Estimation of Bonding Nature Using Diamagnetic Susceptibility: Supplementary Information

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The numerical data used for generating the plot of $\Delta\chi_{EN}$ versus α [Fig. 1] is given in Table 1. Non-magnetic insulating materials, which are appropriate for LDS measurements, are selected because the LDS is too small to be extracted in materials with magnetic atoms or ions. The extraction of the LDS in metals, too, is difficult because metals exhibit Pauli paramagnetism and Landau diamagnetism in addition to Larmor diamagnetism.

Table 1 Experimental (χ_{LD}) and theoretical (χ_{ref}) Larmor diamagnetic susceptibilities, their difference ($\Delta\chi_{LD}$), summation of theoretical susceptibilities for atoms constituting dominant bonds ($\sum_i' \chi_{ref}(i)$), the deviation rate (α), and the electronegativity difference ($\Delta\chi_{EN}$). For example, in the case of KCl, $\Delta\chi_{LD} = (-39.3) - (-45.7) = 6.4$ and $\alpha = -|6.4/(-45.7)| = 0.14$. All the susceptibilities are in units of emu mol^{-1}. For simple substances, e.g., C (diamond), Si, Ge, and H_2, the referential values are set to those for the virtual ionic states, e.g., $\chi_{ref} = \{\chi_{ref}(C^{4+}) + \chi_{ref}(C^{4-})\}/2$ and $\{\chi_{ref}(H^+) + \chi_{ref}(H^-)\}/2$. Superscript [a] means data measured in this study.

materials	χ_{LD}	χ_{ref}	$\Delta\chi_{LD}$	$\sum_i' \chi_{ref}(i)$	α	$\Delta\chi_{EN}$
LiF	-10.1	-8.4	-1.7	-8.4	-0.21	3.00
LiCl	-24.3	-29.3	5.0	-29.3	0.17	2.18
LiBr	-34.3	-54.3	20.0	-54.3	0.37	1.98
LiI	-50.0	-80.3	30.3	-80.3	0.38	1.68
NaF	-16.4	-12.3	-4.1	-12.3	-0.33	3.05
NaCl	-30.3	-33.2	2.9	-33.2	0.09	2.23
NaBr	-41.0	-58.2	17.2	-58.2	0.30	2.03
NaI	-57.0	-84.2	27.2	-84.2	0.32	1.73
KF	-23.6	-24.8	1.2	-24.8	0.05	3.16
KCl	-39.3	-45.7	6.4	-45.7	0.14	2.34
KBr	-49.1	-70.7	21.6	-70.7	0.31	2.14
KI	-63.8	-96.7	32.9	-96.7	0.34	1.84
RbF	-31.9	-43.1	11.2	-43.1	0.26	3.16
RbBr	-56.4	-89.0	32.6	-89.0	0.37	2.14
RbI	-72.2	-115.0	42.8	-115.0	0.37	1.84
CsF	-44.5	-63.1	18.6	-63.1	0.29	3.19
CsCl	-56.7	-84.0	27.3	-84.0	0.32	2.37
CsBr	-67.2	-109.0	41.8	-109.0	0.38	2.17
CsI	-82.6	-135.0	52.4	-135.0	0.39	1.87
BeO	-11.9	-12.9	1.0	-12.9	0.08	1.87
MgO	-10.2	-15.8	5.6	-15.8	0.35	2.13
CaS	-45.5	-53.3	7.8	-53.3	0.15	1.58
CaSe	-61.2	-83.3	22.2	-83.3	0.27	1.55
CaTe	-84.4	-118.3	33.9	-118.3	0.29	1.10
SrS	-58.0	-68.0	10.0	-68.0	0.15	1.63
SrSe	-75.5	-98.0	22.5	-98.0	0.23	1.60
SrTe	-93.0	-133.0	40.0	-133.0	0.30	1.15
BaS	-75.8	-86.0	10.2	-86.0	0.12	1.69
Al_2O_3	-37.0	-42.8	5.8	-42.8	0.14	1.83
In_2O_3	-56.0	-101.8	45.8	-101.8	0.45	1.66
ZnS	-25.0	-51.0	26.0	-51.0	0.51	0.93
CdS	-50.0	-77.0	27.0	-77.0	0.35	0.89
AgBr	-61.0	-98.0	37.0	-98.0	0.38	1.03
AgCl	-49.0	-73.0	24.0	-73.0	0.33	1.23
AgF	-36.5	-52.1	15.6	-52.1	0.30	2.05
AgI	-80.0	-124.0	44.0	-124.0	0.35	0.73
GaP	-30.0	-74.5	44.5	-74.5	0.60	0.38
GaAs	-33.3	-104.5	71.2	-104.5	0.68	0.37
GaSb	-38.4	-139.5	101.1	-139.5	0.72	0.24
InP	-45.6	-97.0	51.4	-97.0	0.53	0.41
InAs	-55.3	-127.0	71.7	-127.0	0.56	0.40
InSb	-65.9	-162.0	96.1	-162.0	0.59	0.27
ZnSe	-46.5	-81.0	34.5	-81.0	0.43	0.90
ZnTe	-67.0	-118.0	51.0	-118.0	0.43	0.45
CdSe	-63.9	-107.0	43.1	-107.0	0.40	0.86
CdTe	-84.0	-142.0	58.0	-142.0	0.41	0.41
HgSe	-58.7	-125.0	66.3	-125.0	0.53	0.55
HgTe	-75.8	-160.0	84.2	-160.0	0.53	0.10
C (diamond)	-5.9	-25.1	19.2	-25.1	0.76	0
Si	-3.1	-56.0	52.9	-56.0	0.94	0
Ge	-11.6	-76.2	64.7	-76.2	0.85	0
BCl_3	-59.9	-87.2	27.3	-87.2	0.31	1.12
CO_2	-21.0	-25.4	4.4	-25.4	0.17	0.89
CCl_4	-66.8	-116.2	49.3	-116.2	0.42	0.61
CBr_4	-93.7	-216.1	122.4	-216.1	0.57	0.41
CI_4	-136.0	-310.1	174.1	-310.1	0.56	0.11
$GaCl_3$	-63.0	-96.5	33.5	-96.5	0.35	1.35
$GeCl_4$	-72.0	-124.5	52.5	-124.5	0.42	1.15
GeF_4	-50.0	-40.9	-9.1	-40.9	-0.22	1.97

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SF_6	-44.0	-50.0	6.0	-50.0	0.12	1.40
SeF_6	-51.0	-55.1	4.1	-55.1	0.07	1.43
$SiBr_4$	-126.0	-218.1	92.1	-218.1	0.42	1.06
$SiCl_4$	-87.5	-118.1	30.6	-118.1	0.26	1.26
TeF_6	-66.0	-68.6	2.6	-68.6	0.04	1.88
H_2	-4.0	-8.0	4.0	-8.0	0.50	0.00
HCl	-22.6	-29.0	6.4	-29.0	0.22	0.96
HF	-8.6	-8.1	-0.5	-8.1	-0.06	1.78
HI	-48.3	-80.0	31.7	-80.0	0.40	0.46
H_2O	-13.0	-12.6	-0.4	-12.6	-0.03	1.24
H_2S	-25.5	-40.0	14.5	-40.0	0.36	0.38
NH_3	-16.3	-22.0	5.7	-22.0	0.26	0.84
CH_4	-17.4	-50.0	32.6	-50.0	0.65	0.35
LiF	-8.7±0.2[a]	-8.7	0.0±0.2	-8.7	0.00±0.01	3.00
NaF	-11.0±0.2[a]	-12.3	1.3±0.2	-12.3	0.11±0.01	3.05
KF	-20.0±0.2[a]	-24.8	4.8±0.2	-24.8	0.19±0.01	3.16
AlF_3	-22.5±0.6[a]	-26.8	4.3±0.6	-26.8	0.16±0.02	2.37
LiH	-4.6	-8.6	4.0	-8.6	0.47	1.22
B_2H_6	-21.0	-48.4	27.4	-48.4	0.57	0.16
SiH_4	-20.4	-34.1	13.7	-34.1	0.40	0.30
GeH_4	-29.7	-40.5	10.8	-40.5	0.27	0.19
NaH	-6.9±0.6[a]	-12.2	5.3±0.6	-12.2	0.43±0.05	1.27
AlH_3	-5.0±4.0[a]	-26.5	21.5±4.0	-26.5	0.81±0.14	0.59
AlD_3	-7.0±2.5[a]	-26.5	19.5±2.5	-26.5	0.74±0.10	0.59
$LiAlD_4$	-14.8±0.5[a]	-35.1	20.3±0.5	-34.5	0.59±0.02	0.59
$LiAlH_4$	-15.1±0.5[a]	-35.1	20.0±0.5	-34.5	0.58±0.02	0.59
$NaAlH_4$	-15.7±0.5[a]	-38.7	23.0±0.5	-34.5	0.67±0.02	0.59
$LiBH_4$	-16.7±0.5[a]	-32.8	16.1±0.5	-32.2	0.50±0.02	0.16
$NaBH_4$	-19.5±0.5[a]	-36.4	16.9±0.5	-32.2	0.52±0.02	0.16