Supplementary Information for the article “**Intermolecular interactions, spectroscopic and theoretical investigation of 4-aminoacetophenone”** by Mariana Rocha1, Alejandro Di Santo1, Aída Ben Altabef1,+ and Diego M. Gil1,+,\*

**Figure S1:** Dipolar moment vector for PAAP at B3LYP/6-311++G(d,p) level.

Dipole moment.tif

**Figure S2:** Optimized molecular structure of a dimer structure of PAAP calculated at B3LYP/6-311++G(d,p) level of theory.

Dimero-Opt.tif

**Figure S3:** Molecular graph of 4-aminoacetophenone molecule calculated at B3LYP/6-311++G(d,p) approximation using AIM program.

Figure S1.tif

**Figure S4:** AIM Molecular graph of a dimer structure of PAAP.

aim-dimer.tif

**Figure S5:** MEP plot for PAAP computed at B3LYP/6-311++G(d,p) approximation.

Figure 4.tif

**Table S1:** Total atomic charges obtained using NPA approach, computed at B3LYP/6-311++G(d,p) approximation.

Atom Charge Core Valence Rydberg Total

C 1 0.19235 1.99902 3.78912 0.01951 5.80765

C 2 -0.25969 1.99907 4.24388 0.01674 6.25969

C 3 -0.14718 1.99911 4.13301 0.01507 6.14718

C 4 -0.19476 1.99893 4.17739 0.01844 6.19476

C 5 -0.12543 1.99909 4.10808 0.01825 6.12543

C 6 -0.25319 1.99906 4.23786 0.01628 6.25319

H 7 0.20073 0.00000 0.79635 0.00291 0.79927

H 8 0.20613 0.00000 0.79202 0.00185 0.79387

H 9 0.22933 0.00000 0.76841 0.00226 0.77067

H 10 0.20234 0.00000 0.79566 0.00200 0.79766

N 11 -0.77692 1.99942 5.76162 0.01588 7.77692

H 12 0.37787 0.00000 0.61970 0.00243 0.62213

H 13 0.37851 0.00000 0.61899 0.00250 0.62149

C 14 0.55170 1.99928 3.40942 0.03960 5.44830

O 15 -0.57498 1.99976 6.56121 0.01400 8.57498

C 16 -0.66687 1.99926 4.65932 0.00828 6.66687

H 17 0.22719 0.00000 0.77057 0.00225 0.77281

H 18 0.21628 0.00000 0.78187 0.00185 0.78372

H 19 0.21659 0.00000 0.78156 0.00185 0.78341

**Table S2:** Enrichment ratios Exy of the main intermolecular interactions of PAAP.

|  |  |
| --- | --- |
| Interaction | Enrichment Ratio |
| H···H  C···H  N···H  O···H | 0.87  1.34  1.36  1.30 |