Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Table S1 Selected geometric bond lengths, bond angles and dihedral angles of the optimized p-N-dimethyl-2-aminopyrazine Schiff base (donor), Picric, 3,5-dinitrosalicylic and 3,5-dinitrobenzoic acids (acceptors) and their CT complex usingB3LYP/6-311G(d,p)

Ligand/ complexes	Bond lengths (Å)		Bond angles		Dihedral angles	
Donor	C5-C6	1.409	N1-C5-C6	122.643	C5-C6- N7-C8	180.000
	C6-N4	1.341	C5-C6-N4	120.354	C6- N7-C8-C9	180.000
	C6-N7	1.396	C5-C6-N7	117.261	N7-C8-C9-C10	0.000
	C8-N7	1.288	N4-C6-N7	122.385	N7-C8-C9-C14	180.000
	C8-C9	1.448	C6-N7-C8	119.115	N4-C6-N7-C8	0.000
	C9-C10	1.406	N7-C8-C9	122.656		
	C9-C14	1.402	C8-C9-C10	122.488		
			C8-C9-C14	120.475		
Acceptor (PA)	C1-C2	1.428	O9-C1-C2	122.861	O9-C1-C2-C5	180.000
	C3-N11	1.387	C1-C2-N13	120.403	C1-C2-N13-O18	0.000
	C2-N13	1.467	C2-N13-O18	117.728	C1-C2-N13-O19	180.000
	N13-O18	1.244	C2-N13-O19	118.825	O9-C1-C3-N11	0.000
	N13-O19	1.212	N13-C2-C5	30.603	C1-C3-C4-C6	0.000
			O9-C1-C3	121.521	N7-C8-C9-C10	-0.418
CT complex	C8-N7	1.272	N4-C6-N7	116.574	N5-C6-N7-C8	134.297
	C6-N7	1.381	C5-C6-N7	29.047	C6-N7-C8-C9	176.716
	C6-N5	1.336	C6-N7-C8	120.238	N1-C4-C6-N7	-178.565
	C6-C4	1.407	N7-C8-C9	31.414	N5-C6-N7-N42	-52.660
	C33-N44	1.473	C6-N7-N42	160.509	N42-C34-C32-O40	-1.282
	C34-C32	1.439	C33-N44-O49	118.411	N42-C34-C35-C37	178.957
	C34-O35	1.3968	C33-N44-O50	116.752		
	C35-C37	1.390				
Acceptor						

3,5-dinitro salicylic acid						
	C2-C5	1.417	C2-C5-C6	121.715	C1-C2-C5-N15	-179.987
	C5-C6	1.389	C2-C5-N15	120.693	C2-C5-N15-O17	0.011
	C5-N15	1.464	C5-C2-O13	122.269	C2-C5-N15-O18	-179.980
	C2-O13	1.337	C5-N15-O17	117.593	O13-C2-C5-N15	0.023
	N15-O17	1.247	C5-N15-O18	119.091	C6-C5-N15-O17	179.983
	N15-O18	1.211			C6-C5-N15-O18	0.026
CT complex	C6-N7	1.393	N4-C6-N7	117.375	C3-N4-C6-N7	-179.487
	N7-C8	1.285	C6-N7-C8	119.087	N4-C6-N7-C8	-136.956
	C8-C9	1.451	C5-C6-N4	120.291	C6-N7-C8-C9	-174.021
	C6-N4	1.340	C5-C6-N7	122.253	N4-C6-N7-N38	-12.355
	C5-C6	1.412	N7-C8-C9	124.117	C9-C8-N7-N38	105.256
	C9-C10	1.403	C8-C9-C10	119.893	C8-N7-N38-O39	11.362
	C9-C14	1.406	C8-C9-C14	122.431	C8-N7-N38O40	146.777
	N7-N38	5.62	C8-N7-N38	130.984	C25-C26-N38-O39	-0.975
	N38-O39	1.222	C6-N7-N38	64.837	C25-C26-N38-O40	179.103
	N38-O40	1.226	O39-N38-O40	124.933	O34- C25-C28-N38	0.568
	C26-N38	1.471	C26-N38-O39	117.568	C23-C25-C26-N38	-178.988
	C26-C28	1.381	C26-N38-O40	117.500	C27-C28-C26-N38	179.379
	C28-C27	1.386	C25-C26-N38	119.556	C25-C23-C29-O30	-1.620
	C27-O35	1.459	C28-C26-N38	119.123		
			C25-C26-C28	121.314		
Acceptor 3,5-dinitro						

benzoic acid						
	C3-C5	1.389	C3-C5-C6	122.546	C1-C3-C5-N14	180.000
	C5-C6	1.387	C3-C5-N14	118.873	C4-C6-C5-N14	180.000
	C5-N14	1.486	C5-C6-N14	118.581	C3-C5-N15-O16	0.000
	N14-O16	1.221	C5-N14-O16	117.168	C3-C5-N15-O17	180.000
	N14-O17	1.2205	C5-N14-O16	117.229		
CT complex						
	C3-N4	1.333	N4-C6-N7	117.061	C3-N4-C6-N7	-178.713
	N4-C6	1.341	C6-N7-C8	119.790	N4-C6-N7-C8	-134.315
	C5-C6	1.412	C5-C6-N4	120.421	C6-N7-C8-C9	-176.598
	C6-N7	1.391	C5-C6-N7	122.438	N4-C6-N7-N33	37.075
	N7-C8	1.285	C8-C9-C10	120.154	C8-N7-N33O35	-62.696
	C8-C9	1.450	C8-C9-C14	122.160	C8-N7-N34O36	170.316
	C9-C10	1.403	C6-N7-N33	102.868	C24-C26-N33-O35	163.743
	C9-C14	1.407	C8-N7-N33	136.542	C24-C26-N33-O36	-16.979
	N7-N33	3.558	O35-N33-O36	125.504	C28-C26-N33-O35	-15.454
	N33-O35	1.224	C26-N33-O35	117.085	C28-C26-N33-O36	163.825
	N33-O36	1.218	C26-N33-O36	117.407	C23-C24-C26-N33	-179.562
	C26-N33	1.491	C25-C27-C28	122.228	C27-C28-C24-N33	179.047
	C26-C24	1.388				
	C26-C28	1.385				

Table S2 Total energy, energy of HOMO and LUMO, energy gap (E_g, eV), ionization energy (I, eV), electron affinity (A, eV), absolute electronegativities, (χ, eV), absolute hardness (η, eV), global softness (S, eV^{-1}) chemical potential (π, eV^{-1}) global electrophilicity (ω, eV), additional electronic charge, $\Delta N_{max,}$ of the studied p-N-dimethyl-2-aminopyrazine Schiff base (donor, Picric, 3,5-dinitrosalicylic and 3,5-dinitrobenzoic acids (acceptors) and their CT complex usingB3LYP/6-311G(d,p)

Parameter	Donor	Acceptor	CT complex	Acceptor	CT complex	Acceptor	CT complex
	p-$N(CH_3)_2$	PA		3,5-dNSA		3,5-DNBA	
E_T, a.u.	-722.97	-921.20	-1664.20	-904.97	-1627.90	-829.85	-1552.68
E_{HOMO}, a.u.	-0.1988	-0.3117	-0.1652	-0.3129	-0.2135	-0.3280	-0.2107
E_{LUMO}, a.u.	-0.0694	-0.1506	-0.1182	-0.1610	-0.1249	-0.1352	-0.1217
E_g, eV	3.5228	4.3832	1.2800	4.1334	2.4129	5.2464	2.4226
I, eV	5.4099	8.4824	4.4964	8.5145	5.8108	8.9265	5.7343
A, eV	1.8871	4.0992	3.2164	4.3811	3.3979	3.6801	3.3117
χ, eV	3.6485	6.2908	3.8564	6.4478	4.6043	6.3033	4.5230
η, eV	1.7614	2.1916	0.6400	2.0667	1.2064	2.6232	1.2113
S, eV	0.2839	0.2281	0.7812	0.2419	0.4144	0.1906	0.4128
π eV	-3.6485	-6.2908	-3.8564	-6.4478	-4.6043	-6.3033	-4.5230
(ω, eV)	4.1238	9.1353	11.6186	10.0566	8.7857	12.2387	8.4326
$\Delta N_{max.}$	2.0714	2.8704	6.0256	3.1198	3.8166	2.4029	3.7340

Table S3 NBO charges calculated for the of the studied p-N-dimethyl-2-aminopyrazine Schiff base donor, Picric, 3,5-dinitrosalicylic and 3,5-dinitrobenzoic acids (acceptors) and their CT complex using B3LYP/6-311G(d,p)

Parameter	Donor	Acceptor	CT complex	Acceptor	CT complex	Acceptor	CT complex
	p-N$(CH_3)_2$	PA		3,5-dNSA		3,5-DNBA	
N1	-0.419		-0.407		-0.410		-0.41
N4	-0.472		-0.411		-0.452		-0.445
N7	-0.527		-0.408		-0.483		-0.485
N23	-0.426						
N42		0.515	0.344				
N43		0.518	0.500				
N44		0.521	0.500				
N35				0.476	0.520		
N38				0.472	0.504		
N33						0.502	0.507
N34						0.502	0.507

Table S4 Calculated natural charge, natural population and natural electronic configuration of the studied p-N-dimethyl-2-aminopyrazine Schiff base donor, Picric, 3,5-dinitrosalicylic and 3,5-dinitrobenzoic acids (acceptors) and their CT complex usingB3LYP/6-31G+(d,p)

Complex	Natural charge	Core	Natural population			Natural electronic configuration
			Valence	Rydberg	Total	
Donor (f), (N7)	-0.527	1.9993	5.5092	0.0186	7.5271	[core]$2s^{1.37}2p^{4.14}3p^{0.01}3d^{0.01}$
PA (1), (N13)	0.521	1.9994	4.4286	0.0513	6.4792	[core]$2s^{1.07}2p^{3.36}3s^{0.01}3p^{0.03)}3d^{0.02}$
CT complex (N7)	-0.438	1.9993	5.4554	0.0285	7.4832	[core]$2s^{1.35}2p^{4.10}3p^{0.01}3d^{0.01}$
(N35)	0.520	1.9995	4.4326	0.0480	6.4801	[core]$2s^{1.10}2p^{3.34}3s^{0.01}3d^{0.01}4p^{0.03}$
3,5-DNSA (2), (N15)	0.476	1.9994	4.4898	0.0350	6.5242	[core]$2s^{1.08}2p^{3.41}3s^{0.01}3p^{0.03}$
CT complex, (N7)	-0.483	1.9993	5.4554	0.0285	7.4832	[core]$2s^{1.35}2p^{4.10}3p^{0.01}3d^{0.01}$
(N35)	0.520	1.9995	4.4326	0.0480	6.4801	[core]$2s^{1.10}2p^{3.34}3s^{0.01}3d^{0.01}4p^{0.03}$
3,5-DNBA (3), (N14)	0.502	1.9996	4.4426	0.0563	6.4985	[core]$2s^{1.10}2p^{3.35}3d^{0.02}4p^{0.03}$
CT complex (N7)	-0.485	1.9993	5.4576	0.02858	7.4854	[core]$2s^{1.35}2p^{4.11}3p^{0.01}3d^{0.01}$
(N33)	0.507	1.9996	4.4374	0.0557	6.49263	[core]$2s^{1.09)}2p^{3.34}3s^{0.01}3d^{0.02}4p^{0.03}$

Table S5 Calculated total static dipole moment (μ), the mean polarizability <α>, anisotropy of the polarizability Δα and the first-order hyperpolarizability <β > configuration for the studied p-N-dimethyl-2-aminopyrazine Schiff base donor, Picric, 3,5-dinitrosalicylic and 3,5-dinitrobenzoic acids (acceptors) and their CT complex using B3LYP/6-311G(d,p)

Property		Donor	Acceptor	CT complex	Acceptor	CT complex	Acceptor	CT complex
	Urea	p-N(CH_3)$_2$ (f)	PA (1)		3,5-dNSA (2)		3,5-DNBA (3)	
μ, D	1.3197	6.1717	1.8975	20.8480	3.9698	9.6823	3.7529	2.7038
αxx, a.u.	-	-79.5137	-106.1316	-243.751	-105.9304	-167.1929	-108.0481	-159.0539
αyy	-	-92.2189	-108.2568	-168.8421	-118.8258	-198.766	-87.0213	-191.8124
αzz	-	-104.1396	-84.3036	-195.6793	-86.5795	-196.6617	-81.495	-196.5906
αxy	-	-11.4706	3.4958	-4.8814	4.9395	9.3347	-7.5274	-25.1649
αxz	-	0	-0.0036	16.0001	0.0039	10.8413	0	9.766
αyz	-	0	0.0006	-19.1557	-0.0048	-10.5663	0	9.0787
<α> esu	-	$-1.3628xq0^{-23}$	$-1.4755x10^{-23}$	$-3.0049x10^{-23}$	$-1.538x10^{-23}$	$-2.7794x10^{-23}$	$-1.3662x10^{-23}$	$-2.7044x10^{-23}$
Δα, esu	-	$3.1611x10^{-24}$	$3.4033x10^{-24}$	$9.7421x10^{-24}$	$4.1662x10^{-24}$	$4.5313x10^{-24}$	$3.5963x10^{-24}$	$5.2449x10^{-24}$
βxxx	-	-19.8405	-58.2773	575.3357	71.581	-425.5192	-2.765	79.9354
βxxy	-	12.8082	-0.7731	43.673	25.9008	-12.5359	35.5277	-0.6102
βxyy	-	-45.6068	20.0168	178.3933	-30.791	-36.5143	-36.5708	11.3865
βyyy	-	178.6939	-14.9933	261.2411	38.4414	-138.2668	69.4985	65.0427
βxxz	-	0	-0.0089	-36.4279	0.024	26.1764	0	-56.0454
βxyz	-	0	-0.0004	15.4904	-0.0007	-18.3411	0	34.8468
βyyz	-	0	0.0041	36.2127	0.0334	21.2741	0	12.1622
βxzz	-	-1.5918	-1.8796	20.9318	-0.7307	-33.484	0.1683	22.1173
βyzz	-	-0.1705	0.1695	29.6825	3.2008	-9.0052	-3.0908	-12.0357
βzzz	-	0	-0.0012	-24.7883	-0.0087	-5.6371	0	-23.6182
<β>, esu	$0.1947x10^{-30}$	$1.7515x10^{-30}$	$0.3720x10^{-30}$	$7.2933x10^{-30}$	$0.6784x10^{-30}$	$4.5125x10^{-30}$	$0.9434x10^{-30}$	$1.2270x10^{-30}$