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## Trends in the stability of covalent dative bonds with variable solvent polarity depend on the charge transfer in the Lewis electron-pair system†

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**In general, the stability of neutral complexes with dative bonds increases as the polarity of the solvent increases. This is based on the fact that the dipole moment of the complex increases as the charge transferred from the donor to the acceptor increases. As a result, the solvation energy of the complex becomes greater than that of subsystems, causing an increase in the stabilization energy with increasing solvent polarity. Our research confirms this assumption, but only when the charge transfer is sufficiently large. If it is below a certain threshold, the increase in the complex's dipole moment is insufficient to result in a higher solvation energy than subsystems. Thus, the magnitude of the charge transfer in the Lewis electron-pair system determines the stability trends of dative bonds with varying solvent polarity. We used molecular dynamics (MD) simulations based on an explicit solvent model, which is considered more reliable, to verify the results obtained with a continuous solvent model.**

The covalent dative bond (DB), also called the coordinate, coordinate covalent, or donor-acceptor bond, shares similarities with a covalent bond in that it involves an electron pair facilitating the binding process.<sup>1,2</sup> However, unlike a covalent bond where each fragment contributes one electron to the bond, in a DB, one fragment, specifically the electron donor, provides the electron pair. The transfer of charge from an electron donor (Lewis base) to an electron acceptor (Lewis acid) gives origin to the ionic character in the bond (see eqn (1)).<sup>3,4</sup>

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The resulting covalent-ionic nature of the DB highlights the importance of the solvent in determining the strength of the dative bond.

$$\Psi_{\text{dative}} (D^+ - A^-) = a\Psi_{\text{covalent}} (D - A) + b\Psi_{\text{ionic}} (D^+, A^-) \quad (1)$$

Previously, we studied complexes with covalent dative bonds in both neutral and charged systems and observed varying stability trends in solvents as the dielectric constants of the solvents changed.<sup>5-12</sup> We have shown that the stability of DB in neutral complexes increases systematically with increasing solvent polarity.<sup>5-10</sup> However, the opposite trend is observed for DB in charged coordinate complexes.<sup>11,12</sup>

The effect of solvent was also studied in hydrogen-bonded complexes. As expected, a decrease in stability with increasing solvent polarity was observed in most complexes.<sup>13,14</sup> However, our research has shown that certain hydrogen-bonded complexes unexpectedly stabilize with increased solvent polarity.

This surprising behavior was attributed to a larger charge transfer within the Lewis electron-pair system, resulting in an increase in dipole moment and, consequently, in the solvation energy. Based on these findings, we decided to conduct a detailed study on the effects of solvent on the stability of neutral complexes with DB. Two families of DB complexes are considered: (i) systems with  $\text{InCl}_3$  as an electron acceptor and a series of electron donors and (ii) systems with  $\text{NCl}_3$  as an electron donor and a series of electron acceptors. In addition to the gas phase, we investigated the effects of four aprotic solvents, carbon disulfide, chloroform, dichloromethane and o-dichlorobenzene.

**Subsystems.** Fig. S1 and S2 (ESI†) illustrate the optimized structures of all the subsystems; Table 1 collects ESP characteristics ( $V_{s,\text{max}}$  and  $V_{s,\text{min}}$ ) of complexes.  $\text{NH}_3$  is the strongest and  $\text{OF}_2$  the weakest electron donor;  $\text{InCl}_3$  is the strongest and  $\text{BF}_3$  the weakest electron acceptor among the studied systems.

**Complexes.** Fig. S3 and S4 (ESI†) illustrate the optimized structures of all the complexes containing  $\text{InCl}_3$  as an electron acceptor ( $\text{Y} \rightarrow \text{InCl}_3$ ) or  $\text{NCl}_3$  as an electron donor ( $\text{NCl}_3 \rightarrow \text{X}$ ).



**Table 1** The maximum ( $V_{s,\max}$ ) and minimum ( $V_{s,\min}$ ) electrostatic potentials of acceptor and donor molecules respectively

Donor molecules	$V_{s,\min}$ (kcal mol <sup>-1</sup> )	$V_{s,\max}$ (kcal mol <sup>-1</sup> )
NH <sub>3</sub>	-37.73	—
NMe <sub>3</sub>	-30.33	—
NH <sub>2</sub> Ph(4-Me)	-26.59	—
NH <sub>2</sub> Ph	-24.93	—
NCl <sub>3</sub>	-11.35	—
NHPhPh(3-Me)	-9.91	—
NHPh <sub>2</sub>	-9.08	—
NPh <sub>3</sub>	-5.61	—
NHClCOMe	-4.77	—
NHPhCOMe	-1.56	—
OF <sub>2</sub>	-1.03	—
Acceptor molecules	—	—
InCl <sub>3</sub>	—	71.38
GaCl <sub>3</sub>	—	60.93
BF <sub>3</sub>	—	52.47

The properties of these complexes are summarized in Tables 2 and 3. Notably, the complexes in both families either increase or decrease their stabilities as solvent polarity increases. Used DFT methods are further validated by inclusion of relativistic effects for heavy elements (Table S1, ESI<sup>†</sup>) and MP2 calculations (Table S2, ESI<sup>†</sup>).

The gas phase stabilization energies of all complexes demonstrate a strong correlation with the DB length (as shown in Fig. S5, ESI<sup>†</sup>) and are generally high, ranging from 12 to 36 kcal mol<sup>-1</sup>. This suggests that the complexes contain both moderate and strong DBs. The InCl<sub>3</sub>·OF<sub>2</sub> complex represents one exception – its significantly lower gas phase stabilization energy of 3.08 kcal mol<sup>-1</sup> indicates its vdW character.

The Wiberg bond indexes, which provide estimates of bond strength, are listed in Table 2. Their values range between 0.13 and 0.31, further supporting moderately strong DB. In contrast, the Wiberg bond index (WBI) for InCl<sub>3</sub>·OF<sub>2</sub> complex is smaller, only 0.08. For comparison, WBI for single and double covalent bonds in ethane and ethylene are 1.0 and 2.0, respectively. For the heavier elements such as In and Ga considered in this study, the Mayer bond order also supports the formation of moderately strong DB (Table S3, ESI<sup>†</sup>).

The most significant findings of this study concern the influence of solvent polarity on the stability of the DB. Table 2 shows that for the strongest complexes (those with gas phase binding energy greater than 27 kcal mol<sup>-1</sup>), both  $\Delta E$  and  $\Delta G$  increase as solvent polarity increases. The increase in stability is particularly significant in the InCl<sub>3</sub>·NH<sub>3</sub> system, where it accounts for more than 5 kcal mol<sup>-1</sup> due to a shift of 10 in the value of  $\epsilon$ .

Conversely, for weaker complexes with gas phase binding energy less than 24 kcal mol<sup>-1</sup>, the relationship between  $\Delta E$  and  $\Delta G$  and solvent polarity is reversed, transitioning from an increase to a decrease. It is worth noting that in previous studies on neutral dative bond complexes, only an increase in the stability of the DB with increasing solvent polarity was observed.<sup>5–10</sup> However, only strong DB complexes were investigated in those studies.

Table 2 emphasizes that  $\Delta E_{\text{solv}}$  accurately reflects the different behavior of all the complexes. Negative and positive  $\Delta E_{\text{solv}}$

consistently correspond to an increase or decrease in  $\Delta E$ , respectively, as the solvent polarity increases. This is predictable since  $\Delta E_{\text{solv}}$  is obtained from the stabilization energies calculated in the solvent (see Computation in ESI<sup>†</sup>).

Table 2 also shows that the charge transfer (CT) in complexes manifesting an increase in stability with increasing solvent polarity is greater than that of complexes showing the opposite trend. The CT for the former and latter complexes ranges between 0.191–0.179 e and 0.168–0.132 e, respectively. Notably, the CT for the vdW complex, InCl<sub>3</sub>·OF<sub>2</sub>, is much smaller at 0.052 e.

At approximately 0.174 e, a CT acts as a limiting factor between the two types of complexes. This value is not constant and varies based on the electron donors and acceptors involved. The correlation between  $\Delta E$  and CT is presented in Fig. S6 (ESI<sup>†</sup>) and shows a strong relationship ( $R^2 = 0.88$ ). The dipole moment values of the complex obtained with and without CT (refer to Table 2 for full DFT and constrained DFT (cDFT) calculations) highlight the importance of CT in explaining complex stability in solvents of different polarities. In all cases, the dipole moment value decreases when CT is ignored, resulting in reduced solvent stabilization (as compared to  $\Delta E_{\text{solv}}$  calculated using the full and cDFT approach).

The impact of solvation on H-bonded complexes was effectively analyzed, among others, in terms of the solvent-accessible surfaces.<sup>15</sup> The alterations in solvent accessible surface area (SASA) upon complex formation are recorded in Table 2. These values for all the complexes are negative, indicating a smaller SASA in the complex than in the subsystems. As a result, the corresponding contribution to the overall solvation energy should be consistently positive. It cannot predict differences in the stability of the complexes when solvent polarity increases. The electrostatic contributions to the solvation energy are thus responsible for the distinct responses of the stabilization energy to changes in solvent polarity.

Table 3 presents energy and other relevant characteristics for the second DB complex family, which uses the same electron donor, NCl<sub>3</sub>. The previous paragraph's conclusions are also applicable to this family of complexes. Specifically, the changes in the stability of the DB complexes with solvent polarity depend on the CT's magnitude. The NCl<sub>3</sub>·BH<sub>3</sub> complex, which manifests an increased stability, has a larger CT (0.236 e) than the other DB complexes (0.120 e, 0.036 e), whose stabilities decrease in the solvent. The CT limit separating the two types of DB complexes using InCl<sub>3</sub> as an acceptor (0.174 e) also applies to the present complexes. The calculated Löwdin charge transfer are higher in absolute value but it follows the same trends (Table 3). As in the previous case, the complex dipole moments are systematically smaller when the CT is neglected, demonstrating the significant role of CT. Additionally, solvation energies evaluated without considering CT are larger than those calculated while allowing for CT. The  $\Delta$ SASA values for all the complexes in Table 3 are negative, indicating a positive contribution to the overall solvation energy, similar to the previous case.

The stability trends of the DB complexes with varying solvent polarity, as discussed earlier, were analysed using the continuous solvent model, where the solvent is characterized by its dielectric constant. An explicit solvent model provides an



**Table 2** Interaction energy ( $\Delta E$ ), binding free energy ( $\Delta G$ ) (in kcal mol<sup>-1</sup>,  $T = 298$  K), dative bond length (Å), charge transfer (CT, calculated from NBO charges), Wiberg bond index (WBI) and changes in the solvent accessible surface area ( $\Delta\text{SASA}$ , Å<sup>2</sup>) of  $\text{InCl}_3$  complexes in various solvents. Changes of solvation energy ( $\Delta E_{\text{solv}}$ ) values and dipole moments of DB complexes are calculated in DFT and cDFT methods

	$\varepsilon$	$\Delta E$	$\Delta G$	CT	WBI	$\Delta\text{SASA}$	$\Delta E_{\text{solv}}$ (DFT)	$\Delta E_{\text{solv}}$ (cDFT)	Dipole moment (DFT)	Dipole moment (cDFT)	DB length (Å)
<b>NH<sub>3</sub></b>	1.0	-30.16	-18.23	0.191	0.308						2.284
	2.6	-32.93	-20.96	0.229	0.363	-21.181	-2.18	3.22	7.422	3.305	2.226
	4.8	-34.29	-22.86	0.244	0.385	-21.392	-3.31	4.11	8.142	3.784	2.205
	8.9	-35.33	-23.60	0.255	0.400	-21.416	-6.34	4.85	9.014	3.875	2.192
	9.99	-35.47	-23.78	0.256	0.401	-21.322	-4.49	4.66	8.878	3.974	2.191
<b>NMe<sub>3</sub></b>	1.0	-35.74	-21.17	0.187	0.268						2.282
	2.6	-35.67	-21.88	0.212	0.294	-36.499	-1.40	2.22	8.173	2.744	2.254
	4.8	-35.87	-22.08	0.223	0.305	-34.268	-2.37	3.02	9.198	3.056	2.242
	8.9	-36.15	-22.15	0.231	0.313	-32.134	-3.04	3.62	9.877	3.284	2.236
	9.99	-36.17	-22.14	0.232	0.314	-32.009	-2.92	3.98	9.985	3.319	2.234
<b>NH<sub>2</sub>Ph(4-Me)</b>	1.0	-27.99	-16.48	0.183	0.282						2.301
	2.6	-29.14	-16.30	0.212	0.320	-27.459	0.06	2.68	6.895	2.868	2.261
	4.8	-29.81	-16.98	0.224	0.335	-27.513	-2.02	3.46	9.764	3.298	2.246
	8.9	-30.35	-16.99	0.234	0.346	-26.709	-3.00	3.67	10.587	3.352	2.235
	9.99	-30.42	-17.00	0.235	0.348	-26.684	-2.52	3.74	9.930	3.446	2.234
<b>NH<sub>2</sub>Ph</b>	1.0	-27.06	-12.87	0.179	0.278						2.307
	2.6	-28.16	-15.35	0.209	0.316	-27.925	-0.94	2.51	7.799	2.601	2.265
	4.8	-28.86	-15.63	0.221	0.331	-26.922	-1.66	3.47	8.863	3.008	2.249
	8.9	-29.38	-16.28	0.229	0.342	-27.467	-2.36	3.80	9.629	3.340	2.239
	9.99	-29.45	-16.32	0.230	0.343	-27.424	-2.46	4.02	9.731	3.449	2.238
<b>NHPhPh(3-Me)</b>	1.0	-23.92	-9.95	0.168	0.255						2.330
	2.6	-23.62	-10.37	0.191	0.280	-39.495	-2.01	1.84	8.414	3.248	2.296
	4.8	-23.67	-9.69	0.200	0.289	-39.271	-2.06	2.66	9.396	3.563	2.284
	8.9	-23.78	-9.77	0.207	0.296	-38.061	-2.59	2.92	10.104	3.759	2.276
	9.99	-23.79	-9.75	0.208	0.297	-37.942	-2.59	2.95	10.193	3.784	2.275
<b>NCl<sub>3</sub></b>	1.0	-12.06	0.13	0.090	0.132						2.534
	2.6	-10.68	1.23	0.100	0.141	-30.065	1.14	0.03	3.552	0.908	2.521
	4.8	-10.21	1.97	0.104	0.145	-28.901	1.36	1.98	3.806	0.981	2.519
	8.9	-9.91	2.38	0.107	0.147	-28.362	1.66	2.45	3.939	1.011	2.514
	9.99	-9.89	2.28	0.107	0.147	-28.982	1.66	2.45	3.971	1.054	2.513
<b>NHPh<sub>2</sub></b>	1.0	-23.38	-9.66	0.167	0.252						2.336
	2.6	-23.15	-9.27	0.186	0.273	-38.777	-0.52	2.15	8.043	3.198	2.305
	4.8	-23.16	-9.48	0.200	0.289	-36.857	-0.98	2.86	9.043	3.594	2.284
	8.9	-23.26	-9.60	0.206	0.294	-36.739	-1.24	3.34	9.637	3.725	2.278
	9.99	-23.28	-9.51	0.207	0.295	-36.589	-1.32	3.54	9.740	3.893	2.276
<b>NPh<sub>3</sub></b>	1.0	-16.91	-1.99	0.149	0.203						2.445
	2.6	-15.10	0.05	0.176	0.221	-58.495	-0.22	2.47	9.488	4.327	2.401
	4.8	-14.59	0.75	0.188	0.228	-57.877	-0.51	2.51	10.615	4.521	2.385
	8.9	-14.37	0.83	0.197	0.233	-56.694	-0.75	3.01	11.475	4.760	2.372
	9.99	-14.33	1.24	0.197	0.234	-58.805	-0.81	3.85	11.573	4.888	2.371
<b>NHPhCOMe</b>	1.0	-15.14	-1.67	0.143	0.213						2.414
	2.6	-13.39	-0.37	0.164	0.235	-34.686	1.55	2.78	5.724	3.321	2.382
	4.8	-12.02	1.32	0.178	0.252	-35.182	1.80	3.77	8.477	4.962	2.356
	8.9	-11.80	2.25	0.185	0.258	-34.667	1.20	4.97	9.121	5.474	2.345
	9.99	-12.88	1.10	0.180	0.252	-34.213	1.81	4.00	7.155	4.243	2.359
<b>NHClCOMe</b>	1.0	-14.59	-1.74	0.132	0.202						2.454
	2.6	-11.93	1.41	0.149	0.218	-36.352	2.34	3.64	4.594	3.727	2.428
	8.9	-10.83	2.93	0.161	0.231	-33.877	3.94	5.26	5.731	4.064	2.415
	9.99	-10.79	2.84	0.162	0.231	-33.810	3.44	5.33	5.846	4.112	2.414
vdW complexes											
<b>OF<sub>2</sub></b>	1.0	-3.08	6.30	0.052	0.081						2.840
	8.9	-1.71	6.52	0.016	0.024	-6.157	0.26	0.59	0.661	0.791	3.483
	9.99	-1.70	6.66	0.015	0.024	-6.005	-0.17	0.58	1.058	0.800	3.489



**Table 3** Interaction energy ( $\Delta E$ ), binding free energy ( $\Delta G$ ) (in kcal mol<sup>-1</sup>,  $T = 298$  K), dative bond length (Å), charge transfer (CT, calculated from NBO charges), Wiberg bond index (WBI) and changes in the solvent accessible surface area ( $\Delta\text{SASA}$ , Å<sup>2</sup>) of  $\text{NCl}_3$  complexes in various solvents. Changes of solvation energy ( $\Delta E_{\text{solv}}$ ) values and dipole moments of DB complexes are calculated in DFT and cDFT methods. The  $\Delta E_{\text{solv}}$  values and dipole moments of DB complexes calculated at PBE0-D3/def2-QZVP level are given in parenthesis. The Löwdin charge transfer (in e) values are given in [·]

	$\varepsilon$	$\Delta E$	$\Delta G$	CT	WBI	$\Delta\text{SASA}$	$\Delta E_{\text{solv}}$ (DFT)	$\Delta E_{\text{solv}}$ (cDFT)	Dipole moment (DFT)	Dipole moment (cDFT)	DB length (Å)
$\text{GaCl}_3$	1.0	-12.62	-0.41	0.120	0.189						2.306
	2.6	-12.48	-0.13	0.140 [0.40]	0.209	-37.194	0.16 (0.15)	1.79	4.725 (4.671)	0.652	2.265
	4.8	-12.47	-0.08	0.147 [0.42]	0.217	-37.554	0.08 (0.07)	2.28	5.071 (5.028)	0.716	2.251
	8.9	-12.48	-0.07	0.152 [0.44]	0.222	-37.427	0.04 (0.04)	2.74	5.312 (5.278)	0.747	2.240
	9.99	-12.46	-0.18	0.152 [0.44]	0.222	-38.248	0.02 (0.02)	2.87	5.344 (5.312)	0.750	2.239
$\text{BF}_3$	1.0	-4.47	6.78	0.036	0.109						2.404
	2.6	-4.23	7.20	0.051 [0.25]	0.082	-28.077	0.24 (0.24)	0.75	2.141 (2.096)	0.754	2.318
	4.8	-4.19	7.34	0.073	0.119	-30.455	0.08	1.00	2.679	0.913	2.210
	8.9	-4.28	8.70	0.152 [0.49]	0.247	-34.519	-1.12 (-1.08)	1.26 (1.17)	4.157 (4.123)	1.335 (1.410)	1.960
	9.99	-4.32	8.71	0.152	0.247	-34.652	-1.14	1.29	4.175	1.337	1.960
$\text{BH}_3$	1.0	-18.13	-3.10	0.235	0.567						1.661
	2.6	-19.42	-4.28	0.260 [0.68]	0.573	-32.425	-1.39 (-1.33)	-1.04 (-1.08)	3.887 (3.797)	3.359 (3.438)	1.657
	4.8	-19.90	-4.71	0.268 [0.68]	0.576	-32.744	-1.94 (-1.87)	-1.42 (-1.48)	4.121 (4.040)	3.507 (3.601)	1.655
	8.9	-20.21	-4.98	0.273 [0.70]	0.578	-32.725	-2.11 (-2.02)	-1.65 (-1.71)	4.236 (4.161)	3.582 (3.687)	1.654
	9.99	-20.24	-5.05	0.274 [0.69]	0.578	-32.932	-2.30 (-2.22)	-1.67 (-1.73)	4.274 (4.199)	3.597 (3.704)	1.655

alternative and more reliable approach to studying the solvation process. We chose two complexes,  $\text{InCl}_3\text{-NH}_3$  and  $\text{NCl}_3\text{-BH}_3$ , which showed an increase in DB stability with a rise in polarity and conducted simulations of 10 ps in the gas phase,  $\text{CS}_2$ , and DCB. Both complexes remained stable throughout the simulations (Fig. S7 and S8, ESI<sup>†</sup>). In contrast, complexes that destabilize in polar solvents, such as  $\text{InCl}_3\text{-NCl}_3$  and  $\text{GaCl}_3\text{-NCl}_3$ , remained stable in the gas phase and  $\text{CS}_2$  and decomposed into fragments within 10 ps in more polar DCB (Fig. S9 and S10, ESI<sup>†</sup>). In fact, the solvent molecule (such as acetone) displaces the donor  $\text{NCl}_3$  molecule and forms  $\text{InCl}_3\cdots\text{Acetone}$  complex (Fig. S11, ESI<sup>†</sup>). The results including the CT values determined from selected snapshots of the MD trajectories are presented in ESI<sup>†</sup>. This finding is crucial as it verifies the results obtained from the continuous solvent model. It was also demonstrated that the variation in stability trends of the DB complexes with changing solvent polarity depends on the CT in the Lewis electron-pair system.

All the DB complexes studied in the present work exhibit a sizable donor  $\rightarrow$  acceptor CT; with varying values. In complexes with higher CT, the dipole moment within the complex increases compared to its fragments, leading to increased solvation energy and stability in polar solvents. On the other hand, in complexes with lower CT values, the dipole moment is smaller than that of the isolated fragments, resulting in a decrease in solvation energy and destabilization of the complexes in polar solvents.

All these findings, obtained through the continuous solvent model, were confirmed by more reliable MD simulations using an explicit solvent model.

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## Conflicts of interest

There are no conflicts to declare.

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