Responses to Reviewers and Editors Point by Point

Page / Line **Initial version**	**Initial manuscript text**	**Corrections / Additions / Responses by the authors**	**Type of correction/ Editors/ Reviewers and authors**
P3 / L97 – L98	The molecules are linked by a small C—H···O contact (Figure 3) and by short C—H···N contacts to form a long chain along the a-axis (Figure 4).	The molecules are linked by a small C—H···O contact (Figure 3, see SM) and by short C—H···N contacts to form a long chain along the a-axis (Figure 4, see SM)	1./ The packing diagrams of 5 are very important for the SCXRD analysis, but Figure 3-5 should be inserted into the SM.
P4 – P5		Figures 3-5 have been displaced to SM	1./ The packing diagrams of 5 are very important for the SCXRD analysis, but Figure 3-5 should be inserted into the SM.
P5 / L117		Table 1 has been inserted into the SM	2./ Table 1 is also important but move it to the SM.
P5 / L103 - L104	interactions, which are represented by black dotted lines (with centroids shown as of pink	interactions, which are represented by black dotted lines (with centroids shown as of pink spheres) (Figure 5 and Table 1, see SM).	2./ Table 1 is also important but move it to the SM.

	spheres) (Figure 5 and Table 1, see SM).		
P5 / L 124 - L125	The most important red spots and the corresponding interactions are shown in Figure 7 (See SM).	The most important red spots and the corresponding interactions are shown in Figure 7 (See SM).	3/ Figure 7-8 should be inserted into SM, the manuscript is long.
P6 / L137 - L138	Figure 7 depicts the existence of multiple brilliant red spots on the three-dimensional dnorm surfaces of the crystal structure, which are hydrogen bonding interactions.	Figure 7 (See SM) depicts the existence of multiple brilliant red spots on the three-dimensional dnorm surfaces of the crystal structure, which are hydrogen bonding interactions.	3/ Figure 7-8 should be inserted into SM, the manuscript is long.
P6 - P7		Figures 7-8 have been displaced to SM	3/ Figure 7-8 should be inserted into SM, the manuscript is long.
P6 / L 142 – L144	Figure 8a displays the entire two-dimensional fingerprint pattern [34], while those divided into H···O/O···H, H···H, H···C/C···H, H···Cl/Cl···H, H···N/N···H, C···C, Cl···O/O···Cl and O···C/C···O contacts are illustrated in Figure 8b–I,……..	Figure 8a (See SM) displays the entire two-dimensional fingerprint pattern [34], while those divided into H···O/O···H, H···H, H···C/C···H, H···Cl/Cl···H, H···N/N···H, C···C, Cl···O/O···Cl and O···C/C···O contacts are illustrated in Figure 8b–i (See SM),	3/ Figure 7-8 should be inserted into SM, the manuscript is long.
P7-P8 /L174 – L176	Table 2 provides an overview of the experimental and theoretical findings regarding angles and bond lengths.	Table 2 (See SM) provides an overview of the experimental and theoretical findings regarding angles and bond lengths.	4./ Instead of Table 2, it would be better to have a figure overlaid with the DFT calculations and the SCXRD data. Move the Table 2 to the SM.

P8 / L187		- The software that generates the DFT calculations cannot provide bond length and angle datas in the figure form. - Table 2 has been moved into the SM	4./ Instead of Table 2, it would be better to have a figure overlaid with the DFT calculations and the SCXRD data. Move the Table 2 to the SM.
P8 / L176	Table 3 summarizes the results for the title compound, which include hardness (η),……	Table 3 (See SM) summarizes the results for the title compound, which include hardness (η),…..	5./ Table 3-4 and Figure 9 put to the SM.
P8 / L180	Figure 9 depicts the electron's change in energy level from HOMO to LUMO.	Figure 9 (See SM) depicts the electron's change in energy level from HOMO to LUMO.	5./ Table 3-4 and Figure 9 put to the SM.
P10 / L228	Table 4 provides data collection, crystal data and refined structural informations.	Table 4 (See SM) provides data collection, crystal data and refined structural informations.	5./ Table 3-4 and Figure 9 put to the SM.
SM		It's done	6./ In the SM, the ESI-MS spectrum shows only 1 decimal digit; it is not necessary to present.
SM		Following the displacement of the Figures and Tables, we have renumbered the SM pages and inserted two titles marked in red	The referees' comments of 1/ to 5/