

## What can $pK_a$ and NBO charges of the ligands tell us about the water and thermal stability of metal organic frameworks?

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### SUPPORTING INFORMATION

Taking the H<sub>2</sub>BDC for example, we give the calculation input files of the Gas phase geometries, the Solvation Gibbs energies ( $\Delta G_{\text{solv}}$ ) and the NBO charges as follows:

#### 1. the input file of the Gas phase geometries

```
%chk=freqH2BDC
```

```
%mem=20000000
```

```
%nproc=8
```

```
# B3LYP/6-31+g(d,p) opt freq
```

```
freqH2BDC
```

```
0 1
```

```
6          0.665594    1.230542   -0.000019
```

```
6         -0.726121    1.198900   -0.000004
```

```
6         -1.397219   -0.034047    0.000011
```

```
6         -0.665594   -1.230542    0.000018
```

```
6          0.726121   -1.198900    0.000002
```

6	1.397219	0.034047	-0.000013
1	1.201341	2.174228	-0.000026
1	-1.294009	2.122594	-0.000025
1	-1.201341	-2.174228	0.000024
1	1.294009	-2.122594	0.000024
6	-2.884608	-0.123018	0.000000
8	-3.518330	-1.160535	-0.000017
8	-3.489973	1.092519	0.000014
1	-4.451317	0.928524	-0.000007
6	2.884608	0.123018	-0.000001
8	3.518330	1.160535	0.000019
8	3.489973	-1.092519	-0.000012
1	4.451317	-0.928524	0.000011

## 2. The input file of the calculated $\Delta G_{\text{solv}}$

%chk=solH<sub>2</sub>BDC

%mem=20000000

%nproc=8

# B3LYP/6-31+g(d,p) SCF=Tight SCRF=(SMD,solvent=water,externalIteration,dovacuum)

solH<sub>2</sub>BDC

0 1

6	-0.666105	1.230188	0.000011
6	0.725474	1.199321	0.000012
6	1.396807	-0.033338	-0.000001
6	0.666105	-1.230188	-0.000012
6	-0.725474	-1.199321	-0.000014
6	-1.396807	0.033338	-0.000001
1	-1.203172	2.172391	0.000019
1	1.293233	2.122316	0.000019

1	1.203172	-2.172391	-0.000021
1	-1.293233	-2.122316	-0.000021
6	2.884385	-0.122404	-0.000004
8	3.516888	-1.160610	0.000010
8	3.490691	1.092017	-0.000002
1	4.448388	0.926573	0.000007
6	-2.884385	0.122404	0.000001
8	-3.516888	1.160610	-0.000007
8	-3.490691	-1.092017	0.000005
1	-4.448388	-0.926573	-0.000001

### 3. The input file of the calculated NBO charges

First we did the optimization and frequency calculation of BDC<sup>2-</sup> using the same method as we did with H<sub>2</sub>BDC (1), then we did the NBO charges based on the obtained geometry as follows:

```
%chk=nboBDC
```

```
%mem=20000000
```

```
%nproc=8
```

```
# B3LYP/6-31+g(d,p) pop=nbo
```

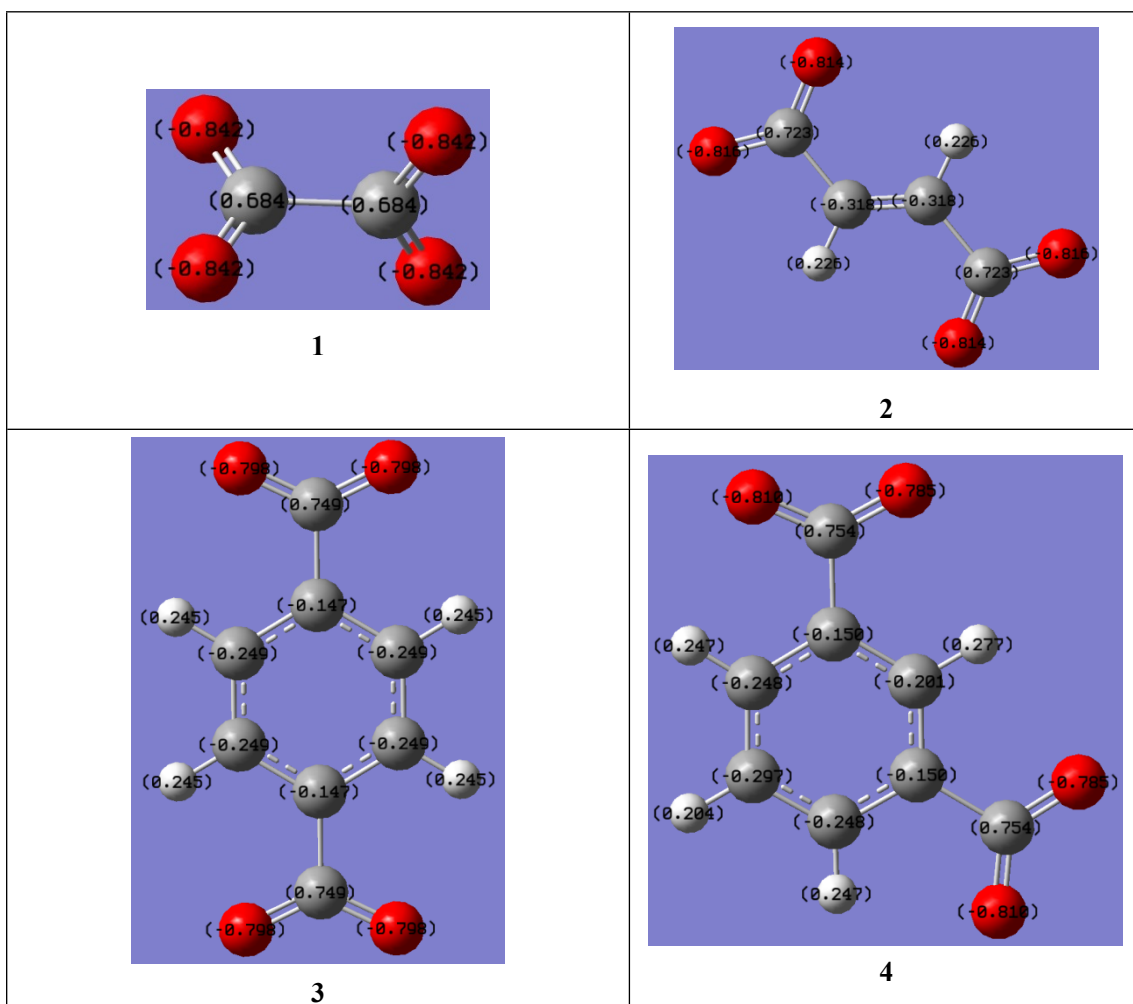
```
nboBDC
```

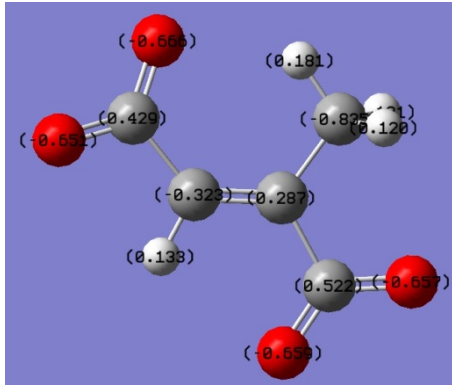
```
-2 1
```

6	-0.700019	-1.199425	0.000014
6	0.700017	-1.199444	0.000061
6	1.430691	-0.000013	0.000080
6	0.700006	1.199424	0.000054
6	-0.700031	1.199444	0.000014
6	-1.430700	0.000013	-0.000009
1	-1.262233	-2.129660	-0.000006
1	1.262226	-2.129679	0.000080

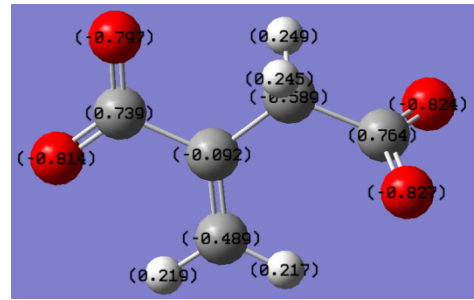
1	1.262218	2.129659	0.000070
1	-1.262241	2.129679	-0.000002
6	2.977795	-0.000001	0.000129
8	3.538983	1.134412	-0.000124
8	3.539111	-1.134359	-0.000135
6	-2.977795	-0.000001	-0.000058
8	-3.538970	-1.134418	0.000061
8	-3.539093	1.134367	-0.000032

### NBO Charges of all the ligands

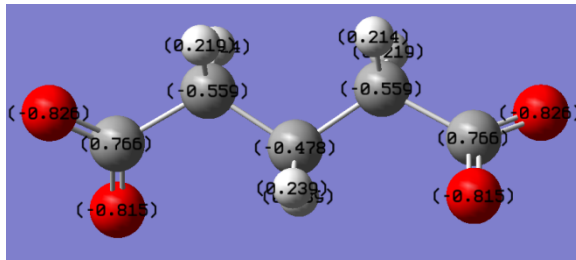




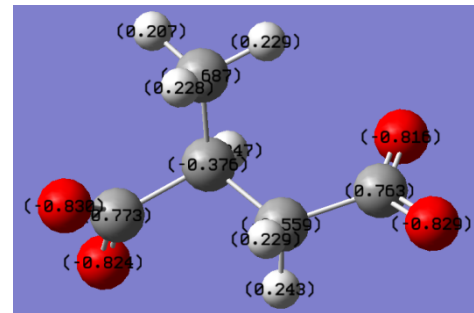
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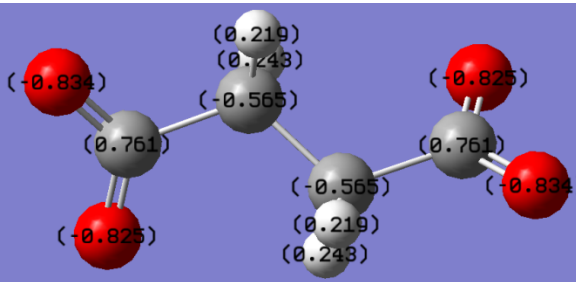
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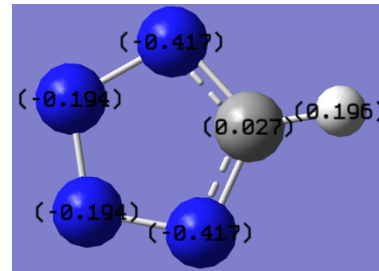
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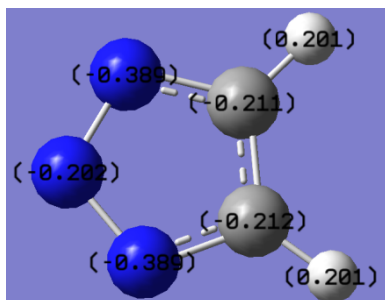
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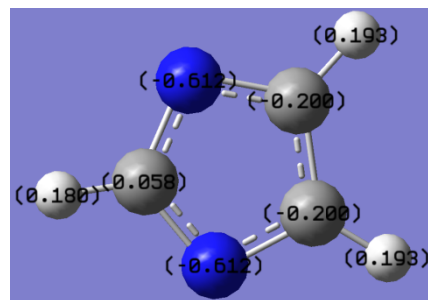
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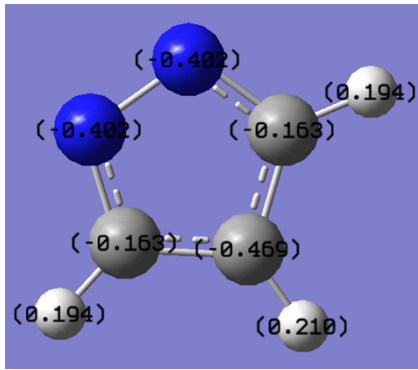
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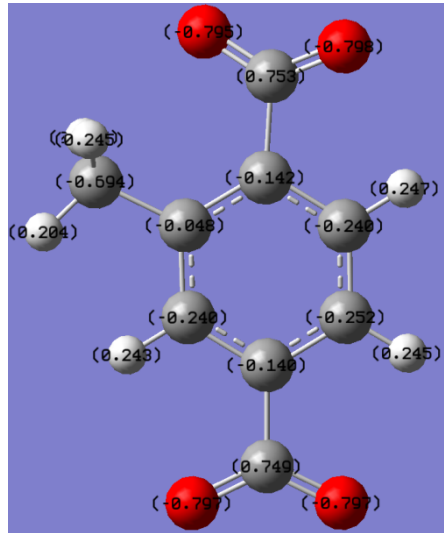
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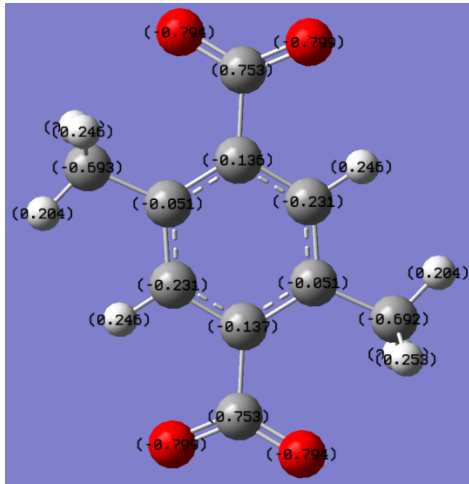
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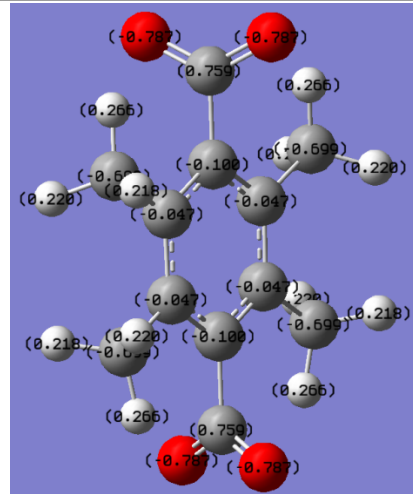
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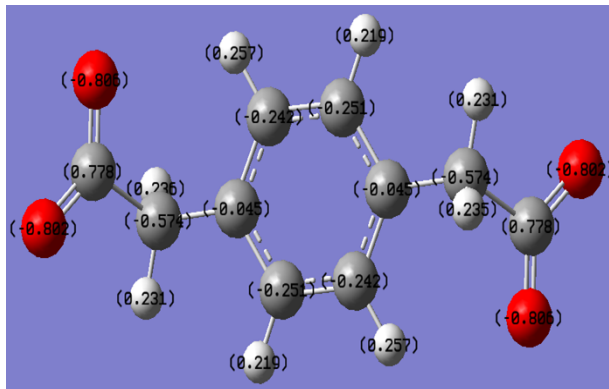
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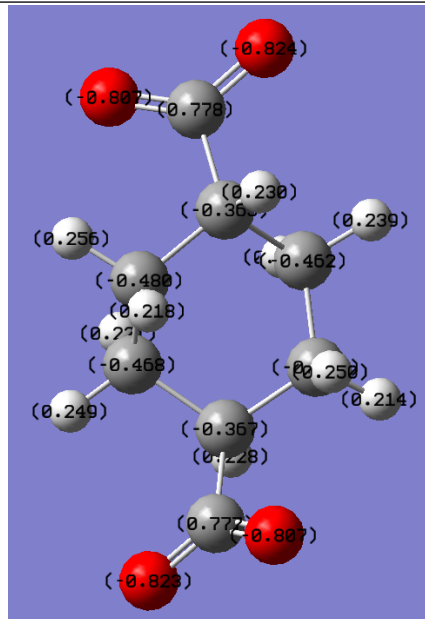
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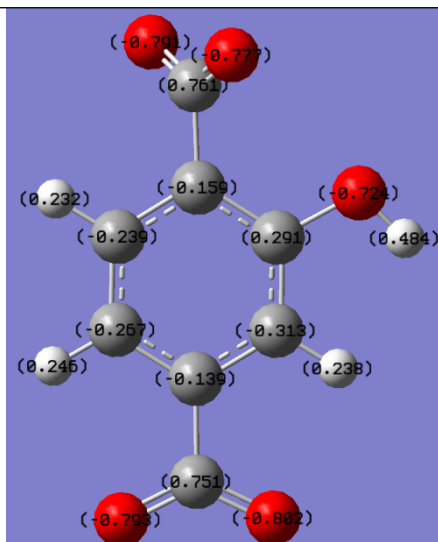
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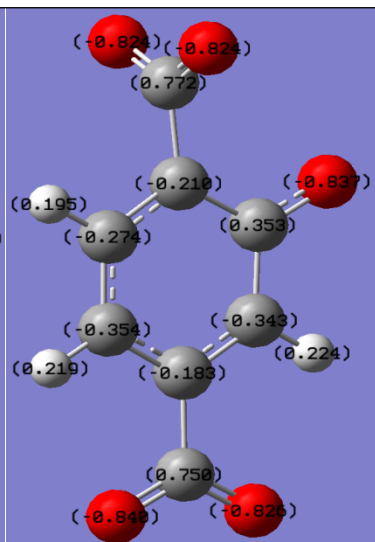
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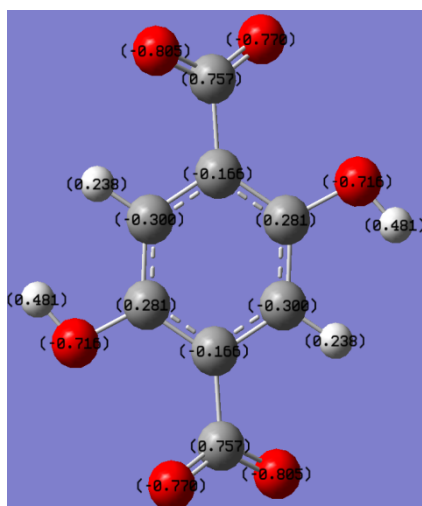
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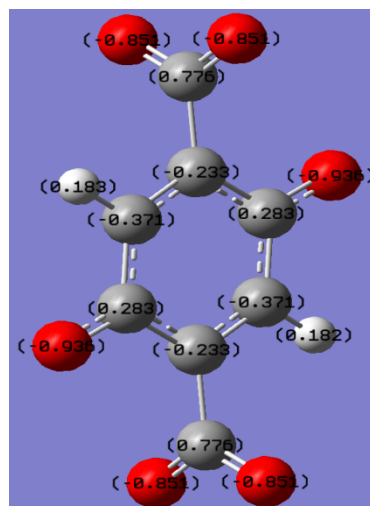
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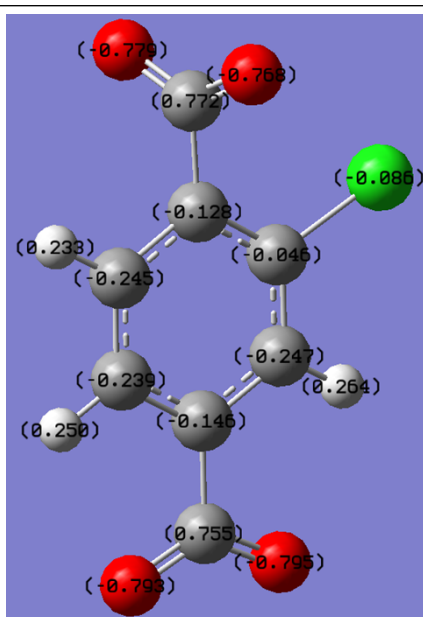
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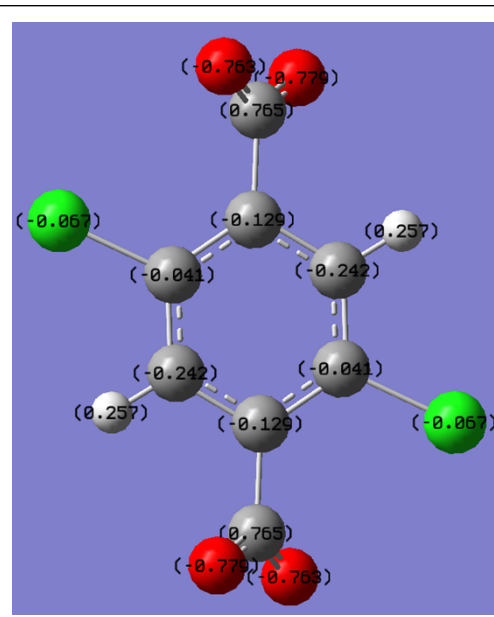
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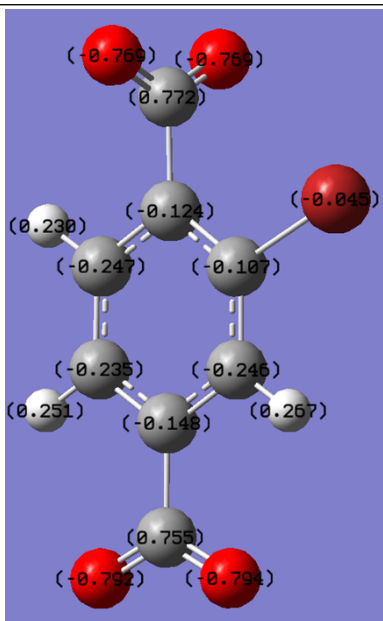
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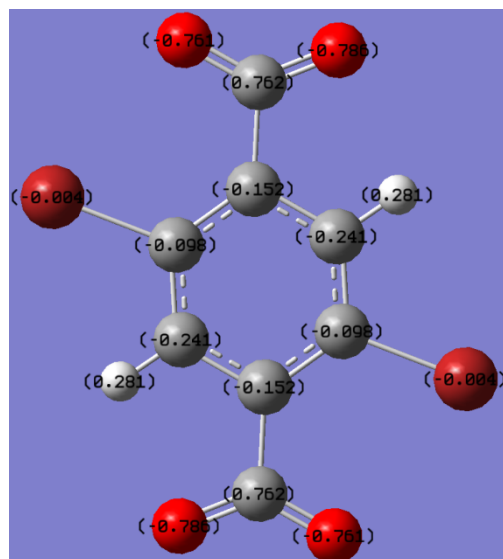
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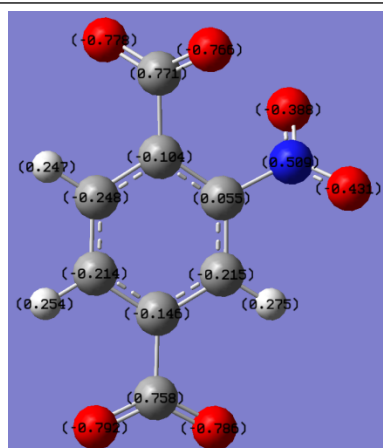
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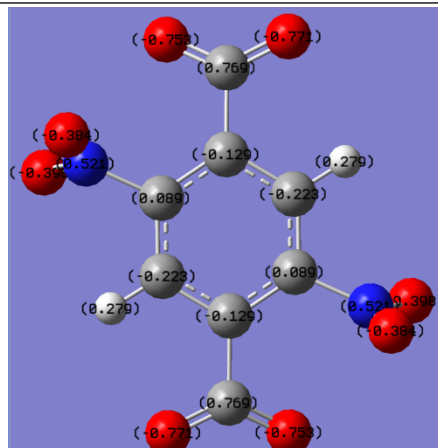
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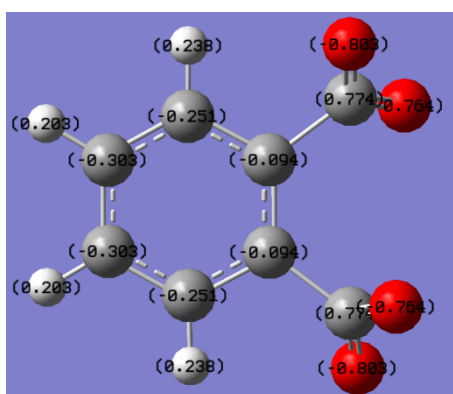
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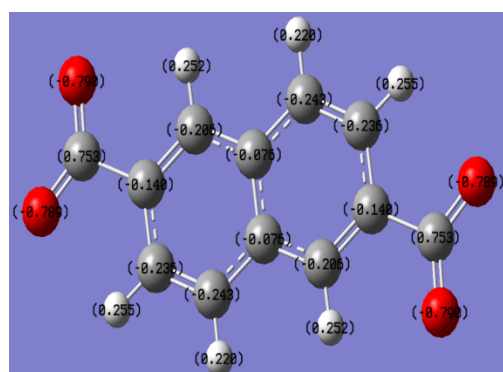
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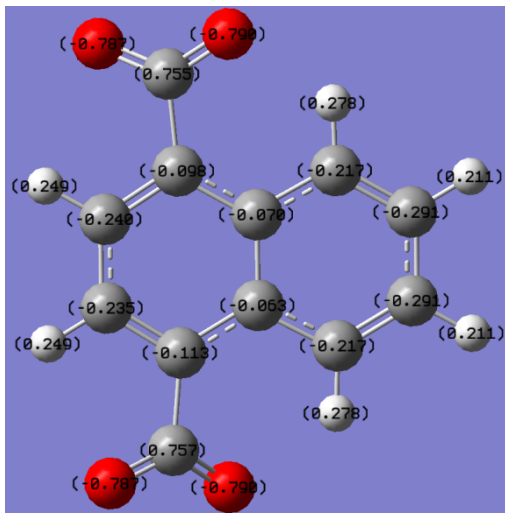


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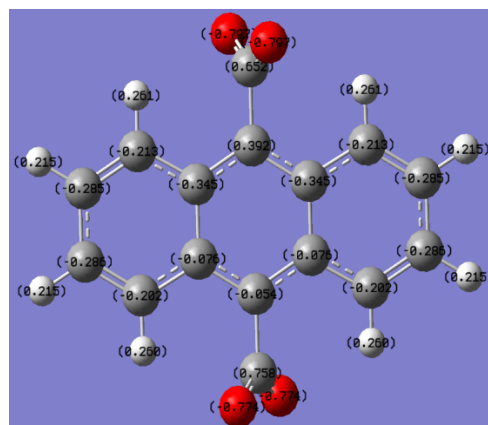


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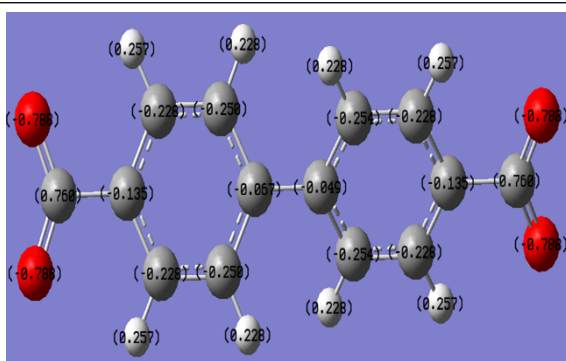




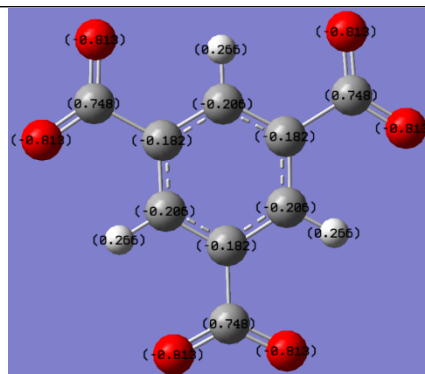
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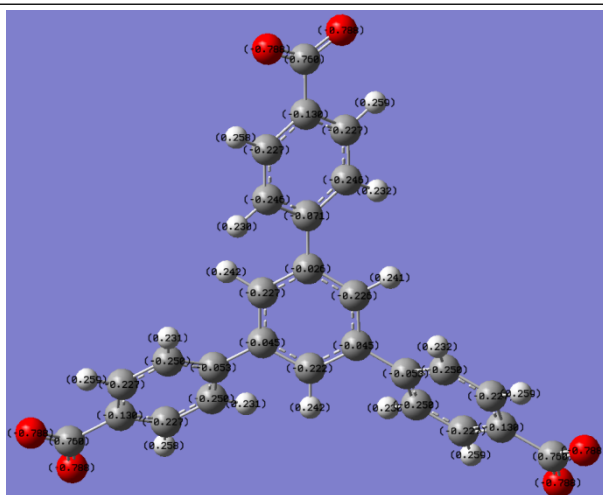
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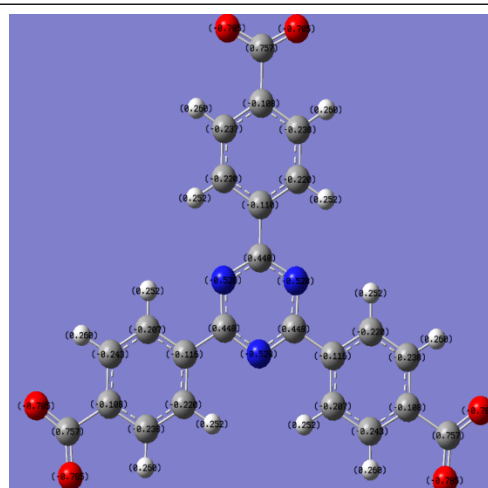
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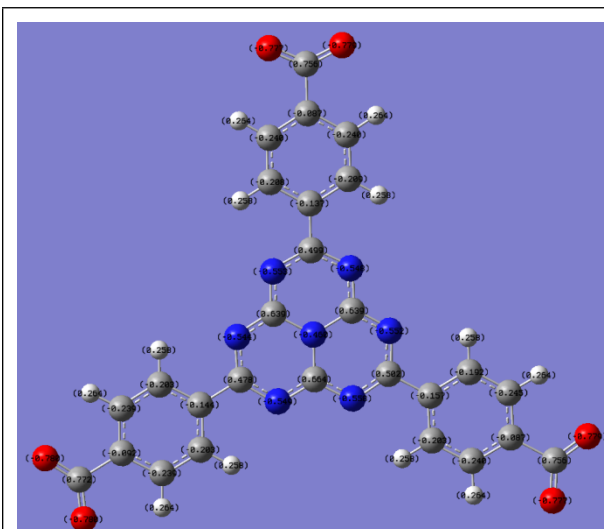
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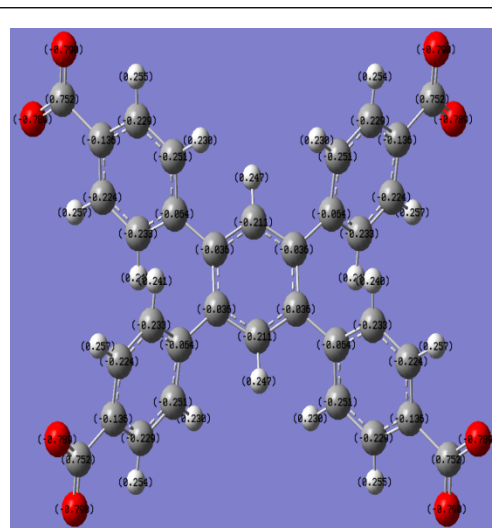
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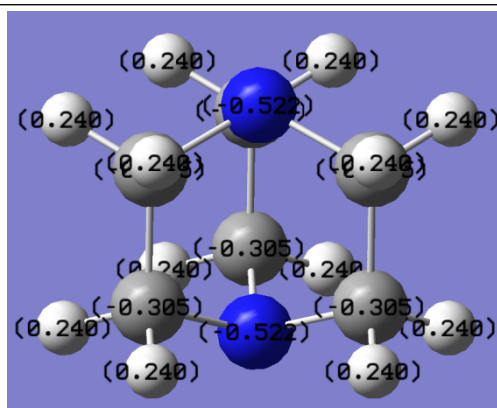
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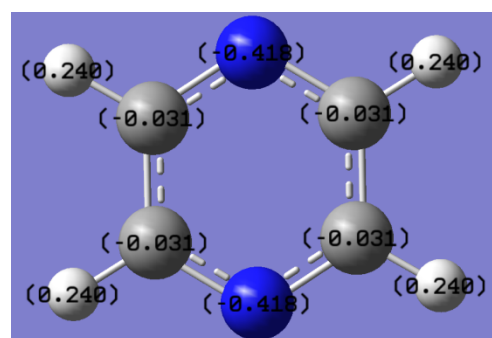
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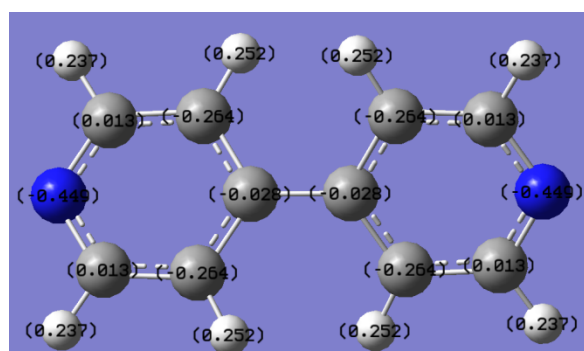
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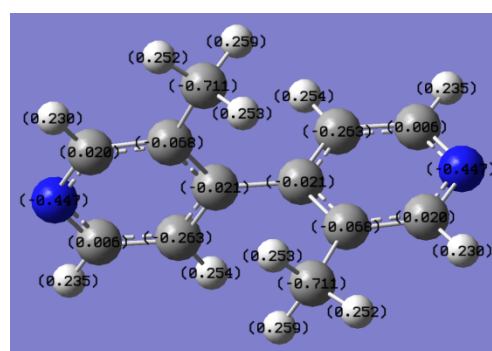
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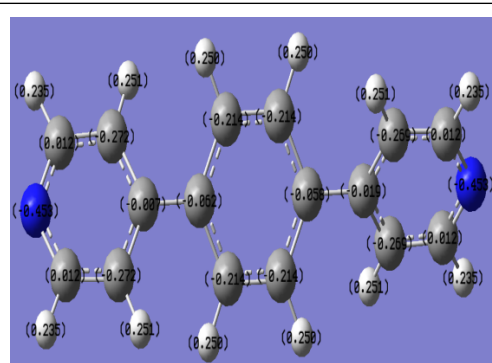
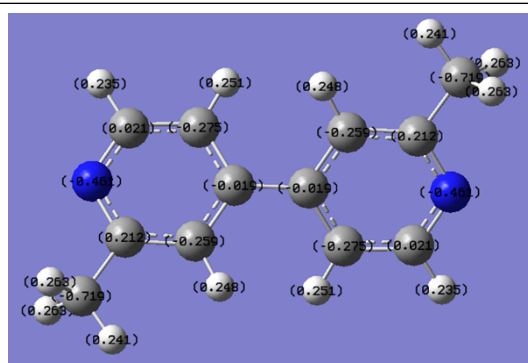
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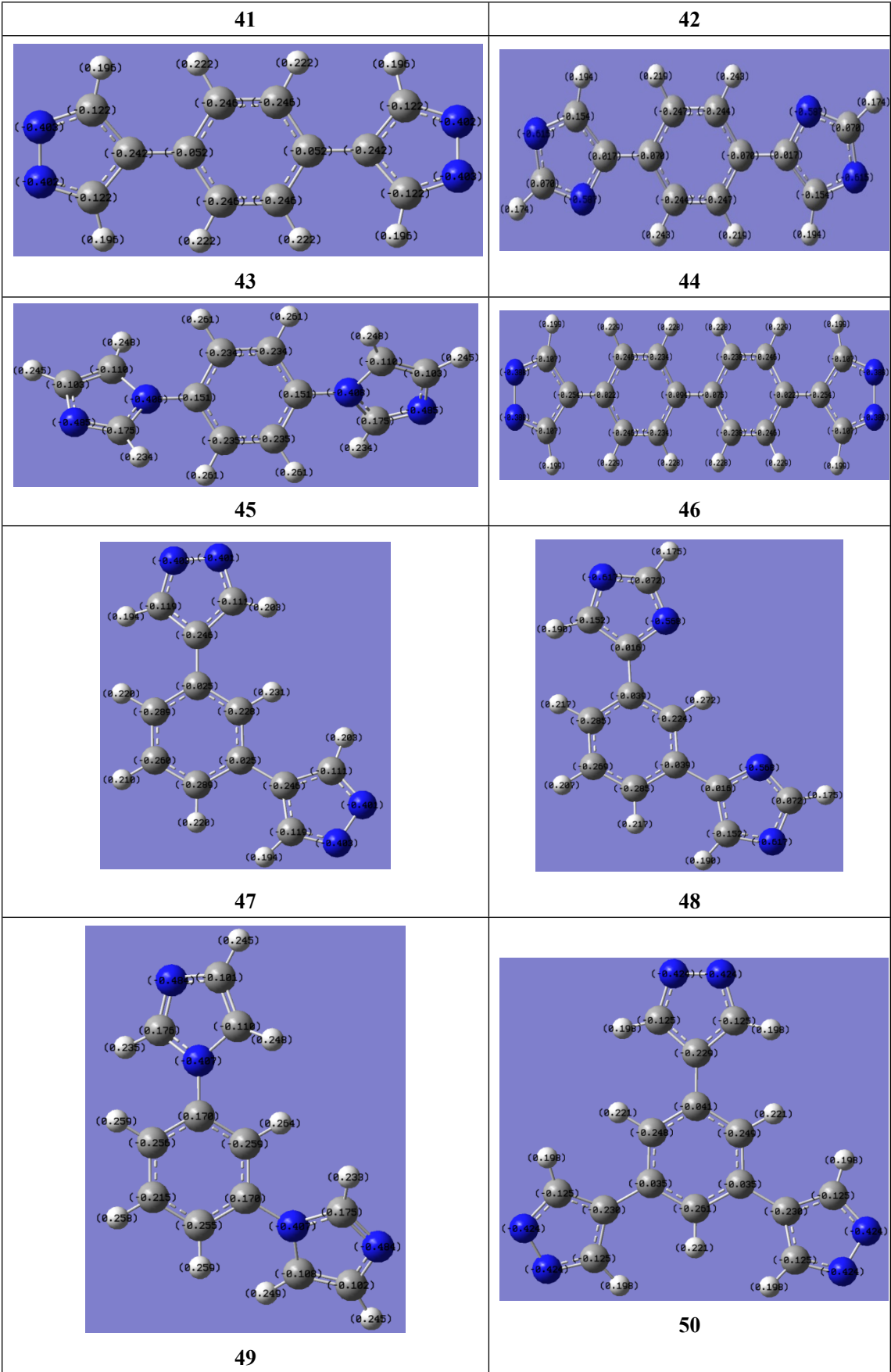


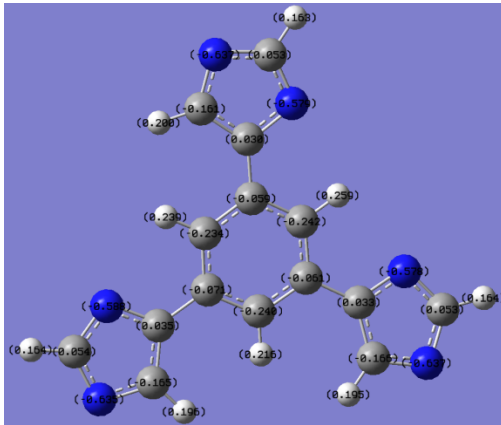
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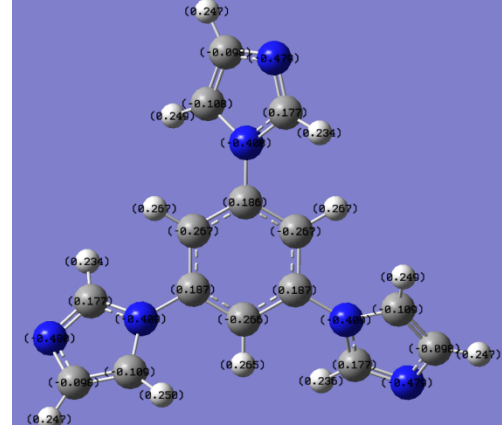
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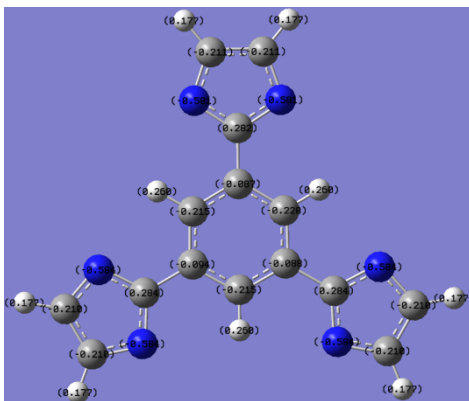




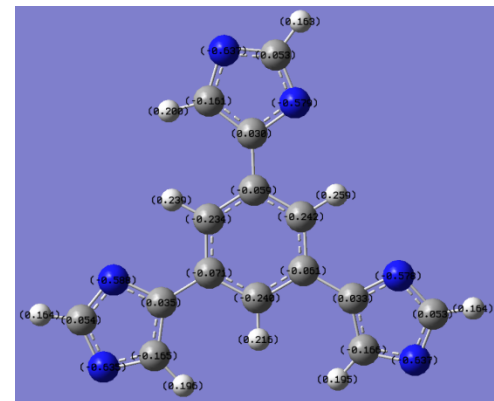
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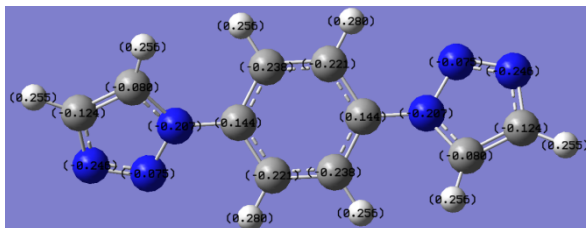
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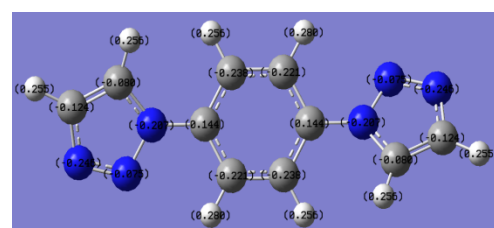
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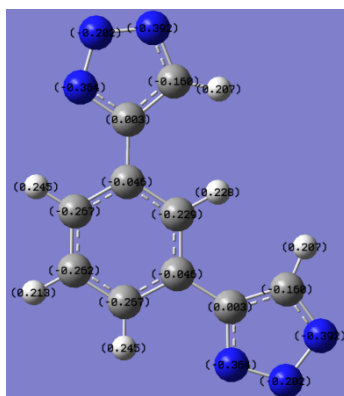
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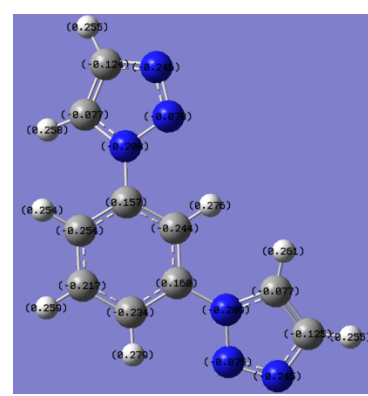
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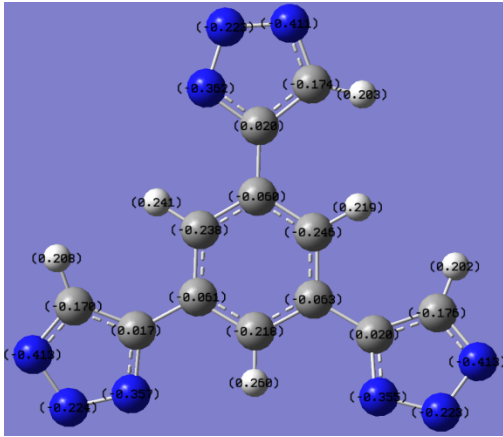
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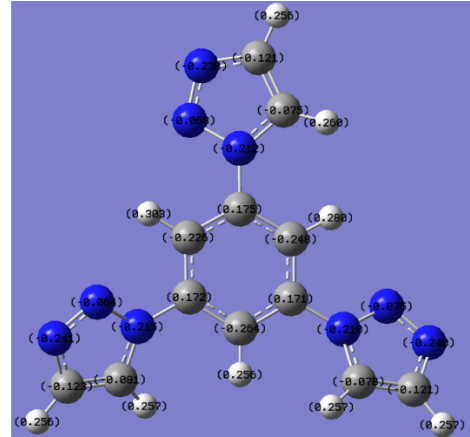
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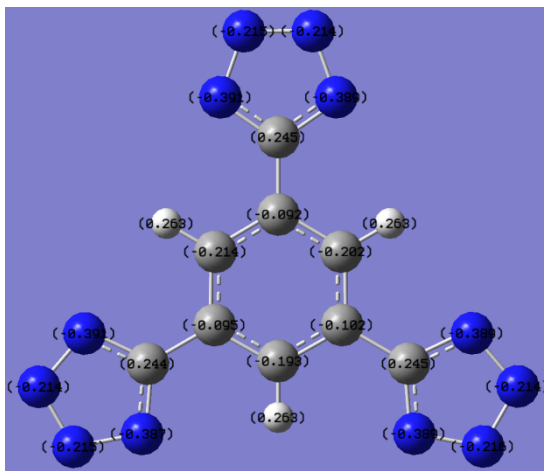
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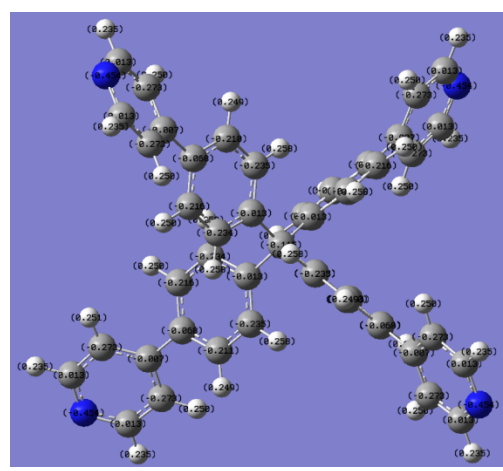
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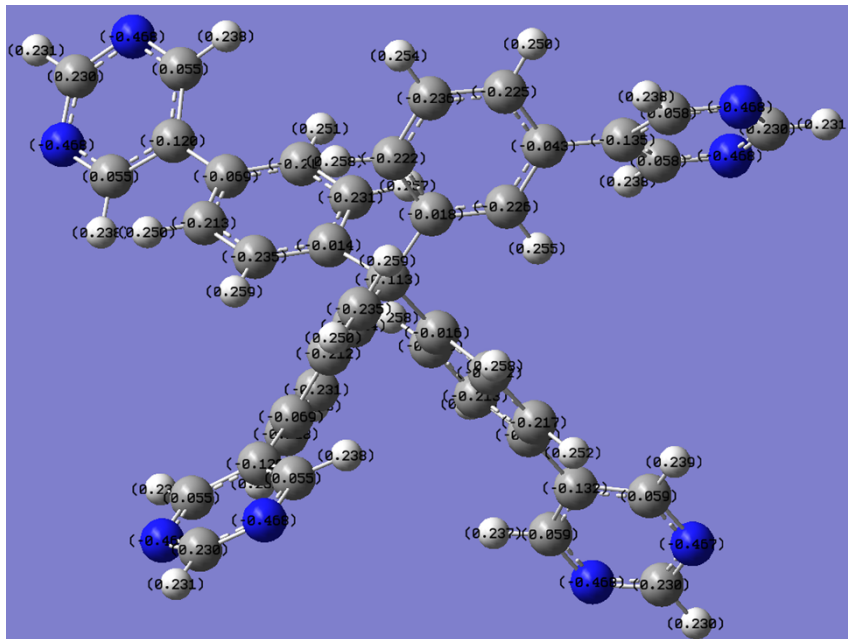
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