



STRUCTURAL  
CHEMISTRY

**Volume 74 (2018)**

**Supporting information for article:**

**Structural and optical profile of a multifunctionalized 2-pyridone derivative in a crystal engineering perspective**

**Monu Joy, E. R. Anabha, Subash Gopi, Bijo Mathew, Ajeesh Kumar S and Annie Mathews**

**Table S1:** Second-order perturbation theory analysis of Fock matrix in NBO basis for P1.

Donor Orbitals		Acceptor Orbitals		Interaction Energy [ $E(2)$ ] in Kcal/mol
$\sigma$	O2 – C13	$\sigma^*$	N1 – H1 <sup>#</sup>	1051.85
$\sigma$	O2 – C13	$\sigma^*$	C14 – H14A <sup>#</sup>	906.67
$\pi$	O2 – C13	$\sigma^*$	N1 – H1 <sup>#</sup>	1243.39
$\pi$	O2 – C13	$\pi^*$	C6 – C1	812.77
$\pi$	O2 – C13	$n^*$	N2 – C12	1240.72
$\pi$	O2 – C13	$\sigma^*$	C14 – H14A <sup>#</sup>	4076.5
$\sigma$	N1 – C13	$\pi^*$	C6 – C1	1384.24
$\sigma$	N1 – C13	$n^*$	N2 – C12	1560.57
$\sigma$	N1 – C13	$\sigma^*$	C14 – H14A <sup>#</sup>	7317.63
$\sigma$	N1 – C7	$\pi^*$	C6 – C1	1204.64
$\sigma$	N1 – C7	$n^*$	N2 – C12	1146.88
$\sigma$	N1 – C7	$\sigma^*$	C14 – H14A <sup>#</sup>	3528.77
$\sigma$	C13 – C11	$\sigma^*$	N1 – H1 <sup>#</sup>	3007.04
$\sigma$	C13 – C11	$n^*$	N2 – C12	1714.62
$\sigma$	C13 – C11	$\sigma^*$	C14 – H14A <sup>#</sup>	6336.87
$\sigma$	C11 – C10	$n^*$	N2 – C12	1569.22
$\sigma$	C11 – C10	$\sigma^*$	C14 – H14A <sup>#</sup>	2122.54
$\sigma$	C4 – C5	$n^*$	N2 – C12	3462.72
$\sigma$	C4 – C5	$\sigma^*$	C14 – H14A <sup>#</sup>	10361.15
$\pi$	C4 – C5	$\pi^*$	C6 – C1	1038.52
$\pi$	C4 – C5	$n^*$	N2 – C12	1097.12
$\pi$	C4 – C5	$\sigma^*$	C14 – H14A <sup>#</sup>	3263.61
$\sigma$	C4 – C3	$n^*$	N2 – C12	1583.77
$\sigma$	C4 – C3	$\sigma^*$	C14 – H14A <sup>#</sup>	5018.86
$\sigma$	C3 – C2	$n^*$	N2 – C12	3512.81
$\sigma$	C3 – C2	$\sigma^*$	C14 – H14A <sup>#</sup>	4188.74
$\sigma$	C9 – H9	$\pi^*$	C6 – C1	2229.26
$\sigma$	C9 – H9	$n^*$	N2 – C12	11664.7
$\sigma$	C9 – H9	$\sigma^*$	C14 – H14A <sup>#</sup>	13881.27
$\sigma$	S1	$\sigma^*$	N1 – H1	1160.06
$\sigma$	C9 – H9	$\pi^*$	C6 – C1	2229.26
$\sigma$	C9 – H9	$n^*$	N2 – C12	11664.7
$\sigma$	C9 – H9	$\sigma^*$	C14 – H14A <sup>#</sup>	13881.27
$\sigma$	S1	$\sigma^*$	N1 – H1	1160.06
$\sigma$	O2	$\sigma^*$	C14 – H14A <sup>#</sup>	29553.21

<sup>#</sup>The atom names involved in the table S1 are based on figure 2 (see paper), but the hydrogen atoms present in the image are not numbered. Hence, the readers are advised to use the associated CIF while considering this table.