 7.90 – 8.06 |
| **9c** |  | 167 |  | 7.85 |  |  | 7.77 – 7.93 | 7.74 – 7.90 |
| **9d** |  | 163 |  | 8.03 |  |  | 7.95 – 8.11 | 7.92 – 8.08 |
|  |  |  |  |  |  | Average  -0.05 ± 0.03 | Average  +0.05 ± 0.03 |  |  |
|  |  |  |  |  |  | Combined error limits  -0.08 – +0.08 | |  |  |

**Table S2.** Cartesian coordinates (Å) and vibrational frequencies (cm−1) of neutral C3H6O2 molecules (shown in Figure 2) as well as their respective monocations computed at the ωB97X-D/cc-pVTZ theory level.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Isomer** | Vibration frequencies (cm−1) | | |  | Cartesian coordinates (Å) | |
|  |  |  | | | Atom X Y Z |
| **1a** | 94.4637 136.2090 301.0849  414.9140 424.9803 491.5268  630.5218 822.1221 871.1799  987.6416 1106.6050 1156.1980  1224.2324 1272.3170 1333.2071  1410.3897 1460.1763 1477.7245  1483.2724 1497.5457 1829.8264  3004.0753 3034.4374 3060.0203  3129.4864 3174.7052 3768.5339 | | |  | O 1.923732 -0.076789 -0.026575  C 0.721458 -0.771708 0.023641  C -0.471189 0.162776 0.010883  C -1.839411 -0.456274 -0.012366  O -0.287257 1.356272 0.009979  H 1.683742 0.858701 -0.014535  H 0.653540 -1.384281 0.932737  H 0.628527 -1.461188 -0.824740  H -2.595438 0.300574 0.175832  H -1.914576 -1.256596 0.724271  H -2.012740 -0.901834 -0.993751 | |
| **1a+** | 53.9942 132.0517 226.4620  257.5249 356.7191 410.0558  493.6897 563.7727 859.2452  904.9423 1028.2806 1051.6044  1155.3179 1214.7028 1320.7059  1376.5964 1406.1416 1442.6025  1459.6626 1522.9662 2034.1208  3058.8810 3067.8286 3149.1734  3181.8238 3192.6749 3804.2336 | | |  | O -1.947452 -0.047088 -0.266845  C -0.921590 -0.707354 0.211640  C 0.651734 0.272764 0.029237  C 1.813196 -0.649977 -0.082409  O 0.491557 1.416648 0.038882  H -2.351043 0.556575 0.369728  H -0.655547 -1.557770 -0.410840  H -0.849983 -0.843406 1.292361  H 2.721273 -0.082730 0.111606  H 1.819619 -1.041255 -1.102190  H 1.702798 -1.480494 0.612233 | |
| **1b** | 71.0699 143.9319 221.3558  267.2098 480.2743 505.0050  519.1578 773.6081 877.2936  990.2226 1102.9486 1125.6325  1207.4991 1264.3880 1280.5690  1399.5617 1439.7425 1466.3958  1466.5342 1499.6904 1839.7204  3021.4424 3065.9481 3068.4918  3137.9511 3178.9983 3926.8632 | | |  | O 1.753876 0.296593 0.053975  C 0.791856 -0.727232 -0.048334  H 2.625785 -0.090143 -0.010455  H 0.870344 -1.456973 0.763632  H 0.873898 -1.274503 -0.994524  C -0.618144 -0.158377 -0.000582  C -0.774528 1.335183 -0.017645  O -1.551234 -0.919755 0.034630  H -1.830671 1.587718 0.004608  H -0.299639 1.748524 -0.908279  H -0.255962 1.773232 0.835537 | |
| **1b+** | 61.0310 106.2159 224.7380  287.3063 383.9959 454.6613  519.0423 565.7702 877.7412  900.8322 1023.2735 1046.9213  1159.6282 1241.5619 1297.8170  1373.2427 1392.4877 1438.2443  1452.0603 1516.4891 1987.0285  3065.8483 3077.0634 3152.1547  3190.2786 3193.9398 3810.2911 | | |  | O -1.788749 0.325985 -0.132450  C -0.980262 -0.636973 0.282889  H -2.159875 0.152014 -1.006280  H -1.039975 -1.601158 -0.215041  H -0.903248 -0.669516 1.370540  C 0.732182 -0.158864 -0.002182  C 0.932409 1.314820 0.058144  O 1.427919 -1.072639 -0.164337  H 1.998822 1.523227 0.030677  H 0.464155 1.702703 0.961970  H 0.420779 1.752058 -0.800672 | |
| **2a** | 84.8082 151.1990 177.4381  288.5871 434.6598 622.0374  655.2598 878.4947 1007.3458  1081.5626 1105.1944 1182.3983  1214.5710 1305.5818 1418.9417  1477.9026 1486.7541 1492.1968  1494.3425 1497.4243 1845.7077  3071.1502 3078.5091 3148.6650  3151.9216 3180.2273 3189.3541 | | |  | C 1.860090 -0.161213 -0.006254  O 0.547129 -0.715181 0.010198  C -0.456774 0.174682 0.006867  C -1.790823 -0.515059 -0.002782  O -0.286395 1.363230 0.001015  H 2.018940 0.477765 0.860891  H 2.016756 0.426578 -0.909502  H 2.540557 -1.006914 0.016282  H -2.577049 0.219055 0.139636  H -1.830987 -1.274051 0.776117  H -1.929050 -1.017295 -0.960116 | |
| **2a+** | 88.2572 110.3716 189.1791  233.4367 352.9049 528.6926  608.8274 826.7270 940.8484  1001.9162 1020.7731 1170.9137  1210.7400 1280.1206 1399.4517  1427.2349 1454.2020 1475.2436  1479.0304 1499.4012 1617.4133  3047.6393 3087.4797 3139.2600  3171.7428 3193.1602 3233.4881 | | |  | C -1.932769 -0.103316 -0.000017  O -0.575083 -0.684959 0.000023  C 0.438317 0.067797 0.000018  C 1.820044 -0.494826 -0.000005  O 0.368580 1.322686 0.000006  H -2.053635 0.489671 -0.902691  H -2.053427 0.490352 0.902240  H -2.589612 -0.963320 0.000385  H 2.576366 0.286590 0.000853  H 1.909670 -1.110765 -0.897258  H 1.909107 -1.112277 0.896257 | |
| **2b** | 49.8617 146.0928 221.4032  329.1654 485.9250 584.2199  590.2017 810.0946 1009.6333  1067.7498 1133.8802 1183.4882  1200.2872 1298.7857 1407.2398  1472.1619 1485.0626 1496.4193  1504.6862 1520.2206 1870.3551  3049.1286 3074.7957 3120.7244  3143.7639 3168.6956 3189.5677 | | |  | C 1.803082 0.023083 -0.005105  O 0.616636 -0.751659 0.010023  C -0.599415 -0.167399 -0.000125  C -0.655968 1.340151 0.001290  O -1.571826 -0.863405 -0.004952  H 1.863199 0.692142 0.854313  H 1.893827 0.601598 -0.925742  H 2.621327 -0.689281 0.044275  H -1.698651 1.636698 -0.029966  H -0.133270 1.757275 -0.859220  H -0.191114 1.747073 0.899413 | |
| **2b+** | 75.1273 183.4823 200.9268  269.6716 390.8456 529.8808  574.3197 793.7364 955.1417  1018.3433 1025.2366 1172.8726  1183.4692 1313.8283 1399.2286  1439.9480 1460.6382 1478.4954  1494.9936 1505.3992 1649.0201  3047.1793 3092.6985 3136.8674  3167.2205 3202.1545 3227.4819 | | |  | C -1.865197 0.115971 0.000000  O -0.646508 -0.702722 0.000000  C 0.500294 -0.177867 0.000000  C 0.831458 1.278922 0.000000  O 1.515408 -0.923259 0.000000  H -1.886628 0.719358 -0.902805  H -1.886628 0.719358 0.902805  H -2.666488 -0.612348 0.000000  H 1.907083 1.440149 0.000000  H 0.391071 1.719587 0.896981  H 0.391071 1.719587 -0.896982 | |
| **3a** | 69.1359 169.3452 195.2418  265.4509 394.4626 671.5594  696.3177 885.6646 911.8908  1066.8267 1090.8967 1115.2822  1198.8613 1307.0138 1332.5754  1400.0761 1419.4270 1429.7300  1455.8101 1507.8797 1846.8219  2906.7044 3037.7362 3048.6470  3076.4800 3131.1557 3903.6093 | | |  | O 2.230064 -0.094728 -0.097205  C 0.869593 -0.460149 0.012061  C -0.050375 0.750511 -0.016508  C -1.512671 0.409349 -0.003805  O -1.950640 -0.708472 0.016000  H 2.500536 0.332452 0.715444  H 0.681647 -1.051631 0.912491  H 0.654127 -1.103530 -0.838949  H 0.147530 1.354883 -0.907302  H 0.140829 1.415393 0.833679  H -2.199348 1.279776 -0.016213 | |
| **3a+** | 58.6881 168.0469 197.1825  343.9818 388.2061 616.7882  716.4249 796.7869 853.1887  944.3064 1048.0166 1109.9059  1145.4510 1165.2397 1220.8938  1250.7024 1319.7252 1377.8238  1438.2230 1486.9940 1816.8818  2876.2797 2909.2011 3055.6709  3127.0200 3144.3591 3813.6356 | | |  | O 2.099424 -0.088082 -0.223341  C 0.841704 -0.433692 0.194557  C -0.029447 0.834049 -0.000927  C -1.484925 0.376448 0.041933  O -1.844260 -0.740423 -0.096365  H 2.750493 -0.126243 0.487253  H 0.799765 -0.793078 1.221576  H 0.411109 -1.195198 -0.481799  H 0.094773 1.264287 -1.001376  H 0.158779 1.620470 0.729525  H -2.220225 1.196974 0.189086 | |
| **3b** | 118.6755 167.0018 252.6354  405.1319 509.5012 638.0279  781.2550 855.1836 968.8091  976.0824 1101.0780 1129.0956  1229.3515 1261.1491 1392.6073  1407.5722 1429.1483 1430.5703  1450.3713 1522.8620 1838.6246  2924.2348 3026.7682 3047.0124  3086.1803 3113.1877 3856.1846 | | |  | O -1.473770 -0.774794 -0.348909  C -1.123471 0.363748 0.399124  H -0.762385 -1.409492 -0.232521  H -0.953163 0.111317 1.451655  H -1.975506 1.041642 0.358816  C 0.108117 1.065731 -0.155777  C 1.347517 0.219464 -0.115939  O 1.367669 -0.938919 0.210912  H 0.314848 1.995946 0.382781  H -0.052296 1.351743 -1.200691  H 2.284331 0.724889 -0.420507 | |
| **3b+** | 202.3424 236.2652 282.9530  432.6065 489.4112 622.0639  823.2014 874.0702 910.4074  934.9053 1033.9475 1094.3661  1177.0993 1211.3810 1246.7789  1280.9404 1322.5030 1411.2164  1436.2497 1480.7505 1727.3114  2991.3282 3026.7166 3049.4743  3128.9817 3144.9763 3806.2497 | | |  | O -1.086415 -0.850869 -0.299345  C -1.139871 0.429772 0.274930  H -1.419833 -1.532949 0.297544  H -1.235617 0.386382 1.358972  H -2.001143 0.962320 -0.145173  C 0.125385 1.156485 -0.155539  C 1.277304 0.206905 0.026730  O 1.130499 -0.981914 0.097378  H 0.295636 2.087747 0.382746  H 0.127882 1.391911 -1.226667  H 2.303494 0.607883 0.071593 | |
| **3c** | 51.3197 108.4122 258.4542  297.5555 409.3541 534.3087  791.6465 880.6215 982.9770  1086.5876 1094.5673 1126.6553  1202.1773 1275.3035 1327.3808  1406.6444 1434.0684 1440.2754  1467.6000 1515.9315 1855.8562  2894.1817 3029.6848 3061.4502  3093.8072 3129.1624 3900.1258 | | |  | O -2.318906 -0.079441 0.008134  C -1.031817 0.470163 0.168507  C 0.072040 -0.488164 -0.285793  H -2.413306 -0.818936 0.608961  H -0.853571 0.772573 1.205730  H -1.014958 1.374225 -0.441865  H -0.170384 -0.823223 -1.297776  H 0.132804 -1.354714 0.373021  C 1.408876 0.197549 -0.317135  O 2.335230 -0.076472 0.393894  H 1.494224 1.020088 -1.057764 | |
| **3c+** | 81.0826 120.1017 229.1921  364.8197 384.7461 451.1540  725.5454 833.0987 843.2946  926.8765 1048.8268 1099.2554  1159.3631 1208.1622 1234.7825  1252.7785 1372.5788 1387.6553  1449.5912 1508.8735 1819.3825  2947.7813 3051.9982 3064.1490  3133.2616 3176.3637 3827.4534 | | |  | O 2.231172 -0.192011 0.071859  C 1.080825 0.519171 -0.191637  C -0.058825 -0.458551 0.241824  H 2.590996 -0.603817 -0.721431  H 0.974017 0.815069 -1.234480  H 1.053566 1.396119 0.459651  H 0.069905 -0.755656 1.287688  H -0.126234 -1.339200 -0.391585  C -1.399239 0.314204 0.216255  O -2.339638 -0.192263 -0.283048  H -1.431093 1.312723 0.691012 | |
| **4a** | 73.1820 192.3983 199.9454  225.9139 379.6684 740.5766  740.7899 885.2256 1071.9594  1117.9250 1189.6411 1197.5402  1266.2870 1269.0145 1411.0242  1417.4533 1460.6093 1495.4526  1501.1341 1513.0545 1875.3866  2890.6938 2948.5780 2969.8026  2991.8437 3043.1358 3153.4251 | | |  | C 2.139134 -0.153757 0.000099  O 0.764340 -0.436900 -0.000294  C -0.018354 0.704660 0.000062  C -1.487963 0.377762 -0.000070  O -1.956898 -0.721179 0.000126  H 2.432394 0.415493 0.890562  H 2.432770 0.416215 -0.889776  H 2.664286 -1.105635 -0.000176  H 0.172568 1.341718 -0.880232  H 0.172480 1.341196 0.880773  H -2.130940 1.283657 -0.000359 | |
| **4a+** | 140.0509 150.9182 198.6729  321.6099 419.9067 528.5268  585.4359 794.4346 929.4614  1018.3422 1073.4145 1146.6190  1183.1428 1254.7707 1293.6732  1329.9494 1437.7435 1450.3564  1476.4894 1507.3591 1938.9873  2954.6264 2974.1263 3008.2483  3107.9171 3160.9494 3200.7860 | | |  | C 1.551395 -0.696351 0.168239  O 0.997558 0.463785 -0.432852  C -0.017436 1.067843 0.174136  C -1.414632 0.168566 0.023983  O -1.401115 -0.991622 -0.082719  H 0.848038 -1.524143 -0.018040  H 1.681667 -0.557842 1.241536  H 2.489271 -0.895953 -0.338714  H -0.243685 2.018734 -0.304098  H 0.042671 1.123076 1.269924  H -2.305470 0.818471 0.075805 | |
| **4b** | 72.8997 97.0171 218.5364  224.1303 436.6979 533.8941  748.9404 1020.2769 1063.6042  1121.0318 1192.0707 1195.3313  1251.1494 1260.2454 1368.0402  1420.0753 1475.6902 1496.2055  1498.0770 1517.7063 1862.1869  2932.5434 2982.3739 2996.1370  3017.2028 3049.1603 3147.1058 | | |  | C -2.257104 -0.116179 0.000001  O -0.996986 0.502197 -0.000001  C 0.058161 -0.412299 -0.000001  H -2.395393 -0.741779 0.889620  H -2.395394 -0.741782 -0.889617  H -3.006971 0.671201 0.000000  H 0.037408 -1.064230 -0.884458  H 0.037408 -1.064230 0.884457  C 1.361651 0.350321 0.000000  O 2.434362 -0.182459 0.000000  H 1.247688 1.451853 0.000001 | |
| **4b+** | 140.0407 150.9074 198.6319  321.6099 419.9047 528.5118  585.4278 794.4392 929.4557  1018.3402 1073.4111 1146.6159  1183.1376 1254.7683 1293.6730  1329.9469 1437.7443 1450.3458  1476.4891 1507.3602 1938.9900  2954.6253 2974.1294 3008.2524  3107.9150 3160.9507 3200.7909 | | |  | C -1.551400 0.696351 -0.168232  O -0.997554 -0.463785 0.432856  C 0.017431 -1.067841 -0.174147  H -1.681764 0.557799 -1.241513  H -0.847999 1.524126 0.017952  H -2.489230 0.896001 0.338785  H -0.042678 -1.123053 -1.269935  H 0.243679 -2.018742 0.304070  C 1.414638 -0.168567 -0.023974  O 1.401117 0.991622 0.082709  H 2.305476 -0.818475 -0.075758 | |
| **4c** | 139.8263 181.8839 208.7365  275.7590 409.2846 715.0985  781.1193 844.3143 1006.8608  1112.4478 1194.5975 1206.6082  1257.9213 1325.7732 1396.9984  1413.7874 1452.7267 1491.7178  1510.8111 1520.8226 1864.7329  2875.9706 2960.7834 3006.8149  3066.0016 3095.2346 3157.3026 | | |  | C -1.610794 -0.619923 0.259395  O -0.985246 0.364378 -0.534378  C 0.082888 0.992796 0.084364  C 1.356904 0.183164 0.180087  O 1.489802 -0.948708 -0.186523  H -2.000509 -0.182749 1.186771  H -0.929356 -1.437211 0.502814  H -2.442745 -1.011392 -0.320683  H -0.161097 1.331667 1.105576  H 0.321695 1.895101 -0.487630  H 2.201589 0.743002 0.637286 | |
| **4c+** | 140.0410 150.9076 198.6337  321.6098 419.9047 528.5104  585.4273 794.4392 929.4554  1018.3400 1073.4115 1146.6161  1183.1376 1254.7680 1293.6731  1329.9470 1437.7446 1450.3466  1476.4892 1507.3603 1938.9906  2954.6262 2974.1295 3008.2527  3107.9151 3160.9506 3200.7908 | | |  | C -1.551401 -0.696351 0.168232  O -0.997554 0.463785 -0.432856  C 0.017431 1.067841 0.174147  C 1.414638 0.168567 0.023974  O 1.401118 -0.991622 -0.082708  H -1.681765 -0.557799 1.241513  H -0.848001 -1.524127 -0.017952  H -2.489231 -0.896000 -0.338785  H -0.042678 1.123052 1.269936  H 0.243679 2.018742 -0.304070  H 2.305476 0.818476 0.075757 | |
| **5a** | 143.8182 180.6507 227.3979  267.8834 326.6453 429.9584  461.6546 602.2858 835.8788  847.9006 1022.2487 1067.2558  1153.9428 1215.7779 1267.8192  1334.4367 1395.9248 1442.3518  1486.6675 1494.8503 1829.3201  3036.2911 3094.5663 3169.1391  3192.5049 3905.5716 3924.3180 | | |  | C 0.786869 -0.636227 0.023685  C -0.426720 -0.100579 0.016777  C -0.719227 1.360918 0.005531  O -1.503660 -0.951641 -0.054084  O 1.914659 0.143537 -0.073406  H 0.918178 -1.711599 0.025521  H -1.215898 1.647494 -0.923969  H 0.198189 1.934946 0.102458  H -1.382970 1.627770 0.833704  H -2.273572 -0.501805 0.293618  H 2.622544 -0.276650 0.412633 | |
| **5a+** | 62.6447 236.5430 275.0202  454.8116 462.9097 590.2355  602.9597 621.8014 844.6352  904.7267 1034.5995 1037.2931  1163.5127 1245.3273 1347.7542  1405.0949 1438.4250 1474.3604  1494.6164 1506.4500 1707.2744  3048.6179 3113.6800 3188.8438  3199.4991 3797.9464 3811.6156 | | |  | C -0.843999 -0.614987 0.000000  C 0.459337 -0.093262 0.000000  C 0.790667 1.345393 0.000000  O 1.385255 -1.009353 0.000000  O -1.845789 0.211030 0.000000  H -1.005362 -1.687403 0.000000  H 1.389200 1.582035 0.883235  H -0.101217 1.963462 0.000003  H 1.389195 1.582036 -0.883238  H 2.279047 -0.642313 0.000000  H -2.702622 -0.234091 0.000000 | |
| **5b** | 31.1694 175.7496 189.5341  250.4499 294.4122 404.7745  570.6562 613.1712 773.3806  892.1996 1022.5178 1072.0251  1171.4978 1217.8243 1260.8758  1366.4931 1409.4060 1436.6023  1475.0052 1500.6099 1843.5779  3024.3968 3075.5382 3148.6917  3212.6553 3924.8840 3946.0157 | | |  | C -0.766422 -0.628937 -0.000631  C 0.402164 0.002236 -0.001691  C 1.714012 -0.707937 0.000856  O 0.436054 1.369596 -0.001371  O -1.955943 0.045180 0.007818  H -0.797643 -1.709867 0.001408  H 2.304095 -0.439324 -0.880166  H 1.577418 -1.787257 -0.002433  H 2.298361 -0.444405 0.887224  H 1.348024 1.657407 -0.004234  H -2.669665 -0.586936 -0.044572 | |
| **5b+** | 106.7504 213.4116 274.5017  415.4064 489.0560 603.6277  614.1362 641.3666 881.0570  905.3805 1028.7800 1037.9820  1162.8592 1253.9394 1354.4376  1393.8587 1411.5868 1469.4024  1483.7036 1540.5250 1713.5196  3046.1218 3111.5043 3175.8085  3212.0761 3796.2144 3810.4236 | | |  | C -0.791719 -0.657066 0.000000  C 0.436223 0.029781 0.000000  C 1.737480 -0.670860 0.000000  O 0.359060 1.325245 0.000000  O -1.891903 0.026336 0.000000  H -0.812542 -1.739949 0.000000  H 2.312622 -0.380726 -0.882915  H 1.616985 -1.750300 -0.000001  H 2.312621 -0.380727 0.882916  H 1.224338 1.755177 0.000000  H -2.683188 -0.527252 0.000000 | |
| **6a** | 97.0146 254.7402 311.6938  430.6451 435.3465 492.2096  669.4799 734.0767 842.5031  887.4645 991.3490 1007.2916  1101.4758 1202.7813 1232.1521  1368.0982 1399.3536 1438.9509  1468.5478 1518.7153 1741.2167  3047.0658 3114.8691 3168.2845  3267.8699 3884.0951 3894.2515 | | |  | O -1.827862 -0.079110 -0.390591  C -0.855047 0.368466 0.528999  C 0.546836 0.037964 0.104533  C 1.459835 0.958464 -0.191664  O 0.752353 -1.299912 0.052455  H -1.631617 0.310923 -1.243322  H -1.072473 -0.142313 1.467456  H -0.927195 1.446025 0.702145  H 2.467542 0.695107 -0.487785  H 1.215361 2.007142 -0.126564  H 1.642715 -1.474077 -0.258053 | |
| **6a+** | 123.7252 259.8412 265.4658  394.8745 419.5021 470.7771  604.9479 684.4994 842.3477  866.3429 964.3778 1017.2253  1169.1192 1204.8010 1226.0635  1251.7649 1379.6503 1423.1509  1484.5694 1555.5295 1580.8500  2940.4189 2957.5051 3165.3781  3283.0024 3759.4114 3889.7554 | | |  | O 1.810552 0.165359 -0.000127  C 0.760578 -0.716649 -0.000006  C -0.529577 0.011537 0.000042  C -1.752285 -0.690086 -0.000023  O -0.461735 1.291308 0.000074  H 2.647317 -0.304322 0.000455  H 0.731686 -1.387831 0.877383  H 0.731562 -1.387659 -0.877512  H -2.701680 -0.169993 -0.000786  H -1.750629 -1.771102 0.000609  H -1.321087 1.738757 0.000191 | |
| **6b** | 131.6878 283.1143 319.2329  417.7636 456.6699 511.2188  552.3192 747.0573 841.0009  883.0383 986.7304 1015.4857  1128.5875 1194.6617 1228.7025  1353.7263 1398.3076 1436.8108  1462.7407 1511.5856 1747.7709  3024.0963 3101.9883 3176.6993  3280.9698 3888.9680 3890.7619 | | |  | O 1.911331 0.087144 -0.008553  C 0.760297 -0.710475 -0.083557  C -0.531122 0.058999 -0.021618  C -0.632036 1.381683 -0.041594  O -1.574886 -0.805515 0.064033  H 1.916893 0.525522 0.843434  H 0.734501 -1.473489 0.703193  H 0.806334 -1.240562 -1.036149  H -1.589992 1.880884 0.020545  H 0.254608 1.985369 -0.150469  H -2.396743 -0.311991 0.056216 | |
| **6b+** | 90.3883 222.1437 293.2617  353.8600 474.9293 501.7447  535.3016 657.9967 838.8289  893.9896 992.7164 1007.9638  1153.8361 1190.3632 1235.9273  1262.7409 1418.5356 1442.1187  1471.4192 1542.1685 1579.9951  2986.9843 3020.1197 3164.0211  3291.3452 3762.7833 3903.9067 | | |  | O -1.791463 0.223629 0.000023  C -0.777800 -0.723244 -0.000001  C 0.530312 -0.015786 -0.000003  C 0.634205 1.392388 -0.000005  O 1.560933 -0.785520 0.000002  H -2.650214 -0.202405 -0.000113  H -0.782147 -1.380777 -0.881590  H -0.782136 -1.380804 0.881568  H 1.600187 1.882301 -0.000001  H -0.273242 1.978836 -0.000009  H 2.411492 -0.322173 0.000000 | |
| **7a** | 60.4569 164.9025 313.1222  353.8027 460.8909 597.5912  683.3247 689.3536 762.7790  882.3683 968.0916 1139.2577  1184.5805 1190.2841 1241.1128  1392.2744 1445.7690 1493.6536  1511.4721 1517.8162 1750.7594  3051.5714 3130.5640 3168.5730  3198.3411 3298.6812 3911.3731 | | |  | C -1.809941 -0.078727 0.164978  O -0.605615 -0.694121 -0.270248  C 0.542888 -0.042894 -0.051542  C 1.695356 -0.684974 0.122648  O 0.386780 1.301956 -0.071417  H -2.016212 0.835882 -0.388606  H -1.770055 0.145487 1.232646  H -2.593290 -0.807209 -0.023204  H 2.626698 -0.145277 0.198964  H 1.706525 -1.761167 0.155627  H 1.227189 1.709175 0.141386 | |
| **7a+** | 128.2496 193.3851 277.8373  362.2752 429.6274 563.6709  627.9115 678.2364 833.9955  869.6061 1000.7210 1068.3834  1171.7281 1175.8053 1236.2728  1457.8979 1460.4379 1477.7032  1495.2918 1549.9620 1653.8264  3090.2840 3182.5614 3192.6856  3231.2139 3308.3108 3814.6472 | | |  | C -1.873737 -0.095055 0.000005  O -0.548835 -0.712274 -0.000005  C 0.504696 -0.000723 -0.000002  C 1.757441 -0.670043 0.000003  O 0.366030 1.287248 -0.000002  H -1.980225 0.509220 -0.896764  H -1.980107 0.509477 0.896614  H -2.559482 -0.932303 0.000162  H 2.682962 -0.112926 0.000004  H 1.767383 -1.749327 0.000005  H 1.201500 1.771000 0.000003 | |
| **7b** | 130.8340 219.8431 342.5042  349.3954 502.2975 576.4462  669.0707 691.2296 737.8298  913.7090 992.4845 1140.9392  1189.0510 1232.1175 1247.0948  1426.6203 1454.0049 1500.9595  1501.1763 1521.8420 1727.2126  3037.0166 3104.0485 3173.6287  3204.4777 3296.8309 3917.3321 | | |  | C 1.845017 -0.029622 0.000005  O 0.609716 -0.709914 -0.000005  H 1.948760 0.592733 0.891708  H 1.948386 0.593293 -0.891353  H 2.612474 -0.797634 -0.000451  C -0.497789 0.033825 0.000030  C -0.582174 1.367502 -0.000056  O -1.545928 -0.810931 0.000017  H -1.549114 1.846415 0.000048  H 0.291066 1.995700 0.000176  H -2.352197 -0.293975 -0.000104 | |
| **7b+** | 161.8218 170.2566 301.3365  312.1209 483.5010 544.6361  569.2381 650.4236 823.0167  869.6860 1012.4465 1076.6247  1176.5890 1197.2247 1238.3917  1451.7482 1474.0295 1498.5841  1511.9919 1552.2176 1655.8664  3085.4687 3185.3558 3189.2281  3222.4017 3305.5043 3824.8116 | | |  | C 1.895672 -0.017827 -0.000020  O 0.595234 -0.670789 -0.000087  H 2.000589 0.578101 0.902934  H 2.000575 0.578314 -0.902835  H 2.605810 -0.835166 -0.000122  C -0.503598 -0.032669 0.000001  C -0.622933 1.389875 0.000172  O -1.532164 -0.814033 -0.000082  H -1.600878 1.849416 0.000240  H 0.252051 2.020479 0.000235  H -2.377548 -0.348851 -0.000018 | |
| **8a** | 64.6582 237.6108 244.3931  300.5175 351.5775 554.3538  669.5933 780.6919 939.7753  976.6085 1033.6934 1076.3135  1137.0712 1214.2796 1279.0394  1306.9926 1377.0872 1415.6436  1464.8527 1519.0809 1775.9709  3053.3193 3101.7066 3177.1025  3214.8937 3896.6861 3942.7437 | | |  | O 2.120370 -0.210038 -0.379408  C 1.014105 -0.223865 0.510903  C -0.018710 0.792878 0.141324  C -1.292170 0.528943 -0.118421  O -1.818044 -0.723399 -0.038475  H 1.778399 -0.335290 -1.265173  H 1.434428 0.001752 1.491870  H 0.563341 -1.218037 0.566851  H 0.304794 1.821691 0.055878  H -1.984750 1.314501 -0.400362  H -2.734166 -0.704859 -0.308833 | |
| **8a+** | 87.8981 198.4431 287.7799  318.2963 401.7578 576.1844  645.9103 686.6192 924.1631  995.3877 1018.0033 1140.2462  1183.9055 1227.4894 1231.5608  1277.8782 1353.4716 1378.4272  1408.8966 1534.3609 1654.3537  2901.8621 2904.5694 3187.6537  3210.6474 3782.0523 3894.2415 | | |  | O 2.239607 0.056599 -0.000067  C 0.945912 -0.418442 0.000046  C 0.005850 0.698910 0.000023  C -1.381511 0.548422 0.000003  O -1.890679 -0.638114 -0.000025  H 2.867567 -0.668447 0.000078  H 0.709110 -1.062302 0.870586  H 0.709015 -1.062459 -0.870349  H 0.400528 1.708270 0.000021  H -2.041070 1.410494 0.000010  H -2.858082 -0.646773 -0.000042 | |
| **8b** | 98.7854 200.6151 205.7684  300.5409 330.0333 456.8743  579.0849 858.5369 962.8745  966.9740 1036.1007 1108.0939  1184.2016 1206.6897 1264.0211  1358.0496 1379.3347 1385.8284  1438.4124 1528.3686 1784.4047  3011.3410 3098.1864 3158.8987  3178.3046 3901.3130 3933.3531 | | |  | C 0.064225 -0.198441 0.442904  C 1.136445 0.303815 -0.150163  O 2.359811 -0.276238 -0.065085  C -1.283263 0.438744 0.334809  O -2.186204 -0.275873 -0.497681  H 0.160046 -1.116270 1.013304  H 1.079522 1.219425 -0.732063  H 2.993191 0.233763 -0.567208  H -1.193876 1.429412 -0.112043  H -1.718438 0.570500 1.332336  H -2.213738 -1.184654 -0.197496 | |
| **8b+** | 68.3266 153.0461 291.3394  356.3396 407.0350 553.3973  642.4269 864.4920 939.3832  999.2784 1032.7281 1080.6450  1176.4599 1191.5819 1334.9815  1362.7272 1367.4024 1391.1035  1403.7749 1524.1482 1657.7419  3112.2048 3175.6538 3176.5481  3203.6335 3781.7175 3838.4633 | | |  | C -0.005506 0.585126 0.272423  C 1.038934 -0.099973 -0.343469  O 2.199317 -0.104258 0.215515  C -1.377861 0.529150 -0.302900  O -1.738697 -0.772288 0.142857  H 0.171189 1.021730 1.248711  H 0.898333 -0.622701 -1.286102  H 2.873672 -0.580457 -0.289368  H -1.396369 0.527371 -1.389671  H -2.030091 1.312688 0.073396  H -2.135090 -0.732088 1.019739 | |
| **8c** | 120.6660 198.5723 217.0376  256.3596 304.1060 424.6977  659.2196 817.8103 939.4492  959.2825 1058.7264 1136.1233  1178.2541 1197.9462 1255.7937  1279.0773 1345.9956 1375.1882  1474.7746 1532.7600 1795.6396  2987.8410 3008.4112 3196.1734  3197.9619 3929.9157 3937.9806 | | |  | C 0.092691 0.741371 0.000254  C 0.947079 -0.267684 -0.000052  O 2.294990 -0.071354 -0.000352  H 0.466241 1.758090 0.000629  H 0.602583 -1.294595 -0.000428  H 2.735141 -0.919214 0.002154  C -1.390235 0.567355 -0.000107  O -1.720133 -0.807622 0.000040  H -1.813734 1.065536 -0.882273  H -1.814131 1.065752 0.881736  H -2.672164 -0.890011 0.000104 | |
| **8c+** | 174.7030 203.9833 216.5708  293.2733 433.7589 640.8905  654.5660 741.2238 930.3489  943.3505 1017.2778 1156.8861  1202.7036 1228.7662 1230.3402  1333.8118 1377.2159 1378.0832  1399.5251 1482.1213 1672.1978  2929.5477 2941.6854 3198.3115  3209.9440 3775.3071 3902.4504 | | |  | C -0.068722 0.756061 0.000000  C -0.968312 -0.312651 0.000000  O -2.229864 -0.051217 0.000000  H -0.458565 1.767161 0.000000  H -0.619762 -1.340748 0.000000  H -2.788285 -0.842082 0.000000  C 1.376600 0.550686 0.000000  O 1.684512 -0.800102 0.000000  H 1.779132 1.097548 0.872763  H 1.779132 1.097548 -0.872762  H 2.633763 -0.933450 0.000000 | |
| **9a** | 50.0062 175.8441 189.8915  214.1431 376.4038 556.6746  732.1704 743.7586 873.0733  1001.2402 1117.8894 1177.8169  1187.9572 1238.8081 1286.9462  1338.4199 1436.0783 1497.2379  1499.6333 1520.2127 1810.4127  3011.2833 3070.3305 3148.1341  3179.2381 3213.1960 3944.5756 | | |  | C -2.171098 -0.162403 0.156993  O -0.845968 -0.386732 -0.260644  C -0.015263 0.670651 -0.082876  C 1.298515 0.538796 0.043894  O 1.920051 -0.672804 0.050845  H -2.607141 0.706356 -0.348312  H -2.229124 -0.007691 1.238564  H -2.742557 -1.048659 -0.107580  H -0.459906 1.659653 -0.087873  H 1.912119 1.426081 0.126883  H 2.861023 -0.541712 0.148651 | |
| **9a+** | 65.2727 162.1638 202.3358  368.7642 397.6631 604.2091  723.5442 857.9728 957.1083  973.1150 1103.3521 1175.4129  1190.0437 1262.0083 1322.4065  1408.7952 1465.2460 1472.6056  1504.6209 1576.5713 1706.7606  3081.4958 3179.8175 3192.8684  3200.1762 3209.3347 3808.5580 | | |  | C -2.227389 -0.179008 0.000046  O -0.785311 -0.332575 -0.000086  C -0.021602 0.692132 -0.000016  C 1.366174 0.519246 0.000012  O 1.856802 -0.678965 0.000015  H -2.496881 0.874623 -0.000892  H -2.588494 -0.680710 0.892612  H -2.588769 -0.682326 -0.891492  H -0.439903 1.694012 0.000010  H 2.016686 1.385877 0.000032  H 2.822335 -0.693368 0.000040 | |
| **9b** | 67.4699 166.4594 232.5707  288.5221 360.5425 543.3503  754.4810 817.4407 912.6913  929.1195 1059.3113 1186.2776  1200.1250 1239.1480 1282.9224  1377.6573 1439.0930 1498.0464  1503.7580 1520.6406 1794.3464  3044.4461 3120.0321 3152.1352  3189.7580 3224.6146 3934.4915 | | |  | C -1.423719 -0.848368 0.058886  O -1.245060 0.548306 -0.085688  C 0.001181 1.055534 0.016866  C 1.195272 0.469668 0.038817  O 1.431228 -0.875880 -0.093145  H -1.031109 -1.195787 1.016231  H -0.936502 -1.400761 -0.744207  H -2.497173 -1.017409 0.022888  H -0.021723 2.134881 0.067154  H 2.063093 1.111120 0.122829  H 2.297667 -1.072451 0.258360 | |
| **9b+** | 143.9061 157.4608 237.5777  354.0160 431.6083 596.4565  814.4140 845.7470 861.2983  959.2039 1058.7612 1168.5557  1204.0945 1270.8714 1330.4869  1431.8143 1468.2154 1475.9352  1500.9379 1572.5838 1702.0557  3089.9462 3193.2349 3197.0161  3212.3013 3224.2530 3801.3968 | | |  | C -1.485951 -0.824430 0.000000  O -1.155968 0.592310 0.000000  C 0.027188 1.071695 0.000000  C 1.257944 0.402752 0.000000  O 1.340028 -0.895403 0.000000  H -1.083251 -1.285191 0.897602  H -1.083254 -1.285190 -0.897604  H -2.568409 -0.848417 0.000002  H 0.053922 2.155413 0.000000  H 2.161348 1.001835 0.000000  H 2.252073 -1.213804 0.000000 | |
| **9c** | 86.1553 169.0090 212.6304  219.6140 359.9220 471.4661  553.4236 856.0451 932.7003  1041.8701 1149.4549 1194.6210  1200.4469 1226.1220 1281.5921  1329.0999 1372.8676 1489.2020  1498.4577 1525.8524 1800.2841  3009.7838 3068.8273 3151.4031  3153.6993 3185.2009 3937.3289 | | |  | C 0.027006 0.236792 -0.210932  C 1.168054 -0.365514 0.085541  O 2.357785 0.303191 0.021412  O -1.135632 -0.469309 -0.295471  C -2.248268 0.211090 0.238772  H -0.018020 1.295499 -0.452298  H 1.192255 -1.421502 0.329006  H 3.015733 -0.183397 0.514468  H -3.122294 -0.409463 0.056135  H -2.390847 1.181030 -0.250080  H -2.134804 0.372573 1.314957 | |
| **9c+** | 54.2542 180.2918 215.4140  269.4268 481.4148 525.8216  580.9191 917.1009 946.6657  966.2953 1151.6461 1174.8548  1196.9368 1311.2369 1345.8320  1372.1494 1444.2870 1472.9147  1504.3437 1534.7018 1717.4482  3082.0299 3170.3148 3193.5363  3197.0230 3199.7146 3811.4535 | | |  | C 0.016255 0.263763 -0.000016  C 1.244766 -0.395244 0.000015  O 2.318683 0.333520 0.000002  O -1.049063 -0.448150 -0.000029  C -2.355754 0.182283 0.000021  H -0.037251 1.349580 -0.000053  H 1.301182 -1.478618 0.000040  H 3.131936 -0.186879 0.000019  H -2.865165 -0.167646 -0.892666  H -2.253511 1.264847 0.000934  H -2.865754 -0.169058 0.891818 | |
| **9d** | 163.3422 203.9319 251.6385  260.8815 367.3497 413.1497  645.9309 815.2189 937.5617  999.4135 1169.8382 1185.0474  1190.5504 1247.3297 1302.6965  1334.3529 1364.3270 1489.2160  1493.9941 1514.1261 1768.7035  3008.5542 3066.6272 3159.4579  3188.4032 3225.1520 3907.7703 | | |  | C 0.066766 0.701850 0.026399  C 0.907750 -0.326883 0.001720  O 2.260378 -0.091303 -0.078650  H 0.443565 1.715191 0.044431  H 0.591165 -1.362084 -0.026990  H 2.718906 -0.717172 0.480954  O -1.283897 0.663888 0.004488  C -1.878493 -0.609393 -0.007152  H -2.953588 -0.452864 -0.019957  H -1.605259 -1.181514 0.885552  H -1.582782 -1.175675 -0.896491 | |
| **9d+** | 156.0063 203.3837 236.1437  352.6513 405.6514 578.2037  641.2670 891.9435 902.9284  948.1335 1152.6050 1173.0608  1207.7132 1316.0803 1357.5723  1382.4285 1440.2260 1480.2294  1509.9126 1534.1636 1712.7371  3074.6381 3172.8022 3198.3558  3207.6011 3219.0740 3809.6831 | | |  | C 0.062502 0.724332 0.000000  C 0.943711 -0.362581 0.000000  O 2.211198 -0.074598 0.000000  H 0.460164 1.733858 0.000000  H 0.621168 -1.396962 0.000001  H 2.782748 -0.853070 0.000000  O -1.213860 0.655950 0.000000  C -1.925824 -0.607214 0.000000  H -2.974621 -0.337864 0.000000  H -1.675246 -1.162001 0.902037  H -1.675246 -1.162000 -0.902038 | |

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