Supporting Information

Temperature Dependent Approach to Electronic Charge Transfer

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a) Derivation of equation (20) of our work.

b) Experimental and calculated values of each system considered in the correlations reported in Table 1 of our work.

a) Derivation of equation (20) of our work.

The main goal in this supporting material is to provide a detailed derivation of the result obtained for the chemical potential of the bath at the stoichiometry condition displayed in Eq. (20) of our work, *i.e.*,

$$\mu_{st} = -\frac{\left(I_{\mathrm{X}} + A_{\mathrm{Y}}\right)}{2} \quad \forall \quad I_{\mathrm{Y}} > I_{\mathrm{X}}, \quad A_{\mathrm{Y}} > A_{\mathrm{X}} \tag{1}$$

For this purpose, we begin with the conservation of charge condition of the stoichiometry case (Eq. (18) of our work)

$$\omega_{f\mathrm{X}}(\mu_{Bath} = \mu_{st}) + \omega_{f\mathrm{Y}}(\mu_{Bath} = \mu_{st}) = 0 \quad . \tag{2}$$

Defining $\mu_{0\mathrm{X}} = -(I_{\mathrm{X}} + A_{\mathrm{X}})/2$ and using the expression of the fractional charge given by the Eq. (9) of the our work we have that,

$$\frac{1 - e^{-2\beta\left(\mu_{St} - \mu_{0\mathrm{X}}\right)}}{1 + e^{-2\beta\left(\mu_{St} - \mu_{0\mathrm{X}}\right)} + e^{-\beta(A_{\mathrm{X}} + \mu_{St})}} = -\frac{1 - e^{-2\beta\left(\mu_{St} - \mu_{0\mathrm{X}}\right)}}{1 + e^{-2\beta\left(\mu_{St} - \mu_{0\mathrm{X}}\right)} + e^{-\beta(A_{\mathrm{Y}} + \mu_{St})}} \quad ,$$

$$\frac{e^{\beta(A_{\mathrm{X}} + \mu_{St})} - e^{-\beta\left(I_{\mathrm{X}} + \mu_{St}\right)}}{1 + e^{\beta(A_{\mathrm{X}} + \mu_{St})} + e^{-\beta\left(I_{\mathrm{X}} + \mu_{St}\right)}} = -\frac{e^{\beta(A_{\mathrm{Y}} + \mu_{St})} - e^{-\beta\left(I_{\mathrm{Y}} + \mu_{St}\right)}}{1 + e^{\beta(A_{\mathrm{Y}} + \mu_{St})} + e^{-\beta\left(I_{\mathrm{Y}} + \mu_{St}\right)}} \quad , \tag{3}$$

which can be rearranged as follows,

$$2e^{\beta(A_{\mathrm{X}} + A_{\mathrm{Y}})} e^{4\beta\mu_{St}} + \left(e^{\beta A_{\mathrm{X}}} + e^{\beta A_{\mathrm{Y}}}\right) e^{3\beta\mu_{St}} - \left(e^{\beta I_{\mathrm{X}}} + e^{\beta I_{\mathrm{Y}}}\right) e^{\beta\mu_{St}} - 2e^{-\beta(I_{\mathrm{X}} + I_{\mathrm{Y}})} = 0 \,, \tag{4}$$

that may be written as

$$a_1 x_1^4 + a_2 x_1^3 - a_3 x_1 - a_4 = 0 \quad , \tag{5}$$

with $x_1 = e^{-\beta\mu_{St}}$ and

$$a_1 = 2e^{\beta(A_X + A_Y)}, \quad a_2 = \left(e^{\beta A_X} + e^{\beta A_Y}\right), \quad a_3 = \left(e^{-\beta I_X} + e^{\beta I_Y}\right), \quad a_4 = 2e^{-\beta(I_X + I_Y)} \quad . \tag{6}$$

Multiplying Eq. (4) by $e^{-4\beta\mu_{St}}$ one gets,

$$2e^{-\beta(I_X + I_Y)} e^{-4\beta\mu_{St}} + \left(e^{\beta I_X} + e^{\beta I_Y}\right) e^{-3\beta\mu_{St}} - \left(e^{\beta A_X} + e^{\beta A_Y}\right) e^{-\beta\mu_{St}} - 2e^{\beta(A_X + A_Y)} = 0 \, , \tag{7}$$

which leads to,

$$a_4 x_2^4 + a_3 x_2^3 - a_2 x_2 - a_1 = 0 \quad , \tag{8}$$

with $x_2 = e^{-\beta\mu_{St}}$.

Now, instead of trying to get the eight roots concerning Eqs. (5) and (8), one can take advantage of the fact that ω is a single-valued function of μ_{Bath} and therefore, there exists only one value of μ_{Bath} that fulfills the condition in Eq. (2). Therefore, one can impose the weaker condition

$$\ln(\omega_X / \omega_0) - \ln(\omega_Y / \omega_0) = 0 \quad , \tag{9}$$

which is equivalent to the condition

$$\left|\omega_{fX}(\mu_{St})\right| = \pm\left|\omega_{fY}(\mu_{St})\right| \quad . \tag{10}$$

By making use of the relationship

$$\left|\omega_{f\mathrm{X}}(\mu_{St})-\omega_{f\mathrm{Y}}(\mu_{St})\right| \geq \left\|\omega_{f\mathrm{X}}(\mu_{St})\right|-\left|\omega_{f\mathrm{Y}}(\mu_{St})\right\| \qquad , \tag{11}$$

one can work with the weaker condition in Eq. (10) as follows

$$\left|\omega_{f\mathrm{X}}(\mu_{St})-\omega_{f\mathrm{Y}}(\mu_{St})\right| \geq 0 \tag{12}$$

which through Eq. (9) of our work leads to

$$\left|e^{-2\beta\mu_{St}}\left(e^{\beta(2\mu_{0\mathrm{Y}}-A_{\mathrm{X}})}-e^{\beta(2\mu_{0\mathrm{X}}-A_{\mathrm{Y}})}\right)+2e^{-\beta\mu_{St}}\left(e^{2\beta\mu_{0\mathrm{Y}}}-e^{2\beta\mu_{0\mathrm{X}}}\right)+e^{-\beta A_{\mathrm{Y}}}-e^{-\beta A_{\mathrm{X}}}\right| \geq 0\,. \tag{13}$$

This expression may be written as,

$$\left|b_1x_1^2+b_2x_1+b_3\right| \geq 0 \qquad , \tag{14}$$

with

$$b_1=\left(e^{\beta(2\mu_{0\mathrm{Y}}-A_{\mathrm{X}})}+e^{\beta(2\mu_{0\mathrm{X}}-A_{\mathrm{Y}})}\right) \qquad b_2=2\left(e^{\beta 2\mu_{0\mathrm{Y}}}-e^{\beta 2\mu_{0\mathrm{X}}}\right) \qquad b_3=\left(e^{-\beta A_{\mathrm{Y}}}-e^{-\beta A_{\mathrm{X}}}\right) \tag{15}$$

Since Eq. (14) can be expressed in the form,

$$\left|\left(x_1\sqrt{b_1}+\frac{b_2}{2\sqrt{b_1}}\right)^2-\frac{b_2^2}{4b_1}+b_3\right| \geq 0$$

so that

$$\left|\left(x_1\sqrt{b_1}+\frac{b_2}{2\sqrt{b_1}}\right)^2-\frac{b_2^2}{4b_1}+b_3\right| \geq \left|\left(x_1\sqrt{b_1}+\frac{b_2}{2\sqrt{b_1}}\right)^2-\left|\frac{b_2^2}{4b_1}-b_3\right|\right| \geq 0 \qquad , \tag{16}$$

when the equality holds, one finds that

$$\left(x_1\sqrt{b_1} + \frac{b_2}{2\sqrt{b_1}} \right)^2 - \left| \left(\frac{b_2^2}{4b_1} - b_3 \right) \right| = 0 \quad ,$$

and therefore

$$x_1 = -\frac{1}{\sqrt{b_1}} \left(\frac{b_2}{2\sqrt{b_1}} + \left| \left(\frac{b_2^2}{4b_1} - b_3 \right) \right|^{1/2} \right) \quad . \tag{17}$$

The real solution for x_1 is then

$$x_1 = \frac{-b_2 + \left| b_2^2 - 4b_1b_3 \right|^{1/2}}{2b_1} \tag{18}$$

If Eq. (13) is multiplied by $e^{2\beta\mu_{St}}$ one obtains that,

$$\left| e^{2\beta\mu_{st}} \left(e^{-\beta A_{\mathrm{Y}}} - e^{-\beta A_{\mathrm{X}}} \right) + e^{\beta\mu_{St}} 2\left(e^{2\beta\mu_{0\mathrm{Y}}} - e^{2\beta\mu_{0\mathrm{X}}} \right) + e^{\beta\left(2\mu_{0\mathrm{Y}} - A_{\mathrm{X}}\right)} - e^{\beta\left(2\mu_{0\mathrm{X}} - A_{\mathrm{Y}}\right)} \right| \geq 0 \,, \tag{19}$$

that can be expressed as,

$$\left| b_3x_2^2 + b_2x_2 + b_1 \right| \geq 0 \quad , \tag{20}$$

Thus, applying a similar procedure to the one performed for Eq. (14) one obtains that the real solution for x_2 is given by,

$$x_2 = \frac{-b_2 + \left| b_2^2 - 4b_1b_3 \right|^{1/2}}{2b_3} \tag{21}$$

Now, at any temperature of chemical interest the product,

$$\begin{aligned} b_1 b_3 &= e^{2\beta(\mu_{0\mathrm{Y}}-A_{\mathrm{X}})} + e^{2\beta(\mu_{0\mathrm{X}}-A_{\mathrm{Y}})} + e^{\beta(2\mu_{0\mathrm{Y}}-A_{\mathrm{X}}-A_{\mathrm{Y}})} + e^{\beta(2\mu_{0\mathrm{X}}-A_{\mathrm{X}}-A_{\mathrm{Y}})} \\ &= e^{-\beta(I_{\mathrm{Y}}+A_{\mathrm{Y}}+2A_{\mathrm{X}})} + e^{-\beta(I_{\mathrm{X}}+A_{\mathrm{X}}+2A_{\mathrm{Y}})} + e^{-\beta(I_{\mathrm{Y}}+2A_{\mathrm{Y}}+A_{\mathrm{X}})} + e^{-\beta(I_{\mathrm{X}}+2A_{\mathrm{X}}+A_{\mathrm{Y}})} \end{aligned} \tag{22}$$

is much bigger than b_2^2 since,

$$b_2^2 = 4\left(e^{-4\beta(I_{\mathrm{Y}}+A_{\mathrm{Y}})} - e^{-4\beta(I_{\mathrm{Y}}+A_{\mathrm{Y}})}\right) \quad , \tag{23}$$

and the ionization potentials are in general much bigger than the electron affinities. With the same arguments, $\left|b_1 b_3\right|^{1/2} >> b_2$. Using this two considerations, the root in Eq. (18) can be simplified and rearranged as follows

$$\begin{aligned} \mu_{St} &= -kT\ln\left(\frac{\left|b_1 b_3\right|^{1/2}}{b_1}\right) = \frac{kT}{2}\ln\left(\frac{b_1}{\left|b_3\right|}\right) \\ &= \frac{kT}{2}\ln\left(\frac{e^{\beta(2\mu_{0\mathrm{Y}}+2\mu_{0\mathrm{Y}}+I_{\mathrm{X}}+A_{\mathrm{Y}})}\left(1-e^{\beta(I_{\mathrm{Y}}-I_{\mathrm{X}})}\right)}{\left|\left(1-e^{\beta(A_{\mathrm{Y}}-A_{\mathrm{X}})}\right)\right|}\right) \\ &= -\frac{\left(I_Y + A_X\right)}{2} + \frac{kT}{2}\ln\left(\frac{1-e^{\beta(I_{\mathrm{Y}}-I_{\mathrm{X}})}}{\left|1-e^{\beta(A_{\mathrm{Y}}-A_{\mathrm{X}})}\right|}\right) \end{aligned} \quad . \tag{24}$$

A similar treatment to the root in Eq. (21) leads to,

$$
\begin{aligned}
\mu_{St} &= kT\ln\left(\frac{\left|b_1 b_3\right|^{1/2}}{b_3}\right) = \frac{kT}{2}\ln\left(\frac{\left|b_1\right|}{b_3}\right) \\
&= \frac{kT}{2}\ln\left(\frac{e^{\beta(2\mu_{0\mathrm{Y}}+2\mu_{0\mathrm{Y}}+I_{\mathrm{X}}+A_{\mathrm{Y}})}\left|\left(1-e^{\beta(I_{\mathrm{Y}}-I_{\mathrm{X}})}\right)\right|}{\left(1-e^{\beta(A_{\mathrm{Y}}-A_{\mathrm{X}})}\right)}\right) \\
&= -\frac{\left(I_Y + A_X\right)}{2} + \frac{kT}{2}\ln\left(\frac{\left|1-e^{\beta(I_{\mathrm{Y}}-I_{\mathrm{X}})}\right|}{1-e^{\beta(A_{\mathrm{Y}}-A_{\mathrm{X}})}}\right)
\end{aligned}
\quad . \tag{25}
$$

These expressions, Eqs. (24) and (25) imply that, once $I_{\mathrm{Y}} > I_{\mathrm{X}}$ has been defined, the condition $A_{\mathrm{Y}} > A_{\mathrm{X}}$ must be necessarily fulfilled, since otherwise one gets a negative argument in the logarithmic function of any of these equations. This last statement leads to the desired solution for the chemical potential of the bath at the stoichiometry condition, since one can see that Eqs. (24) and (25) have, in addition to the leading term, a temperature dependent term that is negligible up to temperatures close to 10^4 K, so that they both reduce to Eq. (20) of our work.

b) Experimental and calculated values of each system considered in the correlations reported in Table 1 of our work.

X in the bath of Y (W_X, K_X) and Y in the bath of X (W_Y, K_Y)

	Expt.	W_X	W_Y	$K_{\omega X}$	$K_{\omega Y}$	ΔE	ΔN
Cl_2-Substituted Benzenes							
Benceno	0.00	-28.56	-40.32	-28.18	-39.35	-0.21	0.15
Tiofeno	6.91	-23.52	-30.24	-23.14	-29.29	-0.27	0.17
Furano	11.51	-18.48	-30.24	-18.10	-29.29	-0.31	0.18
Pirrol	27.63	-8.40	-21.84	-8.02	-20.92	-0.42	0.21
R^2		**0.990**	**0.892**	**0.990**	**0.892**	**0.997**	**0.982**
Br_2 - Olefins							
CH_2CH_2	0.00	-30.24	-67.20	-29.82	-66.17	-0.12	0.11
$CH_2CHCHCH_2$		-28.56	-43.68	-28.14	-42.71	-0.15	0.13
CH_3CHCH_2	1.79	-21.84	-53.76	-21.42	-52.77	-0.18	0.14
trans-$CH_3CHCHCH_3$	3.23	-15.12	-42.00	-14.70	-41.04	-0.25	0.16
cis-$CH_3CHCHCH_3$	3.30	-14.28	-42.84	-13.86	-41.88	-0.26	0.16
$(CH3)_2CCH_2$	3.73	-15.12	-43.68	-14.70	-42.71	-0.25	0.16
$(CH3)_2CCHCH_3$	5.18	-11.76	-36.96	-11.34	-36.01	-0.29	0.17
$(CH3)_2CC(CH_3)_2$	6.26	-6.72	-28.56	-6.30	-27.64	-0.35	0.19
HCCH	-3.00	-30.24	-80.64	-29.82	-79.58	-0.11	0.10
R^2		**0.911**	**0.982**	**0.911**	**0.982**	**0.918**	**0.943**
Low Spin Ni atoms - Olefins							
Maleic anhydride	8.60	0.00	-31.92	0.76	-31.71	-0.28	0.20
trans-NCCHCHCN	8.20	0.00	-48.72	0.76	-48.94	-0.23	0.17
CH_2CHCN	4.60	-6.72	-62.16	-5.96	-62.86	-0.11	0.12
C_2H_4	2.40	-23.52	-89.04	-22.76	-88.78	-0.02	0.05
CH_2CHF	1.95	-26.88	-90.72	-26.12	-90.44	-0.01	0.04
Styrene	1.00	-28.56	-63.84	-27.80	-64.36	-0.01	0.04
CH_3CHCH_2	-0.30	-31.92	-92.40	-31.16	-92.09	0.00	0.02
Ciclohexene	-3.46	-36.96	-90.72	-36.88	-89.77	0.00	-0.01
$(CH3)_2CCHCH_3$	-3.52	-35.28	-89.04	-35.20	-88.09	0.00	-0.01
R^2		**0.929**	**0.713**	**0.935**	**0.706**	**0.812**	**0.953**
1,3-Cyclopentadiene - Olefins							
$C_2(CN)_4$	8.63	-16.80	-38.64	-16.35	-37.66	-0.30	0.17
$NCCHC(CN)_2$	6.68	-28.56	-47.04	-28.24	-46.06	-0.21	0.14
$CH_2C(CN)_2$	5.66	-36.96	-52.08	-36.75	-51.10	-0.17	0.13
Maleic Anhydride	4.74	-36.96	-55.44	-36.75	-54.46	-0.15	0.12
p-Bezoquinone	3.95	-33.60	-65.52	-33.34	-64.53	-0.09	0.10
Maleonitrile	2.96	-53.76	-57.12	-53.98	-56.14	-0.13	0.11
Fumaronitrile	2.91	-53.76	-57.12	-53.98	-56.14	-0.13	0.11
CH_2CHCN	1.00	-67.20	-70.56	-67.90	-69.57	-0.06	0.07
CH_2CH_2	-3.00	-94.08	-87.36	-93.82	-86.37	-0.01	0.03
R^2		**0.958**	**0.931**	**0.958**	**0.931**	**0.897**	**0.978**

Methyl radical - olefines							
$(CH3)_2CC(CH3)_2$	1.51	-55.44	-83.74	-55.96	-82.83	0.00	-0.02
cis-$CH_3CHCHCH_3$	1.49	-58.46	-86.77	-57.62	-86.50	0.00	0.01
$(CH_3)_2CCHCH_3$	1.90	-60.64	-92.31	-60.08	-91.17	0.00	0.00
$(CH_3)_2CCH_2$	2.87	-57.62	-92.65	-56.78	-92.31	0.00	0.01
CH_3CHCH_2	2.96	-50.90	-89.29	-50.06	-88.99	-0.01	0.03
CH_2CH_2	3.10	-42.50	-85.93	-41.66	-85.67	-0.03	0.06
cis-CHClCHCl	3.13	-44.18	-74.17	-43.34	-74.13	-0.03	0.05
trans-CHClCHCL	3.56	-42.50	-69.13	-41.66	-69.23	-0.03	0.06
CH_2CHOAc	3.62	-43.34	-75.01	-42.50	-74.95	-0.03	0.06
CH_2CHCl	4.22	-42.50	-75.85	-41.66	-75.77	-0.03	0.06
CH_2CCl_2	5.54	-39.14	-67.45	-38.30	-67.60	-0.05	0.07
CH_2CHCN	6.00	-25.70	-59.05	-24.86	-59.75	-0.12	0.11
R^2		**0.806**	**0.671**	**0.816**	**0.658**	**0.750**	**0.840**
H_20 - Electrophiles							
$CH_3COCOCH_3$	0.52	-127.67	-40.32	-126.57	-40.47	-0.07	0.07
CH_2O	3.30	-127.67	-67.20	-126.57	-67.24	-0.06	0.06
$ClCH_2COCH_3$	-0.22	-133.55	-62.16	-132.45	-62.38	-0.04	0.05
CH_3CHO	0.11	-136.07	-72.24	-134.97	-72.16	-0.03	0.05
$(CH3)_2CO$	-2.70	-142.79	-77.28	-141.69	-77.10	-0.02	0.03
HCO_2CH_3	-5.33	-134.39	-82.32	-133.29	-82.06	-0.04	0.05
$HCON(CH3)_2$	-14.14	-154.55	-92.40	-153.45	-92.02	0.00	0.01
HCN	13.00	-115.91	-90.72	-114.81	-90.35	-0.10	0.07
CH_3CN	2.03	-132.71	-99.12	-131.61	-98.67	-0.04	0.05
R^2		**0.875**	**0.005**	**0.875**	**0.05**	**0.800**	**0.766**
Ethylene - Free radicals							
Cl	24.53	-38.64	-13.44	-37.61	-12.88	-0.35	0.18
OH	22.33	-52.08	-43.68	-51.05	-43.42	-0.20	0.13
H	21.42	-57.12	-60.48	-56.09	-60.57	-0.16	0.11
Br	18.42	-50.40	-16.80	-49.37	-16.27	-0.25	0.15
CF_3	15.07	-85.68	-43.68	-84.65	-43.42	-0.03	0.06
O_2H	14.51	-70.56	-53.76	-69.53	-53.68	-0.09	0.09
CCI_3	10.71	-87.36	-33.60	-86.33	-33.22	-0.03	0.05
CH_3	10.71	-94.08	-72.24	-93.05	-73.24	-0.01	0.03
i-C_3H_7	10.00	-90.72	-53.76	-90.46	-52.88	-0.02	-0.04
C_2H_5	10.46	-97.44	-67.20	-97.18	-66.27	0.00	-0.02
t-C_4H_9	11.40	-85.68	-42.00	-85.42	-41.16	-0.03	-0.06
R^2		**0.901**	**0.257**	**0.902**	**0.249**	**0.838**	**0.764**
Trimethylamine - Boron trihalides							
BF_3	1.28	-84.00	-0.30	-26.74	-83.45	-0.34	0.15
BCl_3	1.57	-19.66	-30.83	-29.93	-20.14	-0.42	0.19
BBr_3	1.65	-11.42	-35.87	-34.97	-11.51	-0.39	0.19
BCl_2Br	1.61	-13.61	-31.75	-30.86	-13.77	-0.42	0.19
$BClBr_2$	1.63	-9.41	-32.51	-31.61	-9.43	-0.42	0.19
BI_3	1.74	-6.22	-43.85	-42.95	-6.16	-0.33	0.18
R^2		**0.941**	**0.992**	**0.631**	**0.944**	**0.049**	**0.639**

Stoichiometric quantities

	Expt.	W_{St}	K_{StX}	K_{StY}
Cl_2-Substituted Benzenes				
Benceno	0.00	-58.80	-58.42	-57.82
Tiofeno	6.91	-53.76	-53.38	-52.81
Furano	11.51	-53.76	-53.38	-52.81
Pirrol	27.63	-49.56	-49.18	-48.64
$\mathbf{R^2}$		**0.892**	**0.892**	**0.892**
Br_2 - Olefins				
CH_2CH_2	0.00	-67.31	-66.06	-65.84
CH_3CHCH_2	1.79	-60.48	-60.06	-59.49
trans-$CH_3CHCHCH_3$	3.23	-54.60	-54.18	-53.64
cis-$CH_3CHCHCH_3$	3.30	-55.02	-78.35	-54.06
$(CH3)_2CCH_2$	3.73	-55.44	-77.93	-54.47
$(CH3)_2CCHCH_3$	5.18	-52.08	-81.29	-51.13
$(CH3)_2CC(CH_3)_2$	6.26	-47.88	-85.49	-46.96
HCCH		--	--	--
$\mathbf{R^2}$		**0.964**	**0.454**	**0.961**
1,3-Cyclopentadiene - Olefins				
$C_2(CN)_4$	8.63	-57.12	-56.67	-56.14
$NCCHC(CN)_2$	6.68	-63.00	-62.68	-62.01
$CH_2C(CN)_2$	5.66	-67.20	-66.99	-66.21
Maleic Anhydride	4.74	-67.20	-66.99	-66.21
p-Bezoquinone	3.95	-68.04	-62.74	-67.05
Maleonitrile	2.96	-75.60	-75.82	-74.61
Fumaronitrile	2.91	-75.60	-75.82	-74.61
CH_2CHCN	1.00	-82.32	-83.02	-81.33
CH_2CH_2	-3.00	-95.76	-95.50	-94.77
$\mathbf{R^2}$		**0.980**	**0.926**	**0.980**
Trimethylamine - Boron trihalides				
BF_3	1.28	-94.92	-94.37	-94.02
BCl_3	1.57	-62.75	-63.23	-61.85
BBr_3	1.65	-58.63	-58.72	-57.74
BCl_2Br	1.61	-59.72	-59.88	-58.83
$BClBr_2$	1.63	-57.62	-57.65	-56.73
BI_3	1.74	-56.03	-55.97	-55.13
$\mathbf{R^2}$		**0.941**	**0.946**	**0.946**