Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information for:

Theoretical investigations of positron affinities and their structure-dependent properties of carbon dioxide clusters $(CO_2)_n$ (n = 1 – 5)

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Contents:

S1. All the obtained cluster structures.

All the structures are shown below.

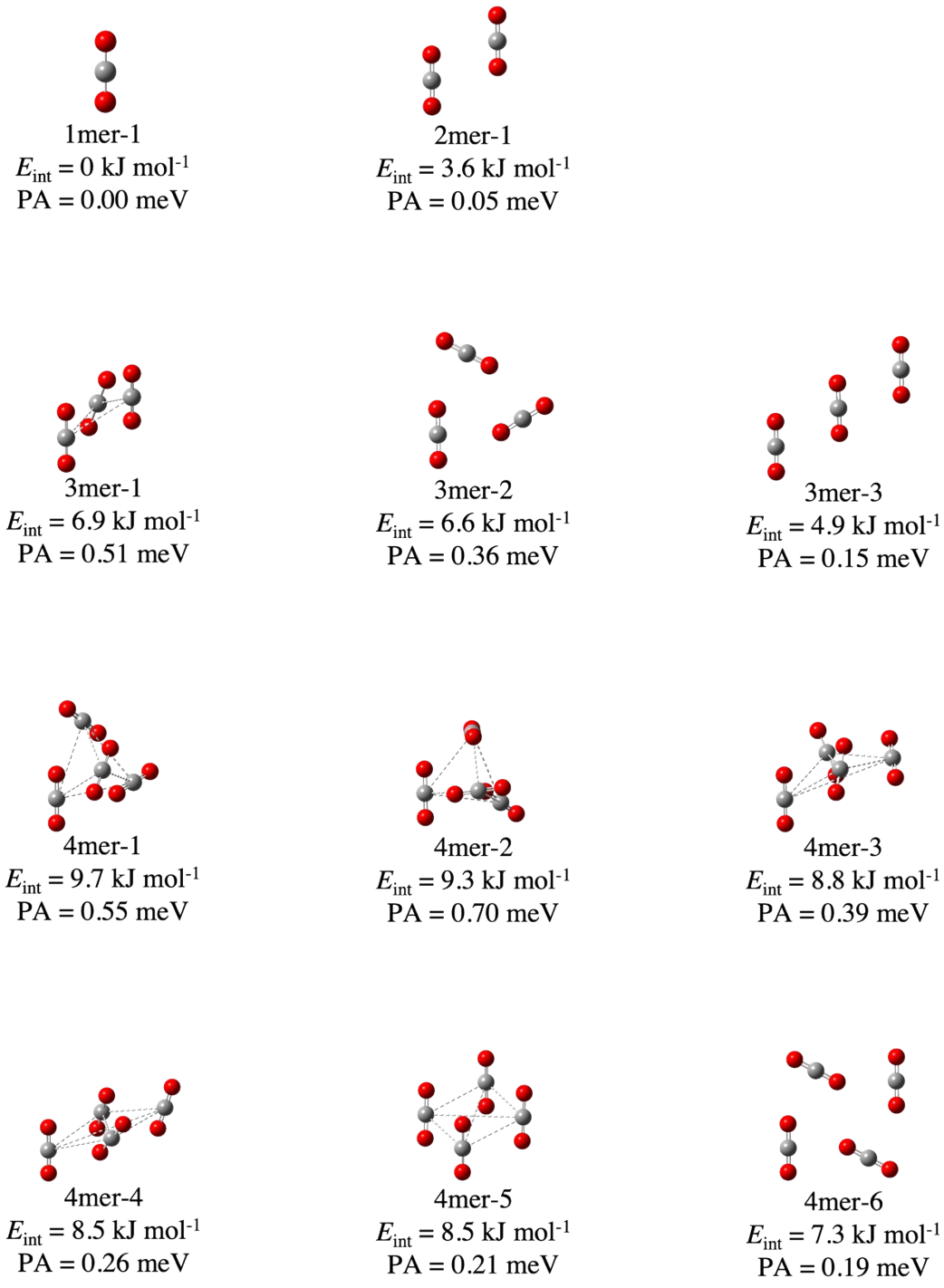
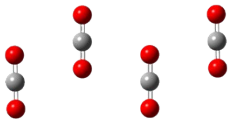


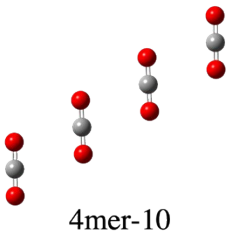
Fig. S1. The obtained $(CO_2)_n$ structures. The name, interaction energy per molecule E_{int}, and PA are shown in the labels. For the three-dimensional structures, dot lines are also shown between carbon atoms.

4mer-7
E_{int} = 6.9 kJ mol^{-1}
PA = 0.61 meV

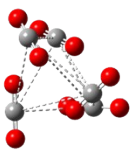


4mer-8
E_{int} = 5.7 kJ mol^{-1}
PA = 0.02 meV

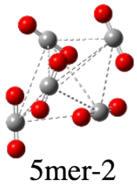
4mer-9
E_{int} = 5.7 kJ mol^{-1}
PA = 0.54 meV



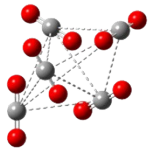
4mer-10
E_{int} = 5.6 kJ mol^{-1}
PA = 0.16 meV



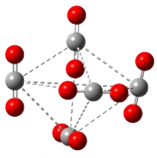
5mer-1
E_{int} = 11.8 kJ mol^{-1}
PA = 0.89 meV



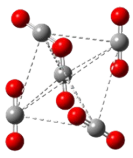
5mer-2
E_{int} = 11.8 kJ mol^{-1}
PA = 0.49 meV



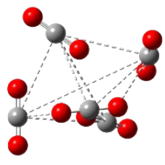
5mer-3
E_{int} = 11.6 kJ mol^{-1}
PA = 0.43 meV



5mer-4
E_{int} = 11.1 kJ mol^{-1}
PA = 0.68 meV

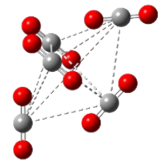


5mer-5
E_{int} = 11.0 kJ mol^{-1}
PA = 0.61 meV



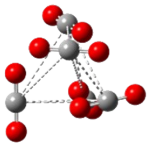
5mer-6
E_{int} = 11.0 kJ mol^{-1}
PA = 0.65 meV

Fig. S1. Continued.

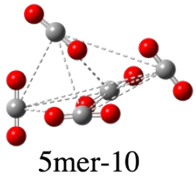


5mer-7
E_{int} = 10.9 kJ mol^{-1}
PA = 0.62 meV

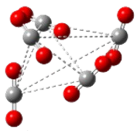
5mer-8
E_{int} = 10.7 kJ mol^{-1}
PA = 0.99 meV



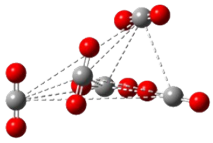
5mer-9
E_{int} = 10.7 kJ mol^{-1}
PA = 0.58 meV



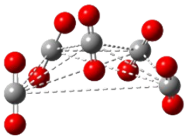
5mer-10
E_{int} = 10.6 kJ mol^{-1}
PA = 0.50 meV



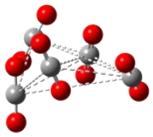
5mer-11
E_{int} = 10.5 kJ mol^{-1}
PA = 0.83 meV



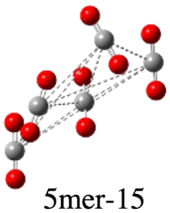
5mer-12
E_{int} = 10.3 kJ mol^{-1}
PA = 1.21 meV



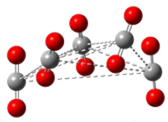
5mer-13
E_{int} = 10.0 kJ mol^{-1}
PA = 1.15 meV



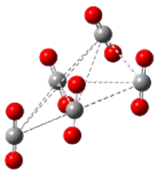
5mer-14
E_{int} = 9.9 kJ mol^{-1}
PA = 0.65 meV



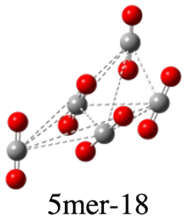
5mer-15
E_{int} = 9.8 kJ mol^{-1}
PA = 1.14 meV



5mer-16
E_{int} = 9.8 kJ mol^{-1}
PA = 1.15 meV

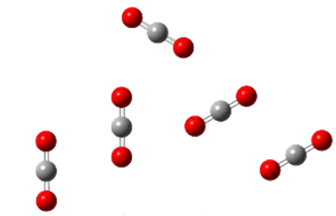


5mer-17
E_{int} = 9.8 kJ mol^{-1}
PA = 0.93 meV

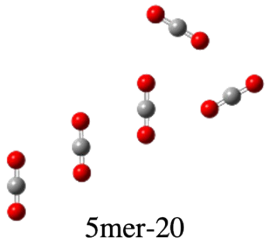


5mer-18
E_{int} = 9.7 kJ mol^{-1}
PA = 1.04 meV

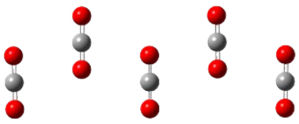
Fig. S1. Continued.



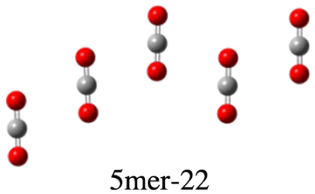
5mer-19
E_{int} = 7.1 kJ mol^{-1}
PA = 1.21 meV



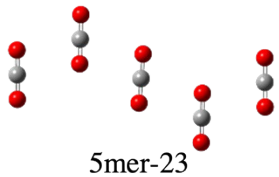
5mer-20
E_{int} = 7.1 kJ mol^{-1}
PA = 1.02 meV



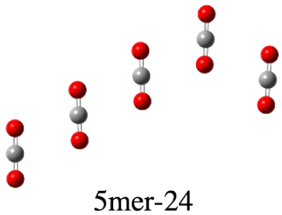
5mer-21
E_{int} = 6.2 kJ mol^{-1}
PA = 0.66 meV



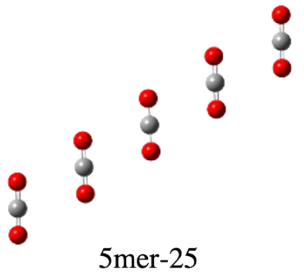
5mer-22
E_{int} = 6.1 kJ mol^{-1}
PA = 1.51 meV



5mer-23
E_{int} = 6.1 kJ mol^{-1}
PA = 0.62 meV



5mer-24
E_{int} = 6.1 kJ mol^{-1}
PA = 0.91 meV



5mer-25
E_{int} = 6.0 kJ mol^{-1}
PA = 0.96 meV

Fig. S1. Continued.

S2. Cartesian coordinates of all the obtained cluster structures.

Table S1. Cartesian coordinates of every CO_2 molecule/cluster in units of Å.

1mer-1

C	0.000000	0.000000	0.000000
O	1.180223	0.000000	0.000000
O	-1.180223	0.000000	0.000000

2mer-1

C	1.710572	0.288876	0.000001
O	0.959910	1.201333	0.000001
O	2.462626	-0.618762	0.000001
C	-1.710572	-0.288876	-0.000001
O	-2.462626	0.618762	-0.000001
O	-0.959910	-1.201333	-0.000001

3mer-1

C	-0.000008	1.909065	0.000005
O	-1.073530	1.908291	-0.490045
O	1.073514	1.908290	0.490055
C	1.737425	-0.952875	-0.387995
O	0.925255	-0.719364	-1.215269
O	2.547353	-1.190154	0.433361
C	-1.737418	-0.952886	0.387990
O	-2.547309	-1.190183	-0.433396
O	-0.925283	-0.719357	1.215293

3mer-2

C	-0.487955	2.252740	0.000045
O	0.243214	3.176935	0.000057
O	-1.230649	1.334614	0.000033
C	-1.706953	-1.548952	-0.000010
O	-2.872913	-1.377838	-0.000023
O	-0.540486	-1.733079	0.000003
C	2.194909	-0.703789	-0.000035
O	2.629699	-1.799097	-0.000054
O	1.771134	0.398466	-0.000016

3mer-3

C	0.000000	0.000007	0.000000
O	0.556939	1.040327	0.000000
O	-0.556940	-1.040313	0.000000
C	-3.467720	-0.062723	0.000000
O	-4.053153	-1.085740	0.000000
O	-2.884098	0.964683	0.000000
C	3.467720	0.062716	0.000000
O	2.884087	-0.964682	0.000000
O	4.053165	1.085726	0.000000

4mer-1

C	-0.906734	2.217580	0.010991
O	1.912284	-0.244714	1.863204
O	-0.393189	-0.746192	1.897129
C	1.923599	-0.224698	-1.266804
O	-1.984304	-0.355186	-0.830775
O	-1.579054	-2.642300	-0.418629
C	-1.776402	-1.498750	-0.621844

O	0.175165	1.743863	0.059117
O	-1.978533	2.702940	-0.032446
C	0.759867	-0.495336	1.878019
O	1.078862	-1.020437	-1.042420
O	2.768521	0.562929	-1.495452

4mer-2

C	0.805334	-1.170430	-1.817459
O	1.381902	1.647992	0.781432
O	0.200420	2.688071	-0.975852
C	0.789574	-0.989547	1.927693
O	-1.203781	-0.002257	-0.005313
O	-3.563307	-0.004845	-0.012179
C	-2.385934	-0.003554	-0.008751
O	1.395141	-0.148470	-1.808159
O	0.212365	-2.189505	-1.838832
C	0.792797	2.163534	-0.101475
O	0.189843	-0.498099	2.816168
O	1.386089	-1.492891	1.042729

4mer-3

C	-0.120567	-1.420599	0.968413
O	3.142307	0.573089	-0.177582
O	2.319040	-1.518562	-0.896923
C	0.260800	1.798663	-0.155374
O	-2.388465	0.579228	0.689816
O	-3.351420	-0.390129	-1.234809
C	-2.869405	0.091534	-0.274378
O	0.596762	-0.720602	1.593357

O	-0.839213	-2.116244	0.344268
C	2.731685	-0.472776	-0.537928
O	0.138927	0.956844	-0.978391
O	0.380178	2.638760	0.659715

4mer-4

C	-0.383180	1.727641	0.002922
O	3.670814	0.336283	-0.902603
O	2.667560	-0.055669	1.197198
C	0.245732	-1.547380	0.251020
O	-2.212215	-0.290945	-1.251220
O	-3.847087	-0.350270	0.450141
C	-3.030212	-0.319400	-0.397508
O	0.573688	1.356894	-0.580986
O	-1.339790	2.097413	0.584781
C	3.167682	0.140646	0.144559
O	-0.470291	-1.148033	1.101524
O	0.957305	-1.946803	-0.599580

4mer-5

C	0.002716	-2.134484	0.403770
O	-0.003915	3.114485	0.206561
O	-0.001512	1.140679	-1.087425
C	2.600596	0.005859	0.016376
O	-2.611067	-1.029937	-0.559711
O	-2.593326	1.029970	0.592170
C	-2.600600	-0.000071	0.016349
O	0.001445	-1.165975	1.083448
O	0.003991	-3.101051	-0.267755

C	-0.002712	2.128600	-0.436229
O	2.613872	-1.024055	-0.559552
O	2.590512	1.035955	0.592065

4mer-6

C	0.038010	2.508762	-0.013745
O	2.489445	-1.041335	0.007942
O	3.731455	0.964467	0.019914
C	-0.038009	-2.508756	-0.013968
O	-2.489441	1.041323	0.007325
O	-3.731461	-0.964466	0.020430
C	-3.105114	0.034382	0.013838
O	-0.550386	3.530055	-0.018759
O	0.634325	1.489673	-0.008826
C	3.105113	-0.034388	0.013890
O	-0.634354	-1.489685	-0.009258
O	0.550416	-3.530032	-0.018781

4mer-7

C	2.439621	2.049455	0.000079
O	1.549949	-1.835721	-0.001279
O	3.900084	-2.043251	0.001740
C	-0.857983	-0.200295	-0.001330
O	-3.642414	1.060264	0.001716
O	-4.976140	-0.887045	0.000330
C	-4.308322	0.084262	0.001019
O	1.947341	3.120075	-0.001154
O	2.944167	0.981654	0.001313
C	2.726861	-1.933231	0.000235

O	-1.532582	-1.168153	-0.002066
O	-0.190539	0.772034	-0.000603

4mer-8

C	-4.551596	-0.262465	0.000191
O	-1.189267	2.235171	-0.000388
O	-1.524285	-0.101123	-0.000133
C	1.356474	-1.069534	-0.000056
O	4.415442	-0.911588	-0.000232
O	4.691136	1.432519	0.000481
C	4.551722	0.262110	0.000123
O	-4.690677	-1.432920	0.000137
O	-4.415650	0.911278	0.000244
C	-1.356600	1.069889	-0.000259
O	1.524273	0.101461	-0.000060
O	1.189028	-2.234798	-0.000049

4mer-9

C	4.240697	-1.261795	0.000167
O	-1.695572	-0.701854	-0.000329
O	-1.140014	1.591868	-0.000149
C	-4.755375	-0.498248	0.000202
O	1.580780	0.185629	-0.000180
O	2.282689	2.439022	-0.000081
C	1.932823	1.315001	-0.000129
O	3.859312	-2.377064	0.000028
O	4.626356	-0.144897	0.000306
C	-1.418061	0.445034	-0.000237
O	-5.058809	-1.637187	-0.000232

O	-4.454805	0.644491	0.000635

4mer-10

C	5.198266	-0.161422	0.000108
O	1.121510	-1.047636	-0.000227
O	2.340171	0.973415	0.000084
C	-1.731070	0.038019	-0.000177
O	-4.556408	1.152658	0.000020
O	-5.841659	-0.826987	0.000261
C	-5.198298	0.160607	0.000139
O	4.555700	-1.153041	0.000356
O	5.842300	0.825738	-0.000143
C	1.731104	-0.037204	-0.000069
O	-2.339864	-0.972762	-0.000382
O	-1.121752	1.048614	0.000029

5mer-1

C	0.183475	-1.204518	2.023275
O	-0.678955	-1.298364	1.221006
O	1.036562	-1.119588	2.830090
C	2.605454	-0.307302	-0.656334
O	3.028088	0.677036	-1.148308
O	2.182178	-1.297745	-0.171815
C	0.476429	2.232467	0.182123
O	0.847408	1.415145	0.951058
O	0.115055	3.050440	-0.583427
C	-2.738719	0.477652	0.146356
O	-3.192707	-0.431667	-0.452582
O	-2.287825	1.390454	0.742723

C	-0.527621	-1.196855	-1.690942
O	-0.758158	-2.344004	-1.812179
O	-0.290911	-0.042791	-1.579925

5mer-2

C	2.837515	0.223970	0.606590
O	2.355631	1.254022	0.921971
O	3.324425	-0.803121	0.292419
C	-0.068985	2.273924	-0.397925
O	-0.754333	1.620219	0.308921
O	0.601832	2.934248	-1.104807
C	-0.632693	-0.853785	1.870283
O	0.406971	-1.147626	1.394660
O	-1.670896	-0.568393	2.349788
C	0.762888	-1.399266	-1.542526
O	0.872407	-0.222677	-1.574536
O	0.659344	-2.571441	-1.518347
C	-2.897524	-0.244363	-0.533150
O	-3.758243	0.537939	-0.349679
O	-2.038039	-1.033530	-0.722845

5mer-3

C	-3.095247	-0.123804	-0.005506
O	-2.392344	0.811109	-0.176911
O	-3.805326	-1.046028	0.171487
C	0.115748	1.829580	-1.283312
O	0.605078	0.792914	-0.992821
O	-0.362611	2.863837	-1.576509
C	0.074349	-2.064968	-0.802865

O	-1.052121	-1.894532	-1.109721
O	1.200405	-2.243739	-0.503435
C	-0.214371	0.500969	1.855955
O	0.006607	1.654386	1.956211
O	-0.450293	-0.651639	1.757001
C	3.121037	-0.145808	0.235037
O	3.659991	-0.244056	-0.808516
O	2.589477	-0.039225	1.283733

5mer-4

C	-2.858826	0.134356	-0.281719
O	-2.996472	1.298391	-0.141071
O	-2.722197	-1.026944	-0.433345
C	-0.000056	0.002416	2.179930
O	1.179504	0.010639	2.181571
O	-1.179617	0.010505	2.181697
C	0.000023	1.943291	-0.851291
O	-0.000037	0.773275	-0.669567
O	0.000081	3.104934	-1.034155
C	0.000040	-2.218340	-0.758586
O	-0.000030	-2.293784	0.419086
O	0.000109	-2.145507	-1.935051
C	2.858821	0.134350	-0.281613
O	2.996410	1.298395	-0.140991
O	2.722248	-1.026960	-0.433215

5mer-5

C	2.397385	1.520163	-0.071678
O	1.313368	1.980472	0.025129

O	3.482211	1.070071	-0.159825
C	0.000287	0.000648	1.802626
O	-1.044497	0.549031	1.805762
O	1.045081	-0.547723	1.805422
C	1.496608	-1.964313	-0.832342
O	1.309475	-0.893467	-1.294672
O	1.685904	-3.033630	-0.375071
C	-1.497062	1.964270	-0.832293
O	-1.309997	0.893165	-1.294036
O	-1.686299	3.033839	-0.375599
C	-2.397218	-1.520766	-0.071092
O	-3.482464	-1.071807	-0.159983
O	-1.312782	-1.979952	0.026457

5mer-6

C	3.005969	-0.360130	-0.128422
O	2.635723	0.595847	-0.713782
O	3.386975	-1.314301	0.448867
C	0.340238	2.379323	-0.886607
O	-0.355672	1.546443	-0.419069
O	1.022589	3.216962	-1.354947
C	-0.000013	-0.000722	2.032218
O	1.139484	0.303385	2.039141
O	-1.139509	-0.304845	2.038769
C	-0.340394	-2.378976	-0.887287
O	-1.023096	-3.216611	-1.355118
O	0.355858	-1.546101	-0.420251
C	-3.005799	0.360507	-0.128352
O	-3.386489	1.314227	0.449890
O	-2.635863	-0.595009	-0.714664

5mer-7

C	3.154062	0.037323	-0.000153
O	2.287558	-0.766704	0.000055
O	4.028043	0.826285	-0.000360
C	-0.000114	-1.140659	-1.798553
O	-0.000068	0.032657	-1.939389
O	-0.000162	-2.310656	-1.663451
C	-0.000021	2.210090	-0.000096
O	1.179342	2.216578	-0.000210
O	-1.179384	2.216620	0.000016
C	0.000154	-1.140261	1.798812
O	0.000112	-2.310243	1.663586
O	0.000197	0.033039	1.939766
C	-3.154082	0.037317	-0.000007
O	-4.028181	0.826149	-0.000327
O	-2.287457	-0.766581	0.000313

5mer-8

C	-0.618612	0.169593	2.081161
O	-0.319479	-0.654665	1.286660
O	-0.917326	0.976262	2.883623
C	2.602482	-0.893858	0.618910
O	2.413013	-0.013706	-0.147082
O	2.795941	-1.767512	1.384663
C	0.774537	2.372278	-0.783080
O	0.189645	2.190256	0.226466
O	1.358504	2.566035	-1.787874
C	-2.886243	-0.460880	-0.318466
O	-2.844745	-1.547780	-0.776349
O	-2.927282	0.623110	0.146698

C	0.126032	-1.187154	-1.605339
O	0.578897	-2.246010	-1.354086
O	-0.325816	-0.125973	-1.857607

5mer-9

C	-3.233908	0.014221	0.019989
O	-3.347867	1.189324	0.044468
O	-3.126182	-1.159651	-0.005619
C	0.574078	-1.968997	-1.180846
O	0.001814	-2.112606	-0.159033
O	1.152947	-1.834837	-2.199658
C	0.023200	-0.330623	2.130277
O	-0.793492	0.330300	1.591759
O	0.839855	-0.979434	2.678492
C	-0.470452	1.652964	-1.028961
O	-0.748304	0.618984	-1.527698
O	-0.188300	2.686943	-0.540156
C	3.107198	0.631435	0.059079
O	4.253403	0.897242	0.097934
O	1.956039	0.364485	0.019858

5mer-10

C	3.538918	0.196987	0.215097
O	3.037994	1.258816	0.334621
O	4.045707	-0.861784	0.098515
C	-0.854595	2.355972	-0.080509
O	-0.098676	1.448129	-0.109720
O	-1.596514	3.269818	-0.050272
C	-0.006111	-0.857548	1.660148

O	1.115890	-1.051493	1.349530
O	-1.127276	-0.668667	1.972482
C	-3.200478	-0.737726	-0.185331
O	-3.012246	0.409743	-0.391407
O	-3.397751	-1.881317	0.018306
C	0.518590	-0.958324	-1.610210
O	-0.542349	-1.370695	-1.294357
O	1.577977	-0.552071	-1.927094

5mer-11

C	3.343247	-0.144221	-0.500324
O	2.853850	-0.978235	-1.178983
O	3.835708	0.689805	0.171204
C	-2.608835	-1.073714	-1.065702
O	-2.254648	0.030190	-0.834839
O	-2.974349	-2.167591	-1.301546
C	0.081843	1.772507	-1.070410
O	0.630703	1.035564	-0.325818
O	-0.456566	2.508956	-1.813759
C	0.686119	-1.680919	0.848541
O	-0.139384	-2.067610	0.099959
O	1.514465	-1.300772	1.596964
C	-1.503989	1.125096	1.790971
O	-1.328003	0.026301	2.183507
O	-1.680565	2.224329	1.401006

5mer-12

C	-3.666022	-0.141870	-0.012984
O	-3.999173	0.180003	-1.097008

O	-3.339054	-0.465556	1.074642
C	2.539619	-0.691325	-1.504270
O	1.540249	-0.258535	-1.043564
O	3.533413	-1.122596	-1.964753
C	-0.666947	-1.645758	0.348578
O	-1.212036	-1.893483	-0.668048
O	-0.115186	-1.407886	1.363263
C	2.075581	0.497066	1.790639
O	2.886698	-0.359834	1.781055
O	1.274321	1.362628	1.796433
C	-0.281739	1.982088	-0.619368
O	-1.103567	1.217308	-0.254827
O	0.533964	2.747801	-0.989137

5mer-13

C	-0.119953	-1.039584	1.117128
O	-0.085823	-0.768245	-0.035716
O	-0.153038	-1.311739	2.260088
C	2.967727	-1.297483	-0.565607
O	2.869613	-1.085934	0.593926
O	3.065556	-1.512923	-1.719169
C	1.713936	1.724377	0.261094
O	1.116365	1.758158	1.279529
O	2.310573	1.685998	-0.754909
C	-2.932824	-1.199186	-0.760859
O	-2.968736	-1.932507	0.163013
O	-2.895274	-0.464649	-1.683664
C	-1.630674	1.815642	-0.052990
O	-2.226717	1.296930	0.824856
O	-1.031177	2.332086	-0.927030

5mer-14

C	1.605340	1.632243	0.743070
O	1.743542	1.884770	1.883843
O	1.465628	1.382771	-0.405635
C	3.289623	-0.982644	-0.587599
O	2.683607	-1.494092	-1.461716
O	3.892729	-0.470918	0.287951
C	-0.000021	-1.304043	0.000247
O	-0.702154	-1.301490	-0.948117
O	0.702115	-1.300781	0.948608
C	-1.605092	1.632330	-0.742987
O	-1.465111	1.382497	0.405598
O	-1.743560	1.885215	-1.883639
C	-3.289851	-0.982427	0.587267
O	-2.684291	-1.494001	1.461627
O	-3.892504	-0.470565	-0.288518

5mer-15

C	3.543347	-0.991050	0.541717
O	4.281552	-1.512428	-0.213110
O	2.803014	-0.469803	1.302817
C	-2.092856	1.719935	-0.027526
O	-1.897845	1.034422	-0.971532
O	-2.290035	2.404162	0.909738
C	1.825644	1.736206	-0.477419
O	2.810473	1.545898	-1.097330
O	0.840533	1.925989	0.144986
C	-3.289923	-1.476567	-0.206007
O	-3.951331	-0.807195	0.505658
O	-2.627563	-2.146456	-0.916926

C	0.013806	-0.987936	0.167478
O	0.689698	-1.119536	-0.790838
O	-0.658507	-0.855493	1.127854

5mer-16

C	3.438917	-0.918554	0.099864
O	3.196397	-0.425912	1.146365
O	3.684766	-1.411955	-0.941332
C	-2.230776	1.474951	-0.175688
O	-1.580064	0.904151	-0.982971
O	-2.880696	2.043440	0.623552
C	1.091746	2.123064	-0.683512
O	1.629691	1.126614	-1.018166
O	0.553870	3.117470	-0.349286
C	-2.511572	-2.084373	-0.274001
O	-2.697716	-1.399136	0.671890
O	-2.331140	-2.767050	-1.216374
C	0.214359	-0.594937	1.035264
O	0.016316	0.403828	1.631478
O	0.406572	-1.591564	0.433398

5mer-17

C	-3.679615	-0.195108	-0.357316
O	-4.435273	-0.793024	0.319424
O	-2.924052	0.408478	-1.038435
C	-0.905712	1.694101	0.798577
O	-1.246223	0.795596	1.485462
O	-0.568980	2.590734	0.111137
C	-0.491591	-1.299216	-0.595267

O	-1.267527	-2.091414	-0.197506
O	0.283791	-0.504677	-1.000280
C	2.319992	1.560076	-0.108149
O	2.023317	1.129129	0.952663
O	2.616169	1.990277	-1.162996
C	2.759517	-1.760351	0.266440
O	3.581712	-1.198614	-0.366487
O	1.935123	-2.326111	0.893805

5mer-18

C	-3.644202	-1.009298	-0.210242
O	-4.317737	-0.813814	0.736437
O	-2.972021	-1.208605	-1.161574
C	1.892998	1.486021	0.733847
O	0.965204	1.403148	1.460265
O	2.818878	1.565577	0.008452
C	-1.218771	2.067881	-0.459351
O	-2.025892	1.439704	0.130384
O	-0.411015	2.695179	-1.046214
C	3.250797	-1.469236	-0.183093
O	2.648230	-1.449969	0.834471
O	3.851283	-1.492996	-1.195784
C	-0.279741	-1.072165	0.118492
O	0.244777	-0.570914	-0.815126
O	-0.802517	-1.569712	1.048947

5mer-19

C	-0.170546	3.449637	0.000102
O	-1.136515	4.124391	0.000610

O	0.804671	2.783456	-0.000411
C	-4.990743	-1.668691	-0.000135
O	-5.073018	-2.844535	-0.000622
O	-4.912546	-0.489734	0.000353
C	-1.873043	-0.161333	0.000276
O	-1.963752	-1.337511	-0.000119
O	-1.790211	1.015214	0.000670
C	4.941046	-1.792437	0.000544
O	6.006658	-1.288590	-0.000172
O	3.874659	-2.301220	0.001261
C	2.093127	0.172941	-0.000781
O	1.032827	-0.343525	-0.000370
O	3.157346	0.681968	-0.001204

5mer-20

C	-3.962684	2.063296	0.000209
O	-3.453920	3.126166	-0.000083
O	-4.483531	1.003331	0.000505
C	-4.307293	-1.914367	0.000244
O	-5.481919	-2.007982	0.001076
O	-3.129114	-1.833322	-0.000588
C	-0.698451	-0.235946	-0.000647
O	-1.351781	0.745868	-0.000463
O	-0.037448	-1.213218	-0.000830
C	6.215954	0.123811	0.000515
O	6.861999	-0.862054	0.000678
O	5.571537	1.114191	0.000354
C	2.752199	-0.036567	-0.000325
O	2.124863	0.962873	-0.000226
O	3.379521	-1.036023	-0.000421

5mer-21

C	5.968788	-0.697916	0.001930
O	5.949788	-1.876447	0.001432
O	5.991307	0.483453	0.002433
C	2.979602	1.048850	-0.000535
O	2.990840	-0.134048	-0.001075
O	2.967868	2.226027	-0.000001
C	-0.000082	-0.701933	-0.002756
O	-0.000108	-1.879152	-0.003402
O	-0.000056	0.481049	-0.002113
C	-5.968655	-0.698080	0.001963
O	-5.949298	-1.876610	0.001740
O	-5.991534	0.483287	0.002190
C	-2.979651	1.049081	-0.000600
O	-2.967830	2.226255	-0.000204
O	-2.990976	-0.133814	-0.001001

5mer-22

C	2.962053	0.447147	0.000053
O	3.204475	-0.707660	0.000083
O	2.718941	1.601888	0.000023
C	6.268982	-0.598232	-0.000089
O	6.003646	0.553203	-0.000123
O	6.537243	-1.745964	-0.000054
C	-0.361411	1.414271	0.000070
O	-0.680775	2.547322	0.000049
O	-0.040370	0.275664	0.000090
C	-6.108913	-0.193118	-0.000089
O	-6.410649	0.946292	-0.000133
O	-5.809749	-1.336210	-0.000045

C	-2.760829	-1.070099	0.000055
O	-2.435773	-2.201553	0.000086
O	-3.086900	0.067042	0.000023

5mer-23

C	3.175967	1.377820	0.000530
O	3.346265	2.542632	0.001008
O	3.004403	0.207350	0.000052
C	5.856053	-0.808766	-0.000536
O	5.651943	-1.969638	-0.001102
O	6.064123	0.354370	0.000029
C	0.000125	0.000710	0.000101
O	-0.100445	-1.175018	-0.000026
O	0.100695	1.176439	0.000238
C	-5.856750	0.807620	-0.000450
O	-6.064067	-0.355657	0.000502
O	-5.653388	1.968628	-0.001402
C	-3.175395	-1.377383	0.000351
O	-3.004387	-0.206829	-0.000248
O	-3.345144	-2.542277	0.000950

5mer-24

C	-3.705982	-1.223171	0.000214
O	-4.184025	-2.298935	0.000915
O	-3.225066	-0.142359	-0.000496
C	-5.695346	1.605782	0.000805
O	-5.184507	2.668008	0.000102
O	-6.210615	0.542436	0.001511
C	-0.277851	-0.730116	-0.001457

O	0.121624	0.380254	-0.002415
O	-0.677247	-1.840469	-0.000505
C	6.549947	0.462539	0.001380
O	6.981886	1.559207	0.000857
O	6.120327	-0.638203	0.001910
C	3.129133	-0.115005	-0.000940
O	2.735751	-1.227597	-0.000251
O	3.521946	0.997637	-0.001629

5mer-25

C	-3.462095	0.042178	-0.000108
O	-4.063481	-0.973001	-0.000849
O	-2.860025	1.057121	0.000628
C	-6.930624	0.139332	0.000144
O	-6.295318	1.135619	0.000955
O	-7.567399	-0.852518	-0.000666
C	-0.000007	0.000557	-0.000113
O	0.597164	1.018320	0.000261
O	-0.597179	-1.017206	-0.000501
C	6.930648	-0.140274	0.000101
O	7.567827	0.851321	-0.001106
O	6.294935	-1.136307	0.001307
C	3.462080	-0.041793	-0.000012
O	2.859626	-1.056510	0.000717
O	4.063848	0.973159	-0.000755

S3. Table of all the properties.

Table S2. Properties of all the structures. The structure name, positron affinity PA (in meV), dipole moment μ (in debye), quadrupole moment Q (in buckingham), dipole polarizability α (in bohr^3), flatness F (dimension-less), surface area S (in Å^2), and interaction energy E_{int} (in kJ mol^{-1}) are shown from left to right.

name	PA	μ	Q	α	F	S	E_{int}
1mer-1	0.00	0.00	3.27	13.93	1.00	0.00	0.00
2mer-1	0.05	0.00	7.05	28.09	1.00	47.61	3.62
3mer-1	0.51	0.02	9.46	42.28	0.82	117.91	6.88
3mer-2	0.36	0.00	5.43	43.34	1.00	221.51	6.61
3mer-3	0.15	0.00	10.42	42.18	1.00	126.05	4.94
4mer-1	0.55	0.15	7.16	57.61	0.46	54.07	9.67
4mer-2	0.70	0.35	0.92	57.77	0.12	56.20	9.26
4mer-3	0.39	0.10	11.65	56.30	0.83	54.02	8.75
4mer-4	0.26	0.15	11.86	56.69	0.90	54.36	8.53
4mer-5	0.21	0.01	13.43	56.50	0.90	65.42	8.53
4mer-6	0.19	0.00	9.26	58.36	1.00	123.45	7.33
4mer-7	0.61	0.02	7.70	57.48	1.00	136.82	6.93
4mer-8	0.02	0.00	13.75	55.90	1.00	108.75	5.72
4mer-9	0.54	0.01	13.67	56.05	1.00	132.86	5.67
4mer-10	0.16	0.00	5.32	56.28	1.00	65.96	5.62
5mer-1	0.89	0.08	8.18	71.68	0.45	67.83	11.78
5mer-2	0.49	0.15	8.91	72.06	0.62	71.97	11.76
5mer-3	0.43	0.25	4.21	72.15	0.68	74.10	11.56
5mer-4	0.68	0.23	6.07	71.52	0.58	70.35	11.11
5mer-5	0.61	0.03	11.16	72.04	0.73	78.72	10.97
5mer-6	0.65	0.06	5.46	73.01	0.68	88.84	10.96
5mer-7	0.62	0.03	8.29	72.03	0.70	76.54	10.87
5mer-8	0.99	0.12	8.02	71.61	0.41	74.56	10.69
5mer-9	0.58	0.57	3.15	72.40	0.64	79.68	10.68
5mer-10	0.50	0.22	9.43	72.58	0.78	84.75	10.60
5mer-11	0.83	0.32	8.31	71.79	0.65	85.24	10.52

5mer-12	1.21	0.46	3.17	72.22	0.71	87.84	10.32
5mer-13	1.15	0.11	13.41	70.15	0.76	83.36	10.01
5mer-14	0.65	0.05	13.30	70.26	0.81	82.91	9.94
5mer-15	1.14	0.28	14.47	70.82	0.92	97.96	9.80
5mer-16	1.15	0.16	14.28	70.62	0.85	98.86	9.79
5mer-17	0.93	0.21	14.57	70.59	0.90	92.73	9.77
5mer-18	1.04	0.17	14.35	70.74	0.89	96.67	9.75
5mer-19	1.21	0.01	9.28	71.63	1.00	308.60	7.14
5mer-20	1.02	0.02	10.54	71.60	1.00	225.70	7.08
5mer-21	0.66	0.01	17.09	69.77	1.00	187.45	6.16
5mer-22	1.51	0.01	17.06	69.94	1.00	191.78	6.11
5mer-23	0.62	0.00	17.02	69.90	1.00	217.23	6.11
5mer-24	0.91	0.01	17.00	70.13	1.00	222.69	6.07
5mer-25	0.96	0.00	17.16	70.39	1.00	105.43	6.03

S4. The result of regression analysis with μ and α (μ-α model).

In the section 3.3 in the main paper, we discuss the relation between PA and several electrostatic and structural properties. The result of linear regression analysis for PA with μ and α is summarized here. Determination coefficient R^2 is 0.45, which indicates that it is an insufficient regression model. Akaike information criterion AIC is 17.1 which shows that it is an inadequate model compared with μ-Q-α model and μ-Q-α-struct model. Obtained regression equation is,

$$PA_{reg} = -0.51 + 0.10\mu + 0.0183\alpha, \quad \text{(s4.1)}$$

where PA_{reg} means fitted PA with linear regression analysis.

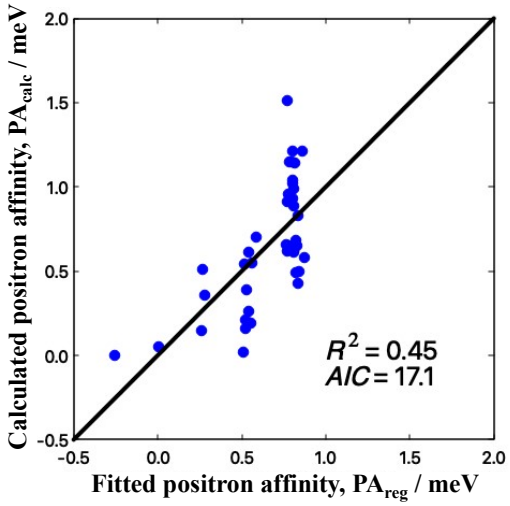


Fig. S2. The result of regression analysis to explain PA with the magnitude of permanent dipole moment μ and polarizability α, refer to as μ-α model. The horizontal axis shows predicted PA by regression analysis (PA_{reg}) and the vertical axis shows first-principle calculated PA (PA_{calc}). The diagonal line indicates the identical line where $PA_{calc} = PA_{reg}$

S5. Discussion on the standardized regression analyses.

In this section, the validity of every explanatory variable in the three regression models (μ-α, μ-Q-α, and μ-Q-α-struct models) are discussed, and thus validities for μ-Q-α and μ-Q-α-struct models are confirmed.

The validities of the variables can be verified by the following standardization process. Every property X is standardized as,

$$X^{\mathrm{std}} = \frac{X - \overline{X}}{\sigma(X)}, \tag{s5.1}$$

where, X^{std}, $\overline{X}$, and $\sigma(X)$ indicate the standardized variable of X, the averaged value of X, and the standard deviation of X respectively, and where X = PA, μ, Q, α, F, and S.

The standardized regression models of μ-α, μ-Q-α, and μ-Q-α-struct are expressed as,

$$PA_{reg}^{std} = 0.04\mu^{\mathrm{std}} + 0.66\alpha^{\mathrm{std}}, \tag{s5.2}$$

$$PA_{reg}^{std} = 0.18\mu^{\mathrm{std}} + 0.23Q^{\mathrm{std}} + 0.54\alpha^{\mathrm{std}}, \tag{s5.3}$$

and,

$$PA_{reg}^{std} = 0.29\mu^{\mathrm{std}} + 0.34Q^{\mathrm{std}} + 0.30\alpha^{\mathrm{std}} - 0.27F^{\mathrm{std}} + 0.40S^{\mathrm{std}}, \tag{s5.4}$$

respectively, where PA_{reg}^{std} is the fitted value for PA^{std}. Generally, the larger values of absolute coefficients, which are to be in the range from 0 to 1, are more meaningful. The absolute coefficients of μ^{std} in μ-α model in Eq. (s5.2) is small reflecting the low accuracy of μ-α model. In the models of μ-Q-α and μ-Q-α-struct, absolute values of all the coefficients are large enough indicating every respective validity. Especially, the absolute coefficients of F and S, which are added in μ-Q-α-struct model, is obviously non-zero indicating the validity of structural parameters.