Level of theory study of magnetic resonance parameters of chalcogen XY^- (X, Y = O, S and Se) defects in alkali halides

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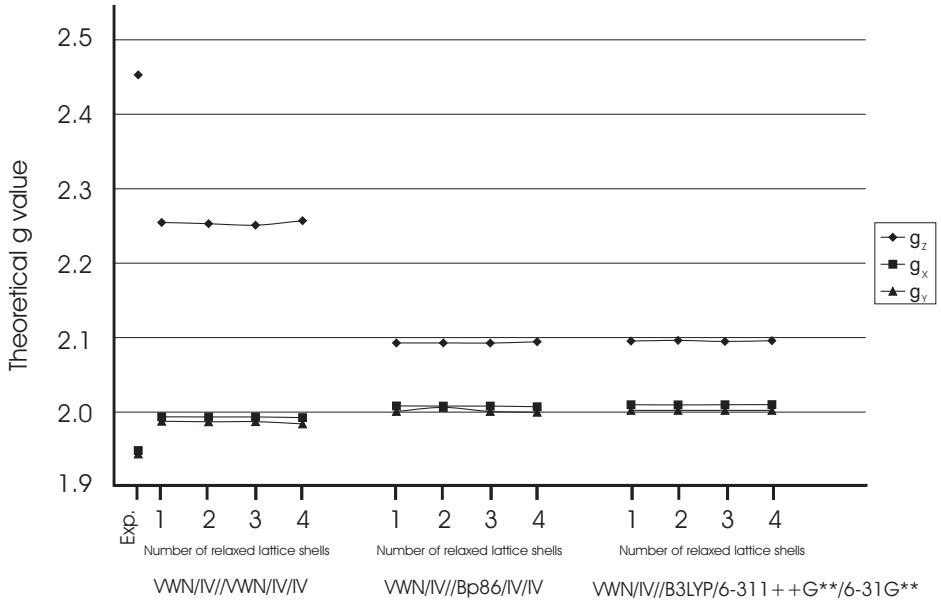
CAPTIONS OF THE SUPPORTING FIGURES

S.Fig. 1: Calculated g values for NaCl:O_2^- using the VWN/IV//VWN/IV/IV (ADF), VWN/IV//Bp86/IV/IV/ (ADF) and VWN/IV//B3LYP/6-311G**/6-31G** (G03) functional form as a function of the number of neighboring lattice shells that are allowed to relax.

S.Fig. 2: Relaxations of the first two lattice shells for the NaCl:O_2^- defect structure as a function of increasing basis set. The same convention as described in the caption of Fig. 4 is used.

S.Fig. 3: Relaxations of the first two lattice shells for the NaCl:Se_2^- defect structure as a function of increasing basis set. The same convention as described in the caption of Fig. 4 is used.



S.Figure 1
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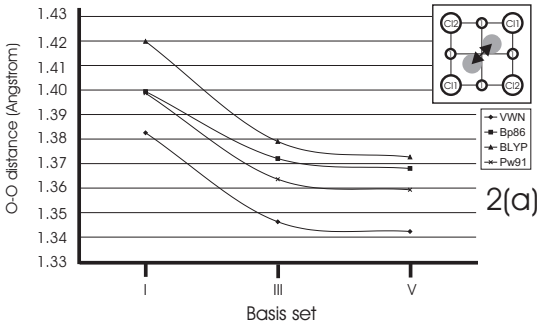

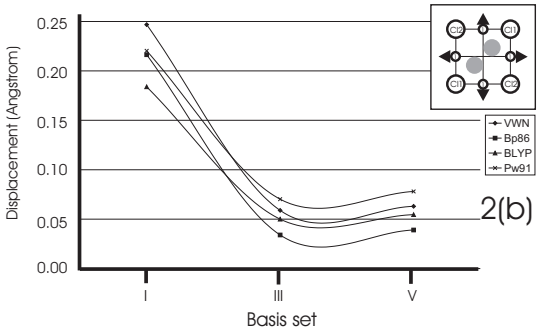

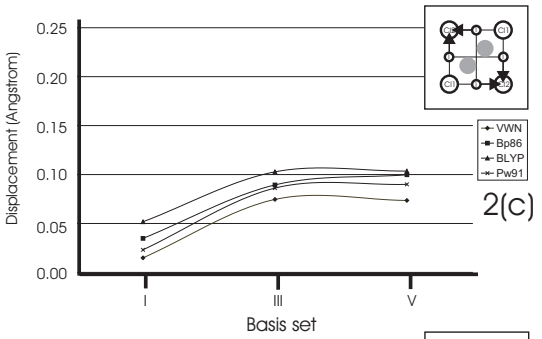

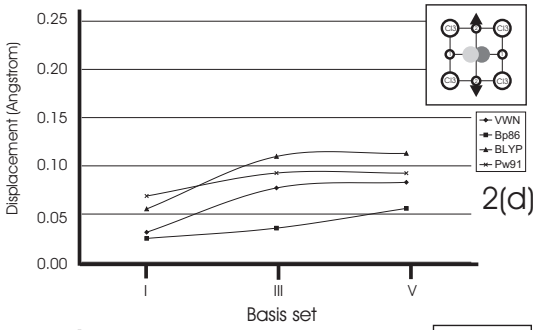

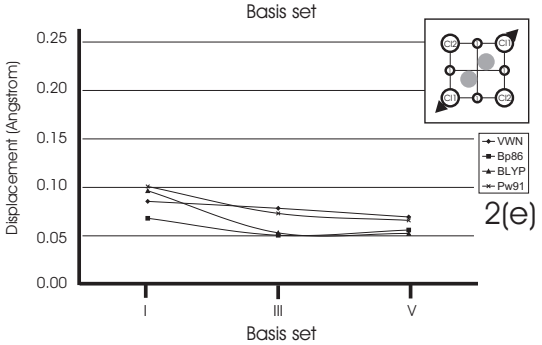

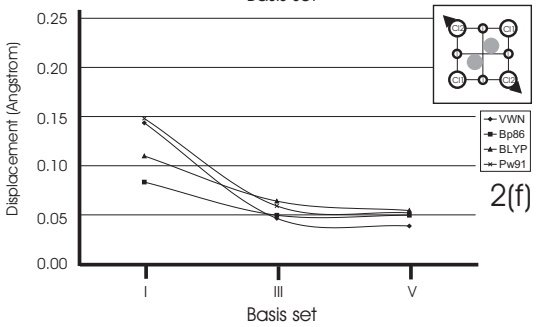

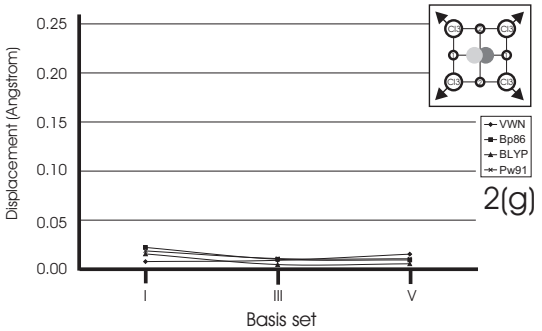

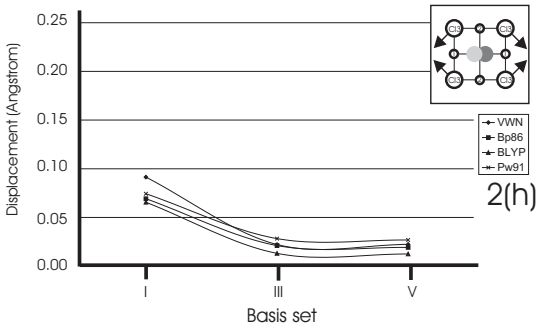

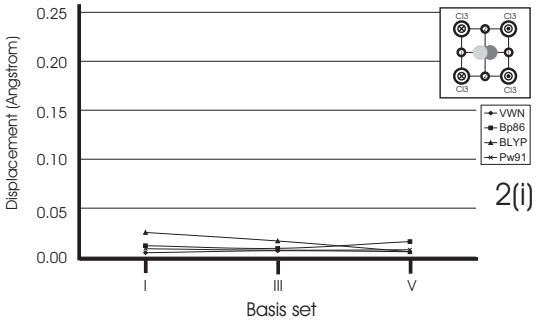

S.Figure 2
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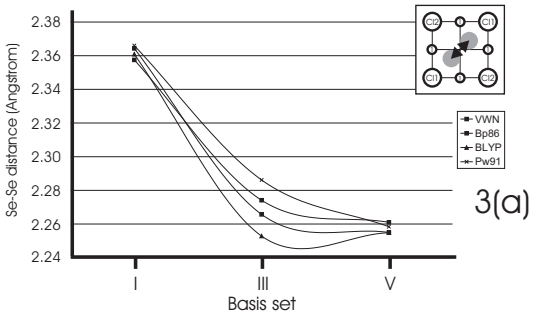

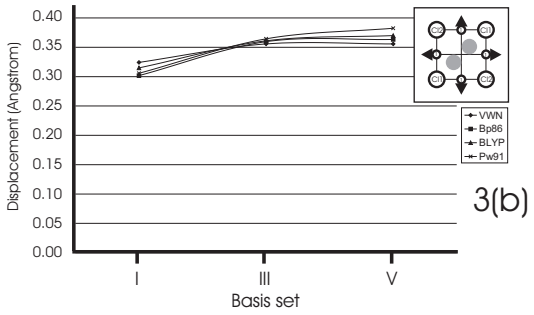

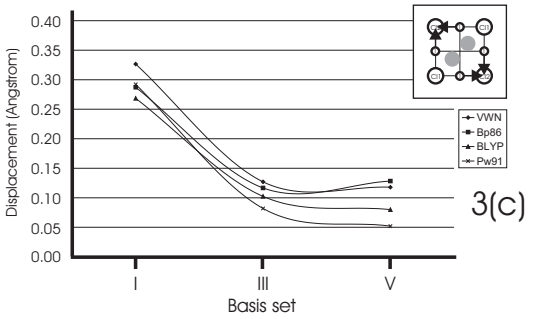

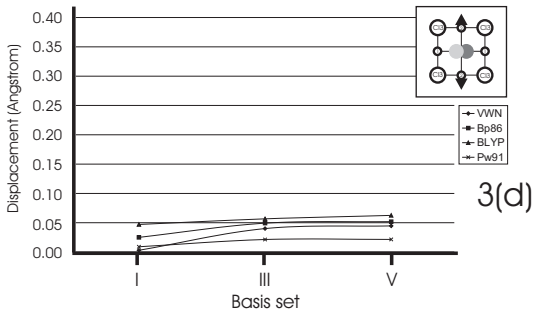

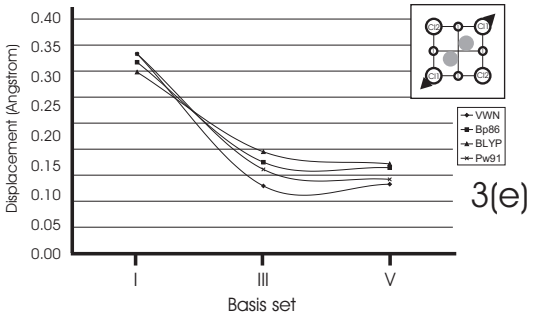

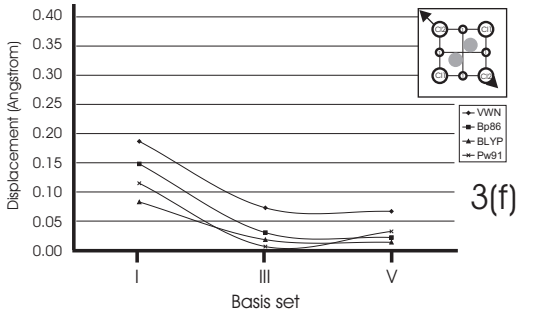

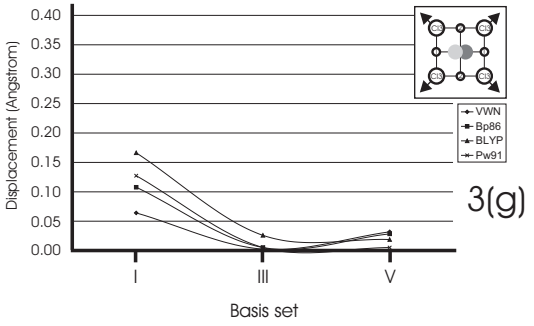

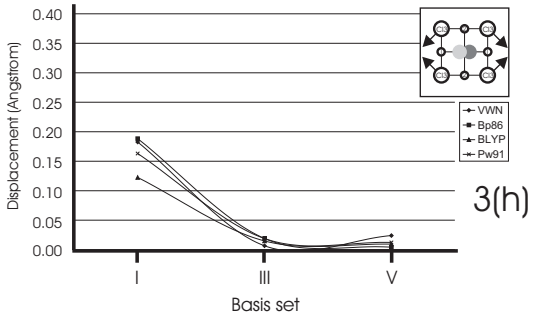

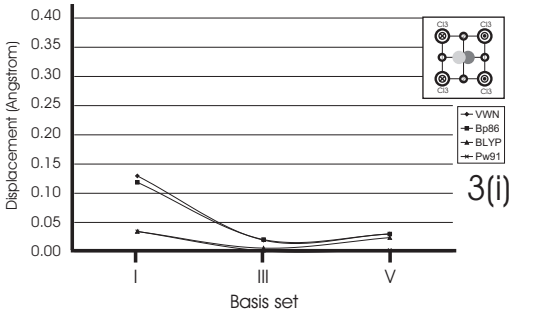

S.Figure 3
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S.Table I. Comparison between experimental and computed g values using a cluster in vacuo model and an embedded cluster approach. All calculations are performed with the ADF program package and basis set IV.

				vacuo		embedded	
lattice	defect		exp	VWN	Bp86	VWN	Bp86
NaCl	O_2^-,[a]	g_x	1,9438	1,9935	2,0080	1,9862	2,0096
		g_y	1,9436	1,9869	2,0063	1,9797	2,0023
		g_z	2,4529	2,2531	2,0928	2,2796	2,1047
NaCl	Se_2^-,[b]	g_x	1,8862	1,9141	1,9899	1,8999	1,9426
		g_y	1,7923	1,8226	1,8844	1,7844	1,8456
		g_z	2,8356	2,7256	2,6352	2,7413	2,6389
KCl	O_2^-,[a]	g_x	1,9512	1,8674	1,9968	0,6022	1,9966
		g_y	1,9551	1,8799	2,0036	0,6029	2,0023
		g_z	2,4360	2,6715	2,1413	3,8352	2,1441
KI	O_2^-,[a]	g_x	1,9370	1,7997	1,9988	1,7456	2,0017
		g_y	1,9420	1,8057	2,0079	1,7509	2,0114
		g_z	2,4859	2,8292	2,1179	3,2581	2,1494
RbBr	S_2^-,[c]	g_x	1,7448	0,3491	0,6418	0,3287	0,5290
		g_y	1,7571	0,3516	0,6465	0,3328	0,5468
		g_z	2,8936	3,7924	3,6644	3,7677	3,5835

[a]Reference[8] [b]Reference[17] [c]Reference[12]

S.Table II. Comparison between experimental and calculated g values for the MZ:XY^- defect structures using various level of theory. Also, the relative error (R.E.) and the deviation from the free electron value for g_z are listed. For the Rb atoms, the Huzinaga (HP,ref.[55]) and Glendening polarization (GP,ref.[56]) are used.

	level of theory: EPR calculation									
				basis lattice		theoretical				
	opt.	XC	basis defect	alkali	halide	g_x	g_y	g_z	R.E.	Δg_z
NaCl:$O_2^{-,a}$						***1,9483***	***1,9436***	***2,4529***		***0,4506***
	VWN/IV	VWN	III	III	III	1,9919	1,9851	2,2605	7,84	0,2582
	VWN/IV	VWN	IV	IV	IV	1,9935	1,9869	2,2531	8,15	0,2508
	VWN/IV	VWN	V	V	V	1,9958	1,9895	2,2363	8,83	0,2340
	VWN/IV	BP86	III	III	III	2,0063	2,0085	2,1055	14,16	0,1032
	VWN/IV	BP86	IV	IV	IV	2,0080	2,0063	2,0928	14,68	0,0905
	VWN/IV	BP86	V	V	V	2,0082	2,0008	2,0858	14,97	0,0835
	VWN/IV	VWN	EPR-II	6-31g**	6-31g**	1,9648	1,9646	2,2145	9,72	0,2122
	VWN/IV	VWN	6-311g**	6-31g**	6-31g**	1,9637	1,9463	2,2248	9,30	0,2225
	VWN/IV	VWN	Sadlej	6-31g**	6-31g**	1,9548	1,9346	2,1946	10,53	0,1923
	VWN/IV	VWN	augg-cc-pV6Z	6-31g**	6-31g**	1,9878	1,9601	2,1999	10,31	0,1976
	VWN/IV	B3LYP	EPR-II	6-31g**	6-31g**	2,0096	2,0022	2,0947	14,60	0,0924
	VWN/IV	B3LYP	6-311g**	6-31g**	6-31g**	2,0097	2,0022	2,0963	14,54	0,0940
	VWN/IV	B3LYP	Sadlej	6-31g**	6-31g**	2,0095	2,0022	2,0907	14,77	0,0884
	VWN/IV	B3LYP	augg-cc-pV6Z	6-31g**	6-31g**	2,0099	2,0022	2,0887	14,85	0,0864
	VWN/IV	VWN	6-311g**	6-311g**	6-31g**	1,9635	1,9467	2,2289	9,13	0,2266
	VWN/IV	VWN	6-311g**	Sadlej	6-31g**	1,9685	1,9468	2,2301	9,08	0,2278
	VWN/IV	B3LYP	6-311g**	6-311g**	6-31g**	2,0097	2,0022	2,0970	14,51	0,0947
	VWN/IV	B3LYP	6-311g**	Sadlej	6-31g**	2,0098	2,0022	2,0980	14,47	0,0957
	VWN/IV	B3PW91	6-311g**	6-31g**	6-31g**	2,0095	2,0022	2,0965	14,53	0,0942
	VWN/IV	B3P86	6-311g**	6-31g**	6-31g**	2,0095	2,0022	2,0987	14,44	0,0964
	VWN/IV	PBE1PBE	6-311g**	6-31g**	6-31g**	2,0096	2,0021	2,0983	14,46	0,0960
	VWN/IV	BHandHLyp	6-311g**	6-31g**	6-31g**	2,0112	2,0021	2,1059	14,15	0,1036
NaCl:$S_2^{-,b}$						***2,0107***	***1,9860***	***2,2531***		***0,2508***
	VWN/IV	VWN	III	III	III	2,0060	1,9817	2,2737	-0,91	0,2714
	VWN/IV	VWN	IV	IV	IV	2,0094	1,9865	2,2642	-0,49	0,2619
	VWN/IV	VWN	V	V	V	2,0146	1,9902	2,2213	1,41	0,2190
	VWN/IV	BP86	III	III	III	2,0285	1,9903	2,2005	2,33	0,1982
	VWN/IV	BP86	IV	IV	IV	2,0191	1,9946	2,1895	2,82	0,1872
	VWN/IV	BP86	V	V	V	2,0217	1,9959	2,1791	3,28	0,1768
	VWN/IV	VWN	6-311g**	6-31g	6-31g**	2,0069	1,9973	2,1985	2,42	0,1962
	VWN/IV	VWN	6-311g**	6-31g*	6-31g**	2,0072	1,9986	2,2053	2,12	0,2030
	VWN/IV	VWN	6-311g**	6-31g**	6-31g**	2,0078	1,9989	2,2364	0,74	0,2341
	VWN/IV	VWN	EPR-II	6-31g**	6-31g**	2,0061	1,9964	2,2365	0,74	0,2342
	VWN/IV	VWN	Sadlej	6-31g**	6-31g**	2,0063	1,9924	2,2296	1,04	0,2273
	VWN/IV	VWN	augg-cc-pV6Z	6-31g**	6-31g**	2,0060	1,9942	2,2292	1,06	0,2269
	VWN/IV	B3LYP	EPR-II	6-31g**	6-31g**	2,0377	2,0036	2,2047	2,15	0,2024
	VWN/IV	B3LYP	6-311g**	6-31g**	6-31g**	2,0362	2,0031	2,2068	2,05	0,2045
	VWN/IV	B3LYP	Sadlej	6-31g**	6-31g**	2,0345	2,0030	2,2058	2,10	0,2035
	VWN/IV	B3LYP	augg-cc-pV6Z	6-31g**	6-31g**	2,0374	2,0031	2,2001	2,35	0,1978
	VWN/IV	VWN	6-311g**	6-311g**	6-31g**	2,0068	1,9931	2,2436	0,42	0,2413
	VWN/IV	VWN	6-311g**	Sadlej	6-31g**	2,0096	1,9903	2,2503	0,12	0,2480
	VWN/IV	B3LYP	6-311g**	6-311g**	6-31g**	2,0335	2,0030	2,2078	2,01	0,2055
	VWN/IV	B3LYP	6-311g**	Sadlej	6-31g**	2,0315	2,0024	2,2104	1,90	0,2081
	VWN/IV	B3PW91	6-311g**	6-31g**	6-31g**	2,0332	2,0029	2,2077	2,02	0,2054
	VWN/IV	B3P86	6-311g**	6-31g**	6-31g**	2,0333	2,0029	2,2091	1,95	0,2068
	VWN/IV	PBE1PBE	6-311g**	6-31g**	6-31g**	2,0334	2,0028	2,1700	3,69	0,1677
	VWN/IV	BHandHLyp	6-311g**	6-31g**	6-31g**	2,0361	2,0027	2,1927	2,68	0,1904

NaCl:SSe$^{-,c}$						***1,9421***	***1,8818***	***2,6393***		***0,6370***
	VWN/IV	VWN	IV	IV	IV	1,8920	1,8419	2,6812	-1,59	0,6789
	VWN/IV	Bp86	IV	IV	IV	1,9724	1,9095	2,5482	3,45	0,5459
	VWN/IV	B3LYP	6-311g**	6-31g**	6-31g**	2,0846	2,0031	2,4820	5,96	0,4797
NaCl:Se$_2^{-,c}$						***1,8862***	***1,7923***	***2,8356***		***0,8333***
	VWN/IV	VWN	III	III	III	1,8981	1,7992	2,7932	1,50	0,7909
	VWN/IV	VWN	IV	IV	IV	1,9141	1,8226	2,7256	3,88	0,7233
	VWN/IV	VWN	V	V	V	1,9346	1,8654	2,6941	4,99	0,6918
	VWN/IV	BP86	III	III	III	1,9793	1,8774	2,6469	6,65	0,6446
	VWN/IV	BP86	IV	IV	IV	1,9899	1,8844	2,6352	7,07	0,6329
	VWN/IV	BP86	V	V	V	2,0016	1,9354	2,5352	10,59	0,5329
	VWN/IV	VWN	6-311g**	6-31g**	6-31g**	1,9637	1,9463	2,2248	21,54	0,2225
	VWN/IV	BP86	6-311g**	6-31g**	6-31g**	2,0011	2,0006	2,0924	26,21	0,0901
	VWN/IV	B3LYP	6-311g**	6-31g**	6-31g**	2,0097	2,0022	2,0963	26,07	0,0940
	VWN/IV	B3PW91	6-311g**	6-31g**	6-31g**	2,0095	2,0022	2,0965	26,07	0,0942
	VWN/IV	B3P86	6-311g**	6-31g**	6-31g**	2,0095	2,0022	2,0987	25,99	0,0964
	VWN/IV	PBE1PBE	6-311g**	6-31g**	6-31g**	2,0096	2,0021	2,0983	26,00	0,0960
	VWN/IV	BHandHLyp	6-311g**	6-31g**	6-31g**	2,0112	2,0021	2,1059	25,73	0,1036
NaBr:O$_2^{-,a}$						***1,9705***	***1,9663***	***2,3733***		***0,3710***
	VWN/IV	VWN	IV	IV	IV	2,0001	1,9959	2,2739	4,19	0,2716
	VWN/IV	Bp86	IV	IV	IV	2,0115	2,0061	2,0993	11,55	0,0970
NaBr:S$_2^{-,d}$						***2,0114***	***1,9876***	***2,2379***		***0,2356***
	VWN/IV	VWN	IV	IV	IV	2,0187	1,9935	2,2586	-0,92	0,2563
	VWN/IV	Bp86	IV	IV	IV	2,0537	1,9953	2,3528	-5,13	0,3505
NaBr:SSe$^{-,e}$						***1,9365***	***1,8916***	***2,6259***		***0,6236***
	VWN/IV	VWN	IV	IV	IV	1,9359	1,8953	2,6229	0,11	0,6206
	VWN/IV	Bp86	IV	IV	IV	1,9887	1,9356	2,5221	3,95	0,5198
NaBr:Se$_2^{-,e}$						***1,9007***	***1,8079***	***2,8073***		***0,8050***
	VWN/IV	VWN	IV	IV	IV	1,9196	1,8407	2,7344	2,60	0,7321
	VWN/IV	Bp86	IV	IV	IV	1,9785	1,8850	2,6609	5,21	0,6586
NaI:O$_2^{-,a}$						***1,9996***	***2,0004***	***2,1859***		***0,1836***
	VWN/IV	VWN	IV	IV	IV	1,9882	1,9943	2,2849	-4,53	0,2826
	VWN/IV	Bp86	IV	IV	IV	2,0049	2,0116	2,1153	3,23	0,1130
NaI:S$_2^{-,f}$						***2,0178***	***1,9942***	***2,2303***		***0,2280***
	VWN/IV	VWN	IV	IV	IV	2,0189	2,0000	2,2471	-0,75	0,2448
	VWN/IV	Bp86	IV	IV	IV	2,0259	2,0119	2,2026	1,24	0,2003
NaI:SSe$^{-,g}$						***1,9675***	***1,9004***	***2,6064***		***0,6041***
	VWN/IV	VWN	IV	IV	IV	1,9581	1,9238	2,5943	0,46	0,5920
	VWN/IV	Bp86	IV	IV	IV	2,0049	1,9571	2,4924	4,37	0,4901
NaI:Se$_2^{-,g}$						***1,9042***	***1,8148***	***2,8015***		***0,7992***
	VWN/IV	VWN	IV	IV	IV	1,8795	1,8211	2,8013	0,01	0,7990
	VWN/IV	Bp86	IV	IV	IV	1,9538	1,8776	2,7072	3,37	0,7049

KCl:O_2^{-}[a]						***1,9512***	***1,9551***	***2,4360***		***0,4337***
	VWN/IV	VWN	III	III	III	1,6149	1,6180	3,1261	-28,33	1,1238
	VWN/IV	VWN	IV	IV	IV	1,8674	1,8799	2,6715	-9,67	0,6692
	VWN/IV	VWN	V	V	V	1,8964	1,9031	2,6035	-6,88	0,6012
	VWN/IV	BP86	III	III	III	1,9976	2,0039	2,1316	12,50	0,1293
	VWN/IV	BP86	IV	IV	IV	1,9968	2,0036	2,1413	12,10	0,1390
	VWN/IV	BP86	V	V	V	1,9987	2,0057	2,1131	13,26	0,1108
	VWN/IV	B3LYP	6-311g**	6-31g**	6-31g**	2,0019	2,0091	2,1765	10,65	0,1742
KCl:S_2^{-}[f]						***0,9484***	***0,9500***	***3,4303***		***1,428***
	VWN/IV	VWN	III	III	III	0,4090	0,4109	3,7047	-8,00	1,7024
	VWN/IV	VWN	IV	IV	IV	0,5424	0,5439	3,6968	-7,77	1,6945
	VWN/IV	VWN	V	V	V	0,5769	0,5975	3,6164	-5,43	1,6141
	VWN/IV	VWN	6-311g**	6-31g	6-31g**	0,5104	0,5244	3,6984	-7,82	1,6961
	VWN/IV	VWN	6-311g**	6-31g*	6-31g**	0,5801	0,5843	3,6555	-6,57	1,6532
	VWN/IV	VWN	6-311g**	6-31g**	6-31g**	0,5985	0,6002	3,6352	-5,97	1,6329
	VWN/IV	BP86	III	III	III	1,7080	1,7232	2,9563	13,82	0,954
	VWN/IV	BP86	IV	IV	IV	1,5936	1,6064	3,0716	10,46	1,0693
	VWN/IV	BP86	V	V	V	1,5539	1,5955	3,1645	7,75	1,1622
	VWN/IV	B3LYP	6-311g**	6-31g**	6-31g**	2,0024	2,0349	2,3667	31,01	0,3644
KBr:O_2^{-}[a]						***1,9268***	***1,9315***	***2,5203***		***0,5180***
	VWN/IV	VWN	IV	IV	IV	1,4295	1,4329	3,3708	-33,75	1,3685
	VWN/IV	Bp86	IV	IV	IV	1,9990	2,0079	2,1188	15,93	0,1165
KBr:S_2^{-}[f]						***0,9434***	***0,8388***	***3,5037***		***1,5014***
	VWN/IV	VWN	IV	IV	IV	1,1168	1,1119	3,4948	0,25	1,4925
	VWN/IV	Bp86	IV	IV	IV	1,8867	1,8648	2,6793	23,53	0,6770
KI:O_2^{-}[a]						***1,9370***	***1,9420***	***2,4859***		***0,4836***
	VWN/IV	VWN	IV	IV	IV	1,7997	1,8057	2,8292	-13,81	0,8269
	VWN/IV	Bp86	IV	IV	IV	1,9988	2,0079	2,1179	14,80	0,1156
KI:S_2^{-}[f]						***1,6369***	***1,6254***	***3,0629***		***1,0606***
	VWN/IV	VWN	IV	IV	IV	1,5654	1,5537	3,1655	-3,35	1,1632
	VWN/IV	Bp86	IV	IV	IV	1,9617	1,9359	2,5121	17,98	0,5098
KI:SSe^{-}[g]						***0,9681***	***0,9532***	***3,6290***		***1,6267***
	VWN/IV	VWN	IV	IV	IV	1,1042	1,0924	3,5028	3,48	1,5005
	VWN/IV	Bp86	IV	IV	IV	1,5059	1,4764	3,2290	11,02	1,2267
KI:Se_2^{-}[g]						***0,7824***	***0,7698***	***3,7079***		***1,7056***
	VWN/IV	VWN	IV	IV	IV	0,7831	0,7752	3,6229	2,29	1,6206
	VWN/IV	Bp86	IV	IV	IV	1,0101	0,9913	3,5399	4,53	1,5376
RbCl:O_2^{-}[a]						***1,9836***	***1,9846***	***2,2947***		***0,2924***
	VWN/IV	VWN	III	III	III	0,3304	0,3323	3,9419	-71,78	1,9396
	VWN/IV	VWN	IV	IV	IV	0,8615	0,8638	3,7549	-63,63	1,7526
	VWN/IV	VWN	V	V	V	1,5309	1,5344	3,2903	-43,39	1,288
	VWN/IV	BP86	III	III	III	1,9986	2,0058	2,1087	8,11	0,1064
	VWN/IV	BP86	IV	IV	IV	1,9976	2,0059	2,1231	7,48	0,1208
	VWN/IV	BP86	V	V	V	1,9987	2,0065	2,1005	8,46	0,0982
	VWN/IV	BP86	6-311g**	3-21G + GP + HP	6-31g**	1,9874	2,0046	2,1088	8,10	0,1065
	VWN/IV	B3LYP	6-311g**	3-21G + GP + HP	6-31g**	2,0019	2,0094	2,1682	5,51	0,1659

RbCl:S_2^{-}[h]						***1,8728***	***1,8881***	***2,6515***		***0,6492***
	VWN/IV	VWN	III	III	III	1,0329	1,0393	3,5541	-34,04	1,5518
	VWN/IV	VWN	IV	IV	IV	1,0576	1,0641	3,5053	-32,20	1,503
	VWN/IV	VWN	V	V	V	1,4032	1,4555	3,2459	-22,42	1,2436
	VWN/IV	BP86	III	III	III	1,9033	1,9232	2,5711	3,03	0,5688
	VWN/IV	BP86	IV	IV	IV	1,9058	1,9253	2,5528	3,72	0,5505
	VWN/IV	BP86	V	V	V	1,9105	1,9266	2,5073	5,44	0,505
	VWN/IV	VWN	6-311g**	3-21G	6-31g**	1,1091	1,1308	3,4535	-30,25	1,4512
	VWN/IV	VWN	6-311g**	3-21G + GP	6-31g**	1,341	1,3675	3,2513	-22,62	1,249
	VWN/IV	VWN	6-311g**	3-21G + HP	6-31g**	1,2274	1,2985	3,2958	-24,30	1,2935
	VWN/IV	VWN	6-311g**	3-21G + GP + HP	6-31g**	1,4234	1,4824	3,2052	-20,88	1,2029
	VWN/IV	BP86	6-311g**	6-31g**	6-31g**	1,8968	1,9267	2,5635	3,32	0,5612
	VWN/IV	B3LYP	6-311g**	3-21G + GP + HP	6-31g**	2,0016	2,0241	2,1386	19,34	0,1363
RbBr:O_2^{-}[a]						***1,9745***	***1,9763***	***2,3425***		***0,3402***
	VWN/IV	VWN	IV	IV	IV	0,2953	0,2974	3,9416	-68,26	1,9393
	VWN/IV	VWN	V	V	V	1,6459	1,6488	2,8623	-22,19	0,8600
	VWN/IV	Bp86	IV	IV	IV	1,9979	2,0067	2,1172	9,62	0,1149
RbBr:S_2^{-}[f,h]						***1,7448***	***1,7571***	***2,8936***		***0,8913***
	VWN/IV	VWN	IV	IV	IV	0,1673	0,1692	3,8016	-31,38	1,7993
	VWN/IV	VWN	V	V	V	0,3491	0,3516	3,7924	-31,06	1,7901
	VWN/IV	Bp86	IV	IV	IV	0,6418	0,6465	3,6644	-26,64	1,6621
RbI:O_2^{-}[a]						***1,9674***	***1,9695***	***2,3774***		***0,3751***
	VWN/IV	VWN	IV	IV	IV	0,8271	0,8299	3,8101	-60,26	1,8078
	VWN/IV	VWN	V	V	V	1,4363	1,4411	3,3709	-41,79	1,3686
	VWN/IV	Bp86	IV	IV	IV	1,9977	2,0083	2,1334	10,26	0,1311
RbI:S_2^{-}[f]						***1,2895***	***1,2968***	***3,3595***		***1,3572***
	VWN/IV	VWN	IV	IV	IV	0,8728	0,9016	3,6182	-7,70	1,6159
	VWN/IV	VWN	V	V	V	1,5707	1,5877	3,1911	5,01	1,1888
	VWN/IV	Bp86	IV	IV	IV	1,4696	1,4836	3,3056	1,60	1,3033

[a]Reference[8] [b]Reference[15] [c]Reference[17] [d]Reference[18]
[e]Reference[19] [f]Reference[12] [g]Reference[13] [h]Reference[20]

S.TABLE III. Theoretical and experimental ^{17}O, ^{33}S and ^{77}Se hyperfine couplings (in MHz) for the O_2^-, S_2^- and Se_2^- molecular ions doped in NaCl using various functional forms.

			VWN		Bp86		B3LYP	B3Pw91	B3P86	PBE1PBE	BHandHLYP
		exp.	ADF	G03	ADF	G03	G03	G03	G03	G03	G03
	A_x	n.a.	22,8	82,9	46,7	58,6	55,1	63,7	63,7	52,9	31,2
O_2^-	A_y	n.a.	-128,4	-149,1	-181,2	-174,3	-193,1	-183,1	-182,6	-194,3	-227,7
	A_z	n.a.	58,7	86,2	48,0	62,3	58,1	66,1	65,8	55,3	35,3
	A_x	< A_y[a]	-10,0	-11,3	-47,9	-45,6	-41,1	-46,9	-47,4	-48,1	-30,3
S_2^-	A_y	108,5	71,4	71,9	81,7	82,3	96,6	93,8	93,6	93,0	108,9
	A_z	< A_y	-30,0	-36,3	-48,9	-46,2	-42,3	-47,2	-48,7	-49,5	-32,4
	A_x	63[b]	-40,8	-23,5	-244,2	-260,8	-252,8	-256,6	-256,9	-260,4	-229,2
Se_2^-	A_y	350,0	271,0	292,7	337,4	364,4	374,4	402,5	404,5	399,7	478,4
	A_z	287,0	234,0	240,7	-266,5	-264,4	-258,4	-262,7	-262,3	-266,2	-237,2

[a]Reference[15] [b]Reference[17]

S.Table IV. Experimental and theoretical ^{17}O, ^{33}S and ^{77}Se hyperfine couplings (MHz) using ADF and the VWN functional form and basis set IV for the NaZ and KZ lattices. For the RbZ lattices basis set V was used.

		experimental					theoretical				
				SSe$^-$					SSe$^-$		
		O_2^-[a]	S_2^-	S	Se	Se_2^-	O_2^-	S_2^-	S	Se	Se_2^-
	A_x	n.a.	< A_y[b]	< A_z[d]	69[d]	63[f]	25,9	-10,0	-7,5	-95,7	-40,8
NaCl	A_y	n.a.	108,5	80,0	432,0	350,0	-128,9	71,4	50,4	293,7	271,9
	A_z	n.a.	< A_y	60,0	200,0	287,0	59,4	-30,0	35,7	232,8	234,7
	A_x	n.a.	n.a.	n.a.	n.a.	60[g]	24,9	-13,8	-10,8	-107,6	-46,6
NaBr	A_y	n.a.	n.a.	n.a.	n.a.	357,0	-125,5	71,6	54,1	300,0	267,3
	A_z	n.a.	n.a.	n.a.	n.a.	275,0	57,9	-31,7	26,5	173,3	220,5
	A_x	n.a.	n.a.	n.a.	n.a.	n.a.	-123,7	-15,9	-13,1	-13,6	-44,5
NaI	A_y	n.a.	n.a.	n.a.	n.a.	n.a.	28,1	72,9	57,7	-315,4	257,8
	A_z	n.a.	n.a.	n.a.	n.a.	n.a.	-57,5	-32,4	18,7	127,8	239,0
	A_x	189,3	< A_z[c]	n.a.	n.a.	n.a.	-156,4	-29,9	3,3	12,9	19,7
KCl	A_y	< A_z	< A_z	n.a.	n.a.	n.a.	15,4	-28,0	4,6	21,4	30,7
	A_z	55,1	137,0	n.a.	n.a.	n.a.	-72,9	115,0	156,8	854,6	820,4
	A_x	181,3	< A_z[c]	n.a.	n.a.	n.a.	-143,4	1,3	5,3	14,8	20,3
KBr	A_y	< A_z	< A_z	n.a.	n.a.	n.a.	16,2	22,3	14,5	69,4	33,7
	A_z	71,1	145,0	n.a.	n.a.	n.a.	-73,2	122,6	137,8	775,9	806,4
	A_x	184,3	< A_y[c]	< A_y[e]	< A_y[e]	< A_y[e]	-113,2	-5,6	4,7	5,6	62,7
KI	A_y	< A_z	64,0	< A_z	< A_z	< A_z	26,1	37,5	20,8	102,4	24,5
	A_z	64,2	93,0	141,0	749,0	740,0	-45,5	90,4	123,0	698,6	732,8
	A_x	201,6	n.a.	n.a.	n.a.	n.a.	-177,3	-21,6	4,7	-2,5	17,6
RbCl	A_y	< A_x	n.a.	n.a.	n.a.	n.a.	4,0	61,8	27,1	160,7	47,3
	A_z	< A_x	n.a.	n.a.	n.a.	n.a.	-46,2	238,8	120,9	791,4	889,0
	A_x	n.a.	n.a.	n.a.	n.a.	n.a.	-239,3	4,6	6,0	7,6	14,5
RbBr	A_y	n.a.	n.a.	n.a.	n.a.	n.a.	18,3	6,5	13,3	19,6	18,6
	A_z	n.a.	n.a.	n.a.	n.a.	n.a.	-57,2	168,1	136,5	964,3	908,5
	A_x	193,7	< A_z[c]	n.a.	n.a.	n.a.	-187,3	3,2	4,8	19,9	20,9
RbI	A_y	< A_x	< A_z	n.a.	n.a.	n.a.	7,6	15,6	5,9	50,2	31,7
	A_z	< A_x	105,0	n.a.	n.a.	n.a.	-57,3	144,3	156,0	999,3	890,5

[a]Reference[8] [b]Reference[15] [c]Reference[12] [d]Reference[21]
[e]Reference[13] [f]Reference[17] [g]Reference[19]