Electronic Supplementary Material (ESI) for Materials Advances.

Experimental and theoretical exploration of the new stilbazolium family single crystal grown by the integration of novel anion for optical limiting and optoelectronic applications

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Atoms	Bond length
C(1)-C(2)	1.381(3)
C(1)-C(6)	1.396(3)
C(1)-N(1)	1.426(3)
C(2)-C(3)	1.368(3)
C(2)-H(2)	0.9300
C(3)-C(4)	1.389(3)
C(3)-H(3)	0.9300
C(4)-N(3)	1.367(3)
C(4)-C(5)	1.400(3)
C(5)-C(6)	1.376(3)
C(5)-H(5)	0.9300
C(6)-H(6)	0.9300
C(7)-C(8)	1.377(3)
C(7)-C(12)	1.390(3)
C(7)-N(2)	1.448(2)
C(8)-C(9)	1.375(3)
C(8)-H(8)	0.9300
C(9)-C(10)	1.383(3)
C(9)-H(9)	0.9300
C(10)-C(11)	1.385(3)
C(10)-S(1)	1.7764(19)
C(11)-C(12)	1.393(3)
C(11)-H(11)	0.9300
C(12)-H(12)	0.9300
N(1)-N(2)	1.232(2)
N(3)-H(3B)	0.87(3)
N(3)-H(3A)	0.81(3)
O(1)-S(1)	1.370(6)
O(2)-S(1)	1.588(4)
O(3)-S(1)	1.355(4)
C(13)-N(5)	1.476(3)
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600

Atoms	Bond length
C(14)-C(15)	1.360(3)
C(14)-H(14)	0.9300
C(15)-C(16)	1.397(3)
C(15)-H(15)	0.9300
C(16)-C(17)	1.402(3)
C(16)-C(19)	1.446(3)
C(17)-C(18)	1.358(3)
C(17)-H(17)	0.9300
C(18)-N(5)	1.349(3)
C(18)-H(18)	0.9300
C(19)-C(20)	1.337(3)
C(19)-H(19)	0.9300
C(20)-C(21)	1.444(3)
C(20)-H(20)	0.9300
C(21)-C(22)	1.390(3)
C(21)-C(26)	1.398(3)
C(22)-C(23)	1.370(3)
C(22)-H(22)	0.9300
C(23)-C(24)	1.402(3)
C(23)-H(23)	0.9300
C(24)-N(4)	1.368(2)
C(24)-C(25)	1.408(3)
C(25)-C(26)	1.373(3)
C(25)-H(25)	0.9300
C(26)-H(26)	0.9300
C(27)-N(4)	1.453(3)
C(27)-H(27A)	0.9600
C(27)-H(27B)	0.9600
C(27)-H(27C)	0.9600
C(28)-N(4)	1.446(3)
C(28)-H(28A)	0.9600
C(28)-H(28B)	0.9600
C(28)-H(28C)	0.9600

Table 1: Bond lengths of DMMA crystal

Atoms	Angle
C(2)-C(1)-C(6)	118.82(19)
C(2)-C(1)-N(1)	115.23(19)
C(6)-C(1)-N(1)	125.95(19)
C(3)-C(2)-C(1)	121.1(2)
C(3)-C(2)-H(2)	119.5
C(1)-C(2)-H(2)	119.5
C(2)-C(3)-C(4)	120.8(2)
C(2)-C(3)-H(3)	119.6
C(4)-C(3)-H(3)	119.6
N(3)-C(4)-C(3)	120.9(2)
N(3)-C(4)-C(5)	120.7(2)
C(3)-C(4)-C(5)	118.38(19)
C(6)-C(5)-C(4)	120.6(2)
C(6)-C(5)-H(5)	119.7
C(4)-C(5)-H(5)	119.7
C(5)-C(6)-C(1)	120.3(2)
C(5)-C(6)-H(6)	119.8
C(1)-C(6)-H(6)	119.8
C(8)-C(7)-C(12)	120.00(18)
C(8)-C(7)-N(2)	114.62(19)
C(12)-C(7)-N(2)	125.37(19)
C(9)-C(8)-C(7)	120.5(2)
C(9)-C(8)-H(8)	119.7
C(7)-C(8)-H(8)	119.7
C(8)-C(9)-C(10)	120.1(2)
C(8)-C(9)-H(9)	120.0
C(10)-C(9)-H(9)	120.0
C(9)-C(10)-C(11)	119.85(18)
C(9)-C(10)-S(1)	119.41(16)
C(11)-C(10)-S(1)	120.67(16)
C(10)-C(11)-C(12)	120.0(2)
C(10)-C(11)-H(11)	120.0
C(12)-C(11)-H(11)	120.0
C(7)-C(12)-C(11)	119.4(2)

Atoms	Angle
C(11)-C(12)-H(12)	120.3
N(1)-N(2)-C(7)	112.46(18)
C(4)-N(3)-H(3B)	118(2)
C(4)-N(3)-H(3A)	114(2)
H(3B)-N(3)-H(3A)	125(3)
O(3)-S(1)-O(1)	121.2(4)
O(3)-S(1)-O(2)	106.5(3)
O(1)-S(1)-O(2)	107.4(4)
O(1)-S(1)-C(10)	108.3(3)
O(2)-S(1)-C(10)	103.13(17)
N(5)-C(13)-H(13A)	109.5
N(5)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
N(5)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
N(5)-C(14)-C(15)	120.91(19)
N(5)-C(14)-H(14)	119.5
C(15)-C(14)-H(14)	119.5
C(14)-C(15)-C(16)	121.6(2)
C(14)-C(15)-H(15)	119.2
C(16)-C(15)-H(15)	119.2
C(15)-C(16)-C(17)	115.65(18)
C(15)-C(16)-C(19)	120.45(19)
C(18)-C(17)-C(16)	121.0(2)
C(18)-C(17)-H(17)	119.5
N(5)-C(18)-C(17)	121.4(2)
N(5)-C(18)-H(18)	119.3
C(17)-C(18)-H(18)	119.3
C(20)-C(19)-H(19)	117.9
C(16)-C(19)-H(19)	117.9
C(19)-C(20)-C(21)	129.3(2)
C(19)-C(20)-H(20)	115.3
C(21)-C(20)-H(20)	115.3

Atoms	Angle
C(22)-C(21)-C(20)	118.59(19)
C(26)-C(21)-C(20)	124.94(18)
C(23)-C(22)-C(21)	122.94(19)
C(23)-C(22)-H(22)	118.5
C(21)-C(22)-H(22)	118.5
C(22)-C(23)-C(24)	120.55(19)
C(22)-C(23)-H(23)	119.7
C(24)-C(23)-H(23)	119.7
N(4)-C(24)-C(23)	120.89(18)
N(4)-C(24)-C(25)	122.03(18)
C(23)-C(24)-C(25)	117.06(18)
C(26)-C(25)-C(24)	121.31(19)
C(26)-C(25)-H(25)	119.3
C(18)-N(5)-C(13)	120.15(19)
C(25)-C(26)-H(26)	119.2
C(21)-C(26)-H(26)	119.2

N(4)-C(27)-H(27A)	109.5
Atoms	**Angle**
H(27A)-C(27)-H(27B)	109.5
N(4)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
N(4)-C(28)-H(28A)	109.5
N(4)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
N(4)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(24)-N(4)-C(28)	120.26(17)
C(24)-N(4)-C(27)	119.54(17)
C(28)-N(4)-C(27)	115.68(17)
C(14)-N(5)-C(18)	119.42(18)
C(14)-N(5)-C(13)	120.39(18)
C(18)-N(5)-C(13)	120.15(19)

Table 2: Bond angle of DMMA crystal

Faces (hkl)	d_{hkl} (Å)	Calculated relative growth rates from BFDH law	Morphological importance (M.I.) by BFDH law
$(00\bar{1})$, (001)	26.99	1.000	1.000
$(\bar{1}00)$, (100)	12.12	2.226	0.449
$(\bar{1}01)$, $(10\bar{1})$	11.05	2.442	0.409
$(0\bar{1}0)$, (010)	7.552	3.573	0.279
$(0\bar{1}1)$, (011)	7.275	3.709	0.269

Table 3: Morphological importance planes of DMMA crystal

Sample	E_d (eV)	E_0(eV)	F $(eV)^2$	n_0	M_{-1}	M_{-3}

name						
DMMA	3.753	1.987	7.459	1.699	1.888	0.4780

Table 4: Dispersive parameters of DMMA crystal

Donor	Acceptor	E(2) (kcal/mol)
$\pi(C_1\text{-}C_9)$	$\pi^*(C_2\text{-}C_4)$	23.68
	$\pi^*(C_6\text{-}C_7)$	18.12
	$\pi^*(N_{21}\text{-}N_{22})$	19.14
$\pi(C_2\text{-}C_4)$	$\pi^*(C_1\text{-}C_9)$	14.64
	$\pi^*(C_6\text{-}C_7)$	23.03
$\pi\ (C_6\text{-}C_7)$	$\pi\ ^*(C_1\text{-}C_9)$	26.65
	$\pi\ ^*(C_2\text{-}C_4)$	14.64
$\pi\ (C_{11}\text{-}C_{12})$	$\pi\ ^*(C_{14}\text{-}C_{16})$	20.92
	$\pi\ ^*(C_{17}\text{-}C1_9)$	18.36
	$\pi\ ^*(N_{21}\text{-}N_{22})$	21.97
$\pi\ (C_{14}\text{-}C_{16})$	$\pi\ ^*(C_{11}\text{-}C_{12})$	19.35
	$\pi\ ^*(C_{17}\text{-}C1_9)$	19.66
LP(2) O_{25}	$\sigma^*(C_{16}\text{-}S_{27})$	10.10
	$\sigma^*(O_{24}\text{-}S_{27})$	11.61
π(C38 – C43)	$\pi^*(C_{34}\text{-}C_{36})$	16.68
	$\pi^*(C_{39}\text{-}C_{41})$	14.91
	$\pi^*(C_{45}\text{-}C_{47})$	26.97
$\pi(C_{45} – C_{47})$	$\pi^*(C_{38}\text{-}C_{43})$	18.38
	$\pi^*(C_{48}\text{-}C_{50})$	20.70
	$\pi^*(C_{38}\text{-}C_{43})$	18.66
$\pi(C_{48} – C_{50})$	LP*(1) C_{52}	42.88
$\pi(C_{53} – C_{55})$	LP*(1) C_{52}	41.29
LP(1) N_{66}	$\pi^*\ (C_{34}\text{-}C_{36})$	35.80
LP(1) N_{66}	$\pi^*\ (C_{39}\text{-}C_{41})$	36.27

Table 5: Second order perturbation interaction energy values computed from the NBO analysis

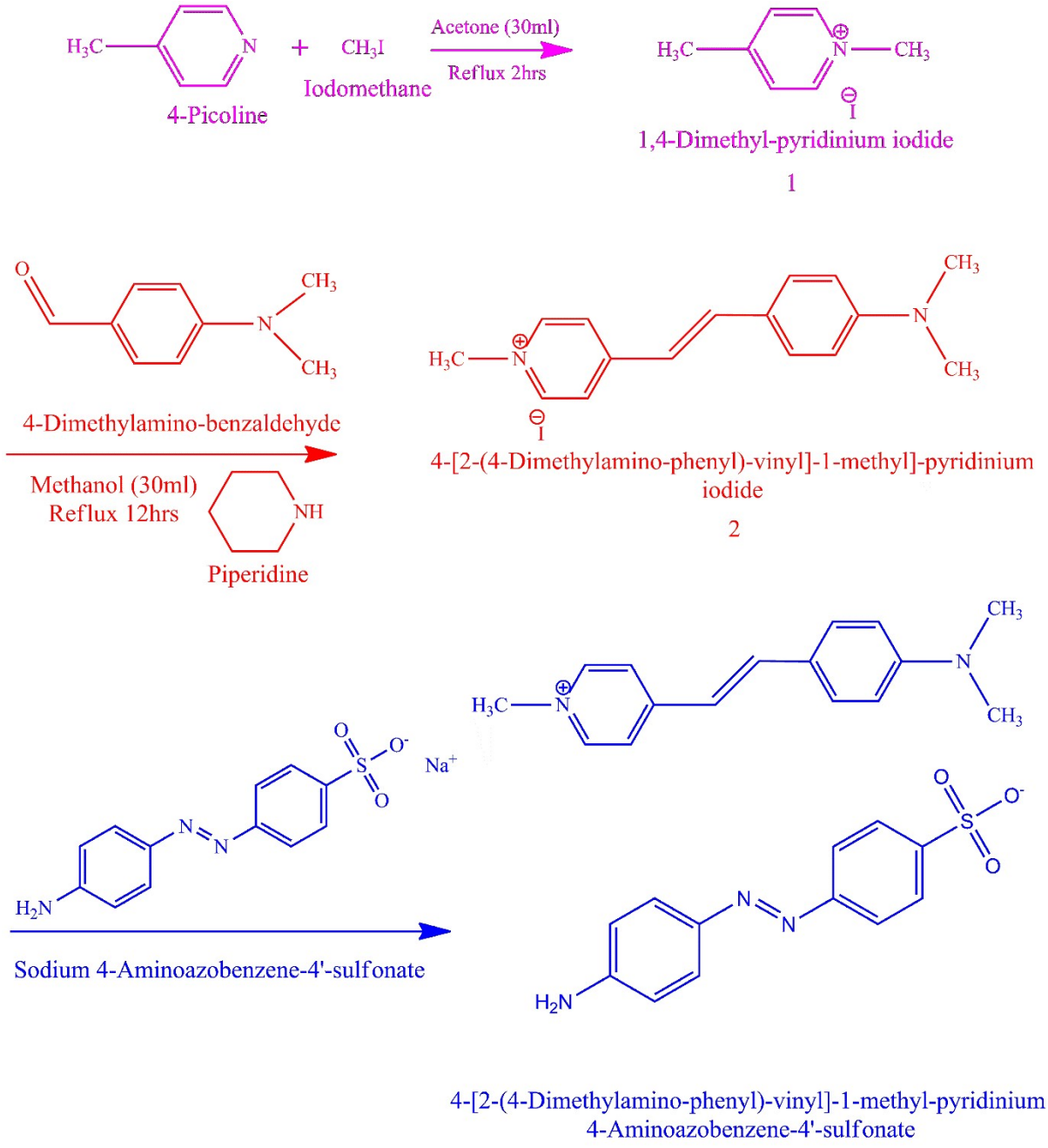


Figure 1: Synthesis of DMMA powder

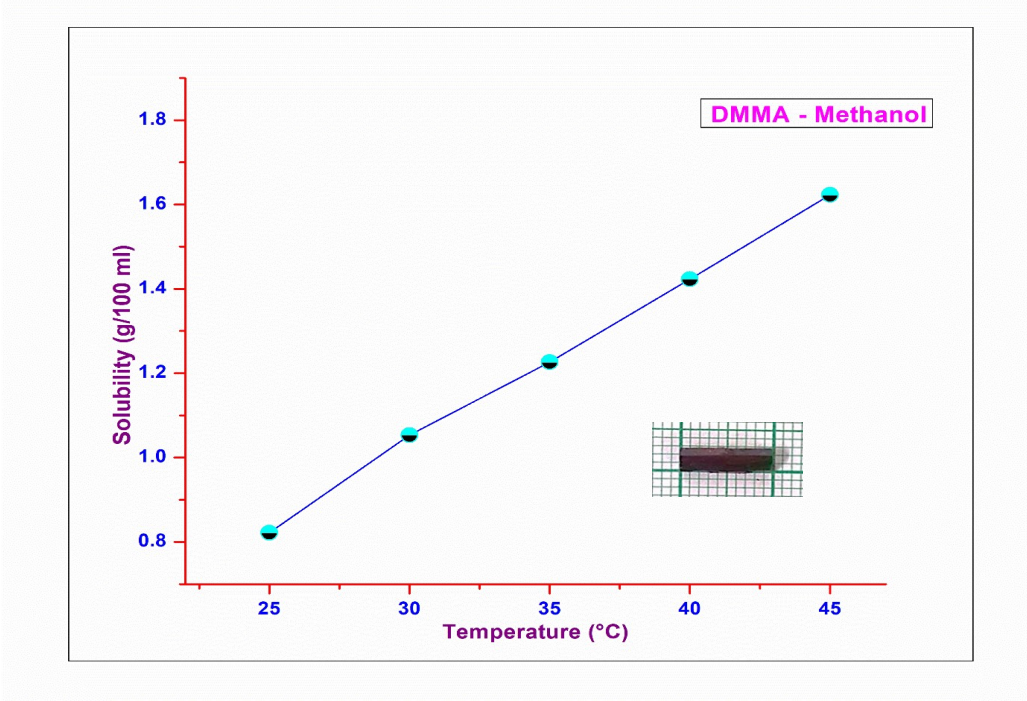
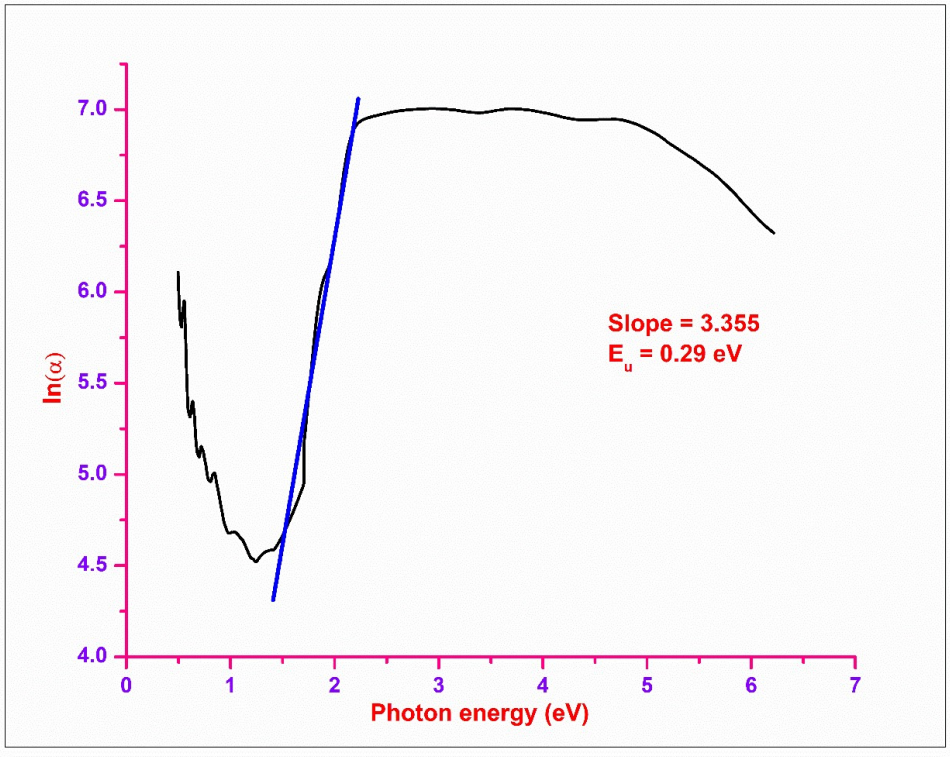


Figure 2: Solubility trace of DMMA and image of the grown crystal

Figure 3: Urbach energy of DMMA crystal



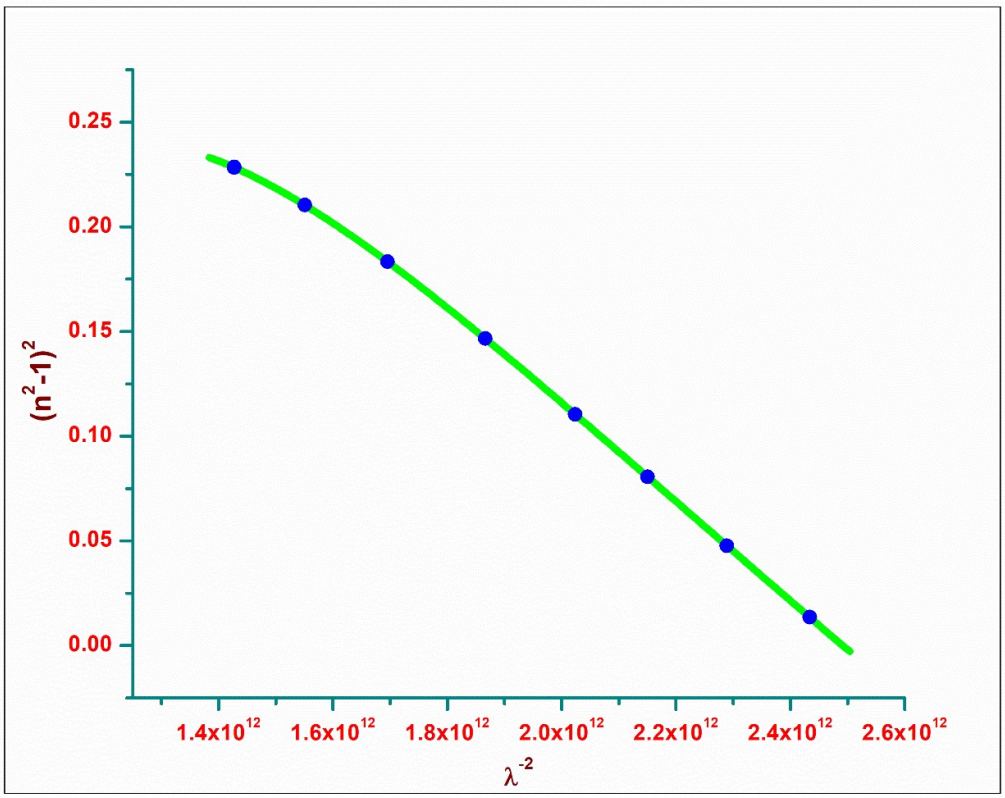


Figure 4: Refractive index dispersion plot of DMMA crystal using Sellmeier model

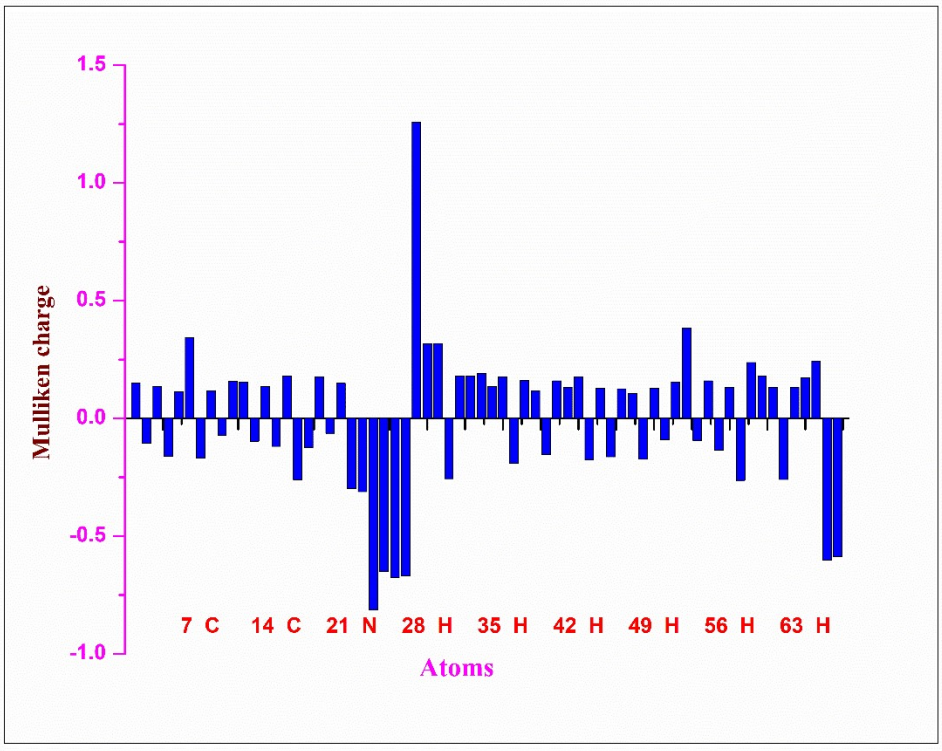


Figure 5: Mulliken atomic charge diagram