

Electronic Supplementary Information

Unexpectedly Strong Xe Binding by Host-Guest Interaction

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Supplementary Figures (Figure S1 to Figure S3)

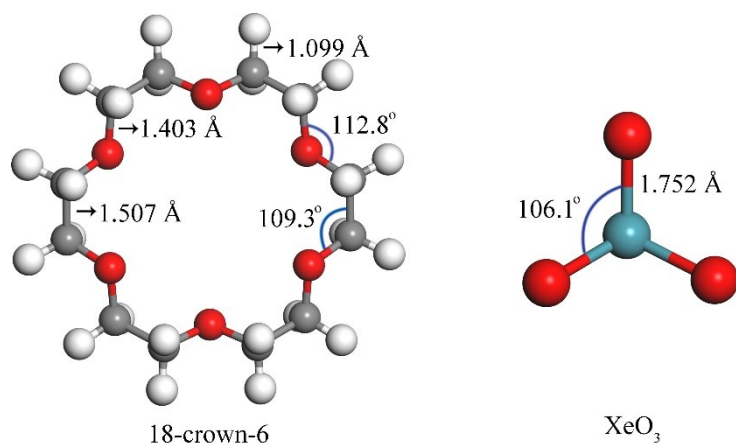


Figure S1. Optimized geometries and key structural parameters of 18-crown-6 and XeO₃ at M06-2X/def2-TZVPP level.

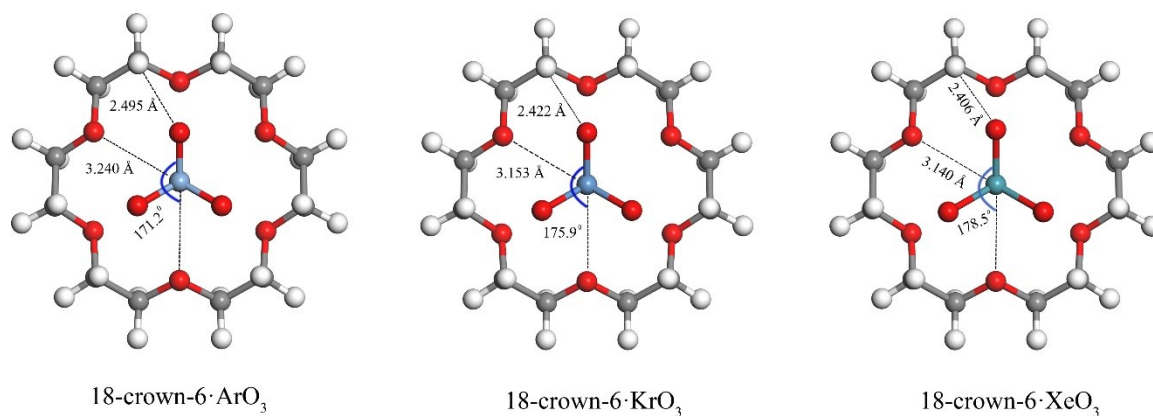


Figure S2. Several key parameters showing the change of the binding between host and guest for the optimized geometries of 18-crown-6·ArO₃, 18-crown-6·KrO₃ and 18-crown-6·XeO₃ at M06-2X/aug-cc-pVTZ-pp level of theory.

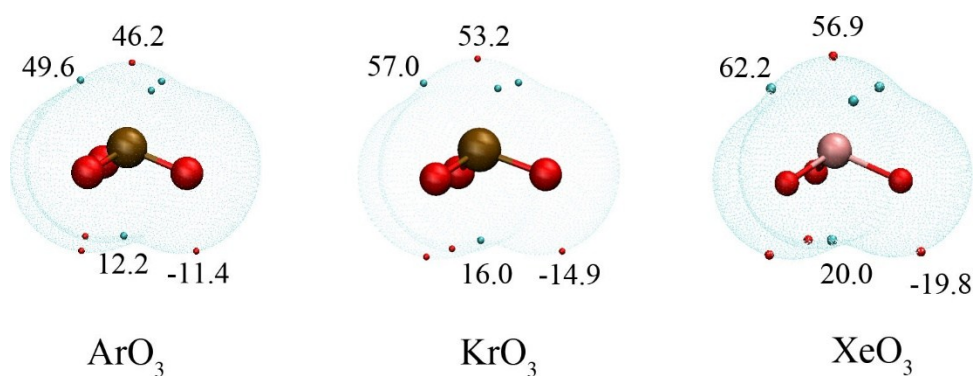


Figure S3. The distribution of minima and maxima of molecular electrostatic potential on vdW isosurfaces (isovalue = 0.001 a.u.) for ArO₃, KrO₃ and XeO₃ calculated at M06-2X/aug-cc-pVTZ-pp level of theory. Unit for numeric values on the isosurface is kcal mol⁻¹. Small red spheres, minima; small cyan spheres, maxima.

Supplementary Table

Table S1. δg (unit: a.u.) of some atom pairs in 18-crown-6·XeO₃ calculated at M06-2X/aug-cc-pVTZ-pp level of theory and the corresponding geometry with atomic labels.

Atom index	Atom index	δg
3	43	0.161
1	43	0.161
24	43	0.160
25	43	0.096
23	43	0.095
2	43	0.096
33	44	0.090
31	44	0.090
15	46	0.091
17	46	0.092
40	45	0.090
22	45	0.091
27	44	0.077
7	46	0.077
27	43	0.074
7	43	0.074
4	44	0.072
8	46	0.072
10	43	0.071
30	43	0.071
10	45	0.071
30	45	0.071
25	45	0.071

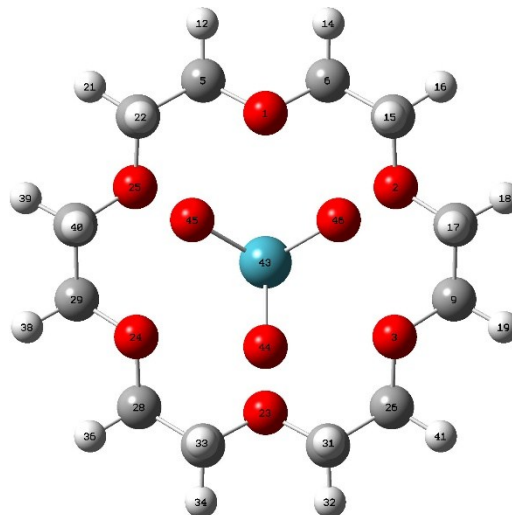


Table S2. δg (unit: a.u.) of some atom pairs in 18-crown-6·KrO₃ calculated at M06-2X/aug-cc-pVTZ-pp level of theory and the corresponding geometry with atomic labels.

Atom index	Atom index	δg
1	29	0.111
3	45	0.103
4	25	0.103
1	5	0.100
1	15	0.100
3	39	0.091
4	32	0.091
2	11	0.089
2	18	0.089
3	41	0.079
4	21	0.079
4	27	0.073
3	35	0.073
2	8	0.073
2	13	0.073
2	7	0.073
3	36	0.071
4	22	0.071

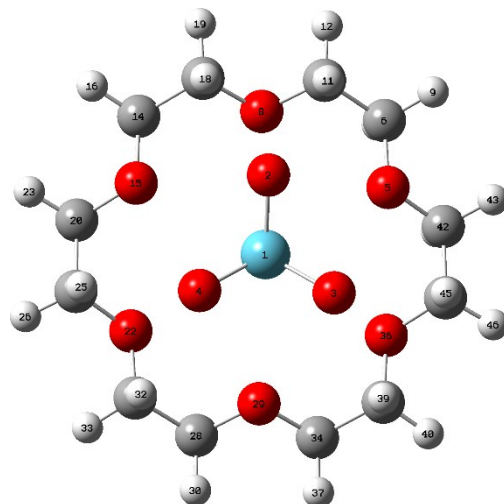
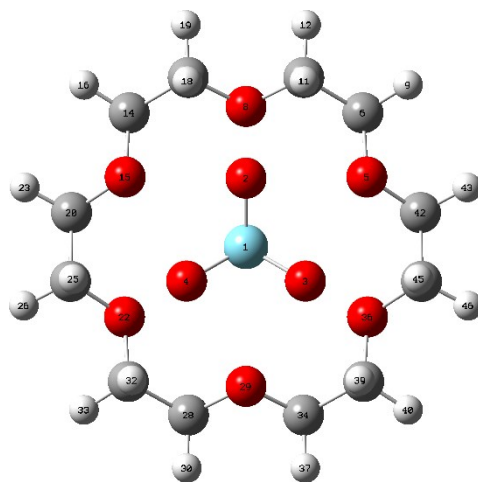


Table S3. δg (unit: a.u.) of some atom pairs in 18-crown-6 \cdot ArO₃ calculated at M06-2X/aug-cc-pVTZ-pp level of theory and the corresponding geometry with atomic labels.

Atom index	Atom index	δg
3	45	0.092
4	25	0.092
4	32	0.081
3	39	0.081
2	11	0.080
2	18	0.080
3	41	0.070
4	21	0.070
1	29	0.070



The optimized coordinates for species under study

18-crown-6

O	2.169803	-1.874039	0.258258
O	-0.536936	-2.814873	-0.258957
O	-2.706578	-0.939928	0.257631
C	-3.345408	1.345416	0.294912
C	3.345398	-1.345422	-0.294892
C	1.817467	-3.113180	-0.296631
C	0.508375	-3.568707	0.294836
C	-1.786180	-3.127638	0.296755
C	-2.835274	-2.222460	-0.295607
C	3.604670	0.016128	0.296754
H	3.251038	-1.253124	-1.384041
H	4.197665	-2.005191	-0.079097
H	1.711613	-3.031643	-1.385589
H	2.594333	-3.860760	-0.082581
H	0.541043	-3.440494	1.383929
H	0.363058	-4.636750	0.079415
H	-1.767966	-2.993809	1.385534
H	-2.045660	-4.174528	0.084516
H	-3.832744	-2.631377	-0.080832
H	-2.707509	-2.187017	-1.384684
H	4.640144	0.315948	0.081951
H	3.482069	-0.034920	1.385817
O	-2.169811	1.874032	-0.258233
O	0.536927	2.814865	0.258986
O	2.706569	0.939922	-0.257606
C	-3.604677	-0.016135	-0.296733
C	-1.817475	3.113172	0.296659
C	-0.508383	3.568701	-0.294805
C	1.786172	3.127633	-0.296722
C	2.835265	2.222452	0.295636
H	-3.251053	1.253119	1.384062
H	-4.197674	2.005184	0.079113
H	-1.711624	3.031633	1.385617
H	-2.594341	3.860753	0.082609
H	-0.541050	3.440493	-1.383898
H	-0.363066	4.636744	-0.079379
H	1.767959	2.993808	-1.385503
H	2.045651	4.174522	-0.084479

H	3.832735	2.631370	0.080862
H	2.707501	2.187006	1.384713
H	-4.640152	-0.315955	-0.081935
H	-3.482071	0.034912	-1.385797

XeO₃

Xe	0.000000	0.000000	0.207721
O	0.000000	1.616918	-0.467373
O	1.400292	-0.808459	-0.467373
O	-1.400292	-0.808459	-0.467373

KrO₃

Kr	-4.142822	-2.032789	-0.591526
O	-2.779261	-1.359544	-0.016992
O	-4.238632	-3.550598	-0.017150
O	-5.406183	-1.191106	-0.010515

ArO₃

Ar	0.000000	0.000000	1.444353
O	0.000000	1.395771	1.933563
O	1.208773	-0.697885	1.933563
O	-1.208773	-0.697885	1.933563

18-crown-6·XeO₃

O	-2.409647	-1.391210	0.099853
O	-2.430795	1.403420	-0.341834
O	-0.000000	2.782421	0.099853
C	2.378840	2.719382	0.152853
C	-2.356428	-2.702352	-0.414072
C	-3.518520	-0.689550	-0.414072
C	-3.544474	0.700445	0.152853
C	-2.378840	2.719382	0.152853
C	-1.162092	3.391903	-0.414072
C	-1.165634	-3.419827	0.152853
H	-2.283363	-2.670662	-1.507962
H	-3.270883	-3.245662	-0.144582
H	-3.454543	-0.642120	-1.507962
H	-4.446267	-1.209837	-0.144582
H	-3.510693	0.661599	1.245807
H	-4.473745	1.196279	-0.158164
H	-2.328308	2.709549	1.245807
H	-3.272880	3.276238	-0.158164
H	-1.175384	4.455499	-0.144582
H	-1.171179	3.312782	-1.507962

H	-1.200865	-4.472516	-0.158164
H	-1.182384	-3.371149	1.245807
O	2.430795	1.403420	-0.341834
O	2.409647	-1.391210	0.099853
O	0.000000	-2.806840	-0.341834
C	1.162092	3.391903	-0.414072
C	3.544474	0.700445	0.152853
C	3.518520	-0.689550	-0.414072
C	2.356428	-2.702352	-0.414072
C	1.165634	-3.419827	0.152853
H	2.328308	2.709549	1.245807
H	3.272880	3.276238	-0.158164
H	3.510693	0.661599	1.245807
H	4.473745	1.196279	-0.158164
H	3.454543	-0.642120	-1.507962
H	4.446267	-1.209837	-0.144582
H	2.283363	-2.670662	-1.507962
H	3.270883	-3.245662	-0.144582
H	1.200865	-4.472516	-0.158164
H	1.182384	-3.371149	1.245807
H	1.175384	4.455499	-0.144582
H	1.171179	3.312782	-1.507962
Xe	0.000000	-0.000000	1.554864
O	1.364834	0.787987	2.325957
O	0.000000	-1.575974	2.325957
O	-1.364834	0.787987	2.325957

18-crown-6·KrO₃

Kr	0.000000	0.000000	1.126325
O	0.000000	1.490804	1.777821
O	1.291075	-0.745402	1.777821
O	-1.291075	-0.745402	1.777821
O	2.417865	1.395955	-0.338469
C	2.359427	2.702755	-0.858396
C	1.166680	3.424989	-0.297447
O	0.000000	2.833723	-0.809587
H	3.272039	3.252159	-0.592954
H	2.285490	2.668279	-1.952145
H	1.175772	3.365746	0.795479
H	1.218472	4.481910	-0.592327
C	-1.166680	3.424989	-0.297447
C	-2.359427	2.702755	-0.858396
O	-2.417865	1.395955	-0.338469
H	-3.272039	3.252159	-0.592954

H	-2.285490	2.668279	-1.952145
H	-1.175772	3.365746	0.795479
H	-1.218472	4.481910	-0.592327
C	-3.520368	0.691946	-0.858396
C	-3.549468	-0.702120	-0.297447
O	-2.454076	-1.416861	-0.809587
H	-4.452471	1.207590	-0.592954
H	-3.453543	0.645153	-1.952145
H	-3.502708	-0.664624	0.795479
H	-4.490684	-1.185727	-0.592327
C	-2.382787	-2.722869	-0.297447
C	-1.160942	-3.394701	-0.858396
O	0.000000	-2.791910	-0.338469
H	-1.180432	-4.459748	-0.592954
H	-1.168052	-3.313432	-1.952145
H	-2.326936	-2.701122	0.795479
H	-3.272212	-3.296183	-0.592327
C	1.160942	-3.394701	-0.858396
C	2.382787	-2.722869	-0.297447
O	2.454076	-1.416861	-0.809587
H	1.180432	-4.459748	-0.592954
H	1.168052	-3.313432	-1.952145
H	2.326936	-2.701122	0.795479
H	3.272212	-3.296183	-0.592327
C	3.549468	-0.702120	-0.297447
C	3.520368	0.691946	-0.858396
H	4.452471	1.207590	-0.592954
H	3.453543	0.645153	-1.952145
H	3.502708	-0.664624	0.795479
H	4.490684	-1.185727	-0.592327

18-crown-6·ArO₃

Ar	0.000000	0.000000	1.417037
O	0.000000	1.385257	1.942248
O	1.199668	-0.692629	1.942248
O	-1.199668	-0.692629	1.942248
O	2.440638	1.409103	-0.182036
C	2.361468	2.706205	-0.718154
C	1.167207	3.419309	-0.145748
O	0.000000	2.834673	-0.661895
H	3.272215	3.270582	-0.476005
H	2.267645	2.659439	-1.810281
H	1.181869	3.345455	0.947377
H	1.215391	4.481563	-0.423056

C	-1.167207	3.419309	-0.145748
C	-2.361468	2.706205	-0.718154
O	-2.440638	1.409103	-0.182036
H	-3.272215	3.270582	-0.476005
H	-2.267645	2.659439	-1.810281
H	-1.181869	3.345455	0.947377
H	-1.215391	4.481563	-0.423056
C	-3.524376	0.691989	-0.718154
C	-3.544812	-0.698823	-0.145748
O	-2.454899	-1.417337	-0.661895
H	-4.468515	1.198530	-0.476005
H	-3.436964	0.634118	-1.810281
H	-3.488184	-0.649200	0.947377
H	-4.488843	-1.188222	-0.423056
C	-2.377605	-2.720485	-0.145748
C	-1.162908	-3.398194	-0.718154
O	0.000000	-2.818206	-0.182036
H	-1.196300	-4.469112	-0.476005
H	-1.169319	-3.293557	-1.810281
H	-2.306315	-2.696256	0.947377
H	-3.273452	-3.293341	-0.423056
C	1.162908	-3.398194	-0.718154
C	2.377605	-2.720485	-0.145748
O	2.454899	-1.417337	-0.661895
H	1.196300	-4.469112	-0.476005
H	1.169319	-3.293557	-1.810281
H	2.306315	-2.696256	0.947377
H	3.273452	-3.293341	-0.423056
C	3.544812	-0.698823	-0.145748
C	3.524376	0.691989	-0.718154
H	4.468515	1.198530	-0.476005
H	3.436964	0.634118	-1.810281
H	3.488184	-0.649200	0.947377
H	4.488843	-1.188222	-0.423056

18-crown-6·XeO₃ (TS)

O	-0.000000	2.758408	-0.637646
O	2.344598	1.353654	-0.752116
O	2.388852	-1.379204	-0.637646
C	1.177833	-3.362605	-0.339548
C	-1.181731	3.385817	-1.046115
C	1.181731	3.385817	-1.046115
C	2.323185	2.701336	-0.339548
C	3.501018	0.661269	-0.339548

C	3.523069	-0.669500	-1.046115
C	-2.323185	2.701336	-0.339548
H	-1.309112	3.306756	-2.133264
H	-1.170440	4.449107	-0.772658
H	1.309112	3.306756	-2.133264
H	1.170440	4.449107	-0.772658
H	2.178155	2.765053	0.744812
H	3.266474	3.194313	-0.604832
H	3.483684	0.503811	0.744812
H	4.399593	1.231693	-0.604832
H	4.438259	-1.210922	-0.772658
H	3.518291	-0.519654	-2.133264
H	-3.266474	3.194313	-0.604832
H	-2.178155	2.765053	0.744812
O	-0.000000	-2.707309	-0.752116
O	-2.388852	-1.379204	-0.637646
O	-2.344598	1.353654	-0.752116
C	2.341338	-2.716317	-1.046115
C	-1.177833	-3.362605	-0.339548
C	-2.341338	-2.716317	-1.046115
C	-3.523069	-0.669500	-1.046115
C	-3.501018	0.661269	-0.339548
H	1.305529	-3.268864	0.744812
H	1.133119	-4.426006	-0.604832
H	-1.305529	-3.268864	0.744812
H	-1.133119	-4.426006	-0.604832
H	-2.209179	-2.787102	-2.133264
H	-3.267819	-3.238184	-0.772658
H	-3.518291	-0.519654	-2.133264
H	-4.438259	-1.210922	-0.772658
H	-4.399593	1.231693	-0.604832
H	-3.483684	0.503811	0.744812
H	3.267819	-3.238184	-0.772658
H	2.209179	-2.787102	-2.133264
Xe	-0.000000	0.000000	1.125201
O	1.365893	-0.788599	1.897808
O	-1.365893	-0.788599	1.897808
O	-0.000000	1.577198	1.897808