Analysis of the chemical reactivity of aminocyclopyrachlor herbicide through the Fukui function

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TABLE S-I. Values of the condensed Fukui function for the neutral aminocyclopyrachlor conformers computed from *MEP* charges according to Eqs. (9)–(11)

Position	*cisoid* Conformer			*transoid* Conformer		
	$f^-(\bar{r})$	$f^+(\bar{r})$	$f^0(\bar{r})$	$f^-(\bar{r})$	$f^+(\bar{r})$	$f^0(\bar{r})$
1C	0.091	0.067	0.079	0.084	0.031	0.058
2C	***0.203***	–0.008	0.097	0.196	–0.038	0.079
3C	0.112	***0.237***	***0.174***	0.083	***0.206***	0.145
4C	0.032	–0.046	–0.007	0.034	0.02	0.027
5N	–0.139	0.173	0.017	–0.171	0.106	–0.032
6N	0.151	0.052	0.102	0.199	0.151	***0.175***
7N	0.182	0.077	0.129	***0.217***	0.1	0.159
8H	0.039	0.014	0.026	0.036	0.016	0.026
9H	–0.001	–0.007	–0.004	–0.007	–0.007	–0.007
10Cl	0.155	0.140	0.148	0.150	0.124	0.137
11C	–0.088	–0.050	–0.069	–0.083	–0.052	–0.067
12°	0.028	0.075	0.051	0.028	0.071	0.049
13°	0.071	0.155	0.113	0.068	0.145	0.107
14C	–0.067	0.001	–0.033	–0.052	0.012	–0.020
15H	0.056	0.020	0.038	0.033	0.021	0.027
16C	0.023	0.004	0.014	0.033	–0.009	0.012
17H	0.033	0.02	0.027	0.023	0.018	0.020
18H	0.019	0.013	0.016	0.026	0.027	0.027
19C	0.014	–0.015	0.000	0.029	–0.016	0.007
20H	0.034	0.021	0.027	0.024	0.019	0.022
21H	0.028	0.031	0.029	0.025	0.025	0.025
22H	0.025	0.029	0.027	0.024	0.028	0.026

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TABLE S-II. Values of the condensed Fukui function for the anionic aminocyclopyrachlor conformers computed from *MEP* charges according to Eqs. (9)–(11)

Position	*cisoid* Conformer			*transoid* Conformer		
	$f^-(\bar{r})$	$f^+(\bar{r})$	$f^0(\bar{r})$	$f^-(\bar{r})$	$f^+(\bar{r})$	$f^0(\bar{r})$
1C	0.279	0.169	***0.224***	0.244	***0.221***	***0.232***
2C	***0.400***	–0.046	0.177	***0.362***	0.005	0.183
3C	0.061	0.126	0.093	0.036	0.088	0.062
4C	0.223	–0.049	0.087	0.198	–0.037	0.080
5N	–0.410	***0.253***	–0.078	–0.416	0.154	–0.131
6N	0.154	0.141	0.147	0.209	0.166	0.188
7N	–0.346	0.115	–0.116	–0.225	0.049	–0.088
8H	0.108	0.025	0.066	0.099	0.029	0.064
9H	0.038	–0.011	0.013	0.027	–0.014	0.006
10Cl	0.199	0.107	0.153	0.184	0.136	0.160
11C	–0.160	–0.178	–0.169	–0.148	–0.186	–0.167
12O	0.117	0.129	0.123	0.109	0.135	0.122
13O	0.117	0.130	0.123	0.110	0.135	0.123
14C	–0.099	–0.011	–0.055	–0.073	0.010	–0.031
15H	0.083	0.031	0.057	0.041	0.020	0.031
16C	0.022	–0.013	0.004	0.040	–0.020	0.010
17H	0.052	0.023	0.038	0.034	0.028	0.031
18H	0.037	0.025	0.031	0.045	0.036	0.040
19C	0.052	–0.010	0.021	0.068	–0.009	0.029
20H	0.046	0.023	0.035	0.030	0.026	0.028
21H	0.027	0.024	0.025	0.025	0.030	0.028

TABLE S-III. Values of the condensed Fukui function for the cationic aminocyclopyrachlor conformers computed from *MEP* charges according to Eqs. (9)–(11)

Position	*cisoid* Conformer			*transoid* Conformer		
	$f^-(\bar{r})$	$f^+(\bar{r})$	$f^0(\bar{r})$	$f^-(\bar{r})$	$f^+(\bar{r})$	$f^0(\bar{r})$
1C	0.091	0.028	0.060	0.089	0.020	0.054
2C	–0.067	0.008	–0.030	–0.048	0.009	–0.020
3C	0.055	***0.224***	0.140	0.048	***0.218***	0.133
4C	–0.259	0.089	–0.085	–0.259	0.133	–0.063
5N	0.264	0.087	0.176	0.256	0.033	0.145
6N	0.251	–0.007	0.122	0.244	0.017	0.130
7N	***0.646***	0.070	***0.358***	***0.659***	0.045	***0.352***
8H	–0.035	0.027	–0.004	–0.037	0.034	–0.001
9H	–0.042	0.011	–0.016	–0.045	0.013	–0.016
10Cl	0.092	0.139	0.115	0.089	0.143	0.116
11C	–0.077	0.088	0.005	–0.077	0.083	0.003
12O	0.011	0.003	0.007	0.012	0.007	0.010
13O	0.049	0.114	0.082	0.046	0.117	0.081
14C	–0.046	–0.005	–0.025	–0.067	0.004	–0.032
15H	0.019	0.022	0.021	0.030	0.013	0.021
16C	–0.001	–0.002	–0.001	0.001	–0.005	–0.002
17H	0.014	0.013	0.013	0.015	0.014	0.015

TABLE S-III. Continued

Position	cisoid Conformer			transoid Conformer		
	$f^-(\bar{r})$	$f^+(\bar{r})$	$f^0(\bar{r})$	$f^-(\bar{r})$	$f^+(\bar{r})$	$f^0(\bar{r})$
18H	0.009	0.015	0.012	0.004	0.019	0.011
19C	–0.001	–0.002	–0.001	0.000	–0.005	–0.002
20H	0.014	0.013	0.013	0.015	0.014	0.015
21H	0.009	0.015	0.012	0.004	0.019	0.012
22H	0.017	0.035	0.026	0.017	0.034	0.026
23H	–0.012	0.015	0.002	0.003	0.022	0.012

Table S-IV. Values of the condensed Fukui function for the dipolar aminocyclopyrachlor conformers computed from *MEP* charges according to Eqs. (9)–(11)

Position	cisoid Conformer			transoid Conformer		
	$f^-(\bar{r})$	$f^+(\bar{r})$	$f^0(\bar{r})$	$f^-(\bar{r})$	$f^+(\bar{r})$	$f^0(\bar{r})$
1C	0.147	–0.055	0.046	0.145	–0.037	0.054
2C	–0.082	0.030	–0.026	–0.065	0.014	–0.026
3C	–0.007	***0.246***	0.119	–0.016	***0.228***	0.106
4C	–0.254	0.151	–0.051	–0.251	0.195	–0.028
5N	0.238	0.101	0.170	0.227	0.043	0.135
6N	0.290	0.032	0.161	0.283	0.059	0.171
7N	***0.634***	0.126	***0.380***	***0.646***	0.088	***0.367***
8H	–0.026	0.025	0.000	–0.027	0.034	0.004
9H	–0.037	0.022	–0.008	–0.040	0.021	–0.009
10Cl	0.097	0.096	0.096	0.094	0.104	0.099
11C	–0.078	–0.017	–0.047	–0.075	–0.014	–0.044
12°	0.045	0.079	0.062	0.045	0.082	0.064
13°	0.052	0.087	0.069	0.046	0.085	0.066
14C	–0.043	–0.018	–0.031	–0.060	0.001	–0.030
15H	0.021	0.030	0.026	0.029	0.017	0.023
16C	–0.002	–0.002	–0.002	–0.001	–0.010	–0.006
17H	0.013	0.016	0.014	0.014	0.018	0.016
18H	0.009	0.019	0.014	0.005	0.025	0.015
19C	–0.002	–0.002	–0.002	–0.001	–0.010	–0.006
20H	0.013	0.016	0.014	0.014	0.018	0.016
21H	0.009	0.019	0.014	0.005	0.025	0.015
23H	–0.039	0.001	–0.019	–0.019	0.015	–0.002