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Supporting Information

Effect of Hydration on the Organo-Noble Gas Molecule HKrCCH: Role of Krypton in the Stabilization of Hydrated HKrCCH Complexes

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TableS1: Electron density (ρ), Laplacian (∇^2), total electronic energy density (H), local electronic kinetic energy density (G) and local potential energy density (V) for the different complexes of HKrCCH-$(H_2O)_n$ calculated at the MP2/aug-cc-pVDZ level of theory. All the parameters are in atomic units.

	Bond	BCP Type	ρ(r)	∇^2 ρ(r)	G(r)	V(r)	H(r)
			1W				
a	C≡C….HOH	(3,-1)	0.0182	0.0498	0.0118	-0.0111	0.0007
	Kr…..OH2	(3,-1)	0.0094	0.0396	0.0085	-0.0071	0.0014
	Ring	(3,+1)	0.0891	0.0413	0.0087	-0.0070	0.0017
b	C-H….O	(3,-1)	0.0133	0.0415	0.0100	-0.0098	0.0002
c	Kr-H….O	(3,-1)	0.0406	0.1104	0.0288	-0.0299	-0.0011
			2W				
d	C≡C..HOH	(3,-1)	0.0227	0.0581	0.0139	-0.0132	0.0007
	Kr……OH2	(3,-1)	0.0128	0.0505	0.0112	-0.0097	0.0015
	HOH…..OH2	(3,-1)	0.0314	0.1159	0.0268	-0.0245	0.0023
	Ring	(3,+1)	0.00511	0.0235	0.0047	-0.0035	0.0012
e	C≡C…..HOH	(3,-1)	0.0191	0.0517	0.0123	-0.0116	0.0007
			0.0190	0.0515	0.0122	-0.0116	0.0006
	Kr……OH2	(3,-1)	0.041	0.041	0.0088	-0.0073	0.0015
			0.041	0.041	0.0088	-0.0073	0.0015
	Ring	(3,+1)	0.0424	0.0424	0.0089	-0.0072	0.0017
			0.0424	0.0424	0.0089	-0.0072	0.0017
f	C≡C…..HOH	(3,-1)	0.0114	0.0324	0.0076	-0.0071	0.0005
			0.0204	0.0547	0.0131	-0.0125	0.0006
	Kr……OH2	(3,-1)	0.0101	0.0336	0.0076	-0.0068	0.0008
	HOH……OH2	(3,-1)	0.0199	0.0547	0.0155	-0.0151	0.0004
	Ring	(3,+1)	0.0084	0.0299	0.0065	-0.0057	0.0008
			0.0059	0.0259	0.0052	-0.0039	0.0013
g	C-H….OH2	(3,-1)	0.0134	0.042	0.0100	-0.0096	0.0004
	C≡C ….HOH	(3,-1)	0.01846	0.0504	0.0119	-0.0112	0.0007
	Kr…..OH2	(3,-1)	0.0089	0.0378	0.0081	-0.0067	0.0014
	Ring	(3,+1)	0.0086	0.0399	0.0083	-0.0068	0.0015
			3W				
h	C≡C …..HOH	(3,-1)	0.0236	0.0595	0.0144	-0.0139	0.0005
			0.0207	0.0552	0.0131	-0.0125	0.0006
	Kr……OH2	(3,-1)	0.0135	0.0547	0.0121	-0.0104	0.0017
			0.0100	0.0426	0.0091	-0.0075	0.0016
	HOH……OH2	(3,-1)	0.0304	0.1125	0.0258	-0.0235	0.0023
	Ring	(3,+1)	0.0062	0.0282	0.0057	-0.0044	0.0013
			0.0093	0.0437	0.0092	-0.0076	0.0016
	C≡C…..HOH	(3,-1)	0.0115	0.0322	0.0076	-0.0071	0.0005
			0.0214	0.0569	0.0137	-0.0132	0.0005
			0.0200	0.0534	0.0127	-0.0121	0.0006
	Kr……OH2	(3,-1)	0.0102	0.0339	0.0077	-0.0069	0.0008
			0.0100	0.0421	0.0090	-0.0074	0.0016
	HOH……OH2	(3,-1)	0.0198	0.0637	0.0155	-0.0151	0.0004
	Ring	(3,+1)	0.0082	0.0064	0.0064	-0.0055	0.0009

			0.0060	0.0262	0.0053	-0.0040	0.0013
			0.0093	0.0433	0.0091	-0.0074	0.0023
	Kr-C…..HOH	(3,-1)	0.0200	0.0523	0.0127	0.0120	0.0007
			0.0200	0.0532	0.0127	-0.0120	0.0007
			0.0200	0.0532	0.0127	-0.0120	0.0007
	Kr……OH2	(3,-1)	0.0100	0.0422	0.009	-0.0015	0.0075
			0.0100	0.0422	0.009	-0.0075	0.0015
			0.0100	0.0422	0.009	-0.0075	0.0015
	Ring	(3,+1)	0.0092	0.0423	0.009	-0.0073	0.0017
			0.0092	0.0423	0.009	-0.0073	0.0017
			0.0092	0.0423	0.009	-0.0073	0.0017
	C-H….OH2	(3,-1)	0.0133	0.042	0.0100	-0.0096	0.0004
	KrC….HOH	(3,-1)	0.0195	0.0527	0.0125	-0.0119	0.0006
			0.0193	0.0524	0.0124	-0.0117	0.0007
	Kr…..OH2	(3,-1)	0.0092	0.0396	0.0084	-0.007	0.0014
			0.0092	0.0393	0.0084	-0.007	0.0014
	Ring	(3,+1)	0.0090	0.0418	0.0088	-0.007	0.0018
			0.0088	0.0414	0.0087	-0.007	0.0018
			4W				
l	C≡C…..HOH	(3,-1)	0.0122	0.0334	0.0080	-0.0075	0.0005
			0.0214	0.0569	0.0136	-0.0131	0.0005
			0.0122	0.0333	0.0080	-0.0075	0.0005
			0.0213	0.0568	0.0136	-0.0130	0.0006
	Kr……OH_2	(3,-1)	0.0130	00342	0.0078	-0.0069	0.0009
			0.0076	0.0323	0.0068	-0.0055	0.0013
			0.0103	0.0342	0.0078	-0.0069	0.0009
			0.0076	0.0322	0.0068	-0.0055	0.0013
	HOH……OH_2	(3,-1)	0.0189	0.0598	0.0148	0.0146	0.0002
			0.0190	0.0568	0.0148	-0.0146	0.0002
	Ring	(3,+1)	0.0083	0.0296	0.0065	-0.0055	0.0010
			0.0076	0.0337	0.0071	-0.0057	0.0014
			0.0060	0.0268	0.0054	-0.0041	0.0013
			0.0082	0.0295	0.0065	-0.0055	0.0010
			0.0076	0.0337	0.0070	-0.0057	0.0013
			0.0060	0.0267	0.0054	-0.0041	0.0013
			5W				
m	C≡C…..HOH	(3,-1)	0.0201	0.0540	0.0129	-0.0123	0.0006
			0.0108	0.0309	0.0071	-0.0066	0.0005
			0.0211	0.0559	0.0135	-0.0130	0.0005
			0.0165	0.0427	0.0105	-0.0104	0.0001
	Kr……OH2	(3,-1)	0.0078	0.0314	0.0067	-0.0056	0.0011
			0.0108	0.0359	0.0082	-0.0074	0.0009
			0.0074	0.0316	0.0067	-0.0054	0.0013
			0.0085	0.0300	0.0066	-0.0057	0.0011
	HOH……OH2	(3,-1)	0.0199	0.0646	0.0157	-0.0153	0.0004
			0.0211	0.0674	0.0166	-0.0163	0.0003
			0.0279	0.1028	0.0233	-0.0210	0.0023
	Ring	(3,+1)	0.0760	0.0331	0.070	0.0057	0.0013
			0.0081	0.0281	0.0061	-0.0053	0.0008
			0.0050	0.0231	0.0047	-0.0036	0.0011
			0.0074	0.0324	0.0068	-0.0055	0.0013

			0.0081	0.0310	0.0067	-0.0055	0.0012
			0.0068	0.0313	0.0064	-0.0049	0.0015
			6W				
n	C≡C…..HOH	(3,-1)	0.0201	0.0540	0.0130	-0.0125	0.0005
			0.0141	0.0377	0.0091	-0.0088	0.0003
			0.0202	0.0541	0.0130	-0.0126	0.0004
			0.0141	0.0378	0.0091	-0.0088	0.0003
	Kr……OH2	(3,-1)	0.0078	0.0319	0.0068	-0.0057	0.0011
			0.0091	0.0312	0.0069	-0.0061	0.0008
			0.0078	0.0319	0.0068	-0.0057	0.0011
			0.0091	0.0311	0.0069	-0.0061	0.0008
	HOH……OH2	(3,-1)	0.0231	0.0761	0.0183	-0.0176	0.0007
			0.0231	0.0760	0.0183	-0.0176	0.0007
			0.0274	0.1003	0.0228	-0.0205	0.0023
			0.0274	0.1003	0.0228	-0.0204	0.0023
	Ring	(3,+1)	0.0076	0.0335	0.0071	-0.0058	0.0013
			0.0081	0.0298	0.0064	-0.0055	0.0011
			0.0065	0.0291	0.0059	-0.0046	0.0013
			0.0076	0.0336	0.0071	-0.0058	0.0013
			0.0081	0.0298	0.0065	-0.0055	0.0010
			0.0065	0.0292	0.0060	-0.0046	0.0014

TableS2: The values of absolute and change in the bond length of the C-H, Kr-H, C≡C, Kr-C and OH (angstrom) group of the HKrCCH-$(H_2O)_n$ calculated at the MP2/aug-cc-pVDZ level of calculation.

	Kr-C(ΔKr-C)	**C-C(ΔC-C)**	**Kr-H(ΔKr-H)**	**C-H(ΔC-H)**	**O-H(ΔO-H)**
HKrCCH	2.2638	1.2491	1.5926	1.0778	
H_2O					0.9659
			1W		
a	2.3178(0.05)	1.2524(0.0033)	1.5458(-0.0468)	1.0786(0.0008)	0.9757(0.0098)
b	2.2519(-0.0119)	1.2491(0)	1.6092(0.0166)	1.0822(0.0044)	0.9662(0.0003)
c	2.4383(0.17)	1.2576(0.0085)	1.5259(-0.0667)	1.0790(0.0012)	0.9684(0.0025)
			2W		
d	2.3792(0.1154)	1.2555(0.0064)	1.5067(-0.0859)	1.0792(0.0014)	0.9828(0.0169) 0.9816(0.0157)
e	2.3885(0.1247)	1.2557(0.0066)	1.5035(-0.0891)	1.0794(0.0016)	0.9763(0.0104) 0.9763(0.0104)
f	2.3618(0.098)	1.2550(0.0059)	1.5170(-0.0756)	1.0792(0.0014)	0.9702(0.0043) 0.9787(0.0128)
g	2.2996(0.0358)	1.2522(0.0031)	1.5614(-0.0312)	1.0828(0.0050)	0.9761(0.0102) 0.9662(0.0003)
			3W		
h	2.4724(0.2086)	1.2587(0.0096)	1.4707(-0.1219)	1.0798(0.0020)	0.9839(0.0180) 0.9778(0.0119) 0.9815(0.0156)
i	2.4449(0.1811)	1.2579(0.0088)	1.4798(-0.1128)	1.0800(0.0022)	0.9766(0.0107) 0.9703(0.0044) 0.9794(0.0135)
j	2.4772(0.2134)	1.2587(0.0096)	1.4692(-0.1234)	1.0801(0.0023)	0.9767(0.0108) 0.9767(0.0108) 0.9767(0.0108)
k	2.3663(0.1025)	1.2555(0.0064)	1.5160(-0.0766)	1.0834(0.0056)	0.9768(0.0109) 0.9766(0.0107) 0.9660(0.0101)
			4W		
l	2.5065(0.2427)	1.2597(0.0106)	1.4610(-0.1316)	1.0806(0.0028)	0.9788(0.0129) 0.9706(0.0047) 0.9788(0.0129) 0.9706(0.0047)
			5W		
m	2.4843(0.2205)	1.2594(0.0103)	1.4664(-0.1262)	1.0803(0.0031)	0.9755(0.0096) 0.9698(0.0039) 0.9805(0.0146) 0.9687(0.0028)
			6W		

n	2.4977(0.2339)	1.2595(0.0104)	1.4644(-0.1282)	1.0808(0.0030)	0.9779(0.0120) 0.9722(0.0063) 0.9779(0.0120) 097220(0.006)

TableS3: The C-H, Kr-H and C≡C stretching frequencies (cm^{-1}) of HKrCCH-$(H_2O)_n$ calculated at the MP2/aug-cc-pVDZ level of calculation.

	$\nu_{(Kr-H)}$	$\nu_{(C-H)}$	$\nu_{(C-C)}$
Monomer	1542	3443	1928
a	1736(194)	3435(-8)	1909(-19)
b	1484(-58)	3389(-54)	1926(-2)
c	1822(280)	3425(-18)	1882(-46)
d	1956(414)	3428(-15)	1890(-38)
e	1966(424)	3426(-17)	1888(-40)
f	1884(342)	3428(-15)	1898(-30)
g	1664(122)	3381(-62)	1909(-19)
h	2197(655)	3419(-24)	1869(-59)
i	2123(581)	3419(-24)	1874(-54)
j	2197(655)	3418(-25)	1868(-60)
k	1892(350)	3377(-66)	1886(-42)
l	2261(719)	3412(-31)	1861(-67)
m	2219(677)	3414(-29)	1864(-64)
n	2238(696)	3411(-32)	1862(-66)

TableS4: Scaled OH stretching frequencies (cm^{-1}) of water as well as HKrCCH-$(H_2O)_n$ [n=1-6] complexes and the charge on the hydrogen atom of the water molecule in the hydrated HKrCCH complexes calculated at the MP2/ aug-cc-pVDZ level of calculation.

	Scaled OH stretching frequency/*Charge on hydrogen atom*
Monomer	3780, 3651 *0.482,0.482*
a	3742.1, 3507 *0.485, 0.495*
b	3772.8, 3646 *0.487, 0.487*
c	3738.2, 3616 *0.507, 0.507*
d	3715, 3364, 3738, 3415 *0.492, 0.510, 0.487, 0.507*
e	3737, 3499, 3736, 3492 *0.485, 0.496,0.485, 0.496*
f	3725, 3453, 3672, 3572 *0.495, 0.484, 0.501, 0.491*
g	3772, 3646, 3737, 3500 *0.484, 0.496, 0.487, 0.487*
h	3714, 3347, 3739, 3412, 3735, 3466 *0.493, 0.510, 0.485, 0.497, 0.490, 0.509*
i	3735, 3482, 3735, 3482, 3736 , 3493 *0.486, 0.495, 0.495, 0.484, 0.501, 0.492*
j	3671, 3571, 3724, 3438, 3735 ,3486 *0.485, 0.496, 0.485, 0.496, 0.496,0.485*
k	3772, 3646, 3736, 3483, 3735, 3491 *0.484, 0.496, 0.484, 0.496, 0.488, 0.487*
l	3724, 3441, 3671, 3576, 3723, 3453, 3669, 3575 *0.492, 0.500, 0.495, 0.485, 0.500, 0.492, 0.495, 0.485*
m	3675, 3564, 3722, 3414, 3683, 3468, 3587, 3512,3769, 3645 *0.511, 0.499, 0.496, 0.484, 0.501, 0.492, 0.497, 0.481, 0.495, 0.496*
n	3721, 3469, 3628, 3491, 3720, 3539, 3625, 3458, 3744, 3539, 3744, 3490 *0.497, 0.503, 0.497, 0.506, 0.497 ,0.503,0.497, 0.507, 0.500, 0.473, 0.500*

TableS5: The occupancy of bonding and antibonding orbitals (atomic unit) of C-H, Kr-H, C≡C and OH group of HKrCCH-$(H_2O)_n$ calculated at the MP2/aug-cc-pVDZ level of calculation. The values shown in italics correspond to the occupancies of antibonding orbitals.

	C-H	**Kr-H**	**C≡C**	**OH**
	1W			
Monomer	1.9895	1.9558	1.9972	1.9989, 1.9989
	0.0114	*0.4136*	*0.0060*	*0.0002, 0.0002*
a	1.9896	1.9933	1.9852	1.9978, 1.9953
	0.0123	*0.3444*	*0.0078*	*0.0009, 0.0170*
b	1.9884	1.9921	1.9971	1.99834, 1.99835
	0.0203	*0.4363*	*0.0062*	*0.00006, 0.00005*
c	1.9911	1.9916	1.9975	1.9981, 1.9981
	0.0147	*0.3067*	*0.0077*	*0.0020, 0.0019*
	2W			
d	1.9902	1.9934	1.9742	1.9976, 1.9952, 1.9982, 1.9977
	0.0132	*0.2827*	*0.0084*	*0.0006, 0.0323, 0.0013, 0.0317*
e	1.9897	1.9943	1.9813	1.9978, 1.9945,1.9978, 1.9945
	0.0132	*0.2749*	*0.0093*	*0.0009, 0.0180, 0.0009, 0.0180*
f	1.9896	1.9939	1.9804	1.9980, 1.9969, 1.9948, 1.9976
	0.0130	*0.2976*	*0.0079*	*0.0130, 0.0048, 0.0231, 0.0014*
g	1.9873	1.9930	1.9840	1.9978, 1.9956, 1.9983, 1.9983
	0.0205	*0.3672*	*0.0084*	*0.0008, 0.0177, 0.0001, 0.00001*
	3W			
h	1.9902	1.9944	1.9756	1.9974, 1.9935, 1.9977, 1.9938, 1.9981, 1.9974
	0.0142	*0.2118*	*0.0097*	*0.0006, 0.0339, 0.0010, 0.0216, 0.0013, 0.0302*
i	1.9898	1.9950	1.9866	1.9973, 1.9936, 1.9980, 1.9969, 1.9939, 1.9976
	0.0138	*0.2303*	*0.0102*	*0.0009, 0.0190, 0.0129, 0.0045, 0.0243, 0.0014*
j	1.9899	1.9954	1.9822	1.9973, 1.9940, 1.9973, 1.9940, 1.9940, 1.9973
	0.0140	*0.2091*	*0.0100*	*0.0010, 0.0191, 0.0010, 0.0191, 0.0191, 0.0010*
k	1.9887	1.9940	1.9900	1.9978, 1.9945, 1.9978, 1.9948, 1.9982, 1.9982
	0.0219	*0.2955*	*0.0074*	*0.0009, 0.0191, 0.0009, 0.0187, 0.0001, 0.0001*
	4W			
l	1.9902	1.9956	1.9890	1.9971, 1.9936, 1.9980, 1.9962, 1.9935, 1.9971, 1.9980, 1.9962
	0.0145	*0.1899*	*0.0119*	*0.0014, 0.0230, 0.0116, 0.0052, 0.0231, 0.0014, 0.0116, 0.0051*
	5W			
m	1.9902	1.9953	1.9952	1.9970,1.9949,1.9979,1.9969,1.9925,1.9971, 1.9979,1.9974,1.9984, 1.9985
	0.0145	*0.2039*	*0.0091*	*0.0213, 0.0164, 0.0146, 0.0034, 0.0273, 0.0013, 0.0245, 0.0019, 0.0004, 0.0002*
	6W			
n	1.9901	1.9955	1.9895	1.9971,1.9941, 1.9974, 1.9955, 1.9941, 1.9971, 1.9974, 1.9955, 1.9979, 1.9987,
	0.0141	*0.1947*	*0.0111*	1.9979,1.9987
				0.0014, 0.0198, 0.0179, 0.0079, 0.0198, 0.0014, 0.0179, 0.0080, 0.0240,0.0001, 0.0001, 0.0240