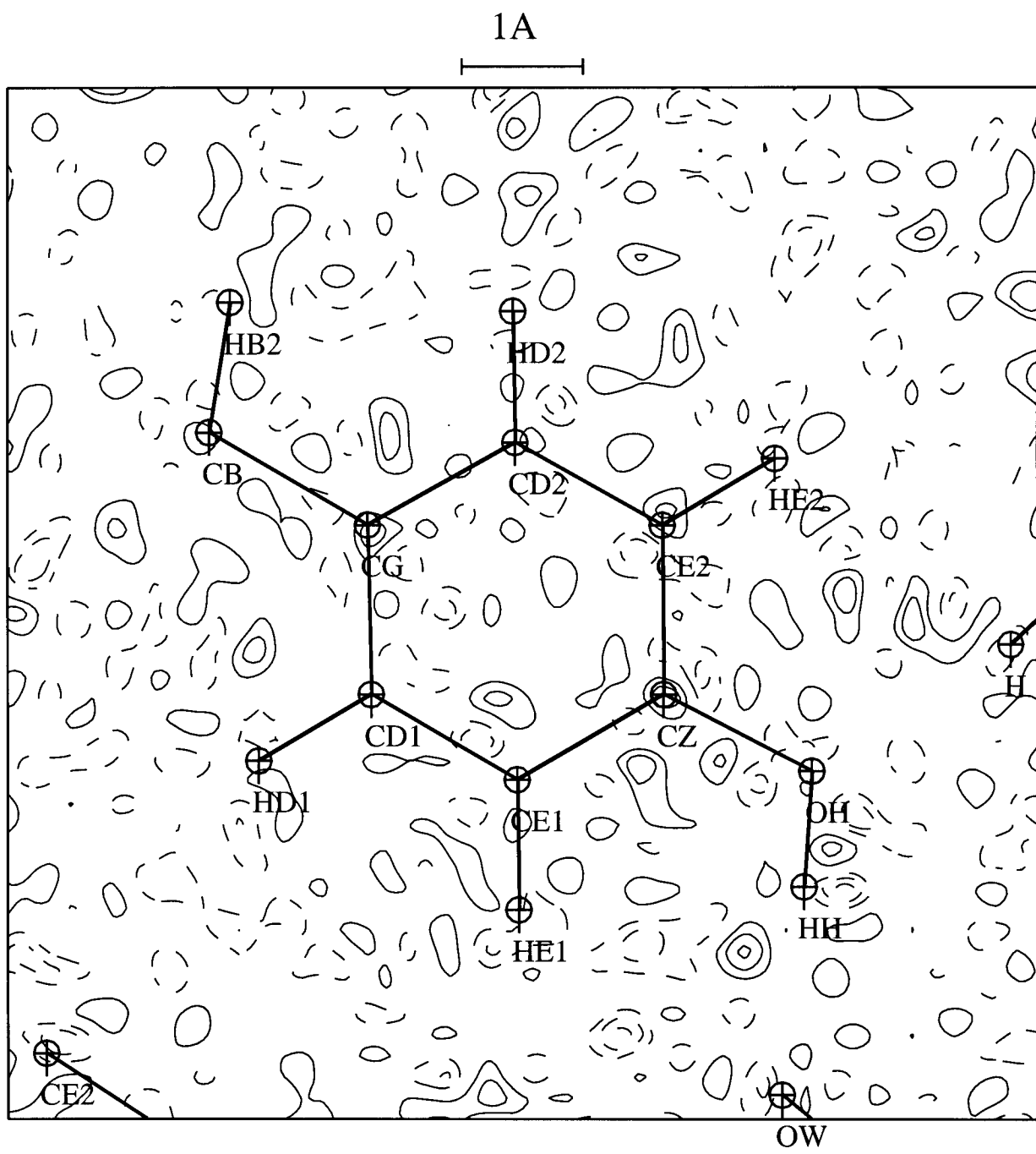


CHARGE DENSITY PARAMETERS (Pv + P1m) [MULTIPOLAR REFINEMENT]

Atom	Pv	P11+	P11-	P10	P20	P21+	P21-	P22+	P22-	P30	P31+	P31-	P32+	P32-	P33+	P33-	kappa1	kappa2
O1	6.018	-.048	-.013	.086	-.053	.018	.017	-.053	.010	.042	-.003	.008	-.056	-.006	.032	.000	1.0050	.8822
O	6.281	-.087	-.051	.018	-.069	.014	-.012	-.080	-.016	.012	-.038	.022	-.029	.005	.026	-.012	.9942	.8540
O2	6.148	-.042	-.055	.014	-.048	-.001	-.024	-.034	-.025	-.010	.013	.035	-.009	.026	.083	.017	1.0053	.9982
OH	6.558	-.032	-.006	-.017	.026	.010	.024	.057	-.001	-.023	.008	.009	-.017	-.030	.107	.052	.9838	.9093
HH	.667	.064	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	1.2437	1.2175
N	5.154	-.025	-.042	.028	-.028	-.002	.003	.055	.009	-.053	.014	.023	-.008	.016	.241	.010	1.0037	.9126
H	4.787	.094	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	1.2496	1.2496
CA	4.100	-.058	-.017	.162	.020	-.033	.103	.074	-.017	.029	.264	.333	.003	.031	.211	.041	1.0010	.8742
HA	.670	.072	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	1.2399	1.1078
C	4.161	.139	.015	-.012	-.313	.035	.000	.131	.012	.023	.010	.009	-.039	.023	.408	.026	.9842	.9289
C2	4.401	.078	.028	-.009	-.329	.001	.024	.096	-.021	-.010	.012	.030	-.022	-.008	.491	.036	.8919	.8999
CG	3.881	-.024	.039	.006	-.225	-.022	.015	.025	.019	.029	.020	.014	-.001	-.010	.349	.023	1.0060	.9444
CD1	4.323	-.007	.070	.048	-.254	-.019	.017	.003	.036	.007	.010	.042	.010	.067	.346	.039	.9730	.8747
HD1	.809	.111	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	1.1168	1.1430
C3	4.311	-.030	-.205	.018	.092	.020	.008	.079	.114	.069	.116	.200	.059	.042	.234	.106	.9851	.9328
H31	.777	.060	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	1.3257	1.3257
H32	.777	.060	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	1.1526	1.1526
CB	4.349	-.065	-.091	.019	.074	-.029	.007	.015	.057	-.022	.134	.224	.038	-.071	.319	.027	.9870	.8638
HB1	.737	.101	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	1.2140	1.0360
HB2	.737	.101	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	1.2140	1.0360
Cl	4.816	-.165	.102	.028	.086	.011	.026	.099	.080	-.079	.354	.012	.010	.058	.365	.100	.9529	.7624
HL1	.693	.087	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	1.0639	1.2740
HL2	.693	.087	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	1.0639	1.2740
HL3	.693	.087	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	1.0639	1.2740
CZ	3.721	.099	-.009	.006	-.153	.012	.020	.068	-.008	.047	.059	.016	-.027	.003	.259	.006	1.0236	1.0411
CE2	4.320	-.039	.020	.022	-.204	-.017	.005	.017	.021	-.015	.038	.022	.003	.005	.340	.026	.9799	.9428
HE2	.809	.111	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	1.1168	1.1430
CE1	4.216	.011	.003	.001	-.262	-.015	.038	.046	.036	.022	.017	.023	.040	.001	.415	.059	.9906	.8692
HE1	.809	.111	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	1.1168	1.1430
CD2	4.222	.046	.006	.057	-.285	.020	.002	.010	-.002	.026	.022	.010	.018	-.030	.375	.027	.9916	.8343
HD2	.809	.111	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	1.1168	1.1430
C4	4.410	-.083	.007	.028	.022	.032	-.034	.051	.038	.155	.318	.261	.184	.129	.358	.115	.9567	.7030
H41	.708	.145	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	1.1172	1.1448
H42	.708	.145	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	1.1172	1.1448
H43	.708	.145	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	1.1172	1.1448
OW	6.420	-.042	-.075	.014	.096	-.009	.033	.019	.046	-.071	.001	.042	-.039	.000	.053	.081	.9873	.7561
HW1	.747	.123	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	1.1945	1.3534
HW2	.826	.163	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	1.0977	1.2892

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