Fog. 1



Fig. 2



Fig. 3



Fig. 4



Fig. 5



Fig. 6



Fig. 7



Fig. 8



Fig. 9

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| C:\Users\toshiba\Desktop\R. KERKOUR Calculs\P4\Gas phase\Optimized strucure.tif(a)Optimized molecular structure |
| **C:\Users\toshiba\Desktop\R. KERKOUR Calculs\P4\Gas phase\HOMO.tif**(b) HOMO |
| **C:\Users\toshiba\Desktop\R. KERKOUR Calculs\P4\Gas phase\LUMO.tif**( c) LUMO |
| C:\Users\toshiba\Desktop\R. KERKOUR Calculs\P4\Gas phase\Electron density from total SCF density mapped withe ESP.tif( d) MEP |

Fig. 10