

Negative Solvatochromism of the Intramolecular Charge Transfer Band in Two Structurally Related Pyridazinium – Ylids

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Table S1. Solvent parameters for the Abe model

	Solvent	$\mu(D)$	$\alpha (\text{\AA}^3)$	$I_g(eV)$	$\mu(g/mol)$	$\rho (g/cm^3)$
1	Cyclohexane	0.00	10.85	11.0	84.16	0.779
2	Toluene	0.38	12.4	8.72	92.14	0.867
3	Anisole	1.38	13.10	8.20	108.14	0.995
4	Diethyl ether	1.15	8.85	9.53	74.12	0.713
5	Chloroform	1.15	8.23	11.50	119.38	1.446
6	Bytyl acetate	1.84	13.42	10.00	116.16	0.883
7	Ethyl acetate	1.78	9.70	10.11	88.11	0.902
8	Pyridine	2.20	2.41	9.34	79.1	0.978
9	Tetrahydrofuran	1.75	8.14	9.40	72.06	0.888
10	1,2 Dichloroethane	1.43	8.68	10.49	173.84	2.447
11	1-Pentanol	1.70	11.58	10.42	88.15	0.814
12	1-Butanol	1.66	8.88	9.99	74.12	0.810
13	Iso-Butanol	1.76	9.07	19.12	74.12	0.802
14	2-Propanol	1.66	6.67	9.90	60.1	0.786
15	Acetophenone	3.81	14.37	9.77	120.14	1.028
16	1-Propanol	1.68	6.67	10.58	60.10	0.803
17	Acetone	2.80	6.27	9.89	58.08	0.805
18	Ethanol	1.69	5.06	10.70	46.07	0.789
19	Acetonitril	3.92	4.30	12.20	41.05	0.786
20	Methanol	1.70	3.21	10.85	32.04	0.792
21	DMF	3.86	7.91	9.12	73.94	0.944
22	DMSO	4.1	8.0	9.10	78.13	1.100
23	Water	1.85	1.5	12.59	18.0	1.0
24	Formamide	3.73	4.08	10.20	45.04	1.133

Table S2. PPPyNiP in the binary solvent MeOH (1) + DMF (2): percent concentration (C_1 , %), MeOH molar fraction (x_1 , %), the average statistic weight of MeOH in the first solvation sphere of PPPyNiP (p_1 , %) and the wavenumber of the ICT band (ν_i , cm^{-1})

$C_1\%$	$x_1\%$	$\ln \frac{x_1}{1-x_1}$	$\nu_i (\text{cm}^{-1})$	$p_1\%$	$\ln \frac{p_1}{1-p_1}$	ϵ
0	0	-	20530	0	-	37.6
10	17.7	-1.537	20800	29.0	-0.895	37.2
20	32.6	-0.726	21000	50.5	0.020	36.7
30	45.4	-0.185	21150	66.7	0.695	36.3
40	56.4	0.257	21270	79.6	1.361	35.6
50	65.9	0.659	21320	84.9	1.726	35.0
60	74.4	1.067	21370	90.3	2.231	33.5
70	81.9	1.510	21400	93.5	2.666	32.8
80	88.6	2.051	21420	95.6	3.078	32.3
90	99.4	5.110	21440	97.8	3.794	31.7
100	100	-	21460	100	-	31.0

Table S3. PPPyNiP in the Binary solvent MeOH (1) + DMSO (2): percent concentration (C_1 , %), MeOH molar fraction (x_1 , %), the average statistic weight of MeOH in the first solvation sphere of PPPyNiP (p_1 , %) and the wavenumber of the ICT band (ν_i , cm^{-1})

$C_1\%$	$x_1\%$	$\ln \frac{x_1}{1-x_1}$	$\nu_i (\text{cm}^{-1})$	$p_1\%$	$\ln \frac{p_1}{1-p_1}$	ϵ
0	0	-	20600	0	-	54.0
10	16.3	-1.636	20850	29.1	-0.891	52.0
20	30.5	-0.824	21020	48.8	-0.048	50.4
30	42.9	-0.286	21170	66.2	0.672	48.2
40	53.9	0.156	21260	76.7	1.191	46.0
50	63.7	0.562	21320	83.7	1.636	44.0
60	72.5	0.969	21390	91.9	2.428	41.5
70	80.3	1.405	21420	95.3	3.009	38.8
80	87.5	1.946	21425	95.9	3.152	36.0
90	94.0	2.752	21440	97.7	3.748	33.6
100	100	-	21460	100	-	31.0

Table S4. PyNiP in the binary solvent MeOH (1) + DMF (2): percent concentration (C_1 , %), MeOH molar fraction (x_1 , %), the average statistic weight of MeOH in the first solvation sphere of PyNiP (p_1 , %) and the wavenumber of the ICT band (ν_i , cm^{-1})

$C_1\%$	$x_1\%$	$\ln \frac{x_1}{1-x_1}$	$\nu_i (\text{cm}^{-1})$	$p_1\%$	$\ln \frac{p_1}{1-p_1}$	ϵ
0	0	-	20700	0	-	37.6
10	17.7	-1.537	20936	25.1	-1.093	37.2
20	32.6	-0.726	21100	42.6	-0.299	36.7
30	45.4	-0.185	21240	57.4	0.299	36.3
40	56.4	0.257	21388	73.2	1.004	35.6

50	65.9	0.659	21464	81.3	1.468	35.0
60	74.4	1.067	21520	87.2	1.921	33.5
70	81.9	1.510	21560	91.5	2.375	32.8
80	88.6	2.051	21588	94.5	2.838	32.3
90	99.4	5.110	21620	98.8	3.838	31.7
100	100	-	21640	100	-	31.0

Table S5. PyNiP in the binary solvent MeOH (1) + DMSO (2): percent concentration (C_1 , %), MeOH molar fraction (x_1 , %), the average statistic weight of MeOH in the first solvation sphere of PyNiP (p_1 , %) and the wavenumber of the ICT band (ν_t , cm^{-1})

$C_1\%$	$x_1\%$	$\ln \frac{x_1}{1-x_1}$	$\nu_t (\text{cm}^{-1})$	$p_1\%$	$\ln \frac{p_1}{1-p_1}$	ϵ
0	0	-	20700	0	-	54.0
10	16.3	-1.636	21100	42.6	-0.299	52.0
20	30.5	-0.824	21280	61.7	0.477	50.4
30	42.9	-0.286	21420	76.6	1.186	48.2
40	53.9	0.156	21518	87.0	1.903	46.0
50	63.7	0.562	21562	91.7	2.403	44.0
60	72.5	0.969	21580	93.6	2.685	41.5
70	80.3	1.405	21620	97.8	3.828	38.8
80	87.5	1.946	21628	98.7	4.348	36.0
90	94.0	2.752	21633	99.3	4.893	33.6
100	100	-	21640	100	-	31.0

Table S6. PPPyNiP in the binary solvent Water (1) + MeOH (2): percent concentration (C_1 , %), Water molar fraction (x_1 , %), the average statistic weight of Water in the first solvation sphere of PPPyNiP (p_1 , %) (p_1 , %) and the wavenumber of the ICT band (ν_t , cm^{-1})

$x_1\%$	$\ln \frac{x_1}{1-x_1}$	$\nu_t (\text{cm}^{-1})$	$p_1\%$	$\ln \frac{p_1}{1-p_1}$	π^*	β	α
0	-	21460	0	-	0.58	0.74	1.14
10	-2.20	21508	25.3	-1.083	0.64	0.74	1.12
20	-1.39	21545	44.7	-0.212	0.60	0.74	1.09
30	-0.85	21576	61.1	0.450	0.76	0.74	1.06
40	-0.41	21596	71.6	0.924	0.82	0.72	1.04
50	0.00	21615	81.6	1.488	0.88	0.70	1.03
60	0.41	21624	86.3	1.842	0.95	0.66	1.01
70	0.85	21632	93.7	2.257	1.01	0.63	1.01
80	1.39	21640	94.7	2.890	1.06	0.59	1.06
90	2.20	21645	97.4	3.611	1.11	0.54	1.13
100	-	21650	100	-	1.14	0.49	1.23

Table S7. PPPyNiP in the binary solvent Water (1) + EtOH (2): percent concentration (C_i , %), Water molar fraction (x_1 , %), the average statistic weight of Water in the first solvation sphere of PPPyNiP (p_1 , %) and the wavenumber of the ICT band (ν_i , cm^{-1})

$x_1\%$	$\ln \frac{x_1}{1-x_1}$	$\nu_t (\text{cm}^{-1})$	$p_1\%$	$\ln \frac{p_1}{1-p_1}$	π^*	β	α
0	-	21350	0	-	0.51	0.83	0.98
10	-2.20	21420	23.3	-1.190	0.57	0.84	0.96
20	-1.39	21484	46.7	-0.170	0.63	0.83	0.93
30	-0.85	21532	60.7	0.434	0.68	0.82	0.92
40	-0.41	21570	73.3	1.011	0.73	0.80	0.91
50	0.00	21598	82.7	1.563	0.77	0.79	0.90
60	0.41	21616	93.3	2.057	0.82	0.77	0.89
70	0.85	21632	96.0	3.178	0.90	0.74	0.88
80	1.39	21640	96.7	3.368	1.00	0.67	0.87
90	2.20	21646	98.3	4.304	1.11	0.59	0.97
100	-	21650	100	-	1.13	0.50	1.26

Table S8. PyNiP in the binary solvent Water (1) + MeOH (2): percent concentration (C_i , %), Water molar fraction (x_1 , %), the average statistic weight of Water in the first solvation sphere of PyNiP (p_1 , %) and the wavenumber of the ICT band (ν_i , cm^{-1})

$x_1\%$	$\ln \frac{x_1}{1-x_1}$	$\nu_t (\text{cm}^{-1})$	$p_1\%$	$\ln \frac{p_1}{1-p_1}$	π^*	β	α
0	-	21640	0	-	0.58	0.74	1.14
10	-2.20	21700	27.3	-0.980	0.64	0.74	1.12
20	-1.39	21740	45.5	-0.181	0.60	0.74	1.09
30	-0.85	21766	57.3	0.293	0.76	0.74	1.06
40	-0.41	21805	75.0	1.099	0.82	0.72	1.04
50	0.00	21826	84.5	1.699	0.88	0.70	1.03
60	0.41	21840	90.9	2.302	0.95	0.66	1.01
70	0.85	21850	95.5	3.045	1.01	0.63	1.01
80	1.39	21858	99.1	4.691	1.06	0.59	1.06
90	2.20	21860	1.00	-	1.11	0.54	1.13
100	-	21860	100	-	1.14	0.49	1.23

Table S9. PyNiP in the binary solvent Water (1) + EtOH (2): percent concentration (C_1 , %), Water molar fraction (x_1 , %), the average statistic weight of Water in the first solvation sphere of PyNiP (p_1 , %) and the wavenumber of the ICT band (ν_t , cm^{-1})

$x_1\%$	$\ln \frac{x_1}{1-x_1}$	$\nu_t (\text{cm}^{-1})$	$p_1\%$	$\ln \frac{p_1}{1-p_1}$	π^*	β	α
0	-	21410	0	-	0.51	0.83	0.98
10	-2.20	21518	24.0	-1.153	0.57	0.84	0.96
20	-1.39	21628	48.4	-0.063	0.63	0.83	0.93
30	-0.85	21704	65.3	0.633	0.68	0.82	0.92
40	-0.41	21766	79.1	1.331	0.73	0.80	0.91
50	0.00	21800	86.7	1.872	0.77	0.79	0.90
60	0.41	21826	92.4	2.504	0.82	0.77	0.89
70	0.85	21842	96.0	3.178	0.90	0.74	0.88
80	1.39	21852	98.2	4.012	1.00	0.67	0.87
90	2.20	21858	99.6	5.412	1.11	0.59	0.97
100	-	21860	100	-	1.13	0.50	1.26

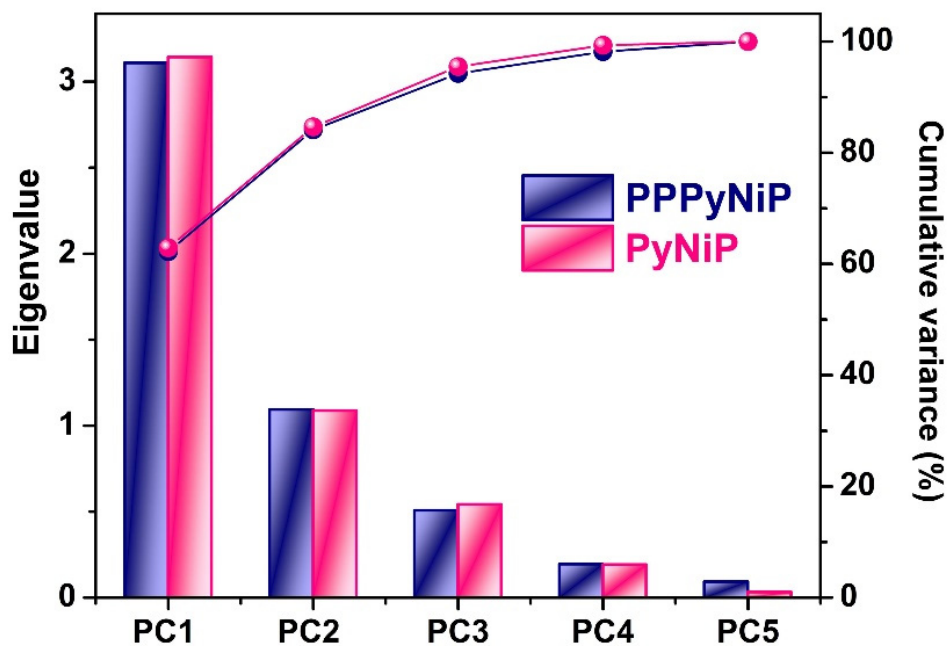


Figure S1. Scree plot of the PC eigenvalues and the cumulative variance for PPPyNiP and PyNiP.