

ESI for manuscript:

**Noble Gas Bonds Facilitate Anion···Anion Supramolecular Assemblies: Insights
from CSD and DFT Analysis**

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1. Table S1

Table S1. CSD reference codes of ion pairs involving organoxenon derivatives

COLNAU	DAMROY	ESOSIQ	EZAKIB	EZAKEX	EZAKOH	EZAKUN	IDUQED	JAQCOT
JORDUS	JORFAA	JORFEE	JORHIK	KAZLUV	KAZMAC	KAZMEG	KAZMIC	KAZMIK
KEDMUB	LUYSEG	LUYSIK	MOFHOF	MOFHUL	MOFJAT	MOFJEX	MOFHOF	QEZVUQ
QOYRAZ	QOYRED	QOYRIH	ROQQET	SOBWA H	TUKFAH	VIFKUT	VIFLAA	VIFLEE
VIFLII	WADHIS	WEJBES	ZHGKA	ZOGPIV	COGTUR			

2. Cartesian Coordinates:

MOFJEZ optimized using periodic boundary conditions

Xe	3.1254408	8.3969680	9.5713155
C	3.3137974	7.2791577	7.7590488
C	4.3925470	7.5656013	6.9267770
C	2.3301293	6.3624523	7.4074166
C	2.4609204	5.6709891	6.2017835
C	3.5583288	5.9157807	5.3731266
C	4.5161783	6.8726485	5.7198548
F	1.2671001	6.1452378	8.1827248
F	5.5485478	7.1084527	4.9012059
F	1.5526510	4.7492729	5.8530607
F	5.3000913	8.4854289	7.2662850
F	3.7097853	5.2060916	4.2535066
N	3.0205527	9.8929125	11.7839451
C	3.1179797	10.2672741	12.8786812
B	3.1696852	10.6679402	14.4199471
C	1.6782430	10.5981286	14.9472084
N	0.5689053	10.5525402	15.2916379
C	4.0614754	9.5869630	15.1623933
N	4.6958481	8.7558913	15.6746612
C	3.7289224	12.1318720	14.6462355
N	4.1032912	13.2124281	14.8587391
F	6.2260428	6.0564871	8.6002595
C	7.2891904	5.8392565	9.3755633
C	7.4198914	6.5307537	10.5811902
C	8.5173873	6.2859437	11.4098765
C	8.2728109	4.9226527	9.0239681
F	6.5116369	7.4524685	10.9299606
F	8.6688003	6.9956617	12.5294700
C	9.3515643	4.6361652	9.8562303
C	9.4751801	5.3290826	11.0631099
F	10.5075453	5.0932798	11.8817786
F	10.2590528	3.7163104	9.5166978
Xe	8.0844193	3.8047210	7.2116627
N	7.9795462	2.3088443	4.9991331
C	8.0769963	1.9344726	3.9042656
B	8.1287178	1.5338252	2.3630698
C	6.6372383	1.6036315	1.8357753
N	5.5279444	1.6492048	1.4913633
C	9.0204575	2.6147479	1.6206212

N	9.6548798	3.4458582	1.1082836
C	8.6879302	0.0698828	2.1367850
N	9.0622543	-1.0106319	1.9242797
C	-0.8342956	13.0571339	16.1505263
C	0.1492322	13.9737223	15.7988973
C	0.0186011	14.6652511	14.5933082
C	-1.0788717	14.4204471	13.7646299
F	1.2124346	14.1909783	16.5741993
F	0.9268727	15.5869509	14.2445331
F	-1.2302909	15.1301509	12.6450380
C	-1.9129882	12.7707446	15.3183053
C	-2.0366882	13.4635713	14.1113999
F	-3.0690403	13.2277921	13.2927239
F	-2.8205564	11.8508642	15.6577918
Xe	-0.6459372	11.9392576	17.9627961
N	-0.5410413	10.4433032	20.1754989
C	-0.6384781	10.0689905	21.2701264
B	-0.6902395	9.6683533	22.8114478
C	0.8012797	9.7381270	23.3387152
N	1.9105433	9.7837060	23.6831235
C	-1.5819599	10.7492661	23.5539010
N	-2.2163321	11.5803061	24.0661993
C	-1.2494337	8.2043592	23.0377320
N	-1.6237602	7.1238833	23.2502006
N	6.8695704	2.4180321	9.8829055
C	5.7602973	2.4636409	10.2272723
B	4.2687962	2.5334182	10.7545932
C	3.7095920	3.9973807	10.5282501
N	3.3352144	5.0779020	10.3158118
C	4.3205224	2.1327522	12.2958225
N	4.4179268	1.7584172	13.3904213
C	3.3770214	1.4524538	10.0120711
N	2.7426837	0.6214422	9.4998758
Xe	4.3130441	0.2624458	15.6032132
C	4.1247333	-0.8553115	17.4154338
C	3.0459809	-0.5689378	18.2477165
C	5.1083574	-1.7720152	17.7671151
C	4.9775872	-2.4635000	18.9727187
C	3.8801614	-2.2187091	19.8013560
C	2.9223143	-1.2618557	19.4546247
F	6.1713754	-1.9892472	16.9918268
F	1.8899215	-1.0260890	20.2732698
F	5.8858670	-3.3852303	19.3214468
F	2.1384239	0.3508464	17.9082076
F	3.7287043	-2.9284112	20.9209539
Xe	3.1254323	3.8048063	1.1797937
C	3.3138288	4.9225953	-0.6324563
C	4.3924985	4.6361973	-1.4646922
C	2.3301776	5.8392606	-0.9840762
C	2.4609367	6.5307471	-2.1897125
C	3.5583241	6.2859707	-3.0183591
C	4.5161866	5.3290735	-2.6716124
F	1.2670753	6.0565084	-0.2087975
F	5.5485416	5.0933078	-3.4902823
F	1.5526237	7.4525058	-2.5384664
F	5.3000373	3.7163611	-1.1252150
F	3.7098014	6.9956763	-4.1379957
N	3.0205713	2.3088203	3.3923764
C	3.1180017	1.9344363	4.4872800
B	3.1697119	1.5338531	6.0284455
C	4.0614098	2.6147225	6.7708638

N	4.6958583	3.4458711	7.2832409
C	1.6782034	1.6036333	6.5557343
N	0.5690192	1.6492215	6.9001528
C	3.7289275	0.0698812	6.2547305
N	4.1032600	-1.0106117	6.4672015
F	6.2260581	6.1452466	0.2087630
C	7.2892198	6.3624820	0.9840926
C	7.4199209	5.6709915	2.1897040
C	8.5173743	5.9158084	3.0183580
C	8.2727853	7.2791106	0.6324661
F	6.5116484	4.7492962	2.5384537
F	8.6687969	5.2060950	4.1379878
C	9.3515198	7.5655600	1.4647276
C	9.4751632	6.8726333	2.6716328
F	10.5075510	7.1084571	3.4902824
F	10.2590959	8.4854717	1.1252023
Xe	8.0844288	8.3969914	-1.1798203
N	7.9795325	9.8928911	-3.3923816
C	8.0769930	10.2672961	-4.4872412
B	8.1287088	10.6679141	-6.0284366
C	6.6372036	10.5981308	-6.5557259
N	5.5279088	10.5525403	-6.9001596
C	9.0204599	9.5869798	-6.7708748
N	9.6548685	8.7558441	-7.2831716
C	8.6879426	12.1319246	-6.2547241
N	9.0622894	13.2124471	-6.4671624
N	6.8695215	9.7837298	1.4913593
C	5.7602948	9.7381322	1.8357699
B	4.2687887	9.6683583	2.3630476
C	3.3770702	10.7492410	1.6206079
N	2.7426500	11.5803780	1.1082734
C	3.7095823	8.2044137	2.1367682
N	3.3352042	7.1238135	1.9242710
C	4.3205064	10.0689378	3.9042280
N	4.4179567	10.4433300	4.9991204
Xe	4.3130588	11.9392878	7.2116944
C	4.1246598	13.0571195	9.0239792
C	3.0459789	12.7706895	9.8562044
C	5.1083189	13.9737743	9.3755893
C	4.9775714	14.6652581	10.5812331
C	3.8801569	14.4204645	11.4098899
C	2.9222977	13.4635679	11.0631259
F	6.1714087	14.1910032	8.6002902
F	1.8899831	13.2278008	11.8817907
F	5.8858686	15.5869679	10.9299695
F	2.1384533	11.8508637	9.5167260
F	3.7287171	15.1301448	12.5294918
C	8.0049442	15.7000709	6.9267515
C	7.8813214	15.0071224	5.7198523
F	6.8489272	15.2429319	4.9012154
F	7.0973907	16.6199843	7.2663115
C	9.0837042	15.4135573	7.7590224
C	8.8391153	14.0503028	5.3730821
C	9.9366292	13.8054845	6.2017692
C	10.0673054	14.4969594	7.4073965
F	11.1304570	14.2797434	8.1827344
F	10.8448475	12.8838268	5.8530070
F	8.6877096	13.3406156	4.2535058
Xe	9.2720698	16.5315092	9.5713481
N	9.3769654	18.0274007	11.7839921
C	9.2795095	18.4017766	12.8787316

B	9.2278017	18.8024208	14.4199560
C	8.3360281	17.7214705	15.1624207
N	7.7016557	16.8903656	15.6746116
C	10.7192739	18.7326388	14.9472503
N	11.8285730	18.6870245	15.2916546
C	8.6685801	20.2663767	14.6462494
N	8.2941984	21.3469650	14.8586895

Dimer A in water

B	0.0061270	-0.0540446	2.3888191
N	-2.3823335	-1.4032046	2.1760805
N	1.7730641	-0.9112141	0.4629190
C	0.6301851	-0.3880890	3.8162158
C	-1.3784271	-0.8208941	2.2474261
N	1.0870693	-0.6335099	4.8574631
C	1.0162012	-0.5427484	1.2651563
C	-0.2055890	1.5167262	2.2781413
N	-0.3334367	2.6710412	2.2222497
B	-0.0061270	0.0540446	-2.3888191
N	2.3823335	1.4032046	-2.1760805
N	-1.7730641	0.9112141	-0.4629190
C	-0.6301851	0.3880890	-3.8162158
C	1.3784271	0.8208941	-2.2474261
N	-1.0870693	0.6335099	-4.8574631
C	-1.0162012	0.5427484	-1.2651563
C	0.2055890	-1.5167262	-2.2781413
N	0.3334367	-2.6710412	-2.2222497

Dimer B in water

B	-0.0000000	-0.0000000	3.0332789
N	-0.0004318	2.6234293	2.2024763
N	-2.2717405	-1.3120886	2.2024763
C	-0.0000000	-0.0000000	4.6271159
C	0.0016809	1.5074718	2.5294093
N	-0.0000000	-0.0000000	5.7903854
C	-1.3063493	-0.7522803	2.5294093
C	1.3046685	-0.7551916	2.5294093
N	2.2721723	-1.3113407	2.2024763
B	-0.0000000	0.0000000	-3.0718267
N	-0.2794155	2.5813965	-3.9874907
N	-0.0000000	0.0000000	-0.3212688
C	-1.2106591	-0.8840720	-3.6022549
C	-0.1602992	1.4904976	-3.6022549
N	-2.0958472	-1.5326792	-3.9874907
C	-0.0000000	0.0000000	-1.4841045
C	1.3709584	-0.6064256	-3.6022549
N	2.3752627	-1.0487173	-3.9874907

Dimer C in water

Xe	0.2216402	-0.3383508	-7.5361904
F	-2.3244221	-0.5613375	-9.4482068
F	-0.4595641	0.5174601	-13.6531429
C	-1.2700948	-0.2174194	-10.1920159
F	-2.6154268	-0.1847153	-12.1388006
F	2.2958442	0.4776255	-9.8151090
C	-0.0127786	-0.0448432	-9.6225898
C	-0.3142181	0.3351279	-12.3406093
C	-1.4197672	-0.0251720	-11.5659132
C	1.0968046	0.3147633	-10.3803682
F	1.9911965	0.8509786	-12.5044687

C	0.9421885	0.5059668	-11.7537656
B	0.5970881	-0.8027694	-2.2181256
N	-0.4036732	-3.2274095	-1.3917110
N	-0.9168891	1.2458483	-1.1802813
C	0.5373412	-0.7300850	-3.8082790
C	0.0172908	-2.2022300	-1.7429682
N	0.4926884	-0.6755819	-4.9653194
C	-0.2764240	0.3805224	-1.6192657
C	2.1075408	-0.6578894	-1.7510376
N	3.2130593	-0.5562813	-1.4058973

Dimer ion-pair in water

Xe	0.2207062	-0.3326028	-7.5174991
F	-2.3226487	-0.5626220	-9.4304961
F	-0.4590226	0.5134876	-13.6363688
C	-1.2684872	-0.2187123	-10.1748929
F	-2.6144376	-0.1899166	-12.1213859
F	2.2968750	0.4788176	-9.7985937
C	-0.0115282	-0.0443009	-9.6053144
C	-0.3131967	0.3321326	-12.3237126
C	-1.4187413	-0.0281656	-11.5488533
C	1.0977250	0.3152212	-10.3636297
F	1.9922332	0.8484636	-12.4887871
C	0.9433166	0.5045113	-11.7372984
B	0.6035866	-0.8111009	-2.2068155
N	-0.4395542	-3.2413129	-1.4587491
N	-0.9273679	1.2630352	-1.2545667
C	0.5422016	-0.7340711	-3.7992247
C	0.0100249	-2.2111176	-1.7549047
N	0.4901100	-0.6704743	-4.9556097
C	-0.2745606	0.3795578	-1.6351556
C	2.1174574	-0.6561600	-1.7586319
N	3.2347331	-0.5304618	-1.4635752
Xe	-0.2204546	0.3331934	7.5174284
F	2.3232807	0.5605515	9.4303493
F	0.4588634	-0.5136717	13.6362476
C	1.2688540	0.2175009	10.1747586
F	2.6149640	0.1876758	12.1211911
F	-2.2973927	-0.4762531	9.7989091
C	0.0115495	0.0446883	9.6054097
C	0.3131664	-0.3323633	12.3235966
C	1.4190292	0.0271116	11.5487548
C	-1.0980738	-0.3135526	10.3638360
F	-1.9928585	-0.8464399	12.4890160
C	-0.9437384	-0.5030538	11.7374821
B	-0.6035585	0.8110149	2.2067449
N	0.9257158	-1.2645540	1.2550318
N	0.4408878	3.2402398	1.4573371
C	-0.5417747	0.7344559	3.7991724
C	0.2737196	-0.3803911	1.6354447
N	-0.4895284	0.6711985	4.9555583
C	-0.0093286	2.2104820	1.7540566
C	-2.1176471	0.6566976	1.7591068
N	-3.2350997	0.5312611	1.4646333

Dimer ion-pair gas phase

Xe	0.1817926	-0.2615284	-7.3229959
F	-2.3305894	-0.5474786	-9.3089450
F	-0.4155027	0.4332915	-13.5153677

C	-1.2646785	-0.2144825	-10.0470282
F	-2.5893584	-0.2388411	-12.0115641
F	2.2870858	0.5054899	-9.6391596
C	-0.0203339	-0.0222162	-9.4550893
C	-0.2873914	0.2866403	-12.1985269
C	-1.4036566	-0.0596428	-11.4283726
C	1.0925514	0.3227835	-10.2156318
F	2.0175499	0.8119643	-12.3416908
C	0.9620550	0.4798649	-11.5977397
B	0.6165823	-0.8401308	-2.1891100
N	-0.4240677	-3.3376992	-1.7394379
N	-0.8979753	1.2121519	-1.1782959
C	0.4918047	-0.6625486	-3.7828240
C	0.0269660	-2.2746229	-1.8773865
N	0.4030477	-0.5331118	-4.9343830
C	-0.2466684	0.3315721	-1.5694247
C	2.1610825	-0.7106235	-1.8722832
N	3.3106811	-0.6011029	-1.7345545
Xe	-0.1817926	0.2615284	7.3229959
F	2.3305894	0.5474786	9.3089450
F	0.4155027	-0.4332915	13.5153677
C	1.2646785	0.2144825	10.0470282
F	2.5893584	0.2388411	12.0115641
F	-2.2870858	-0.5054899	9.6391596
C	0.0203339	0.0222162	9.4550893
C	0.2873914	-0.2866403	12.1985269
C	1.4036566	0.0596428	11.4283726
C	-1.0925514	-0.3227835	10.2156318
F	-2.0175499	-0.8119643	12.3416908
C	-0.9620550	-0.4798649	11.5977397
B	-0.6165823	0.8401308	2.1891100
N	0.8979753	-1.2121519	1.1782959
N	0.4240677	3.3376992	1.7394379
C	-0.4918047	0.6625486	3.7828240
C	0.2466684	-0.3315721	1.5694247
N	-0.4030477	0.5331118	4.9343830
C	-0.0269660	2.2746229	1.8773865
C	-2.1610825	0.7106235	1.8722832
N	-3.3106811	0.6011029	1.7345545

Dimer ion-pair-K in water

B	0.6025165	-0.8135613	-2.2143393
N	-0.4315936	-3.2432220	-1.4456258
N	-0.9341705	1.2644602	-1.2762832
C	0.5475108	-0.7417999	-3.8052663
C	0.0116176	-2.2119783	-1.7487663
N	0.4957759	-0.6745687	-4.9638016
C	-0.2781436	0.3780453	-1.6449635
C	2.1136908	-0.6589635	-1.7516652
N	3.2302692	-0.5385148	-1.4510364
B	-0.6024477	0.8134157	2.2142431
N	0.9320881	-1.2664218	1.2768608
N	0.4330071	3.2418660	1.4438338
C	-0.5470004	0.7423553	3.8051676
C	0.2770182	-0.3791616	1.6451872
N	-0.4950375	0.6754822	4.9637147
C	-0.0107616	2.2111347	1.7477030
C	-2.1139431	0.6596635	1.7523356
N	-3.2308127	0.5398233	1.4524403
K	0.2142473	-0.3198429	-7.7175253
K	-0.2135622	0.3206782	7.7175690