

**ESI Table 1.** Cartesian coordinates of phenyl  $\beta$ -D-galactopyranoside conformers at the B3LYP/6-31+G(d) level of theory.

**ESI Table 1A**


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**tttG+g-** SCF energy: -918.245957  
 $\Omega_{\text{phe}} = 106.6^\circ$

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|   | Coordinates (Å) |           |           |
|---|-----------------|-----------|-----------|
|   | X               | Y         | Z         |
| C | -0.427304       | -0.085734 | -1.966444 |
| C | -0.444562       | -0.076202 | -0.437099 |
| O | 0.882557        | -0.036332 | 0.051737  |
| C | 1.661265        | -1.187169 | -0.319769 |
| C | 1.760575        | -1.340591 | -1.843449 |
| C | 0.355078        | -1.300142 | -2.460550 |
| O | -1.115042       | 1.091352  | -0.036308 |
| C | -1.499202       | 1.169086  | 1.302004  |
| C | -2.610900       | 0.456394  | 1.756101  |
| C | -3.012618       | 0.591595  | 3.088128  |
| C | -2.314075       | 1.439586  | 3.952752  |
| C | -1.208559       | 2.154813  | 3.481587  |
| C | -0.794624       | 2.020500  | 2.153585  |
| C | 3.008599        | -1.021757 | 0.376312  |
| O | 2.861276        | -1.016698 | 1.791504  |
| H | 2.205616        | -2.325758 | -2.059010 |
| O | 0.514670        | -1.275015 | -3.877027 |
| O | -1.737651       | -0.187233 | -2.520864 |
| H | -0.351740       | -1.073399 | -4.269096 |
| H | 2.244365        | -0.300285 | 2.014775  |
| H | -0.190468       | -2.210355 | -2.164744 |
| O | 2.581052        | -0.310981 | -2.376398 |
| H | 1.168829        | -2.089413 | 0.080828  |
| H | 3.654545        | -1.871456 | 0.136000  |
| H | -2.234943       | 0.606675  | -2.265048 |
| H | -0.961695       | -0.967021 | -0.040713 |
| H | 0.068007        | 0.834819  | -2.300826 |
| H | 3.491826        | -0.104065 | 0.020215  |
| H | 0.060942        | 2.565168  | 1.766587  |
| H | -0.663765       | 2.817765  | 4.148779  |
| H | -2.631982       | 1.545576  | 4.986391  |
| H | -3.878180       | 0.040029  | 3.445948  |
| H | -3.157852       | -0.185594 | 1.070718  |
| H | 2.441026        | -0.310666 | -3.339351 |

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**ESI Table 1B****tffTg+** SCF energy: -918.244931 $\Omega_{\text{phe}} = 96.1^\circ$ 

|   | Coordinates (Å) |           |           |
|---|-----------------|-----------|-----------|
|   | X               | Y         | Z         |
| O | 0.111900        | -0.019462 | -0.844394 |
| C | 0.113485        | -0.021667 | 0.569629  |
| C | 1.557604        | -0.022921 | 1.072155  |
| C | 2.256358        | 1.237397  | 0.573889  |
| C | 2.148157        | 1.380351  | -0.949229 |
| C | 0.702305        | 1.153619  | -1.420543 |
| O | -0.489354       | -1.203948 | 1.030681  |
| C | -1.881866       | -1.263239 | 0.969066  |
| C | -2.637793       | -0.761092 | 2.030010  |
| C | -4.030756       | -0.873330 | 1.992094  |
| C | -4.657460       | -1.487741 | 0.903854  |
| C | -3.887004       | -1.990577 | -0.149628 |
| C | -2.494276       | -1.879845 | -0.122622 |
| O | 1.640845        | -0.002552 | 2.495554  |
| O | 3.645505        | 1.231538  | 0.898864  |
| O | 3.007601        | 0.458356  | -1.618208 |
| C | 0.607433        | 0.949097  | -2.942790 |
| O | 1.386400        | 1.891104  | -3.667526 |
| H | -0.440207       | 0.855001  | 0.949251  |
| H | 2.053389        | -0.913980 | 0.665158  |
| H | 1.222704        | -0.812260 | 2.831316  |
| H | 1.770708        | 2.107260  | 1.043774  |
| H | 0.116209        | 2.038672  | -1.122117 |
| H | 3.729368        | 0.974794  | 1.832692  |
| H | 2.433507        | 2.407413  | -1.218718 |
| H | 0.910863        | -0.079895 | -3.167246 |
| H | -0.428964       | 1.082573  | -3.263743 |
| H | 2.315263        | 1.617918  | -3.581834 |
| H | 3.848913        | 0.451534  | -1.128429 |
| H | -1.877573       | -2.259716 | -0.930461 |
| H | -4.370081       | -2.470298 | -0.996969 |
| H | -5.740167       | -1.577262 | 0.878358  |
| H | -4.623658       | -0.486347 | 2.816851  |
| H | -2.135425       | -0.297326 | 2.874775  |

**ESI Table 1C****tttG-g-** SCF energy: -918.244931 $\Omega_{\text{phe}} = 83.9^\circ$ 

|   | Coordinates (Å) |           |           |
|---|-----------------|-----------|-----------|
|   | X               | Y         | Z         |
| C | -2.349294       | 1.195474  | -0.933485 |
| C | -2.390224       | 1.156838  | 0.599156  |
| C | -0.982220       | 1.143006  | 1.185485  |
| C | -0.191021       | -0.012371 | 0.569411  |
| O | -0.119446       | 0.158490  | -0.832753 |
| C | -1.395246       | 0.115316  | -1.474829 |
| O | 1.102184        | 0.038713  | 1.114185  |
| O | -1.127687       | 1.015788  | 2.598017  |
| O | -3.127402       | 2.299971  | 1.028846  |
| C | -1.174849       | 0.186921  | -2.990951 |
| O | -0.461975       | 1.320958  | -3.439999 |
| O | -1.931461       | 2.482319  | -1.389056 |
| H | -0.657300       | -0.985830 | 0.806188  |
| H | -0.462054       | 2.075337  | 0.929716  |
| C | 1.912982        | -1.080553 | 0.919243  |
| H | -0.239952       | 1.032443  | 2.991597  |
| H | -2.909466       | 0.239683  | 0.918697  |
| H | -1.874020       | -0.859405 | -1.265950 |
| H | -3.002078       | 2.389290  | 1.988827  |
| H | -3.359411       | 0.983689  | -1.317233 |
| H | -0.590587       | -0.685924 | -3.298300 |
| H | -2.165660       | 0.116276  | -3.472483 |
| H | -0.829058       | 2.101798  | -2.988733 |
| H | -2.398602       | 3.144159  | -0.848996 |
| C | 2.637123        | -1.223349 | -0.266175 |
| C | 3.486510        | -2.323265 | -0.413336 |
| C | 3.613097        | -3.265102 | 0.613107  |
| C | 2.885845        | -3.106139 | 1.796303  |
| C | 2.031787        | -2.010494 | 1.953444  |
| H | 2.525860        | -0.481761 | -1.049797 |
| H | 4.053394        | -2.441293 | -1.333259 |
| H | 4.278181        | -4.116121 | 0.492678  |
| H | 2.983698        | -3.831422 | 2.600007  |
| H | 1.464249        | -1.867081 | 2.868944  |

**ESI Table 1D****gggG-g+** SCF energy: -918.245541 $\Omega_{\text{phe}} = 114.9^\circ$ 

|   | Coordinates (Å) |           |           |
|---|-----------------|-----------|-----------|
|   | X               | Y         | Z         |
| C | -2.426280       | 1.283680  | -0.812636 |
| C | -2.318090       | 1.137259  | 0.707756  |
| C | -0.852809       | 1.081795  | 1.170965  |
| C | -0.091221       | 0.002634  | 0.403991  |
| O | -0.214300       | 0.221057  | -1.004883 |
| C | -1.556392       | 0.209958  | -1.493180 |
| O | 1.268173        | 0.080549  | 0.710753  |
| O | -0.790139       | 0.761125  | 2.554184  |
| O | -3.004209       | 2.183486  | 1.389619  |
| C | -1.442934       | 0.371208  | -3.009070 |
| O | -0.786659       | 1.594318  | -3.362893 |
| O | -2.053642       | 2.626090  | -1.117010 |
| H | -0.487166       | -0.995724 | 0.649339  |
| H | -0.364297       | 2.045188  | 0.969709  |
| C | 1.992372        | -1.104294 | 0.737814  |
| H | -1.411311       | 1.354906  | 3.009579  |
| H | -2.812084       | 0.208488  | 1.019861  |
| H | -2.022311       | -0.770688 | -1.287197 |
| H | -2.799573       | 3.008475  | 0.912476  |
| H | -3.472653       | 1.116029  | -1.116261 |
| H | -0.903104       | -0.486526 | -3.429897 |
| H | -2.437315       | 0.416207  | -3.462851 |
| H | 0.112018        | 1.553513  | -2.992317 |
| H | -1.660892       | 2.651211  | -2.012059 |
| C | 3.003389        | -1.292385 | -0.205638 |
| C | 3.785206        | -2.449606 | -0.150806 |
| C | 3.552940        | -3.412856 | 0.835850  |
| C | 2.539992        | -3.209578 | 1.778480  |
| C | 1.759552        | -2.051030 | 1.739478  |
| H | 3.166537        | -0.532870 | -0.964040 |
| H | 4.574554        | -2.598737 | -0.883257 |
| H | 4.161728        | -4.312206 | 0.874658  |
| H | 2.364496        | -3.947154 | 2.557581  |
| H | 0.992509        | -1.863335 | 2.485582  |

**ESI Table 1E**

| <sup>1</sup> C <sub>4</sub> SCF energy: -918.239442 |           |           |           |
|---|-----------|-----------|-----------|
| $\Omega_{\text{phe}} = 20.8^\circ$                  |           |           |           |
| Coordinates (Å)                                     |           |           |           |
|   | X         | Y         | Z         |
| C   | 1.869419  | -0.609621 | -1.837213 |
| C   | 1.873179  | -0.572453 | -0.440017 |
| C   | 3.070170  | -0.434960 | 0.269404  |
| C   | 4.275121  | -0.341294 | -0.426572 |
| C   | 4.291204  | -0.390664 | -1.824712 |
| C   | 3.088446  | -0.525962 | -2.519846 |
| O   | 0.719550  | -0.651812 | 0.331479  |
| C   | -0.464062 | -1.211068 | -0.231232 |
| O   | -1.164998 | -0.321752 | -1.069548 |
| C   | -1.696239 | 0.901834  | -0.485526 |
| C   | -2.482887 | 0.616391  | 0.826526  |
| C   | -1.848146 | -0.454593 | 1.740561  |
| C   | -1.355304 | -1.665308 | 0.931170  |
| O   | -0.814437 | 0.122101  | 2.548373  |
| H   | -3.483846 | 0.265764  | 0.550450  |
| C   | -0.643261 | 2.022885  | -0.387643 |
| O   | -1.277082 | 3.295108  | -0.397430 |
| O   | -2.448816 | -2.415659 | 0.414111  |
| H   | 0.017753  | 0.111041  | 2.041217  |
| H   | -1.903055 | 3.297317  | 0.349672  |
| H   | -2.610215 | -0.795896 | 2.447336  |
| O   | -2.666247 | 1.819175  | 1.575417  |
| H   | -2.408778 | 1.240722  | -1.243323 |
| H   | -0.008382 | 1.981856  | -1.276703 |
| H   | -2.768509 | -1.979678 | -0.394523 |
| H   | -0.204004 | -2.060269 | -0.870529 |
| H   | -0.798571 | -2.340978 | 1.586571  |
| H   | 0.002132  | 1.914376  | 0.493607  |
| H   | 3.044966  | -0.412643 | 1.355112  |
| H   | 5.204136  | -0.236259 | 0.127505  |
| H   | 5.231155  | -0.319951 | -2.364604 |
| H   | 3.086633  | -0.554625 | -3.606342 |
| H   | 0.938449  | -0.677465 | -2.388509 |
| H   | -1.995192 | 1.796187  | 2.286008  |

**ESI Table 1F****tttG+g-** SCF energy: -918.247742 $\Omega_{\text{phe}} = 12.9^\circ$ 

|   | Coordinates (Å) |           |           |
|---|-----------------|-----------|-----------|
|   | X               | Y         | Z         |
| C | -1.250022       | -1.518746 | 0.062152  |
| C | -0.121881       | -0.512962 | -0.180843 |
| O | -0.506149       | 0.756540  | 0.312300  |
| C | -1.661258       | 1.302382  | -0.347491 |
| C | -2.885501       | 0.386105  | -0.213186 |
| C | -2.516603       | -1.040350 | -0.644099 |
| O | 0.994094        | -0.965686 | 0.534531  |
| C | 2.252156        | -0.476118 | 0.228909  |
| C | 2.484773        | 0.641045  | -0.579261 |
| C | 3.803789        | 1.037553  | -0.829341 |
| C | 4.879206        | 0.342951  | -0.273958 |
| C | 4.629895        | -0.764623 | 0.544533  |
| C | 3.322247        | -1.176934 | 0.796168  |
| C | -1.867326       | 2.691585  | 0.250165  |
| O | -0.742608       | 3.530993  | 0.014034  |
| H | -3.668570       | 0.762033  | -0.891730 |
| O | -3.629759       | -1.876265 | -0.338249 |
| O | -0.950401       | -2.807370 | -0.468872 |
| H | -3.345550       | -2.799713 | -0.445834 |
| H | 0.015255        | 3.134976  | 0.474243  |
| H | -2.333598       | -1.049239 | -1.730353 |
| O | -3.354490       | 0.408364  | 1.127208  |
| H | -1.434157       | 1.411686  | -1.421597 |
| H | -2.720904       | 3.175593  | -0.233663 |
| H | -0.168554       | -3.152625 | -0.008139 |
| H | 0.120147        | -0.448777 | -1.255859 |
| H | -1.425112       | -1.571649 | 1.144291  |
| H | -2.079721       | 2.598951  | 1.321420  |
| H | 3.113319        | -2.035857 | 1.427349  |
| H | 5.456762        | -1.313702 | 0.987570  |
| H | 5.898840        | 0.662266  | -0.470141 |
| H | 3.981787        | 1.906418  | -1.457858 |
| H | 1.660947        | 1.212439  | -0.991170 |
| H | -3.973238       | -0.336740 | 1.221370  |

**ESI Table 1G****tffTg+** SCF energy: -918.246409 $\Omega_{\text{phe}} = 16.8^\circ$ 

|   | Coordinates (Å) |           |           |
|---|-----------------|-----------|-----------|
|   | X               | Y         | Z         |
| O | -0.421028       | 0.752833  | 0.296882  |
| C | 0.086939        | -0.478608 | -0.177069 |
| C | -0.938079       | -1.585410 | 0.081150  |
| C | -2.231468       | -1.250991 | -0.653948 |
| C | -2.751256       | 0.140638  | -0.276797 |
| C | -1.625242       | 1.183488  | -0.354815 |
| O | 1.237053        | -0.813796 | 0.550980  |
| C | 2.448416        | -0.221385 | 0.239419  |
| C | 2.577016        | 0.939699  | -0.528349 |
| C | 3.855744        | 1.446432  | -0.786996 |
| C | 4.992952        | 0.817689  | -0.277683 |
| C | 4.847091        | -0.334372 | 0.503365  |
| C | 3.580590        | -0.856840 | 0.761292  |
| O | -0.506860       | -2.851755 | -0.410453 |
| O | -3.264736       | -2.184548 | -0.345850 |
| O | -3.306346       | 0.148306  | 1.037255  |
| C | -2.001800       | 2.507585  | 0.332595  |
| O | -3.306015       | 2.948471  | -0.018668 |
| H | 0.330755        | -0.408802 | -1.251563 |
| H | -1.120525       | -1.626779 | 1.162938  |
| H | 0.308284        | -3.096875 | 0.056849  |
| H | -2.026532       | -1.269167 | -1.736089 |
| H | -1.416424       | 1.360303  | -1.423315 |
| H | -2.889251       | -3.077890 | -0.423720 |
| H | -3.525433       | 0.427264  | -1.003019 |
| H | -1.900677       | 2.370515  | 1.415020  |
| H | -1.307841       | 3.291419  | 0.017566  |
| H | -3.936378       | 2.404693  | 0.482647  |
| H | -3.827170       | -0.669101 | 1.128083  |
| H | 3.451933        | -1.751776 | 1.363296  |
| H | 5.722943        | -0.832362 | 0.911282  |
| H | 5.980650        | 1.222580  | -0.479437 |
| H | 3.953724        | 2.350120  | -1.383235 |
| H | 1.699982        | 1.462218  | -0.891442 |

**ESI Table 1H****tttG-g-** SCF energy: -918.245765 $\Omega_{\text{phe}} = 20.7^\circ$ 

|   | Coordinates (Å) |           |           |
|---|-----------------|-----------|-----------|
|   | X               | Y         | Z         |
| C | -2.798626       | 0.221498  | -0.439112 |
| C | -2.331660       | -1.220064 | -0.666801 |
| C | -1.066697       | -1.517098 | 0.131146  |
| C | 0.004753        | -0.475722 | -0.203962 |
| O | -0.470228       | 0.819816  | 0.108420  |
| C | -1.628795       | 1.201701  | -0.638675 |
| O | 1.114542        | -0.771285 | 0.599387  |
| O | -0.667123       | -2.839683 | -0.218857 |
| O | -3.406133       | -2.076258 | -0.284820 |
| C | -1.973200       | 2.654545  | -0.285955 |
| O | -2.210725       | 2.900606  | 1.083549  |
| O | -3.337779       | 0.371787  | 0.873667  |
| H | 0.290639        | -0.532834 | -1.269552 |
| H | -1.277635       | -1.444244 | 1.205876  |
| C | 2.361157        | -0.272982 | 0.261330  |
| H | 0.125761        | -3.062424 | 0.295723  |
| H | -2.109877       | -1.358480 | -1.736692 |
| H | -1.387068       | 1.182609  | -1.717945 |
| H | -3.063477       | -2.985519 | -0.252101 |
| H | -3.574800       | 0.461679  | -1.182220 |
| H | -1.130324       | 3.291730  | -0.571533 |
| H | -2.840102       | 2.944757  | -0.904960 |
| H | -2.786872       | 2.191578  | 1.419954  |
| H | -3.906766       | -0.400026 | 1.042029  |
| C | 2.558429        | 0.830920  | -0.573084 |
| C | 3.864849        | 1.247852  | -0.852021 |
| C | 4.962144        | 0.586968  | -0.297559 |
| C | 4.747885        | -0.505861 | 0.549937  |
| C | 3.452431        | -0.939248 | 0.829202  |
| H | 1.712002        | 1.379822  | -0.968508 |
| H | 4.016972        | 2.108363  | -1.498656 |
| H | 5.972186        | 0.922674  | -0.515176 |
| H | 5.592356        | -1.027116 | 0.993414  |
| H | 3.270556        | -1.787485 | 1.482888  |



**ESI Table 1I**

| <b>gggG-g+</b> SCF energy: -918.247007 |           |           |           |
|--|-----------|-----------|-----------|
| $\Omega_{\text{phe}} = 23.0^\circ$     |           |           |           |
| Coordinates (Å)                        |           |           |           |
|  | X         | Y         | Z         |
| C                                      | -2.828804 | 0.233559  | -0.426004 |
| C                                      | -2.367891 | -1.208671 | -0.651799 |
| C                                      | -1.076090 | -1.520670 | 0.121840  |
| C                                      | 0.004615  | -0.488789 | -0.201094 |
| O                                      | -0.487918 | 0.832171  | 0.050606  |
| C                                      | -1.654226 | 1.192250  | -0.693240 |
| O                                      | 1.090012  | -0.706653 | 0.643869  |
| O                                      | -0.588068 | -2.803194 | -0.241221 |
| O                                      | -3.380398 | -2.147115 | -0.299626 |
| C                                      | -1.942885 | 2.647066  | -0.320474 |
| O                                      | -2.168336 | 2.798099  | 1.085110  |
| O                                      | -3.347340 | 0.291051  | 0.900871  |
| H                                      | 0.316587  | -0.568526 | -1.255533 |
| H                                      | -1.272586 | -1.466807 | 1.201729  |
| C                                      | 2.345134  | -0.261757 | 0.277540  |
| H                                      | -1.342132 | -3.415219 | -0.187106 |
| H                                      | -2.177022 | -1.368046 | -1.720453 |
| H                                      | -1.435757 | 1.151848  | -1.775788 |
| H                                      | -3.775033 | -1.832219 | 0.534220  |
| H                                      | -3.631109 | 0.471506  | -1.143536 |
| H                                      | -1.108762 | 3.283165  | -0.643212 |
| H                                      | -2.855876 | 2.991326  | -0.815069 |
| H                                      | -1.350089 | 2.529327  | 1.538011  |
| H                                      | -3.210240 | 1.191127  | 1.257389  |
| C                                      | 3.418402  | -0.907358 | 0.901795  |
| C                                      | 4.724089  | -0.518249 | 0.607266  |
| C                                      | 4.968981  | 0.508307  | -0.312577 |
| C                                      | 3.890925  | 1.147172  | -0.927087 |
| C                                      | 2.573972  | 0.775376  | -0.632472 |
| H                                      | 3.209064  | -1.711101 | 1.601117  |
| H                                      | 5.554183  | -1.025370 | 1.092466  |
| H                                      | 5.987805  | 0.806907  | -0.543337 |
| H                                      | 4.067063  | 1.952967  | -1.635492 |
| H                                      | 1.742948  | 1.304835  | -1.084441 |

**ESI Table 1J**

| <b>tttG-g+</b> SCF energy: -918.2414377 |           |           |           |
|---|-----------|-----------|-----------|
| $\Omega_{\text{phe}} = 19.5^\circ$      |           |           |           |
| Coordinates (Å)                         |           |           |           |
|   | X         | Y         | Z         |
| O                                       | -0.486450 | 0.825108  | 0.084353  |
| C                                       | -0.031847 | -0.484363 | -0.217158 |
| C                                       | -1.117449 | -1.512540 | 0.112427  |
| C                                       | -2.397654 | -1.179889 | -0.649573 |
| C                                       | -2.840862 | 0.260482  | -0.352697 |
| C                                       | -1.667530 | 1.209924  | -0.640237 |
| O                                       | 1.071095  | -0.786692 | 0.591715  |
| C                                       | 2.326061  | -0.308791 | 0.252774  |
| C                                       | 2.543199  | 0.768751  | -0.610781 |
| C                                       | 3.856714  | 1.165413  | -0.886537 |
| C                                       | 4.941174  | 0.510600  | -0.300687 |
| C                                       | 4.706925  | -0.555706 | 0.574882  |
| C                                       | 3.404387  | -0.968847 | 0.851715  |
| O                                       | -0.738541 | -2.830880 | -0.277215 |
| O                                       | -3.465215 | -2.042488 | -0.267011 |
| O                                       | -3.271060 | 0.381367  | 0.991474  |
| C                                       | -1.886937 | 2.695137  | -0.336209 |
| O                                       | -1.969602 | 3.012850  | 1.038041  |
| H                                       | 0.255432  | -0.545459 | -1.281046 |
| H                                       | -1.309337 | -1.464298 | 1.191613  |
| H                                       | 0.037249  | -3.092272 | 0.244808  |
| H                                       | -2.204190 | -1.286140 | -1.728926 |
| H                                       | -1.463026 | 1.133813  | -1.723575 |
| H                                       | -3.126958 | -2.953888 | -0.275499 |
| H                                       | -3.660704 | 0.522653  | -1.041856 |
| H                                       | -1.062034 | 3.252095  | -0.809080 |
| H                                       | -2.824580 | 3.021863  | -0.799592 |
| H                                       | -1.358501 | 2.432477  | 1.520495  |
| H                                       | -3.858953 | -0.374809 | 1.163829  |
| H                                       | 3.206798  | -1.796798 | 1.526459  |
| H                                       | 5.541312  | -1.072216 | 1.042270  |
| H                                       | 5.956734  | 0.830257  | -0.516612 |
| H                                       | 4.024350  | 2.004691  | -1.556762 |
| H                                       | 1.707506  | 1.312873  | -1.034905 |

**ESI Table 2.** Cartesian coordinates of phenyl  $\beta$ -D-galactopyranoside conformers at the B3LYP/6-311++G(d,p) level of theory.

**ESI Table 2A**

| <b>tttG+g-</b> SCF energy: -918.498275 |                 |           |           |
|--|-----------------|-----------|-----------|
| $\Omega_{\text{phe}} = 109.5^\circ$    |                 |           |           |
|  | Coordinates (Å) |           |           |
|  | X               | Y         | Z         |
| C                                      | -0.449113       | -0.053529 | -1.960265 |
| C                                      | -0.451421       | -0.060402 | -0.432399 |
| O                                      | 0.878884        | -0.070031 | 0.044839  |
| C                                      | 1.614345        | -1.240997 | -0.347786 |
| C                                      | 1.697916        | -1.374221 | -1.872362 |
| C                                      | 0.290757        | -1.283425 | -2.475698 |
| O                                      | -1.076578       | 1.124017  | -0.013791 |
| C                                      | -1.445023       | 1.203898  | 1.326969  |
| C                                      | -2.538171       | 0.483540  | 1.803001  |
| C                                      | -2.921004       | 0.624993  | 3.135990  |
| C                                      | -2.223233       | 1.487175  | 3.980653  |
| C                                      | -1.137583       | 2.210657  | 3.488232  |
| C                                      | -0.741908       | 2.069292  | 2.159402  |
| C                                      | 2.969483        | -1.135143 | 0.339030  |
| O                                      | 2.835326        | -1.152713 | 1.753974  |
| H                                      | 2.108187        | -2.367804 | -2.105032 |
| O                                      | 0.437185        | -1.246871 | -3.892061 |
| O                                      | -1.766076       | -0.106172 | -2.502000 |
| H                                      | -0.419152       | -1.013601 | -4.270545 |
| H                                      | 2.254991        | -0.421504 | 1.995027  |
| H                                      | -0.278659       | -2.177532 | -2.184087 |
| O                                      | 2.544448        | -0.363258 | -2.396585 |
| H                                      | 1.095112        | -2.130460 | 0.041337  |
| H                                      | 3.582861        | -1.998366 | 0.072582  |
| H                                      | -2.228627       | 0.698392  | -2.241443 |
| H                                      | -0.994386       | -0.937106 | -0.044372 |
| H                                      | 0.072993        | 0.852968  | -2.285156 |
| H                                      | 3.477504        | -0.229397 | -0.005654 |
| H                                      | 0.098468        | 2.620138  | 1.755578  |
| H                                      | -0.593929       | 2.885354  | 4.139846  |
| H                                      | -2.526797       | 1.597982  | 5.015105  |
| H                                      | -3.772239       | 0.067691  | 3.510344  |
| H                                      | -3.088146       | -0.168404 | 1.133857  |
| H                                      | 2.400185        | -0.345981 | -3.351542 |

**ESI Table 2B****tffTg+** SCF energy: -918.496950 $\Omega_{\text{phe}} = 97.7^\circ$ 

|   | Coordinates (Å) |           |           |
|---|-----------------|-----------|-----------|
|   | X               | Y         | Z         |
| O | 0.111596        | -0.018355 | -0.838178 |
| C | 0.115932        | -0.022782 | 0.574358  |
| C | 1.558538        | -0.025082 | 1.076269  |
| C | 2.259453        | 1.231123  | 0.575344  |
| C | 2.151190        | 1.368829  | -0.946539 |
| C | 0.703453        | 1.154298  | -1.410893 |
| O | -0.486915       | -1.204515 | 1.032010  |
| C | -1.877733       | -1.262635 | 0.964793  |
| C | -2.639415       | -0.732305 | 2.003058  |
| C | -4.028493       | -0.843539 | 1.957978  |
| C | -4.646380       | -1.484716 | 0.885312  |
| C | -3.871067       | -2.015835 | -0.145231 |
| C | -2.482222       | -1.905766 | -0.111084 |
| O | 1.641315        | -0.004219 | 2.498275  |
| O | 3.646869        | 1.223986  | 0.901627  |
| O | 3.000345        | 0.438440  | -1.613165 |
| C | 0.597242        | 0.960731  | -2.931122 |
| O | 1.356035        | 1.918052  | -3.655489 |
| H | -0.433886       | 0.852935  | 0.956718  |
| H | 2.049870        | -0.915412 | 0.668051  |
| H | 1.235050        | -0.812443 | 2.831496  |
| H | 1.774279        | 2.100745  | 1.040971  |
| H | 0.126218        | 2.039851  | -1.104897 |
| H | 3.729097        | 0.968492  | 1.828431  |
| H | 2.442336        | 2.391173  | -1.218230 |
| H | 0.911630        | -0.060425 | -3.162998 |
| H | -0.443073       | 1.079396  | -3.236852 |
| H | 2.280013        | 1.646637  | -3.603971 |
| H | 3.837505        | 0.428475  | -1.130464 |
| H | -1.861046       | -2.307573 | -0.901283 |
| H | -4.347574       | -2.517092 | -0.980139 |
| H | -5.726161       | -1.573356 | 0.854434  |
| H | -4.625640       | -0.435158 | 2.765452  |
| H | -2.144687       | -0.248496 | 2.837657  |

**ESI Table 2C****tttG-g-** SCF energy: -918.496994 $\Omega_{\text{phe}} = 83.7^\circ$ 

|   | Coordinates (Å) |           |           |
|---|-----------------|-----------|-----------|
|   | X               | Y         | Z         |
| C | -2.366366       | 1.172623  | -0.900827 |
| C | -2.371319       | 1.174694  | 0.631235  |
| C | -0.951562       | 1.173754  | 1.184095  |
| C | -0.177567       | 0.002269  | 0.581131  |
| O | -0.139301       | 0.133242  | -0.825003 |
| C | -1.429637       | 0.076257  | -1.434451 |
| O | 1.127685        | 0.066038  | 1.090752  |
| O | -1.061248       | 1.085866  | 2.601231  |
| O | -3.097385       | 2.327575  | 1.048922  |
| C | -1.246054       | 0.104648  | -2.954646 |
| O | -0.538937       | 1.220434  | -3.451961 |
| O | -1.958146       | 2.444087  | -1.401745 |
| H | -0.639806       | -0.960865 | 0.857151  |
| H | -0.436613       | 2.094318  | 0.887333  |
| C | 1.932150        | -1.056173 | 0.896497  |
| H | -0.170929       | 1.119216  | 2.969467  |
| H | -2.880380       | 0.267210  | 0.985266  |
| H | -1.905635       | -0.888369 | -1.188438 |
| H | -2.949011       | 2.441527  | 1.995604  |
| H | -3.383624       | 0.951374  | -1.252062 |
| H | -0.677700       | -0.780353 | -3.249403 |
| H | -2.246736       | 0.025748  | -3.408097 |
| H | -0.889019       | 2.009251  | -3.015984 |
| H | -2.405290       | 3.118579  | -0.873454 |
| C | 2.619817        | -1.223590 | -0.303080 |
| C | 3.462018        | -2.323952 | -0.452455 |
| C | 3.617481        | -3.242659 | 0.585613  |
| C | 2.926678        | -3.060081 | 1.782508  |
| C | 2.080095        | -1.963746 | 1.941910  |
| H | 2.485013        | -0.499391 | -1.095785 |
| H | 4.001052        | -2.460625 | -1.383188 |
| H | 4.276708        | -4.094361 | 0.463329  |
| H | 3.047587        | -3.767534 | 2.595097  |
| H | 1.540993        | -1.801933 | 2.868342  |

**ESI Table 2D****gggG-g+** SCF energy: -918.497029 $\Omega_{\text{phe}} = 118.0^\circ$ 

|   | Coordinates (Å) |           |           |
|---|-----------------|-----------|-----------|
|   | X               | Y         | Z         |
| C | 2.799262        | 0.134572  | 0.523447  |
| C | 2.314625        | -1.314453 | 0.458375  |
| C | 1.059128        | -1.454334 | -0.416365 |
| C | -0.018579       | -0.472739 | 0.034544  |
| O | 0.499957        | 0.859357  | 0.053042  |
| C | 1.622214        | 1.045322  | 0.914099  |
| O | -1.071040       | -0.488805 | -0.879377 |
| O | 0.529904        | -2.766830 | -0.304124 |
| O | 3.332629        | -2.192858 | -0.008503 |
| C | 1.942878        | 2.536631  | 0.863308  |
| O | 2.262272        | 2.968694  | -0.462875 |
| O | 3.375452        | 0.425439  | -0.746313 |
| H | -0.373270       | -0.734667 | 1.042168  |
| H | 1.309845        | -1.217771 | -1.457378 |
| C | -2.340188       | -0.189297 | -0.406456 |
| H | 1.264585        | -3.377932 | -0.439874 |
| H | 2.066457        | -1.657904 | 1.468310  |
| H | 1.346196        | 0.794615  | 1.951999  |
| H | 3.770355        | -1.745072 | -0.746042 |
| H | 3.567723        | 0.219548  | 1.306006  |
| H | 1.092303        | 3.103562  | 1.255409  |
| H | 2.818393        | 2.754556  | 1.478067  |
| H | 1.475104        | 2.829092  | -1.004528 |
| H | 3.300553        | 1.377637  | -0.915147 |
| C | -2.992349       | 0.927309  | -0.921989 |
| C | -4.294203       | 1.210085  | -0.512833 |
| C | -4.937265       | 0.386419  | 0.410412  |
| C | -4.276235       | -0.732893 | 0.915079  |
| C | -2.978527       | -1.031314 | 0.503443  |
| H | -2.475092       | 1.554323  | -1.637690 |
| H | -4.804766       | 2.078208  | -0.914532 |
| H | -5.949078       | 0.610098  | 0.727999  |
| H | -4.776779       | -1.387606 | 1.619682  |
| H | -2.470090       | -1.919442 | 0.860304  |

**Table 3.** Calculated frequencies ( $\text{cm}^{-1}$ ) and intensities ( $\text{km mol}^{-1}$ ) for conformers of phenyl  $\beta$ -D-galactopyranoside at the B3LYP/6-31+G(d) level of theory.

| $\text{ttfG}+\text{g}^-$<br>( $\Omega_{\text{phte}} = 106.6^\circ$ ) |        | $\text{ttfTg}^+$<br>( $\Omega_{\text{phte}} = 96.1^\circ$ ) |        | $\text{ttfG}-\text{g}^-$<br>( $\Omega_{\text{phte}} = 83.9^\circ$ ) |        | $\text{gggG}-\text{g}^+$<br>( $\Omega_{\text{phte}} = 114.9^\circ$ ) |        | ${}^1\text{C}_4$<br>( $\Omega_{\text{phte}} = 20.8^\circ$ ) |        | $\text{ttfG}+\text{g}^-$<br>( $\Omega_{\text{phte}} = 12.9^\circ$ ) |        | $\text{ttfTg}^+$<br>( $\Omega_{\text{phte}} = 16.8^\circ$ ) |        | $\text{ttfG}-\text{g}^-$<br>( $\Omega_{\text{phte}} = 20.7^\circ$ ) |        | $\text{gggG}-\text{g}^+$<br>( $\Omega_{\text{phte}} = 23.0^\circ$ ) |        | $\text{ttfG}-\text{g}^+$<br>( $\Omega_{\text{phte}} = 19.5^\circ$ ) |        |
|--|--------|---|--------|---|--------|--|--------|---|--------|---|--------|---|--------|---|--------|---|--------|---|--------|
| Freq.  | Inten. | Freq.   | Inten. | Freq.   | Inten. | Freq.  | Inten. | Freq.   | Inten. | Freq.   | Inten. | Freq.   | Inten. | Freq.   | Inten. | Freq.   | Inten. | Freq.   | Inten. |
| 21.3   | 0.3    | 14.7  | 0.1    | 13.0  | 0.1    | 11.1   | 0.4    | 30.9  | 0.3    | 32.8  | 0.4    | 30.9  | 0.4    | 30.3  | 0.9    | 28.5  | 0.2    | 31.4  | 0.7    |
| 29.5   | 0.3    | 31.2  | 0.5    | 34.8  | 1.6    | 16.2   | 0.1    | 49.8  | 0.0    | 48.6  | 0.3    | 43.5  | 0.6    | 42.3  | 0.4    | 41.8  | 0.1    | 43.6  | 0.8    |
| 48.2   | 0.1    | 53.6  | 0.2    | 56.0  | 0.4    | 49.0   | 0.6    | 63.9  | 1.0    | 54.7  | 0.2    | 58.9  | 0.1    | 60.6  | 0.3    | 52.5  | 0.8    | 52.3  | 0.6    |
| 86.8   | 0.6    | 72.0  | 4.0    | 83.1  | 0.7    | 79.9   | 1.4    | 107.2   | 0.5    | 94.9  | 0.6    | 71.5  | 3.8    | 88.5  | 1.3    | 82.4  | 2.6    | 68.9  | 0.9    |
| 103.1  | 5.2    | 97.7  | 0.0    | 99.7  | 3.1    | 100.1  | 4.8    | 112.1   | 0.7    | 107.0   | 5.1    | 109.3   | 0.0    | 104.8   | 3.1    | 104.9   | 4.7    | 99.5  | 0.8    |
| 121.4  | 2.5    | 114.4   | 5.1    | 120.8   | 1.2    | 117.7  | 6.4    | 156.6   | 5.7    | 123.1   | 2.5    | 114.0   | 5.5    | 120.3   | 1.3    | 116.8   | 7.8    | 120.3   | 4.0    |
| 138.7  | 1.5    | 147.2   | 3.6    | 162.1   | 2.0    | 165.7  | 5.8    | 160.2   | 9.0    | 151.0   | 2.1    | 147.8   | 3.4    | 170.1   | 4.0    | 169.3   | 5.6    | 145.2   | 7.5    |
| 178.9  | 3.7    | 176.5   | 1.3    | 191.8   | 7.1    | 205.2  | 0.6    | 186.5   | 1.8    | 178.7   | 3.1    | 192.1   | 4.0    | 200.2   | 2.4    | 203.3   | 0.3    | 199.5   | 2.5    |
| 195.6  | 4.9    | 199.6   | 7.9    | 216.2   | 1.4    | 213.2  | 0.5    | 229.1   | 0.9    | 202.6   | 2.8    | 199.7   | 3.6    | 235.0   | 4.3    | 237.5   | 1.1    | 228.2   | 19.6   |
| 216.2  | 0.8    | 216.3   | 3.3    | 238.2   | 2.9    | 244.4  | 3.8    | 236.6   | 2.1    | 237.4   | 2.2    | 237.0   | 1.5    | 240.9   | 3.0    | 243.5   | 1.9    | 232.0   | 8.3    |
| 256.3  | 5.4    | 258.9   | 4.0    | 266.2   | 12.5   | 273.9  | 11.8   | 256.4   | 3.4    | 255.3   | 13.7   | 257.4   | 13.9   | 259.2   | 2.1    | 261.9   | 4.7    | 247.2   | 4.5    |
| 260.1  | 11.1   | 264.4   | 10.6   | 276.6   | 10.4   | 280.8  | 3.7    | 305.4   | 3.7    | 266.1   | 6.8    | 269.1   | 5.6    | 269.8   | 14.0   | 280.0   | 9.8    | 262.7   | 15.7   |
| 302.0  | 2.7    | 292.0   | 2.0    | 287.5   | 1.1    | 285.6  | 4.8    | 308.6   | 3.7    | 278.3   | 8.0    | 275.8   | 6.4    | 289.3   | 9.5    | 293.8   | 0.9    | 271.8   | 12.6   |
| 335.2  | 14.1   | 333.4   | 13.6   | 318.2   | 6.0    | 323.6  | 3.2    | 324.6   | 10.8   | 314.5   | 0.6    | 300.4   | 3.2    | 294.7   | 3.3    | 297.8   | 6.4    | 283.3   | 41.3   |
| 371.6  | 55.5   | 368.7   | 4.4    | 372.3   | 3.1    | 375.7  | 56.3   | 361.6   | 10.2   | 350.0   | 25.9   | 345.4   | 9.9    | 338.1   | 7.5    | 342.7   | 2.4    | 286.1   | 26.4   |
| 375.9  | 47.3   | 386.0   | 109.4  | 381.8   | 82.2   | 387.6  | 0.2    | 385.0   | 101.8  | 370.7   | 91.9   | 375.5   | 72.3   | 379.2   | 92.7   | 387.0   | 60.2   | 335.8   | 28.8   |
| 396.0  | 77.2   | 407.3   | 73.0   | 396.2   | 38.9   | 393.5  | 46.0   | 402.0   | 14.1   | 390.9   | 90.0   | 397.9   | 60.4   | 396.1   | 44.7   | 392.5   | 68.7   | 374.3   | 94.8   |
| 409.4  | 54.8   | 410.7   | 31.8   | 403.9   | 47.7   | 409.4  | 76.1   | 423.7   | 0.0    | 396.1   | 60.8   | 409.0   | 98.3   | 410.3   | 70.9   | 397.1   | 29.7   | 396.6   | 47.3   |
| 412.8  | 102.0  | 422.6   | 55.4   | 414.4   | 105.3  | 424.2  | 0.6    | 442.9   | 13.2   | 408.7   | 68.2   | 421.8   | 0.1    | 421.8   | 16.7   | 423.4   | 0.5    | 409.8   | 67.9   |
| 423.7  | 0.5    | 424.8   | 1.2    | 424.8   | 0.1    | 433.8  | 17.1   | 481.8   | 44.0   | 425.1   | 1.7    | 433.8   | 55.3   | 424.8   | 61.2   | 438.3   | 53.3   | 422.0   | 31.0   |
| 428.7  | 49.3   | 456.3   | 33.5   | 449.4   | 151.6  | 455.7  | 16.5   | 497.4   | 1.6    | 432.1   | 105.7  | 467.4   | 76.2   | 444.2   | 136.0  | 487.4   | 16.3   | 425.1   | 36.4   |
| 447.9  | 116.6  | 465.0   | 73.7   | 482.3   | 33.6   | 498.3  | 21.7   | 512.1   | 22.0   | 444.2   | 122.5  | 488.4   | 98.2   | 489.5   | 45.3   | 501.6   | 41.4   | 455.7   | 100.4  |
| 470.4  | 52.5   | 493.7   | 49.9   | 493.4   | 38.1   | 512.0  | 117.6  | 521.0   | 0.7    | 474.2   | 14.4   | 495.6   | 24.8   | 492.9   | 24.5   | 515.8   | 71.9   | 491.2   | 14.2   |
| 475.9  | 5.9    | 504.4   | 122.5  | 507.3   | 56.3   | 526.5  | 71.4   | 549.1   | 12.6   | 511.7   | 22.7   | 508.5   | 80.1   | 512.2   | 67.2   | 522.8   | 67.3   | 508.1   | 36.3   |
| 521.2  | 4.6    | 537.6   | 18.0   | 516.9   | 25.9   | 573.4  | 8.4    | 567.9   | 89.5   | 519.2   | 5.5    | 521.0   | 1.2    | 518.8   | 12.9   | 581.9   | 2.4    | 519.0   | 9.0    |
| 576.1  | 3.4    | 580.7   | 3.5    | 582.1   | 4.4    | 592.9  | 9.4    | 604.8   | 1.1    | 581.6   | 3.1    | 581.1   | 2.4    | 586.4   | 7.3    | 598.5   | 7.3    | 584.0   | 3.7    |
| 604.9  | 1.2    | 610.9   | 3.2    | 606.2   | 21.0   | 629.1  | 0.1    | 622.2   | 0.7    | 606.4   | 0.4    | 612.5   | 4.6    | 604.2   | 11.4   | 630.6   | 7.5    | 603.4   | 9.5    |
| 626.4  | 12.1   | 628.5   | 6.5    | 632.1   | 0.9    | 641.5  | 18.0   | 662.3   | 0.8    | 628.1   | 1.7    | 627.8   | 1.3    | 631.8   | 2.9    | 645.2   | 19.2   | 632.1   | 1.8    |
| 629.8  | 0.3    | 635.1   | 5.3    | 634.8   | 14.8   | 668.8  | 111.3  | 676.9   | 141.9  | 636.7   | 1.4    | 646.4   | 6.5    | 643.8   | 15.5   | 662.9   | 121.2  | 645.4   | 21.5   |
| 696.9  | 61.9   | 658.4   | 47.6   | 704.6   | 36.7   | 704.8  | 33.5   | 700.8   | 25.5   | 697.7   | 23.6   | 663.3   | 47.1   | 698.9   | 19.4   | 699.7   | 25.0   | 697.7   | 18.3   |
| 705.4  | 29.7   | 704.3   | 38.5   | 742.9   | 16.7   | 754.9  | 19.6   | 707.9   | 14.9   | 699.5   | 54.3   | 696.2   | 19.2   | 742.0   | 18.9   | 752.9   | 23.3   | 743.6   | 16.8   |
| 776.2  | 37.8   | 765.5   | 13.2   | 780.9   | 45.2   | 779.7  | 57.9   | 755.6   | 16.9   | 764.8   | 67.5   | 764.9   | 64.4   | 766.3   | 65.3   | 765.3   | 61.8   | 765.4   | 66.6   |
| 786.8  | 36.8   | 782.7   | 32.3   | 800.7   | 40.6   | 799.5  | 18.2   | 765.7   | 72.1   | 780.8   | 37.4   | 766.7   | 18.0   | 797.3   | 55.7   | 801.8   | 18.9   | 789.9   | 39.7   |

|        |       |        |       |        |       |        |       |        |       |        |       |        |       |        |       |        |       |        |       |
|--------|-------|--------|-------|--------|-------|--------|-------|--------|-------|--------|-------|--------|-------|--------|-------|--------|-------|--------|-------|
| 836.3  | 21.3  | 824.8  | 34.2  | 826.5  | 25.1  | 827.8  | 3.4   | 823.6  | 7.8   | 832.3  | 22.1  | 819.6  | 34.5  | 822.4  | 22.1  | 825.0  | 6.2   | 823.4  | 26.9  |
| 845.5  | 0.3   | 844.9  | 0.1   | 847.3  | 0.3   | 846.0  | 0.1   | 836.8  | 13.7  | 837.0  | 0.6   | 834.4  | 0.3   | 836.5  | 0.2   | 836.2  | 0.5   | 836.7  | 0.3   |
| 878.7  | 17.8  | 859.1  | 0.9   | 861.1  | 3.1   | 870.2  | 12.2  | 841.6  | 5.8   | 880.5  | 18.7  | 860.4  | 1.0   | 862.9  | 2.5   | 867.2  | 12.7  | 863.6  | 2.8   |
| 895.2  | 24.0  | 923.1  | 31.4  | 901.4  | 11.3  | 904.0  | 24.3  | 908.9  | 11.2  | 896.2  | 26.6  | 904.1  | 3.9   | 901.1  | 11.7  | 904.2  | 25.6  | 903.5  | 5.3   |
| 926.1  | 4.5   | 927.6  | 16.9  | 929.5  | 5.3   | 923.4  | 5.2   | 915.5  | 39.6  | 905.3  | 3.4   | 925.0  | 46.3  | 906.6  | 5.4   | 905.2  | 2.9   | 906.7  | 4.7   |
| 954.1  | 24.2  | 976.6  | 0.3   | 955.5  | 16.2  | 956.3  | 44.7  | 945.0  | 17.3  | 954.2  | 23.9  | 969.8  | 0.2   | 955.3  | 16.1  | 956.0  | 49.9  | 962.7  | 74.5  |
| 976.1  | 0.1   | 984.2  | 44.5  | 973.2  | 18.8  | 966.4  | 16.9  | 974.1  | 0.1   | 971.8  | 0.3   | 983.4  | 40.8  | 970.4  | 0.2   | 965.8  | 19.0  | 971.0  | 0.1   |
| 998.1  | 0.2   | 998.2  | 0.2   | 978.9  | 0.4   | 975.4  | 0.2   | 993.9  | 57.6  | 993.4  | 0.0   | 992.2  | 0.2   | 973.8  | 19.5  | 969.5  | 0.3   | 985.5  | 6.8   |
| 1017.5 | 7.6   | 1017.2 | 13.9  | 999.8  | 0.2   | 995.5  | 0.1   | 995.8  | 1.3   | 1014.3 | 1.3   | 1014.9 | 2.4   | 992.6  | 0.1   | 991.0  | 0.1   | 992.9  | 0.2   |
| 1035.1 | 14.4  | 1018.3 | 18.0  | 1017.7 | 6.1   | 1016.7 | 9.6   | 1008.5 | 159.3 | 1036.5 | 10.1  | 1016.3 | 24.1  | 1015.7 | 1.6   | 1015.1 | 1.1   | 1015.3 | 1.7   |
| 1042.7 | 15.7  | 1041.9 | 10.2  | 1042.8 | 18.3  | 1036.4 | 88.5  | 1019.1 | 64.0  | 1043.5 | 8.7   | 1043.2 | 3.8   | 1043.5 | 10.2  | 1033.3 | 224.7 | 1044.2 | 5.9   |
| 1050.1 | 43.2  | 1049.0 | 25.2  | 1049.2 | 24.7  | 1040.5 | 241.8 | 1036.1 | 59.3  | 1055.8 | 15.9  | 1055.2 | 9.4   | 1054.7 | 11.4  | 1040.6 | 73.4  | 1055.3 | 3.0   |
| 1067.8 | 172.6 | 1071.3 | 41.4  | 1067.2 | 30.2  | 1047.5 | 15.6  | 1052.4 | 31.0  | 1067.4 | 170.4 | 1072.6 | 21.6  | 1067.3 | 32.3  | 1052.8 | 34.5  | 1059.4 | 40.5  |
| 1081.7 | 76.5  | 1087.7 | 405.7 | 1077.0 | 249.6 | 1074.3 | 139.3 | 1072.8 | 54.8  | 1081.8 | 69.6  | 1088.9 | 343.8 | 1077.0 | 270.6 | 1075.5 | 148.3 | 1072.8 | 365.6 |
| 1093.7 | 149.8 | 1094.2 | 255.4 | 1094.0 | 184.6 | 1078.7 | 77.0  | 1074.6 | 192.6 | 1094.4 | 139.2 | 1095.9 | 248.7 | 1095.2 | 161.9 | 1078.8 | 70.9  | 1090.3 | 87.3  |
| 1098.0 | 213.5 | 1097.9 | 79.1  | 1100.6 | 3.3   | 1099.0 | 44.8  | 1083.5 | 114.8 | 1099.7 | 164.2 | 1098.5 | 135.4 | 1102.5 | 206.5 | 1103.7 | 156.7 | 1096.8 | 191.1 |
| 1101.1 | 53.8  | 1100.4 | 23.3  | 1103.0 | 187.1 | 1102.9 | 111.6 | 1090.0 | 100.6 | 1107.1 | 84.0  | 1107.1 | 34.1  | 1109.3 | 18.0  | 1105.7 | 7.9   | 1108.6 | 0.5   |
| 1109.3 | 62.9  | 1106.3 | 25.6  | 1124.8 | 98.8  | 1113.6 | 135.8 | 1105.3 | 18.2  | 1114.1 | 153.2 | 1110.9 | 84.1  | 1129.1 | 102.3 | 1117.2 | 134.5 | 1125.1 | 125.1 |
| 1136.6 | 79.5  | 1130.7 | 11.7  | 1140.2 | 77.5  | 1121.8 | 33.0  | 1112.3 | 12.3  | 1139.3 | 69.8  | 1132.1 | 15.4  | 1139.3 | 88.4  | 1124.1 | 20.5  | 1141.8 | 5.8   |
| 1144.7 | 9.5   | 1145.2 | 22.4  | 1145.1 | 9.2   | 1147.2 | 9.3   | 1139.3 | 110.1 | 1146.0 | 11.6  | 1144.2 | 12.1  | 1142.8 | 5.1   | 1148.1 | 8.5   | 1148.1 | 21.5  |
| 1154.4 | 2.0   | 1154.5 | 16.1  | 1157.0 | 12.0  | 1160.5 | 30.6  | 1172.8 | 10.6  | 1155.7 | 3.7   | 1154.6 | 26.8  | 1157.8 | 10.7  | 1159.9 | 38.5  | 1156.7 | 53.3  |
| 1188.8 | 0.7   | 1188.6 | 0.1   | 1188.4 | 0.4   | 1187.5 | 1.1   | 1189.3 | 2.9   | 1188.3 | 2.8   | 1188.1 | 2.2   | 1188.1 | 2.3   | 1187.5 | 2.1   | 1188.3 | 3.1   |
| 1193.1 | 19.0  | 1192.6 | 14.7  | 1193.8 | 13.5  | 1193.6 | 14.6  | 1206.7 | 19.3  | 1205.6 | 17.0  | 1203.7 | 29.9  | 1203.4 | 14.6  | 1202.0 | 14.3  | 1203.9 | 17.6  |
| 1217.0 | 95.2  | 1204.2 | 61.4  | 1218.3 | 89.8  | 1239.1 | 64.8  | 1213.2 | 10.2  | 1216.1 | 96.8  | 1205.0 | 44.9  | 1217.5 | 92.3  | 1239.3 | 42.7  | 1216.0 | 63.2  |
| 1234.1 | 46.3  | 1226.1 | 29.0  | 1235.1 | 16.5  | 1246.1 | 30.3  | 1238.3 | 298.6 | 1234.9 | 23.5  | 1225.4 | 33.6  | 1234.1 | 18.6  | 1247.0 | 37.2  | 1249.0 | 130.8 |
| 1245.8 | 212.9 | 1243.3 | 266.7 | 1243.0 | 251.8 | 1258.1 | 254.9 | 1244.1 | 40.9  | 1248.8 | 61.3  | 1256.7 | 357.6 | 1258.9 | 270.2 | 1262.7 | 90.0  | 1256.3 | 124.5 |
| 1250.2 | 13.2  | 1263.2 | 16.4  | 1263.1 | 11.6  | 1263.8 | 8.0   | 1265.2 | 31.5  | 1262.6 | 316.5 | 1266.6 | 35.1  | 1262.5 | 114.3 | 1269.1 | 268.5 | 1264.5 | 120.6 |
| 1267.8 | 18.9  | 1267.3 | 12.2  | 1284.0 | 23.9  | 1280.2 | 54.6  | 1292.4 | 17.5  | 1268.6 | 10.9  | 1267.8 | 23.6  | 1284.4 | 17.7  | 1281.0 | 58.4  | 1267.1 | 72.8  |
| 1303.0 | 36.7  | 1304.1 | 40.2  | 1303.8 | 39.4  | 1310.9 | 14.8  | 1310.4 | 8.5   | 1308.3 | 29.2  | 1306.6 | 37.5  | 1304.3 | 35.7  | 1309.4 | 12.4  | 1305.1 | 31.8  |
| 1310.4 | 14.2  | 1333.5 | 0.4   | 1329.5 | 27.2  | 1332.3 | 2.8   | 1343.9 | 0.6   | 1312.8 | 13.4  | 1335.8 | 24.7  | 1329.5 | 26.3  | 1335.9 | 2.7   | 1321.2 | 34.5  |
| 1334.4 | 0.3   | 1337.2 | 28.4  | 1333.9 | 2.1   | 1334.5 | 0.8   | 1348.2 | 7.4   | 1347.0 | 3.9   | 1346.5 | 5.7   | 1345.8 | 3.2   | 1338.6 | 17.9  | 1345.9 | 3.0   |
| 1356.9 | 11.6  | 1354.5 | 15.6  | 1353.0 | 11.1  | 1337.9 | 17.6  | 1366.2 | 1.3   | 1356.5 | 26.9  | 1353.5 | 21.4  | 1354.9 | 15.5  | 1344.0 | 0.9   | 1355.9 | 21.7  |
| 1359.3 | 8.5   | 1357.8 | 0.6   | 1358.2 | 0.1   | 1358.3 | 0.6   | 1372.1 | 8.6   | 1366.9 | 5.5   | 1366.3 | 6.7   | 1366.0 | 6.6   | 1365.7 | 0.5   | 1366.3 | 5.3   |
| 1373.0 | 18.3  | 1374.2 | 8.2   | 1372.5 | 12.7  | 1370.8 | 10.6  | 1378.3 | 19.4  | 1373.8 | 20.6  | 1374.4 | 6.1   | 1372.5 | 11.9  | 1370.5 | 20.5  | 1369.6 | 6.4   |
| 1375.7 | 7.1   | 1382.2 | 6.2   | 1382.7 | 6.2   | 1382.1 | 45.0  | 1385.7 | 20.6  | 1378.9 | 3.2   | 1380.1 | 8.6   | 1382.9 | 9.8   | 1379.7 | 60.4  | 1373.5 | 6.1   |
| 1392.2 | 6.1   | 1404.6 | 10.8  | 1390.0 | 5.2   | 1398.4 | 17.7  | 1401.5 | 26.6  | 1395.4 | 5.8   | 1403.4 | 9.1   | 1390.8 | 4.8   | 1397.3 | 13.2  | 1389.9 | 6.8   |
| 1410.3 | 60.2  | 1410.8 | 6.5   | 1411.1 | 33.1  | 1405.5 | 30.8  | 1411.8 | 24.1  | 1410.5 | 50.4  | 1410.1 | 13.0  | 1413.4 | 39.3  | 1405.8 | 37.3  | 1409.4 | 16.0  |
| 1417.1 | 12.1  | 1413.0 | 61.4  | 1414.4 | 32.5  | 1410.3 | 9.1   | 1416.2 | 19.2  | 1416.9 | 13.8  | 1411.9 | 58.4  | 1417.2 | 23.8  | 1409.8 | 3.1   | 1422.0 | 29.4  |
| 1425.4 | 13.6  | 1425.0 | 8.9   | 1426.8 | 13.3  | 1428.3 | 55.4  | 1432.1 | 25.5  | 1429.9 | 13.2  | 1427.5 | 10.8  | 1426.9 | 18.8  | 1428.1 | 57.4  | 1430.3 | 13.8  |
| 1436.5 | 8.1   | 1431.5 | 16.2  | 1437.9 | 3.5   | 1438.1 | 81.4  | 1445.9 | 45.3  | 1437.2 | 31.1  | 1432.2 | 15.1  | 1438.9 | 3.4   | 1439.5 | 77.6  | 1442.1 | 8.1   |



|        |      |        |      |        |       |        |       |        |       |        |      |        |      |        |       |        |       |        |      |
|--------|------|--------|------|--------|-------|--------|-------|--------|-------|--------|------|--------|------|--------|-------|--------|-------|--------|------|
| 1443.8 | 31.0 | 1437.4 | 18.5 | 1449.3 | 33.2  | 1450.0 | 7.2   | 1451.8 | 55.1  | 1444.1 | 12.2 | 1439.6 | 18.5 | 1448.6 | 34.4  | 1450.8 | 5.5   | 1447.9 | 89.4 |
| 1449.8 | 24.8 | 1449.1 | 33.1 | 1469.4 | 88.1  | 1463.7 | 26.3  | 1454.5 | 16.0  | 1449.1 | 29.4 | 1448.4 | 34.5 | 1469.7 | 89.4  | 1463.4 | 25.6  | 1450.7 | 20.0 |
| 1493.0 | 1.6  | 1492.8 | 1.5  | 1492.7 | 1.4   | 1493.1 | 1.9   | 1499.0 | 0.6   | 1498.8 | 0.5  | 1498.8 | 0.5  | 1498.7 | 0.5   | 1497.5 | 0.4   | 1498.6 | 0.5  |
| 1516.4 | 2.1  | 1521.8 | 2.1  | 1517.3 | 5.7   | 1515.6 | 4.6   | 1526.8 | 0.6   | 1515.4 | 1.9  | 1523.3 | 2.5  | 1517.7 | 4.2   | 1515.9 | 4.8   | 1520.6 | 2.4  |
| 1534.1 | 65.5 | 1533.7 | 63.3 | 1534.0 | 63.9  | 1534.0 | 76.8  | 1535.9 | 95.4  | 1536.4 | 95.8 | 1536.2 | 95.9 | 1536.1 | 95.4  | 1536.2 | 98.9  | 1536.2 | 94.7 |
| 1641.7 | 8.5  | 1641.5 | 5.6  | 1641.0 | 5.0   | 1639.8 | 9.2   | 1641.3 | 25.8  | 1640.7 | 24.2 | 1641.0 | 23.1 | 1641.0 | 22.2  | 1639.3 | 20.5  | 1641.0 | 22.5 |
| 1646.9 | 37.7 | 1646.1 | 36.4 | 1646.0 | 35.2  | 1647.5 | 47.3  | 1651.6 | 53.5  | 1652.9 | 59.2 | 1652.7 | 60.1 | 1652.7 | 59.0  | 1652.9 | 66.1  | 1652.7 | 58.3 |
| 2983.0 | 14.8 | 2977.1 | 19.6 | 2958.9 | 7.6   | 2971.1 | 18.3  | 3045.7 | 43.1  | 2983.1 | 15.1 | 2980.8 | 17.2 | 2954.8 | 13.4  | 2969.9 | 18.0  | 2965.4 | 9.4  |
| 2990.5 | 9.5  | 2995.0 | 19.3 | 2967.4 | 33.2  | 2998.2 | 61.2  | 3066.4 | 16.3  | 2989.4 | 13.2 | 2990.4 | 24.8 | 2972.6 | 26.8  | 2997.7 | 43.8  | 2984.9 | 22.7 |
| 2997.9 | 28.6 | 3010.2 | 24.9 | 2982.0 | 70.8  | 3006.0 | 20.8  | 3095.9 | 20.4  | 2998.4 | 27.9 | 3009.4 | 26.3 | 2980.5 | 73.5  | 2999.5 | 42.9  | 2993.6 | 32.9 |
| 3015.3 | 77.1 | 3034.1 | 52.5 | 3007.4 | 22.7  | 3046.5 | 9.4   | 3100.7 | 14.3  | 3015.4 | 76.9 | 3033.9 | 51.2 | 3007.5 | 22.2  | 3043.5 | 13.1  | 2999.9 | 59.5 |
| 3066.1 | 13.6 | 3061.5 | 24.1 | 3021.1 | 84.0  | 3056.3 | 42.5  | 3101.9 | 39.4  | 3067.0 | 20.4 | 3062.7 | 24.7 | 3021.2 | 82.2  | 3054.5 | 43.3  | 3012.6 | 89.9 |
| 3066.8 | 35.0 | 3068.8 | 32.1 | 3062.8 | 23.0  | 3068.8 | 45.9  | 3113.2 | 17.5  | 3071.2 | 27.5 | 3071.8 | 30.5 | 3064.2 | 22.9  | 3069.9 | 42.4  | 3069.3 | 20.7 |
| 3123.2 | 25.1 | 3130.5 | 24.8 | 3104.2 | 30.6  | 3124.1 | 21.2  | 3124.6 | 20.2  | 3126.2 | 23.4 | 3129.9 | 24.2 | 3102.2 | 31.7  | 3124.1 | 22.2  | 3091.4 | 35.1 |
| 3184.4 | 1.6  | 3183.8 | 1.1  | 3183.4 | 0.6   | 3182.5 | 0.7   | 3187.6 | 1.2   | 3185.4 | 1.3  | 3184.7 | 1.3  | 3184.6 | 1.2   | 3182.5 | 1.4   | 3185.1 | 1.2  |
| 3192.5 | 7.4  | 3192.2 | 8.4  | 3192.2 | 9.9   | 3191.3 | 13.5  | 3195.4 | 9.9   | 3193.2 | 10.9 | 3192.6 | 11.7 | 3192.4 | 11.9  | 3191.1 | 15.5  | 3192.9 | 11.5 |
| 3201.9 | 23.1 | 3201.7 | 24.9 | 3202.1 | 26.6  | 3203.8 | 27.5  | 3206.7 | 21.4  | 3206.1 | 23.6 | 3205.6 | 25.0 | 3205.4 | 25.3  | 3206.5 | 29.2  | 3206.0 | 24.2 |
| 3210.4 | 17.1 | 3210.3 | 16.7 | 3210.3 | 14.9  | 3211.5 | 9.3   | 3214.4 | 12.3  | 3213.4 | 13.8 | 3213.1 | 13.7 | 3212.9 | 13.6  | 3216.9 | 6.5   | 3213.4 | 13.0 |
| 3220.5 | 3.0  | 3226.9 | 2.4  | 3232.4 | 0.6   | 3217.5 | 4.9   | 3231.1 | 0.7   | 3232.6 | 3.2  | 3236.4 | 3.3  | 3237.7 | 2.4   | 3228.7 | 5.4   | 3235.7 | 2.6  |
| 3710.1 | 61.3 | 3705.4 | 78.0 | 3698.0 | 186.3 | 3607.9 | 255.3 | 3627.9 | 76.5  | 3710.3 | 61.9 | 3706.9 | 77.2 | 3699.9 | 187.2 | 3606.9 | 261.2 | 3708.1 | 53.6 |
| 3730.2 | 53.0 | 3725.6 | 34.1 | 3709.7 | 8.2   | 3691.7 | 55.8  | 3678.8 | 1.7   | 3730.5 | 53.6 | 3728.5 | 34.4 | 3710.9 | 5.5   | 3690.7 | 55.6  | 3729.3 | 53.1 |
| 3736.5 | 38.4 | 3731.6 | 53.5 | 3729.6 | 54.8  | 3717.9 | 49.8  | 3681.1 | 288.5 | 3743.5 | 32.5 | 3729.8 | 54.0 | 3730.1 | 54.9  | 3715.9 | 50.0  | 3745.7 | 39.3 |
| 3745.7 | 46.5 | 3743.4 | 46.6 | 3744.1 | 46.5  | 3725.4 | 42.6  | 3711.7 | 29.0  | 3747.4 | 43.4 | 3747.0 | 42.3 | 3745.4 | 43.1  | 3724.4 | 43.7  | 3747.5 | 39.0 |

**Table 4.** Calculated frequencies ( $\text{cm}^{-1}$ ) and intensities ( $\text{km mol}^{-1}$ ) for conformers of phenyl  $\beta$ -D-galactopyranoside at the B3LYP/6-311++G(d,p) level of theory.

| <i>tttG+g-</i><br>( $\Omega_{\text{phe}} = 109.5^\circ$ ) |        | <i>tttTg+</i><br>( $\Omega_{\text{phe}} = 97.7^\circ$ ) |        | <i>tttG-g-</i><br>( $\Omega_{\text{phe}} = 83.7^\circ$ ) |        | <i>gggG-g+</i><br>( $\Omega_{\text{phe}} = 118.0^\circ$ ) |        |
|---|--------|---|--------|--|--------|---|--------|
| Freq.   | Inten. | Freq.   | Inten. | Freq.  | Inten. | Freq.   | Inten. |
| 14.5  | 0.2    | 18.1  | 0.1    | 13.9   | 0.1    | 9.1   | 0.1    |
| 26.8  | 0.4    | 29.5  | 0.6    | 34.7   | 1.6    | 25.1  | 0.4    |
| 48.2  | 0.1    | 52.9  | 0.3    | 55.5   | 0.4    | 47.5  | 0.6    |
| 87.2  | 0.6    | 66.6  | 4.1    | 82.9   | 0.6    | 82.5  | 1.2    |
| 103.2   | 5.1    | 97.8  | 0.0    | 99.2   | 3.2    | 101.8   | 5.3    |
| 121.3   | 2.9    | 113.2   | 4.7    | 119.6  | 1.3    | 115.1   | 6.7    |
| 139.1   | 1.5    | 145.6   | 3.7    | 160.0  | 2.3    | 162.4   | 5.2    |
| 179.2   | 3.9    | 176.3   | 1.3    | 191.4  | 7.0    | 201.9   | 0.4    |
| 195.7   | 4.5    | 199.6   | 8.0    | 216.2  | 1.2    | 213.2   | 0.6    |
| 215.5   | 0.7    | 215.9   | 2.9    | 238.0  | 2.5    | 243.1   | 3.7    |
| 256.1   | 4.1    | 257.9   | 3.4    | 266.9  | 10.4   | 271.7   | 5.2    |
| 261.8   | 10.1   | 266.2   | 8.7    | 275.8  | 9.8    | 277.7   | 11.6   |
| 302.3   | 2.6    | 290.8   | 1.9    | 284.9  | 2.0    | 280.8   | 5.9    |
| 334.6   | 14.0   | 332.5   | 13.3   | 316.8  | 5.4    | 319.0   | 3.4    |
| 370.0   | 56.5   | 367.9   | 5.3    | 371.9  | 2.4    | 367.5   | 83.1   |
| 375.1   | 44.5   | 385.5   | 105.9  | 380.1  | 81.1   | 386.2   | 9.7    |
| 396.0   | 82.7   | 411.7   | 20.4   | 395.6  | 46.6   | 388.4   | 31.5   |
| 406.3   | 42.3   | 413.1   | 51.4   | 404.3  | 39.4   | 402.1   | 57.3   |
| 417.1   | 99.7   | 423.4   | 30.8   | 419.7  | 84.5   | 422.6   | 0.4    |
| 421.7   | 0.6    | 424.2   | 39.2   | 423.7  | 0.1    | 436.0   | 9.0    |
| 428.5   | 36.1   | 456.0   | 34.4   | 438.6  | 169.9  | 456.6   | 10.9   |
| 443.9   | 123.3  | 466.5   | 95.2   | 482.3  | 28.9   | 496.0   | 37.4   |
| 468.1   | 45.3   | 476.9   | 125.8  | 486.5  | 41.5   | 503.3   | 127.1  |
| 474.2   | 5.6    | 493.9   | 29.4   | 505.6  | 47.1   | 522.4   | 37.3   |
| 520.5   | 4.3    | 536.5   | 11.5   | 515.8  | 15.6   | 573.7   | 12.7   |
| 575.9   | 3.1    | 580.3   | 3.3    | 582.3  | 4.0    | 593.7   | 14.5   |
| 604.3   | 1.6    | 611.4   | 3.5    | 606.4  | 20.6   | 630.1   | 1.9    |
| 626.5   | 12.2   | 628.9   | 6.9    | 633.1  | 5.7    | 632.9   | 74.8   |
| 630.6   | 0.1    | 635.4   | 4.3    | 634.4  | 9.5    | 645.0   | 37.5   |
| 696.5   | 61.5   | 656.8   | 46.6   | 706.4  | 40.2   | 707.4   | 36.9   |
| 705.6   | 33.6   | 705.8   | 41.8   | 740.8  | 16.5   | 748.8   | 21.0   |
| 775.2   | 35.4   | 762.4   | 13.0   | 781.8  | 40.6   | 779.4   | 48.6   |
| 786.3   | 34.6   | 783.9   | 27.4   | 798.5  | 39.1   | 798.1   | 19.8   |
| 834.4   | 22.5   | 823.4   | 35.5   | 825.0  | 27.3   | 825.4   | 5.4    |
| 842.3   | 0.4    | 843.4   | 0.2    | 845.7  | 0.3    | 842.2   | 0.0    |
| 876.8   | 15.5   | 857.0   | 0.6    | 858.5  | 2.7    | 867.5   | 10.8   |
| 891.4   | 26.4   | 919.0   | 40.9   | 897.6  | 11.4   | 898.9   | 25.5   |
| 925.0   | 5.2    | 927.5   | 9.6    | 930.7  | 7.3    | 921.9   | 5.8    |
| 949.8   | 23.6   | 978.2   | 41.9   | 950.9  | 15.5   | 949.8   | 48.4   |
| 978.2   | 0.1    | 979.9   | 3.3    | 967.9  | 21.4   | 961.2   | 16.0   |
| 996.2   | 0.4    | 997.1   | 0.5    | 983.3  | 0.5    | 978.0   | 0.2    |
| 1017.2  | 11.9   | 1010.9  | 20.9   | 999.0  | 0.7    | 994.4   | 0.2    |
| 1027.4  | 17.4   | 1017.9  | 11.7   | 1017.7   | 8.8    | 1016.2  | 24.9   |
| 1037.5  | 27.8   | 1036.4  | 19.2   | 1036.4   | 27.4   | 1029.3  | 307.7  |
| 1044.2  | 51.4   | 1043.3  | 27.2   | 1043.6   | 21.6   | 1032.4  | 65.0   |
| 1057.3  | 192.3  | 1060.8  | 82.1   | 1060.4   | 36.7   | 1042.8  | 11.0   |
| 1073.5  | 112.8  | 1076.6  | 456.5  | 1064.9   | 294.2  | 1064.2  | 102.6  |

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|               |       |               |       |               |       |               |       |
|---------------|-------|---------------|-------|---------------|-------|---------------|-------|
| <b>1084.0</b> | 131.5 | <b>1084.1</b> | 181.5 | <b>1085.5</b> | 179.1 | <b>1072.7</b> | 73.8  |
| <b>1089.7</b> | 211.8 | <b>1089.2</b> | 86.7  | <b>1093.9</b> | 62.8  | <b>1092.9</b> | 80.3  |
| <b>1094.4</b> | 22.3  | <b>1093.5</b> | 9.0   | <b>1094.2</b> | 84.9  | <b>1095.2</b> | 70.1  |
| <b>1102.6</b> | 39.9  | <b>1099.5</b> | 7.9   | <b>1115.5</b> | 92.0  | <b>1106.4</b> | 129.6 |
| <b>1129.3</b> | 79.2  | <b>1122.7</b> | 13.0  | <b>1132.9</b> | 80.7  | <b>1114.4</b> | 26.7  |
| <b>1137.6</b> | 7.5   | <b>1138.0</b> | 18.8  | <b>1138.1</b> | 8.3   | <b>1139.9</b> | 9.6   |
| <b>1147.6</b> | 1.4   | <b>1148.4</b> | 17.5  | <b>1149.3</b> | 6.3   | <b>1152.4</b> | 33.0  |
| <b>1180.3</b> | 1.4   | <b>1180.2</b> | 0.2   | <b>1179.9</b> | 0.8   | <b>1179.0</b> | 1.9   |
| <b>1183.8</b> | 23.6  | <b>1183.0</b> | 19.2  | <b>1184.2</b> | 17.3  | <b>1184.8</b> | 19.9  |
| <b>1211.2</b> | 92.2  | <b>1199.7</b> | 60.9  | <b>1212.5</b> | 85.9  | <b>1233.3</b> | 100.5 |
| <b>1228.1</b> | 94.4  | <b>1219.5</b> | 30.0  | <b>1231.1</b> | 3.6   | <b>1241.5</b> | 44.7  |
| <b>1237.1</b> | 150.1 | <b>1232.5</b> | 235.5 | <b>1231.9</b> | 241.6 | <b>1246.0</b> | 191.9 |
| <b>1244.5</b> | 7.9   | <b>1256.8</b> | 19.7  | <b>1256.4</b> | 10.4  | <b>1250.5</b> | 10.0  |
| <b>1262.3</b> | 19.4  | <b>1260.8</b> | 12.9  | <b>1278.1</b> | 25.0  | <b>1274.1</b> | 48.3  |
| <b>1294.7</b> | 33.4  | <b>1296.0</b> | 36.0  | <b>1296.0</b> | 35.1  | <b>1301.4</b> | 12.2  |
| <b>1302.7</b> | 11.4  | <b>1320.2</b> | 0.2   | <b>1320.2</b> | 0.5   | <b>1321.1</b> | 0.2   |
| <b>1321.2</b> | 0.5   | <b>1328.5</b> | 23.3  | <b>1322.2</b> | 25.0  | <b>1323.8</b> | 3.5   |
| <b>1345.2</b> | 1.0   | <b>1344.2</b> | 2.2   | <b>1343.8</b> | 6.5   | <b>1330.3</b> | 17.4  |
| <b>1349.7</b> | 15.0  | <b>1347.0</b> | 11.1  | <b>1345.8</b> | 1.2   | <b>1346.1</b> | 0.3   |
| <b>1364.1</b> | 21.4  | <b>1366.1</b> | 11.2  | <b>1364.2</b> | 15.6  | <b>1359.8</b> | 9.9   |
| <b>1367.0</b> | 1.6   | <b>1373.0</b> | 3.9   | <b>1372.2</b> | 3.4   | <b>1371.2</b> | 41.3  |
| <b>1384.2</b> | 6.4   | <b>1396.3</b> | 21.7  | <b>1379.9</b> | 4.7   | <b>1391.0</b> | 6.3   |
| <b>1403.0</b> | 66.1  | <b>1399.9</b> | 7.3   | <b>1402.8</b> | 12.1  | <b>1392.8</b> | 41.6  |
| <b>1407.2</b> | 5.4   | <b>1405.2</b> | 48.3  | <b>1404.0</b> | 54.7  | <b>1399.7</b> | 2.8   |
| <b>1415.5</b> | 12.7  | <b>1414.8</b> | 10.4  | <b>1416.4</b> | 10.8  | <b>1417.5</b> | 49.5  |
| <b>1426.0</b> | 6.7   | <b>1420.0</b> | 12.8  | <b>1426.7</b> | 4.3   | <b>1425.8</b> | 57.0  |
| <b>1432.8</b> | 24.6  | <b>1426.7</b> | 16.5  | <b>1438.0</b> | 28.9  | <b>1436.5</b> | 6.8   |
| <b>1438.2</b> | 22.5  | <b>1437.0</b> | 27.4  | <b>1458.3</b> | 73.4  | <b>1451.2</b> | 31.7  |
| <b>1482.0</b> | 2.1   | <b>1481.8</b> | 2.0   | <b>1481.9</b> | 1.9   | <b>1482.1</b> | 2.3   |
| <b>1498.5</b> | 2.7   | <b>1502.5</b> | 2.8   | <b>1497.6</b> | 6.1   | <b>1497.3</b> | 5.1   |
| <b>1521.1</b> | 69.1  | <b>1520.7</b> | 66.2  | <b>1520.9</b> | 66.7  | <b>1521.2</b> | 78.6  |
| <b>1630.0</b> | 9.9   | <b>1630.1</b> | 6.6   | <b>1629.5</b> | 5.4   | <b>1628.4</b> | 10.9  |
| <b>1635.3</b> | 37.7  | <b>1634.5</b> | 35.9  | <b>1634.3</b> | 34.8  | <b>1636.2</b> | 47.1  |
| <b>2963.7</b> | 15.5  | <b>2956.9</b> | 19.3  | <b>2944.6</b> | 2.5   | <b>2954.6</b> | 15.6  |
| <b>2974.6</b> | 7.2   | <b>2978.0</b> | 16.3  | <b>2948.0</b> | 33.1  | <b>2981.3</b> | 53.4  |
| <b>2982.3</b> | 24.1  | <b>2993.1</b> | 22.9  | <b>2965.3</b> | 67.4  | <b>2985.9</b> | 22.6  |
| <b>2998.9</b> | 71.9  | <b>3016.7</b> | 48.0  | <b>2990.7</b> | 18.8  | <b>3028.6</b> | 7.1   |
| <b>3044.6</b> | 23.9  | <b>3043.6</b> | 22.2  | <b>3004.7</b> | 79.7  | <b>3036.0</b> | 39.7  |
| <b>3048.7</b> | 21.8  | <b>3051.2</b> | 30.1  | <b>3044.2</b> | 21.4  | <b>3049.1</b> | 43.8  |
| <b>3099.0</b> | 23.5  | <b>3108.4</b> | 21.9  | <b>3080.0</b> | 29.0  | <b>3099.8</b> | 19.9  |
| <b>3166.4</b> | 1.3   | <b>3166.0</b> | 0.9   | <b>3165.3</b> | 0.5   | <b>3164.8</b> | 0.9   |
| <b>3174.4</b> | 5.8   | <b>3174.2</b> | 6.6   | <b>3173.8</b> | 7.6   | <b>3173.3</b> | 9.8   |
| <b>3183.7</b> | 17.4  | <b>3183.6</b> | 18.7  | <b>3183.8</b> | 19.7  | <b>3185.2</b> | 19.8  |
| <b>3192.4</b> | 12.1  | <b>3192.4</b> | 12.0  | <b>3192.2</b> | 10.9  | <b>3192.5</b> | 8.5   |
| <b>3201.3</b> | 1.9   | <b>3206.8</b> | 1.4   | <b>3211.2</b> | 0.3   | <b>3199.2</b> | 3.5   |
| <b>3787.5</b> | 71.8  | <b>3781.3</b> | 86.7  | <b>3761.4</b> | 175.0 | <b>3689.1</b> | 247.7 |
| <b>3809.2</b> | 61.8  | <b>3806.9</b> | 40.3  | <b>3782.1</b> | 41.3  | <b>3767.3</b> | 62.7  |
| <b>3814.4</b> | 47.2  | <b>3810.0</b> | 63.3  | <b>3807.8</b> | 64.5  | <b>3799.9</b> | 46.9  |
| <b>3823.9</b> | 55.8  | <b>3821.9</b> | 55.5  | <b>3822.2</b> | 55.5  | <b>3800.8</b> | 63.3  |

**Table 5.** Relative energies of phenyl  $\beta$ -D-galactopyranoside conformers in  $\text{kJ mol}^{-1}$ .

|   | $\text{ttG}^+\text{g}^-$<br>( $\Omega_{\text{phe}} \sim 110^\circ$ ) | $\text{ttTg}^+$<br>( $\Omega_{\text{phe}} \sim 100^\circ$ ) | $\text{ttG}^+\text{g}^-$<br>( $\Omega_{\text{phe}} \sim 85^\circ$ ) | $\text{gggG}^+\text{g}^+$<br>( $\Omega_{\text{phe}} \sim 115^\circ$ ) | $\text{ttG}^+\text{g}^-$<br>( $\Omega_{\text{phe}} \sim 13^\circ$ ) | $\text{ttTg}^+$<br>( $\Omega_{\text{phe}} \sim 17^\circ$ ) | $\text{ttG}^+\text{g}^-$<br>( $\Omega_{\text{phe}} \sim 21^\circ$ ) | $\text{gggG}^+\text{g}^+$<br>( $\Omega_{\text{phe}} \sim 23^\circ$ ) |
|---|--|---|---|---|---|--|---|--|
| B3LYP/6-31+G(d) full opt.                           | 0  | 2.7   | 2.7   | 1.1   | -4.7  | -1.2   | 0.5   | -2.8   |
| 6-311++G(d,p)//6-31+G(d)                            | 0  | 3.6   | 3.4   | 3.5   |   |  |   |  |
| 6-311++G(d,p) full opt.                             | 0  | 3.5   | 3.4   | 3.3   |   |  |   |  |
| MP2/6-311+G(d,p)//B3LYP/6-31+G(d)                   | 0  | 3.4   | 4.5   | 6.5   |   |  |   |  |
| 6-311++G(d,p)//B3LYP/6-31+G(d)                      | 0  | 3.5   | 4.5   | 6.6   | -1.6  | 2.7  | 5.8   | 3.7  |
| 6-311++G(d,p)//<br>B3LYP/6-311++G(d,p)              | 0  | 3.3   | 4.3   | 6.4   |   |  |   |  |
| B3LYP/6-31+G(d) zero-point energy                   | 0  | 0.8   | 0.7   | 1.8   | 0.8   | 1.3  | 1.0   | 2.1  |
| B3LYP/6-311++G(d,p) full opt. <sup>a</sup>          | 0  | 4.3   | 4.0   | 5.1   |   |  |   |  |
| MP2/6-311++G(d,p)//B3LYP/6-311++G(d,p) <sup>a</sup> | 0  | 4.1   | 5.0   | 8.2   |   |  |   |  |

<sup>a</sup>Values include B3LYP/6-31+G(d) zero-point energy correction.