**Supplementary Material**

# Adsorption of Helium and Hydrogen on Triphenylene and 1,3,5-Triphenylbenzene

Stefan Bergmeister[1], Siegfried Kollotzek[1], Florent Calvo[2*], Elisabeth Gruber[1], Fabio Zappa[1], Paul Scheier[1], Olof Echt[1,3*]

[1] Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, A-6020 Innsbruck, Austria
[2] Université Grenoble Alpes, CNRS, LiPhy, F-38000 Grenoble, France
[3] Department of Physics, University of New Hampshire, Durham NH 03824, USA
[*] Corresponding authors:
florent.calvo@univ-grenoble-alpes.fr (Florent Calvo), olof.echt@unh.edu (Olof Echt)

Experimental and theoretical results for triphenylene (TPL, $C_{18}H_{12}$) and 1,3,5-triphenylbenzene (TPB, $C_{24}H_{18}$). The two nearly isoenergetic isomers of $TPB^+$ are labeled (s) and (a).

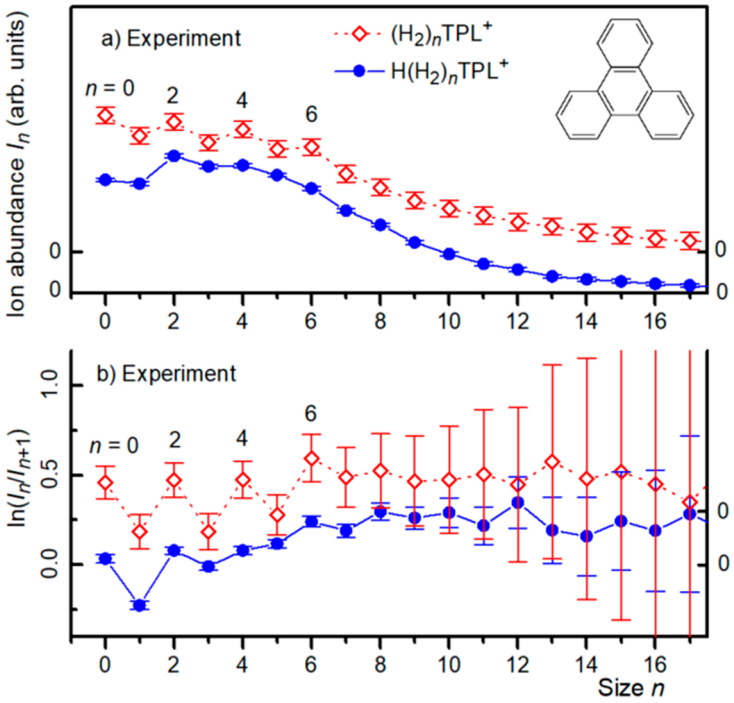



**Figure S1**. Panel a: Ion abundance $I_n$ of $(H_2)_nTPL^+$ and $H(H_2)_nTPL^+$ versus size $n$. Panel b: The 1st derivative of the logarithm of $I_n$. The data sets are stacked for better visibility.

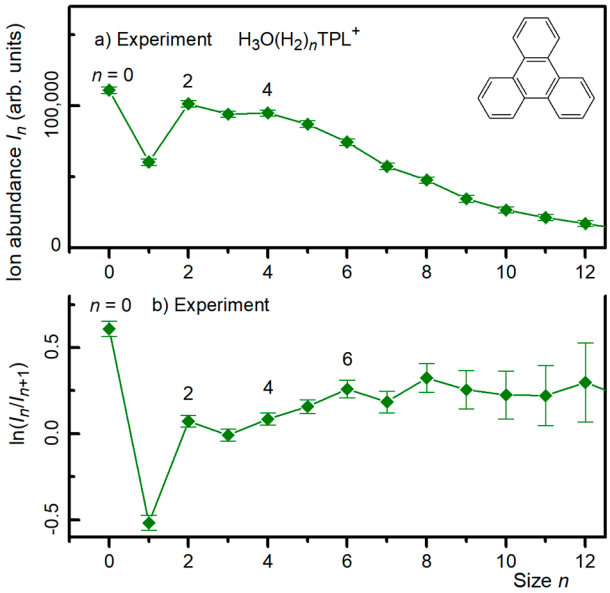



**Figure S2**. Panel a: Ion abundance $I_n$ of $H_3O(H_2)_nTPL^+$ versus size $n$. Panel b: The 1st derivative of ln $I_n$.

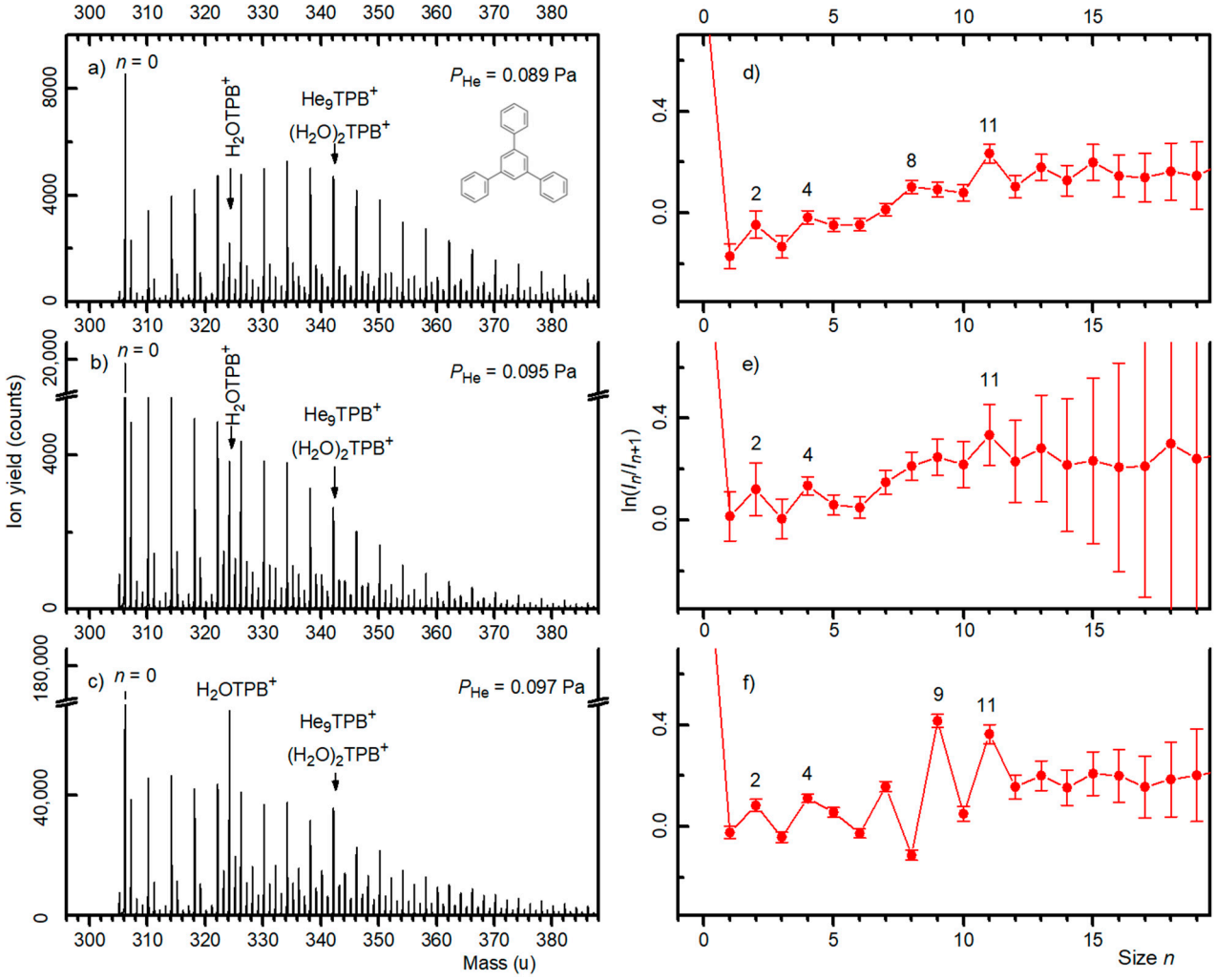



**Figure S3**. Panels a, b, c: Mass spectra of 1,3,5-triphenylbenzene (TPB, $C_{24}H_{18}$, mass 306.141 u) complexed with helium. The $H_2OTPB^+$ mass peak shows that the degree of water contamination increases from a to c. Panels d, e, f: The first derivatives of the logarithm of the ion abundance extracted from the respective mass spectra shown on the left. The local maximum at $n = 9$ in panel f is due to the strong contribution of $(H_2O)_2TPB^+$ which cannot be distinguished from the $He_9TPB^+$ mass peak, but this contribution becomes negligible in panel d as the degree of water contamination decreases.

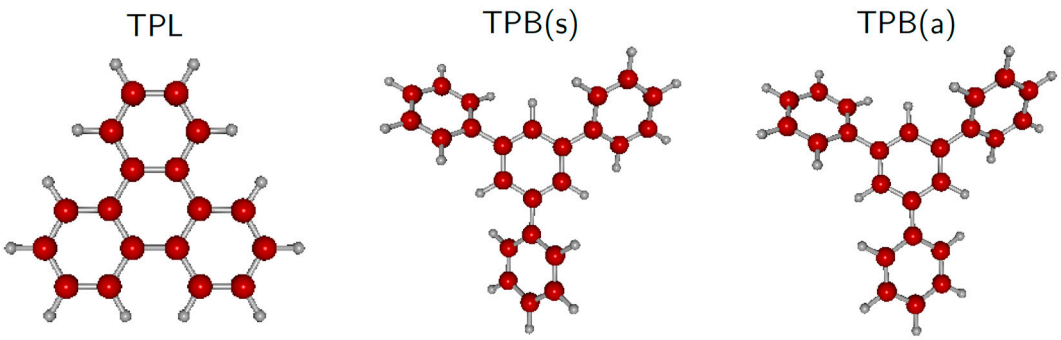
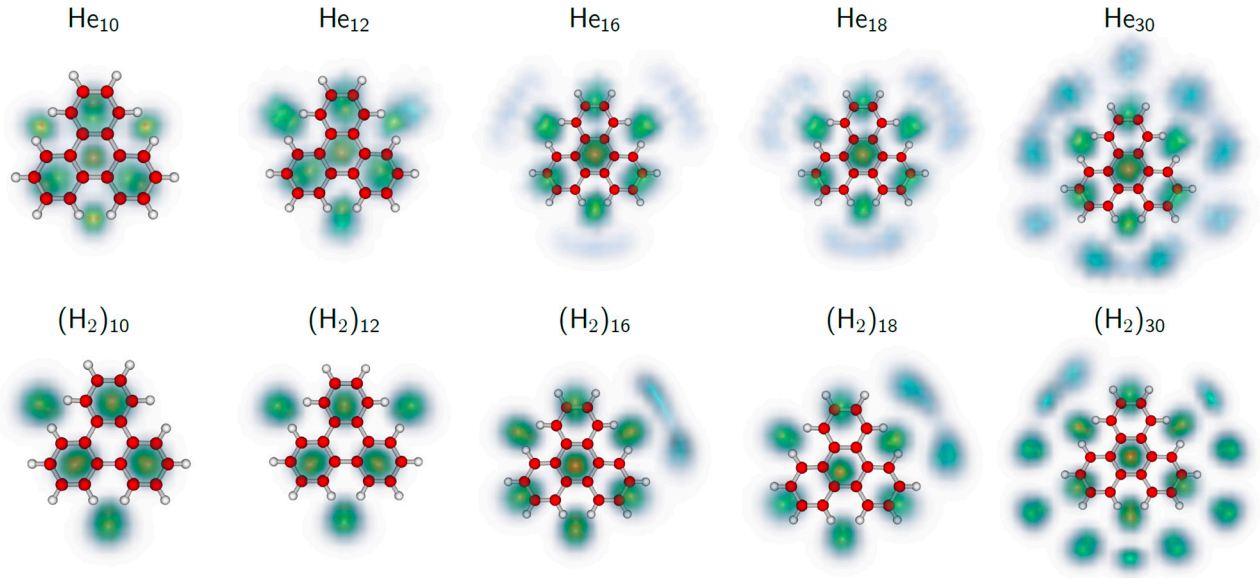



**Figure S4**. Calculated structures of cationic TPL (planar), and the two non-planar isomers of TPB.




**FigureS5.** Selected structures of $He_nTPL^+$ and $(H_2)_nTPL^+$ clusters with $n$ = 10, 12, 16, 18, and 30. For each size, the He and $H_2$ densities obtained from the PIMD simulations are superimposed on the structure of $TPL^+$.

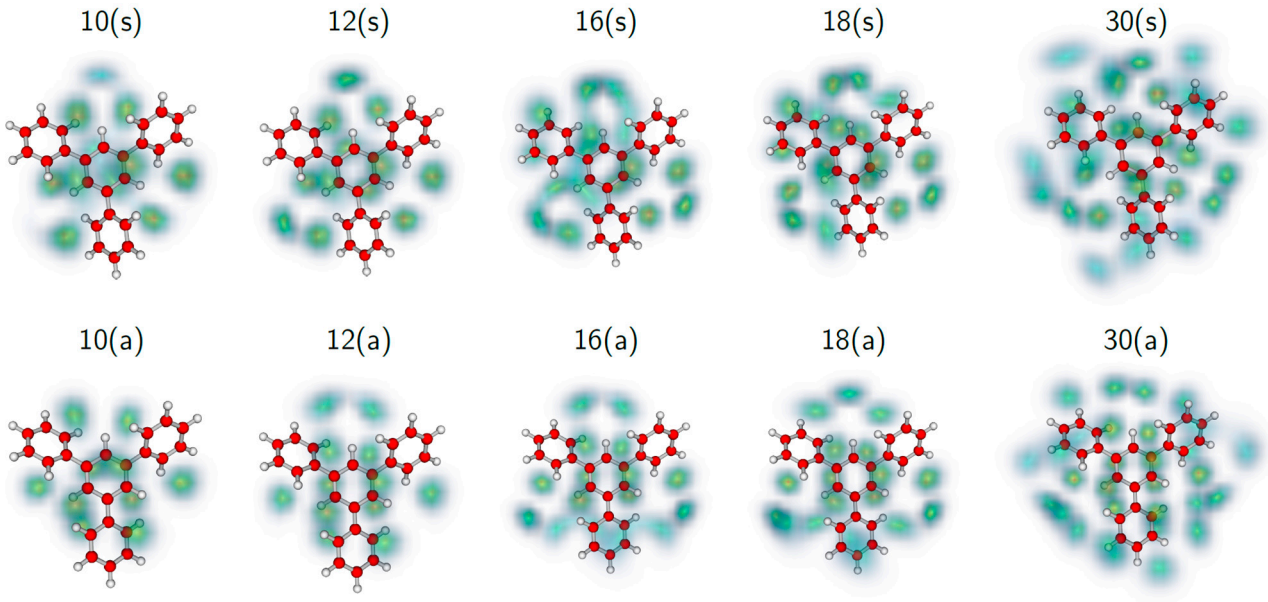


**Figure S6.** Selected structures of $He_nTPB^+$ clusters with $n$ = 10, 12, 16, 18, and 30, for isomers (s) and (a). For each size, the He densities obtained from the PIMD simulations are superimposed on the structure of $TPB^+$. 10(s) denotes $He_{10}TPB(s)^+$, etc.

**Table S1**. Cartesian coordinates ($x$,$y$,$z$) and partial charge ($q$) on each atom of the bare hydrocarbon ion computed with the DFT/wB97xD/6-31+G* method.

**Triphenylene $TPL^+$**

| | *x* | *y* | *z* | *q* |
|---|---|---|---|---|
| C | 1.435823 | 0.005108 | 0.000000 | 0.127033 |
| C | 0.706972 | 1.273432 | 0.000000 | -0.007716 |
| C | -0.706972 | 1.273432 | 0.000000 | -0.007716 |
| C | -1.435823 | 0.005108 | 0.000000 | 0.127033 |
| C | -0.710788 | -1.244503 | 0.000000 | 0.084518 |
| C | 0.710788 | -1.244503 | 0.000000 | 0.084518 |
| C | 2.834163 | -0.044914 | 0.000000 | -0.237909 |
| C | 1.382609 | 2.502772 | 0.000000 | -0.091613 |
| C | -1.382609 | 2.502772 | 0.000000 | -0.091613 |
| C | -2.834163 | -0.044914 | 0.000000 | -0.237909 |
| C | -1.456158 | -2.471008 | 0.000000 | -0.148277 |
| C | 1.456158 | -2.471008 | 0.000000 | -0.148277 |
| C | 0.694465 | 3.711162 | 0.000000 | -0.098722 |
| C | -0.694465 | 3.711162 | 0.000000 | -0.098722 |
| C | -2.821726 | -2.477326 | 0.000000 | -0.137357 |
| C | 2.821726 | -2.477326 | 0.000000 | -0.137357 |
| C | -3.518169 | -1.249832 | 0.000000 | 0.074069 |
| C | 3.518169 | -1.249832 | 0.000000 | 0.074069 |
| H | -3.367187 | -3.414628 | 0.000000 | 0.165842 |
| H | 3.367187 | -3.414628 | 0.000000 | 0.165842 |
| H | 2.464760 | 2.541461 | 0.000000 | 0.141797 |
| H | -2.464760 | 2.541461 | 0.000000 | 0.141797 |
| H | -4.603876 | -1.246213 | 0.000000 | 0.138686 |
| H | -0.940704 | -3.421492 | 0.000000 | 0.163753 |
| H | 0.940704 | -3.421492 | 0.000000 | 0.163753 |
| H | 4.603876 | -1.246213 | 0.000000 | 0.138686 |
| H | 3.417729 | 0.866154 | 0.000000 | 0.167297 |
| H | 1.246141 | 4.645373 | 0.000000 | 0.158599 |
| H | -1.246141 | 4.645373 | 0.000000 | 0.158599 |
| H | -3.417729 | 0.866154 | 0.000000 | 0.167297 |

**1,3,5-triphenylbenzene $TPB(s)^+$**

| | | | | |
|---|---|---|---|---|
| C | 0.595686 | 1.303911 | -0.002677 | 0.095249 |
| C | -1.413338 | -0.091574 | 0.035623 | -0.079394 |
| C | 0.848501 | -1.128688 | -0.031828 | -0.034756 |
| C | -0.821488 | 1.154509 | 0.054149 | -0.076271 |
| C | 1.406184 | 0.132773 | -0.057453 | -0.106144 |
| C | -0.566155 | -1.228065 | 0.005220 | 0.119711 |
| C | 1.198721 | 2.615524 | -0.003488 | 0.038678 |
| C | -2.882571 | -0.260280 | 0.022923 | 0.101480 |
| C | 1.679702 | -2.351236 | -0.019267 | 0.059581 |
| C | 2.498214 | 2.821598 | -0.543632 | 0.012182 |
| C | -3.683924 | 0.584288 | -0.756958 | -0.138572 |
| C | 2.860622 | -2.394571 | 0.734119 | -0.118425 |
| C | 0.512951 | 3.737098 | 0.539592 | -0.164864 |
| C | -3.490666 | -1.264224 | 0.788427 | -0.157242 |
| C | 1.301272 | -3.478360 | -0.761660 | -0.144457 |
| C | 3.069270 | 4.077980 | -0.549411 | -0.033022 |
| C | -5.065685 | 0.429153 | -0.767951 | -0.133514 |

| | | | | |
|---|---|---|---|---|
| C | 3.648653 | -3.540066 | 0.740809 | -0.158424 |
| C | 1.101932 | 4.985161 | 0.553475 | -0.138522 |
| C | -4.873272 | -1.411276 | 0.781885 | -0.137821 |
| C | 2.095743 | -4.619469 | -0.759485 | -0.136842 |
| C | 2.378249 | 5.163476 | 0.004214 | -0.057884 |
| C | -5.662819 | -0.566912 | 0.002576 | -0.089108 |
| C | 3.269363 | -4.652927 | -0.007988 | -0.089591 |
| H | -1.453883 | 2.034681 | 0.081633 | 0.132387 |
| H | 2.485305 | 0.227819 | -0.092400 | 0.143667 |
| H | -1.019486 | -2.215546 | 0.009276 | 0.104006 |
| H | 3.034156 | 1.998257 | -1.002389 | 0.103914 |
| H | -3.224093 | 1.341552 | -1.386904 | 0.127326 |
| H | 3.147112 | -1.543624 | 1.346922 | 0.121114 |
| H | -0.462857 | 3.610301 | 0.995162 | 0.164896 |
| H | -2.888204 | -1.913663 | 1.418672 | 0.138334 |
| H | 0.401002 | -3.457621 | -1.370947 | 0.133786 |
| H | 4.050956 | 4.225371 | -0.986895 | 0.115377 |
| H | -5.676179 | 1.078765 | -1.387204 | 0.152722 |
| H | 4.555019 | -3.567673 | 1.337534 | 0.162166 |
| H | 0.577949 | 5.827492 | 0.992592 | 0.181239 |
| H | -5.335612 | -2.183159 | 1.389009 | 0.157465 |
| H | 1.800723 | -5.482052 | -1.348675 | 0.157389 |
| H | 2.834324 | 6.148618 | 0.007235 | 0.172696 |
| H | -6.741404 | -0.688935 | -0.007746 | 0.148545 |
| H | 3.884305 | -5.547540 | -0.002155 | 0.150941 |

**1,3,5-triphenylbenzene TPB(a)$^{+}$**

| | | | | |
|---|---|---|---|---|
| C | 0.051522 | -1.434786 | 0.010963 | -0.250470 |
| C | -1.269371 | 0.624120 | -0.032158 | -0.384564 |
| C | 1.216357 | 0.717422 | 0.051176 | -0.384565 |
| C | -1.201021 | -0.754391 | -0.023621 | 0.207332 |
| C | 1.250270 | -0.662321 | 0.046021 | 0.207338 |
| C | -0.051465 | 1.349864 | 0.009023 | 0.493514 |
| C | 0.106250 | -2.877115 | 0.006044 | 0.309730 |
| C | -2.558496 | 1.344722 | -0.082626 | 0.325885 |
| C | 2.450656 | 1.529706 | 0.090665 | 0.325879 |
| C | 1.267390 | -3.563372 | -0.444949 | -0.205426 |
| C | -3.656340 | 0.888558 | 0.659604 | -0.280277 |
| C | 3.569787 | 1.151994 | -0.663529 | -0.280271 |
| C | -0.999965 | -3.653887 | 0.448573 | -0.205418 |
| C | -2.700499 | 2.490070 | -0.878230 | -0.333282 |
| C | 2.518913 | 2.682899 | 0.884300 | -0.333274 |
| C | 1.311217 | -4.942791 | -0.462914 | -0.104874 |
| C | -4.871588 | 1.561761 | 0.602980 | -0.074061 |
| C | 4.734650 | 1.910062 | -0.621433 | -0.074064 |
| C | -0.939677 | -5.032837 | 0.449764 | -0.104879 |
| C | -3.919223 | 3.155994 | -0.939637 | -0.040304 |
| C | 3.687918 | 3.434129 | 0.931073 | -0.040307 |
| C | 0.211719 | -5.683706 | -0.011302 | 0.029639 |
| C | -5.005896 | 2.694339 | -0.198554 | -0.104249 |
| C | 4.796482 | 3.050351 | 0.177946 | -0.104249 |
| H | -2.118926 | -1.322900 | -0.121129 | 0.011112 |
| H | 2.207482 | -1.161606 | 0.143964 | 0.011109 |
| H | -0.092322 | 2.435850 | 0.008023 | -0.086156 |
| H | 2.116067 | -3.005968 | -0.825022 | 0.200318 |
| H | -3.550797 | 0.024997 | 1.311454 | 0.187325 |
| H | 3.518678 | 0.282233 | -1.313770 | 0.187323 |
| H | -1.887894 | -3.166537 | 0.835356 | 0.200314 |

| | | | | |
|---|---|---|---|---|
| H | -1.868099 | 2.845880 | -1.480278 | 0.218861 |
| H | 1.669643 | 2.979324 | 1.495023 | 0.218858 |
| H | 2.195163 | -5.452078 | -0.831737 | 0.152385 |
| H | -5.711793 | 1.208573 | 1.192536 | 0.136017 |
| H | 5.591254 | 1.616732 | -1.220222 | 0.136018 |
| H | -1.782771 | -5.611931 | 0.811247 | 0.152387 |
| H | -4.022244 | 4.033764 | -1.569723 | 0.128401 |
| H | 3.735253 | 4.317861 | 1.559575 | 0.128402 |
| H | 0.252691 | -6.768588 | -0.018354 | 0.139117 |
| H | -5.955455 | 3.218416 | -0.242795 | 0.141711 |
| H | 5.706527 | 3.641271 | 0.210790 | 0.141712 |

**Table S2.** Computed energies versus size $n$ for $He_nTPL^+$, $(H_2)_nTPL^+$, $(He)_nTPB(s)^+$, and $(He)_nTPB(a)^+$. Classical energies $E_c$ are listed in meV per atom; total quantum energies $E_q$ are listed in hartree.

**$He_nTPL^+$**

| $n$ | $E_c/n$ (meV) | $E_q$ (har) |
|---|---|---|
| 0 | 0 | 0 |
| 1 | -20.8614 | -0.000547358 |
| 2 | -20.8678 | -0.001095238 |
| 3 | -19.69607 | -0.001514117 |
| 4 | -19.4648 | -0.001936031 |
| 5 | -19.05378 | -0.002348133 |
| 6 | -19.00149 | -0.002771806 |
| 7 | -18.77591 | -0.003121484 |
| 8 | -18.60826 | -0.003481267 |
| 9 | -18.40244 | -0.003809949 |
| 10 | -18.315 | -0.00414966 |
| 11 | -18.2363 | -0.00447712 |
| 12 | -18.11477 | -0.004803059 |
| 13 | -18.04015 | -0.005096007 |
| 14 | -18.02801 | -0.005393754 |
| 15 | -17.60911 | -0.005614286 |
| 16 | -17.2611 | -0.00583146 |
| 17 | -16.98442 | -0.006048502 |
| 18 | -16.69997 | -0.006266072 |
| 19 | -16.46539 | -0.006475996 |
| 20 | -16.27226 | -0.006681098 |
| 21 | -16.06232 | -0.006915579 |
| 22 | -15.86881 | -0.007132551 |
| 23 | -15.71507 | -0.007341397 |
| 24 | -15.55713 | -0.007540491 |
| 25 | -15.42019 | -0.007747757 |
| 26 | -15.30321 | -0.007981299 |
| 27 | -15.18128 | -0.008187127 |
| 28 | -15.05327 | -0.00838678 |
| 29 | -14.96136 | -0.008584397 |
| 30 | -14.85699 | -0.008783918 |
| 31 | -14.76973 | -0.008987686 |
| 32 | -14.69859 | -0.009160633 |
| 33 | -14.61674 | -0.009357977 |
| 34 | -14.54055 | -0.009549094 |
| 35 | -14.46776 | -0.009735707 |
| 36 | -14.39982 | -0.009875835 |
| 37 | -14.33292 | -0.010032477 |
| 38 | -14.26869 | -0.010185185 |
| 39 | -14.20259 | -0.010345545 |
| 40 | -14.14297 | -0.010482762 |
| 41 | -14.07954 | -0.010631475 |
| 42 | -14.01935 | -0.010763064 |
| 43 | -13.96323 | -0.010922564 |
| 44 | -13.90885 | -0.011073517 |
| 45 | -13.81266 | -0.011198673 |
| 46 | -13.71906 | -0.011309316 |
| 47 | -13.64911 | -0.011392151 |
| 48 | -13.56403 | -0.011510629 |
| 49 | -13.4208 | -0.011581119 |
| 50 | -13.27184 | -0.011695085 |

| $(H_2)_n TPL^+$ | | |
|---|---|---|
| 0 | 0 | 0 |
| 1 | -40.24004 | -0.001058501 |
| 2 | -40.30707 | -0.002124176 |
| 3 | -37.60574 | -0.002881821 |
| 4 | -37.29356 | -0.003680061 |
| 5 | -36.44824 | -0.004434703 |
| 6 | -36.32933 | -0.005242985 |
| 7 | -35.87962 | -0.005923754 |
| 8 | -35.56582 | -0.006606863 |
| 9 | -35.12638 | -0.007260163 |
| 10 | -34.79599 | -0.007914293 |
| 11 | -34.49945 | -0.008544275 |
| 12 | -34.27163 | -0.009194343 |
| 13 | -34.02196 | -0.009736447 |
| 14 | -33.81364 | -0.010283942 |
| 15 | -33.1184 | -0.010770767 |
| 16 | -32.58979 | -0.011245971 |
| 17 | -32.25266 | -0.011770618 |
| 18 | -31.97745 | -0.01221868 |
| 19 | -31.67447 | -0.012694915 |
| 20 | -31.27861 | -0.013229421 |
| 21 | -31.04275 | -0.01372147 |
| 22 | -30.79104 | -0.014255316 |
| 23 | -30.59975 | -0.014789229 |
| 24 | -30.41743 | -0.015253224 |
| 25 | -30.2241 | -0.015688048 |
| 26 | -30.07839 | -0.016136315 |
| 27 | -29.91596 | -0.016675612 |
| 28 | -29.72058 | -0.01715919 |
| 29 | -29.59808 | -0.017682648 |
| 30 | -29.51212 | -0.018235005 |
| 31 | -29.4352 | -0.018663137 |
| 32 | -29.36148 | -0.019121178 |
| 33 | -29.20547 | -0.019585011 |
| 34 | -29.0972 | -0.020031517 |
| 35 | -28.97675 | -0.020484282 |
| 36 | -28.8966 | -0.020851754 |
| 37 | -28.78175 | -0.021121692 |
| 38 | -28.71519 | -0.02147632 |
| 39 | -28.61449 | -0.021782685 |
| 40 | -28.54809 | -0.022057304 |
| 41 | -28.44066 | -0.022304596 |
| 42 | -28.33947 | -0.02257148 |
| 43 | -28.22472 | -0.022845181 |
| 44 | -28.11197 | -0.023170903 |
| 45 | -27.98912 | -0.023434787 |
| 46 | -27.87192 | -0.023786507 |
| 47 | -27.64538 | -0.024156059 |
| 48 | -27.48738 | -0.024503527 |
| 49 | -27.38248 | -0.024823783 |
| 50 | -27.22774 | -0.025167675 |

**He$_n$TPB(s)$^+$**

| | | |
|---|---|---|
| 0 | 0 | 0 |
| 1 | -20.25989 | -0.00054031 |
| 2 | -20.19602 | -0.001079057 |
| 3 | -19.88823 | -0.00155473 |
| 4 | -19.71468 | -0.002023737 |
| 5 | -19.49996 | -0.00247013 |
| 6 | -19.44152 | -0.002918442 |
| 7 | -19.37681 | -0.003319861 |
| 8 | -19.29294 | -0.003804082 |
| 9 | -19.26078 | -0.004209689 |
| 10 | -19.22748 | -0.004615411 |
| 11 | -19.10319 | -0.004963977 |
| 12 | -18.99952 | -0.005322297 |
| 13 | -18.71795 | -0.00565743 |
| 14 | -18.47312 | -0.006002205 |
| 15 | -18.25814 | -0.006275776 |
| 16 | -18.06871 | -0.006554958 |
| 17 | -17.89327 | -0.006843786 |
| 18 | -17.74694 | -0.007098658 |
| 19 | -17.5849 | -0.007353675 |
| 20 | -17.41127 | -0.007585567 |
| 21 | -17.26454 | -0.007819499 |
| 22 | -17.1199 | -0.008067557 |
| 23 | -16.95913 | -0.008305041 |
| 24 | -16.84283 | -0.008523977 |
| 25 | -16.68633 | -0.008749012 |
| 26 | -16.56762 | -0.008965266 |
| 27 | -16.42997 | -0.009190869 |
| 28 | -16.2856 | -0.009399621 |
| 29 | -16.16124 | -0.009614626 |
| 30 | -16.03207 | -0.009826197 |
| 31 | -15.92527 | -0.010016702 |
| 32 | -15.81474 | -0.010182927 |
| 33 | -15.68559 | -0.010365035 |
| 34 | -15.55049 | -0.010545762 |
| 35 | -15.42257 | -0.010731735 |
| 36 | -15.31755 | -0.010935995 |
| 37 | -15.21804 | -0.011093011 |
| 38 | -15.11973 | -0.011238642 |
| 39 | -15.01864 | -0.011421468 |
| 40 | -14.91153 | -0.011600522 |
| 41 | -14.82867 | -0.011776797 |
| 42 | -14.74237 | -0.011963397 |
| 43 | -14.65755 | -0.012145241 |
| 44 | -14.55821 | -0.012294772 |
| 45 | -14.47977 | -0.012431973 |
| 46 | -14.41018 | -0.012575623 |
| 47 | -14.34153 | -0.012726256 |
| 48 | -14.25415 | -0.012873228 |
| 49 | -14.15988 | -0.012989036 |
| 50 | -14.05928 | -0.013116044 |

**He$_n$TPB(a)$^+$**

| | | |
|---|---|---|
| 0 | 0 | 0 |
| 1 | -20.28374 | -0.000539961 |
| 2 | -20.26738 | -0.001079358 |
| 3 | -20.0355 | -0.001562377 |
| 4 | -19.88693 | -0.002038663 |
| 5 | -19.79804 | -0.002520117 |
| 6 | -19.72399 | -0.002990341 |
| 7 | -19.58014 | -0.003471211 |
| 8 | -19.49645 | -0.003933237 |
| 9 | -19.39623 | -0.004312556 |
| 10 | -19.32511 | -0.004680517 |
| 11 | -19.18438 | -0.005045411 |
| 12 | -19.06338 | -0.005398148 |
| 13 | -18.82949 | -0.005748929 |
| 14 | -18.64146 | -0.006070642 |
| 15 | -18.45978 | -0.006370628 |
| 16 | -18.32106 | -0.006659893 |
| 17 | -18.16581 | -0.006935685 |
| 18 | -18.05753 | -0.00718876 |
| 19 | -17.8792 | -0.007427514 |
| 20 | -17.70557 | -0.007666182 |
| 21 | -17.49769 | -0.007895204 |
| 22 | -17.33455 | -0.008132428 |
| 23 | -17.16856 | -0.008351251 |
| 24 | -17.03438 | -0.008566937 |
| 25 | -16.8911 | -0.008773608 |
| 26 | -16.75173 | -0.008993611 |
| 27 | -16.6077 | -0.009190753 |
| 28 | -16.47079 | -0.009391346 |
| 29 | -16.31821 | -0.009611487 |
| 30 | -16.18441 | -0.009797021 |
| 31 | -16.05933 | -0.010006887 |
| 32 | -15.94234 | -0.010189926 |
| 33 | -15.81885 | -0.010377213 |
| 34 | -15.70003 | -0.010550935 |
| 35 | -15.56152 | -0.010746968 |
| 36 | -15.43884 | -0.010927416 |
| 37 | -15.31539 | -0.011119454 |
| 38 | -15.206 | -0.011302577 |
| 39 | -15.09393 | -0.011461063 |
| 40 | -14.99226 | -0.011622474 |
| 41 | -14.89381 | -0.011803469 |
| 42 | -14.79963 | -0.011948913 |
| 43 | -14.70622 | -0.01212256 |
| 44 | -14.61358 | -0.012277795 |
| 45 | -14.52531 | -0.012435072 |
| 46 | -14.43951 | -0.012592955 |
| 47 | -14.35404 | -0.012733614 |
| 48 | -14.26712 | -0.012879992 |
| 49 | -14.18234 | -0.013044311 |
| 50 | -14.09481 | -0.013185838 |