Supplemental Information

Adsorption of helium on a charged propeller molecule: Hexaphenylbenzene

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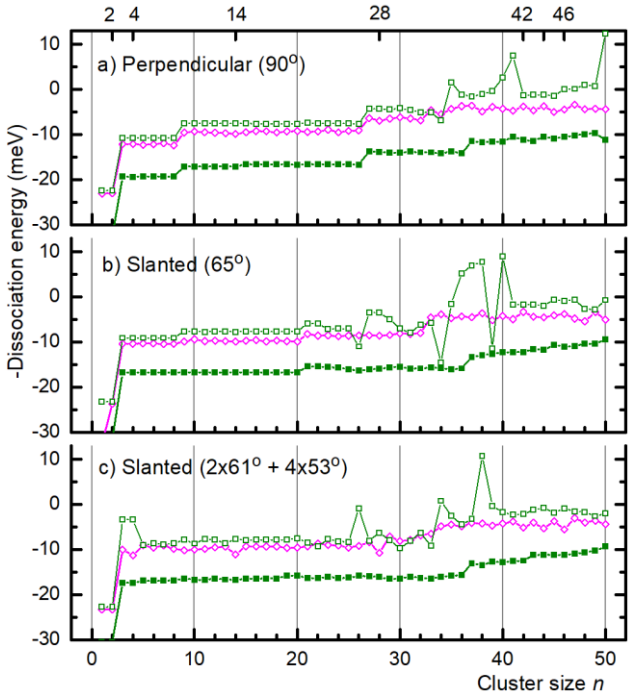

Fig. S1
Negative dissociation energies (=first derivative of the total energy E_n) of He_nHPB^+ clusters calculated from the classical global minima (green full squares), the classical global minima with zero-point energy corrections in the harmonic approximation (green open squares), and the quantum virial energies (magenta open diamonds) for three different orientations of the phenyl groups. Experimentally observed anomalies are indicated along the top ordinate.

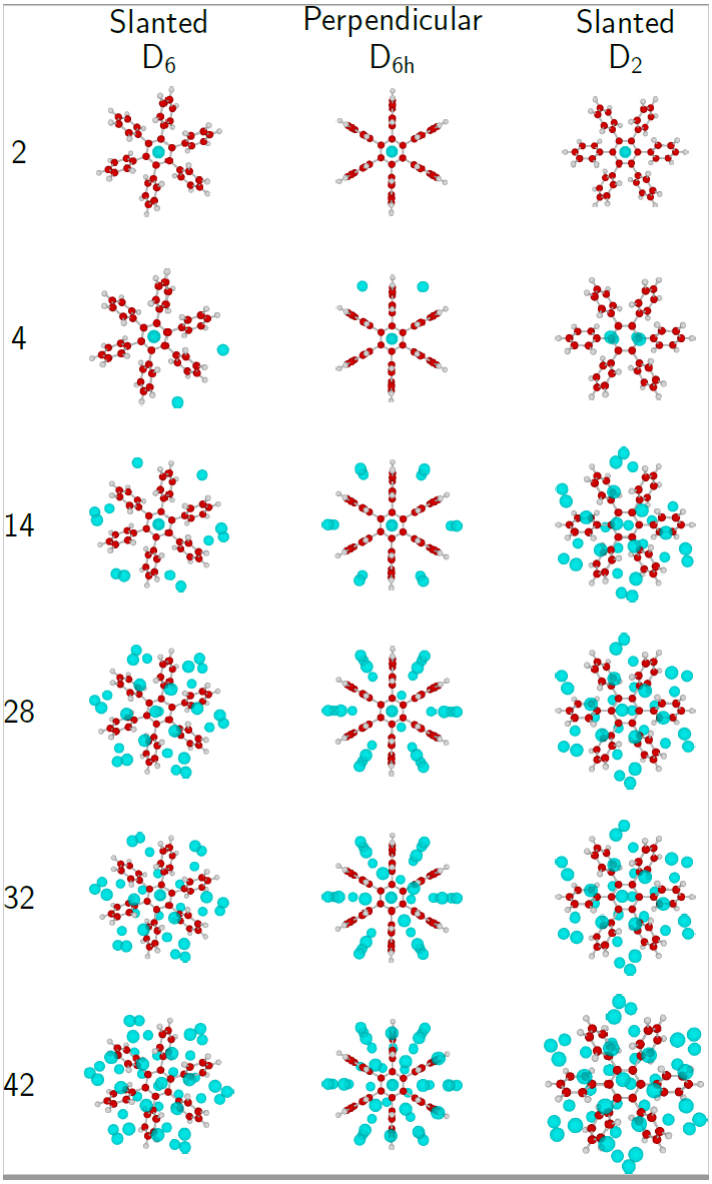

Fig. S2
Selected structures of He_nHPB^+ clusters with n = 2, 4, 14, 28, 32, and 42. For each size, the position of helium atoms (blue) in the classical global minima are shown. In the D_2 slanted cation, the two propeller blades with the angle of 61° are oriented towards the left and right, respectively.

Atomic coordinates and partial charges used for the HPB cations

D6h structure

C	-0.7112	-1.2008	-0.0003	-0.233413
C	-1.3961	0.0143	-0.0002	0.053734
C	0.6836	-1.2154	-0.0004	-0.215919
C	-0.6863	1.2149	-0.0001	-0.184643
C	1.4047	-0.0148	-0.0005	0.121207
C	0.7085	1.2006	-0.0003	-0.249273
C	-1.4538	-2.4560	0.0000	0.468159
C	-2.8543	0.0295	-0.0003	0.356030
C	1.3995	-2.4856	0.0001	0.465792
C	-1.4024	2.4854	-0.0001	0.438836
C	2.8516	-0.0296	-0.0007	0.228050
C	1.4504	2.4556	0.0002	0.453932
C	-1.8029	-3.0462	1.2082	-0.288693
C	-3.5406	0.0365	1.2074	-0.296634
C	1.7360	-3.0832	1.2082	-0.264896
C	-1.7394	3.0830	-1.2079	-0.270647
C	3.5488	-0.0366	-1.2086	-0.196961
C	1.8001	3.0468	-1.2075	-0.261893
C	-1.8032	-3.0466	-1.2078	-0.288773
C	-3.5401	0.0371	-1.2084	-0.296731
C	1.7365	-3.0837	-1.2077	-0.265009
C	-1.7391	3.0827	1.2080	-0.270766
C	3.5490	-0.0365	1.2072	-0.197091
C	1.7991	3.0462	1.2084	-0.261760
C	-2.5133	-4.2467	1.2085	-0.112980
C	-4.9355	0.0511	1.2074	-0.078107
C	2.4208	-4.2986	1.2086	-0.127831
C	-2.4246	4.2981	-1.2077	-0.123403
C	4.9438	-0.0507	-1.2089	-0.152094
C	2.5098	4.2477	-1.2070	-0.121153
C	-2.5136	-4.2470	-1.2075	-0.112882
C	-4.9350	0.0519	-1.2087	-0.078073
C	2.4210	-4.2990	-1.2073	-0.127681
C	-2.4244	4.2977	1.2083	-0.123356
C	4.9439	-0.0504	1.2071	-0.152011
C	2.5087	4.2471	1.2090	-0.121227
C	-2.8686	-4.8470	0.0007	-0.093673
C	-5.6325	0.0589	-0.0008	-0.127402
C	2.7632	-4.9064	0.0008	-0.094395
C	-2.7670	4.9054	0.0003	-0.090207
C	5.6411	-0.0576	-0.0010	-0.054361
C	2.8640	4.8478	0.0013	-0.094403
H	-1.5333	-2.5906	2.1578	0.155314
H	-3.0117	0.0306	2.1572	0.151320
H	1.4762	-2.6221	2.1578	0.144870
H	-1.4797	2.6222	-2.1576	0.150460
H	3.0212	-0.0312	-2.1597	0.132318
H	1.5313	2.5915	-2.1575	0.145561
H	-1.5338	-2.5913	-2.1575	0.155333
H	-3.0109	0.0319	-2.1580	0.151408
H	1.4769	-2.6229	-2.1575	0.144900
H	-1.4792	2.6216	2.1576	0.150479
H	3.0216	-0.0310	2.1583	0.132356

H	1.5296	2.5903	2.1579	0.145527
H	-2.7897	-4.7138	2.1492	0.151153
H	-5.4786	0.0567	2.1478	0.145970
H	2.6871	-4.7714	2.1493	0.154734
H	-2.6913	4.7712	-2.1482	0.153638
H	5.4867	-0.0561	-2.1495	0.158239
H	2.7864	4.7153	-2.1473	0.152186
H	-2.7903	-4.7145	-2.1479	0.151134
H	-5.4778	0.0580	-2.1493	0.145934
H	2.6877	-4.7724	-2.1478	0.154660
H	-2.6911	4.7705	2.1489	0.153643
H	5.4870	-0.0558	2.1476	0.158200
H	2.7845	4.7143	2.1498	0.152183
H	-3.4217	-5.7817	0.0009	0.140408
H	-6.7186	0.0704	-0.0011	0.146341
H	3.2962	-5.8526	0.0010	0.143927
H	-3.3004	5.8514	0.0005	0.141919
H	6.7271	-0.0685	-0.0010	0.135981
H	3.4165	5.7828	0.0017	0.142505

D6 structure

C	3.6319	3.4190	1.0903	-0.150999
C	2.7303	2.3746	1.0959	-0.118134
C	1.8874	2.1789	0.0018	0.104842
C	1.9619	3.0416	-1.0920	-0.083724
C	2.8678	4.0824	-1.0855	-0.171729
C	3.7011	4.2712	0.0026	-0.075197
C	0.9180	1.0599	0.0011	0.047392
C	-0.4589	1.3252	-0.0002	0.096755
C	-1.3771	0.2654	-0.0008	-0.154582
C	-0.9183	-1.0597	-0.0006	0.064933
C	0.4586	-1.3249	-0.0002	0.055403
C	1.3767	-0.2651	-0.0040	-0.147457
C	2.8305	-0.5451	-0.0036	0.144468
C	3.6143	-0.1805	-1.0985	-0.044260
C	4.9687	-0.4438	-1.0919	-0.205507
C	5.5495	-1.0684	-0.0026	-0.095167
C	4.7776	-1.4324	1.0863	-0.182498
C	3.4232	-1.1694	1.0941	-0.110278
C	0.9430	-2.7239	0.0006	0.078806
C	1.6541	-3.2195	-1.0924	-0.052689
C	2.1033	-4.5241	-1.0854	-0.192568
C	1.8493	-5.3403	0.0024	-0.050647
C	1.1446	-4.8547	1.0894	-0.191264
C	0.6951	-3.5502	1.0969	-0.072256
C	-1.8877	-2.1786	-0.0002	0.094912
C	-1.9610	-3.0421	-1.0934	-0.082521
C	-2.8662	-4.0834	-1.0869	-0.183224
C	-3.7004	-4.2718	0.0007	-0.059818
C	-3.6325	-3.4189	1.0879	-0.177687
C	-2.7275	-2.3774	1.0958	-0.077583
C	-2.8308	0.5454	-0.0012	0.126852
C	-3.6146	0.1775	-1.0950	-0.109915
C	-4.9690	0.4408	-1.0891	-0.172623
C	-5.5499	1.0687	-0.0018	-0.100667
C	-4.7779	1.4360	1.0860	-0.189626

C	-3.4235	1.1730	1.0946	-0.054490
C	-0.9433	2.7242	-0.0005	0.048528
C	-1.6532	3.2194	-1.0945	-0.099845
C	-2.1023	4.5239	-1.0886	-0.159337
C	-1.8496	5.3406	-0.0008	-0.065439
C	-1.1462	4.8554	1.0872	-0.173317
C	-0.6967	3.5509	1.0957	-0.069626
H	4.2820	3.5743	1.9387	0.155367
H	2.6776	1.7098	1.9454	0.119470
H	1.3122	2.8950	-1.9421	0.110722
H	2.9267	4.7508	-1.9318	0.156904
H	4.4082	5.0875	0.0031	0.144547
H	3.1618	0.3064	-1.9498	0.084778
H	5.5765	-0.1621	-1.9390	0.157747
H	6.6100	-1.2729	-0.0025	0.144527
H	5.2368	-1.9200	1.9335	0.156487
H	2.8216	-1.4540	1.9447	0.107016
H	1.8524	-2.5835	-1.9425	0.097023
H	2.6539	-4.9089	-1.9310	0.160681
H	2.2023	-6.3610	0.0028	0.140420
H	0.9492	-5.4969	1.9354	0.160123
H	0.1451	-3.1723	1.9460	0.108342
H	-1.3109	-2.8956	-1.9433	0.108770
H	-2.9240	-4.7526	-1.9326	0.160152
H	-4.4078	-5.0879	0.0008	0.142665
H	-4.2866	-3.5709	1.9337	0.158867
H	-2.6755	-1.7122	1.9451	0.104886
H	-3.1622	-0.3121	-1.9447	0.109151
H	-5.5769	0.1565	-1.9353	0.153460
H	-6.6103	1.2733	-0.0022	0.144225
H	-5.2371	1.9262	1.9317	0.153872
H	-2.8219	1.4603	1.9443	0.090614
H	-1.8504	2.5830	-1.9446	0.118412
H	-2.6520	4.9085	-1.9349	0.156338
H	-2.2027	6.3613	-0.0011	0.141682
H	-0.9517	5.4979	1.9333	0.155260
H	-0.1476	3.1733	1.9456	0.109275

D2 structure

C	0.7050	4.9733	0.9847	-0.150999
C	0.7265	3.5891	0.9731	-0.118134
C	0.0017	2.8732	0.0001	0.104842
C	-0.7222	3.5903	-0.9725	-0.083724
C	-0.6989	4.9745	-0.9837	-0.171729
C	0.0034	5.6693	0.0006	-0.075197
C	0.0008	1.4055	-0.0000	0.047392
C	-1.2427	0.6948	-0.0146	0.096755
C	-1.2435	-0.6933	0.0145	-0.154582
C	-0.0007	-1.4055	0.0000	0.064933
C	1.2427	-0.6948	-0.0143	0.055403
C	1.2436	0.6932	0.0145	-0.147457
C	2.5301	1.4457	0.0308	0.144468
C	2.8601	2.3048	-1.0213	-0.044260
C	4.0664	2.9949	-1.0114	-0.205507
C	4.9470	2.8439	0.0552	-0.095167
C	4.6222	1.9927	1.1091	-0.182498

C	3.4242	1.2905	1.0940	-0.110278
C	2.5284	-1.4488	-0.0308	0.078806
C	3.4224	-1.2947	-1.0942	-0.052689
C	4.6197	-1.9982	-1.1094	-0.192568
C	4.9438	-2.8495	-0.0556	-0.050647
C	4.0632	-2.9994	1.0113	-0.191264
C	2.8577	-2.3080	1.0214	-0.072256
C	-0.0017	-2.8733	-0.0000	0.094912
C	0.7218	-3.5901	-0.9732	-0.082521
C	0.6985	-4.9743	-0.9847	-0.183224
C	-0.0035	-5.6693	-0.0003	-0.059818
C	-0.7046	-4.9736	0.9842	-0.177687
C	-0.7261	-3.5893	0.9730	-0.077583
C	-2.5301	-1.4457	0.0311	0.126852
C	-2.8605	-2.3046	-1.0211	-0.109915
C	-4.0668	-2.9945	-1.0108	-0.172623
C	-4.9471	-2.8435	0.0562	-0.100667
C	-4.6218	-1.9925	1.1100	-0.189626
C	-3.4237	-1.2905	1.0946	-0.054490
C	-2.5284	1.4487	-0.0312	0.048528
C	-3.4222	1.2945	-1.0947	-0.099845
C	-4.6195	1.9979	-1.1101	-0.159337
C	-4.9438	2.8493	-0.0563	-0.065439
C	-4.0634	2.9993	1.0107	-0.173317
C	-2.8579	2.3080	1.0210	-0.069626
H	1.2438	5.5132	1.7552	0.155367
H	1.2832	3.0520	1.7318	0.119470
H	-1.2796	3.0541	-1.7314	0.110722
H	-1.2370	5.5153	-1.7540	0.156904
H	0.0041	6.7541	0.0007	0.144547
H	2.1702	2.4321	-1.8499	0.084778
H	4.3164	3.6535	-1.8362	0.157747
H	5.8860	3.3868	0.0657	0.144527
H	5.3061	1.8720	1.9423	0.156487
H	3.1800	0.6159	1.9085	0.107016
H	3.1787	-0.6200	-1.9088	0.097023
H	5.3035	-1.8783	-1.9428	0.160681
H	5.8822	-3.3935	-0.0661	0.140420
H	4.3127	-3.6583	1.8361	0.160123
H	2.1678	-2.4345	1.8501	0.108342
H	1.2789	-3.0537	-1.7321	0.108770
H	1.2363	-5.5149	-1.7554	0.160152
H	-0.0042	-6.7541	-0.0005	0.142665
H	-1.2432	-5.5137	1.7547	0.158867
H	-1.2826	-3.0524	1.7320	0.104886
H	-2.1708	-2.4319	-1.8498	0.109151
H	-4.3172	-3.6530	-1.8355	0.153460
H	-5.8862	-3.3863	0.0668	0.144225
H	-5.3054	-1.8719	1.9435	0.153872
H	-3.1791	-0.6161	1.9091	0.090614
H	-3.1783	0.6198	-1.9092	0.118412
H	-5.3032	1.8780	-1.9436	0.156338
H	-5.8823	3.3932	-0.0669	0.141682
H	-4.3131	3.6580	1.8354	0.155260
H	-2.1681	2.4345	1.8498	0.109275