**Supplementary Materials**

Effect of Tacticity on London Dispersive Surface Energy, Polar Free Energy and Lewis Acid-Base Surface Energies of Poly Methyl Methacrylate by Inverse Gas Chromatography

Tayssir Hamieh1,2

1Faculty of Science and Engineering, Maastricht University, P.O. Box 616, 6200 MD Maastricht, Netherlands

2Laboratory of Materials, Catalysis, Environment and Analytical Methods Laboratory (MCEMA), Faculty of Sciences, Lebanese University, Hadath, Lebanon

Correspondence: Faculty of Science and Engineering, Maastricht University, P.O. Box 616, 6200 MD Maastricht, The Netherlands, E-mail: [t.hamieh@maastrichtuniversity.nl](mailto:t.hamieh@maastrichtuniversity.nl)

**Table S1.** Values of ( in kJ/mol) of organic solvents adsorbed on PMMA particles as a function of the temperature for the different tacticities.

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Atactic PMMA** | | | | | | | | | | | | |
| **T(K)** | **C5** | **C6** | **C7** | **C8** | **C9** | **CCl4** | **CHCl3** | **CH2Cl2** | **Ether** | **THF** | **Ethyl acetate** | **Toluene** |
| 303.15 | -0.580 | 2.437 | 5.366 | 8.363 | 11.294 | 11.734 | 14.493 | 12.647 | 13.265 | 15.688 | 14.476 | 13.112 |
| 313.15 | -2.014 | 0.843 | 3.602 | 6.125 | 9.175 | 10.256 | 12.474 | 10.689 | 11.493 | 13.917 | 12.705 | 11.210 |
| 323.15 | -4.086 | -1.332 | 1.312 | 4.016 | 6.643 | 8.282 | 9.907 | 8.186 | 9.078 | 11.605 | 10.342 | 8.945 |
| 328.15 | -5.409 | -2.577 | 0.140 | 2.818 | 5.618 | 7.140 | 8.419 | 6.720 | 7.574 | 10.256 | 8.915 | 7.783 |
| 333.15 | -6.601 | -3.560 | -0.643 | 2.339 | 5.242 | 6.320 | 7.179 | 5.480 | 6.185 | 9.176 | 7.681 | 7.115 |
| 338.15 | -2.765 | 0.053 | 2.741 | 5.617 | 8.055 | 9.977 | 10.635 | 8.998 | 9.891 | 12.733 | 11.312 | 10.399 |
| 343.15 | -4.064 | -1.396 | 1.137 | 3.724 | 6.225 | 8.569 | 8.985 | 7.404 | 8.417 | 11.194 | 9.805 | 8.719 |
| 348.15 | -5.545 | -2.983 | -0.562 | 1.908 | 4.290 | 7.045 | 7.201 | 5.673 | 6.777 | 9.524 | 8.150 | 6.965 |
| 353.15 | -6.446 | -3.958 | -1.620 | 0.766 | 3.059 | 6.139 | 6.022 | 4.546 | 5.715 | 8.461 | 7.088 | 5.867 |
| 363.15 | -7.548 | -5.147 | -2.814 | -0.640 | 1.538 | 5.124 | 4.432 | 3.053 | 4.308 | 7.112 | 5.710 | 4.536 |
| 373.15 | -8.631 | -6.162 | -3.888 | -1.577 | 0.631 | 4.282 | 2.940 | 1.627 | 2.863 | 5.886 | 4.375 | 3.549 |
| 378.15 | -9.665 | -6.863 | -4.286 | -1.671 | 0.837 | 3.755 | 1.942 | 0.580 | 1.615 | 5.080 | 3.348 | 3.284 |
| 383.15 | -10.478 | -7.190 | -4.172 | -1.115 | 1.830 | 3.641 | 1.281 | -0.180 | 0.566 | 4.648 | 2.607 | 3.595 |
| 388.15 | -6.265 | -3.528 | -1.054 | 1.448 | 3.835 | 7.236 | 4.846 | 3.583 | 4.700 | 8.226 | 6.463 | 6.450 |
| 393.15 | -3.460 | -1.018 | 1.156 | 3.350 | 5.427 | 9.746 | 7.200 | 6.072 | 7.390 | 10.642 | 9.016 | 8.511 |
| 398.15 | -3.703 | -1.366 | 0.686 | 2.752 | 4.697 | 9.446 | 6.652 | 5.606 | 7.005 | 10.193 | 8.599 | 7.972 |
| 403.15 | -4.538 | -2.277 | -0.323 | 1.639 | 3.477 | 8.590 | 5.534 | 4.566 | 6.028 | 9.180 | 7.604 | 6.905 |
| 408.15 | -5.583 | -3.328 | -1.412 | 0.504 | 2.292 | 7.609 | 4.260 | 3.349 | 4.835 | 8.023 | 6.429 | 5.784 |
| 413.15 | -6.233 | -3.969 | -2.085 | -0.209 | 1.534 | 7.035 | 3.389 | 2.534 | 4.040 | 7.271 | 5.655 | 5.079 |
| 423.15 | -8.207 | -5.553 | -3.467 | -1.411 | 0.494 | 5.631 | 1.239 | 0.380 | 1.753 | 5.438 | 3.596 | 3.740 |
| 433.15 | -10.660 | -7.165 | -4.725 | -2.358 | -0.171 | 4.143 | -1.107 | -2.073 | -0.941 | 3.479 | 1.269 | 2.548 |
| 443.15 | - | -3.536 | -1.387 | 0.550 | 2.301 | 8.216 | 2.668 | 2.058 | 3.537 | 7.328 | 5.432 | 5.737 |
| 453.15 | - | -3.644 | -1.741 | -0.108 | 1.326 | 8.226 | 2.218 | 1.849 | 3.490 | 7.034 | 5.262 | 5.209 |
| 463.15 | - | -4.030 | -2.103 | -0.584 | 0.711 | 8.044 | 1.460 | 1.233 | 2.913 | 6.497 | 4.705 | 4.739 |
| 473.15 | - | - | -2.383 | -0.924 | 0.369 | 8.246 | 1.140 | 1.114 | 2.881 | 6.360 | 4.620 | 4.542 |
| **Isotactic PMMA** | | | | | | | | | | | | |
| **T(K)** | **C5** | **C6** | **C7** | **C8** | **C9** | **CCl4** | **CHCl3** | **CH2Cl2** | **Ether** | **THF** | **Ethyl acetate** | **Toluene** |
| 303.15 | -2.464 | 0.378 | 3.263 | 6.216 | 9.168 | 9.117 | 8.350 | 7.391 | 11.311 | 11.815 | 11.071 | 10.831 |
| 313.15 | -4.015 | -1.032 | 1.706 | 4.137 | 7.077 | 7.758 | 6.811 | 5.775 | 9.612 | 9.983 | 9.340 | 9.068 |
| 323.15 | -5.479 | -3.017 | -0.450 | 1.970 | 5.052 | 6.144 | 4.999 | 3.896 | 7.610 | 7.878 | 7.354 | 7.098 |
| 328.15 | -7.072 | -4.241 | -1.625 | 1.049 | 3.848 | 4.964 | 3.636 | 2.483 | 6.001 | 6.389 | 5.971 | 5.942 |
| 333.15 | -9.473 | -6.179 | -3.110 | 0.027 | 2.936 | 3.250 | 1.604 | 0.358 | 3.472 | 4.268 | 4.025 | 4.579 |
| 338.15 | -6.700 | -4.500 | -1.600 | 1.000 | 3.425 | 5.244 | 3.724 | 2.513 | 5.908 | 6.180 | 5.882 | 5.856 |
| 343.15 | -2.964 | -0.420 | 1.881 | 4.231 | 6.695 | 9.053 | 7.491 | 6.274 | 9.684 | 9.782 | 9.520 | 9.355 |
| 348.15 | -3.301 | -0.845 | 1.371 | 3.633 | 5.756 | 8.712 | 7.089 | 5.864 | 9.257 | 9.217 | 9.004 | 8.752 |
| 353.15 | -3.772 | -2.129 | 0.109 | 2.424 | 4.394 | 7.839 | 6.175 | 4.954 | 8.352 | 8.132 | 7.964 | 7.575 |
| 363.15 | -5.137 | -3.344 | -1.414 | 0.742 | 2.616 | 6.657 | 4.803 | 3.557 | 6.805 | 6.450 | 6.421 | 6.037 |
| 373.15 | -6.750 | -4.500 | -2.800 | -0.850 | 1.106 | 5.459 | 3.364 | 2.073 | 5.094 | 4.717 | 4.851 | 4.607 |
| 378.15 | -7.629 | -5.330 | -3.328 | -1.296 | 0.580 | 4.860 | 2.582 | 1.235 | 4.063 | 3.812 | 4.047 | 4.032 |
| 383.15 | -8.240 | -5.940 | -3.925 | -1.877 | 0.271 | 4.393 | 1.956 | 0.564 | 3.230 | 3.056 | 3.382 | 3.534 |
| 388.15 | -9.079 | -6.444 | -4.250 | -2.259 | -0.200 | 3.947 | 1.338 | -0.108 | 2.381 | 2.314 | 2.734 | 3.086 |
| 393.15 | -9.779 | -6.507 | -4.170 | -2.061 | -0.276 | 3.847 | 1.031 | -0.493 | 1.777 | 1.901 | 2.419 | 3.061 |
| 398.15 | -6.475 | -3.508 | -1.443 | 0.410 | 1.952 | 6.898 | 4.095 | 2.632 | 4.955 | 4.760 | 5.326 | 5.697 |
| 403.15 | -6.419 | -3.576 | -1.646 | 0.074 | 1.486 | 6.904 | 4.044 | 2.602 | 4.886 | 4.533 | 5.166 | 5.446 |
| 408.15 | -6.346 | -4.136 | -2.350 | -0.563 | 1.048 | 6.646 | 3.721 | 2.297 | 4.529 | 4.036 | 4.741 | 4.954 |
| 413.15 | -6.509 | -4.404 | -2.727 | -1.043 | 0.689 | 6.476 | 3.458 | 2.035 | 4.182 | 3.612 | 4.395 | 4.609 |
| 423.15 | -7.152 | -4.915 | -3.250 | -1.610 | -0.220 | 6.120 | 2.882 | 1.441 | 3.375 | 2.728 | 3.677 | 3.979 |
| 433.15 | -7.689 | -5.466 | -3.845 | -2.275 | -0.966 | 5.772 | 2.312 | 0.855 | 2.571 | 1.850 | 2.966 | 3.361 |
| 443.15 | - | -5.872 | -4.202 | -2.859 | -1.692 | 5.839 | 2.266 | 0.889 | 2.494 | 1.432 | 2.714 | 2.935 |
| 453.15 | - | -6.457 | -4.741 | -3.440 | -2.336 | 5.510 | 1.700 | 0.303 | 1.667 | 0.562 | 2.020 | 2.373 |
| 463.15 | - | -7.168 | -5.485 | -4.053 | -2.764 | 4.999 | 0.885 | -0.596 | 0.460 | -0.515 | 1.115 | 1.769 |
| 473.15 | - | - | -5.880 | -4.467 | -3.215 | 5.016 | 0.716 | -0.737 | 0.123 | -1.021 | 0.788 | 1.454 |
| **Syndiotactic PMMA** | | | | | | | | | | | | |
| **T(K)** | **C5** | **C6** | **C7** | **C8** | **C9** | **CCl4** | **CHCl3** | **CH2Cl2** | **Ether** | **THF** | **Ethyl acetate** | **Toluene** |
| 303.15 | -2.757 | 0.994 | 3.757 | 6.086 | 8.645 | 9.581 | 10.438 | 10.189 | 11.628 | 10.578 | 9.609 | 9.609 |
| 313.15 | -3.539 | -0.151 | 2.439 | 4.989 | 7.165 | 8.755 | 9.314 | 9.074 | 10.566 | 9.410 | 8.403 | 8.403 |
| 323.15 | -4.487 | -1.955 | 0.508 | 3.027 | 5.468 | 7.446 | 7.726 | 7.510 | 9.072 | 7.771 | 6.675 | 6.675 |
| 328.15 | -5.754 | -2.711 | -0.233 | 2.110 | 4.207 | 6.584 | 6.692 | 6.483 | 8.024 | 6.717 | 5.684 | 5.684 |
| 333.15 | -6.196 | -3.737 | -1.247 | 1.297 | 3.710 | 5.935 | 5.860 | 5.658 | 7.162 | 5.870 | 4.933 | 4.933 |
| 338.15 | -7.300 | -4.797 | -2.222 | 0.531 | 2.832 | 5.041 | 4.752 | 4.545 | 5.962 | 4.754 | 4.013 | 4.013 |
| 343.15 | -8.329 | -5.686 | -3.030 | -0.318 | 2.409 | 4.267 | 3.738 | 3.516 | 4.812 | 3.742 | 3.271 | 3.271 |
| 348.15 | -5.970 | -3.224 | -0.721 | 1.834 | 4.301 | 6.708 | 6.061 | 5.866 | 7.221 | 6.030 | 5.454 | 5.454 |
| 353.15 | -5.718 | -3.124 | -0.780 | 1.611 | 3.860 | 6.871 | 6.131 | 5.978 | 7.423 | 6.057 | 5.306 | 5.306 |
| 363.15 | -6.489 | -4.056 | -1.888 | 0.319 | 2.380 | 6.112 | 5.106 | 5.014 | 6.517 | 4.964 | 4.112 | 4.112 |
| 373.15 | -6.930 | -4.525 | -2.428 | -0.296 | 1.682 | 5.834 | 4.509 | 4.460 | 5.937 | 4.316 | 3.530 | 3.530 |
| 378.15 | -7.352 | -4.518 | -2.421 | -0.500 | 1.136 | 5.746 | 4.267 | 4.244 | 5.715 | 4.045 | 3.278 | 3.278 |
| 383.15 | -7.642 | -5.298 | -3.269 | -1.213 | 0.684 | 5.263 | 3.622 | 3.623 | 5.077 | 3.375 | 2.648 | 2.648 |
| 388.15 | -8.198 | -5.313 | -3.235 | -1.350 | 0.237 | 5.143 | 3.319 | 3.332 | 4.741 | 3.055 | 2.428 | 2.428 |
| 393.15 | -8.631 | -6.195 | -4.120 | -2.024 | -0.095 | 4.588 | 2.569 | 2.585 | 3.933 | 2.294 | 1.804 | 1.804 |
| 398.15 | -9.334 | -6.897 | -4.615 | -2.318 | -0.194 | 4.132 | 1.852 | 1.828 | 3.038 | 1.595 | 1.419 | 1.419 |
| 403.15 | -9.805 | -6.726 | -4.120 | -3.055 | -0.073 | 4.141 | 1.669 | 1.647 | 2.803 | 1.401 | 1.349 | 1.349 |
| 408.15 | -7.088 | -4.516 | -2.185 | 0.148 | 2.296 | 6.722 | 4.059 | 4.039 | 5.143 | 3.781 | 3.847 | 3.847 |
| 413.15 | -4.226 | -2.076 | 0.056 | 2.180 | 4.115 | 9.285 | 6.579 | 6.669 | 7.890 | 6.217 | 6.005 | 6.005 |
| 423.15 | -5.049 | -2.496 | -0.574 | 1.070 | 2.767 | 8.761 | 5.796 | 5.991 | 7.239 | 5.347 | 5.054 | 5.054 |
| 433.15 | -5.996 | -3.165 | -1.273 | 0.312 | 1.935 | 8.193 | 4.870 | 5.096 | 6.258 | 4.384 | 4.275 | 4.275 |
| 443.15 | - | -3.870 | -1.755 | 0.149 | 1.888 | 9.272 | 5.587 | 5.841 | 6.915 | 5.067 | 5.148 | 5.148 |
| 453.15 | - | -1.975 | 0.044 | 1.781 | 3.334 | 10.238 | 6.289 | 6.658 | 7.738 | 5.676 | 5.708 | 5.708 |
| 463.15 | - | -2.435 | -0.278 | 1.430 | 2.929 | 10.058 | 5.751 | 6.155 | 7.146 | 5.100 | 5.316 | 5.316 |
| 473.15 | - | - | -1.119 | 0.617 | 2.110 | 9.731 | 5.154 | 5.678 | 6.660 | 4.409 | 4.602 | 4.602 |

**Table S2.** Values (in kJ/mol) of polar enthalpy ( of polar solvents adsorbed on the various PMMAS as a function of the temperature different temperatures.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Atactic PMMA** | | | | | | | |
| T(K) | CCl4 | CH2Cl2 | CHCl3 | Diethyl ether | THF | Ethyl acetate | Toluene | |
| 303.15 | 9.422 | 14.973 | 11.160 | 15.214 | 17.783 | 15.139 | 11.652 | |
| 313.15 | 9.579 | 14.564 | 10.848 | 14.812 | 17.121 | 14.694 | 11.374 | |
| 323.15 | 9.760 | 14.259 | 10.605 | 14.441 | 16.553 | 14.331 | 11.174 | |
| 328.15 | 9.943 | 14.504 | 10.689 | 14.334 | 16.646 | 14.457 | 11.401 | |
| 333.15 | 10.269 | 15.363 | 11.071 | 14.330 | 17.328 | 15.059 | 12.148 | |
| 338.15 | 10.120 | 14.192 | 10.454 | 13.969 | 16.068 | 14.088 | 11.188 | |
| 343.15 | 10.147 | 13.788 | 10.220 | 13.741 | 15.539 | 13.712 | 10.874 | |
| 348.15 | 10.198 | 13.485 | 10.041 | 13.539 | 15.103 | 13.414 | 10.639 | |
| 353.15 | 10.231 | 13.105 | 9.833 | 13.329 | 14.592 | 13.058 | 10.338 | |
| 363.15 | 10.401 | 12.806 | 9.635 | 12.975 | 14.011 | 12.701 | 10.129 | |
| 373.15 | 10.625 | 12.735 | 9.544 | 12.655 | 13.652 | 12.521 | 10.117 | |
| 378.15 | 10.804 | 12.970 | 9.615 | 12.537 | 13.740 | 12.637 | 10.338 | |
| 383.15 | 10.955 | 13.096 | 9.636 | 12.400 | 13.722 | 12.671 | 10.471 | |
| 388.15 | 11.121 | 13.277 | 9.678 | 12.268 | 13.759 | 12.745 | 10.649 | |
| 393.15 | 11.326 | 13.611 | 9.781 | 12.161 | 13.952 | 12.936 | 10.956 | |
| 398.15 | 11.297 | 13.014 | 9.509 | 11.928 | 13.210 | 12.416 | 10.465 | |
| 403.15 | 11.344 | 12.718 | 9.363 | 11.737 | 12.768 | 12.127 | 10.232 | |
| 408.15 | 11.400 | 12.466 | 9.238 | 11.556 | 12.367 | 11.872 | 10.034 | |
| 413.15 | 11.482 | 12.320 | 9.155 | 11.384 | 12.074 | 11.698 | 9.930 | |
| 423.15 | 11.687 | 12.183 | 9.055 | 11.068 | 11.642 | 11.467 | 9.850 | |
| 433.15 | 11.891 | 12.051 | 8.958 | 10.751 | 11.213 | 11.241 | 9.776 | |
| 443.15 | 11.933 | 11.393 | 8.645 | 10.315 | 10.245 | 10.615 | 9.277 | |
| 453.15 | 12.152 | 11.328 | 8.582 | 10.009 | 9.880 | 10.440 | 9.259 | |
| 463.15 | 12.437 | 11.521 | 8.595 | 9.719 | 9.789 | 10.457 | 9.468 | |
| 473.15 | 12.492 | 11.059 | 8.311 | 9.232 | 9.025 | 9.972 | 9.163 | |
| **Isotactic PMMA** | | | | | | | |
| T(K) | CCl4 | CH2Cl2 | CHCl3 | Diethyl ether | THF | Ethyl acetate | Toluene | |
| 303.15 | 3.3285 | 21.629 | 17.345 | 26.074 | 32.487 | 24.152 | 15.498 | |
| 313.15 | 3.3285 | 21.629 | 17.345 | 26.074 | 32.487 | 24.152 | 15.498 | |
| 323.15 | 3.3285 | 21.629 | 17.345 | 26.074 | 32.487 | 24.152 | 15.498 | |
| 328.15 | 3.3285 | 21.629 | 17.345 | 26.074 | 32.487 | 24.152 | 15.498 | |
| 333.15 | -11.462 | -41.891 | 5.1977 | 14.601 | -28.137 | -25.022 | -37.646 | |
| 338.15 | 20.203 | 93.415 | 52.202 | 38.366 | 101.31 | 79.733 | 76.14 | |
| 343.15 | 9.645 | 40.645 | 36.23 | 29.332 | 64.23 | 45.23 | 59.32 | |
| 348.15 | 7.123 | 37.568 | 32.25 | 27.22 | 51.23 | 41.741 | 42.236 | |
| 353.15 | 5.779 | 30.616 | 20.211 | 26.876 | 41.738 | 31.032 | 23.639 | |
| 363.15 | 5.322 | 25.612 | 17.541 | 22.687 | 27.23 | 22.841 | 17.852 | |
| 373.15 | -1.5944 | -0.3134 | 6.3913 | 20.78 | 11.408 | 7.28 | -2.7642 | |
| 378.15 | -4.44 | -2.445 | 4.77 | 19.041 | 9.456 | 6.211 | -4.33 | |
| 383.15 | -4.22 | -2.041 | 4.22 | 18.854 | 9.114 | 5.987 | -3.887 | |
| 388.15 | -1.5944 | -0.3134 | 6.3913 | 22.346 | 11.408 | 7.28 | -2.7642 | |
| 393.15 | 8.0203 | 38.06 | 21.694 | 27.291 | 49.946 | 36.561 | 30.353 | |
| 398.15 | 9.014 | 43.225 | 25.845 | 32.456 | 54.23 | 40.574 | 36.236 | |
| 403.15 | 9.225 | 42.885 | 24.621 | 31.224 | 53.687 | 40.025 | 35.879 | |
| 408.15 | 9.452 | 41.23 | 23.784 | 30.487 | 52.489 | 38.456 | 34.215 | |
| 413.15 | 8.712 | 38.06 | 21.694 | 27.291 | 49.946 | 36.561 | 30.353 | |
| 423.15 | 4.5731 | 20.904 | 14.931 | 26.295 | 32.989 | 23.507 | 15.07 | |
| 433.15 | 4.5731 | 20.904 | 14.931 | 26.295 | 32.989 | 23.507 | 15.07 | |
| 443.15 | 4.5731 | 20.904 | 14.931 | 26.295 | 32.989 | 23.507 | 15.07 | |
| 453.15 | 4.5731 | 20.904 | 14.931 | 26.295 | 32.989 | 23.507 | 15.07 | |
| 463.15 | 4.5731 | 20.904 | 14.931 | 26.295 | 32.989 | 23.507 | 15.07 | |
| 473.15 | 4.5731 | 20.904 | 14.931 | 26.295 | 32.989 | 23.507 | 15.07 | |
| **Syndiotactic PMMA** | | | | | | | |
| T(K) | CCl4 | CH2Cl2 | CHCl3 | Diethyl ether | THF | Ethyl acetate | Toluene | |
| 303.15 | 4.5566 | 29.181 | 21.728 | 22.08 | 29.193 | 24.901 | 29.768 | |
| 313.15 | 4.5566 | 29.181 | 21.728 | 22.08 | 29.193 | 24.901 | 29.768 | |
| 323.15 | 4.5566 | 29.181 | 21.728 | 22.08 | 29.193 | 24.901 | 29.768 | |
| 328.15 | 4.5566 | 29.181 | 21.728 | 22.08 | 29.193 | 24.901 | 29.768 | |
| 333.15 | -0.927 | 5.1519 | 9.6491 | 17.906 | 6.2739 | -7.4938 | -218.06 | |
| 338.15 | -0.927 | 5.1519 | 9.6491 | 17.906 | 6.2739 | -7.4938 | -218.06 | |
| 343.15 | 7.9129 | 42.342 | 27.246 | 23.996 | 42.172 | 42.973 | 165.43 | |
| 348.15 | 8.552 | 45.224 | 29.334 | 25.228 | 45.362 | 44.887 | 172.23 | |
| 353.15 | 7.9129 | 42.342 | 27.246 | 23.996 | 42.172 | 42.973 | 165.43 | |
| 363.15 | 3.956 | 24.937 | 18.424 | 20.943 | 25.623 | 19.506 | 44.72 | |
| 373.15 | 3.956 | 24.937 | 18.424 | 20.943 | 25.623 | 19.506 | 44.72 | |
| 378.15 | 3.956 | 24.937 | 18.424 | 20.943 | 25.623 | 19.506 | 44.72 | |
| 383.15 | -0.0151 | 14.621 | 13.921 | 18.906 | 15.429 | 5.5251 | 25.686 | |
| 388.15 | -0.0151 | 14.621 | 13.921 | 18.906 | 15.429 | 5.5251 | 25.686 | |
| 393.15 | -0.0151 | 14.621 | 13.921 | 18.906 | 15.429 | 5.5251 | -221.03 | |
| 398.15 | -0.0151 | 14.288 | 14.1 | 18.906 | 8.2202 | -4.2693 | -256.03 | |
| 403.15 | -0.2151 | 12.288 | 13.1 | 18.937 | 7.2202 | -5.2693 | -251.03 | |
| 408.15 | -0.0151 | 14.288 | 14.1 | 20.937 | 8.2202 | -4.2693 | -251.03 | |
| 413.15 | 4.5067 | 26.228 | 18.259 | 20.937 | 27.222 | -4.2693 | -219.03 | |
| 423.15 | 4.5067 | 26.228 | 18.259 | 20.937 | 27.222 | 9.1422 | -0.1906 | |
| 433.15 | 4.5067 | 26.228 | 18.259 | -24.869 | 27.222 | 9.1422 | -0.1906 | |
| 443.15 | 57.439 | 45.479 | 35.913 | -24.869 | 85.88 | 40.42 | 120.38 | |
| 453.15 | 57.439 | 45.479 | 35.913 | 24.77 | 85.88 | 40.42 | 120.38 | |
| 463.15 | 12.446 | 45.479 | 35.913 | 24.77 | 44.851 | 40.42 | 5.5253 | |
| 473.15 | 12.446 | 45.479 | 35.913 | 24.77 | 44.851 | 40.42 | 5.5253 | |

**Table S3.** Values (in kJ/mol) of polar entropy ( of of polar solvents adsorbed on the various PMMAS as a function of the temperature different temperatures.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Atactic PMMA** | | | | | | | |
| T(K) | CCl4 | CH2Cl2 | CHCl3 | Diethyl ether | THF | Ethyl acetate | Toluene | |
| 303.15 | -15.2 | 64.6 | 49.2 | 39.7 | 36.8 | 35.4 | 16.8 | |
| 313.15 | -15.2 | 64.6 | 49.2 | 39.7 | 36.8 | 35.4 | 16.8 | |
| 323.15 | -15.2 | 64.6 | 49.2 | 39.7 | 36.8 | 35.4 | 16.8 | |
| 328.15 | -15.2 | 64.6 | 49.2 | 39.7 | 36.8 | 35.4 | 16.8 | |
| 333.15 | -41.9 | -51.3 | -9.1 | 18.7 | -73.6 | -14.6 | -80.0 | |
| 338.15 | -13.2 | 69.3 | 48.5 | 39.4 | 42.5 | 37.5 | 33.2 | |
| 343.15 | -10.1 | 71.8 | 51.4 | 41.1 | 44.3 | 39.7 | 33.2 | |
| 348.15 | -9.4 | 75.6 | 53.2 | 42.6 | 46.7 | 41.5 | 35.2 | |
| 353.15 | -10.5 | 73.9 | 52.1 | 41.6 | 44.9 | 39.4 | 35.6 | |
| 363.15 | -13.2 | 69.3 | 48.5 | 39.4 | 42.5 | 37.5 | 33.2 | |
| 373.15 | -62.8 | -128.3 | -34.9 | 12.5 | -154.6 | -47.6 | -149.5 | |
| 378.15 | -67.1 | -135.2 | -37.6 | 13.1 | -167.3 | -51.3 | -153.4 | |
| 383.15 | -63.2 | -127.3 | -35.8 | 12.3 | -155.4 | -48.2 | -150.3 | |
| 388.15 | 27.4 | 231.5 | 114.3 | 61.1 | 204.8 | 107.4 | 161.4 | |
| 393.15 | 27.4 | 231.5 | 114.3 | 61.1 | 204.8 | 107.4 | 161.4 | |
| 398.15 | -6.8 | 91.9 | 54.4 | 41.0 | 66.6 | 47.3 | 42.1 | |
| 403.15 | -6.8 | 91.9 | 54.4 | 41.0 | 66.6 | 47.3 | 42.1 | |
| 408.15 | 44.5 | 116.4 | 99.6 | 96.1 | 91.3 | 92.0 | 71.8 | |
| 413.15 | 44.5 | 116.4 | 99.6 | 96.1 | 91.3 | 92.0 | 71.8 | |
| 423.15 | -42.7 | -49.3 | 3.2 | 25.3 | -78.3 | -13.8 | -79.9 | |
| 433.15 | -42.7 | -49.3 | 3.2 | 25.3 | -78.3 | -13.8 | -79.9 | |
| 443.15 | -5.2 | 87.6 | 50.4 | 42.2 | 64.4 | 47.8 | 37.7 | |
| 453.15 | -5.2 | 87.6 | 50.4 | 42.2 | 64.4 | 47.8 | 37.7 | |
| 463.15 | -5.2 | 87.6 | 50.4 | 42.2 | 64.4 | 47.8 | 37.7 | |
| 473.15 | -5.2 | 87.6 | 50.4 | 42.2 | 64.4 | 47.8 | 37.7 | |
| **Isotactic PMMA** | | | | | | | |
| T(K) | CCl4 | CH2Cl2 | CHCl3 | Diethyl ether | THF | Ethyl acetate | Toluene | |
| 303.15 | -20.0 | 22.3 | 20.6 | 35.9 | 48.8 | 30.0 | 12.9 | |
| 313.15 | -20.0 | 22.3 | 20.6 | 35.9 | 48.8 | 30.0 | 12.9 | |
| 323.15 | -20.0 | 22.3 | 20.6 | 35.9 | 48.8 | 30.0 | 12.9 | |
| 328.15 | -20.0 | 22.3 | 20.6 | 35.9 | 48.8 | 30.0 | 12.9 | |
| 333.15 | -65.2 | -171.9 | -16.7 | 0.8 | -136.5 | -120.3 | -149.5 | |
| 338.15 | 29.8 | 234.3 | 123.5 | 72.1 | 252.1 | 194.1 | 192.1 | |
| 343.15 | 15.2 | 94.3 | 57.6 | 55.7 | 110.2 | 89.5 | 77.3 | |
| 348.15 | 15.0 | 81.2 | 51.7 | 54.7 | 95.3 | 84.4 | 59.2 | |
| 353.15 | 13.9 | 69.5 | 44.7 | 49.6 | 81.6 | 77.6 | 44.3 | |
| 363.15 | 10.2 | 42.2 | 24.3 | 38.3 | 61.3 | 45.8 | 25.5 | |
| 373.15 | -32.8 | -35.0 | -8.5 | 26.0 | -15.4 | -25.4 | -50.6 | |
| 378.15 | -44.2 | -49.2 | -15.2 | 20.1 | -13.6 | -24.3 | -49.1 | |
| 383.15 | -42.2 | -47.3 | -14.2 | 19.2 | -9.2 | -19.3 | -47.2 | |
| 388.15 | -32.8 | -35.0 | -8.5 | 26.0 | -6.1 | -14.1 | -34.6 | |
| 393.15 | -8.3 | 62.6 | 30.5 | 38.5 | 92.0 | 60.4 | 66.2 | |
| 398.15 | -4.2 | 80.4 | 43.1 | 48.7 | 123.4 | 88.7 | 65.4 | |
| 403.15 | -4.3 | 75.2 | 41.5 | 47.3 | 120.3 | 85.6 | 60.2 | |
| 408.15 | -4.6 | 73.5 | 37.6 | 45.6 | 111.8 | 82.1 | 52.6 | |
| 413.15 | -6.4 | 70.6 | 30.5 | 38.5 | 100.5 | 70.5 | 49.7 | |
| 423.15 | -8.3 | 55.7 | 27.3 | 27.2 | 84.3 | 55.6 | 38.7 | |
| 433.15 | -16.8 | 20.8 | 13.9 | 36.0 | 50.6 | 28.6 | 12.5 | |
| 443.15 | -16.8 | 20.8 | 13.9 | 36.0 | 50.6 | 28.6 | 12.5 | |
| 453.15 | -16.8 | 20.8 | 13.9 | 36.0 | 50.6 | 28.6 | 12.5 | |
| 463.15 | -16.8 | 20.8 | 13.9 | 36.0 | 50.6 | 28.6 | 12.5 | |
| 473.15 | -16.8 | 20.8 | 13.9 | 36.0 | 50.6 | 28.6 | 12.5 | |
| **Syndiotactic PMMA** | | | | | | | |
| T(K) | CCl4 | CH2Cl2 | CHCl3 | Diethyl ether | THF | Ethyl acetate | Toluene | |
| 303.15 | -17.0 | 41.5 | 26.7 | 22.7 | 43.1 | 38.2 | 60.0 | |
| 313.15 | -17.0 | 41.5 | 26.7 | 22.7 | 43.1 | 38.2 | 60.0 | |
| 323.15 | -17.0 | 41.5 | 26.7 | 22.7 | 43.1 | 38.2 | 60.0 | |
| 328.15 | -17.0 | 41.5 | 26.7 | 22.7 | 43.1 | 38.2 | 60.0 | |
| 333.15 | -33.6 | -31.3 | -9.9 | 10.0 | -26.2 | -59.9 | -681.5 | |
| 338.15 | -33.6 | -31.3 | -9.9 | 10.0 | -26.2 | -59.9 | -681.5 | |
| 343.15 | -7.8 | 77.0 | 41.4 | 27.8 | 78.3 | 87.1 | 435.8 | |
| 348.15 | -5.2 | 81.4 | 52.3 | 31.5 | 87.6 | 95.8 | 470.6 | |
| 353.15 | -7.8 | 77.0 | 41.4 | 27.8 | 78.3 | 87.1 | 435.8 | |
| 363.15 | -18.9 | 28.4 | 16.7 | 19.3 | 32.1 | 21.6 | 92.5 | |
| 373.15 | -18.9 | 28.4 | 16.7 | 19.3 | 32.1 | 21.6 | 92.5 | |
| 378.15 | -18.9 | 28.4 | 16.7 | 19.3 | 32.1 | 21.6 | 92.5 | |
| 383.15 | -29.2 | 1.5 | 5.0 | 13.9 | 5.5 | -14.9 | 41.4 | |
| 388.15 | -29.2 | 1.5 | 5.0 | 13.9 | 5.5 | -14.9 | 41.4 | |
| 393.15 | -24.3 | 2.5 | 8.7 | 18.6 | 7.8 | -11.2 | -620.3 | |
| 398.15 | -29.2 | -0.1 | 5.1 | 13.9 | -13.1 | -40.2 | -664.7 | |
| 403.15 | -29.2 | -0.1 | 5.1 | 19.1 | -13.1 | -40.2 | -664.7 | |
| 408.15 | -29.2 | -0.1 | 5.1 | 19.1 | -7.4 | -40.2 | -664.7 | |
| 413.15 | -17.8 | 30.4 | 15.8 | 19.1 | 34.9 | -10.8 | -617.0 | |
| 423.15 | -17.8 | 30.4 | 15.8 | 12.8 | 34.9 | -3.9 | -18.3 | |
| 433.15 | -17.8 | 30.4 | 15.8 | -86.7 | 34.9 | -3.9 | -18.3 | |
| 443.15 | 99.1 | 71.7 | 53.8 | -86.7 | 164.3 | 65.2 | 254.6 | |
| 453.15 | 99.1 | 71.7 | 53.8 | 27.6 | 164.3 | 65.2 | 254.6 | |
| 463.15 | -0.7 | 71.7 | 53.8 | 27.6 | 72.4 | 65.2 | 1.6 | |
| 473.15 | -0.7 | 71.7 | 53.8 | 27.6 | 72.4 | 65.2 | 1.6 | |

**Table S4.** Values of (London dispersive free energies of organic solvents adsorbed on the various PMMA particles as a function of the temperature for the different tacticities.

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Atactic PMMA** | | | | | | | | | | | | |
| **T(K)** | **C5** | **C6** | **C7** | **C8** | **C9** | **CCl4** | **CHCl3** | **CH2Cl2** | **Ether** | **THF** | **Ethyl acetate** | **Toluene** |
| 303.15 | 16.739 | 19.815 | 22.470 | 26.101 | 28.384 | 19.013 | 12.568 | 15.481 | 15.343 | 13.237 | 15.175 | 18.487 |
| 313.15 | 15.577 | 18.440 | 20.911 | 24.290 | 26.414 | 17.694 | 11.696 | 14.406 | 14.278 | 12.318 | 14.122 | 17.204 |
| 323.15 | 15.121 | 17.900 | 20.298 | 23.579 | 25.640 | 17.175 | 11.354 | 13.984 | 13.860 | 11.957 | 13.708 | 16.700 |
| 328.15 | 15.475 | 18.320 | 20.774 | 24.131 | 26.241 | 17.578 | 11.620 | 14.312 | 14.185 | 12.238 | 14.030 | 17.091 |
| 333.15 | 16.688 | 19.755 | 22.402 | 26.022 | 28.298 | 18.955 | 12.530 | 15.434 | 15.296 | 13.196 | 15.129 | 18.431 |
| 338.15 | 15.362 | 18.185 | 20.621 | 23.954 | 26.048 | 17.449 | 11.534 | 14.207 | 14.080 | 12.147 | 13.927 | 16.966 |
| 343.15 | 14.497 | 17.162 | 19.461 | 22.606 | 24.583 | 16.467 | 10.885 | 13.407 | 13.288 | 11.464 | 13.143 | 16.011 |
| 348.15 | 13.856 | 16.403 | 18.601 | 21.607 | 23.496 | 15.739 | 10.404 | 12.815 | 12.701 | 10.957 | 12.562 | 15.303 |
| 353.15 | 13.389 | 15.850 | 17.974 | 20.878 | 22.704 | 15.208 | 10.054 | 12.383 | 12.273 | 10.588 | 12.139 | 14.788 |
| 363.15 | 12.791 | 15.142 | 17.170 | 19.945 | 21.689 | 14.529 | 9.604 | 11.830 | 11.724 | 10.115 | 11.596 | 14.127 |
| 373.15 | 13.038 | 15.435 | 17.502 | 20.331 | 22.109 | 14.810 | 9.790 | 12.058 | 11.951 | 10.310 | 11.820 | 14.400 |
| 378.15 | 14.781 | 17.497 | 19.841 | 23.048 | 25.063 | 16.789 | 11.098 | 13.670 | 13.548 | 11.688 | 13.400 | 16.324 |
| 383.15 | 17.316 | 20.498 | 23.244 | 27.001 | 29.362 | 19.668 | 13.002 | 16.014 | 15.872 | 13.693 | 15.698 | 19.124 |
| 388.15 | 14.205 | 16.815 | 19.068 | 22.150 | 24.087 | 16.135 | 10.666 | 13.137 | 13.020 | 11.233 | 12.878 | 15.688 |
| 393.15 | 12.495 | 14.792 | 16.773 | 19.484 | 21.188 | 14.193 | 9.382 | 11.556 | 11.453 | 9.881 | 11.328 | 13.800 |
| 398.15 | 11.805 | 13.975 | 15.847 | 18.409 | 20.018 | 13.409 | 8.864 | 10.918 | 10.821 | 9.335 | 10.703 | 13.038 |
| 403.15 | 11.257 | 13.326 | 15.111 | 17.554 | 19.089 | 12.787 | 8.453 | 10.411 | 10.318 | 8.902 | 10.206 | 12.433 |
| 408.15 | 11.053 | 13.085 | 14.838 | 17.236 | 18.743 | 12.555 | 8.299 | 10.222 | 10.131 | 8.741 | 10.021 | 12.207 |
| 413.15 | 10.890 | 12.892 | 14.619 | 16.982 | 18.467 | 12.370 | 8.177 | 10.072 | 9.982 | 8.612 | 9.873 | 12.028 |
| 423.15 | 12.161 | 14.396 | 16.325 | 18.963 | 20.621 | 13.813 | 9.131 | 11.247 | 11.147 | 9.617 | 11.025 | 13.431 |
| 433.15 | 14.559 | 17.234 | 19.543 | 22.702 | 24.687 | 16.537 | 10.931 | 13.464 | 13.344 | 11.513 | 13.199 | 16.079 |
| 443.15 | 11.031 | 13.059 | 14.808 | 17.201 | 18.706 | 12.530 | 8.283 | 10.202 | 10.111 | 8.723 | 10.001 | 12.183 |
| 453.15 | 9.386 | 11.112 | 12.600 | 14.637 | 15.916 | 10.662 | 7.048 | 8.681 | 8.604 | 7.423 | 8.510 | 10.367 |
| 463.15 | 8.933 | 10.575 | 11.991 | 13.929 | 15.147 | 10.146 | 6.707 | 8.261 | 8.188 | 7.064 | 8.098 | 9.866 |
| 473.15 | 7.692 | 9.106 | 10.326 | 11.994 | 13.043 | 8.737 | 5.776 | 7.114 | 7.051 | 6.083 | 6.974 | 8.495 |
| **Isotactic PMMA** | | | | | | | | | | | | |
| **T(K)** | **C5** | **C6** | **C7** | **C8** | **C9** | **CCl4** | **CHCl3** | **CH2Cl2** | **Ether** | **THF** | **Ethyl acetate** | **Toluene** |
| 303.15 | 16.411 | 19.427 | 22.030 | 25.591 | 27.828 | 18.641 | 12.323 | 15.178 | 15.043 | 12.978 | 14.878 | 18.125 |
| 313.15 | 15.408 | 18.239 | 20.683 | 24.026 | 26.127 | 17.501 | 11.569 | 14.250 | 14.123 | 12.184 | 13.968 | 17.017 |
| 323.15 | 14.661 | 17.356 | 19.681 | 22.862 | 24.861 | 16.653 | 11.008 | 13.559 | 13.438 | 11.594 | 13.292 | 16.192 |
| 328.15 | 15.296 | 18.107 | 20.533 | 23.852 | 25.938 | 17.374 | 11.485 | 14.146 | 14.020 | 12.096 | 13.867 | 16.894 |
| 333.15 | 17.508 | 20.726 | 23.503 | 27.301 | 29.689 | 19.887 | 13.146 | 16.192 | 16.048 | 13.845 | 15.873 | 19.337 |
| 338.15 | 14.525 | 17.194 | 19.498 | 22.649 | 24.630 | 16.498 | 10.906 | 13.433 | 13.313 | 11.486 | 13.168 | 16.042 |
| 343.15 | 13.513 | 15.997 | 18.140 | 21.072 | 22.914 | 15.349 | 10.147 | 12.498 | 12.386 | 10.686 | 12.251 | 14.924 |
| 348.15 | 12.749 | 15.092 | 17.114 | 19.880 | 21.619 | 14.481 | 9.573 | 11.791 | 11.686 | 10.082 | 11.558 | 14.081 |
| 353.15 | 11.787 | 13.954 | 15.823 | 18.380 | 19.988 | 13.389 | 8.851 | 10.901 | 10.804 | 9.321 | 10.686 | 13.018 |
| 363.15 | 11.059 | 13.091 | 14.845 | 17.244 | 18.752 | 12.561 | 8.304 | 10.228 | 10.137 | 8.745 | 10.026 | 12.214 |
| 373.15 | 10.923 | 12.931 | 14.663 | 17.033 | 18.522 | 12.407 | 8.202 | 10.102 | 10.012 | 8.638 | 9.903 | 12.064 |
| 378.15 | 11.543 | 13.664 | 15.495 | 17.999 | 19.573 | 13.111 | 8.667 | 10.675 | 10.580 | 9.128 | 10.465 | 12.748 |
| 383.15 | 11.890 | 14.075 | 15.961 | 18.540 | 20.162 | 13.505 | 8.928 | 10.996 | 10.898 | 9.402 | 10.779 | 13.132 |
| 388.15 | 12.377 | 14.651 | 16.614 | 19.300 | 20.987 | 14.058 | 9.293 | 11.447 | 11.345 | 9.787 | 11.221 | 13.669 |
| 393.15 | 13.249 | 15.684 | 17.785 | 20.660 | 22.466 | 15.049 | 9.948 | 12.253 | 12.144 | 10.477 | 12.011 | 14.633 |
| 398.15 | 11.738 | 13.895 | 15.757 | 18.303 | 19.904 | 13.333 | 8.813 | 10.856 | 10.759 | 9.282 | 10.641 | 12.964 |
| 403.15 | 10.997 | 13.018 | 14.762 | 17.148 | 18.647 | 12.491 | 8.257 | 10.170 | 10.080 | 8.696 | 9.970 | 12.145 |
| 408.15 | 10.366 | 12.271 | 13.915 | 16.164 | 17.577 | 11.774 | 7.783 | 9.587 | 9.501 | 8.197 | 9.397 | 11.448 |
| 413.15 | 10.016 | 11.857 | 13.446 | 15.619 | 16.985 | 11.377 | 7.521 | 9.264 | 9.181 | 7.921 | 9.081 | 11.062 |
| 423.15 | 9.699 | 11.481 | 13.019 | 15.123 | 16.446 | 11.016 | 7.282 | 8.970 | 8.890 | 7.669 | 8.793 | 10.711 |
| 433.15 | 9.399 | 11.127 | 12.617 | 14.657 | 15.938 | 10.676 | 7.058 | 8.693 | 8.615 | 7.433 | 8.521 | 10.381 |
| 443.15 | 7.879 | 9.327 | 10.576 | 12.285 | 13.360 | 8.949 | 5.916 | 7.286 | 7.221 | 6.230 | 7.143 | 8.701 |
| 453.15 | 7.752 | 9.177 | 10.407 | 12.088 | 13.146 | 8.806 | 5.821 | 7.170 | 7.106 | 6.130 | 7.028 | 8.562 |
| 463.15 | 8.307 | 9.833 | 11.151 | 12.953 | 14.086 | 9.435 | 6.237 | 7.682 | 7.614 | 6.569 | 7.531 | 9.174 |
| 473.15 | 7.449 | 8.818 | 9.999 | 11.615 | 12.631 | 8.461 | 5.593 | 6.889 | 6.827 | 5.890 | 6.753 | 8.226 |
| **Syndiotactic PMMA** | | | | | | | | | | | | |
| **T(K)** | **C5** | **C6** | **C7** | **C8** | **C9** | **CCl4** | **CHCl3** | **CH2Cl2** | **Ether** | **THF** | **Ethyl acetate** | **Toluene** |
| 303.15 | 15.732 | 18.624 | 21.119 | 24.532 | 26.677 | 17.870 | 11.813 | 14.550 | 14.420 | 12.441 | 14.263 | 17.375 |
| 313.15 | 14.995 | 17.751 | 20.129 | 23.382 | 25.426 | 17.032 | 11.259 | 13.868 | 13.744 | 11.857 | 13.594 | 16.561 |
| 323.15 | 14.041 | 16.622 | 18.849 | 21.895 | 23.810 | 15.949 | 10.543 | 12.986 | 12.870 | 11.103 | 12.730 | 15.508 |
| 328.15 | 13.970 | 16.538 | 18.753 | 21.784 | 23.689 | 15.868 | 10.490 | 12.920 | 12.805 | 11.047 | 12.665 | 15.429 |
| 333.15 | 14.017 | 16.593 | 18.816 | 21.857 | 23.769 | 15.921 | 10.525 | 12.963 | 12.848 | 11.084 | 12.708 | 15.481 |
| 338.15 | 14.452 | 17.108 | 19.399 | 22.535 | 24.505 | 16.415 | 10.851 | 13.365 | 13.246 | 11.428 | 13.102 | 15.961 |
| 343.15 | 15.137 | 17.919 | 20.320 | 23.604 | 25.668 | 17.194 | 11.366 | 13.999 | 13.875 | 11.970 | 13.723 | 16.718 |
| 348.15 | 14.443 | 17.098 | 19.388 | 22.522 | 24.491 | 16.405 | 10.845 | 13.357 | 13.239 | 11.421 | 13.094 | 15.951 |
| 353.15 | 13.481 | 15.959 | 18.097 | 21.022 | 22.860 | 15.313 | 10.122 | 12.468 | 12.357 | 10.661 | 12.222 | 14.889 |
| 363.15 | 12.479 | 14.772 | 16.751 | 19.459 | 21.160 | 14.174 | 9.370 | 11.541 | 11.438 | 9.868 | 11.313 | 13.782 |
| 373.15 | 12.107 | 14.332 | 16.252 | 18.879 | 20.530 | 13.752 | 9.091 | 11.197 | 11.097 | 9.574 | 10.976 | 13.371 |
| 378.15 | 11.860 | 14.040 | 15.921 | 18.494 | 20.111 | 13.471 | 8.905 | 10.969 | 10.871 | 9.379 | 10.752 | 13.099 |
| 383.15 | 11.705 | 13.856 | 15.712 | 18.251 | 19.847 | 13.295 | 8.788 | 10.825 | 10.728 | 9.256 | 10.611 | 12.927 |
| 388.15 | 11.770 | 13.934 | 15.800 | 18.354 | 19.959 | 13.370 | 8.838 | 10.886 | 10.789 | 9.308 | 10.671 | 13.000 |
| 393.15 | 11.991 | 14.195 | 16.096 | 18.698 | 20.333 | 13.620 | 9.003 | 11.090 | 10.991 | 9.482 | 10.871 | 13.243 |
| 398.15 | 12.899 | 15.270 | 17.315 | 20.114 | 21.873 | 14.652 | 9.685 | 11.930 | 11.823 | 10.200 | 11.694 | 14.246 |
| 403.15 | 12.973 | 15.357 | 17.415 | 20.229 | 21.998 | 14.735 | 9.741 | 11.998 | 11.891 | 10.259 | 11.761 | 14.328 |
| 408.15 | 13.731 | 16.255 | 18.433 | 21.412 | 23.284 | 15.597 | 10.310 | 12.699 | 12.586 | 10.858 | 12.449 | 15.165 |
| 413.15 | 11.817 | 13.988 | 15.862 | 18.426 | 20.037 | 13.422 | 8.873 | 10.929 | 10.831 | 9.344 | 10.713 | 13.051 |
| 423.15 | 10.831 | 12.821 | 14.539 | 16.888 | 18.365 | 12.302 | 8.132 | 10.017 | 9.927 | 8.565 | 9.819 | 11.962 |
| 433.15 | 10.914 | 12.920 | 14.651 | 17.019 | 18.507 | 12.397 | 8.195 | 10.094 | 10.004 | 8.631 | 9.894 | 12.054 |
| 443.15 | 10.876 | 12.874 | 14.599 | 16.959 | 18.442 | 12.353 | 8.166 | 10.058 | 9.969 | 8.600 | 9.860 | 12.011 |
| 453.15 | 10.021 | 11.863 | 13.452 | 15.626 | 16.992 | 11.382 | 7.524 | 9.268 | 9.185 | 7.924 | 9.085 | 11.067 |
| 463.15 | 10.098 | 11.953 | 13.555 | 15.745 | 17.122 | 11.469 | 7.582 | 9.339 | 9.255 | 7.985 | 9.154 | 11.152 |
| 473.15 | 9.035 | 10.696 | 12.129 | 14.089 | 15.321 | 10.263 | 6.784 | 8.356 | 8.282 | 7.145 | 8.191 | 9.979 |

**Table S5.** Values of the dispersion coefficient *A* and separation distance *H* of atactic, isotactic and syndiotactic PMMAs as a function of the temperature.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | Dispersion coefficient | | | Separation distance | | |
| T(K) | Atactic PMMA | Isotactic PMMA | Syndiotactic PMMA | Atactic PMMA | Isotactic PMMA | Syndiotactic PMMA |
| 303.15 | 0.30 | 0.29 | 0.28 | 5.00 | 5.02 | 5.05 |
| 313.15 | 0.28 | 0.27 | 0.27 | 5.06 | 5.07 | 5.09 |
| 323.15 | 0.27 | 0.26 | 0.25 | 5.09 | 5.11 | 5.15 |
| 328.15 | 0.27 | 0.27 | 0.25 | 5.07 | 5.08 | 5.15 |
| 333.15 | 0.30 | 0.31 | 0.25 | 5.00 | 4.96 | 5.15 |
| 338.15 | 0.27 | 0.26 | 0.26 | 5.07 | 5.12 | 5.12 |
| 343.15 | 0.26 | 0.24 | 0.27 | 5.12 | 5.18 | 5.08 |
| 348.15 | 0.25 | 0.23 | 0.26 | 5.16 | 5.23 | 5.12 |
| 353.15 | 0.24 | 0.21 | 0.24 | 5.19 | 5.30 | 5.18 |
| 363.15 | 0.23 | 0.20 | 0.22 | 5.23 | 5.36 | 5.25 |
| 373.15 | 0.23 | 0.19 | 0.21 | 5.21 | 5.37 | 5.28 |
| 378.15 | 0.26 | 0.20 | 0.21 | 5.10 | 5.32 | 5.30 |
| 383.15 | 0.31 | 0.21 | 0.21 | 4.97 | 5.29 | 5.31 |
| 388.15 | 0.25 | 0.22 | 0.21 | 5.14 | 5.26 | 5.30 |
| 393.15 | 0.22 | 0.24 | 0.21 | 5.25 | 5.20 | 5.29 |
| 398.15 | 0.21 | 0.21 | 0.23 | 5.30 | 5.30 | 5.22 |
| 403.15 | 0.20 | 0.20 | 0.23 | 5.34 | 5.36 | 5.22 |
| 408.15 | 0.20 | 0.18 | 0.23 | 5.36 | 5.42 | 5.20 |
| 413.15 | 0.19 | 0.18 | 0.21 | 5.37 | 5.45 | 5.30 |
| 423.15 | 0.22 | 0.17 | 0.19 | 5.27 | 5.48 | 5.38 |
| 433.15 | 0.26 | 0.17 | 0.19 | 5.12 | 5.50 | 5.37 |
| 443.15 | 0.20 | 0.14 | 0.19 | 5.36 | 5.67 | 5.37 |
| 453.15 | 0.17 | 0.14 | 0.18 | 5.51 | 5.68 | 5.45 |
| 463.15 | 0.16 | 0.15 | 0.18 | 5.55 | 5.62 | 5.44 |
| 473.15 | 0.14 | 0.13 | 0.16 | 5.69 | 5.72 | 5.54 |

**Table S6.** Values (in mJ/m2) of the polar free energy of the polar molecules adsorbed on the various PMMAs as a function of the temperature different temperatures.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Atactic PMMA** | | | | | | | |
| T(K) | CCl4 | CH2Cl2 | CHCl3 | Diethyl ether | THF | Ethyl acetate | Toluene | |
| 303.15 | 1.47 | 6.72 | 3.41 | 3.01 | 4.39 | 2.72 | 1.08 | |
| 313.15 | 1.58 | 6.40 | 3.29 | 3.05 | 4.43 | 2.74 | 1.09 | |
| 323.15 | 1.69 | 6.14 | 3.17 | 3.05 | 4.49 | 2.75 | 1.11 | |
| 328.15 | 1.73 | 6.06 | 3.10 | 3.01 | 4.54 | 2.73 | 1.15 | |
| 333.15 | 1.74 | 6.03 | 3.03 | 2.91 | 4.62 | 2.69 | 1.20 | |
| 338.15 | 1.83 | 5.83 | 2.99 | 2.98 | 4.62 | 2.73 | 1.19 | |
| 343.15 | 1.91 | 5.67 | 2.94 | 3.03 | 4.63 | 2.76 | 1.19 | |
| 348.15 | 1.99 | 5.52 | 2.90 | 3.06 | 4.66 | 2.78 | 1.19 | |
| 353.15 | 2.07 | 5.39 | 2.85 | 3.08 | 4.69 | 2.79 | 1.20 | |
| 363.15 | 2.23 | 5.16 | 2.76 | 3.10 | 4.77 | 2.82 | 1.23 | |
| 373.15 | 2.36 | 4.99 | 2.65 | 3.05 | 4.88 | 2.81 | 1.30 | |
| 378.15 | 2.35 | 5.02 | 2.57 | 2.89 | 4.99 | 2.74 | 1.38 | |
| 383.15 | 2.30 | 5.11 | 2.47 | 2.67 | 5.12 | 2.65 | 1.48 | |
| 388.15 | 2.53 | 4.81 | 2.48 | 2.90 | 5.08 | 2.77 | 1.42 | |
| 393.15 | 2.72 | 4.60 | 2.47 | 3.04 | 5.09 | 2.84 | 1.40 | |
| 398.15 | 2.86 | 4.46 | 2.45 | 3.10 | 5.14 | 2.88 | 1.41 | |
| 403.15 | 3.00 | 4.34 | 2.42 | 3.14 | 5.18 | 2.91 | 1.43 | |
| 408.15 | 3.14 | 4.25 | 2.42 | 3.17 | 5.20 | 2.93 | 1.47 | |
| 413.15 | 3.25 | 4.15 | 2.34 | 3.15 | 5.32 | 2.95 | 1.49 | |
| 423.15 | 3.36 | 4.09 | 2.22 | 2.98 | 5.51 | 2.90 | 1.61 | |
| 433.15 | 3.37 | 4.12 | 2.05 | 2.70 | 5.73 | 2.79 | 1.76 | |
| 443.15 | 4.04 | 3.70 | 2.07 | 3.03 | 5.86 | 3.01 | 1.77 | |
| 453.15 | 4.64 | 3.42 | 2.07 | 3.24 | 6.03 | 3.16 | 1.82 | |
| 463.15 | 5.13 | 3.23 | 2.01 | 3.29 | 6.25 | 3.24 | 1.93 | |
| 473.15 | 5.98 | 2.97 | 1.98 | 3.47 | 6.59 | 3.42 | 2.06 | |
| **Isotactic PMMA** | | | | | | | |
| T(K) | CCl4 | CH2Cl2 | CHCl3 | Diethyl ether | THF | Ethyl acetate | Toluene | |
| 303.15 | 1.83 | 5.74 | 2.86 | 4.23 | 5.01 | 3.18 | 1.45 | |
| 313.15 | 1.96 | 5.59 | 2.79 | 4.24 | 4.89 | 3.14 | 1.45 | |
| 323.15 | 2.08 | 5.45 | 2.73 | 4.21 | 4.76 | 3.10 | 1.46 | |
| 328.15 | 2.08 | 5.42 | 2.67 | 4.04 | 4.68 | 3.06 | 1.48 | |
| 333.15 | 1.99 | 5.43 | 2.57 | 3.65 | 4.58 | 2.99 | 1.52 | |
| 338.15 | 2.21 | 5.29 | 2.62 | 4.01 | 4.55 | 3.01 | 1.49 | |
| 343.15 | 2.33 | 5.21 | 2.62 | 4.10 | 4.48 | 3.00 | 1.48 | |
| 348.15 | 2.43 | 5.14 | 2.61 | 4.15 | 4.42 | 2.99 | 1.48 | |
| 353.15 | 2.56 | 5.06 | 2.62 | 4.25 | 4.34 | 2.98 | 1.47 | |
| 363.15 | 2.73 | 4.95 | 2.59 | 4.22 | 4.19 | 2.93 | 1.48 | |
| 373.15 | 2.85 | 4.87 | 2.53 | 4.09 | 4.04 | 2.88 | 1.50 | |
| 378.15 | 2.84 | 4.85 | 2.48 | 3.90 | 3.97 | 2.84 | 1.52 | |
| 383.15 | 2.85 | 4.83 | 2.43 | 3.76 | 3.90 | 2.80 | 1.54 | |
| 388.15 | 2.86 | 4.80 | 2.38 | 3.61 | 3.83 | 2.77 | 1.56 | |
| 393.15 | 2.82 | 4.79 | 2.31 | 3.40 | 3.78 | 2.73 | 1.58 | |
| 398.15 | 3.03 | 4.72 | 2.36 | 3.56 | 3.68 | 2.73 | 1.57 | |
| 403.15 | 3.17 | 4.66 | 2.37 | 3.61 | 3.59 | 2.71 | 1.57 | |
| 408.15 | 3.30 | 4.61 | 2.38 | 3.64 | 3.50 | 2.70 | 1.57 | |
| 413.15 | 3.41 | 4.58 | 2.38 | 3.62 | 3.42 | 2.68 | 1.57 | |
| 423.15 | 3.58 | 4.51 | 2.36 | 3.52 | 3.26 | 2.63 | 1.59 | |
| 433.15 | 3.76 | 4.45 | 2.33 | 3.42 | 3.11 | 2.58 | 1.61 | |
| 443.15 | 4.16 | 4.36 | 2.39 | 3.52 | 2.89 | 2.55 | 1.62 | |
| 453.15 | 4.34 | 4.31 | 2.36 | 3.38 | 2.73 | 2.50 | 1.64 | |
| 463.15 | 4.39 | 4.29 | 2.29 | 3.12 | 2.62 | 2.44 | 1.68 | |
| 473.15 | 4.76 | 4.22 | 2.30 | 3.07 | 2.42 | 2.41 | 1.71 | |
| **Syndiotactic PMMA** | | | | | | | |
| T(K) | CCl4 | CH2Cl2 | CHCl3 | Diethyl ether | THF | Ethyl acetate | Toluene | |
| 303.15 | 1.98 | 7.23 | 4.36 | 4.32 | 4.22 | 2.53 | 1.43 | |
| 313.15 | 2.12 | 7.05 | 4.31 | 4.41 | 4.20 | 2.49 | 1.30 | |
| 323.15 | 2.29 | 6.90 | 4.31 | 4.57 | 4.19 | 2.45 | 1.25 | |
| 328.15 | 2.33 | 6.78 | 4.25 | 4.54 | 4.15 | 2.44 | 1.21 | |
| 333.15 | 2.36 | 6.65 | 4.17 | 4.49 | 4.11 | 2.44 | 1.07 | |
| 338.15 | 2.35 | 6.49 | 4.04 | 4.34 | 4.04 | 2.46 | 1.63 | |
| 343.15 | 2.31 | 6.30 | 3.87 | 4.13 | 3.95 | 2.48 | 2.98 | |
| 348.15 | 2.43 | 6.26 | 3.91 | 4.25 | 3.96 | 2.45 | 2.07 | |
| 353.15 | 2.59 | 6.25 | 4.00 | 4.46 | 3.99 | 2.41 | 1.78 | |
| 363.15 | 2.81 | 6.15 | 4.05 | 4.66 | 3.97 | 2.36 | 1.71 | |
| 373.15 | 2.96 | 5.98 | 4.00 | 4.68 | 3.92 | 2.34 | 1.47 | |
| 378.15 | 3.05 | 5.91 | 3.99 | 4.72 | 3.89 | 2.33 | 1.38 | |
| 383.15 | 3.12 | 5.83 | 3.97 | 4.72 | 3.86 | 2.32 | 1.42 | |
| 388.15 | 3.16 | 5.72 | 3.90 | 4.66 | 3.82 | 2.32 | 1.36 | |
| 393.15 | 3.16 | 5.61 | 3.81 | 4.55 | 3.76 | 2.33 | 1.53 | |
| 398.15 | 3.05 | 5.42 | 3.60 | 4.25 | 3.68 | 2.37 | 2.52 | |
| 403.15 | 3.08 | 5.32 | 3.53 | 4.17 | 3.63 | 2.38 | 2.46 | |
| 408.15 | 3.08 | 5.22 | 3.45 | 4.08 | 3.59 | 2.38 | 1.49 | |
| 413.15 | 3.39 | 5.27 | 3.64 | 4.44 | 3.62 | 2.32 | 0.85 | |
| 423.15 | 3.71 | 5.20 | 3.74 | 4.67 | 3.59 | 2.28 | 0.92 | |
| 433.15 | 3.80 | 5.03 | 3.63 | 4.55 | 3.50 | 2.28 | 0.97 | |
| 443.15 | 3.88 | 4.79 | 3.56 | 4.40 | 3.41 | 2.32 | 0.77 | |
| 453.15 | 4.26 | 4.80 | 3.63 | 4.66 | 3.37 | 2.25 | 0.44 | |
| 463.15 | 4.36 | 4.64 | 3.53 | 4.54 | 3.29 | 2.26 | 0.41 | |
| 473.15 | 4.83 | 4.58 | 3.65 | 4.78 | 3.23 | 2.22 | 0.45 | |