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Which charge definition for describing the crystal polarizing field and the $\chi^{(1)}$ and $\chi^{(2)}$ of organic crystals? - Supplementary Information

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TABLES

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Tab. 1: Atomic charges of the MNA molecule in its crystal environment as obtained within scheme B at the B3LYP/6-311++G(d,p) level of approximation together with Pearson's correlation (r coeff.) with respect to PBC-B3LYP/6-31G(d,p)-Mulliken charges. For a definition of the A-C molecular moieties, see Fig 2.

atom	periodic Mulliken	Mulliken* (a)	Mulliken* (a) (final)	MBS	MBS (final)	NBO	NBO (final)	Hirshfeld	Hirshfeld (final)	CM5	CM5 (final)	MK	MK (final)	CHELPG	CHELPG (final)	HLYGat	HLYGat (final)
C1	0.264	0.308	0.296	0.163	0.174	0.207	0.231	0.067	0.078	0.125	0.139	0.341	0.483	0.418	0.508	0.237	0.415
C2	0.096	0.108	0.089	-0.024	-0.013	-0.076	-0.051	-0.013	-0.007	-0.023	-0.012	0.204	0.172	0.015	0.001	0.314	0.258
C3	-0.143	-0.143	-0.153	-0.083	-0.086	-0.153	-0.156	-0.034	-0.037	-0.079	-0.081	-0.377	-0.483	-0.199	-0.245	-0.466	-0.586
H4	0.127	0.126	0.113	0.144	0.135	0.236	0.227	0.054	0.049	0.119	0.112	0.212	0.249	0.158	0.180	0.231	0.274
C5	0.209	0.255	0.270	0.063	0.061	0.032	0.031	0.015	0.012	0.073	0.072	0.100	0.261	0.003	0.067	0.173	0.364
C6	-0.106	-0.097	-0.074	-0.075	-0.071	-0.157	-0.154	-0.033	-0.035	-0.079	-0.079	-0.274	-0.363	-0.108	-0.152	-0.326	-0.422
H7	0.132	0.134	0.099	0.151	0.134	0.244	0.226	0.058	0.050	0.121	0.114	0.206	0.234	0.143	0.160	0.219	0.247
C8	-0.161	-0.130	-0.158	-0.139	-0.143	-0.249	-0.257	-0.064	-0.060	-0.111	-0.110	-0.231	-0.291	-0.272	-0.307	-0.197	-0.273
H9	0.124	0.086	0.143	0.104	0.125	0.205	0.226	0.049	0.054	0.107	0.116	0.165	0.201	0.146	0.172	0.169	0.208
C10	-0.411	-0.404	-0.406	-0.267	-0.275	-0.598	-0.609	-0.095	-0.092	-0.238	-0.235	-0.421	-0.386	-0.142	-0.151	-0.500	-0.437
H11	0.130	0.130	0.134	0.111	0.112	0.222	0.220	0.052	0.053	0.105	0.105	0.145	0.132	0.078	0.073	0.161	0.141
H12	0.125	0.125	0.157	0.099	0.118	0.208	0.222	0.041	0.052	0.096	0.106	0.128	0.127	0.053	0.069	0.146	0.134
H13	0.134	0.116	0.127	0.091	0.106	0.205	0.226	0.041	0.046	0.093	0.104	0.100	0.124	0.029	0.059	0.121	0.141
N14	-0.646	-0.680	-0.695	-0.534	-0.525	-0.766	-0.745	-0.163	-0.142	-0.623	-0.599	-0.896	-0.991	-0.890	-0.955	-0.844	-0.966
H15	0.299	0.275	0.317	0.284	0.313	0.389	0.413	0.137	0.153	0.328	0.345	0.401	0.471	0.386	0.450	0.394	0.470
H16	0.304	0.276	0.348	0.284	0.330	0.396	0.434	0.133	0.156	0.322	0.348	0.403	0.491	0.401	0.482	0.390	0.486
N17	0.394	0.359	0.357	0.362	0.360	0.472	0.478	0.219	0.212	0.051	0.041	0.748	0.721	0.716	0.730	0.720	0.674
O18	-0.430	-0.421	-0.488	-0.368	-0.428	-0.409	-0.477	-0.232	-0.274	-0.195	-0.242	-0.480	-0.579	-0.468	-0.571	-0.473	-0.568
O19	-0.441	-0.422	-0.479	-0.366	-0.426	-0.406	-0.484	-0.232	-0.269	-0.194	-0.245	-0.476	-0.572	-0.467	-0.566	-0.467	-0.561
r coeff.	1.000	0.996	0.996	0.981	0.979	0.963	0.970	0.932	0.909	0.907	0.918	0.967	0.969	0.931	0.942	0.958	0.961
A	-0.044	-0.129	-0.030	0.033	0.118	0.018	0.103	0.107	0.167	0.028	0.095	-0.091	-0.029	-0.102	-0.023	-0.060	-0.010
B	0.521	0.613	0.639	0.339	0.376	0.325	0.381	0.138	0.164	0.310	0.351	0.299	0.459	0.322	0.430	0.280	0.465
C	-0.478	-0.484	-0.610	-0.372	-0.494	-0.343	-0.483	-0.244	-0.331	-0.337	-0.446	-0.208	-0.430	-0.219	-0.407	-0.219	-0.455

(a) 6-31G(d,p) basis set

Tab. 2: Atomic charges of the MNA molecule in its crystal environment as obtained within scheme B at the MP2/6-311++G(d,p) level of approximation together with Pearson's correlation (r coeff.) with respect to PBC-B3LYP/6-31G(d,p)-Mulliken charges. For a definition of the A-C molecular moieties, see Fig 2.

atom	periodic Mulliken	Mulliken* (a)	Mulliken* (a) (final)	MBS	MBS (final)	NBO	NBO (final)	Hirshfeld	Hirshfeld (final)	CM5	CM5 (final)	MK	MK (final)	CHELPG	CHELPG (final)	HLYGat	HLYGat (final)
C1	0.264	0.354	0.354	0.231	0.246	0.306	0.338	0.099	0.111	0.157	0.172	0.472	0.624	0.550	0.657	0.365	0.546
C2	0.096	-0.055	-0.061	-0.055	-0.049	-0.129	-0.113	-0.022	-0.019	-0.032	-0.025	0.122	0.093	-0.077	-0.093	0.233	0.187
C3	-0.143	-0.089	-0.100	-0.038	-0.041	-0.084	-0.086	-0.010	-0.014	-0.055	-0.058	-0.335	-0.422	-0.154	-0.191	-0.431	-0.527
H4	0.127	0.215	0.202	0.143	0.134	0.228	0.220	0.058	0.054	0.123	0.117	0.238	0.269	0.183	0.202	0.259	0.295
C5	0.209	0.098	0.112	0.034	0.023	-0.025	-0.042	0.006	-0.001	0.064	0.058	0.043	0.161	-0.059	-0.022	0.124	0.262
C6	-0.106	-0.079	-0.055	-0.027	-0.021	-0.086	-0.078	-0.007	-0.009	-0.053	-0.053	-0.219	-0.291	-0.052	-0.084	-0.275	-0.349
H7	0.132	0.222	0.181	0.149	0.133	0.236	0.219	0.062	0.056	0.126	0.119	0.229	0.253	0.163	0.178	0.242	0.266
C8	-0.161	-0.211	-0.250	-0.158	-0.169	-0.293	-0.310	-0.074	-0.072	-0.121	-0.122	-0.352	-0.422	-0.386	-0.435	-0.318	-0.403
H9	0.124	0.158	0.221	0.093	0.116	0.197	0.221	0.044	0.050	0.103	0.111	0.197	0.234	0.176	0.204	0.203	0.242
C10	-0.411	-0.363	-0.372	-0.203	-0.211	-0.519	-0.532	-0.081	-0.079	-0.224	-0.222	-0.407	-0.382	-0.101	-0.113	-0.487	-0.441
H11	0.130	0.143	0.143	0.090	0.089	0.197	0.194	0.046	0.046	0.099	0.098	0.144	0.130	0.069	0.062	0.159	0.141
H12	0.125	0.134	0.164	0.078	0.098	0.182	0.197	0.035	0.044	0.089	0.098	0.128	0.128	0.047	0.062	0.146	0.137
H13	0.134	0.123	0.141	0.069	0.083	0.179	0.199	0.034	0.038	0.086	0.096	0.099	0.121	0.021	0.047	0.120	0.140
N14	-0.646	-0.798	-0.823	-0.589	-0.593	-0.826	-0.826	-0.191	-0.176	-0.650	-0.634	-0.997	-1.114	-0.996	-1.083	-0.943	-1.082
H15	0.299	0.317	0.354	0.285	0.311	0.389	0.412	0.137	0.150	0.328	0.342	0.427	0.493	0.412	0.472	0.419	0.491
H16	0.304	0.325	0.395	0.288	0.333	0.398	0.436	0.135	0.155	0.324	0.347	0.431	0.516	0.431	0.510	0.417	0.508
N17	0.394	0.471	0.482	0.448	0.455	0.605	0.622	0.284	0.282	0.116	0.112	0.802	0.788	0.780	0.799	0.770	0.745
O18	-0.430	-0.483	-0.544	-0.421	-0.470	-0.479	-0.532	-0.277	-0.311	-0.240	-0.278	-0.513	-0.594	-0.505	-0.589	-0.505	-0.583
O19	-0.441	-0.483	-0.544	-0.418	-0.467	-0.475	-0.537	-0.276	-0.306	-0.238	-0.280	-0.508	-0.586	-0.502	-0.583	-0.498	-0.576
r coeff.	1.000	0.979	0.980	0.960	0.959	0.960	0.962	0.904	0.891	0.930	0.937	0.963	0.963	0.902	0.910	0.968	0.967
A	-0.044	-0.157	-0.074	-0.016	0.051	-0.040	0.021	0.081	0.129	0.002	0.056	-0.139	-0.105	-0.152	-0.102	-0.107	-0.082
B	0.521	0.653	0.680	0.407	0.431	0.389	0.426	0.188	0.206	0.360	0.390	0.359	0.496	0.380	0.475	0.340	0.497
C	-0.478	-0.496	-0.606	-0.391	-0.482	-0.349	-0.448	-0.269	-0.335	-0.362	-0.445	-0.219	-0.392	-0.228	-0.373	-0.233	-0.415

(a) 6-31G(d,p) basis set