

甲烷与含氮有机杂环化合物吸附作用的 DFT 研究

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A DFT Study of Methane Adsorption on Nitrogen-Containing Organic Heterocycles

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Table 1S The Mulliken charge (e) of N-containing compounds-CH₄ complexes

| Atom | Configuration | | | | | |
|------|---------------|----------|----------|-----------|-----------|----------|
| | 1 | 2 | 3 | 4 | 5 | 6 |
| 1 | -0.055 | 0.072 | -0.064 | -0.283 | 0.186 | 0.013 |
| 2 | -0.080 | -0.305 | 0.055 | 0.047 | -0.299 | 0.008 |
| 3 | 0.052 | 0.168 | -0.201 | 0.045 | 0.186 | -0.274 |
| 4 | -0.315 | -0.311 | -0.192 | -0.288 | -0.303 | 0.155 |
| 5 | 0.054 | 0.073 | 0.057 | 0.048 | 0.186 | -0.342 |
| 6 | -0.081 | -0.090 | -0.064 | 0.046 | -0.299 | 0.049 |
| 7 | 0.066 | 0.072 | 0.075 | 0.071 | 0.081 | 0.056 |
| 8 | 0.065 | 0.079 | 0.085 | 0.076 | 0.085 | 0.185 |
| 9 | 0.064 | 0.072 | 0.080 | 0.071 | 0.081 | 0.059 |
| 10 | 0.069 | 0.073 | 0.075 | 0.071 | -0.332 | -0.335 |
| 11 | 0.065 | -0.331 | -0.334 | -0.331 | 0.073 | 0.064 |
| 12 | -0.333 | 0.075 | 0.066 | 0.112 | 0.074 | 0.124 |
| 13 | 0.069 | 0.110 | 0.072 | 0.072 | 0.108 | 0.070 |
| 14 | 0.119 | 0.072 | 0.119 | 0.072 | -0.074 | 0.069 |
| 15 | 0.070 | 0.071 | 0.072 | 0.071 | - | - |
| 16 | 0.069 | - | - | - | - | - |
| | 7 | 8 | 9 | 10 | 11 | |
| 1 | -0.225 | 0.029 | -0.090 | 0.307 | 0.202 | |
| 2 | 0.142 | -0.311 | -0.099 | -0.377 | -0.164 | |
| 3 | -0.230 | 0.144 | 0.033 | 0.137 | 0.035 | |
| 4 | 0.009 | -0.350 | -0.352 | -0.382 | -0.384 | |
| 5 | -0.096 | 0.330 | 0.308 | 0.322 | 0.304 | |
| 6 | 0.083 | 0.121 | 0.133 | 0.078 | 0.094 | |
| 7 | 0.209 | -0.335 | -0.345 | -0.363 | -0.372 | |
| 8 | -0.343 | 0.176 | 0.171 | 0.160 | 0.160 | |
| 9 | 0.107 | -0.322 | -0.319 | -0.324 | -0.322 | |

| | | | | | |
|----|-------|--------|--------|--------|--------|
| 10 | 0.072 | 0.074 | 0.072 | -0.393 | -0.415 |
| 11 | 0.085 | 0.069 | 0.066 | 0.060 | 0.056 |
| 12 | 0.087 | 0.074 | 0.063 | 0.066 | 0.062 |
| 13 | - | 0.203 | 0.068 | 0.199 | 0.195 |
| 14 | - | -0.345 | 0.198 | 0.198 | 0.187 |
| 15 | - | 0.062 | -0.345 | 0.210 | 0.209 |
| 16 | - | 0.079 | 0.060 | -0.349 | 0.053 |
| 17 | - | 0.082 | 0.077 | 0.064 | -0.351 |
| 18 | - | 0.120 | 0.078 | 0.080 | 0.128 |
| 19 | - | - | 0.125 | 0.082 | 0.080 |
| 20 | - | - | - | 0.125 | 0.063 |
| 21 | - | - | - | - | 0.079 |

Atom coordinates in initiative N-containing compounds-CH4 complexes

| Atom | Configuration | | | | | | | | |
|------|---------------|----------|----------|----------|----------|----------|----------|----------|----------|
| | 1 | | | 2 | | | 3 | | |
| | x | y | z | x | y | z | x | y | z |
| 1 | -0.95876 | -0.41886 | -0.40935 | -1.23210 | 0.72115 | -0.00187 | -0.96665 | -0.76231 | 0.00454 |
| 2 | 0.22246 | -0.40586 | -1.15192 | -0.00531 | 1.26716 | -0.01257 | 0.24196 | -0.05853 | 0.00430 |
| 3 | 1.42558 | -0.14750 | -0.48832 | 0.03087 | 2.60848 | -0.02095 | 0.32730 | 1.28020 | -0.00113 |
| 4 | 1.51411 | 0.09331 | 0.82980 | -1.01177 | 3.45286 | -0.01846 | -0.79401 | 2.00987 | -0.00416 |
| 5 | 0.36758 | 0.07756 | 1.52885 | -2.22471 | 2.87735 | -0.00689 | -1.98098 | 1.38340 | -0.00181 |
| 6 | -0.88550 | -0.17161 | 0.96307 | -2.39352 | 1.49283 | 0.00069 | -2.12991 | -0.00690 | 0.00160 |
| 7 | -1.91763 | -0.61698 | -0.89067 | -1.27744 | -0.37135 | 0.00528 | -0.98110 | -1.85233 | 0.00649 |
| 8 | 0.21811 | -0.59373 | -2.22618 | 1.02208 | 3.06844 | -0.02988 | 1.20470 | -0.57396 | 0.00788 |
| 9 | 2.36938 | -0.13309 | -1.04016 | -3.08392 | 3.55305 | -0.00328 | -2.84775 | 2.04741 | -0.00321 |
| 10 | 0.45819 | 0.27529 | 2.60098 | -3.38327 | 1.03661 | 0.00796 | -3.11905 | -0.46573 | 0.00099 |
| 11 | -1.77995 | -0.16985 | 1.58701 | 1.89581 | 6.08266 | 0.15276 | 4.16696 | 0.57551 | -0.00267 |
| 12 | 2.32858 | 0.57018 | 3.47021 | 2.57626 | 5.22264 | 0.15232 | 4.00865 | -0.50949 | -0.05275 |
| 13 | 2.61993 | 1.52751 | 3.92350 | 0.86325 | 5.73999 | 0.01437 | 4.79994 | 0.88550 | -0.84264 |
| 14 | 2.65705 | 0.54445 | 2.42481 | 1.98206 | 6.60929 | 1.11138 | 3.20436 | 1.09948 | -0.05461 |
| 15 | 2.80036 | -0.25329 | 4.02385 | 2.17280 | 6.76207 | -0.66310 | 4.66688 | 0.82277 | 0.94186 |
| 16 | 1.23699 | 0.46205 | 3.51590 | - | - | - | - | - | - |
| Atom | 4 | | | 5 | | | 6 | | |
| | x | y | z | x | y | z | x | y | z |
| 1 | -0.56717 | 0.60078 | -0.00564 | -1.44914 | 0.14023 | -0.00104 | -2.05657 | 1.24889 | 0.07926 |
| 2 | 0.56489 | 1.32008 | -0.00564 | -0.88377 | -1.07582 | 0.00396 | -1.77565 | -0.09828 | 0.07926 |
| 3 | 0.55875 | 2.71886 | -0.00564 | 0.45720 | -1.05139 | 0.00923 | -0.39648 | -0.17672 | 0.07926 |
| 4 | -0.57941 | 3.42840 | -0.00564 | 1.22715 | 0.04698 | 0.00975 | 0.08545 | 1.10610 | 0.07926 |
| 5 | -1.71147 | 2.70911 | -0.00564 | 0.53550 | 1.19567 | 0.00381 | -0.89513 | 1.99211 | 0.07926 |
| 6 | -1.70533 | 1.31032 | -0.00564 | -0.80022 | 1.31445 | -0.00173 | -3.03192 | 1.72588 | 0.07926 |
| 7 | 1.50603 | 0.76407 | -0.00564 | -2.54165 | 0.17776 | -0.00500 | -2.40396 | -0.98146 | 0.07926 |
| 8 | 1.49489 | 3.28313 | -0.00564 | 0.97252 | -2.01552 | 0.01353 | 0.15253 | -1.02931 | 0.07926 |
| 9 | -2.65261 | 3.26511 | -0.00564 | 1.11425 | 2.12293 | 0.00301 | 1.14864 | 1.32771 | 0.07926 |
| 10 | -2.64148 | 0.74605 | -0.00564 | 4.17948 | -2.55880 | -0.03959 | 1.78914 | 4.13287 | -0.06519 |
| 11 | 1.85354 | 5.85995 | -0.12677 | 3.42386 | -3.35517 | -0.05521 | 2.24922 | 3.13739 | -0.05732 |
| 12 | 0.77999 | 5.64385 | -0.06742 | 4.77055 | -2.60440 | -0.96187 | 0.69932 | 4.03431 | -0.13791 |
| 13 | 2.10448 | 6.20466 | -1.13718 | 3.68800 | -1.58069 | 0.03342 | 2.04795 | 4.66323 | 0.85995 |
| 14 | 2.11081 | 6.64011 | 0.60076 | 4.83879 | -2.70620 | 0.82409 | 2.16203 | 4.69988 | -0.92598 |
| 15 | 2.42147 | 4.95013 | 0.09944 | - | - | - | - | - | - |
| Atom | 7 | | | 8 | | | 9 | | |
| | x | y | z | x | y | z | x | y | z |
| 1 | -1.59042 | 2.55751 | -0.02100 | 0.42525 | -1.14284 | -0.10678 | 0.59695 | -1.13256 | 0.04021 |
| 2 | -1.11637 | 1.28393 | -0.02100 | 1.59328 | -0.38048 | -0.06599 | 1.73768 | -0.42754 | 0.04021 |
| 3 | 0.21748 | 1.22242 | -0.02100 | 1.53176 | 1.02414 | 0.02183 | 1.65118 | 0.91942 | 0.04021 |
| 4 | 0.51630 | 2.51873 | -0.02100 | 0.39120 | 1.73432 | 0.06558 | 0.54314 | 1.68158 | 0.04021 |
| 5 | -0.53470 | 3.34303 | -0.02100 | -0.70396 | 0.97840 | 0.01947 | -0.56610 | 0.94439 | 0.04021 |

| | | | | | | | | | |
|----|----------|---------|----------|----------|----------|----------|----------|----------|----------|
| 6 | -1.75011 | 0.40430 | -0.02100 | -0.78082 | -0.43656 | -0.06338 | -0.63304 | -0.46983 | 0.04021 |
| 7 | 1.47365 | 2.86185 | -0.02100 | -2.10276 | -0.85353 | -0.08762 | -1.95108 | -0.90223 | 0.04021 |
| 8 | 3.84165 | 1.47933 | 0.24622 | -2.79846 | 0.26305 | -0.02486 | -2.65241 | 0.20967 | 0.04021 |
| 9 | 2.98713 | 0.81865 | 0.05644 | -2.02117 | 1.40041 | 0.04253 | -1.88076 | 1.35910 | 0.04021 |
| 10 | 3.57774 | 2.50923 | -0.02281 | 0.44227 | -2.23070 | -0.17347 | 0.66995 | -2.22309 | 0.04021 |
| 11 | 4.10922 | 1.43571 | 1.30953 | 2.56993 | -0.86345 | -0.09741 | 2.60140 | 1.45735 | 0.04021 |
| 12 | 4.69614 | 1.15251 | -0.35762 | 2.45418 | 1.60720 | 0.05848 | -3.73814 | 0.26030 | 0.04021 |
| 13 | - | - | - | -3.88413 | 0.31812 | -0.02266 | -2.20321 | 2.32170 | 0.04021 |
| 14 | - | - | - | -2.32972 | 2.36655 | 0.09486 | -0.99465 | 4.67707 | -0.17725 |
| 15 | - | - | - | -1.10931 | 5.20059 | 0.17601 | -1.79887 | 3.96604 | 0.04726 |
| 16 | - | - | - | -2.16658 | 4.93836 | 0.32003 | -1.14070 | 5.09321 | -1.18136 |
| 17 | - | - | - | -0.99208 | 5.69826 | -0.79445 | -1.00693 | 5.48889 | 0.56095 |
| 18 | - | - | - | -0.80620 | 5.88671 | 0.97663 | -0.02885 | 4.16051 | -0.13378 |
| 19 | - | - | - | -0.48079 | 4.30151 | 0.20593 | - | - | - |

| Atom | 10 | | | 11 | | |
|------|----------|----------|----------|----------|----------|----------|
| | x | y | z | x | y | z |
| 1 | 0.60482 | -1.31908 | -0.12611 | 0.28862 | -0.51114 | -0.08887 |
| 2 | 1.78050 | -0.54558 | -0.09536 | 1.44332 | 0.18334 | -0.04943 |
| 3 | 1.71867 | 0.85505 | -0.01790 | 1.37897 | 1.52567 | 0.04264 |
| 4 | 0.59144 | 1.58980 | 0.02646 | 0.29587 | 2.31701 | 0.09633 |
| 5 | -0.50663 | 0.82743 | -0.00956 | -0.83046 | 1.59090 | 0.05064 |
| 6 | -0.59301 | -0.57581 | -0.08414 | -0.93401 | 0.19482 | -0.03945 |
| 7 | -1.91049 | -1.00120 | -0.11341 | -2.25608 | -0.21704 | -0.06828 |
| 8 | -2.61072 | 0.11457 | -0.05705 | -2.94075 | 0.90595 | 0.00361 |
| 9 | -1.82758 | 1.24685 | 0.00542 | -2.13953 | 2.03042 | 0.07748 |
| 10 | 0.57598 | -2.68964 | -0.15303 | 0.34152 | -1.86786 | -0.14720 |
| 11 | 2.75652 | -1.03234 | -0.12042 | 2.34437 | 2.03619 | 0.07510 |
| 12 | 2.65247 | 1.42144 | 0.00832 | -4.02489 | 0.97902 | 0.00744 |
| 13 | -3.69586 | 0.17210 | -0.06052 | -2.43610 | 2.99863 | 0.14562 |
| 14 | -2.13257 | 2.21340 | 0.07062 | 1.24038 | -2.29147 | -0.34884 |
| 15 | -0.31958 | -3.11000 | -0.38494 | -0.50713 | -2.38082 | -0.35525 |
| 16 | 1.39750 | -3.18227 | -0.48448 | -1.59050 | 5.18261 | -0.00044 |
| 17 | -1.29048 | 4.88931 | 0.30633 | -2.41582 | 4.48707 | 0.19393 |
| 18 | -0.61122 | 4.03370 | 0.19566 | -1.67734 | 5.58191 | -1.01815 |
| 19 | -1.03027 | 5.65389 | -0.43646 | -1.62960 | 6.00815 | 0.72142 |
| 20 | -2.33719 | 4.59246 | 0.14758 | -0.63605 | 4.65366 | 0.10328 |
| 21 | -1.18842 | 5.30735 | 1.31459 | - | - | - |