Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Photoemission from non-polar aromatic molecules in the gas and liquid phase.

Supplementay Information

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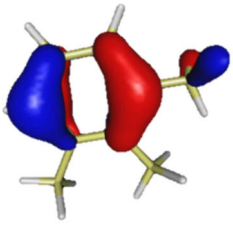
We report the molecular orbital analysis for the three isomers 1,2,3- , 1,2,4- and 1,3,5-trimethylbenzene. In Table SI.1 are summarized the calculated binding energies for the gas phase molecular orbitals, which are showed herein.

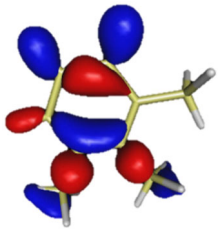
	1,2,3-trimethylbenzene		1,2,4-trimethylbenzene		1,3,5-trimethylbenzene	
Molecular orbital	Energy	Label	Energy	Label	Energy	Label
HOMO	8.82 eV	6a”	8.60 eV	6a”	8.85 eV	2e”
-1	8.84 eV	5a”	9.09 eV	5a”	8.85 eV	2e”
-2	11.71 eV	18a’	11.76 eV	18a’	11.88 eV	6e’
-3	11.80 eV	17a’	11.87 eV	17a’	11.88 eV	6e’
-4	12.36 eV	4a”	12.23 eV	4a”	12.12 eV	2a”
-5	12.93 eV	16a’	12.96 eV	16a’	12.70 eV	6a’
-6	13.73 eV	15a’	13.48 eV	15a’	13.85 eV	5e’
-7	13.93 eV	14a’	13.70 eV	14a’	13.85 eV	5e’
-8	13.96 eV	13a’	14.14 eV	13a’	14.15 eV	4e’
-9	14.29 eV	3a”	14.39 eV	3a”	14.15 eV	4e’
-10	14.29 eV	12a’	14.41 eV	12a’	14.72 eV	1e”
-11	14.77 eV	2a”	14.81 eV	2a”	14.72 eV	1e”
-12	15.07 eV	11a’	15.32 eV	11a’	15.01 eV	5a’
-13	15.65 eV	1a”	15.47 eV	1a”	15.28 eV	1a”
-14	16.68 eV	10a’	16.46 eV	10a’	16.47 eV	4a’
-15	16.78 eV	9a’	16.62 eV	9a’	16.83 eV	3a’

Table SI.1. Calculated gas-phase binding energies of the molecular orbitals for the three isomers of trimethylbenzene.

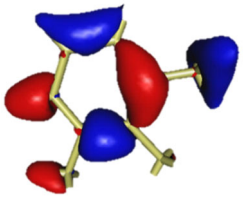
1,2,3-trimethylbenzene – symmetry C_s



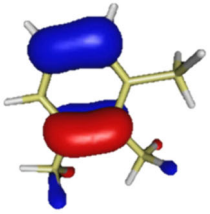
8.82 eV
(HOMO)
a’’



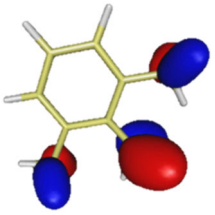
13.96 eV
a’



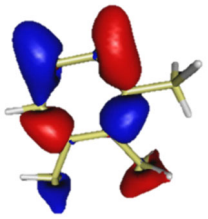
18.94 eV
a’



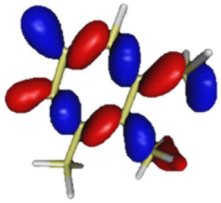
8.84 eV
a’’



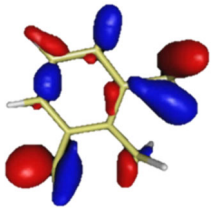
14.29 eV
a’’



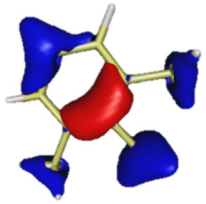
19.01 eV
a’



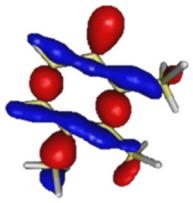
11.71 eV
a’



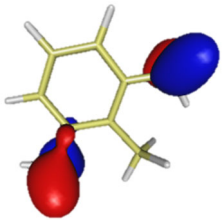
14.29 eV
a’



21.83 eV
a’



11.80 eV
a’



14.77 eV
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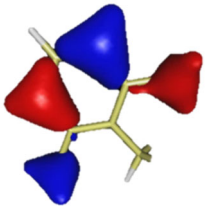
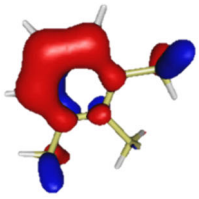
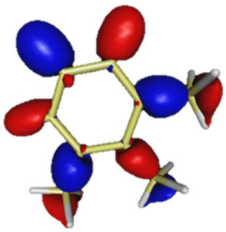


22.09 eV
a’

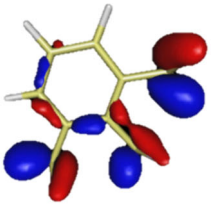


12.36 eV
a’’

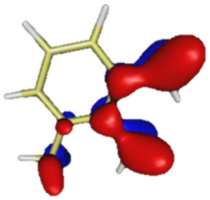


15.07 eV
a’

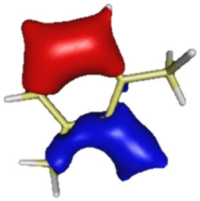
23.44 eV
a’



12.93 eV
a’



15.65 eV
a’’



25.10 eV
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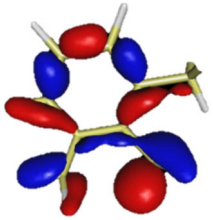
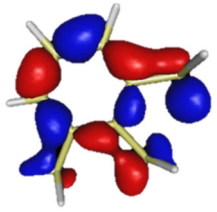


13.73 eV
a’



16.68 eV
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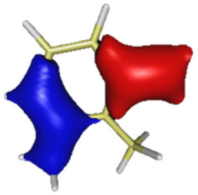
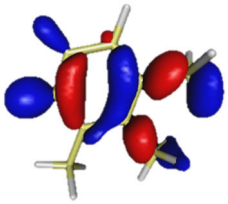
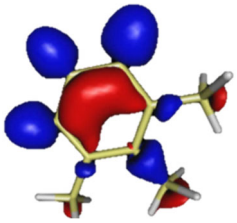


25.44 eV
a’



13.93 eV
a’



16.74 eV
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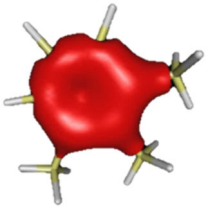
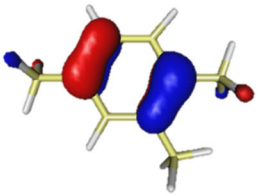
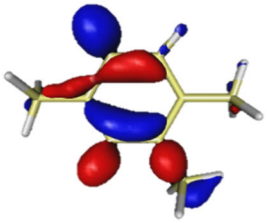


27.50 eV
a’

1,2,4-trimethylbenzene – symmetry C_s



8.60 eV
(HOMO)
a''



14.14 eV
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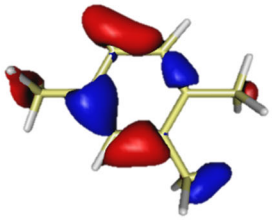
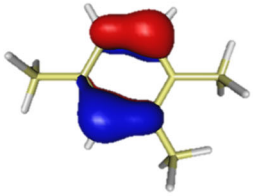


18.49 eV
a'



9.09 eV
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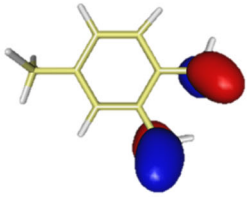

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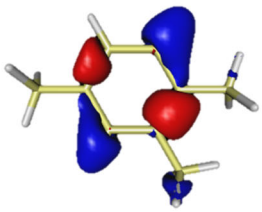

19.79 eV
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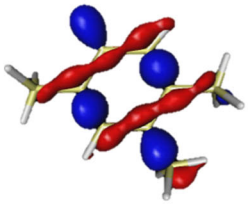

11.76 eV
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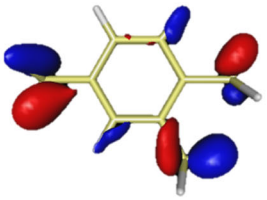

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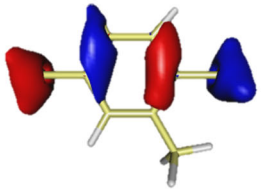

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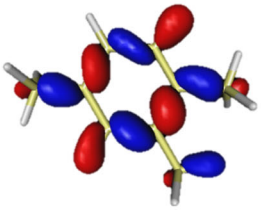

11.87 eV
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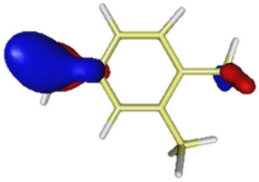

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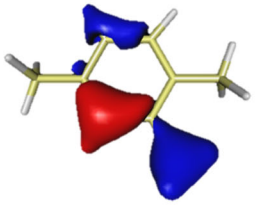

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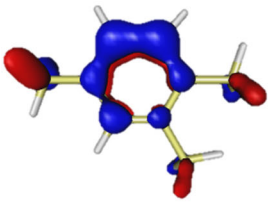

12.23 eV
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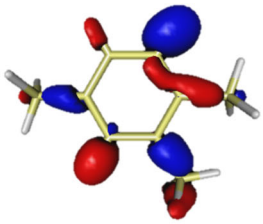

15.32 eV
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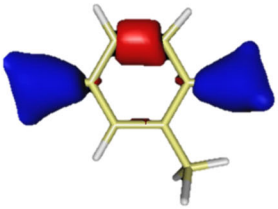

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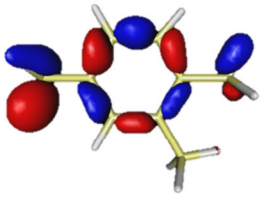

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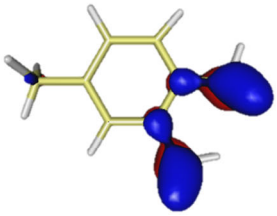

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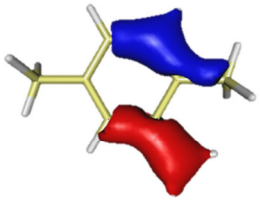

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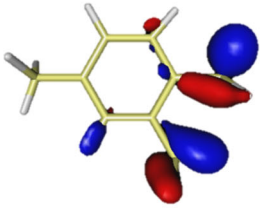

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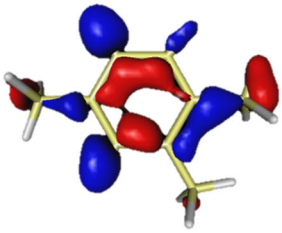

16.46 eV
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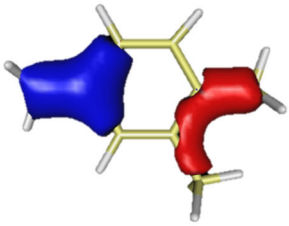

25.71 eV
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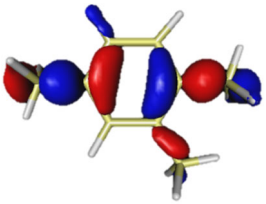

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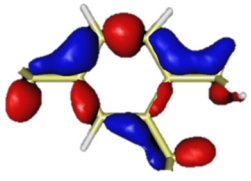
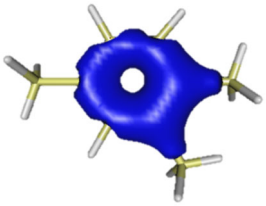
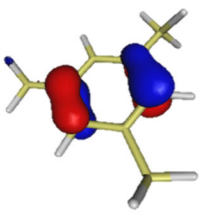


16.62 eV
a'

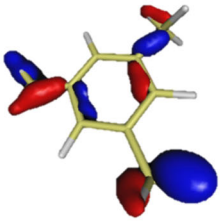


27.42 eV
a'

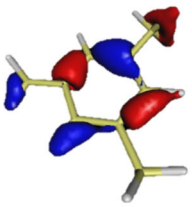
1,3,5-trimethylbenzene – symmetry C_{3h}



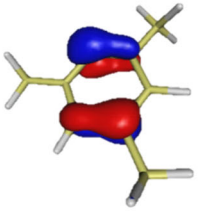
8.85 eV
(HOMO)
e’’



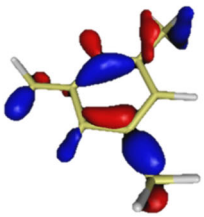
14.15 eV
e’



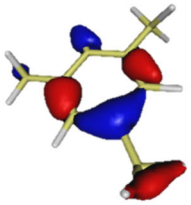
18.90 eV
e’



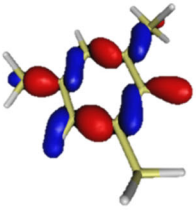
8.85 eV
e’’



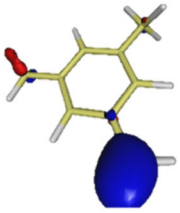
14.15 eV
e’



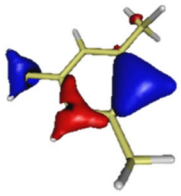
18.90 eV
e’



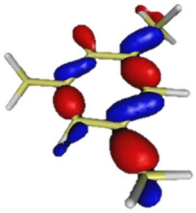
11.88 eV
e’



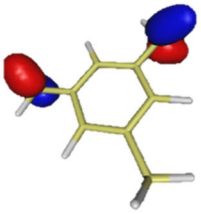
14.72 eV
e’’



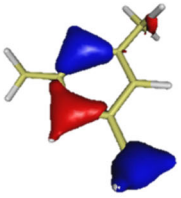
22.13 eV
e’



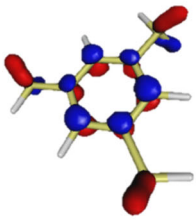
11.88 eV
e’



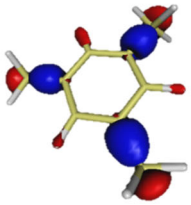
14.72 eV
e’’



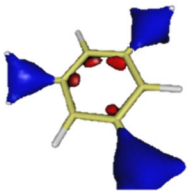
22.13 eV
e’



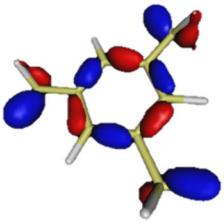
12.12 eV
a’’



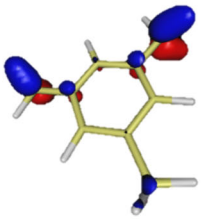
15.01 eV
a’



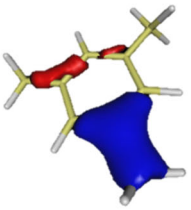
22.94 eV
a’



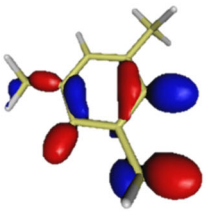
12.70 eV
a’



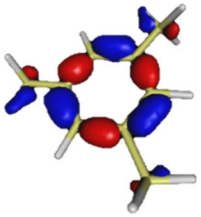
15.28 eV
a’’



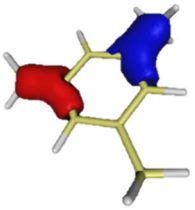
25.37 eV
e’



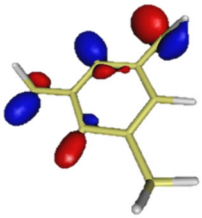
13.85 eV
e’



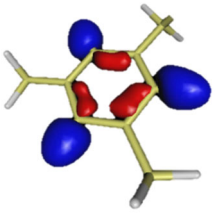
16.47 eV
a’



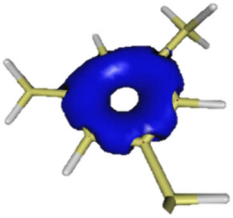
25.37 eV
e’



13.85 eV
e’



16.83 eV
a’



27.37 eV
a’