Supporting information for: Physisorption of bio oil nitrogen compounds onto montmorillonite

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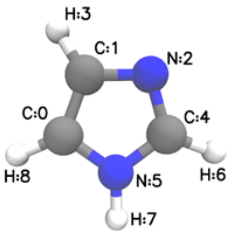
Supporting information

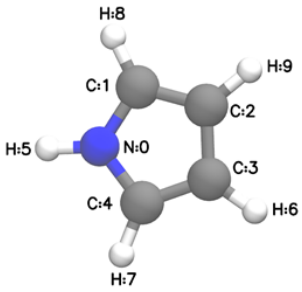
The supporting information consists of partial charge decomposition of the N-heterocycles and fatty acid amides derived from the single point DFT calculations. For further computational details, refer to Section 2.2 of the main article.

Partial charges of N-heterocycles and fatty acid amides

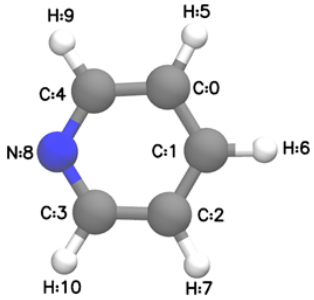
The original Charmm GenFF charges,[1] as well as Hirshfeld,[2] AIM,[3] Merz-Singh-Kollman (MK),[4,5] and ChelpG[6] charges of the studied nitrogen compounds are presented in Figures 1, 2, and 3. The mean, median, and standard deviation of the absolute error for each charge partition scheme compared to Charmm GenFF charges are also presented.



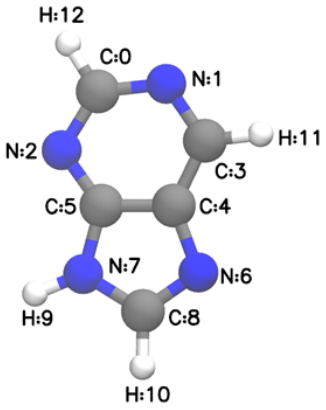
	Charmm GenFF	Hirshfeld	AIM	MK	ChelpG
C:0	-0.048	-0.038	0.355	-0.341	-0.151
C:1	0.225	-0.055	0.401	0.125	0.114
N:2	-0.729	-0.236	-1.168	-0.552	-0.566
H:3	0.102	0.048	0.048	0.106	0.073
C:4	0.277	0.029	1.019	0.141	0.210
N:5	-0.361	-0.039	-1.281	-0.114	-0.215
H:6	0.121	0.064	0.076	0.119	0.087
H:7	0.322	0.165	0.464	0.304	0.315
H:8	0.091	0.062	0.074	0.212	0.134
Error	Average	0.183	0.326	0.122	0.078
	Median	0.157	0.176	0.121	0.067
	SD	0.155	0.307	0.099	0.052



	Charmm GenFF	Hirshfeld	AIM	MK	ChelpG
N:0	-0.359	-0.045	-1.275	-0.150	-0.148
C:1	-0.043	-0.042	0.371	-0.223	-0.181
C:2	-0.262	-0.107	-0.053	-0.207	-0.149
C:3	-0.262	-0.107	-0.053	-0.207	-0.156
C:4	-0.043	-0.042	0.371	-0.224	-0.180
H:5	0.381	0.156	0.451	0.330	0.306
H:6	0.155	0.042	0.033	0.159	0.110
H:7	0.139	0.052	0.056	0.182	0.145
H:8	0.139	0.052	0.056	0.182	0.145
H:9	0.155	0.042	0.033	0.158	0.107
Error	Average	0.125	0.264	0.082	0.089
	Median	0.113	0.165	0.053	0.091
	SD	0.090	0.249	0.073	0.062

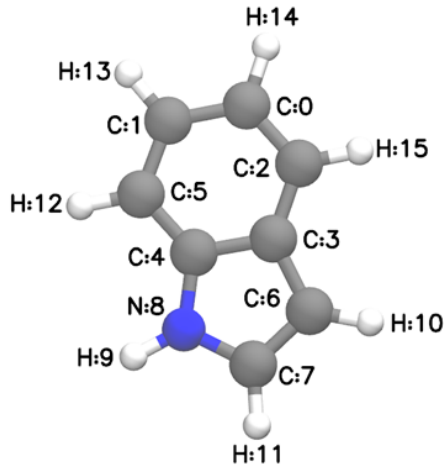


	Charmm GenFF	Hirshfeld	AIM	MK	ChelpG
C:0	-0.116	-0.045	-0.032	-0.508	-0.407
C:1	-0.115	-0.021	-0.017	0.226	0.220
C:2	-0.116	-0.045	-0.032	-0.505	-0.421
C:3	0.181	0.013	0.543	0.454	0.463
C:4	0.181	0.013	0.543	0.452	0.453
H:5	0.115	0.055	0.043	0.199	0.149
H:6	0.115	0.058	0.045	0.098	0.065
H:7	0.115	0.055	0.043	0.197	0.154
N:8	-0.602	-0.178	-1.219	-0.689	-0.683
H:9	0.121	0.047	0.035	0.039	0.005
H:10	0.121	0.047	0.035	0.037	0.002
Error	Average	0.120	0.181	0.191	0.175
	Median	0.074	0.086	0.087	0.119
	SD	0.103	0.174	0.136	0.115

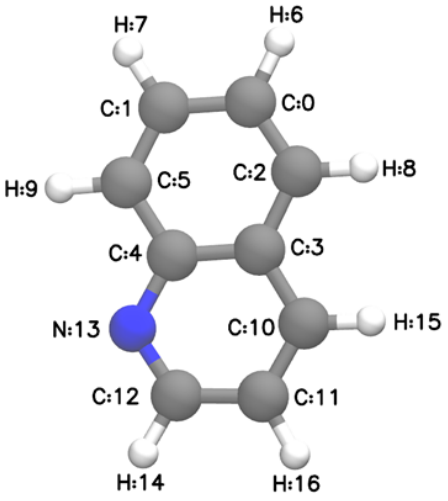


	Charmm GenFF	Hirshfeld	AIM	MK	ChelpG
C:0	0.543	0.064	1.087	0.556	0.625
N:1	-0.743	-0.186	-1.198	-0.683	-0.700
N:2	-0.681	-0.188	-1.208	-0.735	-0.709
C:3	0.079	0.036	0.570	0.218	0.280
C:4	0.284	-0.002	0.394	0.127	0.123
C:5	0.407	0.081	0.985	0.600	0.528
N:6	-0.743	-0.213	-1.142	-0.607	-0.615
N:7	-0.262	-0.035	-1.271	-0.318	-0.295
C:8	0.346	0.078	1.059	0.183	0.244
H:9	0.311	0.174	0.485	0.316	0.301
H:10	0.124	0.080	0.100	0.166	0.132
H:11	0.200	0.062	0.066	0.121	0.081
H:12	0.135	0.051	0.054	0.054	0.005
Error	Average	0.278	0.403	0.091	0.090
	Median	0.268	0.455	0.079	0.102
	SD	0.180	0.277	0.058	0.059

Figure 1: The Charmm GenFF partial charges and the DFT calculation based Hirshfeld, AIM, Merz-Singh-Kollman (MK), and ChelpG charges of imidazole, pyrrole, pyridine, and purine. The charge unit is elementary charge. The average, median, and standard deviation (SD) of absolute error in comparison to Charmm GenFF charges are also presented.

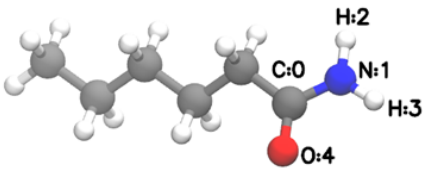


	Charmm GenFF	Hirshfeld	AIM	MK	ChelpG
C:0	-0.214	-0.068	-0.034	-0.143	-0.047
C:1	-0.180	-0.062	-0.029	-0.144	-0.136
C:2	-0.246	-0.055	-0.025	-0.356	-0.334
C:3	0.145	-0.039	-0.029	0.302	0.284
C:4	0.235	0.021	0.392	0.183	0.099
C:5	-0.277	-0.066	-0.021	-0.339	-0.226
C:6	-0.248	-0.101	-0.045	-0.496	-0.391
C:7	-0.082	-0.014	0.384	-0.146	-0.113
N:8	-0.487	-0.052	-1.269	-0.277	-0.254
H:9	0.360	0.157	0.455	0.331	0.307
H:10	0.183	0.047	0.043	0.230	0.169
H:11	0.170	0.060	0.065	0.206	0.172
H:12	0.192	0.047	0.030	0.188	0.141
H:13	0.124	0.042	0.021	0.141	0.102
H:14	0.124	0.040	0.018	0.135	0.076
H:15	0.201	0.045	0.025	0.186	0.152
Error	Average	0.164	0.217	0.073	0.080
	Median	0.146	0.168	0.049	0.051
	SD	0.083	0.169	0.070	0.063

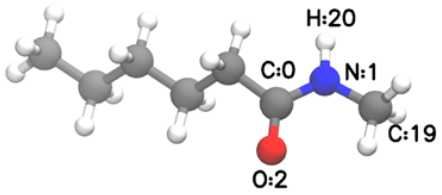


	Charmm GenFF	Hirshfeld	AIM	MK	ChelpG
C:0	-0.114	-0.043	-0.022	-0.198	-0.114
C:1	-0.112	-0.039	-0.023	-0.084	-0.018
C:2	-0.116	-0.041	-0.023	-0.159	-0.203
C:3	-0.005	-0.011	-0.020	-0.173	-0.027
C:4	0.375	0.036	0.460	0.741	0.560
C:5	-0.129	-0.047	-0.023	-0.400	-0.329
H:6	0.115	0.051	0.035	0.161	0.108
H:7	0.115	0.052	0.036	0.154	0.097
H:8	0.115	0.051	0.034	0.150	0.137
H:9	0.115	0.048	0.048	0.182	0.148
C:10	-0.116	-0.019	-0.017	0.030	-0.016
C:11	-0.115	-0.048	-0.033	-0.439	-0.328
C:12	0.155	0.021	0.605	0.392	0.409
N:13	-0.634	-0.173	-1.203	-0.754	-0.701
H:14	0.121	0.049	0.036	0.065	0.023
H:15	0.115	0.058	0.045	0.139	0.114
H:16	0.115	0.055	0.044	0.193	0.142
Error	Average	0.109	0.130	0.125	0.084
	Median	0.071	0.085	0.078	0.067
	SD	0.111	0.141	0.107	0.080

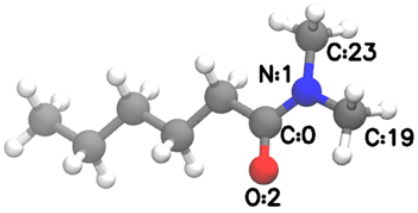
Figure 2: The Charmm GenFF partial charges and the DFT calculation based Hirshfeld, AIM, Merz-Singh-Kollman (MK), and ChelpG charges of indole and quinoline. The charge unit is elementary charge. The average, median, and standard deviation (SD) of absolute error in comparison to Charmm GenFF charges are also presented.



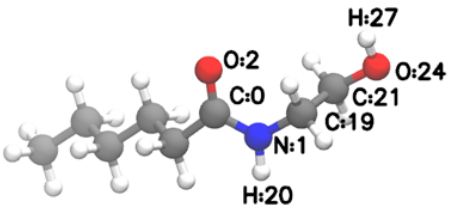
	Charmm GenFF	Hirshfeld	AIM	MK	ChelpG
C:0	0.549	0.159	1.504	0.828	0.836
N:1	-0.623	-0.133	-1.246	-1.007	-0.986
H:2	0.310	0.138	0.436	0.431	0.416
H:3	0.310	0.139	0.441	0.443	0.434
O:4	-0.537	-0.350	-1.244	-0.652	-0.663
Error	Average	0.282	0.509	0.206	0.201
	Median	0.187	0.623	0.133	0.126
	SD	0.133	0.329	0.108	0.104



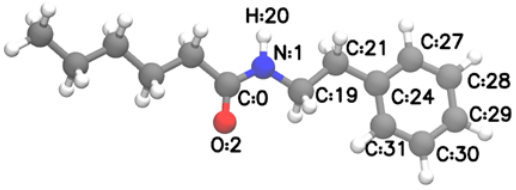
	Charmm GenFF	Hirshfeld	AIM	MK	ChelpG
C:0	0.493	0.155	1.476	0.647	0.688
N:1	-0.489	-0.077	-1.237	-0.417	-0.505
O:2	-0.518	-0.345	-1.255	-0.588	-0.610
C:19	-0.113	-0.038	0.363	-0.084	0.067
H:20	0.369	0.134	0.440	0.320	0.324
Error	Average	0.247	0.603	0.075	0.106
	Median	0.235	0.737	0.070	0.092
	SD	0.119	0.311	0.042	0.071



	Charmm GenFF	Hirshfeld	AIM	MK	ChelpG
C:0	0.440	0.156	1.450	0.520	0.460
N:1	-0.354	-0.035	-1.204	-0.007	-0.089
O:2	-0.529	-0.333	-1.244	-0.618	-0.597
C:19	-0.085	-0.043	0.354	-0.386	-0.120
C:23	-0.085	-0.035	0.355	-0.330	-0.221
Error	Average	0.178	0.691	0.212	0.105
	Median	0.196	0.715	0.245	0.068
	SD	0.115	0.225	0.109	0.089



	Charmm GenFF	Hirshfeld	AIM	MK	ChelpG
C:0	0.506	0.158	1.475	0.741	0.763
N:1	-0.458	-0.074	-1.237	-0.640	-0.669
O:2	-0.512	-0.341	-1.255	-0.592	-0.613
C:19	-0.041	-0.014	0.380	-0.034	0.121
H:20	0.355	0.135	0.443	0.382	0.365
C:21	0.039	0.011	0.538	0.244	0.234
O:24	-0.652	-0.241	-1.172	-0.673	-0.667
H:27	0.419	0.164	0.627	0.421	0.411
Error	Average	0.230	0.528	0.095	0.120
	Median	0.237	0.509	0.054	0.131
	SD	0.140	0.277	0.091	0.094



	Charmm GenFF	Hirshfeld	AIM	MK	ChelpG
C:0	0.506	0.158	1.471	0.813	0.817
N:1	-0.458	-0.083	-1.234	-0.740	-0.811
O:2	-0.512	-0.336	-1.244	-0.673	-0.669
C:19	-0.042	-0.006	0.385	0.325	0.576
H:20	0.355	0.131	0.432	0.328	0.355
C:21	-0.198	-0.051	0.029	-0.227	-0.381
C:24	0.001	0.001	-0.018	0.117	0.174
C:27	-0.117	-0.050	-0.043	-0.207	-0.181
C:28	-0.111	-0.047	-0.039	-0.124	-0.087
C:29	-0.115	-0.052	-0.044	-0.185	-0.126
C:30	-0.111	-0.047	-0.040	-0.147	-0.084
C:31	-0.117	-0.050	-0.043	-0.147	-0.182
Error	Average	0.136	0.299	0.127	0.166
	Median	0.067	0.075	0.080	0.111
	SD	0.117	0.325	0.119	0.176

Figure 3: The Charmm GenFF partial charges and the DFT calculation based Hirshfeld, AIM, Merz-Singh-Kollman (MK), and ChelpG charges of the studied fatty acid amides. The charge unit is elementary charge. The average, median, and standard deviation (SD) of absolute error in comparison to Charmm GenFF charges are also presented.

References

(1) Vanommeslaeghe, K.; Hatcher, E.; Acharya, C.; Kundu, S.; Zhong, S.; Shim, J.; Darian, E.; Guvench, O.; Lopes, P.; Vorobyov, I., et al. CHARMM general force field: A force field for drug-like molecules compatible with the CHARMM all-atom additive biological force fields. *Journal of computational chemistry* **2010**, *31*, 671–690.

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