Electronic Supplementary Material

Local chirality measures in QSPR: IR and VCD spectroscopy.

Piotr F.J. Lipiński*,† and Jan Cz. Dobrowolski‡,§

Mossakowski Medical Research Centre Polish Academy of Sciences, Warsaw, Poland, National Medicines Institute and Institute of Nuclear Chemistry and Technology, Warsaw, Poland

Table of Contents

Substituent used in the study **SI-2**

Calculated global and local chirality measures **SI-3**

Interrelationships of the calculated chirality measures **SI-5**

Spectral parameters of selected modes **SI-126**

ν(CN) in CN-IND **SI-126**

ν(CH) in CN-IND **SI-129**

Coordinates and energies of CN-IND **SI-132**

Substituents used in the study

TABLE S1. Substituents used in the study along with their σ_p and pEDA(I) values.

substituent	σ_p	pEDA(I) [*e*]	substituent	σ_p	pEDA(I) [*e*]
BF_2	0.48	-0.078	$MeSO_2$	0.72	-0.016
Br	0.23	0.057	NH_2	-0.66	0.141
CHO	0.42	-0.088	$NHNH_2$	-0.55	0.133
Cl	0.23	0.064	NMe_2	-0.83	0.177
$COCH_3$	0.50	-0.071	NO	0.91	-0.132
$CONH_2$	0.36	-0.044	NO_2	0.78	-0.069
$COOCH_3$	0.45	-0.062	OCF_3	0.35	0.040
COOH	0.45	-0.069	OH	-0.37	0.114
Et	-0.15	0.011	OMe	-0.27	0.120
F	0.06	0.068	SH	0.15	0.096
H	0.00	0.000	SiH_3	0.10	-0.012
iPr	-0.15	0.007	$SiMe_3$	-0.07	-0.011
Me	-0.17	0.016	tBu	-0.20	0.008

Calculated global and local chirality measures

TABLE S2. Calculated global and local chirality measures

substituent	$^{SR}CM_0$ (f)	$^{SR}CM_L$ (f)	$^{SR}CM_M$ (f)	$^{SR}CM_q$ (f)	$^{SR}CM_0$ (ab)	$^{SR}CM_L$ (ab)	$^{SR}CM_M$ (ab)	$^{SR}CM_q$ (ab)	$^{SR}CM_0$ (a)	$^{SR}CM_L$ (a)	$^{SR}CM_M$ (a)	$^{SR}CM_q$ (a)	CCM (f)	CCM (ab)	CCM (a)
BF_2	0.24892	0.40315	0.42740	0.18012	0.29120	0.47281	0.57289	0.80231	0.47812	0.79126	0.62731	0.67411	2.734	4.072	10.278
Br	0.27447	0.44749	0.37015	0.22050	0.28966	0.47303	0.57396	0.80123	0.47811	0.79200	0.63016	0.67340	3.513	4.077	10.306
CHO	0.24928	0.40429	0.47675	0.17137	0.29071	0.47277	0.57293	0.80078	0.47779	0.79214	0.62752	0.67358	2.798	4.070	10.277
Cl	0.27378	0.44752	0.46334	0.19656	0.29019	0.47312	0.57465	0.80156	0.47729	0.79217	0.63071	0.67334	3.550	4.081	10.315
$COCH_3$	0.22539	0.36124	0.44645	0.15900	0.29120	0.47327	0.57328	0.80209	0.47759	0.79101	0.62821	0.67350	2.045	4.072	10.281
$CONH_2$	0.41902	0.55690	0.57266	0.24505	0.29642	0.47881	0.57468	0.80680	0.47900	0.79168	0.62975	0.67325	2.788	4.072	10.284
$COOCH_3$	0.21496	0.34196	0.41046	0.15386	0.29057	0.47252	0.57327	0.80157	0.48029	0.79144	0.62895	0.67390	1.674	4.071	10.283
COOH	0.24015	0.38581	0.43689	0.16869	0.28991	0.47216	0.57250	0.80045	0.47835	0.79093	0.62666	0.67418	2.434	4.066	10.273
Et	0.56947	0.94038	0.73879	0.55670	0.29013	0.47434	0.57667	0.80728	0.47968	0.79377	0.63055	0.67328	5.311	4.097	10.338
F	0.27470	0.44845	0.50975	0.21445	0.29006	0.47329	0.57591	0.80154	0.47802	0.79351	0.63261	0.67355	3.637	4.092	10.332
H	0.27498	0.44837	0.57137	0.21115	0.29002	0.47341	0.57533	0.80409	0.47727	0.79236	0.63088	0.67425	3.676	4.085	10.306
iPr	0.19402	0.31216	0.45297	0.14148	0.29025	0.47430	0.57765	0.80851	0.47772	0.79377	0.63320	0.67363	1.722	4.105	10.347
Me	0.24497	0.39529	0.52524	0.18898	0.28933	0.47358	0.57703	0.80703	0.47890	0.79376	0.63318	0.67303	2.634	4.099	10.347
MeS	0.23808	0.38195	0.44198	0.19102	0.28949	0.47463	0.57737	0.80736	0.47757	0.79397	0.63279	0.67251	2.147	4.100	10.349
$MeSO_2$	0.65486	1.01834	0.78985	0.56422	0.29982	0.47751	0.57462	0.80456	0.47849	0.79188	0.63004	0.67433	6.555	4.083	10.304
NH_2	0.30246	0.46084	0.53873	0.20839	0.29034	0.47531	0.57841	0.80976	0.47480	0.79626	0.63485	0.67171	2.846	4.110	10.375

$NHNH_2$	0.39028	0.53786	0.55879	0.21828	0.28981	0.47559	0.57970	0.80914	0.47894	0.79565	0.63551	0.67162	2.646	4.114	10.393
NMe_2	0.28963	0.41219	0.49375	0.20619	0.29365	0.47721	0.58076	0.81180	0.47570	0.79709	0.63616	0.67096	1.834	4.121	10.406
NO	0.26181	0.42356	0.47309	0.19719	0.28971	0.47277	0.57176	0.79796	0.47772	0.79103	0.62817	0.67471	3.139	4.060	10.259
NO_2	0.24837	0.40298	0.43326	0.17164	0.29243	0.47244	0.57169	0.79711	0.48021	0.79071	0.62797	0.67360	2.801	4.061	10.268
OCF_3	0.49146	0.66061	0.72262	0.42831	0.29102	0.47387	0.57566	0.80148	0.47792	0.79275	0.63037	0.67348	3.736	4.087	10.313
OH	0.26294	0.42678	0.51796	0.20280	0.28902	0.47442	0.57816	0.80652	0.47815	0.79421	0.63426	0.67253	3.231	4.106	10.370
OMe	0.22848	0.37310	0.47932	0.16718	0.29013	0.47486	0.57878	0.80742	0.47846	0.79478	0.63422	0.67285	2.276	4.112	10.374
SH	0.26398	0.42850	0.46924	0.21206	0.28946	0.47382	0.57638	0.80568	0.47817	0.79446	0.63089	0.67260	3.111	4.094	10.339
SiH_3	0.24047	0.39023	0.47511	0.17058	0.29020	0.47298	0.57440	0.80484	0.47803	0.79164	0.63024	0.67355	2.407	4.077	10.301
$SiMe_3$	0.19262	0.29309	0.39714	0.13410	0.28836	0.47318	0.57526	0.80670	0.47752	0.79367	0.62893	0.67356	1.336	4.088	10.323
tBu	0.16951	0.27498	0.41604	0.10352	0.28954	0.47385	0.57722	0.80877	0.47740	0.79406	0.63325	0.67268	1.505	4.105	10.350
Vin	0.22661	0.36989	0.48578	0.14650	0.28966	0.47356	0.57587	0.80648	0.47802	0.79295	0.63167	0.67288	2.224	4.090	10.322

Interrelationships of the calculated chirality measures

Table S3. Listing of scatter plots presenting relationships between the considered chirality measures. The plots can be found on subsequent pages in the given order.

No.	X	Y
1	$^{SR}CM_0$ (f)	$^{SR}CM_0$ (f)
2	$^{SR}CM_0$ (f)	$^{SR}CM_L$ (f)
3	$^{SR}CM_0$ (f)	$^{SR}CM_M$ (f)
4	$^{SR}CM_0$ (f)	$^{SR}CM_q$ (f)
5	$^{SR}CM_0$ (f)	$^{SR}CM_0$ (ab)
6	$^{SR}CM_0$ (f)	$^{SR}CM_L$ (ab)
7	$^{SR}CM_0$ (f)	$^{SR}CM_M$ (ab)
8	$^{SR}CM_0$ (f)	$^{SR}CM_q$ (ab)
9	$^{SR}CM_0$ (f)	$^{SR}CM_0$ (a)
10	$^{SR}CM_0$ (f)	$^{SR}CM_L$ (a)
11	$^{SR}CM_0$ (f)	$^{SR}CM_M$ (a)
12	$^{SR}CM_0$ (f)	$^{SR}CM_q$ (a)
13	$^{SR}CM_0$ (f)	CCM (f)
14	$^{SR}CM_0$ (f)	CCM (ab)
15	$^{SR}CM_0$ (f)	CCM (a)
16	$^{SR}CM_L$ (f)	$^{SR}CM_0$ (f)
17	$^{SR}CM_L$ (f)	$^{SR}CM_L$ (f)
18	$^{SR}CM_L$ (f)	$^{SR}CM_M$ (f)
19	$^{SR}CM_L$ (f)	$^{SR}CM_q$ (f)
20	$^{SR}CM_L$ (f)	$^{SR}CM_0$ (ab)
21	$^{SR}CM_L$ (f)	$^{SR}CM_L$ (ab)
22	$^{SR}CM_L$ (f)	$^{SR}CM_M$ (ab)
23	$^{SR}CM_L$ (f)	$^{SR}CM_q$ (ab)
24	$^{SR}CM_L$ (f)	$^{SR}CM_0$ (a)
25	$^{SR}CM_L$ (f)	$^{SR}CM_L$ (a)

26	**$^{SR}CM_L$ (f)**	**$^{SR}CM_M$ (a)**
27	**$^{SR}CM_L$ (f)**	**$^{SR}CM_q$ (a)**
28	**$^{SR}CM_L$ (f)**	**CCM (f)**
29	**$^{SR}CM_L$ (f)**	**CCM (ab)**
30	**$^{SR}CM_L$ (f)**	**CCM (a)**
31	**$^{SR}CM_M$ (f)**	**$^{SR}CM_0$ (f)**
32	**$^{SR}CM_M$ (f)**	**$^{SR}CM_L$ (f)**
33	**$^{SR}CM_M$ (f)**	**$^{SR}CM_M$ (f)**
34	**$^{SR}CM_M$ (f)**	**$^{SR}CM_q$ (f)**
35	**$^{SR}CM_M$ (f)**	**$^{SR}CM_0$ (ab)**
36	**$^{SR}CM_M$ (f)**	**$^{SR}CM_L$ (ab)**
37	**$^{SR}CM_M$ (f)**	**$^{SR}CM_M$ (ab)**
38	**$^{SR}CM_M$ (f)**	**$^{SR}CM_q$ (ab)**
39	**$^{SR}CM_M$ (f)**	**$^{SR}CM_0$ (a)**
40	**$^{SR}CM_M$ (f)**	**$^{SR}CM_L$ (a)**
41	**$^{SR}CM_M$ (f)**	**$^{SR}CM_M$ (a)**
42	**$^{SR}CM_M$ (f)**	**$^{SR}CM_q$ (a)**
43	**$^{SR}CM_M$ (f)**	**CCM (f)**
44	**$^{SR}CM_M$ (f)**	**CCM (ab)**
45	**$^{SR}CM_M$ (f)**	**CCM (a)**
46	**$^{SR}CM_q$ (f)**	**$^{SR}CM_0$ (f)**
47	**$^{SR}CM_q$ (f)**	**$^{SR}CM_L$ (f)**
48	**$^{SR}CM_q$ (f)**	**$^{SR}CM_M$ (f)**
49	**$^{SR}CM_q$ (f)**	**$^{SR}CM_q$ (f)**
50	**$^{SR}CM_q$ (f)**	**$^{SR}CM_0$ (ab)**
51	**$^{SR}CM_q$ (f)**	**$^{SR}CM_L$ (ab)**
52	**$^{SR}CM_q$ (f)**	**$^{SR}CM_M$ (ab)**
53	**$^{SR}CM_q$ (f)**	**$^{SR}CM_q$ (ab)**
54	**$^{SR}CM_q$ (f)**	**$^{SR}CM_0$ (a)**

55	**$^{SR}CM_q$ (f)**	**$^{SR}CM_L$ (a)**
56	**$^{SR}CM_q$ (f)**	**$^{SR}CM_M$ (a)**
57	**$^{SR}CM_q$ (f)**	**$^{SR}CM_q$ (a)**
58	**$^{SR}CM_q$ (f)**	**CCM (f)**
59	**$^{SR}CM_q$ (f)**	**CCM (ab)**
60	**$^{SR}CM_q$ (f)**	**CCM (a)**
61	**$^{SR}CM_0$ (ab)**	**$^{SR}CM_0$ (f)**
62	**$^{SR}CM_0$ (ab)**	**$^{SR}CM_L$ (f)**
63	**$^{SR}CM_0$ (ab)**	**$^{SR}CM_M$ (f)**
64	**$^{SR}CM_0$ (ab)**	**$^{SR}CM_q$ (f)**
65	**$^{SR}CM_0$ (ab)**	**$^{SR}CM_0$ (ab)**
66	**$^{SR}CM_0$ (ab)**	**$^{SR}CM_L$ (ab)**
67	**$^{SR}CM_0$ (ab)**	**$^{SR}CM_M$ (ab)**
68	**$^{SR}CM_0$ (ab)**	**$^{SR}CM_q$ (ab)**
69	**$^{SR}CM_0$ (ab)**	**$^{SR}CM_0$ (a)**
70	**$^{SR}CM_0$ (ab)**	**$^{SR}CM_L$ (a)**
71	**$^{SR}CM_0$ (ab)**	**$^{SR}CM_M$ (a)**
72	**$^{SR}CM_0$ (ab)**	**$^{SR}CM_q$ (a)**
73	**$^{SR}CM_0$ (ab)**	**CCM (f)**
74	**$^{SR}CM_0$ (ab)**	**CCM (ab)**
75	**$^{SR}CM_0$ (ab)**	**CCM (a)**
76	**$^{SR}CM_L$ (ab)**	**$^{SR}CM_0$ (f)**
77	**$^{SR}CM_L$ (ab)**	**$^{SR}CM_L$ (f)**
78	**$^{SR}CM_L$ (ab)**	**$^{SR}CM_M$ (f)**
79	**$^{SR}CM_L$ (ab)**	**$^{SR}CM_q$ (f)**
80	**$^{SR}CM_L$ (ab)**	**$^{SR}CM_0$ (ab)**
81	**$^{SR}CM_L$ (ab)**	**$^{SR}CM_L$ (ab)**
82	**$^{SR}CM_L$ (ab)**	**$^{SR}CM_M$ (ab)**
83	**$^{SR}CM_L$ (ab)**	**$^{SR}CM_q$ (ab)**

84	**$^{SR}CM_L$ (ab)**	**$^{SR}CM_0$ (a)**
85	**$^{SR}CM_L$ (ab)**	**$^{SR}CM_L$ (a)**
86	**$^{SR}CM_L$ (ab)**	**$^{SR}CM_M$ (a)**
87	**$^{SR}CM_L$ (ab)**	**$^{SR}CM_q$ (a)**
88	**$^{SR}CM_L$ (ab)**	**CCM (f)**
89	**$^{SR}CM_L$ (ab)**	**CCM (ab)**
90	**$^{SR}CM_L$ (ab)**	**CCM (a)**
91	**$^{SR}CM_M$ (ab)**	**$^{SR}CM_0$ (f)**
92	**$^{SR}CM_M$ (ab)**	**$^{SR}CM_L$ (f)**
93	**$^{SR}CM_M$ (ab)**	**$^{SR}CM_M$ (f)**
94	**$^{SR}CM_M$ (ab)**	**$^{SR}CM_q$ (f)**
95	**$^{SR}CM_M$ (ab)**	**$^{SR}CM_0$ (ab)**
96	**$^{SR}CM_M$ (ab)**	**$^{SR}CM_L$ (ab)**
97	**$^{SR}CM_M$ (ab)**	**$^{SR}CM_M$ (ab)**
98	**$^{SR}CM_M$ (ab)**	**$^{SR}CM_q$ (ab)**
99	**$^{SR}CM_M$ (ab)**	**$^{SR}CM_0$ (a)**
100	**$^{SR}CM_M$ (ab)**	**$^{SR}CM_L$ (a)**
101	**$^{SR}CM_M$ (ab)**	**$^{SR}CM_M$ (a)**
102	**$^{SR}CM_M$ (ab)**	**$^{SR}CM_q$ (a)**
103	**$^{SR}CM_M$ (ab)**	**CCM (f)**
104	**$^{SR}CM_M$ (ab)**	**CCM (ab)**
105	**$^{SR}CM_M$ (ab)**	**CCM (a)**
106	**$^{SR}CM_q$ (ab)**	**$^{SR}CM_0$ (f)**
107	**$^{SR}CM_q$ (ab)**	**$^{SR}CM_L$ (f)**
108	**$^{SR}CM_q$ (ab)**	**$^{SR}CM_M$ (f)**
109	**$^{SR}CM_q$ (ab)**	**$^{SR}CM_q$ (f)**
110	**$^{SR}CM_q$ (ab)**	**$^{SR}CM_0$ (ab)**
111	**$^{SR}CM_q$ (ab)**	**$^{SR}CM_L$ (ab)**
112	**$^{SR}CM_q$ (ab)**	**$^{SR}CM_M$ (ab)**

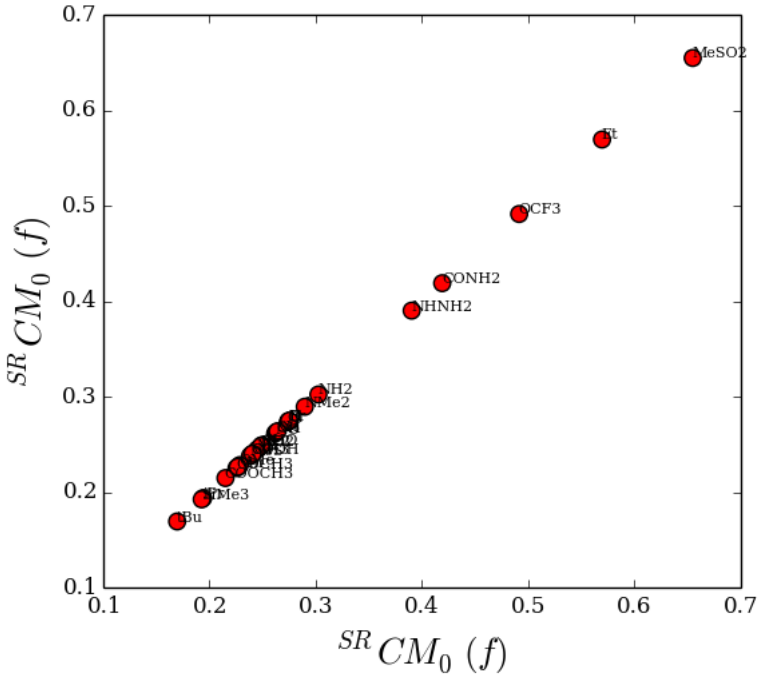
113	**$^{SR}CM_q$ (ab)**	**$^{SR}CM_q$ (ab)**
114	**$^{SR}CM_q$ (ab)**	**$^{SR}CM_0$ (a)**
115	**$^{SR}CM_q$ (ab)**	**$^{SR}CM_L$ (a)**
116	**$^{SR}CM_q$ (ab)**	**$^{SR}CM_M$ (a)**
117	**$^{SR}CM_q$ (ab)**	**$^{SR}CM_q$ (a)**
118	**$^{SR}CM_q$ (ab)**	**CCM (f)**
119	**$^{SR}CM_q$ (ab)**	**CCM (ab)**
120	**$^{SR}CM_q$ (ab)**	**CCM (a)**
121	**$^{SR}CM_0$ (a)**	**$^{SR}CM_0$ (f)**
122	**$^{SR}CM_0$ (a)**	**$^{SR}CM_L$ (f)**
123	**$^{SR}CM_0$ (a)**	**$^{SR}CM_M$ (f)**
124	**$^{SR}CM_0$ (a)**	**$^{SR}CM_q$ (f)**
125	**$^{SR}CM_0$ (a)**	**$^{SR}CM_0$ (ab)**
126	**$^{SR}CM_0$ (a)**	**$^{SR}CM_L$ (ab)**
127	**$^{SR}CM_0$ (a)**	**$^{SR}CM_M$ (ab)**
128	**$^{SR}CM_0$ (a)**	**$^{SR}CM_q$ (ab)**
129	**$^{SR}CM_0$ (a)**	**$^{SR}CM_0$ (a)**
130	**$^{SR}CM_0$ (a)**	**$^{SR}CM_L$ (a)**
131	**$^{SR}CM_0$ (a)**	**$^{SR}CM_M$ (a)**
132	**$^{SR}CM_0$ (a)**	**$^{SR}CM_q$ (a)**
133	**$^{SR}CM_0$ (a)**	**CCM (f)**
134	**$^{SR}CM_0$ (a)**	**CCM (ab)**
135	**$^{SR}CM_0$ (a)**	**CCM (a)**
136	**$^{SR}CM_L$ (a)**	**$^{SR}CM_0$ (f)**
137	**$^{SR}CM_L$ (a)**	**$^{SR}CM_L$ (f)**
138	**$^{SR}CM_L$ (a)**	**$^{SR}CM_M$ (f)**
139	**$^{SR}CM_L$ (a)**	**$^{SR}CM_q$ (f)**
140	**$^{SR}CM_L$ (a)**	**$^{SR}CM_0$ (ab)**
141	**$^{SR}CM_L$ (a)**	**$^{SR}CM_L$ (ab)**

142	**$^{SR}CM_L$ (a)**	**$^{SR}CM_M$ (ab)**
143	**$^{SR}CM_L$ (a)**	**$^{SR}CM_q$ (ab)**
144	**$^{SR}CM_L$ (a)**	**$^{SR}CM_0$ (a)**
145	**$^{SR}CM_L$ (a)**	**$^{SR}CM_L$ (a)**
146	**$^{SR}CM_L$ (a)**	**$^{SR}CM_M$ (a)**
147	**$^{SR}CM_L$ (a)**	**$^{SR}CM_q$ (a)**
148	**$^{SR}CM_L$ (a)**	**CCM (f)**
149	**$^{SR}CM_L$ (a)**	**CCM (ab)**
150	**$^{SR}CM_L$ (a)**	**CCM (a)**
151	**$^{SR}CM_M$ (a)**	**$^{SR}CM_0$ (f)**
152	**$^{SR}CM_M$ (a)**	**$^{SR}CM_L$ (f)**
153	**$^{SR}CM_M$ (a)**	**$^{SR}CM_M$ (f)**
154	**$^{SR}CM_M$ (a)**	**$^{SR}CM_q$ (f)**
155	**$^{SR}CM_M$ (a)**	**$^{SR}CM_0$ (ab)**
156	**$^{SR}CM_M$ (a)**	**$^{SR}CM_L$ (ab)**
157	**$^{SR}CM_M$ (a)**	**$^{SR}CM_M$ (ab)**
158	**$^{SR}CM_M$ (a)**	**$^{SR}CM_q$ (ab)**
159	**$^{SR}CM_M$ (a)**	**$^{SR}CM_0$ (a)**
160	**$^{SR}CM_M$ (a)**	**$^{SR}CM_L$ (a)**
161	**$^{SR}CM_M$ (a)**	**$^{SR}CM_M$ (a)**
162	**$^{SR}CM_M$ (a)**	**$^{SR}CM_q$ (a)**
163	**$^{SR}CM_M$ (a)**	**CCM (f)**
164	**$^{SR}CM_M$ (a)**	**CCM (ab)**
165	**$^{SR}CM_M$ (a)**	**CCM (a)**
166	**$^{SR}CM_q$ (a)**	**$^{SR}CM_0$ (f)**
167	**$^{SR}CM_q$ (a)**	**$^{SR}CM_L$ (f)**
168	**$^{SR}CM_q$ (a)**	**$^{SR}CM_M$ (f)**
169	**$^{SR}CM_q$ (a)**	**$^{SR}CM_q$ (f)**
170	**$^{SR}CM_q$ (a)**	**$^{SR}CM_0$ (ab)**

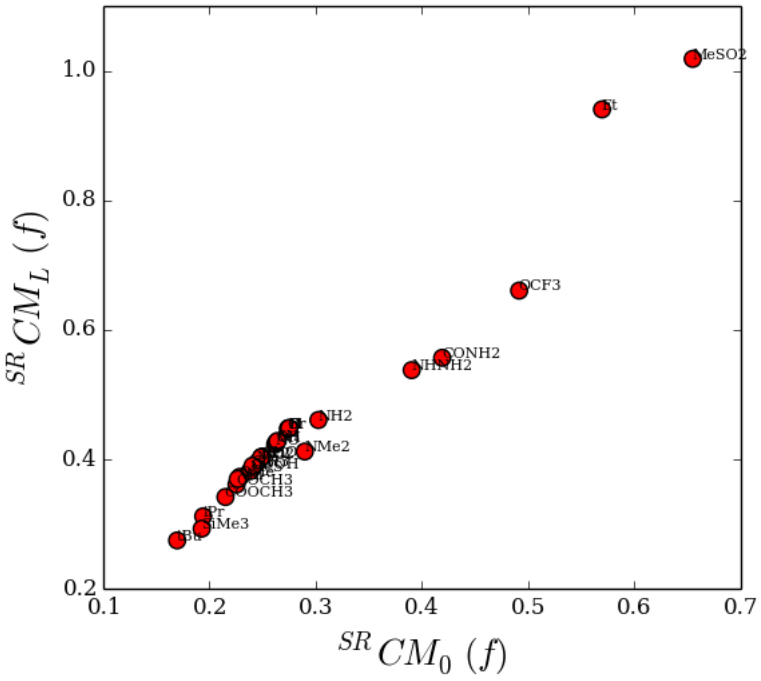
171	**$^{SR}CM_q$ (a)**	**$^{SR}CM_L$ (ab)**
172	**$^{SR}CM_q$ (a)**	**$^{SR}CM_M$ (ab)**
173	**$^{SR}CM_q$ (a)**	**$^{SR}CM_q$ (ab)**
174	**$^{SR}CM_q$ (a)**	**$^{SR}CM_0$ (a)**
175	**$^{SR}CM_q$ (a)**	**$^{SR}CM_L$ (a)**
176	**$^{SR}CM_q$ (a)**	**$^{SR}CM_M$ (a)**
177	**$^{SR}CM_q$ (a)**	**$^{SR}CM_q$ (a)**
178	**$^{SR}CM_q$ (a)**	**CCM (f)**
179	**$^{SR}CM_q$ (a)**	**CCM (ab)**
180	**$^{SR}CM_q$ (a)**	**CCM (a)**
181	**CCM (f)**	**$^{SR}CM_0$ (f)**
182	**CCM (f)**	**$^{SR}CM_L$ (f)**
183	**CCM (f)**	**$^{SR}CM_M$ (f)**
184	**CCM (f)**	**$^{SR}CM_q$ (f)**
185	**CCM (f)**	**$^{SR}CM_0$ (ab)**
186	**CCM (f)**	**$^{SR}CM_L$ (ab)**
187	**CCM (f)**	**$^{SR}CM_M$ (ab)**
188	**CCM (f)**	**$^{SR}CM_q$ (ab)**
189	**CCM (f)**	**$^{SR}CM_0$ (a)**
190	**CCM (f)**	**$^{SR}CM_L$ (a)**
191	**CCM (f)**	**$^{SR}CM_M$ (a)**
192	**CCM (f)**	**$^{SR}CM_q$ (a)**
193	**CCM (f)**	**CCM (f)**
194	**CCM (f)**	**CCM (ab)**
195	**CCM (f)**	**CCM (a)**
196	**CCM (ab)**	**$^{SR}CM_0$ (f)**
197	**CCM (ab)**	**$^{SR}CM_L$ (f)**
198	**CCM (ab)**	**$^{SR}CM_M$ (f)**
199	**CCM (ab)**	**$^{SR}CM_q$ (f)**

200	**CCM (ab)**	**$^{SR}CM_0$ (ab)**
201	**CCM (ab)**	**$^{SR}CM_L$ (ab)**
202	**CCM (ab)**	**$^{SR}CM_M$ (ab)**
203	**CCM (ab)**	**$^{SR}CM_q$ (ab)**
204	**CCM (ab)**	**$^{SR}CM_0$ (a)**
205	**CCM (ab)**	**$^{SR}CM_L$ (a)**
206	**CCM (ab)**	**$^{SR}CM_M$ (a)**
207	**CCM (ab)**	**$^{SR}CM_q$ (a)**
208	**CCM (ab)**	**CCM (f)**
209	**CCM (ab)**	**CCM (ab)**
210	**CCM (ab)**	**CCM (a)**
211	**CCM (a)**	**$^{SR}CM_0$ (f)**
212	**CCM (a)**	**$^{SR}CM_L$ (f)**
213	**CCM (a)**	**$^{SR}CM_M$ (f)**
214	**CCM (a)**	**$^{SR}CM_q$ (f)**
215	**CCM (a)**	**$^{SR}CM_0$ (ab)**
216	**CCM (a)**	**$^{SR}CM_L$ (ab)**
217	**CCM (a)**	**$^{SR}CM_M$ (ab)**
218	**CCM (a)**	**$^{SR}CM_q$ (ab)**
219	**CCM (a)**	**$^{SR}CM_0$ (a)**
220	**CCM (a)**	**$^{SR}CM_L$ (a)**
221	**CCM (a)**	**$^{SR}CM_M$ (a)**
222	**CCM (a)**	**$^{SR}CM_q$ (a)**
223	**CCM (a)**	**CCM (f)**
224	**CCM (a)**	**CCM (ab)**
225	**CCM (a)**	**CCM (a)**

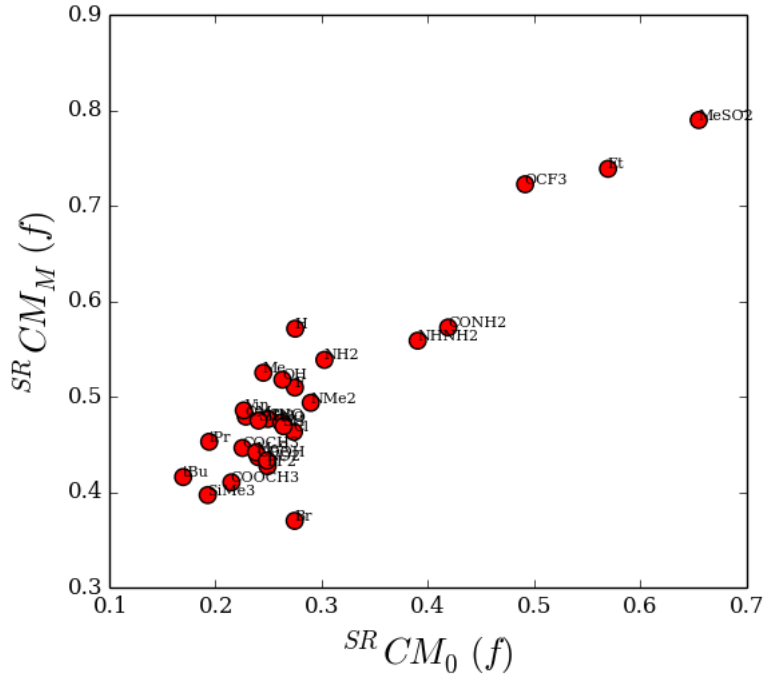
1


MeSO2
Et
OCF3
CONH2
NHNH2
NH2
NMe2
NMe3
tBu
$^{SR}CM_0\ (f)$
$^{SR}CM_0\ (f)$

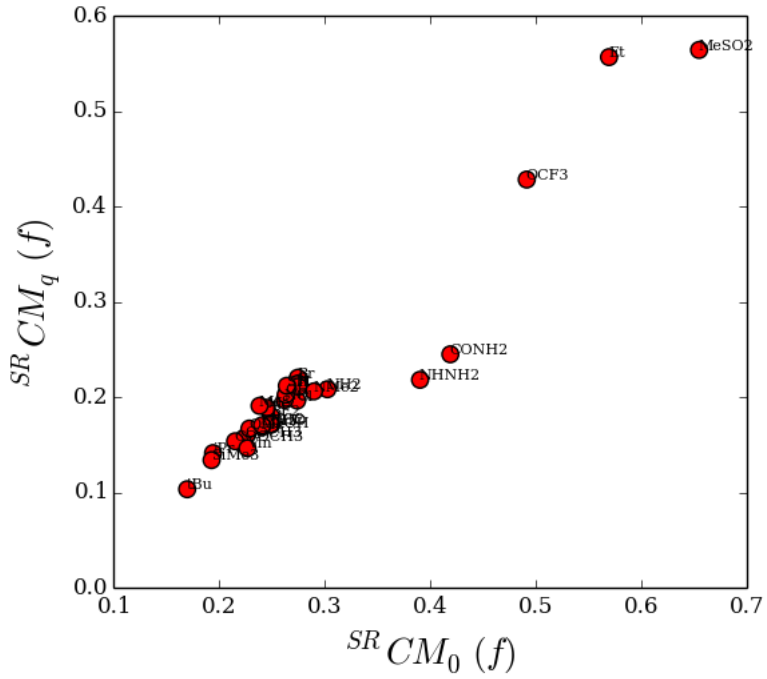
2


MeSO2
Et
OCF3
CONH2
NHNH2
NH2
NMe2
NMe3
tBu
$^{SR}CM_L\ (f)$
$^{SR}CM_0\ (f)$

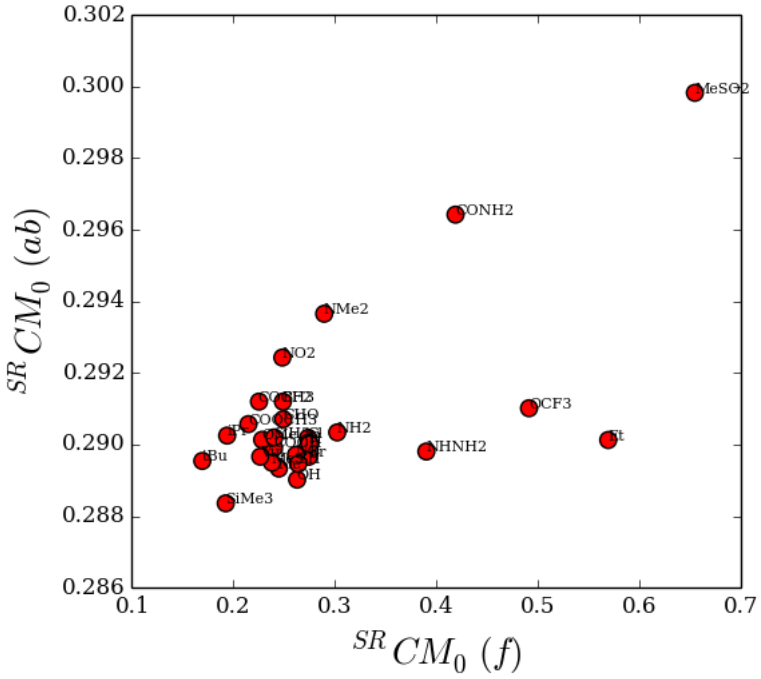
3


0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.1
0.2
0.3
0.4
0.5
0.6
0.7
$^{SR}CM_M\ (f)$
$^{SR}CM_0\ (f)$
MeSO2
OCF3
Et
CONH2
NHNH2
NH2
NMe2
iPr
tBu
COOCH3
SiMe3
Br

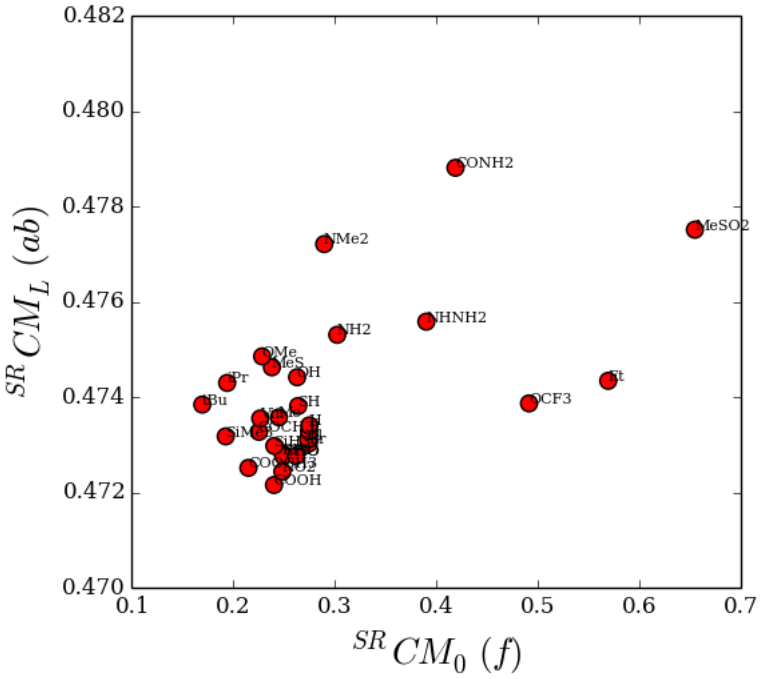
4


0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
$^{SR}CM_q\ (f)$
$^{SR}CM_0\ (f)$
MeSO2
Et
OCF3
CONH2
NHNH2
tBu

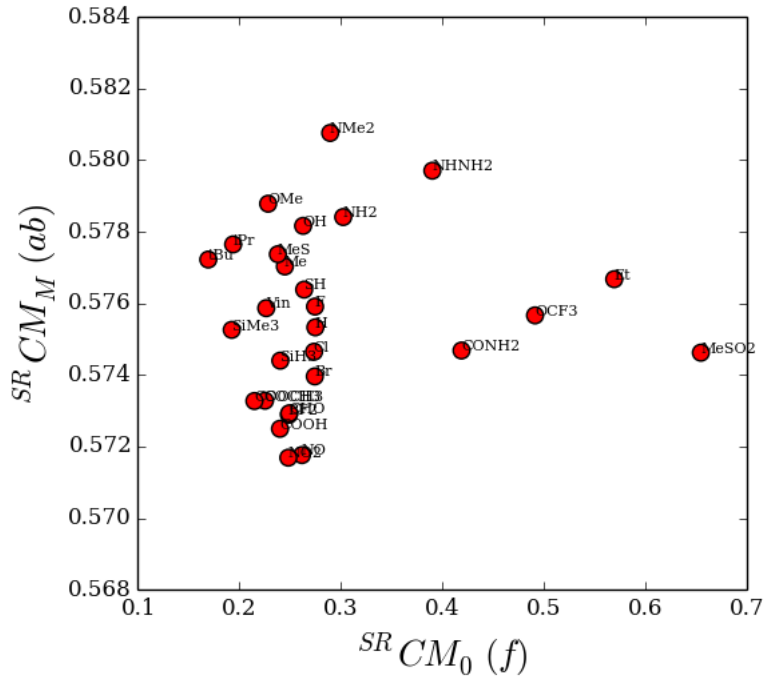
5


0.302
0.300
0.298
0.296
0.294
0.292
0.290
0.288
0.286
0.1
0.2
0.3
0.4
0.5
0.6
0.7
$^{SR}CM_0\ (ab)$
$^{SR}CM_0\ (f)$
SiMe3
OCF3
Et

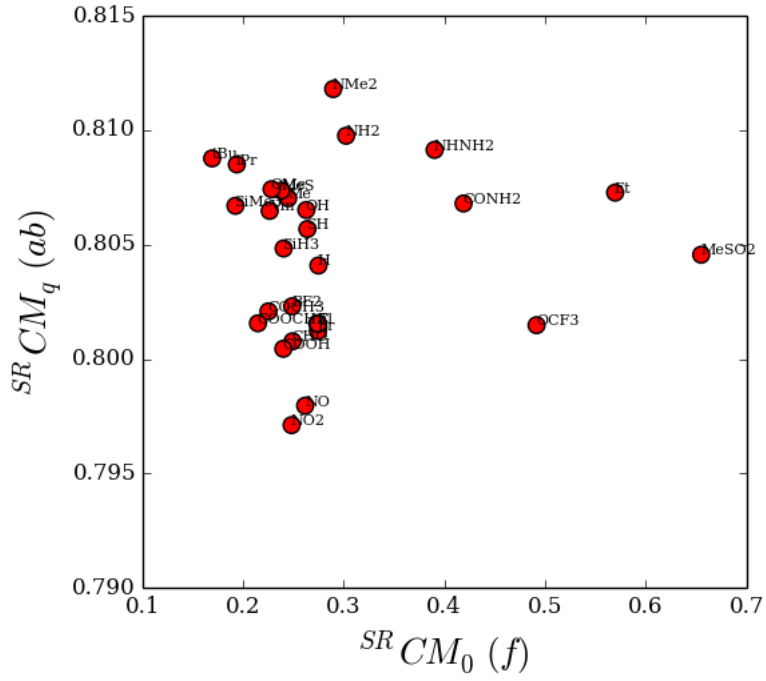
6


0.482
0.480
0.478
0.476
0.474
0.472
0.470
0.1
0.2
0.3
0.4
0.5
0.6
0.7
$^{SR}CM_L\ (ab)$
$^{SR}CM_0\ (f)$
OCF3
Et

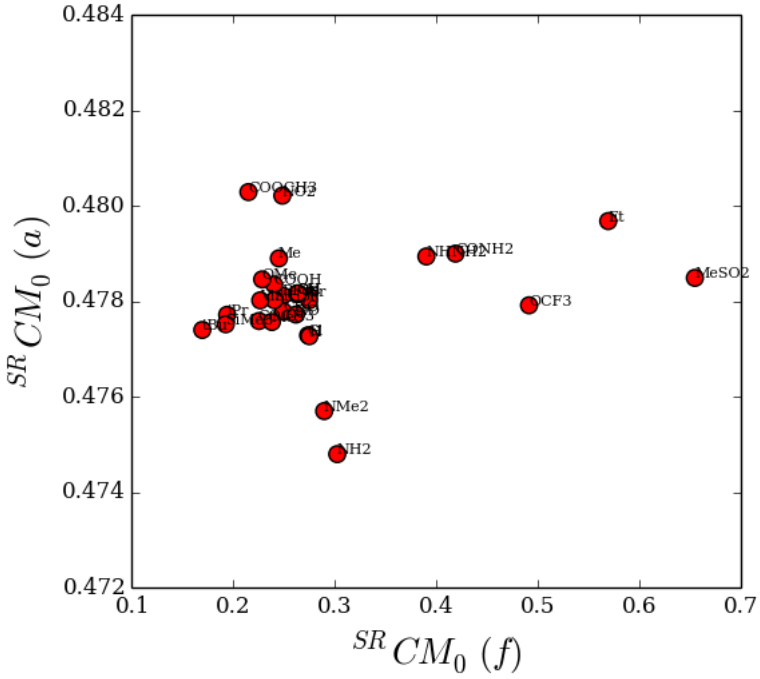
7


0.584
0.582
0.580
0.578
0.576
0.574
0.572
0.570
0.568
0.1
0.2
0.3
0.4
0.5
0.6
0.7
$^{SR}CM_M\ (ab)$
$^{SR}CM_0\ (f)$
NMe2
NHNH2
OMe
NH2
OH
Pr
Bu
MeS
Me
SH
Et
Min
OCF3
SiMe3
CONH2
MeSO2
SiH3
Br
OOH

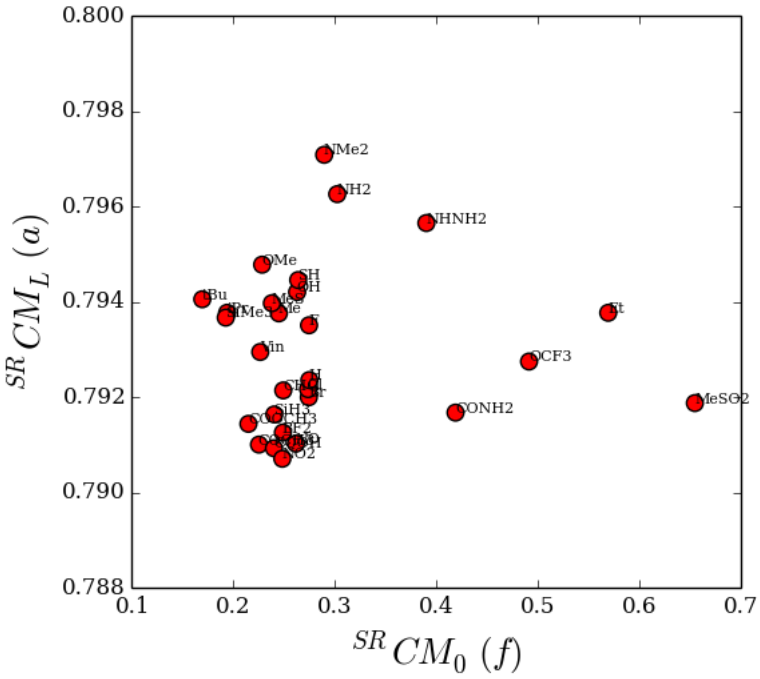
8


0.815
0.810
0.805
0.800
0.795
0.790
0.1
0.2
0.3
0.4
0.5
0.6
0.7
$^{SR}CM_q\ (ab)$
$^{SR}CM_0\ (f)$
NMe2
NH2
NHNH2
Bu
Pr
MeS
Me
SiMe3
OH
SH
SiH3
CONH2
Et
MeSO2
OCF3
OOH
NO
NO2

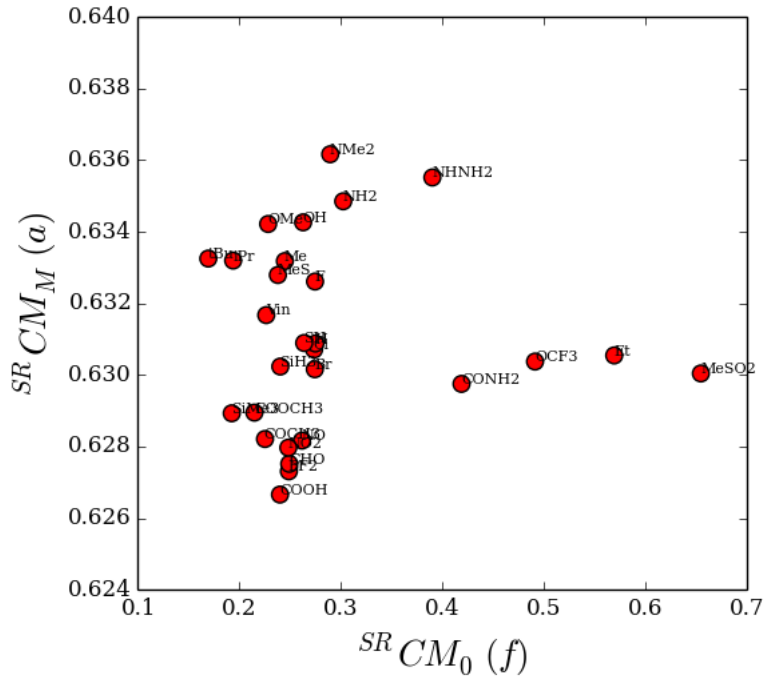
9


0.484
0.482
0.480
0.478
0.476
0.474
0.472
0.1
0.2
0.3
0.4
0.5
0.6
0.7
$^{SR}CM_0\ (a)$
$^{SR}CM_0\ (f)$
Et
MeSO2
OCF3
NMe2
NH2

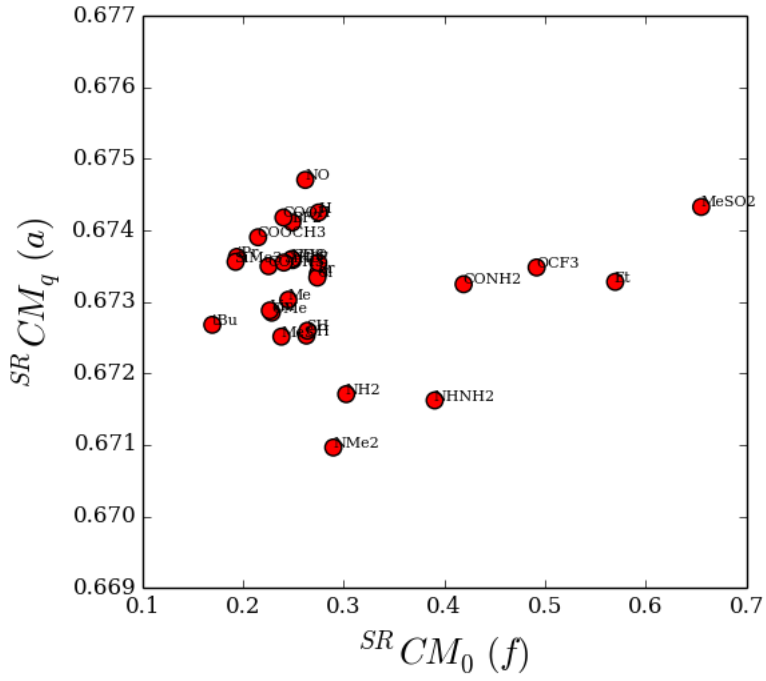
10


0.800
0.798
0.796
0.794
0.792
0.790
0.788
0.1
0.2
0.3
0.4
0.5
0.6
0.7
$^{SR}CM_L\ (a)$
$^{SR}CM_0\ (f)$
NMe2
NH2
NHNH2
OMe
Et
OCF3
MeSO2
CONH2

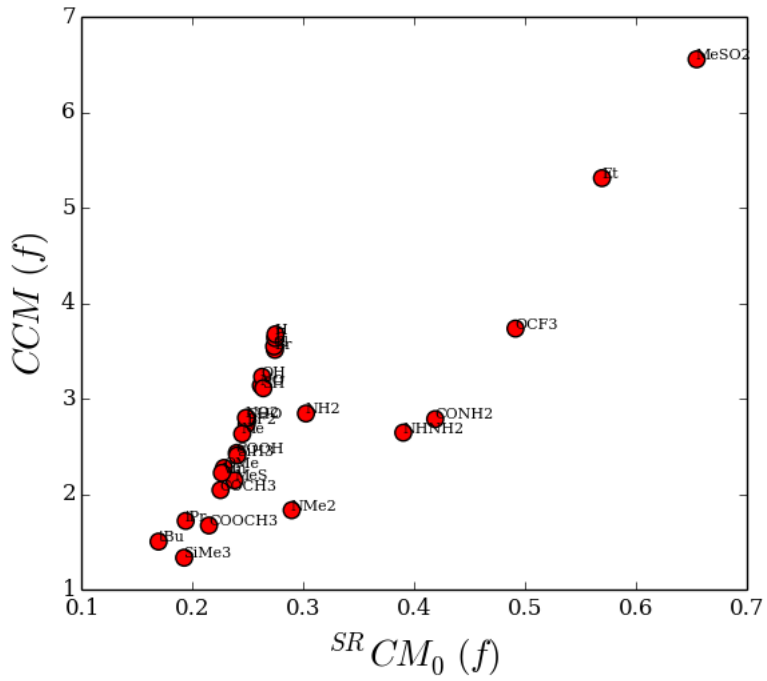
11


0.640
0.638
0.636
0.634
0.632
0.630
0.628
0.626
0.624
0.1
0.2
0.3
0.4
0.5
0.6
0.7
$^{SR}CM_M\ (a)$
$^{SR}CM_0\ (f)$
NMe2
NHNH2
NH2
OCF3
Et
MeSO2
CONH2
COOCH3
COOH

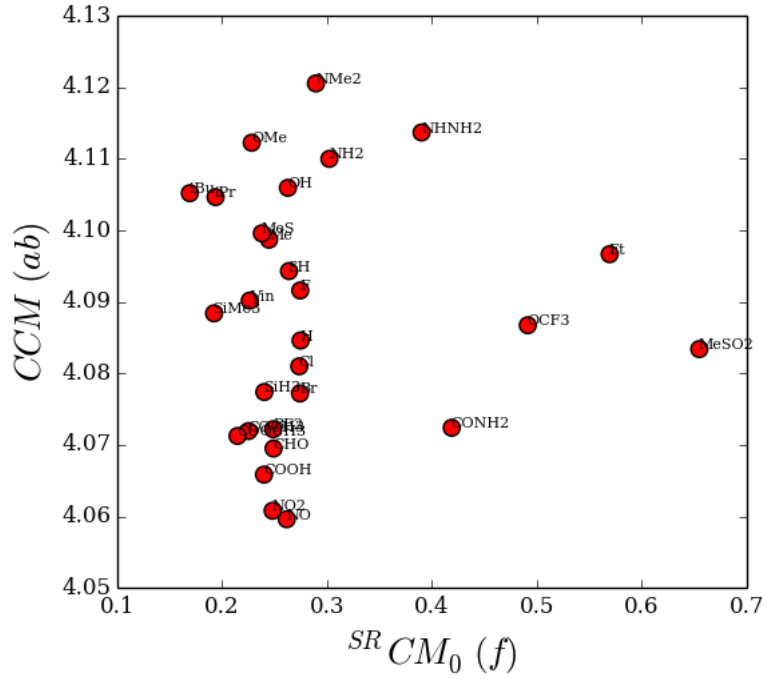
12


0.677
0.676
0.675
0.674
0.673
0.672
0.671
0.670
0.669
0.1
0.2
0.3
0.4
0.5
0.6
0.7
$^{SR}CM_q\ (a)$
$^{SR}CM_0\ (f)$
NO
MeSO2
COOCH3
OCF3
CONH2
Et
Me
tBu
NH2
NHNH2
NMe2

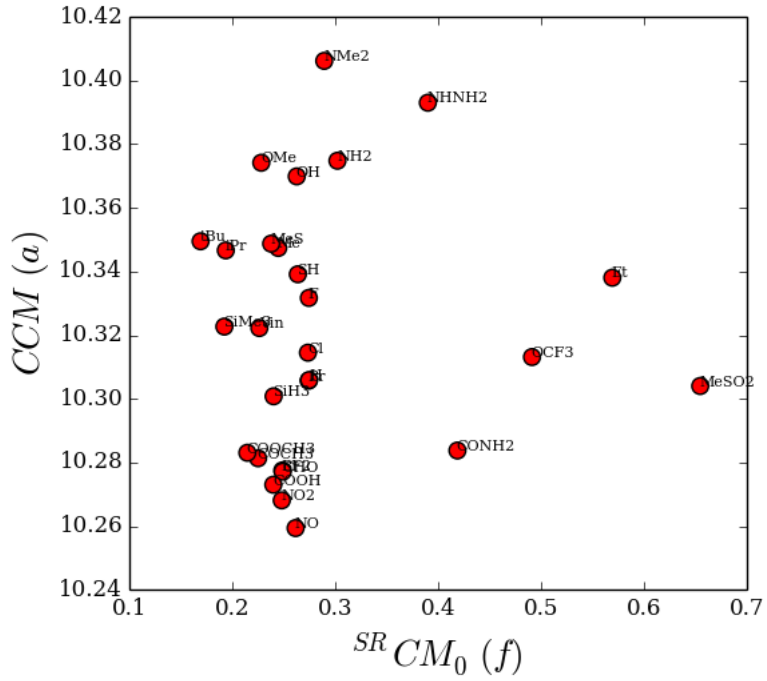
13


CCM (f)
SR CM0 (f)
MeSO2
Et
OCF3
NH2
CONH2
NHNH2
NMe2
OMe
OH
COOCH3
tBu
SiMe3

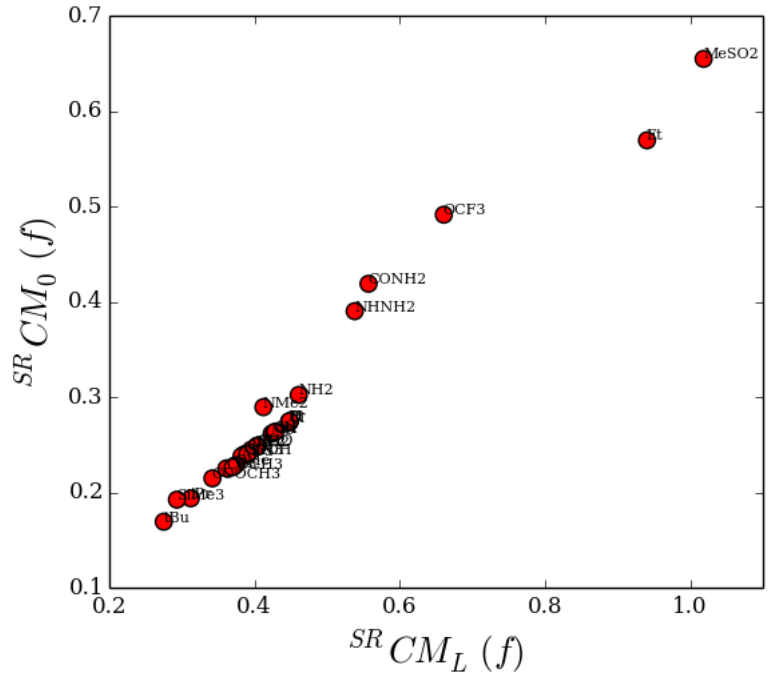
14


CCM (ab)
SR CM0 (f)
NMe2
NHNH2
OMe
NH2
OH
Et
OCF3
MeSO2
CONH2
SiMe3

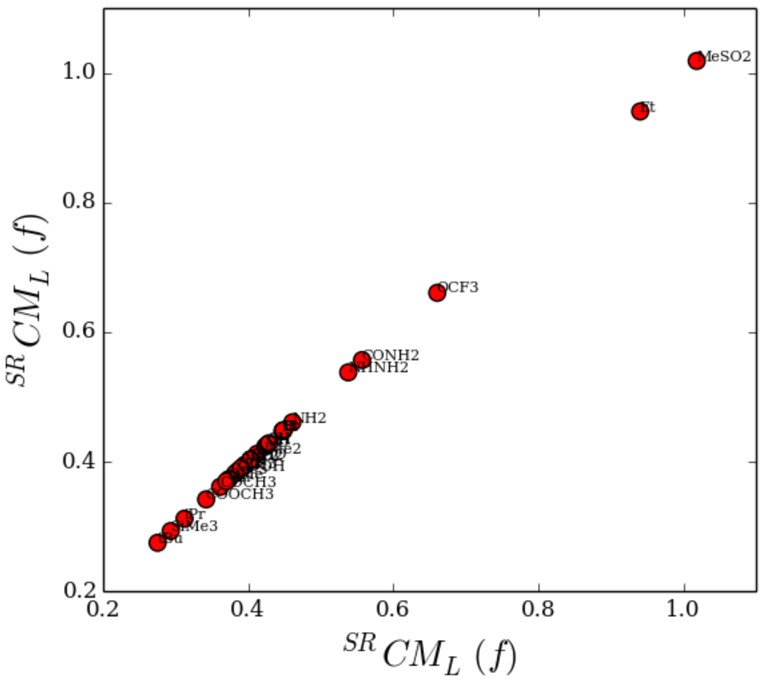
15


10.42
10.40
10.38
10.36
10.34
10.32
10.30
10.28
10.26
10.24
0.1
0.2
0.3
0.4
0.5
0.6
0.7
$CCM\ (a)$
$^{SR}CM_0\ (f)$
NMe2
NHNH2
OMe
NH2
OH
tBu
iPr
MeS
SH
Et
SiMe3
Sn
Cl
OCF3
MeSO2
SiH3
CONH2
COOH
NO2
NO

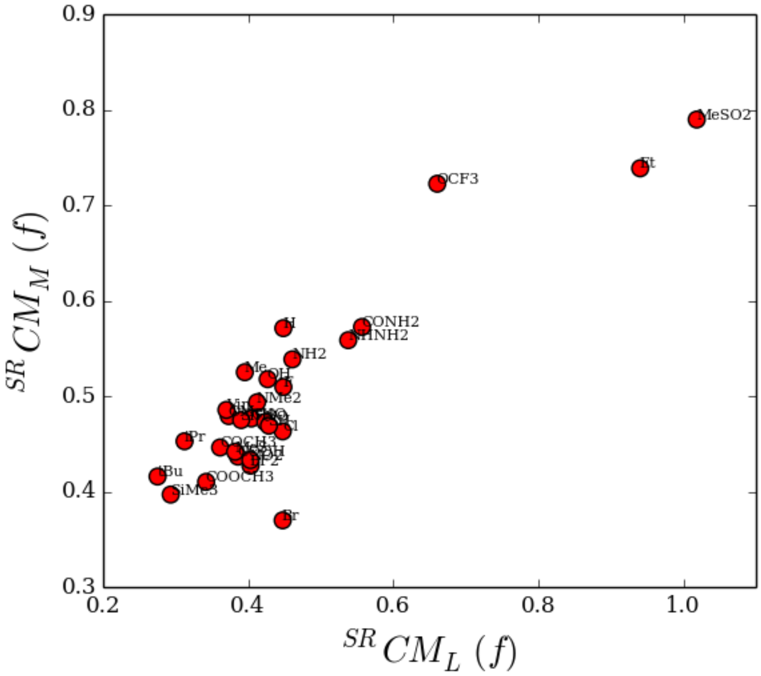
16


0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.2
0.4
0.6
0.8
1.0
$^{SR}CM_0\ (f)$
$^{SR}CM_L\ (f)$
MeSO2
Et
OCF3
CONH2
NHNH2
NH2
NMe2
OCH3
tBu

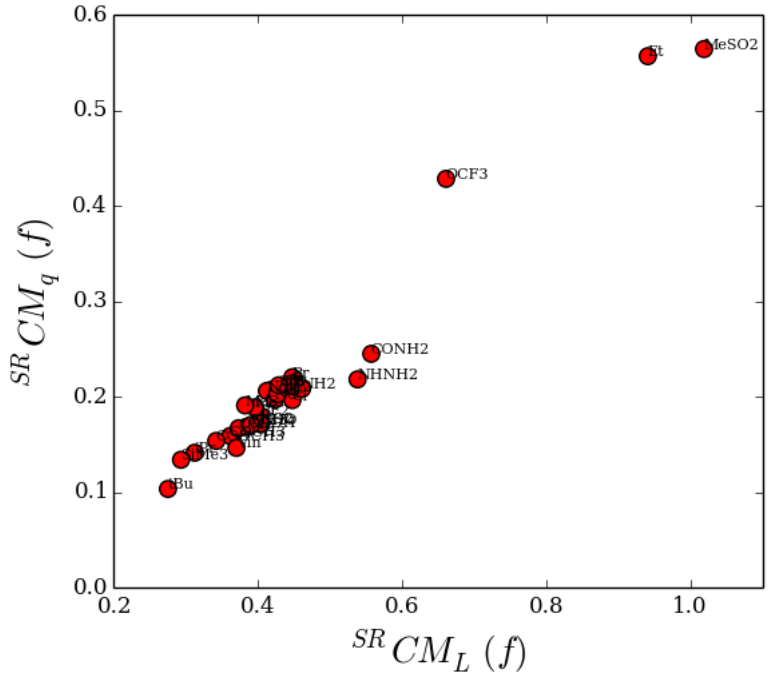
17


MeSO2
OCF3
CONH2
NH2
COOCH3
0.2
0.4
0.6
0.8
1.0
$^{SR}CM_L\ (f)$
$^{SR}CM_L\ (f)$

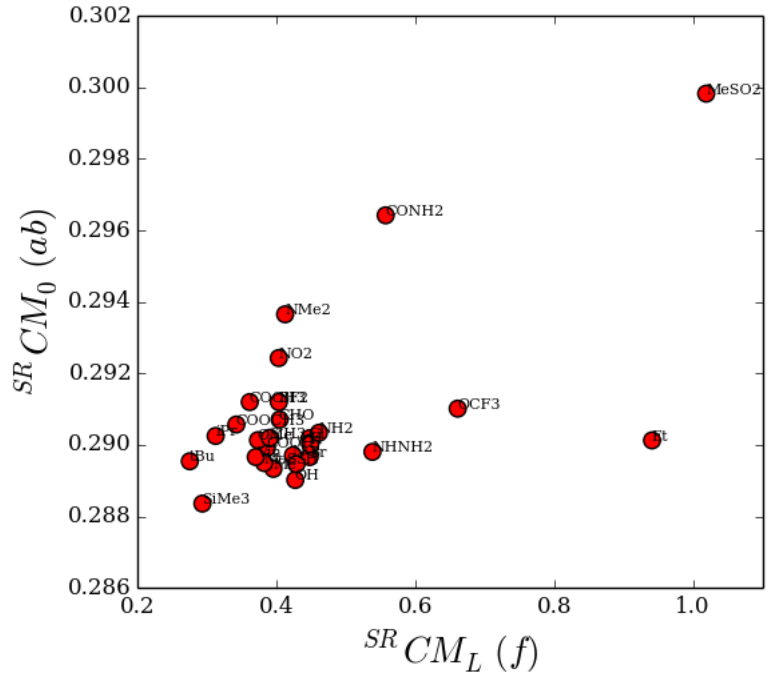
18


MeSO2
OCF3
CONH2
NH2
NMe2
COOCH3
0.3
0.4
0.5
0.6
0.7
0.8
0.9
0.2
0.4
0.6
0.8
1.0
$^{SR}CM_M\ (f)$
$^{SR}CM_L\ (f)$

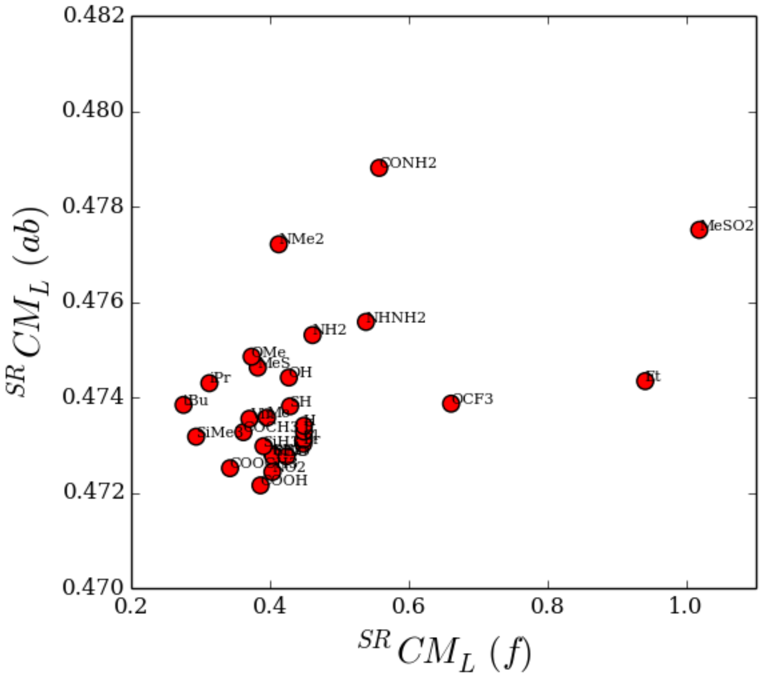
19


0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.2
0.4
0.6
0.8
1.0
$^{SR}CM_q\ (f)$
$^{SR}CM_L\ (f)$
MeSO2
OCF3
CONH2
NHNH2
tBu

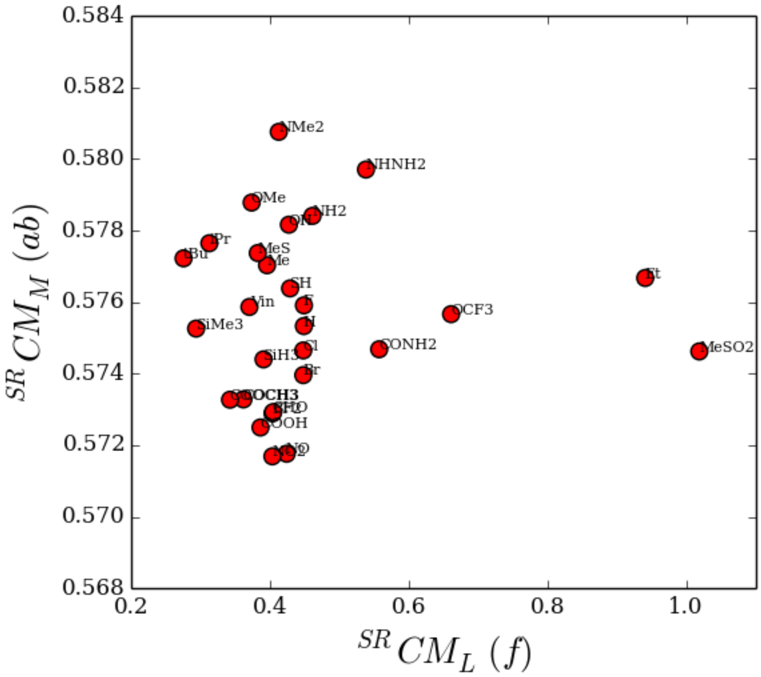
20


0.302
0.300
0.298
0.296
0.294
0.292
0.290
0.288
0.286
0.2
0.4
0.6
0.8
1.0
$^{SR}CM_0\ (ab)$
$^{SR}CM_L\ (f)$
MeSO2
CONH2
NMe2
OCF3
NHNH2
tBu
SiMe3

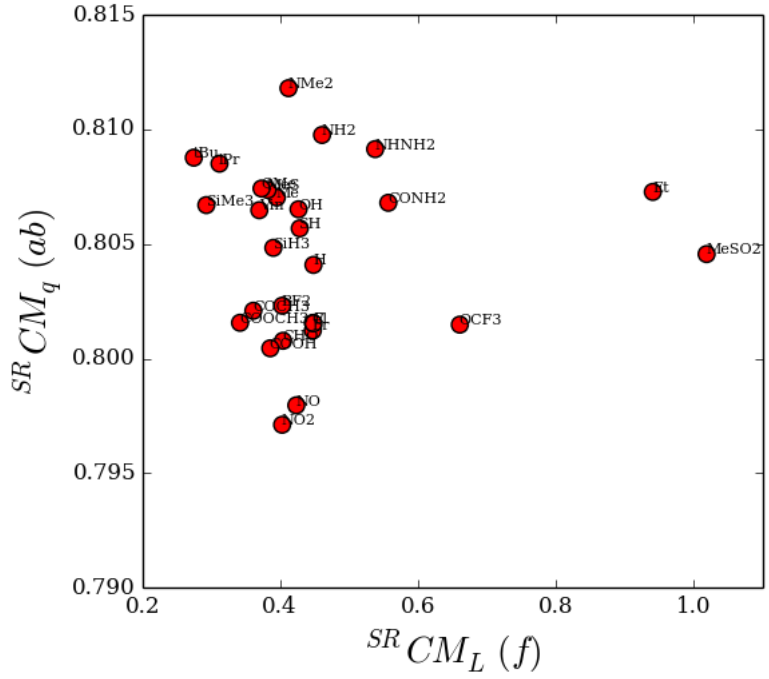
21


0.482
0.480
0.478
0.476
0.474
0.472
0.470
0.2
0.4
0.6
0.8
1.0
$^{SR}CM_L\ (ab)$
$^{SR}CM_L\ (f)$
CONH2
MeSO2
NMe2
NHNH2
NH2
OMe
MeS
OH
iPr
tBu
SH
OCF3
Et
SiMe3
COOH

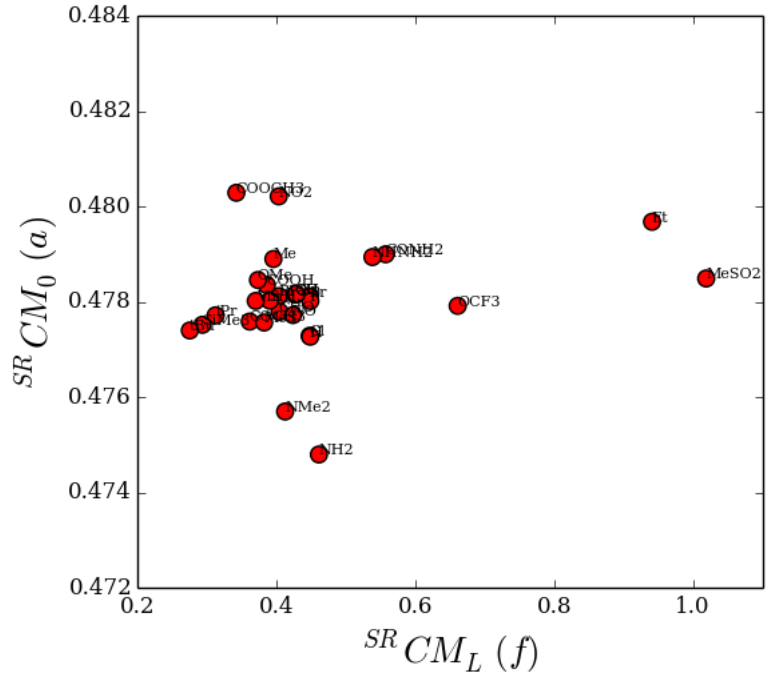
22


0.584
0.582
0.580
0.578
0.576
0.574
0.572
0.570
0.568
0.2
0.4
0.6
0.8
1.0
$^{SR}CM_M\ (ab)$
$^{SR}CM_L\ (f)$
NMe2
NHNH2
OMe
NH2
iPr
tBu
MeS
Me
SH
Vin
Et
OCF3
SiMe3
CONH2
MeSO2
SiH3
Br
COOH

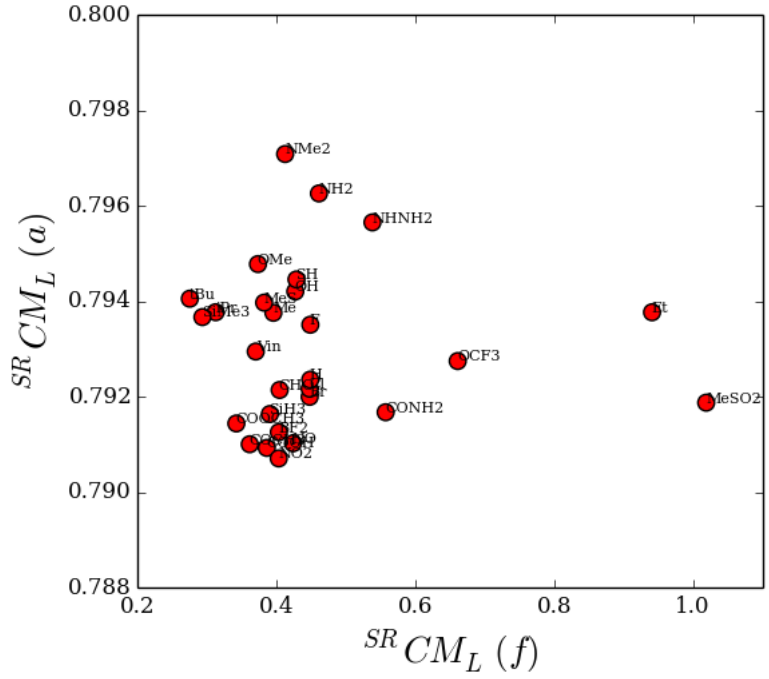
23


0.815
0.810
0.805
0.800
0.795
0.790
0.2
0.4
0.6
0.8
1.0
$^{SR}CM_q\ (ab)$
$^{SR}CM_L\ (f)$
NMe2
NH2
NHNH2
CONH2
Et
MeSO2
OCF3
NO
NO2

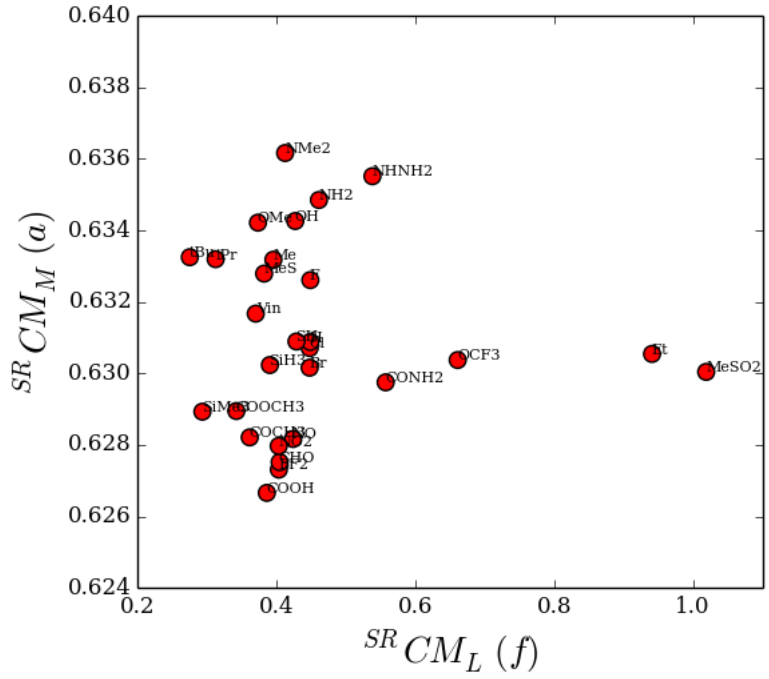
24


0.484
0.482
0.480
0.478
0.476
0.474
0.472
0.2
0.4
0.6
0.8
1.0
$^{SR}CM_0\ (a)$
$^{SR}CM_L\ (f)$
Et
MeSO2
OCF3
NMe2
NH2

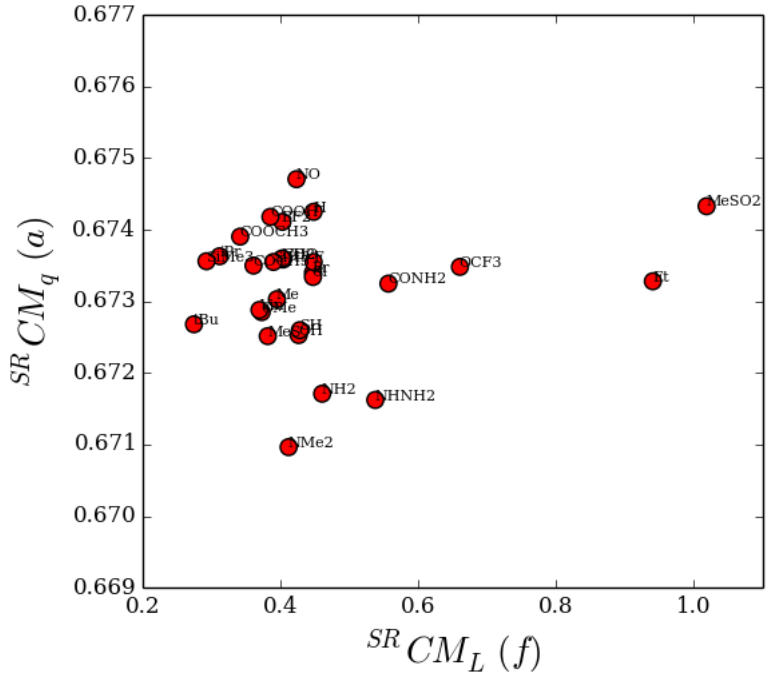
25


0.800
0.798
0.796
0.794
0.792
0.790
0.788
0.2
0.4
0.6
0.8
1.0
$^{SR}CM_L\ (a)$
$^{SR}CM_L\ (f)$
NMe2
NH2
NHNH2
OMe
Et
OCF3
MeSO2
CONH2

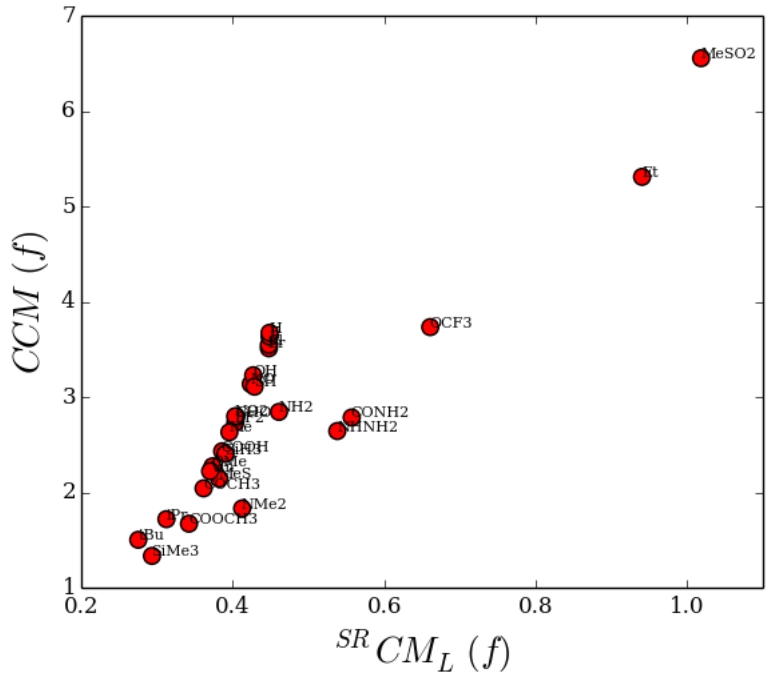
26


0.640
0.638
0.636
0.634
0.632
0.630
0.628
0.626
0.624
0.2
0.4
0.6
0.8
1.0
$^{SR}CM_M\ (a)$
$^{SR}CM_L\ (f)$
NMe2
NHNH2
NH2
Et
OCF3
MeSO2
CONH2
COOH

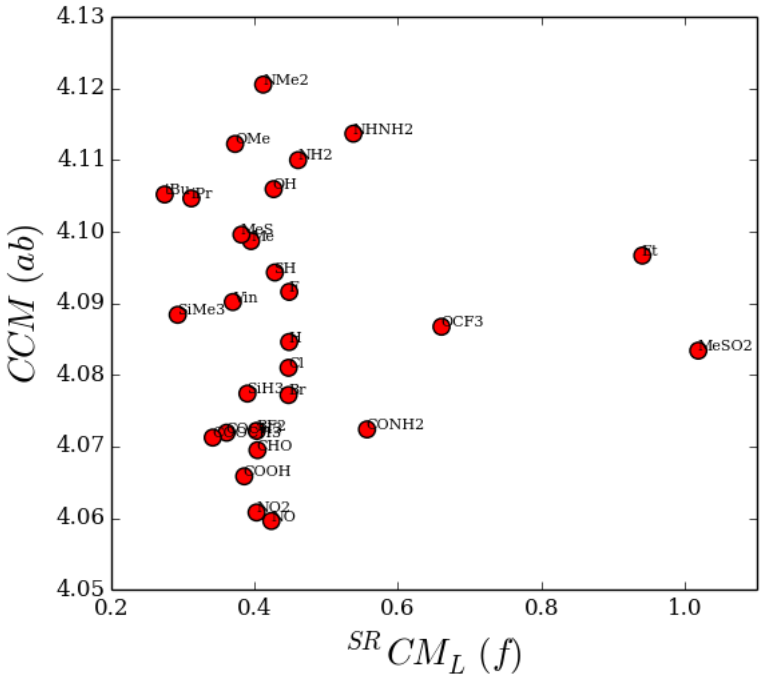
27


0.677
0.676
0.675
0.674
0.673
0.672
0.671
0.670
0.669
0.2
0.4
0.6
0.8
1.0
$^{SR}CM_q\ (a)$
$^{SR}CM_L\ (f)$
NO
MeSO2
COOCH3
OCF3
CONH2
Et
tBu
NHNH2
NMe2

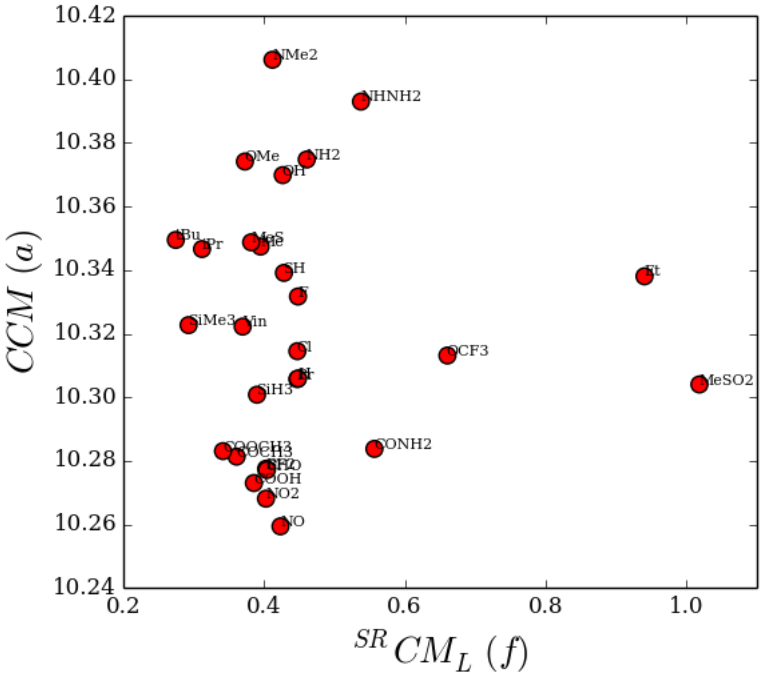
28


7
6
5
4
3
2
1
0.2
0.4
0.6
0.8
1.0
$CCM\ (f)$
$^{SR}CM_L\ (f)$
MeSO2
Et
OCF3
CONH2
NHNH2
CH3
NMe2
COOCH3
tBu
SiMe3

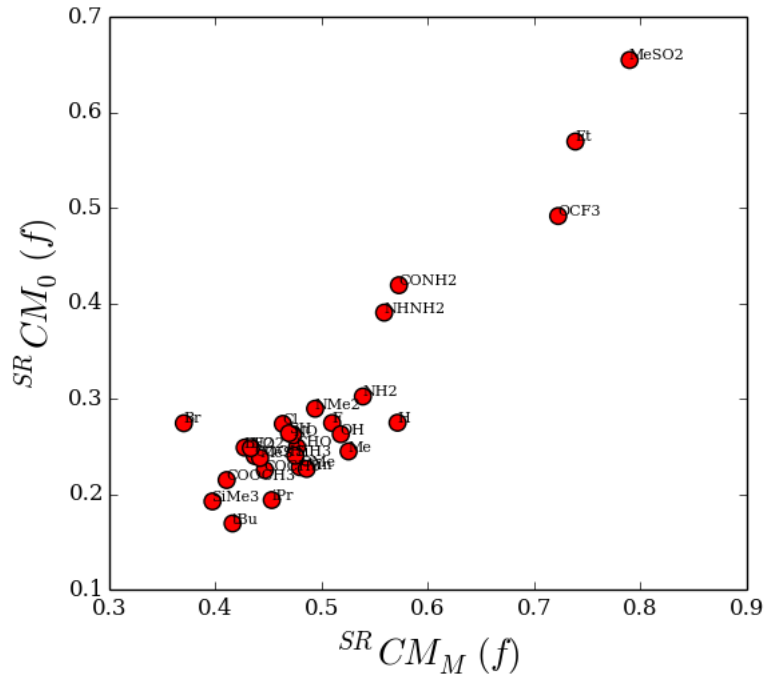
29


4.13
4.12
4.11
4.10
4.09
4.08
4.07
4.06
4.05
0.2
0.4
0.6
0.8
1.0
$CCM\ (ab)$
$^{SR}CM_L\ (f)$
NMe2
NHNH2
OMe
NH2
OH
Et
SiH3
OCF3
MeSO2
CONH2
CHO
COOH
NO2

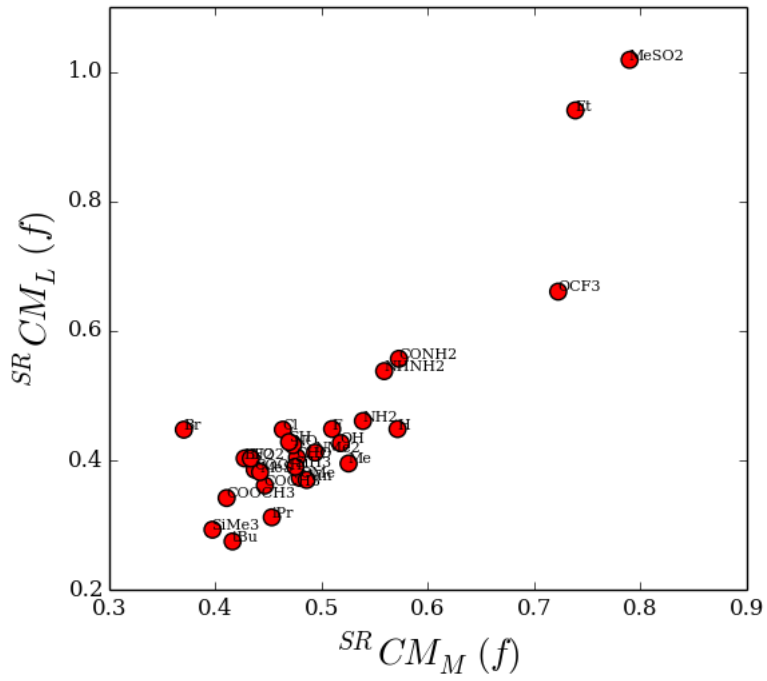
30


10.42
10.40
10.38
10.36
10.34
10.32
10.30
10.28
10.26
10.24
0.2
0.4
0.6
0.8
1.0
$CCM\ (a)$
$^{SR}CM_L\ (f)$
NMe2
NHNH2
OMe
NH2
OH
Et
SiH3
OCF3
MeSO2
CONH2
COOH
NO2

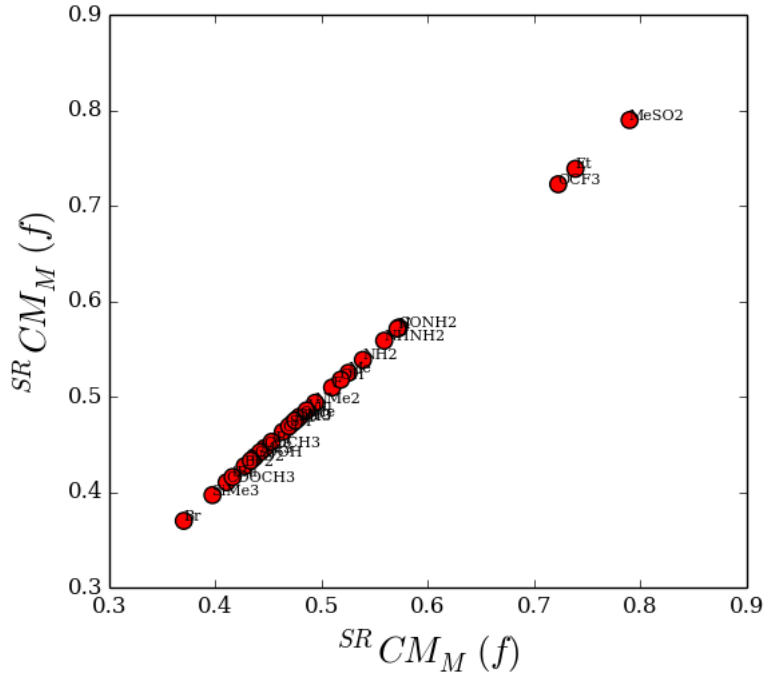
31


0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.3
0.4
0.5
0.6
0.7
0.8
0.9
$^{SR}CM_0\ (f)$
$^{SR}CM_M\ (f)$
MeSO2
Et
OCF3
CONH2
NHNH2
NH2
NMe2
Br
OH
Me
SiMe3
iPr
tBu

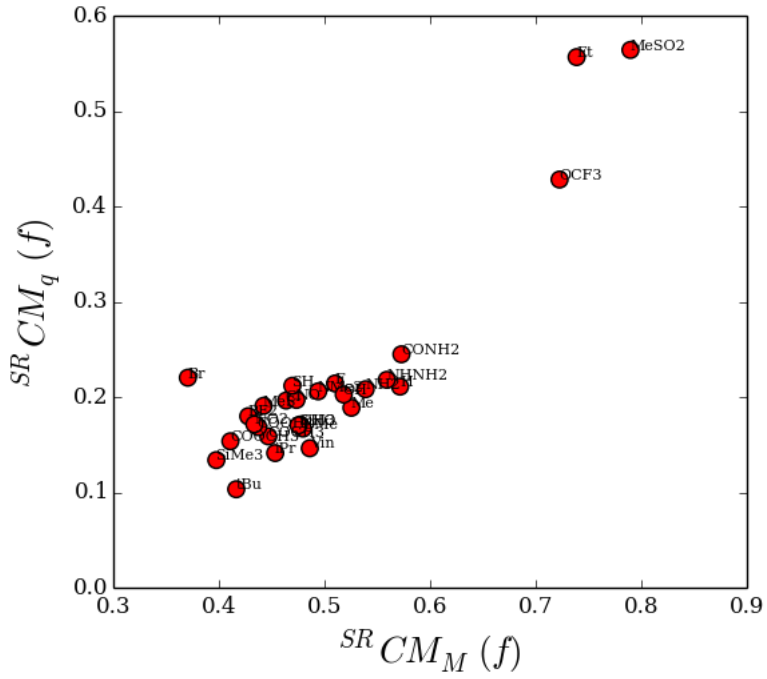
32


1.0
0.8
0.6
0.4
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
$^{SR}CM_L\ (f)$
$^{SR}CM_M\ (f)$
MeSO2
Et
OCF3
CONH2
NHNH2
NH2
Br
OH
Me
iPr
SiMe3
tBu

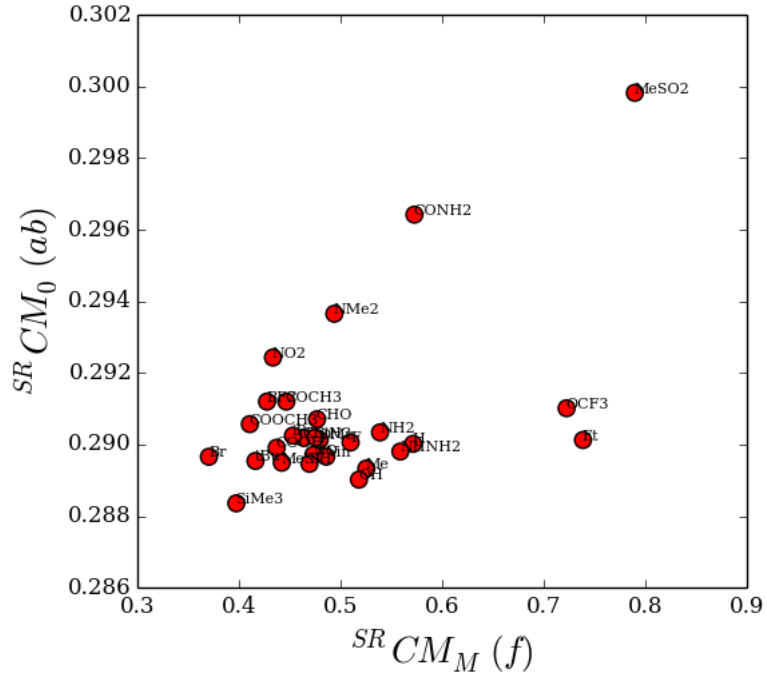
33


0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.3
0.4
0.5
0.6
0.7
0.8
0.9
$^{SR}CM_M\ (f)$
$^{SR}CM_M\ (f)$
MeSO2
Et
OCF3
SONH2
HNH2
NH2
Me2
OCH3
OCH3
SiMe3
Br

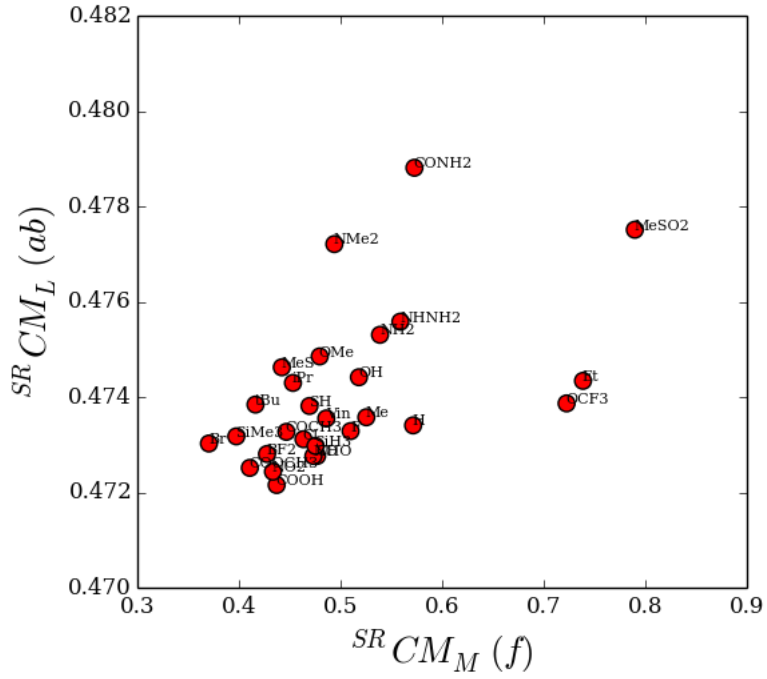
34


0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.3
0.4
0.5
0.6
0.7
0.8
0.9
$^{SR}CM_q\ (f)$
$^{SR}CM_M\ (f)$
Et
MeSO2
OCF3
SONH2
HNH2
Br
SiMe3
tBu

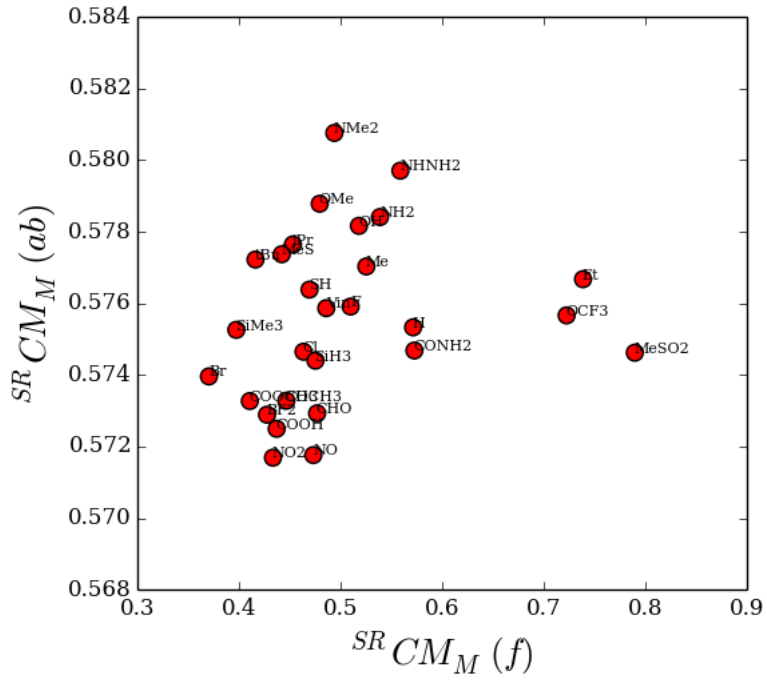
35


0.302
0.300
0.298
0.296
0.294
0.292
0.290
0.288
0.286
0.3
0.4
0.5
0.6
0.7
0.8
0.9
$^{SR}CM_0\ (ab)$
$^{SR}CM_M\ (f)$
MeSO2
CONH2
NMe2
NO2
OCF3
Et
NHNH2
Me
SiMe3

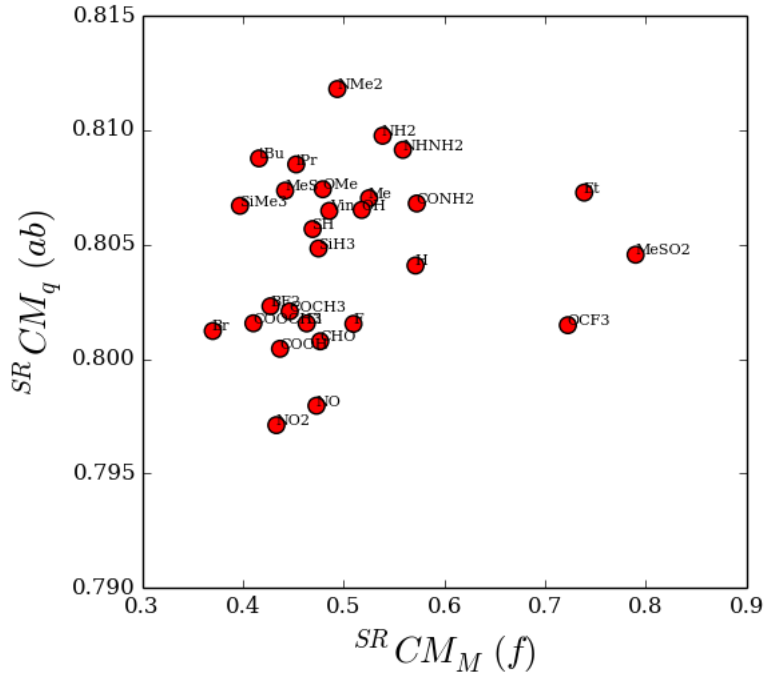
36


0.482
0.480
0.478
0.476
0.474
0.472
0.470
0.3
0.4
0.5
0.6
0.7
0.8
0.9
$^{SR}CM_L\ (ab)$
$^{SR}CM_M\ (f)$
CONH2
MeSO2
NMe2
NHNH2
OMe
OH
Et
OCF3
Me
SiMe3
COOH

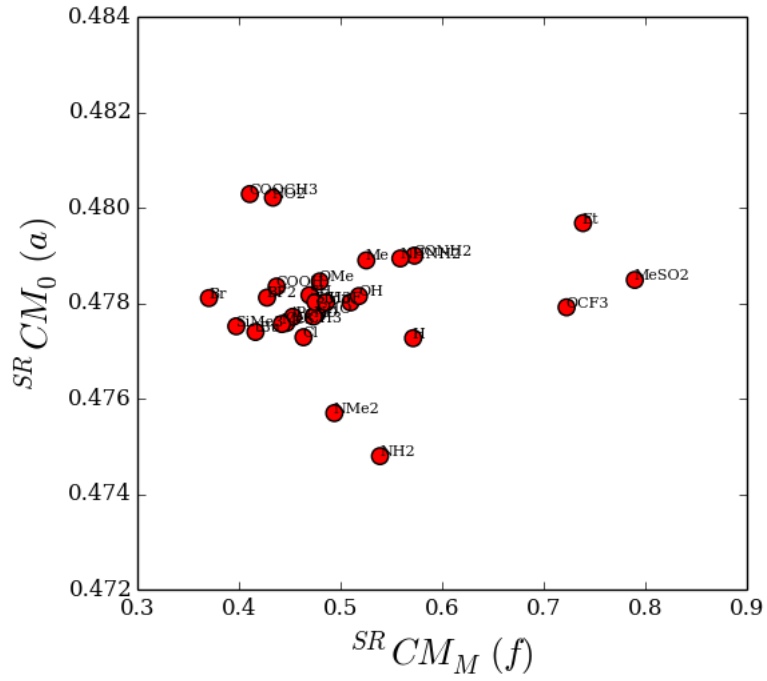
37


0.584
0.582
0.580
0.578
0.576
0.574
0.572
0.570
0.568
0.3
0.4
0.5
0.6
0.7
0.8
0.9
$^{SR}CM_M\ (ab)$
$^{SR}CM_M\ (f)$
NMe2
NHNH2
OMe
NH2
OH
Me
Et
OCF3
SiMe3
CONH2
MeSO2
SiH3
Br
CHO
COOH
NO2
NO

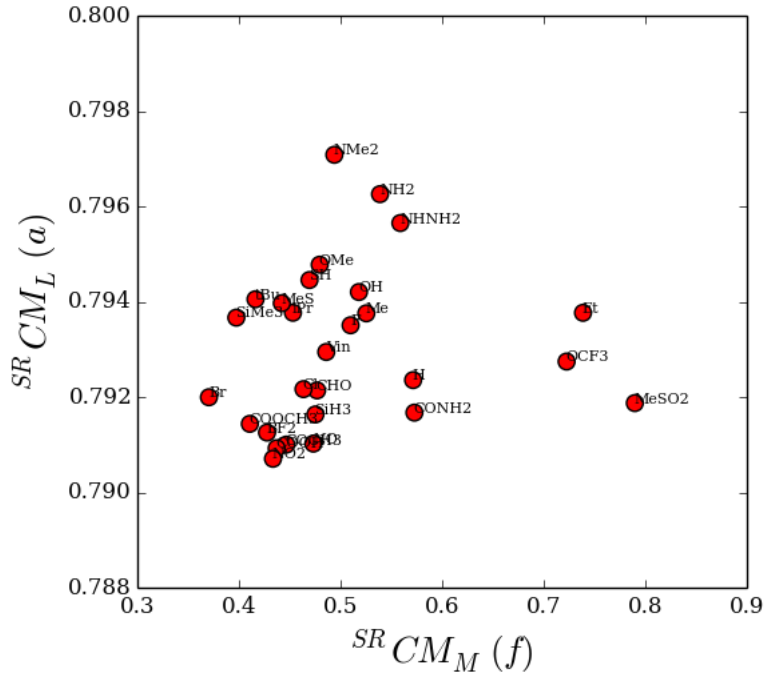
38


0.815
0.810
0.805
0.800
0.795
0.790
0.3
0.4
0.5
0.6
0.7
0.8
0.9
$^{SR}CM_q\ (ab)$
$^{SR}CM_M\ (f)$
NMe2
NH2
NHNH2
OMe
Me
Et
CONH2
SiMe3
SiH3
MeSO2
OCF3
Br
CHO
NO
NO2

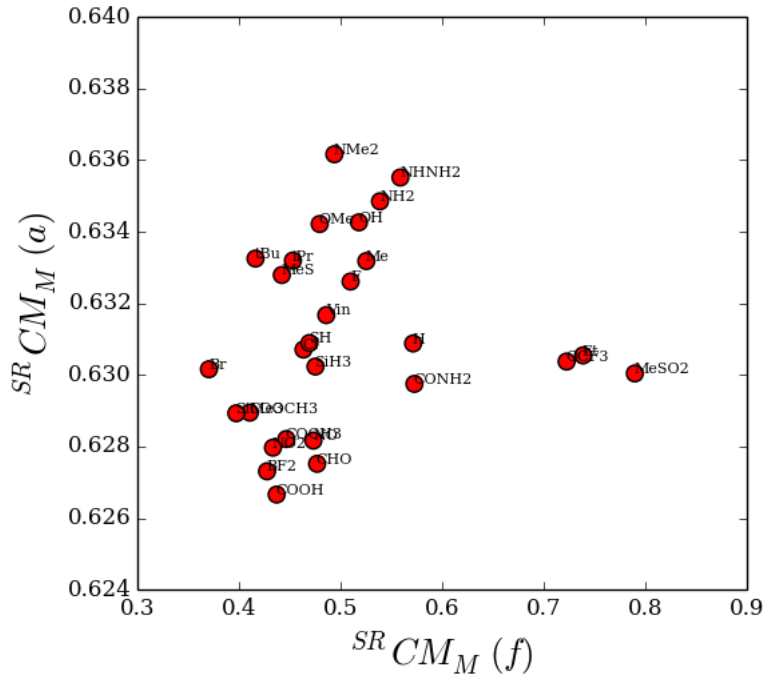
39


0.484
0.482
0.480
0.478
0.476
0.474
0.472
0.3
0.4
0.5
0.6
0.7
0.8
0.9
$^{SR}CM_0\ (a)$
$^{SR}CM_M\ (f)$
Et
MeSO2
OCF3
NMe2
NH2
Br

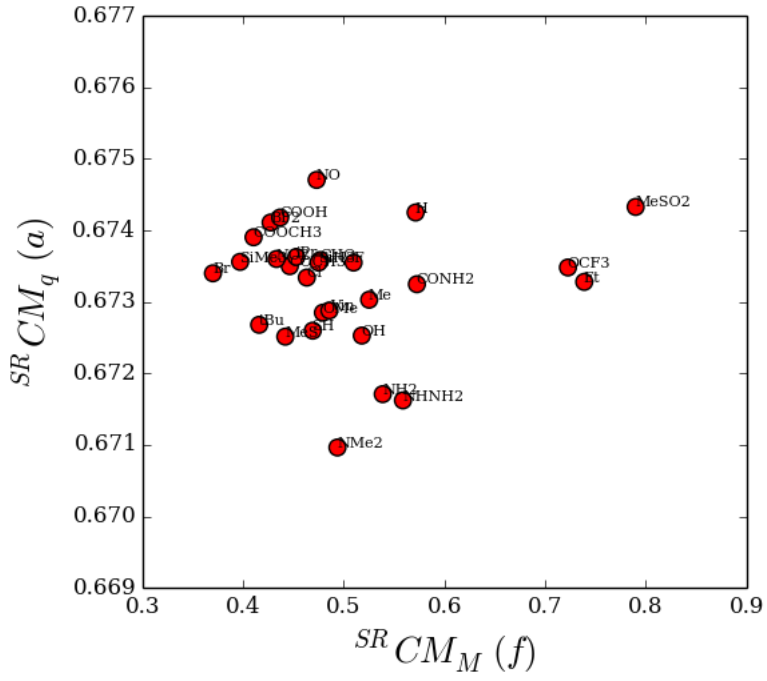
40


0.800
0.798
0.796
0.794
0.792
0.790
0.788
0.3
0.4
0.5
0.6
0.7
0.8
0.9
$^{SR}CM_L\ (a)$
$^{SR}CM_M\ (f)$
NMe2
NH2
NHNH2
OMe
OH
Et
OCF3
MeSO2
Br
CONH2

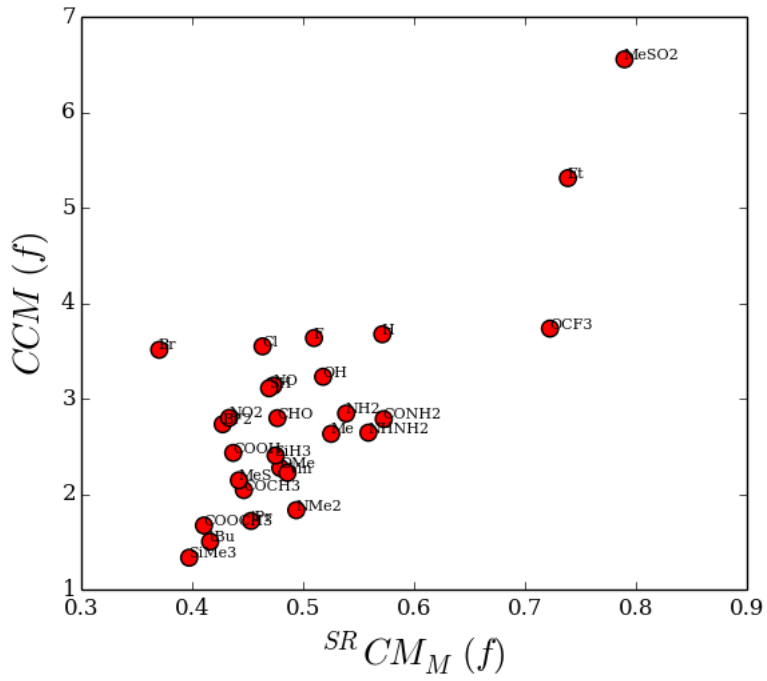
41


0.640
0.638
0.636
0.634
0.632
0.630
0.628
0.626
0.624
0.3
0.4
0.5
0.6
0.7
0.8
0.9
$^{SR}CM_M\ (a)$
$^{SR}CM_M\ (f)$
NMe2
NHNH2
NH2
OMe
OH
tBu
iPr
Me
F
Vin
SH
SiH3
Br
CONH2
MeSO2
COOCH3
CHO
BF2
COOH

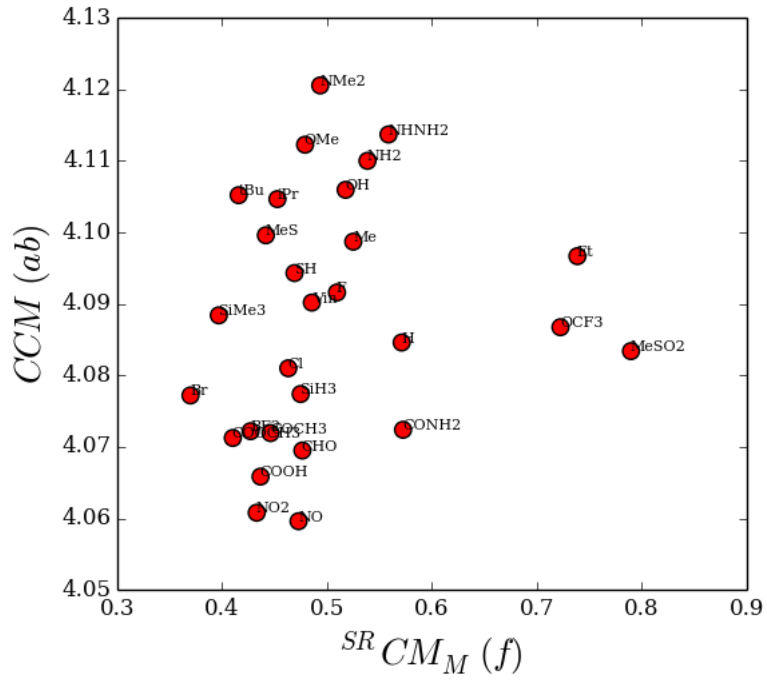
42


0.677
0.676
0.675
0.674
0.673
0.672
0.671
0.670
0.669
0.3
0.4
0.5
0.6
0.7
0.8
0.9
$^{SR}CM_q\ (a)$
$^{SR}CM_M\ (f)$
NO
MeSO2
COOH
COOCH3
Br
CONH2
OCF3
Me
tBu
OH
NH2
NHNH2
NMe2

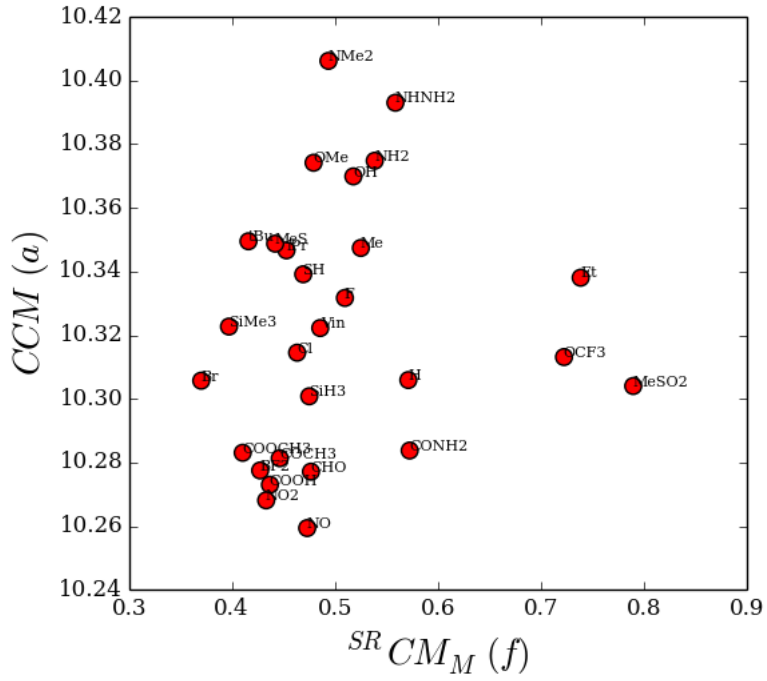
43


MeSO2
Et
OCF3
Br
Cl
F
I
OH
NO2
CHO
NH2
CONH2
Me
NHNH2
COOH
SiH3
OMe
SOCH3
NMe2
tBu
SiMe3
CCM (f)
SR CM_M (f)

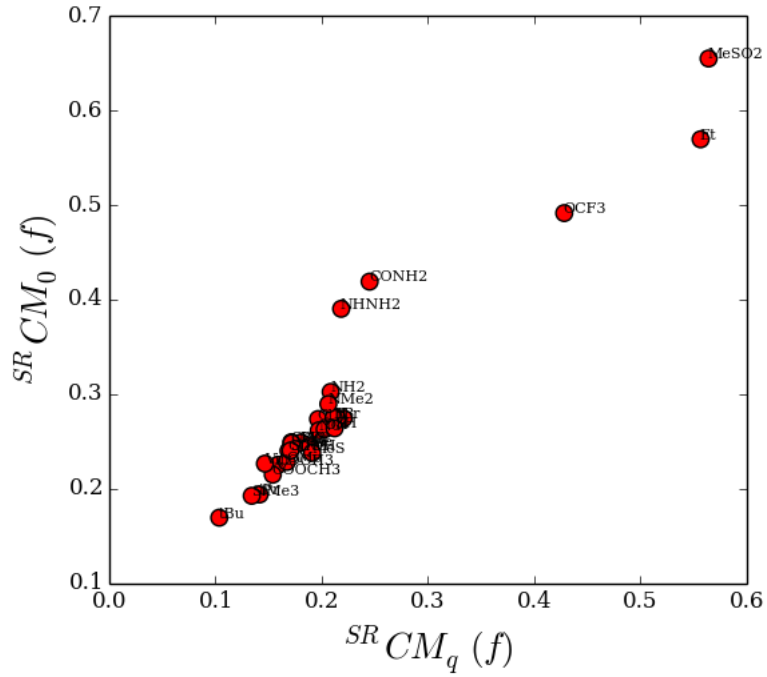
44


NMe2
OMe
NHNH2
NH2
OH
tBu
iPr
MeS
Me
Et
SH
F
SiMe3
OCF3
MeSO2
I
Cl
Br
SiH3
CONH2
SOCH3
CHO
COOH
NO2
NO
CCM (ab)
SR CM_M (f)

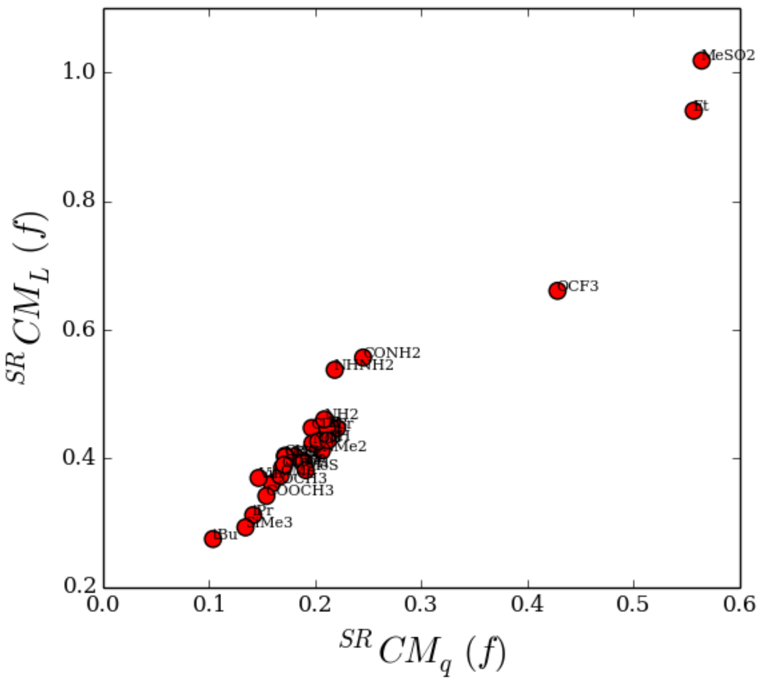
45


10.42
10.40
10.38
10.36
10.34
10.32
10.30
10.28
10.26
10.24
0.3
0.4
0.5
0.6
0.7
0.8
0.9
$CCM\ (a)$
$^{SR}CM_M\ (f)$
NMe2
NHNH2
OMe
NH2
OH
Me
SH
Et
SiMe3
Vin
OCF3
MeSO2
SiH3
CONH2
CHO
NO2
NO

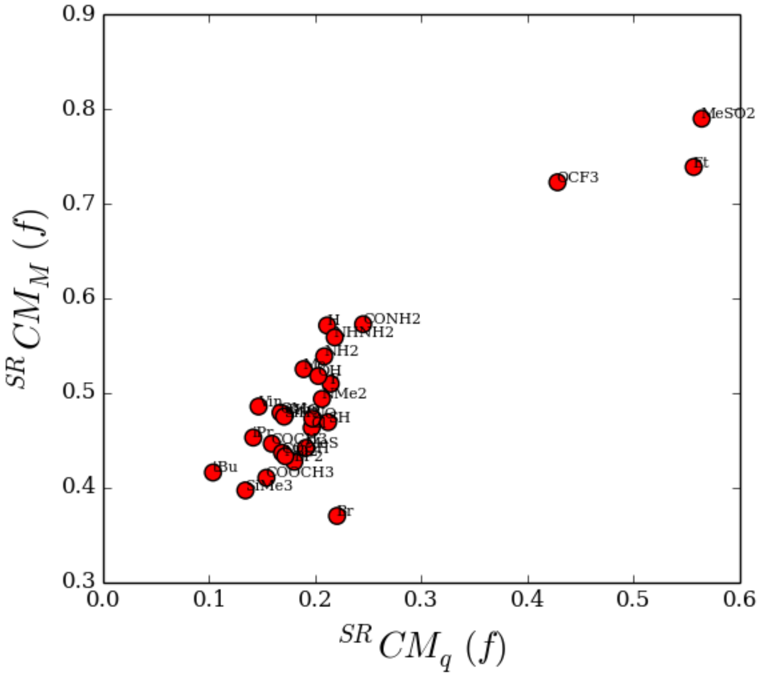
46


0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.1
0.2
0.3
0.4
0.5
0.6
$^{SR}CM_0\ (f)$
$^{SR}CM_q\ (f)$
MeSO2
Et
OCF3
CONH2
NHNH2
NH2
NMe2
tBu

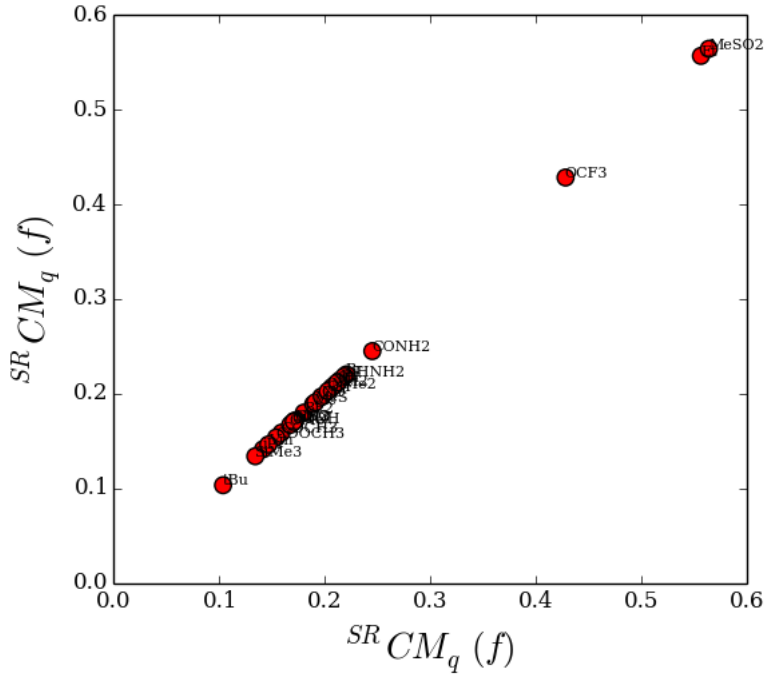
47



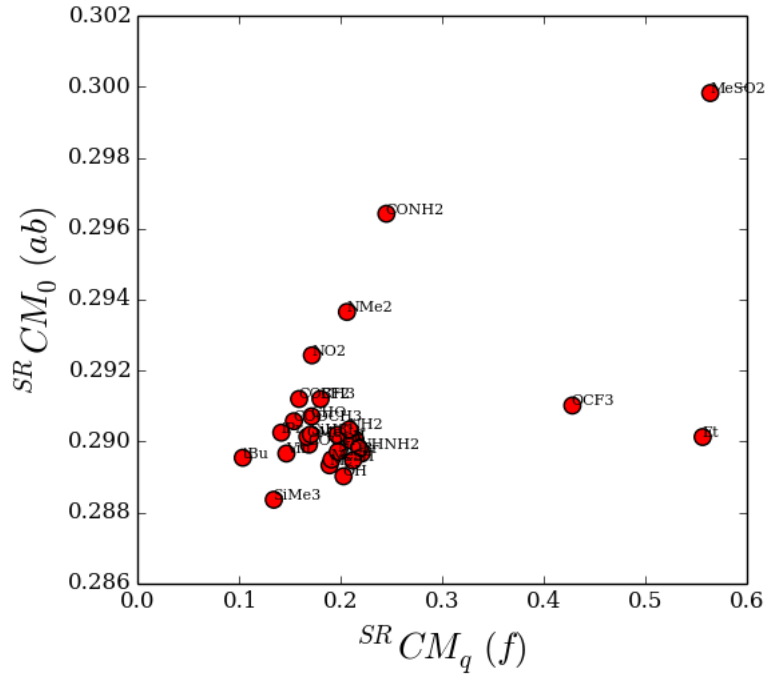
48



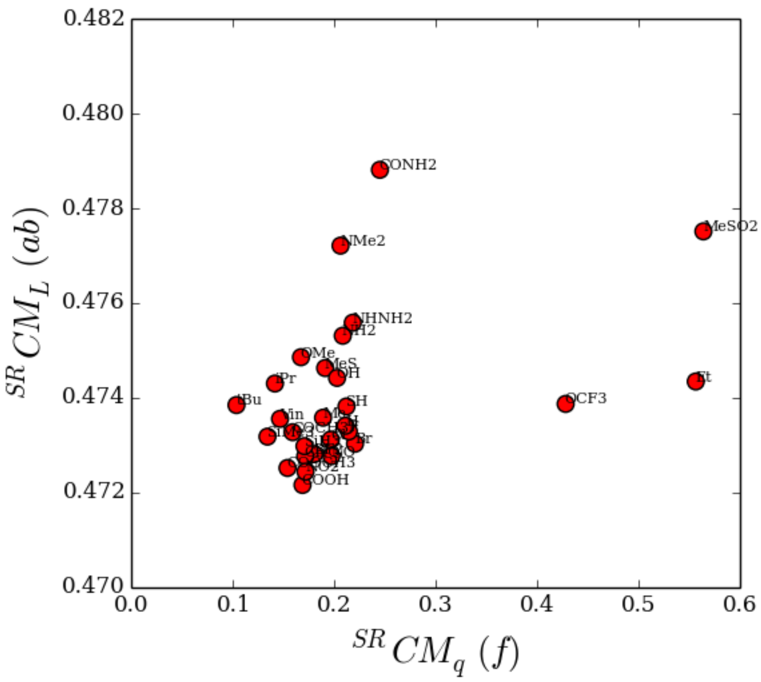
49


0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.0
0.1
0.2
0.3
0.4
0.5
0.6
$^{SR}CM_q\ (f)$
$^{SR}CM_q\ (f)$
MeSO2
OCF3
CONH2
tBu
SiMe3

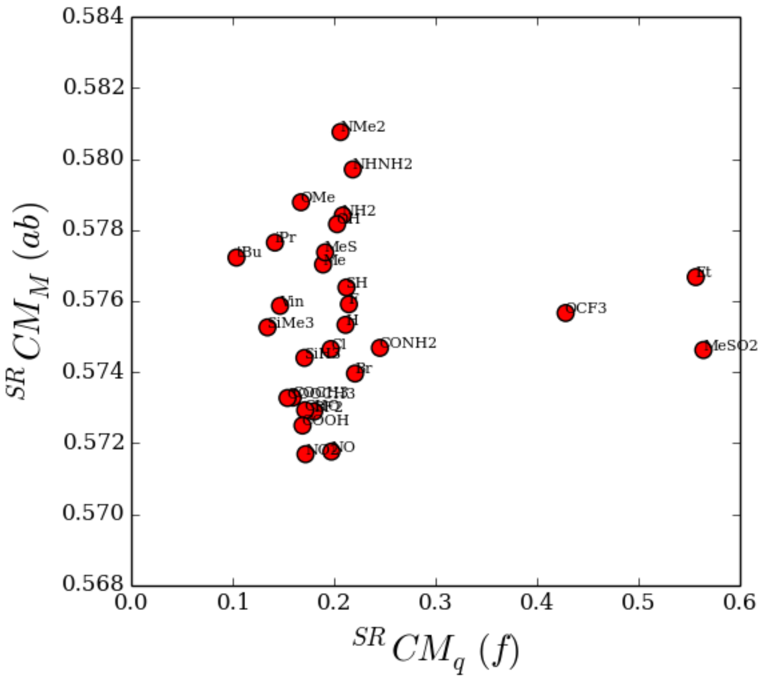
50


0.302
0.300
0.298
0.296
0.294
0.292
0.290
0.288
0.286
0.0
0.1
0.2
0.3
0.4
0.5
0.6
$^{SR}CM_0\ (ab)$
$^{SR}CM_q\ (f)$
MeSO2
CONH2
NMe2
NO2
OCF3
Et
tBu
SiMe3

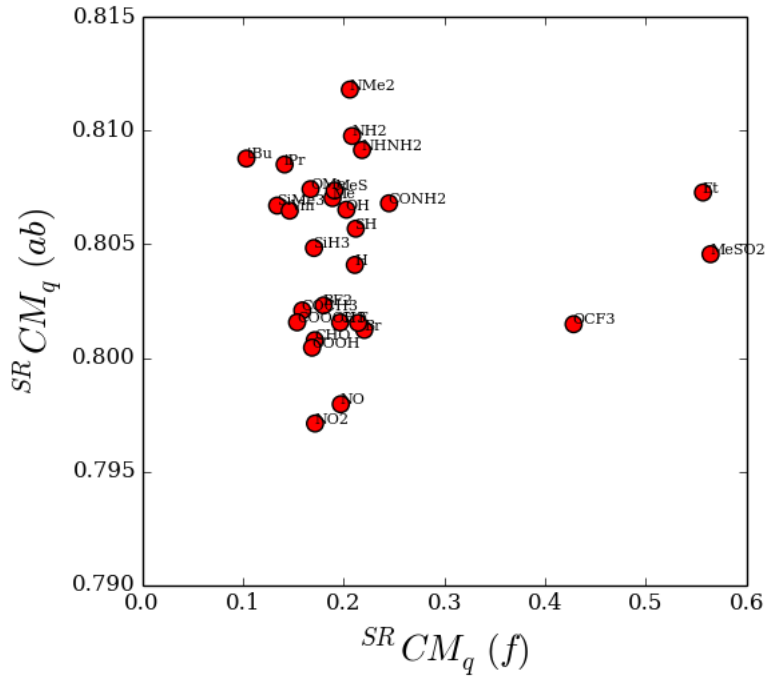
51


0.482
0.480
0.478
0.476
0.474
0.472
0.470
0.0
0.1
0.2
0.3
0.4
0.5
0.6
$^{SR}CM_L\ (ab)$
$^{SR}CM_q\ (f)$
CONH2
MeSO2
NMe2
NHNH2
OMe
OCF3
Et
COOH

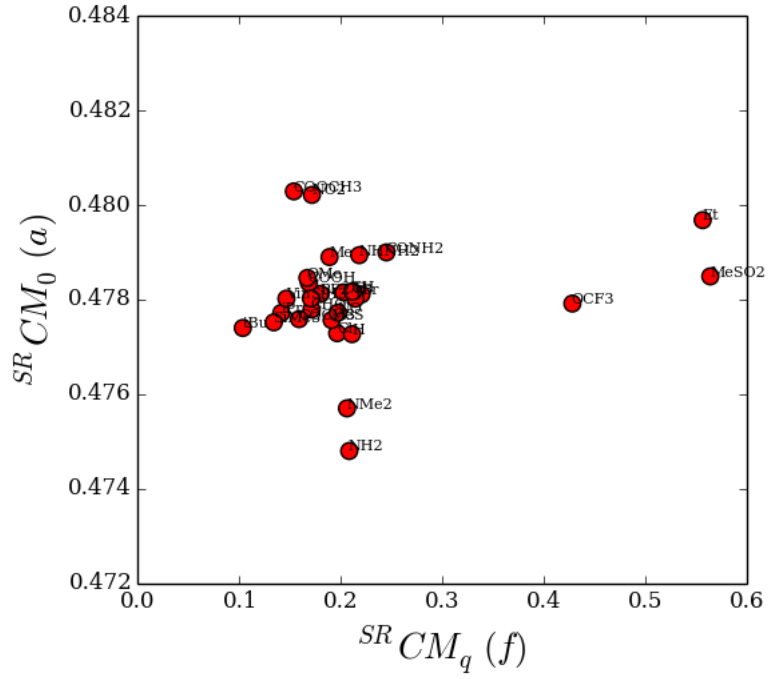
52


0.584
0.582
0.580
0.578
0.576
0.574
0.572
0.570
0.568
0.0
0.1
0.2
0.3
0.4
0.5
0.6
$^{SR}CM_M\ (ab)$
$^{SR}CM_q\ (f)$
NMe2
NHNH2
OMe
NH2
iPr
MeS
tBu
SH
Et
OCF3
SiMe3
CONH2
MeSO2
Br
COOH

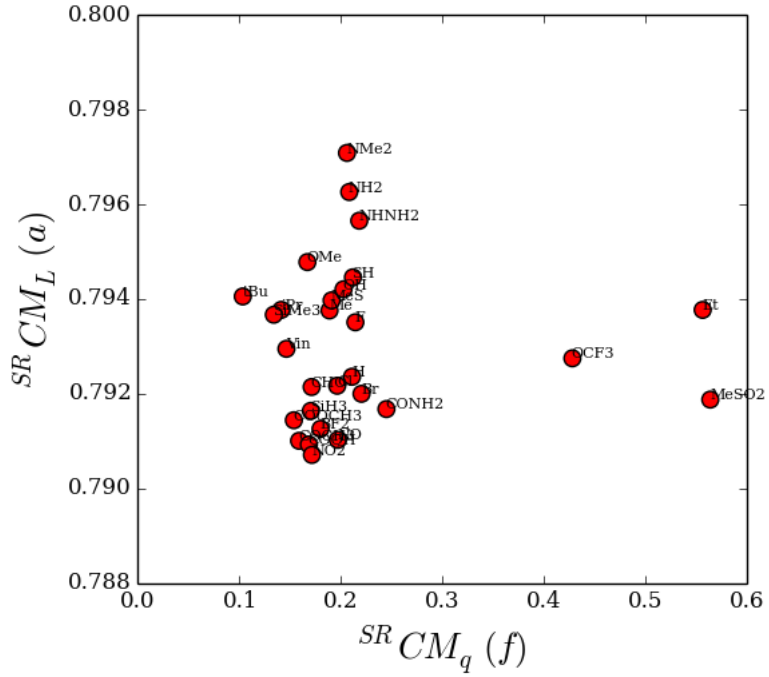
53


0.815
0.810
0.805
0.800
0.795
0.790
0.0
0.1
0.2
0.3
0.4
0.5
0.6
$^{SR}CM_q\ (ab)$
$^{SR}CM_q\ (f)$
NMe2
NH2
NHNH2
tBu
iPr
CONH2
SH
SiH3
Et
MeSO2
OCF3
NO
NO2

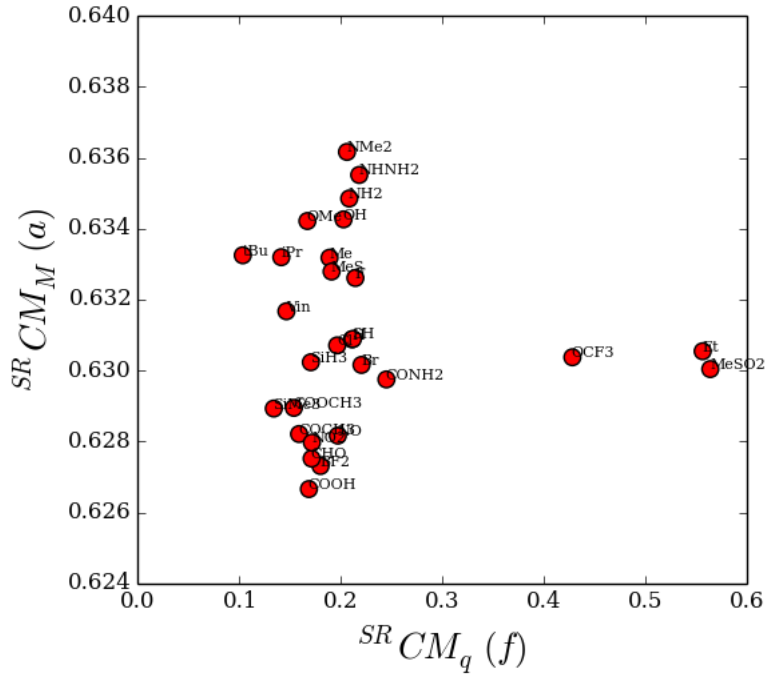
54


0.484
0.482
0.480
0.478
0.476
0.474
0.472
0.0
0.1
0.2
0.3
0.4
0.5
0.6
$^{SR}CM_0\ (a)$
$^{SR}CM_q\ (f)$
Et
MeSO2
OCF3
NMe2
NH2

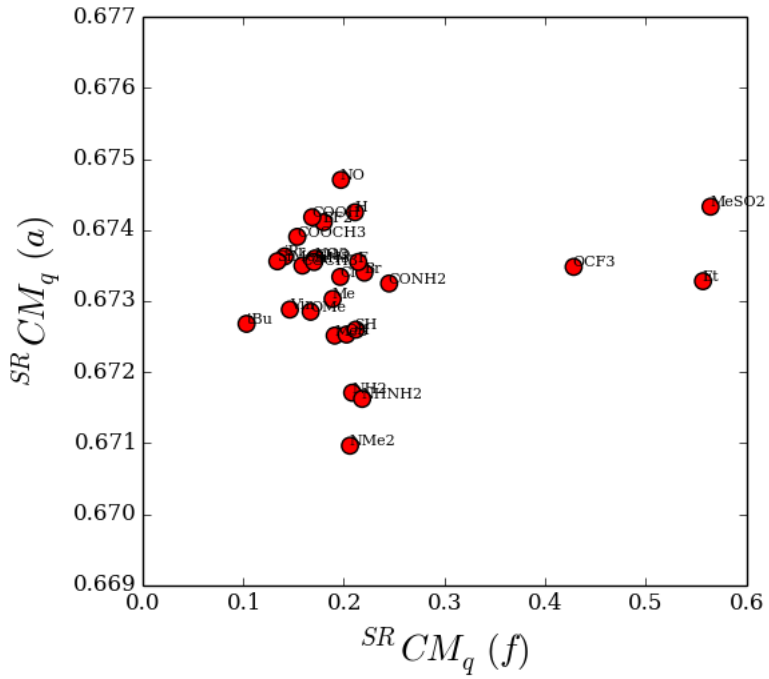
55


0.800
0.798
0.796
0.794
0.792
0.790
0.788
0.0
0.1
0.2
0.3
0.4
0.5
0.6
$^{SR}CM_L\ (a)$
$^{SR}CM_q\ (f)$
NMe2
NH2
NHNH2
OMe
OCF3
MeSO2
CONH2
COOCH3
COOH

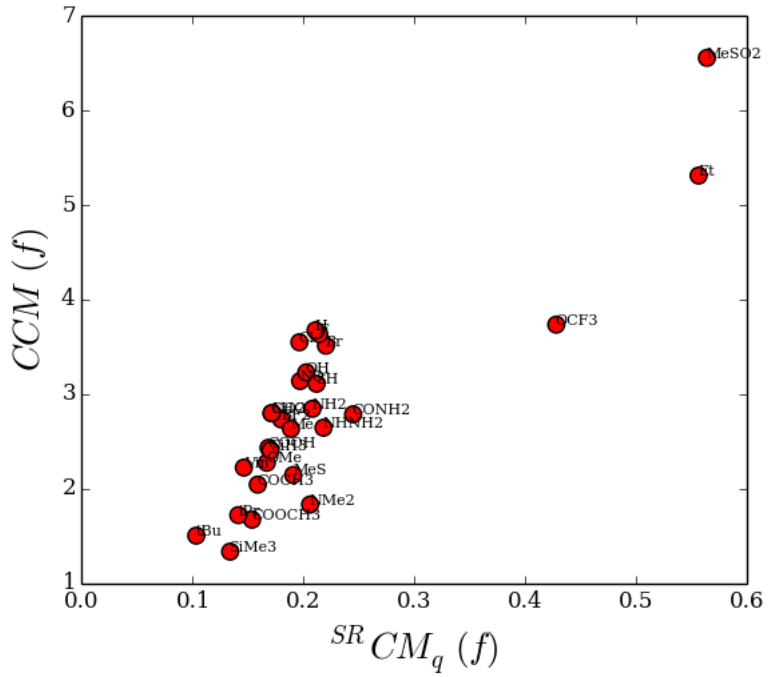
56


0.640
0.638
0.636
0.634
0.632
0.630
0.628
0.626
0.624
0.0
0.1
0.2
0.3
0.4
0.5
0.6
$^{SR}CM_M\ (a)$
$^{SR}CM_q\ (f)$
NMe2
NHNH2
NH2
OCF3
MeSO2
CONH2
COOCH3
COOH

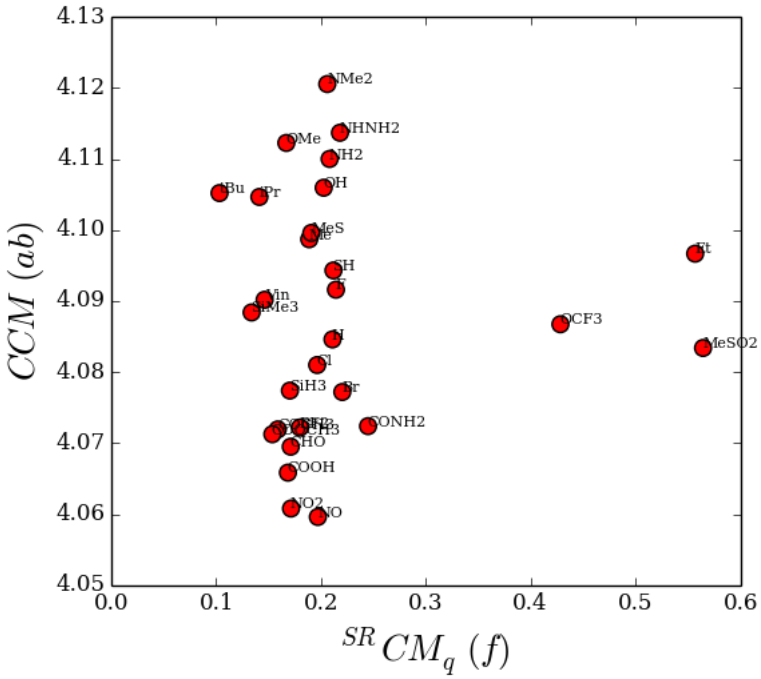
57


0.677
0.676
0.675
0.674
0.673
0.672
0.671
0.670
0.669
0.0
0.1
0.2
0.3
0.4
0.5
0.6
$^{SR}CM_q\ (a)$
$^{SR}CM_q\ (f)$
MeSO2
OCF3
CONH2
NMe2

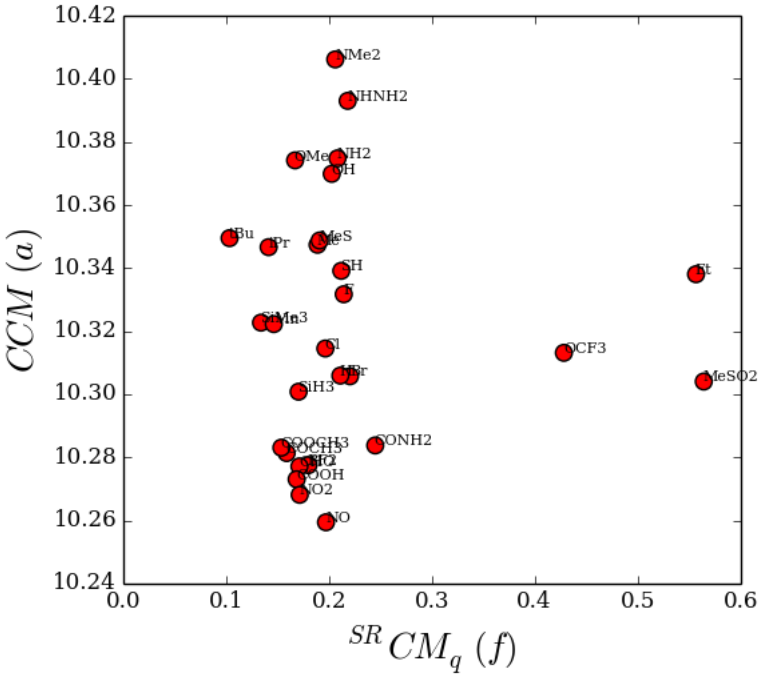
58


7
6
5
4
3
2
1
0.0
0.1
0.2
0.3
0.4
0.5
0.6
$CCM\ (f)$
$^{SR}CM_q\ (f)$
MeSO2
OCF3
CONH2
NMe2
SiMe3

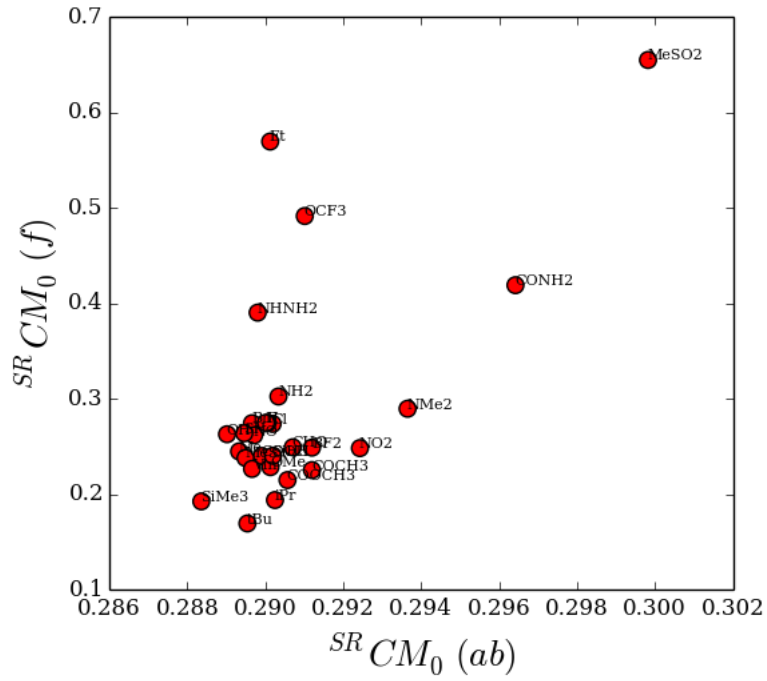
59


4.13
4.12
4.11
4.10
4.09
4.08
4.07
4.06
4.05
0.0
0.1
0.2
0.3
0.4
0.5
0.6
$CCM\ (ab)$
$^{SR}CM_q\ (f)$
NMe2
NHNH2
NH2
OH
Et
OCF3
MeSO2
CONH2
NO2
NO

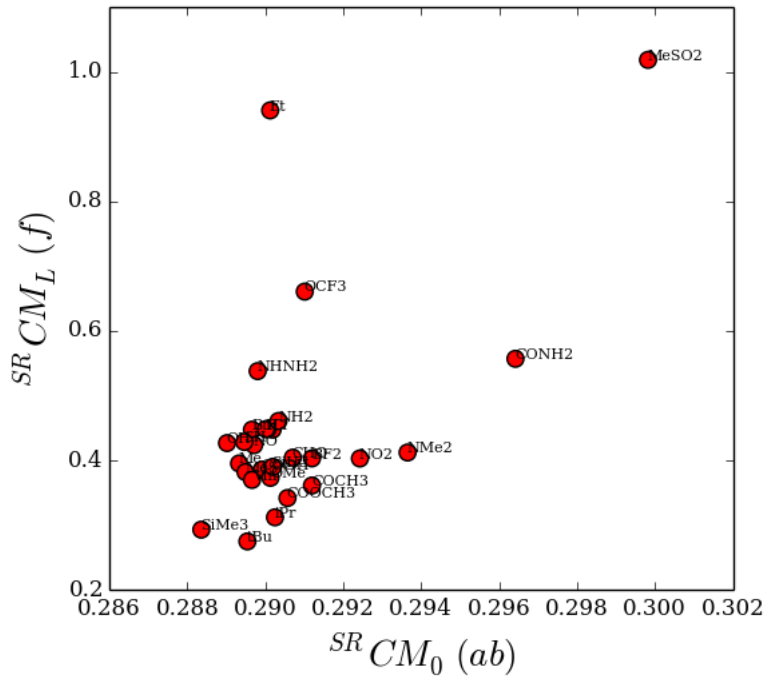
60


10.42
10.40
10.38
10.36
10.34
10.32
10.30
10.28
10.26
10.24
0.0
0.1
0.2
0.3
0.4
0.5
0.6
$CCM\ (a)$
$^{SR}CM_q\ (f)$
NMe2
NHNH2
NH2
Et
OCF3
MeSO2
SiH3
CONH2
NO2
NO

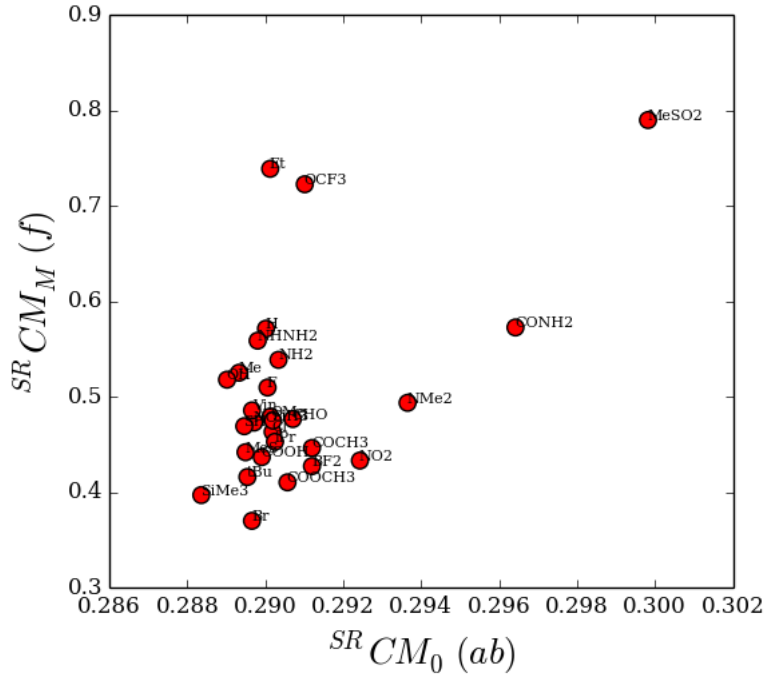
61


0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.286
0.288
0.290
0.292
0.294
0.296
0.298
0.300
0.302
$^{SR}CM_0\ (f)$
$^{SR}CM_0\ (ab)$
MeSO2
OCF3
CONH2
NHNH2
NH2
NMe2
NO2
SiMe3
Bu

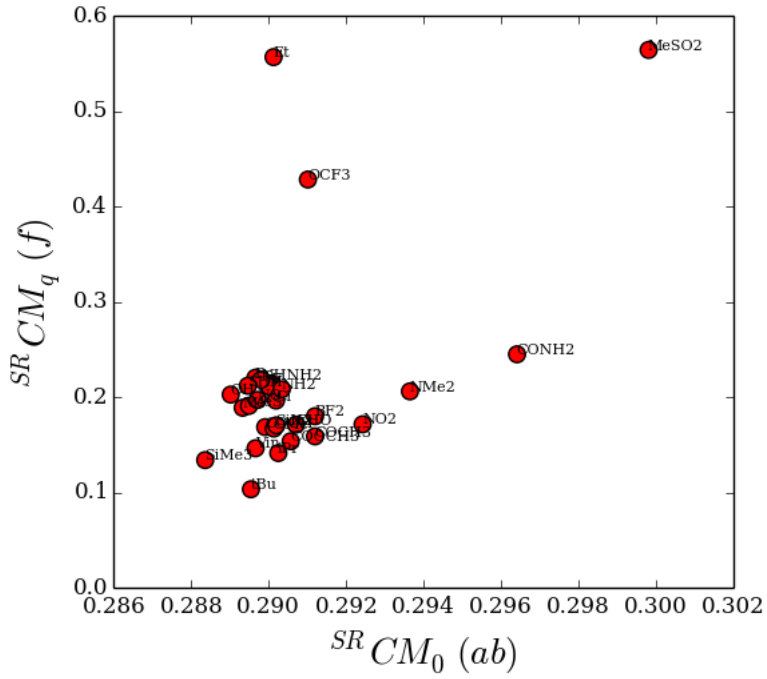
62


1.0
0.8
0.6
0.4
0.2
0.286
0.288
0.290
0.292
0.294
0.296
0.298
0.300
0.302
$^{SR}CM_L\ (f)$
$^{SR}CM_0\ (ab)$
MeSO2
OCF3
CONH2
NHNH2
NH2
NMe2
NO2
SiMe3
Bu

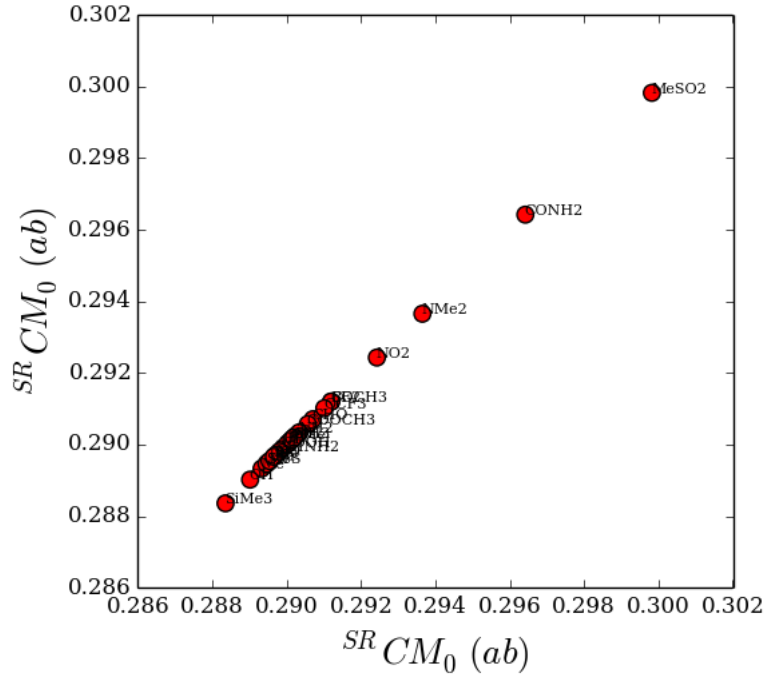
63


0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.286 0.288 0.290 0.292 0.294 0.296 0.298 0.300 0.302
$^{SR}CM_M\ (f)$
$^{SR}CM_0\ (ab)$
MeSO2
CF3
CONH2
NMe2
NO2
SiMe3

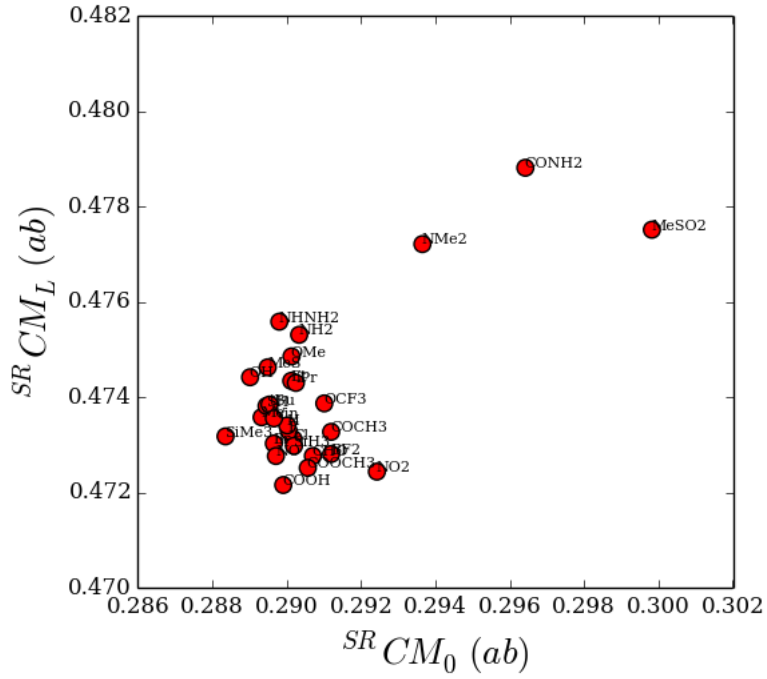
64


0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.286 0.288 0.290 0.292 0.294 0.296 0.298 0.300 0.302
$^{SR}CM_q\ (f)$
$^{SR}CM_0\ (ab)$
MeSO2
CF3
CONH2
NMe2
NO2
SiMe3
tBu

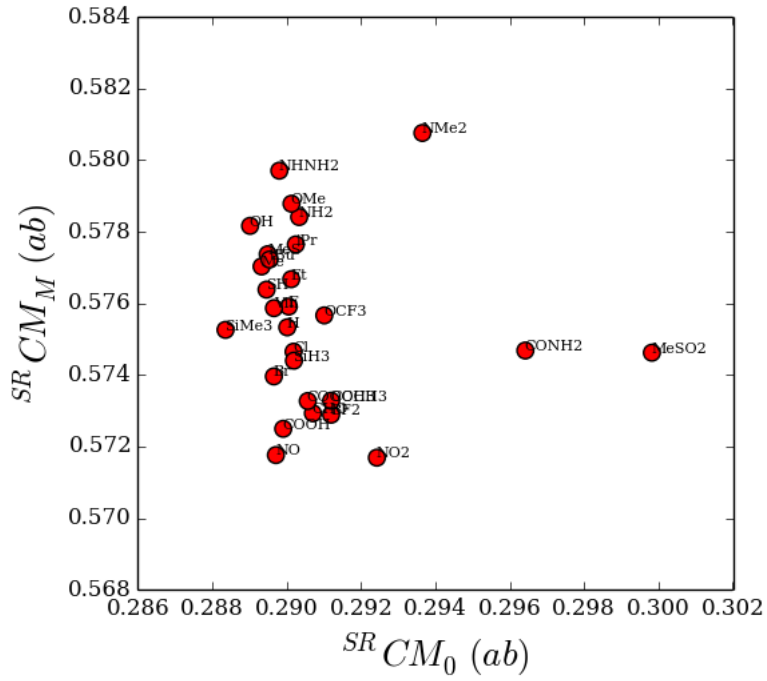
65


0.302
0.300
0.298
0.296
0.294
0.292
0.290
0.288
0.286
0.286 0.288 0.290 0.292 0.294 0.296 0.298 0.300 0.302
$^{SR}CM_0\ (ab)$
$^{SR}CM_0\ (ab)$
MeSO2
CONH2
NMe2
NO2
SiMe3

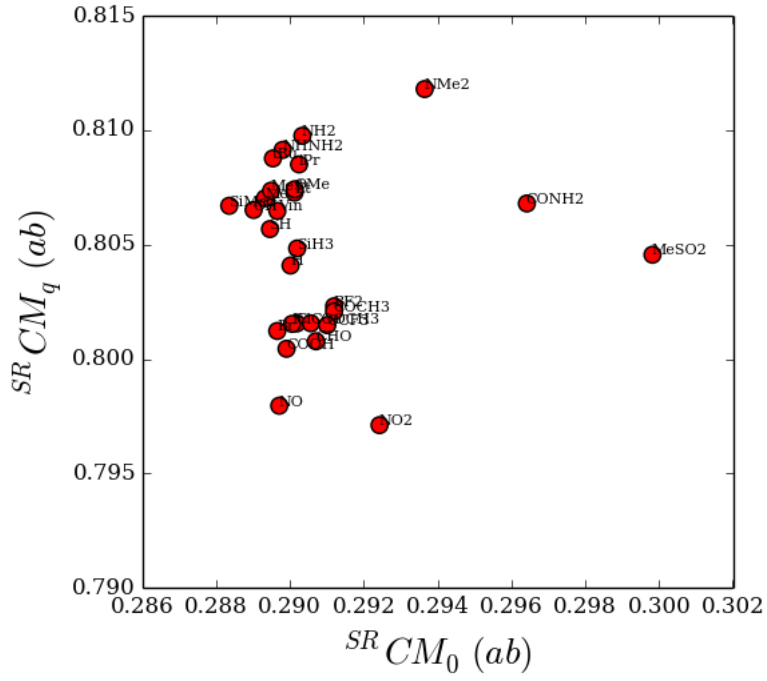
66


0.482
0.480
0.478
0.476
0.474
0.472
0.470
0.286 0.288 0.290 0.292 0.294 0.296 0.298 0.300 0.302
$^{SR}CM_L\ (ab)$
$^{SR}CM_0\ (ab)$
CONH2
MeSO2
NMe2
NO2
SiMe3

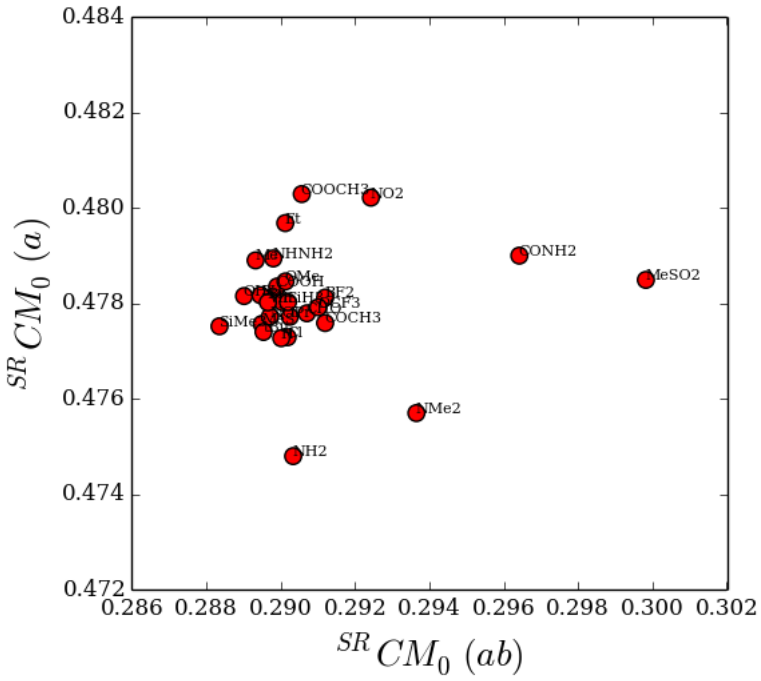
67


0.584
0.582
0.580
0.578
0.576
0.574
0.572
0.570
0.568
0.286 0.288 0.290 0.292 0.294 0.296 0.298 0.300 0.302
$^{SR}CM_M\ (ab)$
$^{SR}CM_0\ (ab)$
NMe2
NHNH2
OMe
NH2
OH
Pr
Et
OCF3
SiMe3
CONH2
MeSO2
SiH3
COOH
NO
NO2

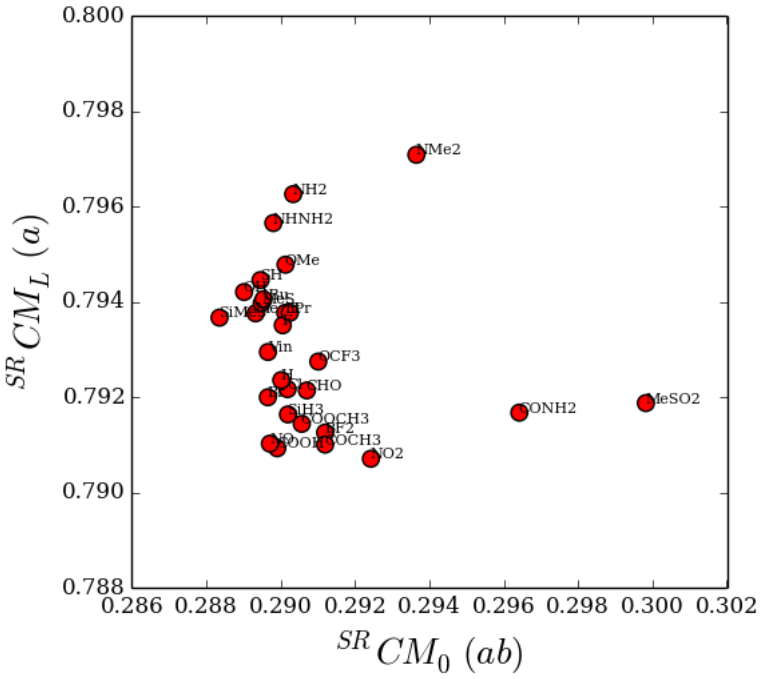
68


0.815
0.810
0.805
0.800
0.795
0.790
0.286 0.288 0.290 0.292 0.294 0.296 0.298 0.300 0.302
$^{SR}CM_q\ (ab)$
$^{SR}CM_0\ (ab)$
NMe2
NH2
NHNH2
Pr
OMe
CONH2
OH
SiH3
MeSO2
COOH
NO
NO2

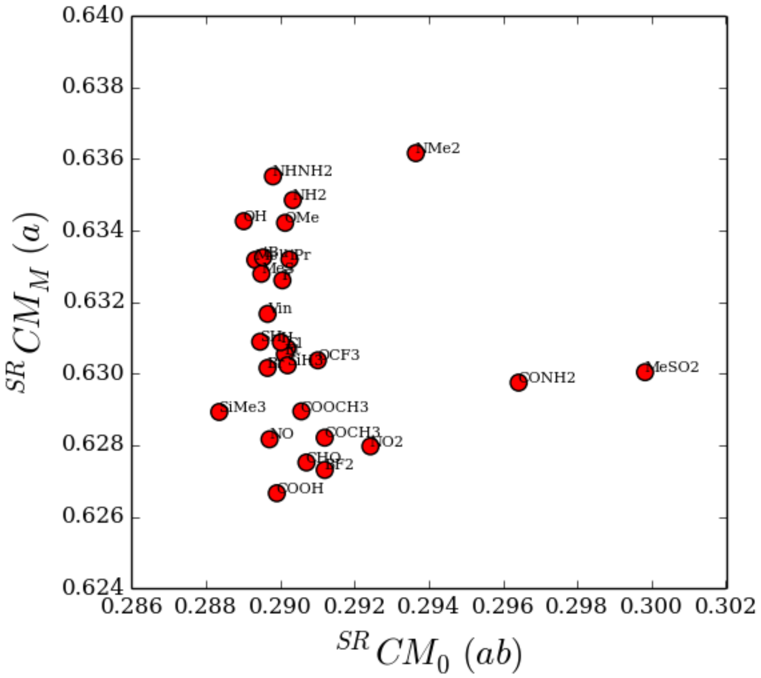
69


0.484
0.482
0.480
0.478
0.476
0.474
0.472
0.286 0.288 0.290 0.292 0.294 0.296 0.298 0.300 0.302
$^{SR}CM_0\ (a)$
$^{SR}CM_0\ (ab)$
SOOCH3
NO2
Et
NHNH2
CONH2
MeSO2
OMe
OCH3
NMe2
NH2

70

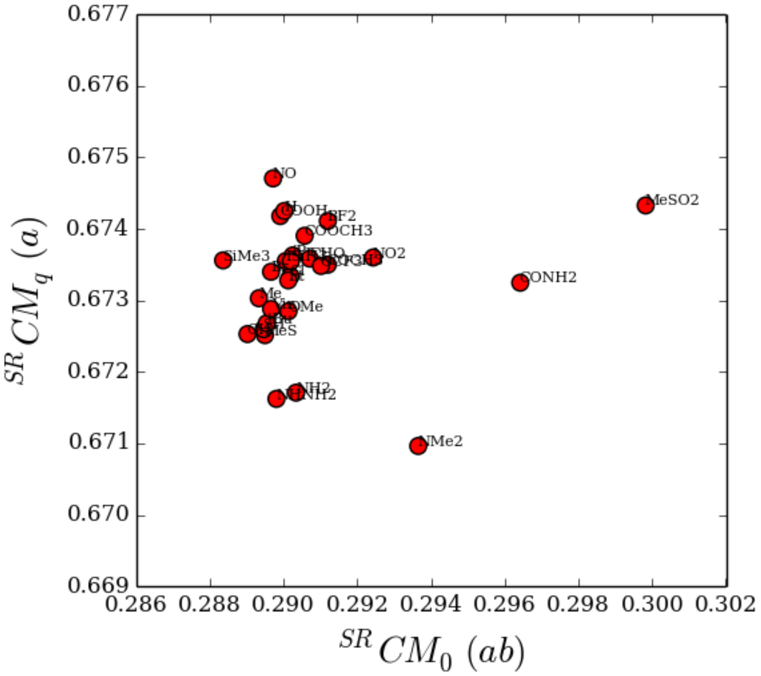

0.800
0.798
0.796
0.794
0.792
0.790
0.788
0.286 0.288 0.290 0.292 0.294 0.296 0.298 0.300 0.302
$^{SR}CM_L\ (a)$
$^{SR}CM_0\ (ab)$
NMe2
NH2
NHNH2
OMe
OCF3
CHO
CONH2
MeSO2
NO2

71



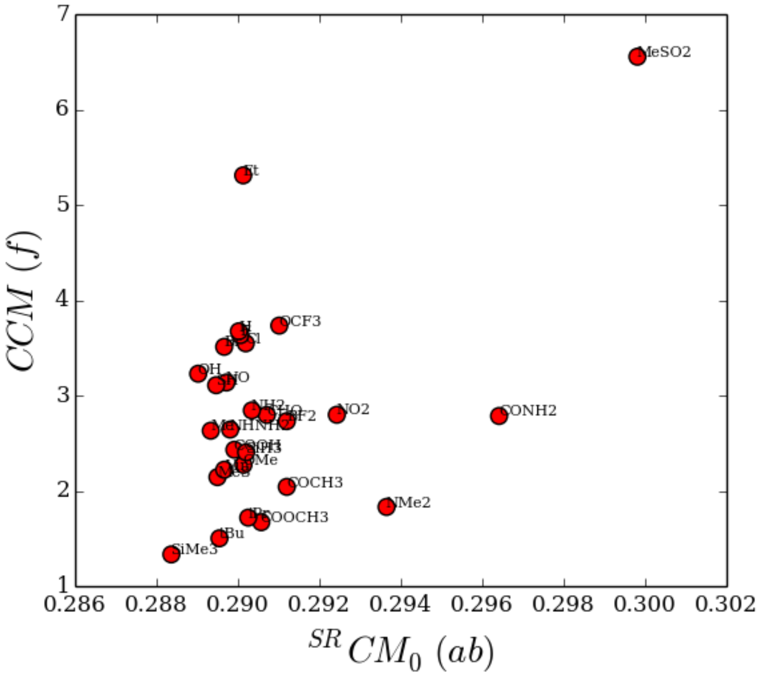
0.640
0.638
0.636
0.634
0.632
0.630
0.628
0.626
0.624
0.286
0.288
0.290
0.292
0.294
0.296
0.298
0.300
0.302
$^{SR}CM_M\ (a)$
$^{SR}CM_0\ (ab)$
NMe2
NHNH2
NH2
OH
OMe
Vin
OCF3
CONH2
MeSO2
SiMe3
COOCH3
NO
COCH3
NO2
CHO
CF2
COOH

72

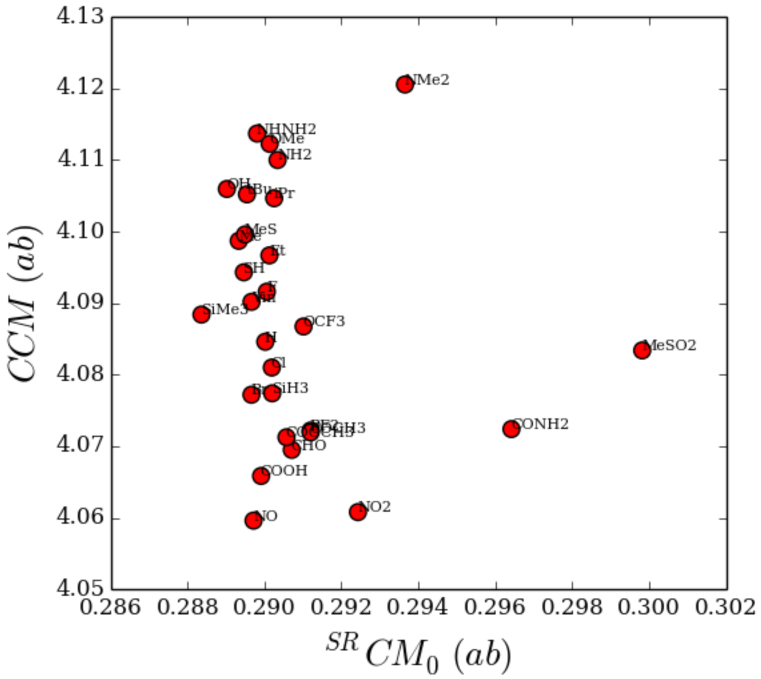


0.677
0.676
0.675
0.674
0.673
0.672
0.671
0.670
0.669
0.286
0.288
0.290
0.292
0.294
0.296
0.298
0.300
0.302
$^{SR}CM_q\ (a)$
$^{SR}CM_0\ (ab)$
NO
MeSO2
CF2
COOCH3
SiMe3
NO2
CONH2
OMe
NH2
NMe2

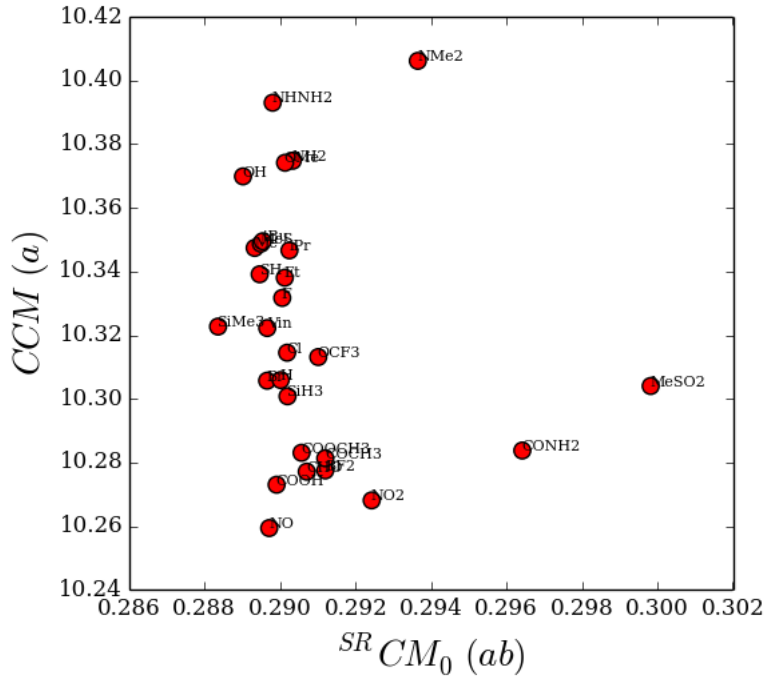
73



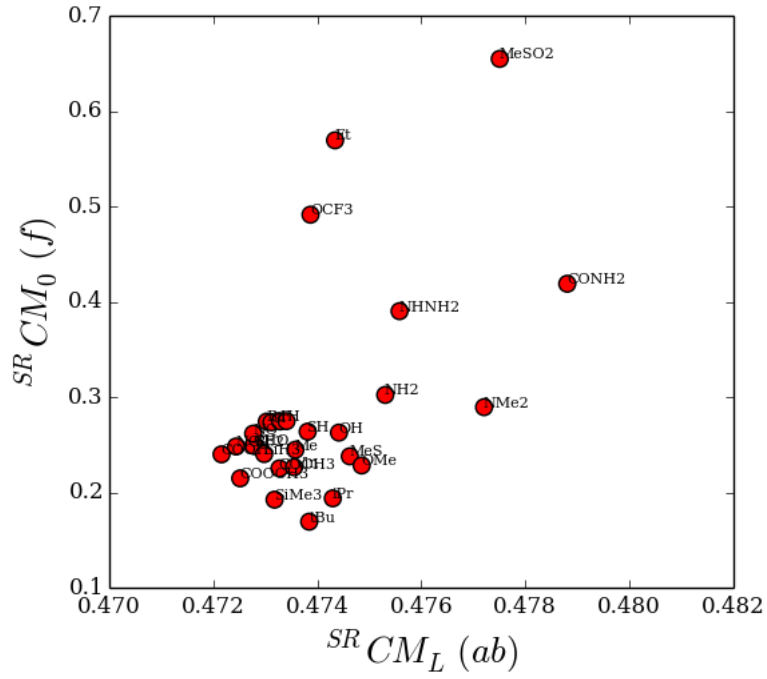
74



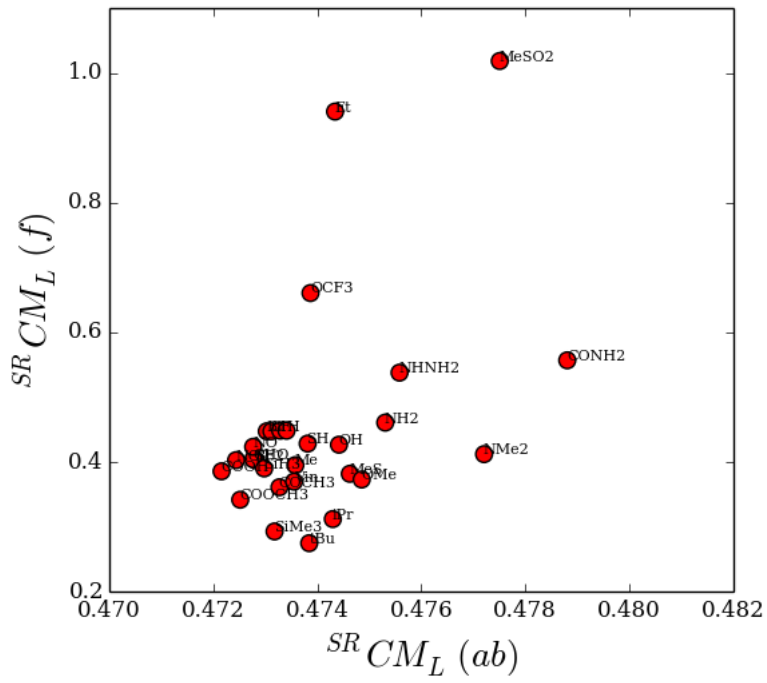
75


10.42
10.40
10.38
10.36
10.34
10.32
10.30
10.28
10.26
10.24
0.286
0.288
0.290
0.292
0.294
0.296
0.298
0.300
0.302
$CCM\ (a)$
$^{SR}CM_0\ (ab)$
NMe2
NHNH2
OH
Pr
Et
Vin
OCF3
SiH3
MeSO2
CONH2
NO2
NO

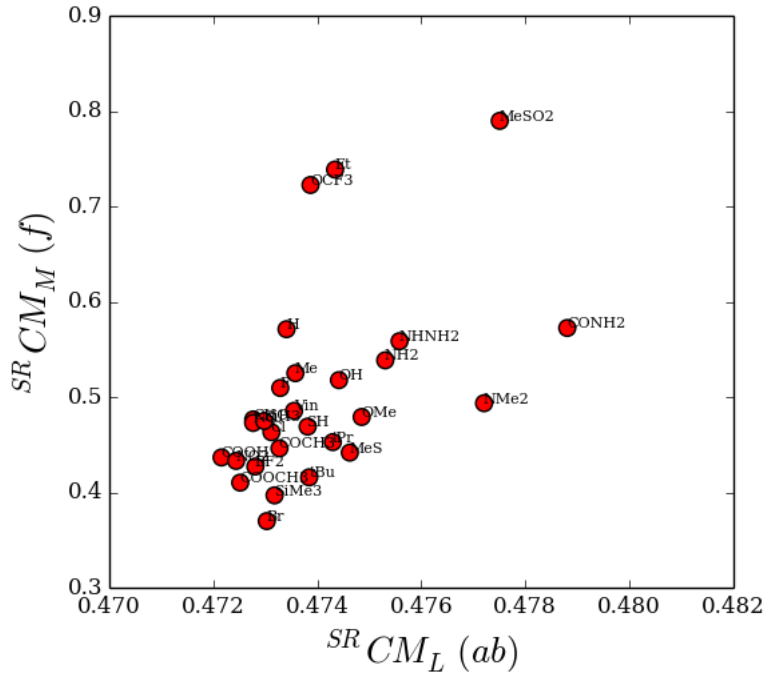
76


0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.470
0.472
0.474
0.476
0.478
0.480
0.482
$^{SR}CM_0\ (f)$
$^{SR}CM_L\ (ab)$
MeSO2
Et
OCF3
CONH2
NHNH2
NH2
NMe2
OH
SiMe3
Pr
tBu

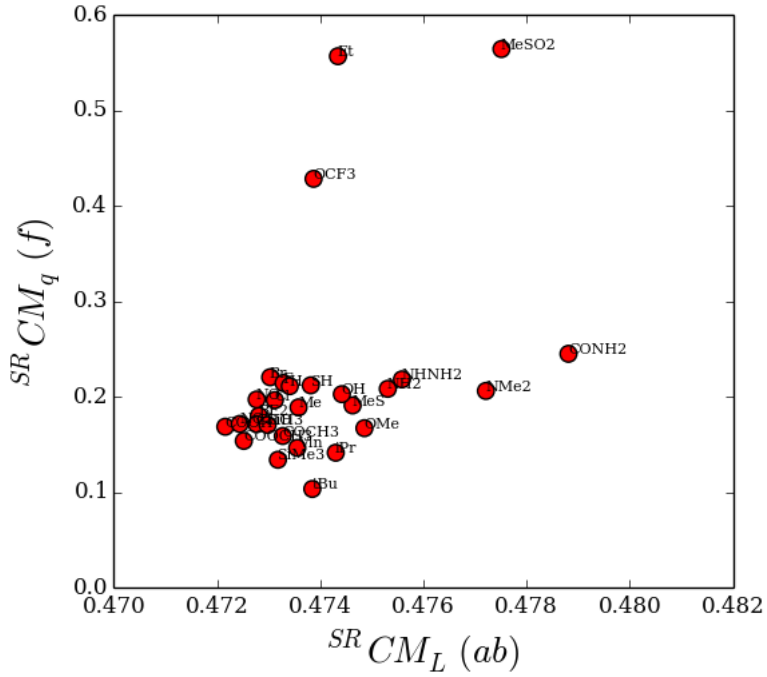
77


MeSO2
Et
OCF3
NHNH2
CONH2
NH2
OH
NMe2
SMe
SiMe3
tBu
1.0
0.8
0.6
0.4
0.2
0.470
0.472
0.474
0.476
0.478
0.480
0.482
$^{SR}CM_L\ (f)$
$^{SR}CM_L\ (ab)$

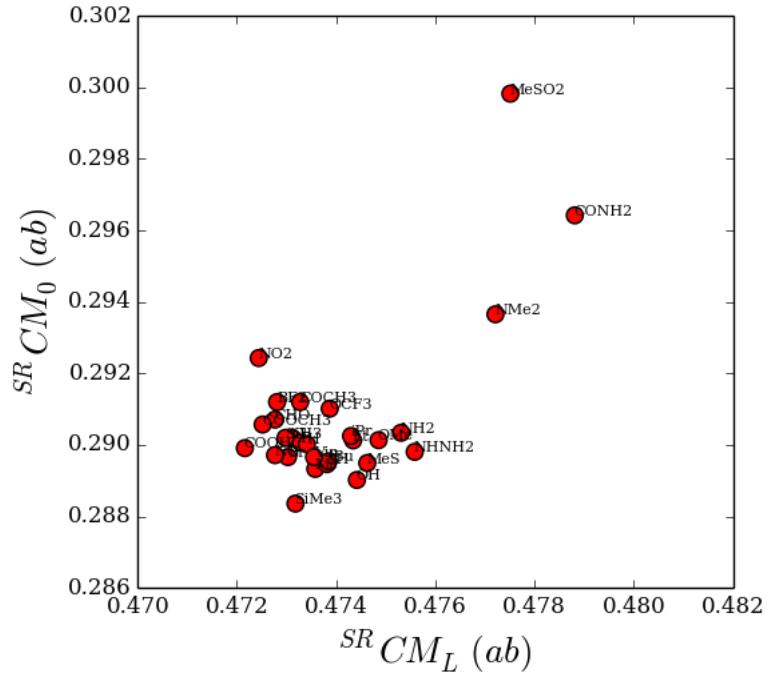
78


MeSO2
Et
OCF3
NHNH2
CONH2
NH2
OH
NMe2
OMe
SiMe3
tBu
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.470
0.472
0.474
0.476
0.478
0.480
0.482
$^{SR}CM_M\ (f)$
$^{SR}CM_L\ (ab)$

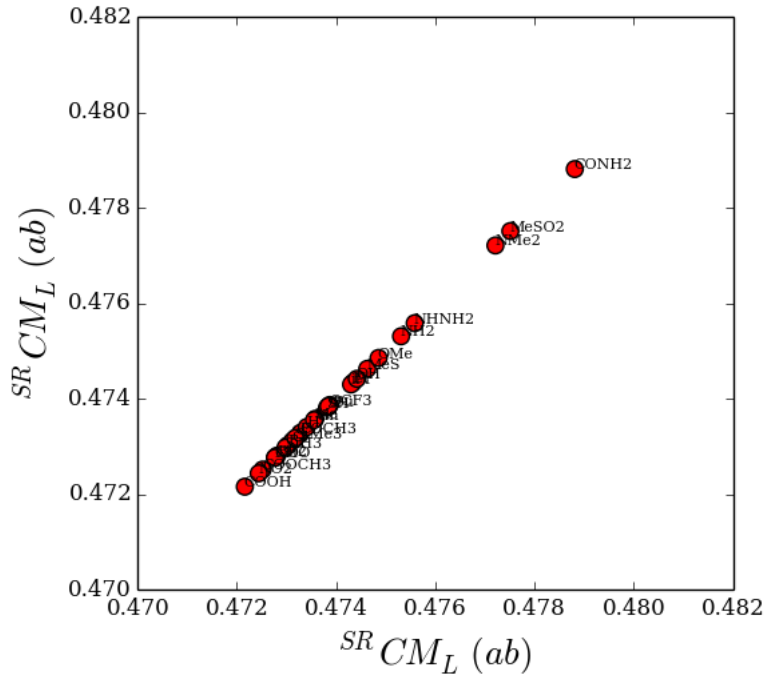
79


0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.470
0.472
0.474
0.476
0.478
0.480
0.482
$^{SR}CM_q\ (f)$
$^{SR}CM_L\ (ab)$
MeSO2
CONH2
NMe2
OCF3
tBu

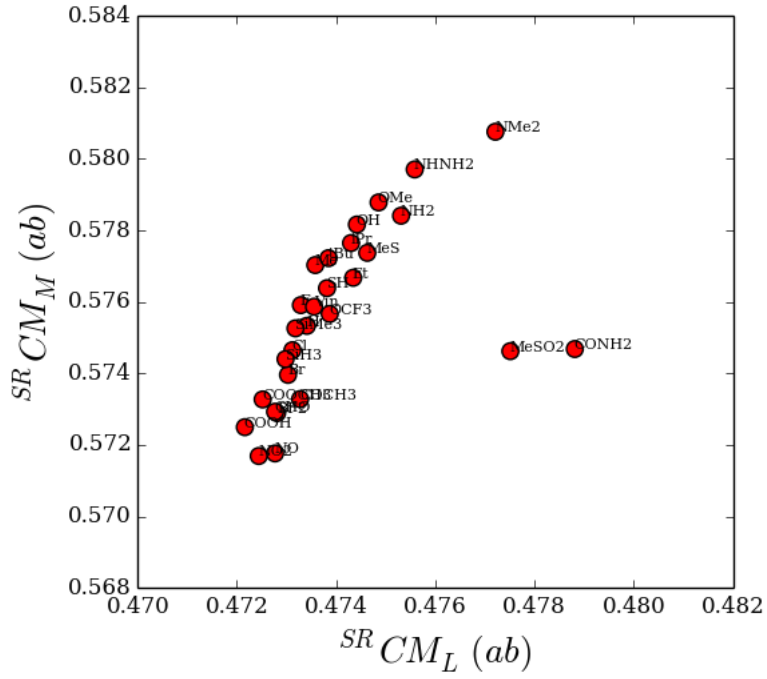
80


0.302
0.300
0.298
0.296
0.294
0.292
0.290
0.288
0.286
0.470
0.472
0.474
0.476
0.478
0.480
0.482
$^{SR}CM_0\ (ab)$
$^{SR}CM_L\ (ab)$
MeSO2
CONH2
NMe2
SiMe3

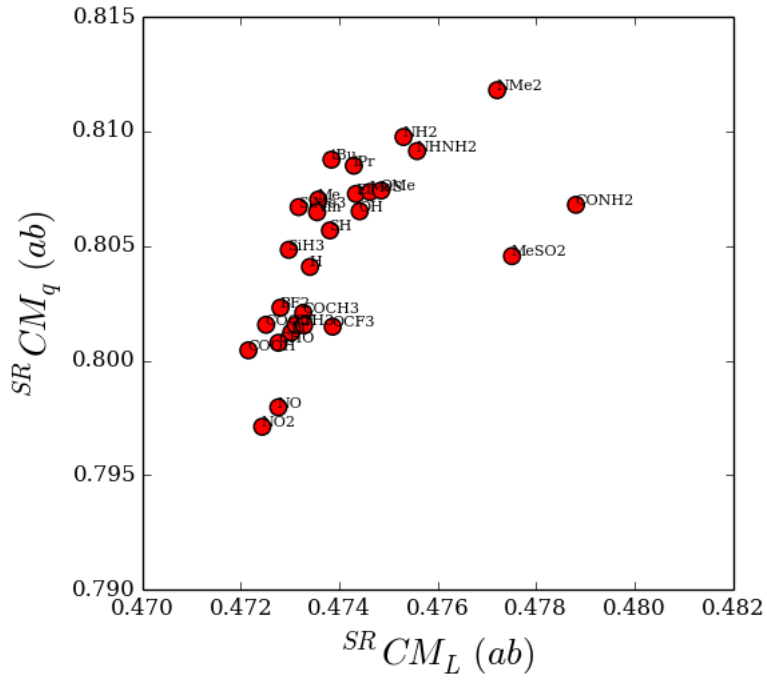
81


0.482
0.480
0.478
0.476
0.474
0.472
0.470
0.470
0.472
0.474
0.476
0.478
0.480
0.482
$^{SR}CM_L\ (ab)$
$^{SR}CM_L\ (ab)$

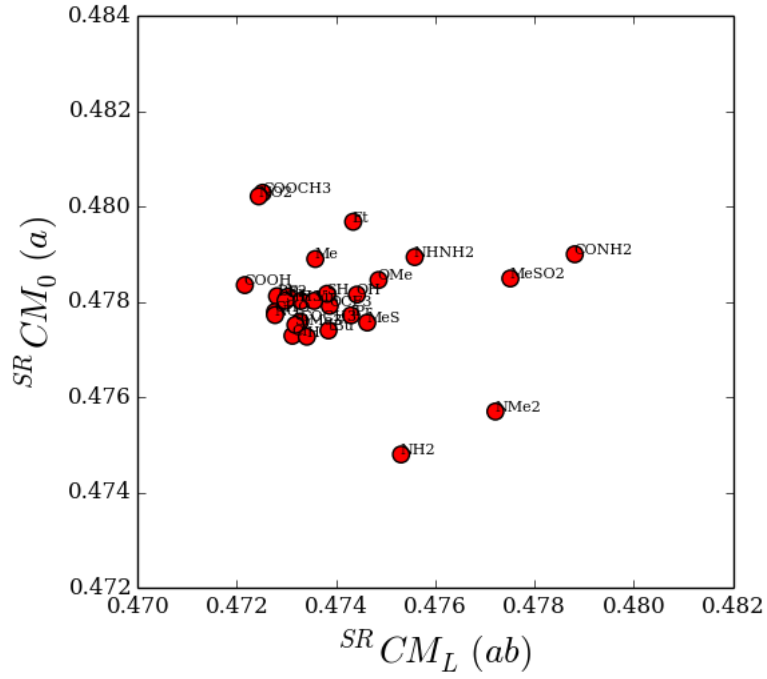
82


0.584
0.582
0.580
0.578
0.576
0.574
0.572
0.570
0.568
0.470
0.472
0.474
0.476
0.478
0.480
0.482
$^{SR}CM_M\ (ab)$
$^{SR}CM_L\ (ab)$

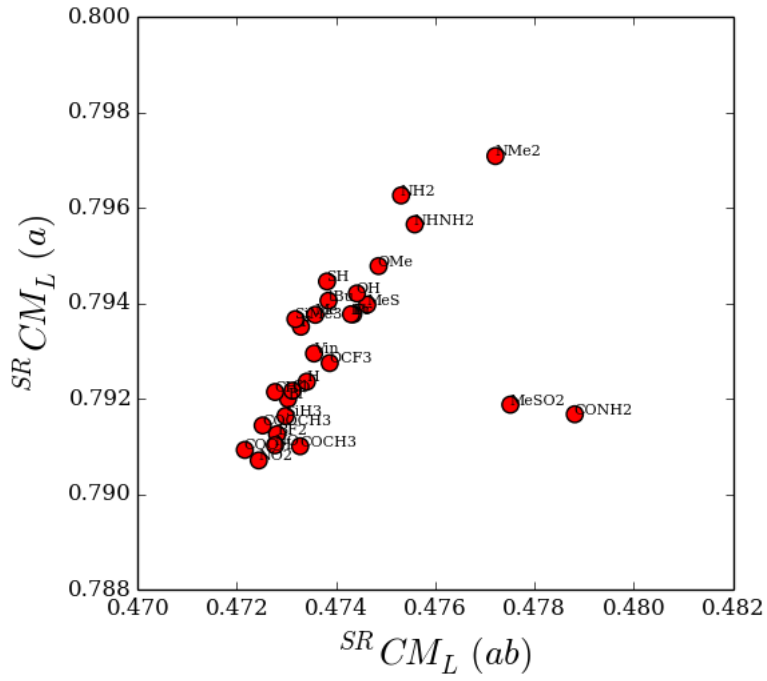
83


0.815
0.810
0.805
0.800
0.795
0.790
0.470
0.472
0.474
0.476
0.478
0.480
0.482
$^{SR}CM_q\ (ab)$
$^{SR}CM_L\ (ab)$
NMe2
NH2
NHNH2
SONH2
MeSO2

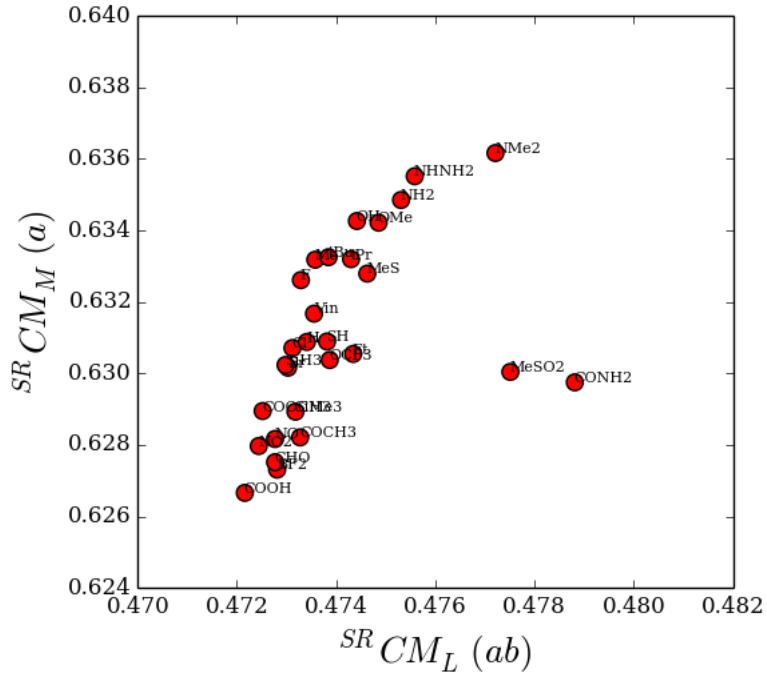
84


0.484
0.482
0.480
0.478
0.476
0.474
0.472
0.470
0.472
0.474
0.476
0.478
0.480
0.482
$^{SR}CM_0\ (a)$
$^{SR}CM_L\ (ab)$
NHNH2
SONH2
MeSO2
NMe2
NH2

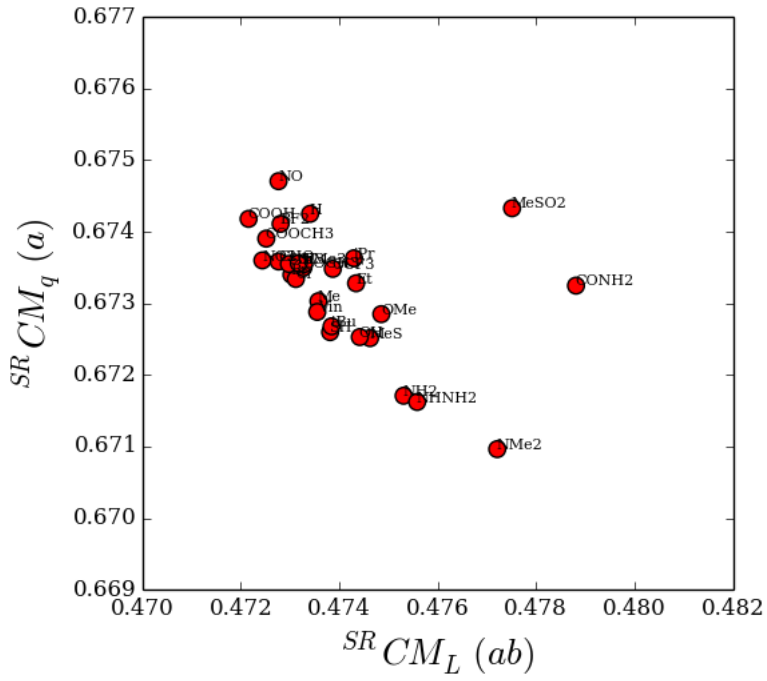
85


0.800
0.798
0.796
0.794
0.792
0.790
0.788
0.470
0.472
0.474
0.476
0.478
0.480
0.482
$^{SR}CM_L\ (a)$
$^{SR}CM_L\ (ab)$
NMe2
NH2
NHNH2
OMe
SH
MeS
CF3
MeSO2
SONH2
COOCH3

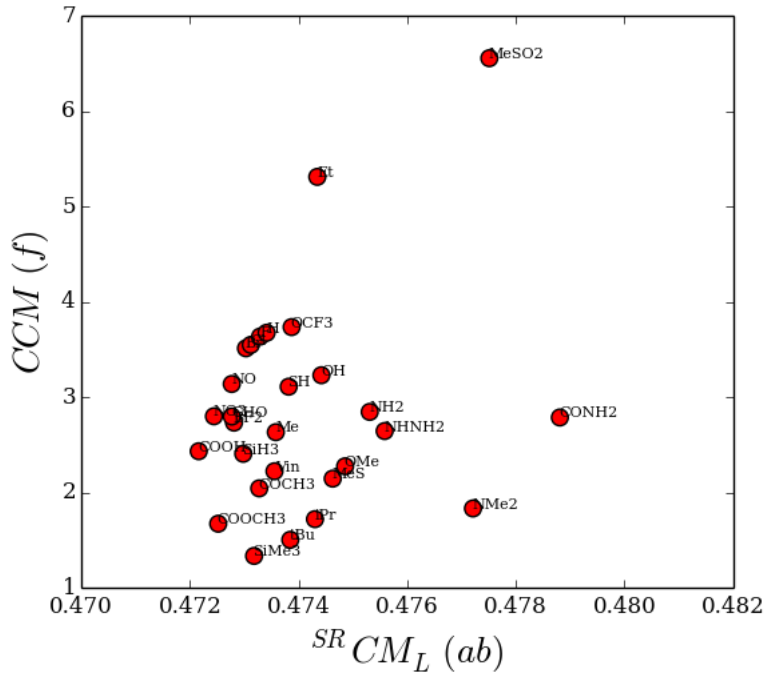
86


0.640
0.638
0.636
0.634
0.632
0.630
0.628
0.626
0.624
0.470
0.472
0.474
0.476
0.478
0.480
0.482
$^{SR}CM_M\ (a)$
$^{SR}CM_L\ (ab)$
NMe2
NHNH2
NH2
OMe
MeS
MeSO2
SONH2
COOCH3
COOH

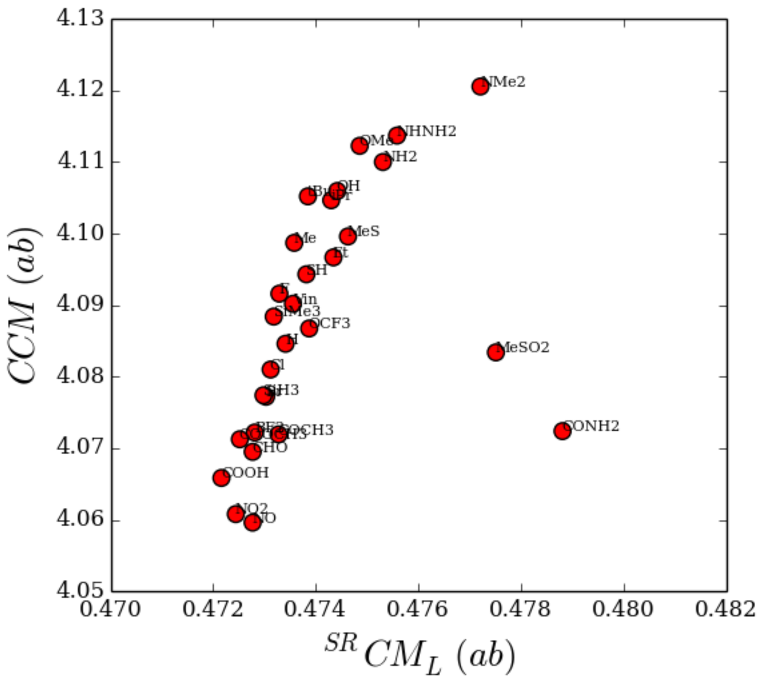
87


0.677
0.676
0.675
0.674
0.673
0.672
0.671
0.670
0.669
0.470
0.472
0.474
0.476
0.478
0.480
0.482
$^{SR}CM_q\ (a)$
$^{SR}CM_L\ (ab)$
NO
MeSO2
COOCH3
CONH2
OMe
SMe
NHNH2
NMe2

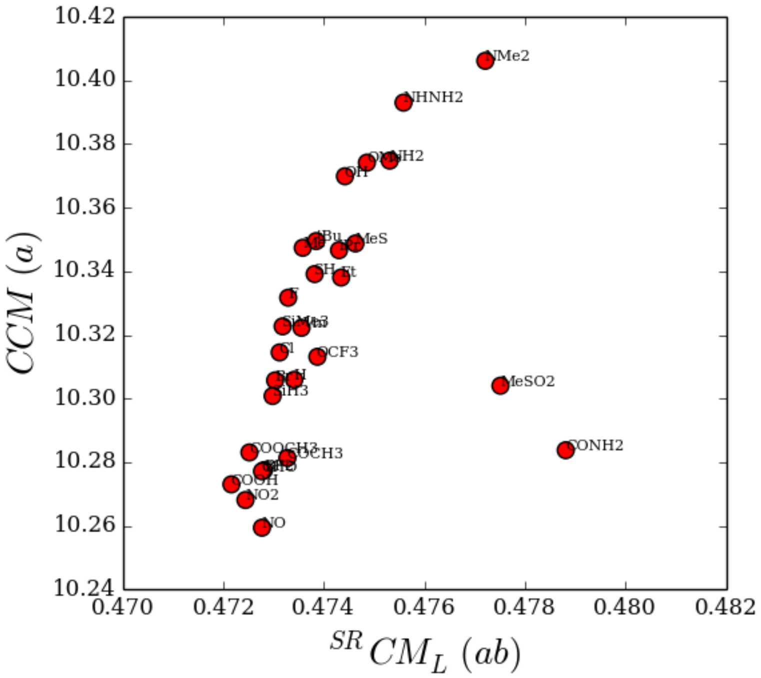
88


7
6
5
4
3
2
1
0.470
0.472
0.474
0.476
0.478
0.480
0.482
$CCM\ (f)$
$^{SR}CM_L\ (ab)$
MeSO2
Et
OCF3
OH
NO
SH
NH2
CONH2
NHNH2
Me
SiH3
Vin
OMe
SMe
COOCH3
NMe2
COOCH3
iPr
tBu
SiMe3

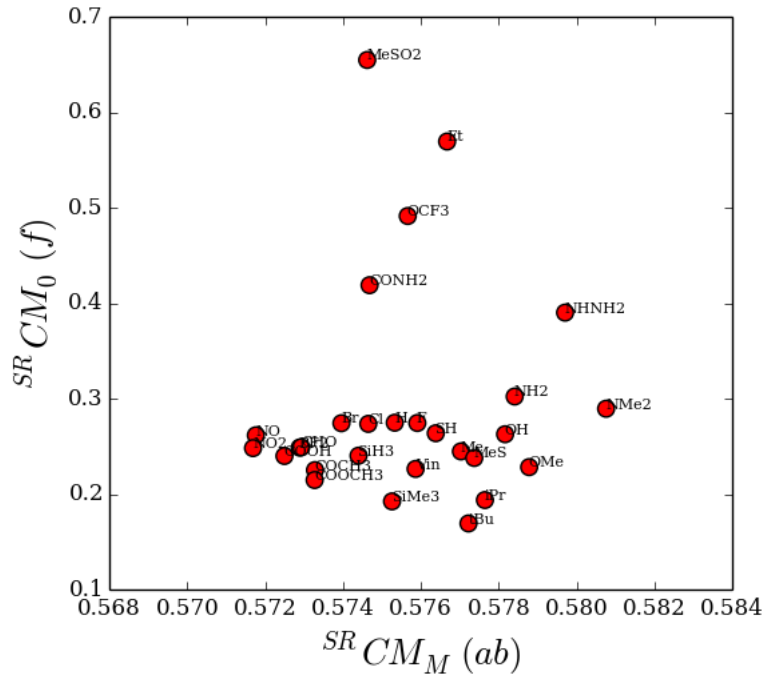
89


4.13
4.12
4.11
4.10
4.09
4.08
4.07
4.06
4.05
0.470
0.472
0.474
0.476
0.478
0.480
0.482
$CCM\ (ab)$
$^{SR}CM_L\ (ab)$
NMe2
NHNH2
NH2
OH
MeS
Et
SH
SiMe3
OCF3
MeSO2
SiH3
CONH2
CHO
COOH
NO2

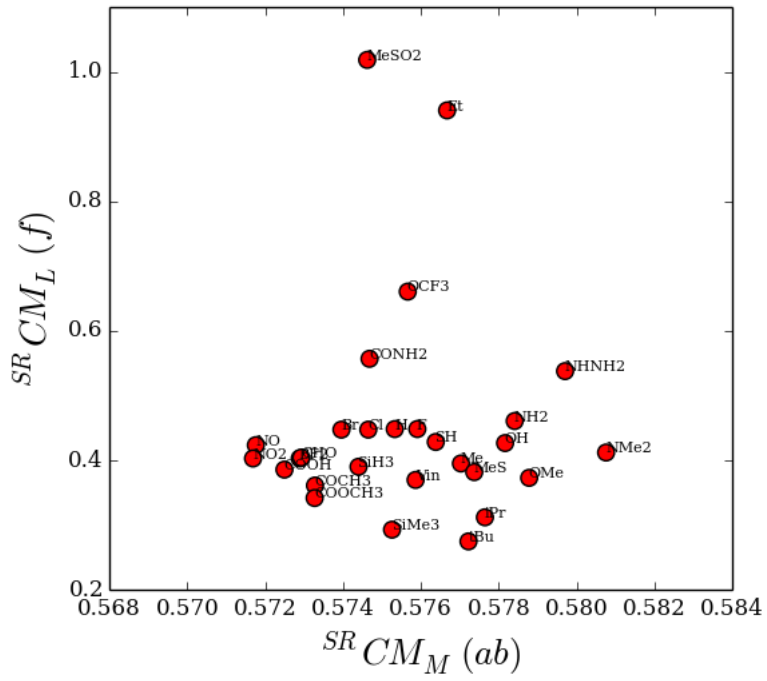
90


10.42
10.40
10.38
10.36
10.34
10.32
10.30
10.28
10.26
10.24
0.470
0.472
0.474
0.476
0.478
0.480
0.482
$CCM\ (a)$
$^{SR}CM_L\ (ab)$
NMe2
NHNH2
MeS
Et
SH
OCF3
MeSO2
SiH3
CONH2
COOH
NO2

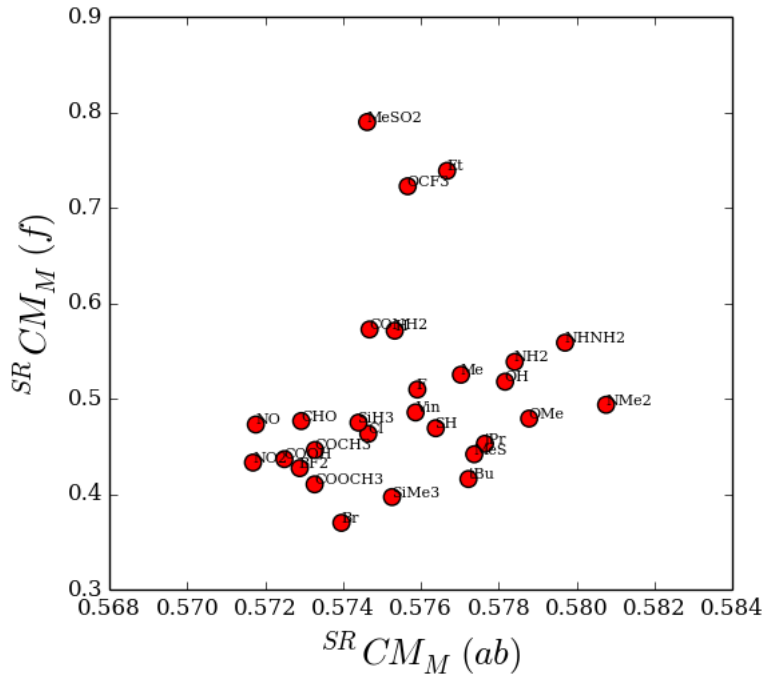
91


0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.568 0.570 0.572 0.574 0.576 0.578 0.580 0.582 0.584
$^{SR}CM_0\ (f)$
$^{SR}CM_M\ (ab)$
MeSO2
Et
OCF3
CONH2
NHNH2
NH2
NMe2
OH
SiH3
Vin
OMe
SiMe3
Pr
Bu

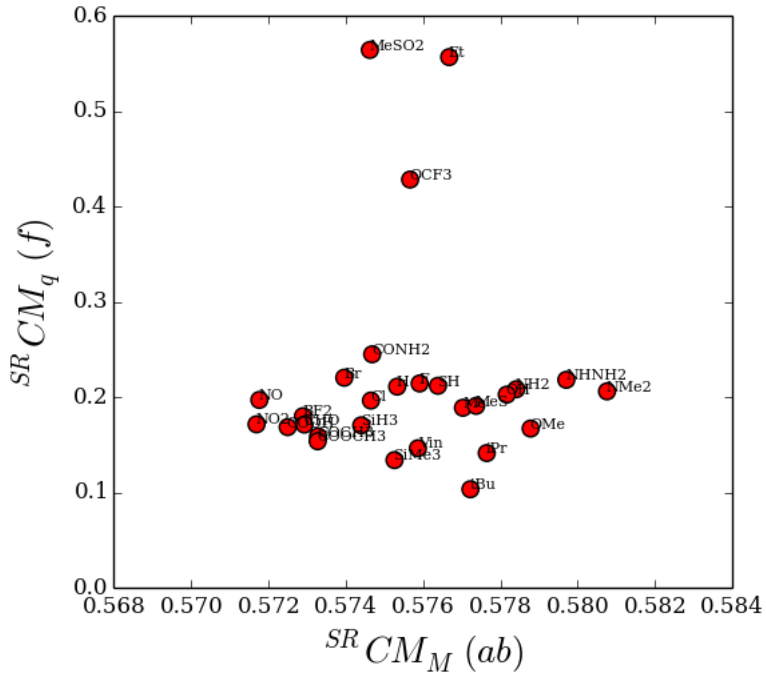
92


1.0
0.8
0.6
0.4
0.2
0.568 0.570 0.572 0.574 0.576 0.578 0.580 0.582 0.584
$^{SR}CM_L\ (f)$
$^{SR}CM_M\ (ab)$
MeSO2
Et
OCF3
CONH2
NHNH2
NH2
NMe2
OH
SiH3
Vin
OMe
SiMe3
Pr
Bu

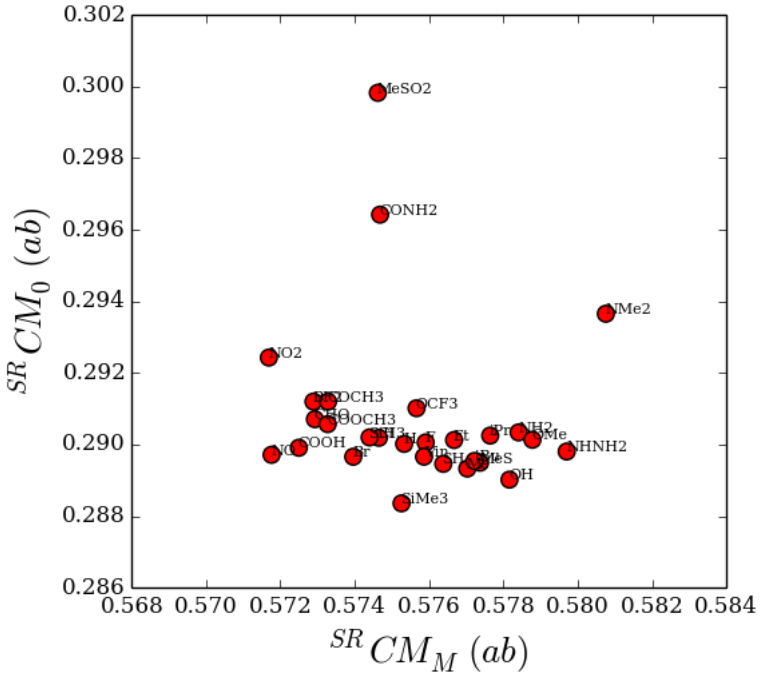
93


0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.568 0.570 0.572 0.574 0.576 0.578 0.580 0.582 0.584
$^{SR}CM_M\ (f)$
$^{SR}CM_M\ (ab)$
MeSO2
Et
OCF3
NHNH2
NH2
Me
NH
NMe2
NO
CHO
SiH3
Vin
SH
OMe
Pr
SMe
tBu
SiMe3
Br

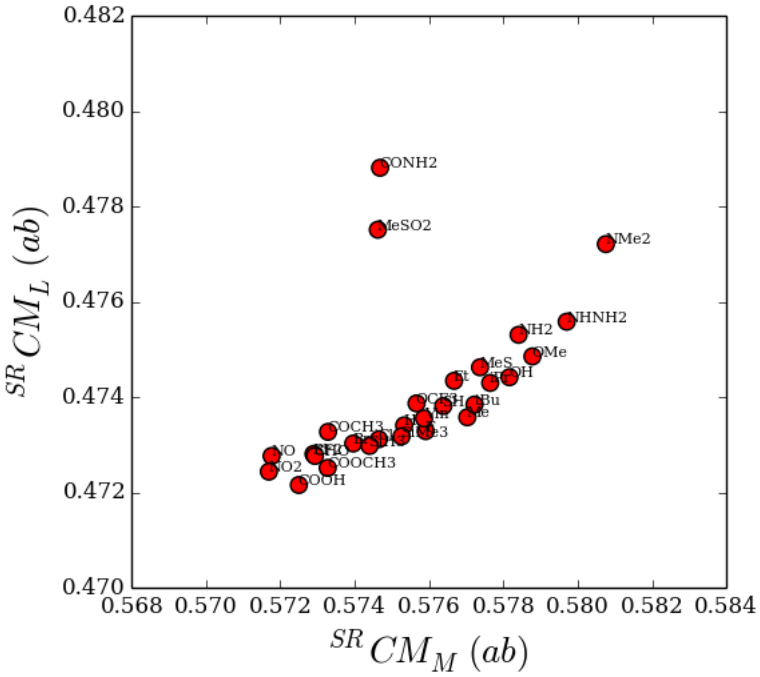
94


0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.568 0.570 0.572 0.574 0.576 0.578 0.580 0.582 0.584
$^{SR}CM_q\ (f)$
$^{SR}CM_M\ (ab)$
MeSO2
Et
OCF3
CONH2
NHNH2
NMe2
NO
SiH3
OMe
Vin
Pr
tBu
SiMe3

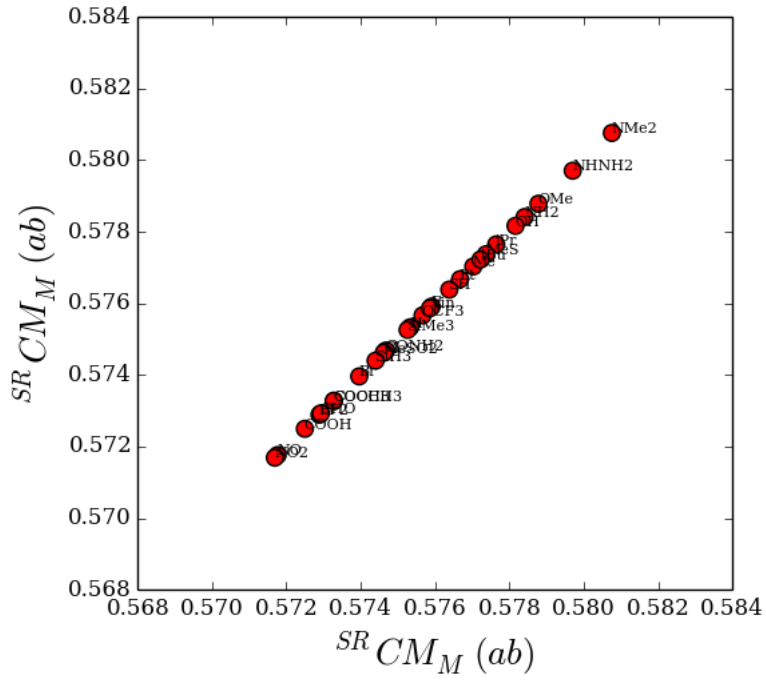
95


0.302
0.300
0.298
0.296
0.294
0.292
0.290
0.288
0.286
0.568 0.570 0.572 0.574 0.576 0.578 0.580 0.582 0.584
$^{SR}CM_0\ (ab)$
$^{SR}CM_M\ (ab)$
MeSO2
CONH2
NMe2
NO2
OCF3
NHNH2
OH
SiMe3

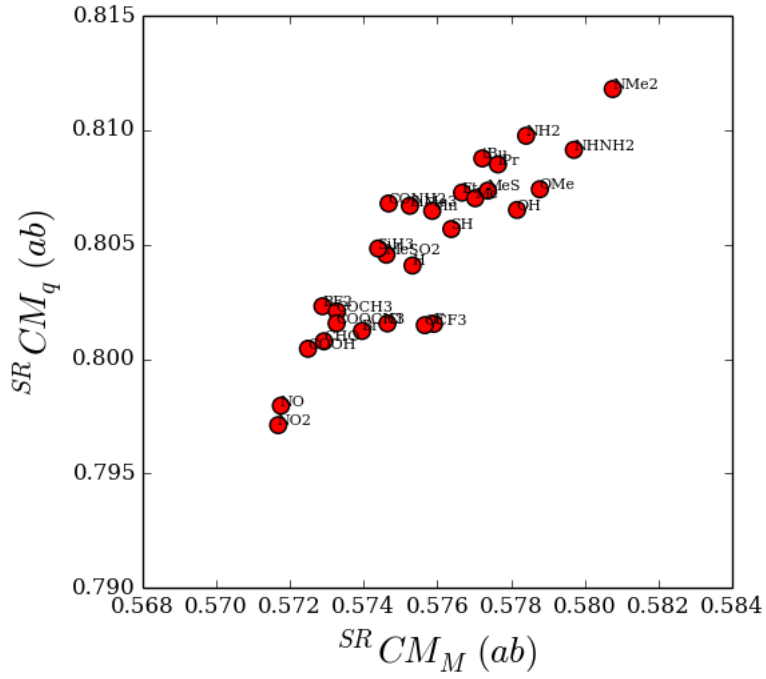
96


0.482
0.480
0.478
0.476
0.474
0.472
0.470
0.568 0.570 0.572 0.574 0.576 0.578 0.580 0.582 0.584
$^{SR}CM_L\ (ab)$
$^{SR}CM_M\ (ab)$
CONH2
MeSO2
NMe2
NHNH2
NH2
OMe
MeS
OH
Et
tBu
COOCH3
COOH

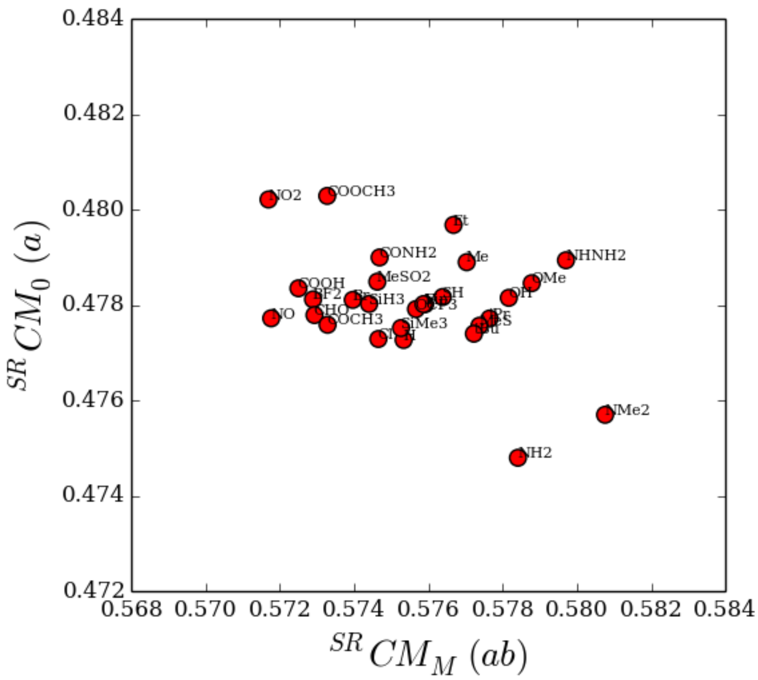
97


0.584
0.582
0.580
0.578
0.576
0.574
0.572
0.570
0.568
0.568 0.570 0.572 0.574 0.576 0.578 0.580 0.582 0.584
$^{SR}CM_M\ (ab)$
$^{SR}CM_M\ (ab)$

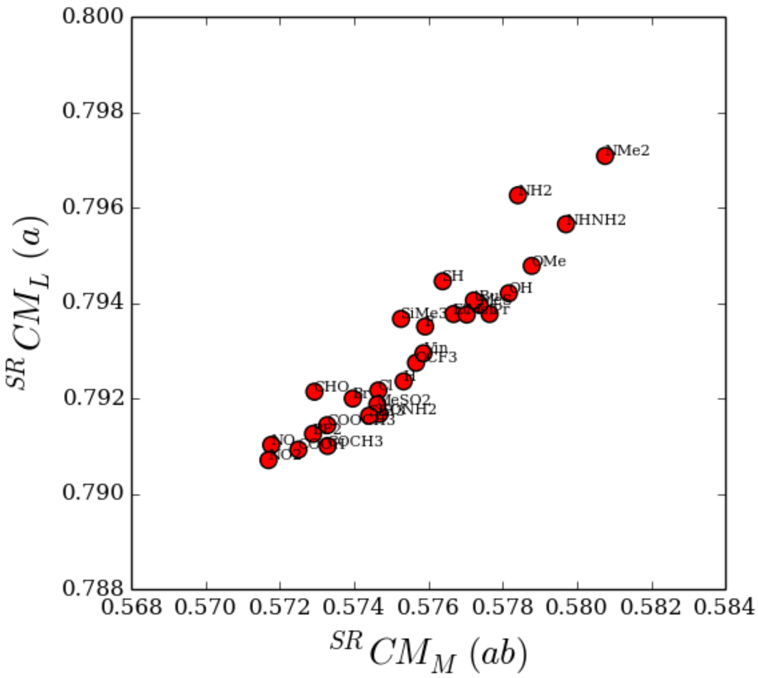
98


0.815
0.810
0.805
0.800
0.795
0.790
0.568 0.570 0.572 0.574 0.576 0.578 0.580 0.582 0.584
$^{SR}CM_q\ (ab)$
$^{SR}CM_M\ (ab)$

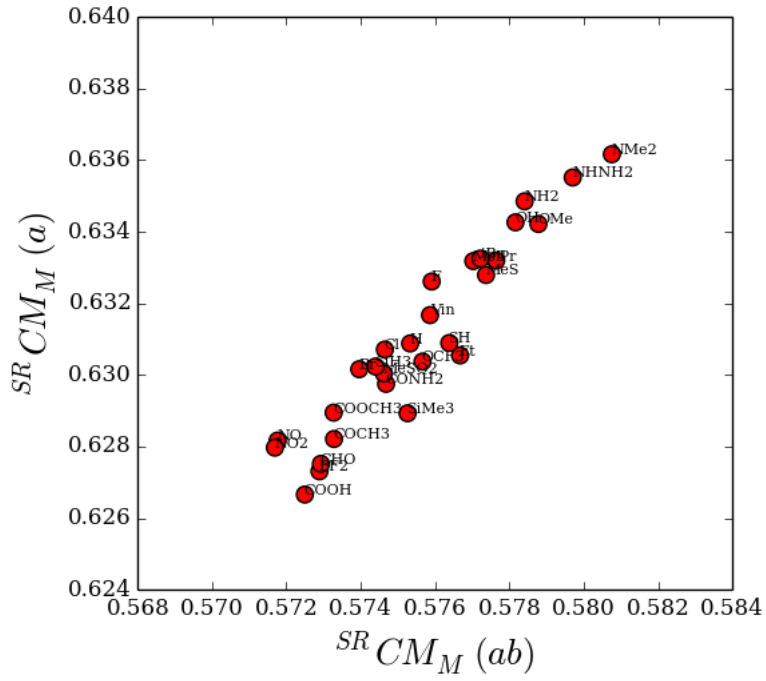
99


0.484
0.482
0.480
0.478
0.476
0.474
0.472
0.568 0.570 0.572 0.574 0.576 0.578 0.580 0.582 0.584
$^{SR}CM_0\ (a)$
$^{SR}CM_M\ (ab)$
NO2
COOCH3
Et
CONH2
Me
NHNH2
MeSO2
OMe
COOH
CF2
SiH3
SH
CF3
OH
NO
CHO
COCH3
SiMe3
NMe2
NH2

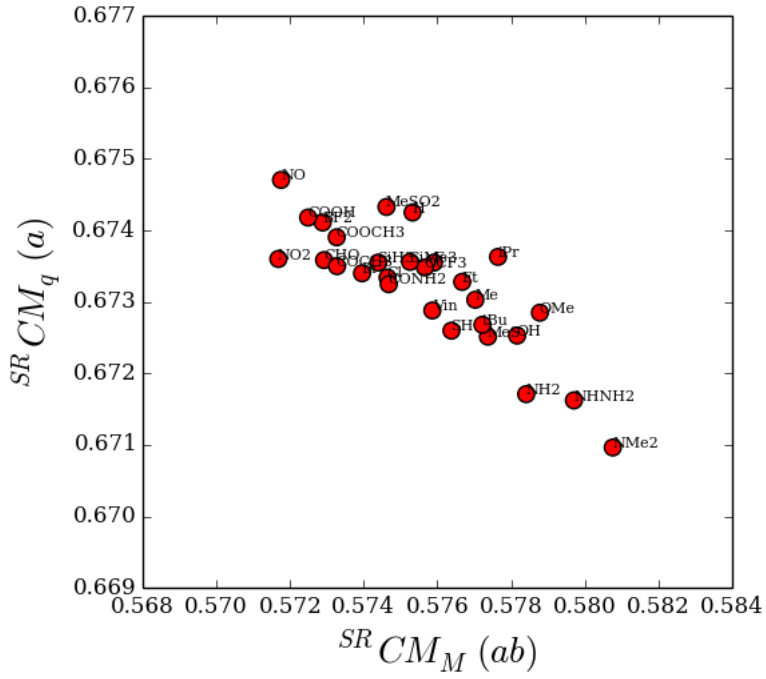
100


0.800
0.798
0.796
0.794
0.792
0.790
0.788
0.568 0.570 0.572 0.574 0.576 0.578 0.580 0.582 0.584
$^{SR}CM_L\ (a)$
$^{SR}CM_M\ (ab)$
NMe2
NH2
NHNH2
OMe
SH
OH
SiMe3
CF3
CHO
MeSO2
CONH2
COOCH3
COCH3
NO

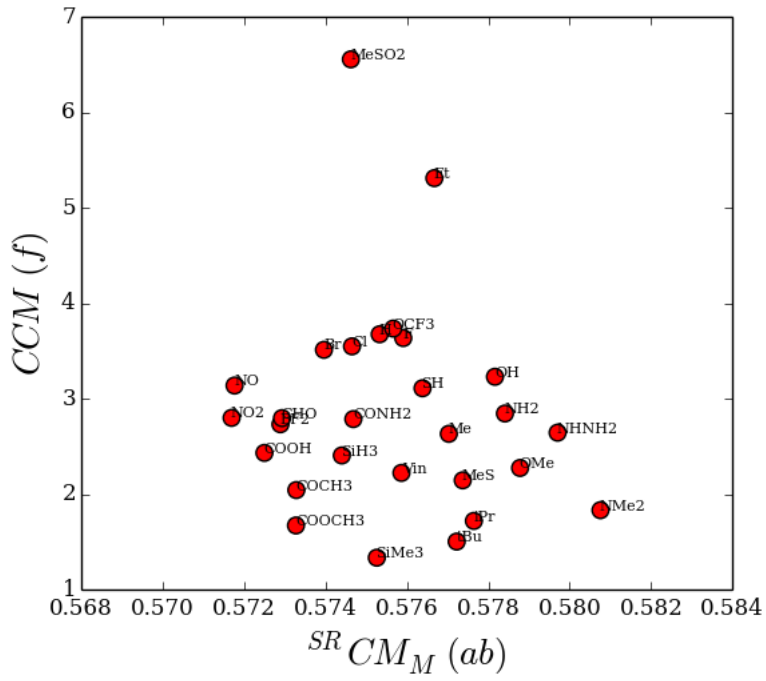
101


0.640
0.638
0.636
0.634
0.632
0.630
0.628
0.626
0.624
0.568 0.570 0.572 0.574 0.576 0.578 0.580 0.582 0.584
$^{SR}CM_M\ (a)$
$^{SR}CM_M\ (ab)$
NMe2
NHNH2
NH2
NHOMe
Vin
COOCH3
SiMe3
NO2
COOH

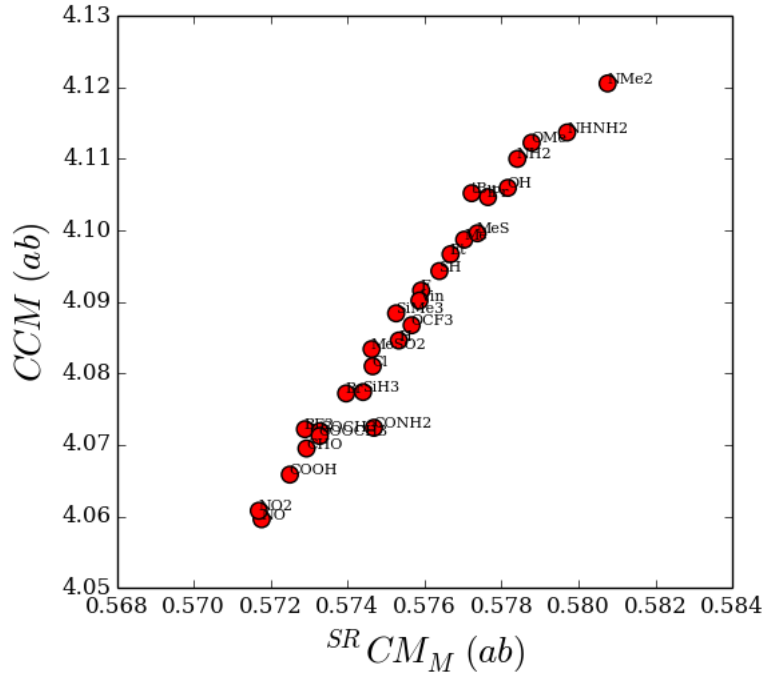
102


0.677
0.676
0.675
0.674
0.673
0.672
0.671
0.670
0.669
0.568 0.570 0.572 0.574 0.576 0.578 0.580 0.582 0.584
$^{SR}CM_q\ (a)$
$^{SR}CM_M\ (ab)$
NO
MeSO2
COOCH3
Et
Me
Vin
OMe
NH2
NHNH2
NMe2

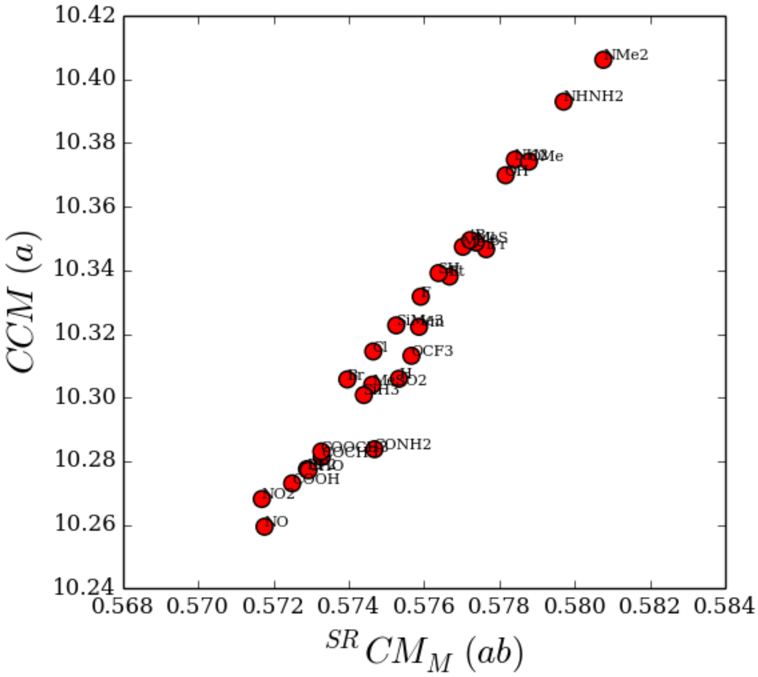
103


MeSO2
Et
OCF3
Br
Cl
NO
SH
OH
NO2
CHO
CONH2
NH2
Me
NHNH2
COOH
SiH3
Vin
OMe
MeS
COCH3
NMe2
COOCH3
iPr
tBu
SiMe3
CCM (f)
SR CM_M (ab)

104

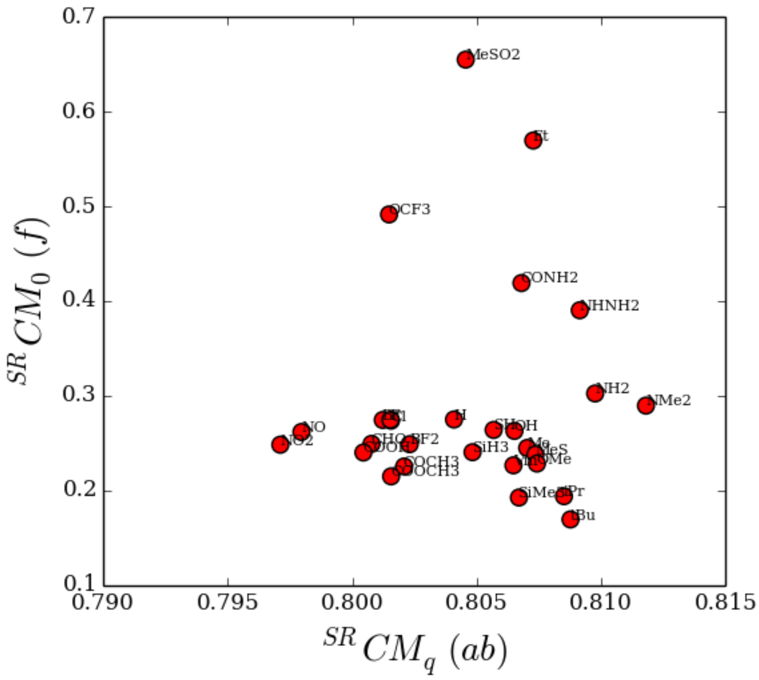

NMe2
NHNH2
OMe
NH2
tBu
OH
MeS
Et
SH
Vin
SiMe3
OCF3
MeSO2
Cl
SiH3
CONH2
CHO
COOH
NO2
NO
CCM (ab)
SR CM_M (ab)

105



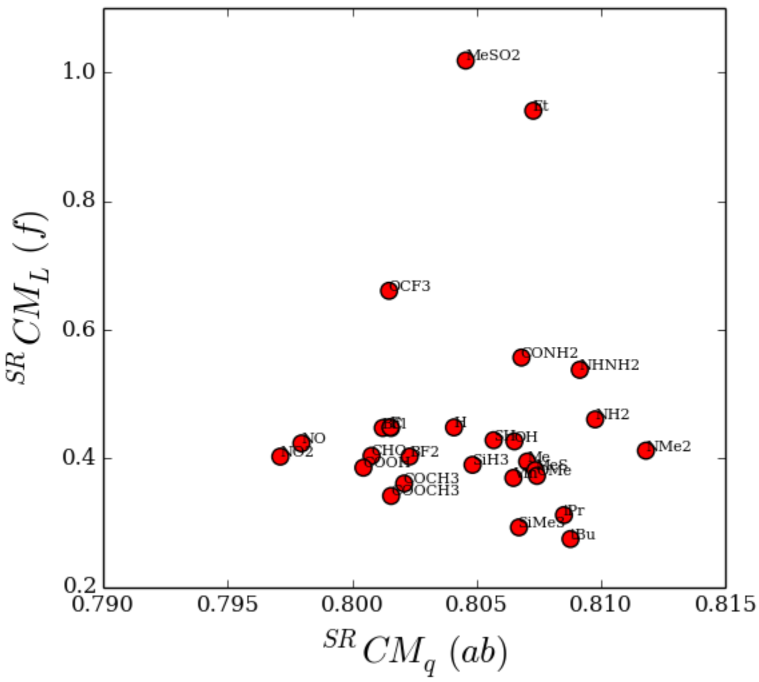
10.42
10.40
10.38
10.36
10.34
10.32
10.30
10.28
10.26
10.24
0.568
0.570
0.572
0.574
0.576
0.578
0.580
0.582
0.584
$CCM\ (a)$
$^{SR}CM_M\ (ab)$
NMe2
NHNH2
OCF3
CONH2
COOH
NO2
NO
Cl
Br

106



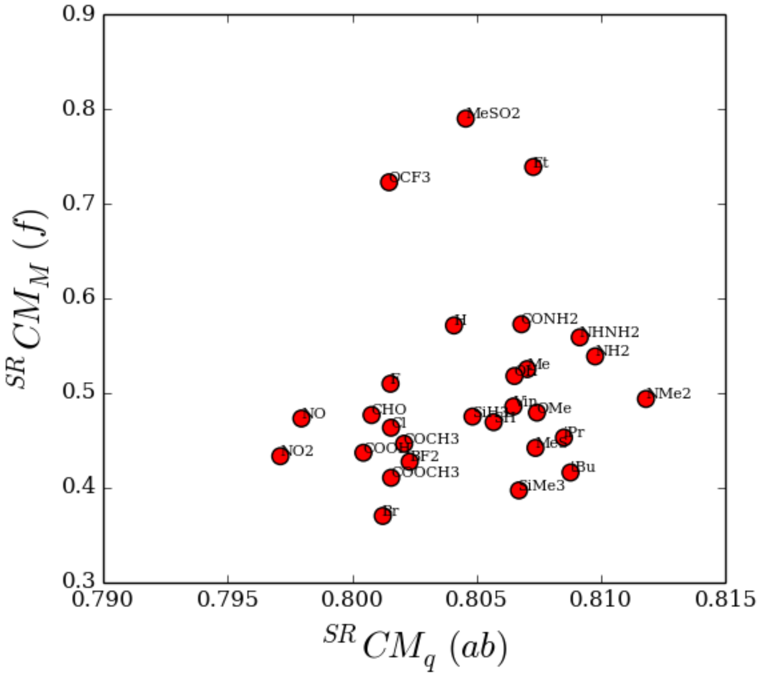
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.790
0.795
0.800
0.805
0.810
0.815
$^{SR}CM_0\ (f)$
$^{SR}CM_q\ (ab)$
MeSO2
Et
OCF3
CONH2
NHNH2
NH2
NMe2
NO
SiH3
CF2
tBu

107



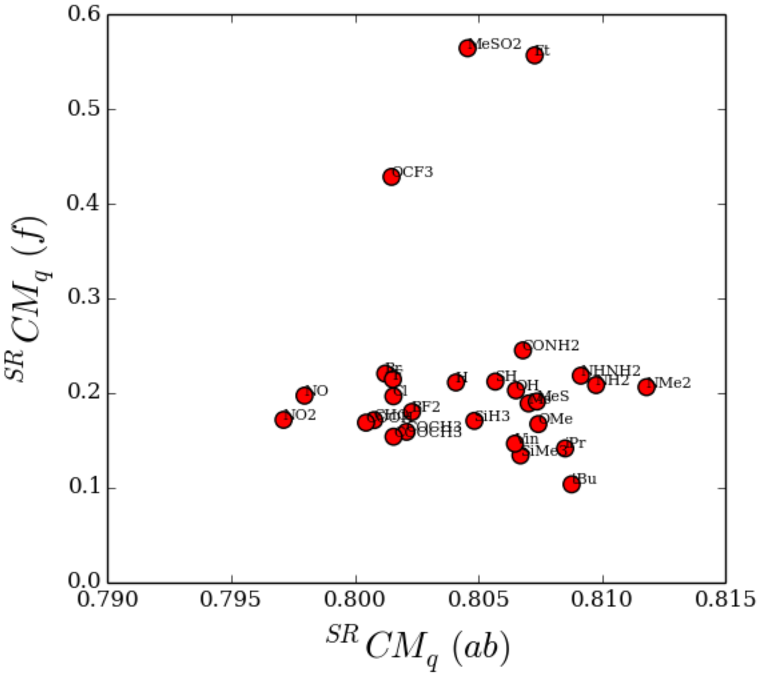
MeSO2
Et
OCF3
CONH2
NHNH2
NH2
NMe2
H
SiH3
SiMe3
tBu
iPr
NO2
1.0
0.8
0.6
0.4
0.2
0.790
0.795
0.800
0.805
0.810
0.815
$^{SR}CM_L\,(f)$
$^{SR}CM_q\,(ab)$

108



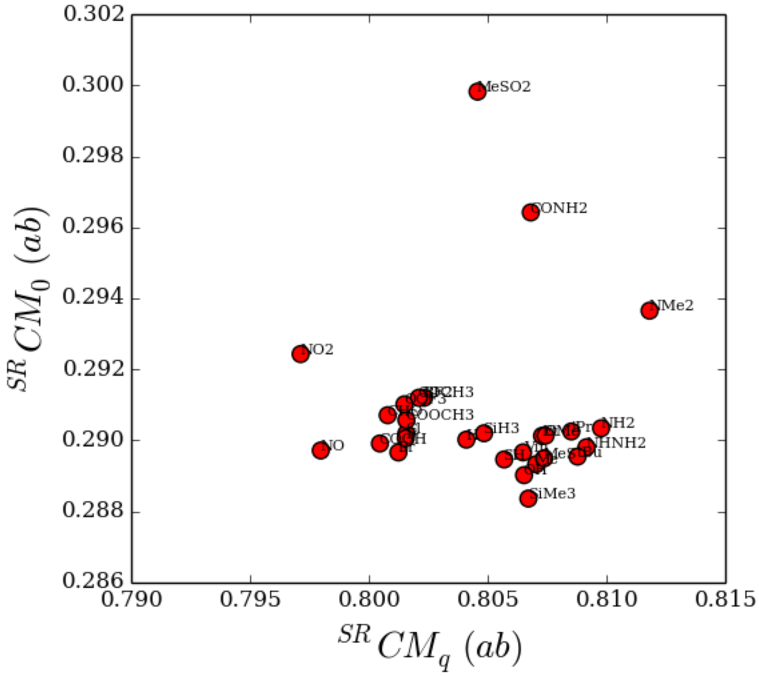
MeSO2
Et
OCF3
H
CONH2
NHNH2
NH2
NMe2
CHO
COCH3
COOCH3
SiMe3
tBu
iPr
OMe
NO2
Br
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.790
0.795
0.800
0.805
0.810
0.815
$^{SR}CM_M\,(f)$
$^{SR}CM_q\,(ab)$

109



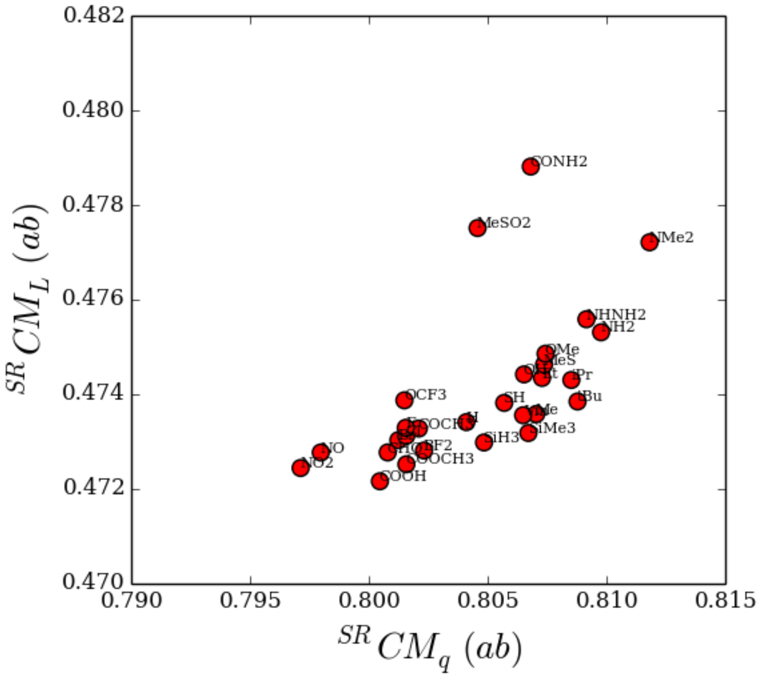
MeSO2
Et
OCF3
CONH2
NHNH2
NMe2
NO
NO2
SH
OH
MeS
SiH3
OMe
iPr
tBu
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.790
0.795
0.800
0.805
0.810
0.815
$^{SR}CM_q\ (f)$
$^{SR}CM_q\ (ab)$

110

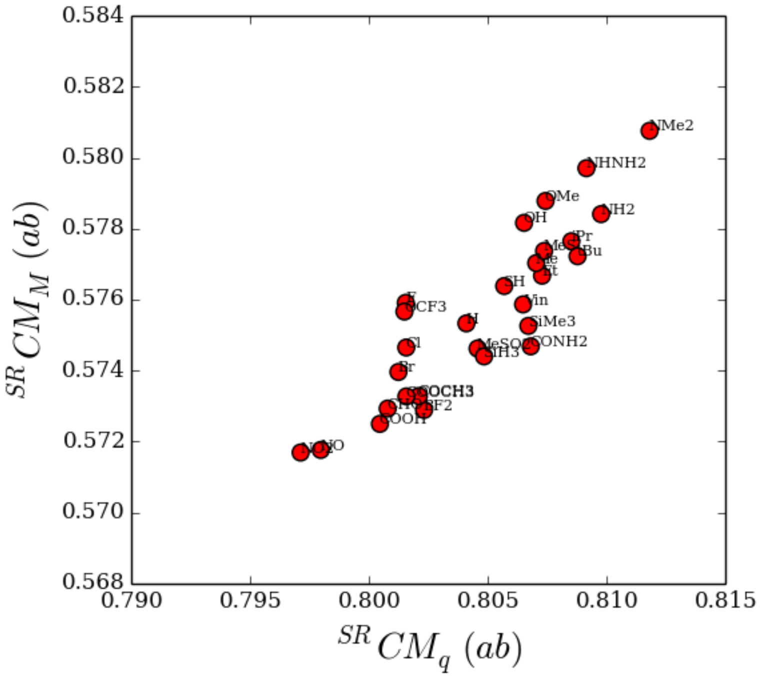


MeSO2
CONH2
NMe2
NO2
NO
SiH3
NH2
NHNH2
SiMe3
COOCH3
0.302
0.300
0.298
0.296
0.294
0.292
0.290
0.288
0.286
0.790
0.795
0.800
0.805
0.810
0.815
$^{SR}CM_0\ (ab)$
$^{SR}CM_q\ (ab)$

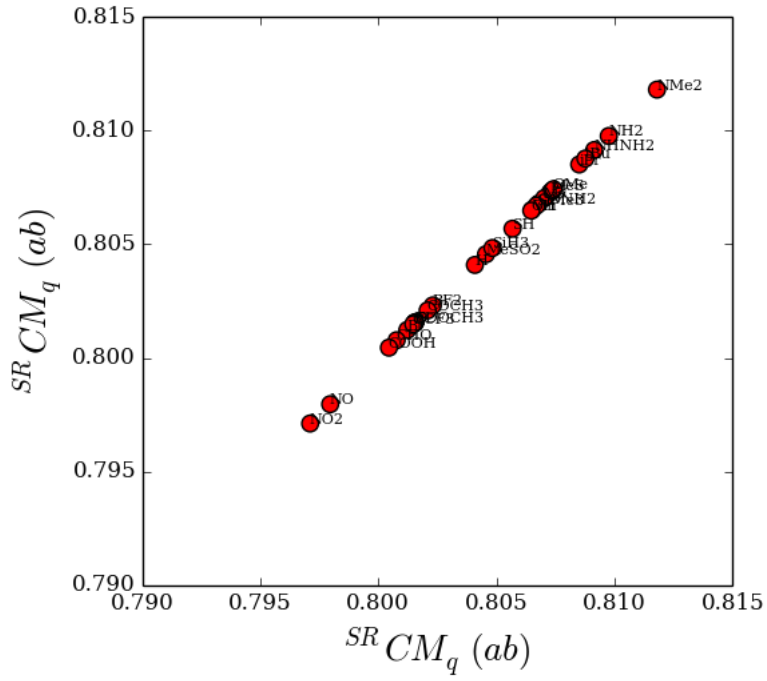
111


0.482
0.480
0.478
0.476
0.474
0.472
0.470
0.790
0.795
0.800
0.805
0.810
0.815
$^{SR}CM_L\ (ab)$
$^{SR}CM_q\ (ab)$
CONH2
MeSO2
NMe2
NHNH2
NH2
OMe
MeS
iPr
tBu
OCF3
SH
Me
SiMe3
SiH3
COCH3
SF2
OCOCH3
NO
NO2
COOH

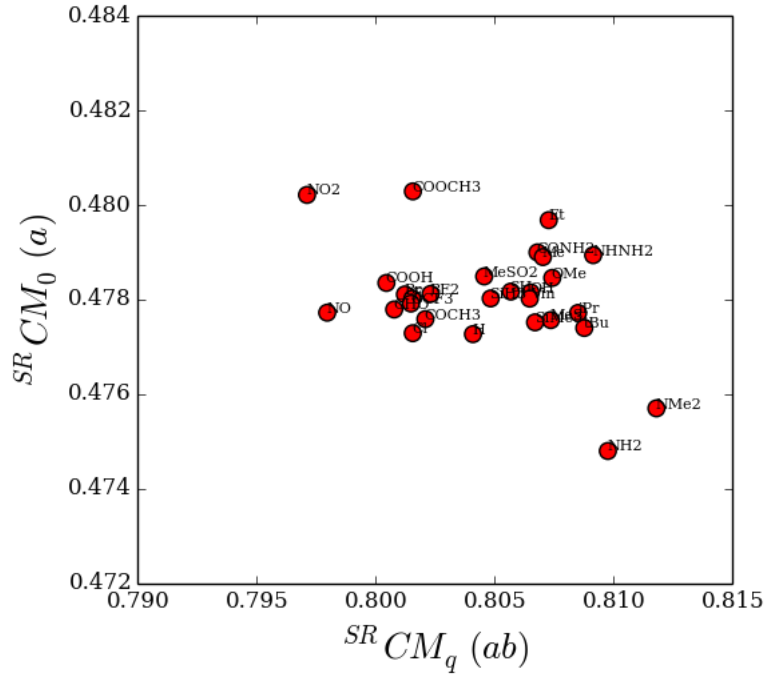
112


0.584
0.582
0.580
0.578
0.576
0.574
0.572
0.570
0.568
0.790
0.795
0.800
0.805
0.810
0.815
$^{SR}CM_M\ (ab)$
$^{SR}CM_q\ (ab)$
NMe2
NHNH2
OMe
OH
NH2
iPr
tBu
SH
F
OCF3
Vin
H
SiMe3
Cl
CONH2
SiH3
Br
COCH3
SF2
COOH
NO

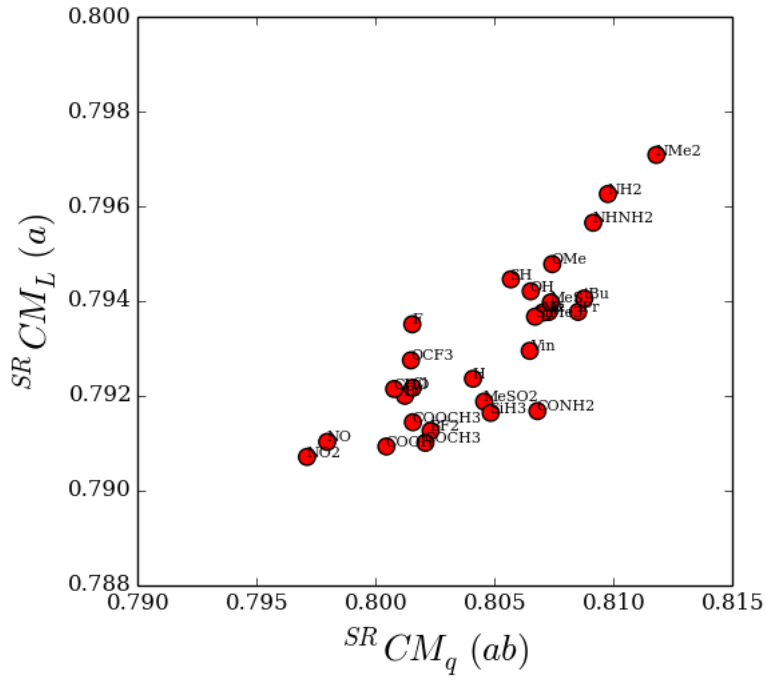
113


0.815
0.810
0.805
0.800
0.795
0.790
0.790
0.795
0.800
0.805
0.810
0.815
$^{SR}CM_q\ (ab)$
$^{SR}CM_q\ (ab)$
NMe2
NH2
NHNH2
OH
SO2
NO
NO2
OOH

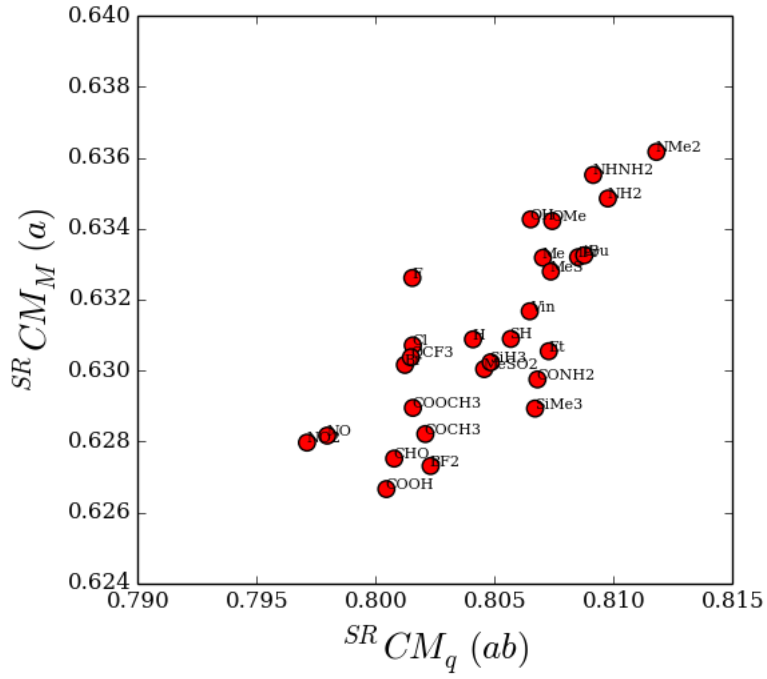
114


0.484
0.482
0.480
0.478
0.476
0.474
0.472
0.790
0.795
0.800
0.805
0.810
0.815
$^{SR}CM_0\ (a)$
$^{SR}CM_q\ (ab)$
NO2
OOCH3
Et
NHNH2
OMe
MeSO2
NO
NMe2
NH2

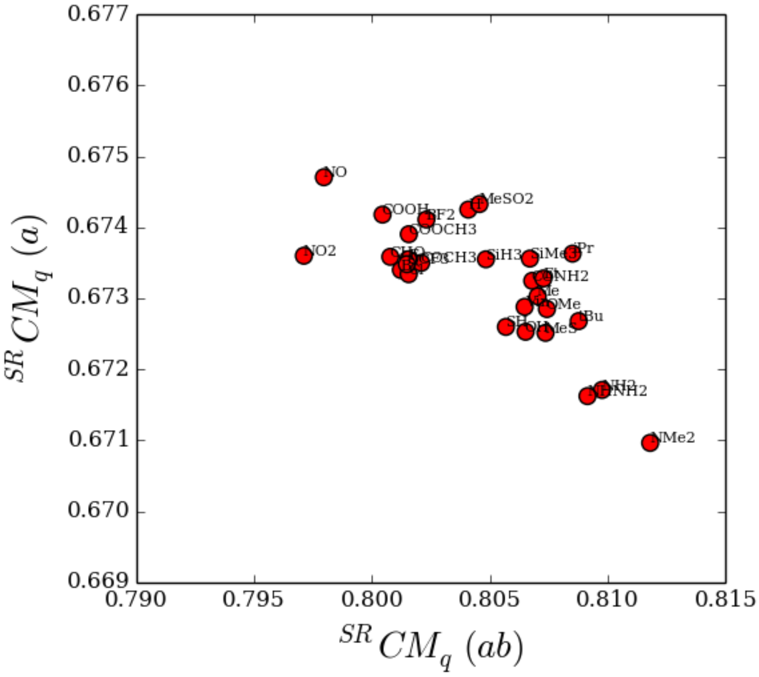
115


0.800
0.798
0.796
0.794
0.792
0.790
0.788
0.790
0.795
0.800
0.805
0.810
0.815
$^{SR}CM_L\ (a)$
$^{SR}CM_q\ (ab)$
NMe2
NH2
NHNH2
OMe
SH
OH
tBu
Br
Vin
OCF3
I
MeSO2
SiH3
CONH2
SOOCH3
CF2
COOCH3
NO
NO2

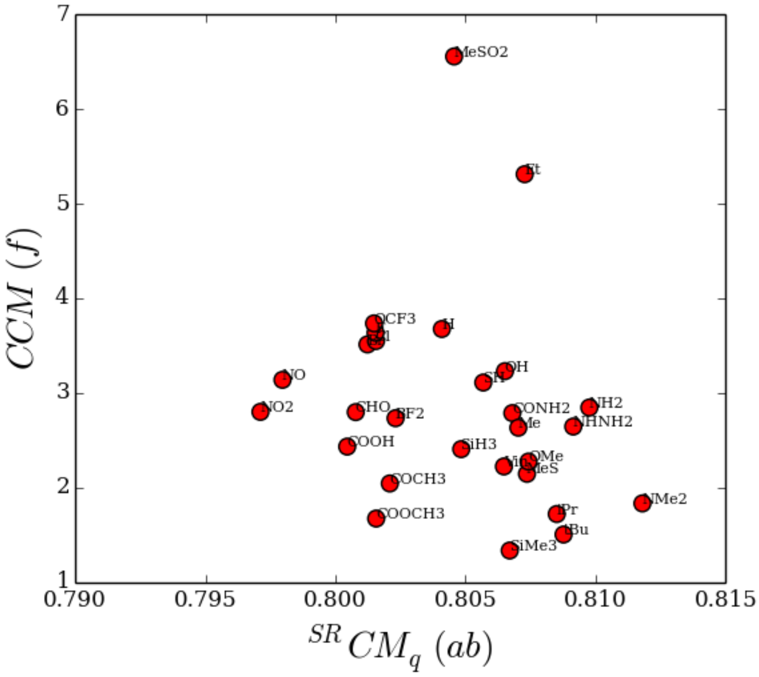
116


0.640
0.638
0.636
0.634
0.632
0.630
0.628
0.626
0.624
0.790
0.795
0.800
0.805
0.810
0.815
$^{SR}CM_M\ (a)$
$^{SR}CM_q\ (ab)$
NMe2
NHNH2
NH2
OH
OMe
tBu
Vin
SH
I
Cl
CF3
SiH3
MeSO2
CONH2
SiMe3
SOOCH3
COCH3
NO
NO2
CHO
CF2
COOH

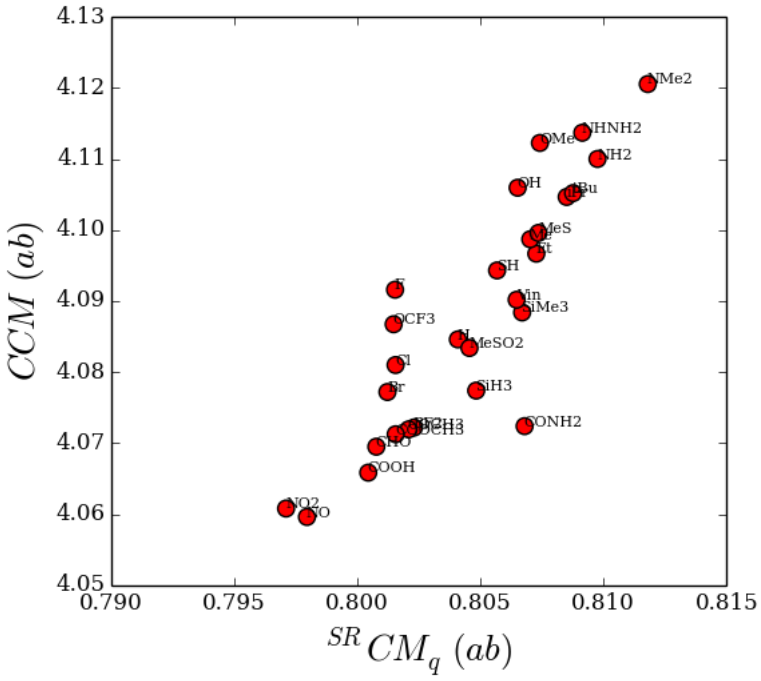
117


NO
COOH
BF2
MeSO2
COOCH3
NO2
CHO
SiH3
NHNH2
OMe
tBu
NH2
NMe2
0.669
0.670
0.671
0.672
0.673
0.674
0.675
0.676
0.677
0.790
0.795
0.800
0.805
0.810
0.815
$^{SR}CM_q\ (a)$
$^{SR}CM_q\ (ab)$

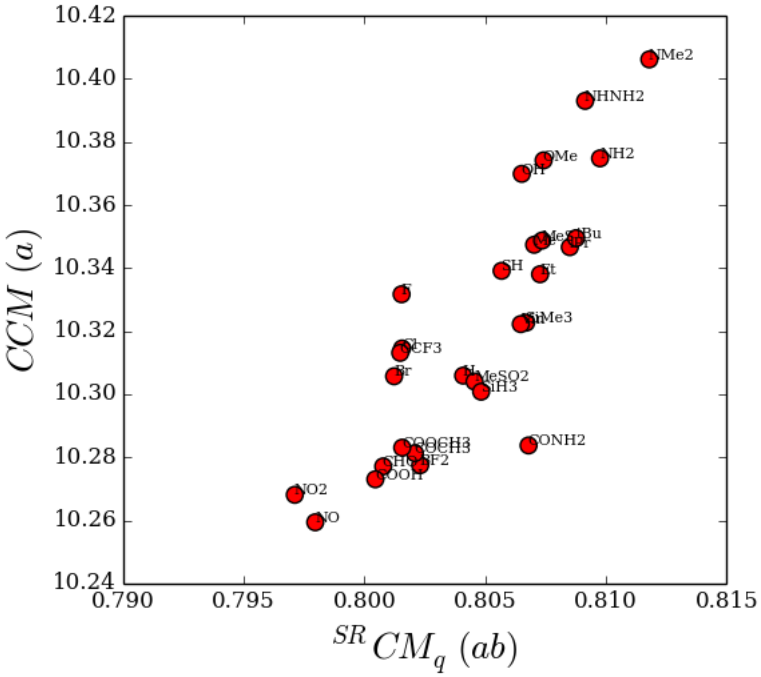
118


MeSO2
Et
OCF3
H
OH
NO
NO2
CHO
BF2
CONH2
NH2
NHNH2
COOH
SiH3
OMe
MeS
COCH3
NMe2
COOCH3
iPr
tBu
SiMe3
1
2
3
4
5
6
7
0.790
0.795
0.800
0.805
0.810
0.815
$CCM\ (f)$
$^{SR}CM_q\ (ab)$

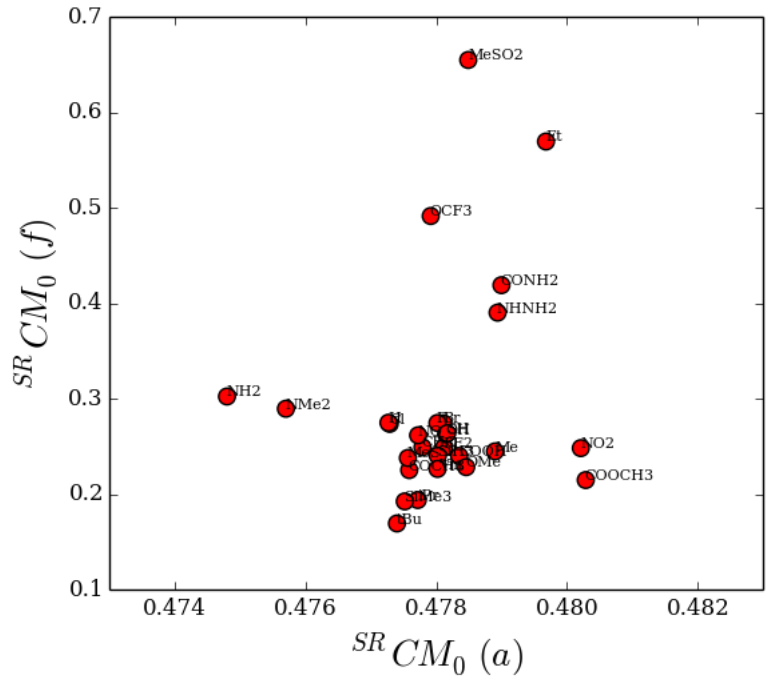
119


4.13
4.12
4.11
4.10
4.09
4.08
4.07
4.06
4.05
0.790
0.795
0.800
0.805
0.810
0.815
$CCM\ (ab)$
$^{SR}CM_q\ (ab)$
NMe2
NHNH2
NH2
OH
SH
SiH3
CONH2
COOH
NO2
NO

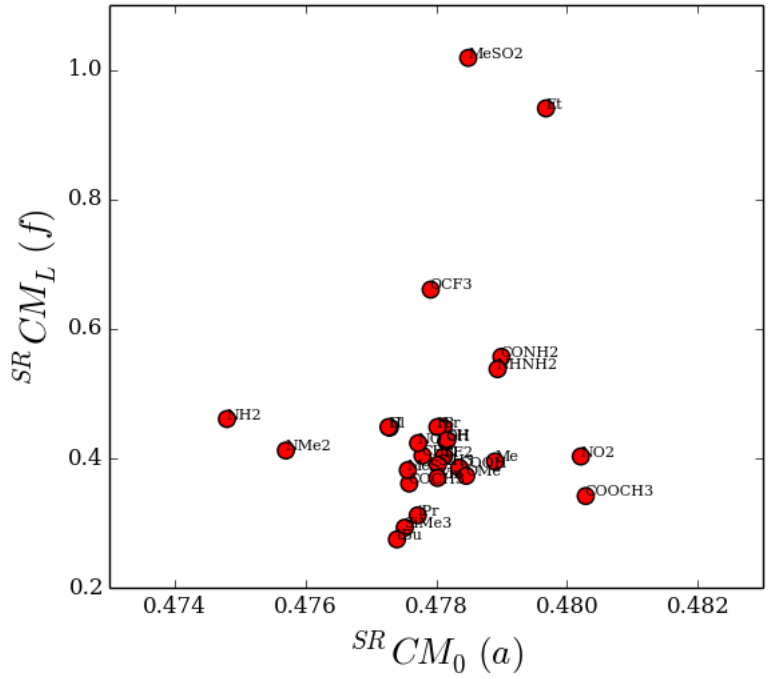
120


10.42
10.40
10.38
10.36
10.34
10.32
10.30
10.28
10.26
10.24
0.790
0.795
0.800
0.805
0.810
0.815
$CCM\ (a)$
$^{SR}CM_q\ (ab)$
NMe2
NHNH2
NH2
OH
SH
SiH3
CONH2
NO2
NO

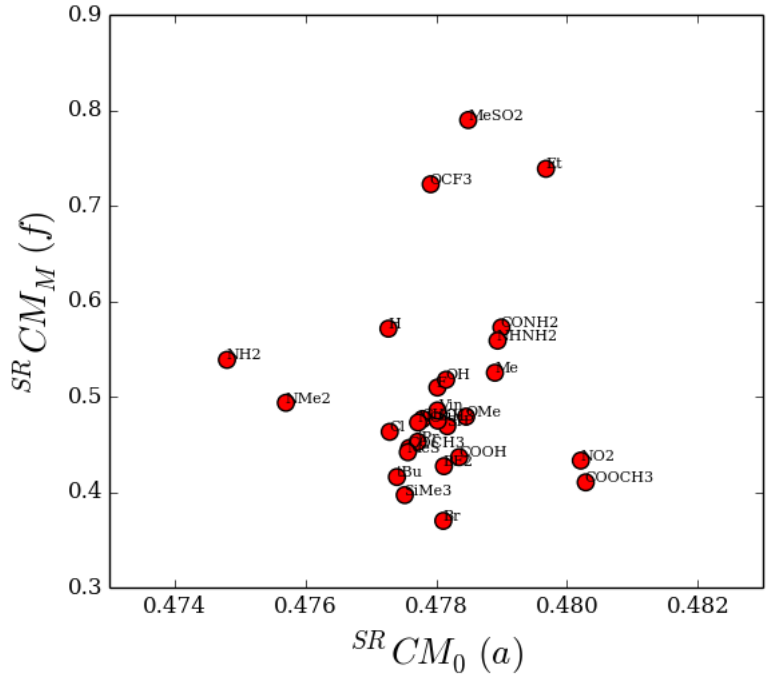
121


0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.474
0.476
0.478
0.480
0.482
$^{SR}CM_0\ (f)$
$^{SR}CM_0\ (a)$
MeSO2
Et
OCF3
CONH2
NHNH2
NH2
NMe2
NO2
COOCH3
tBu

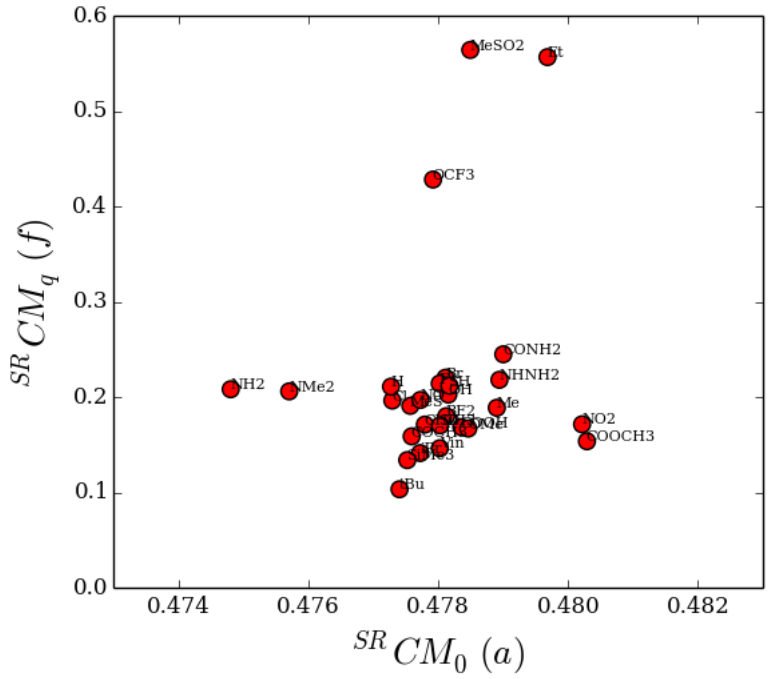
122


1.0
0.8
0.6
0.4
0.2
0.474
0.476
0.478
0.480
0.482
$^{SR}CM_L\ (f)$
$^{SR}CM_0\ (a)$
MeSO2
Et
OCF3
CONH2
NHNH2
NH2
NMe2
NO2
COOCH3
tBu

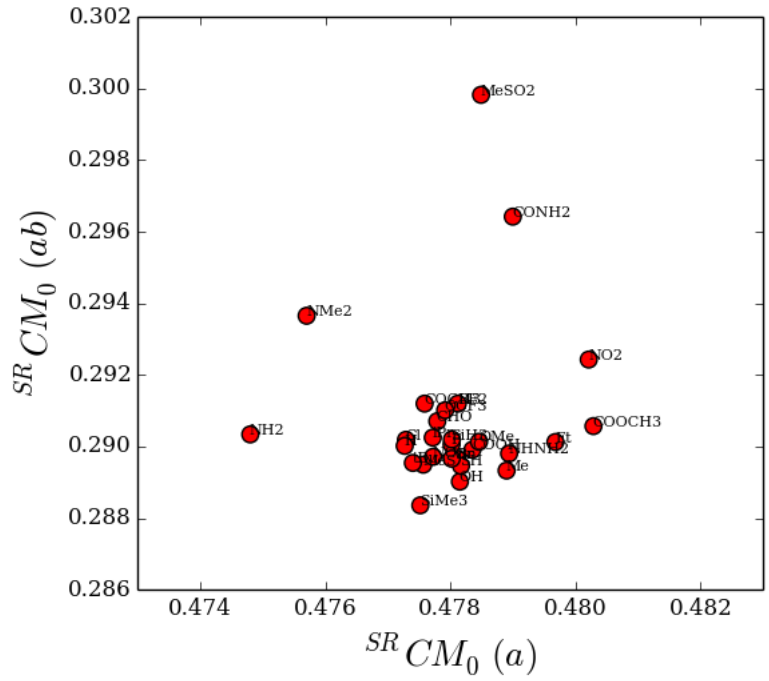
123


0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.474
0.476
0.478
0.480
0.482
$^{SR}CM_M\ (f)$
$^{SR}CM_0\ (a)$
MeSO2
Et
OCF3
H
CONH2
NHNH2
NH2
OH
Me
NMe2
Vin
OMe
Cl
CH3
COOH
NO2
tBu
COOCH3
SiMe3
Br

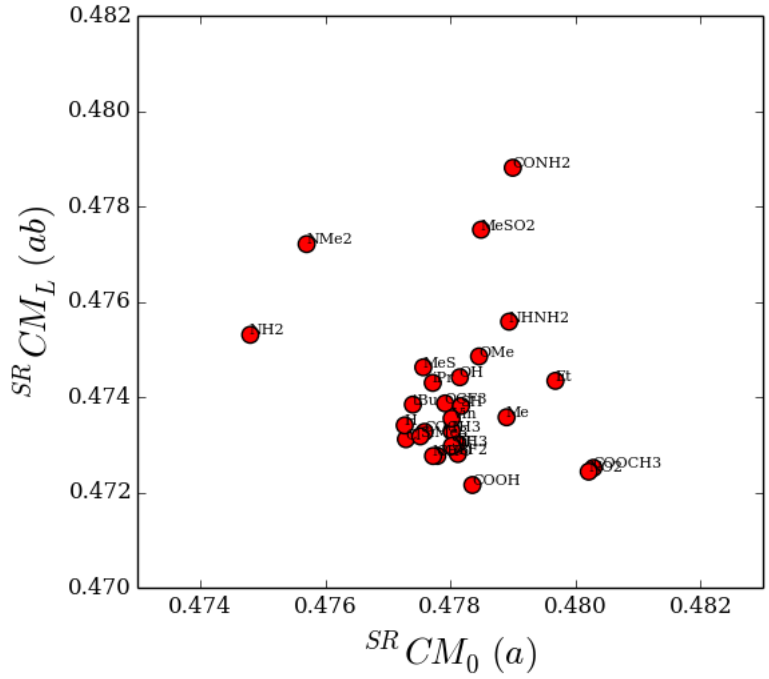
124


0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.474
0.476
0.478
0.480
0.482
$^{SR}CM_q\ (f)$
$^{SR}CM_0\ (a)$
MeSO2
Et
OCF3
CONH2
NHNH2
NH2
NMe2
Me
NO2
COOCH3
tBu

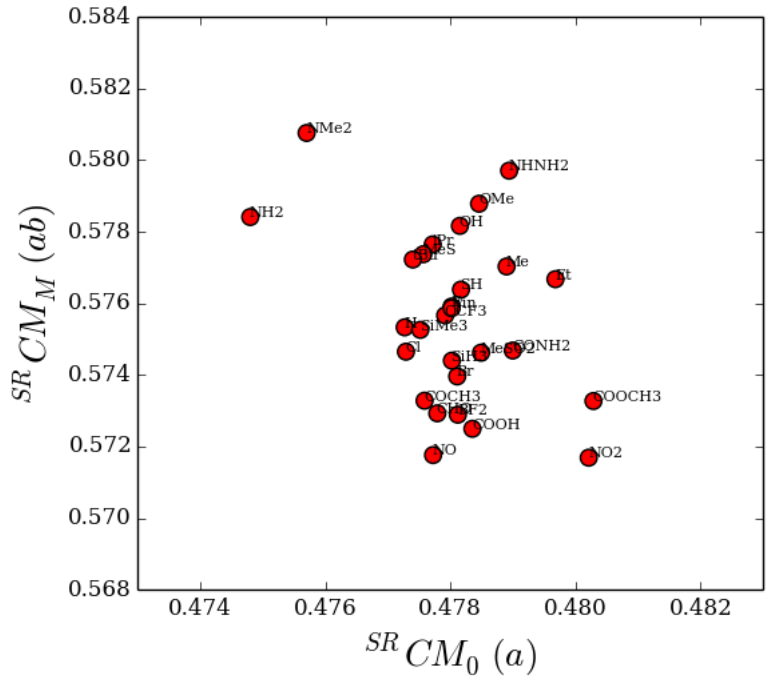
125


0.302
0.300
0.298
0.296
0.294
0.292
0.290
0.288
0.286
0.474
0.476
0.478
0.480
0.482
$^{SR}CM_0\ (ab)$
$^{SR}CM_0\ (a)$
MeSO2
CONH2
NMe2
NO2
NH2
COOCH3
NHNH2
Me
OH
SiMe3

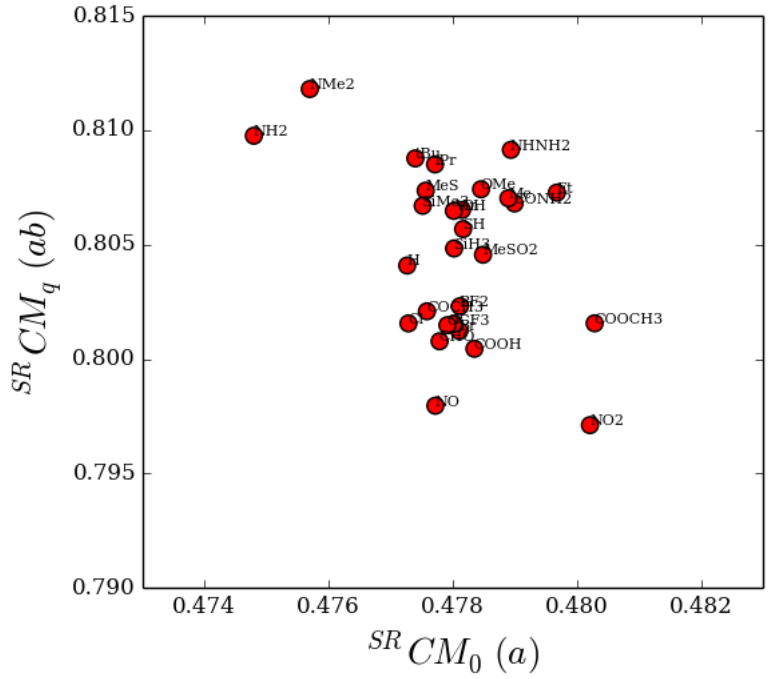
126


0.482
0.480
0.478
0.476
0.474
0.472
0.470
0.474
0.476
0.478
0.480
0.482
$^{SR}CM_L\ (ab)$
$^{SR}CM_0\ (a)$
CONH2
MeSO2
NMe2
NH2
NHNH2
Me
COOH
COOCH3

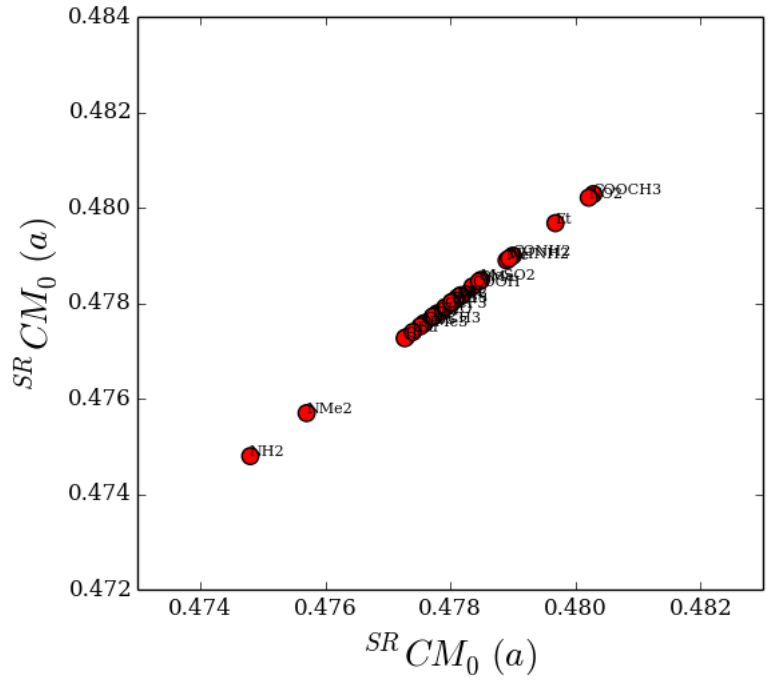
127


0.584
0.582
0.580
0.578
0.576
0.574
0.572
0.570
0.568
0.474
0.476
0.478
0.480
0.482
$^{SR}CM_M\ (ab)$
$^{SR}CM_0\ (a)$
NMe2
NHNH2
OMe
NH2
OH
Me
Et
CH
SiMe3
NO2
COOCH3
COOH
NO

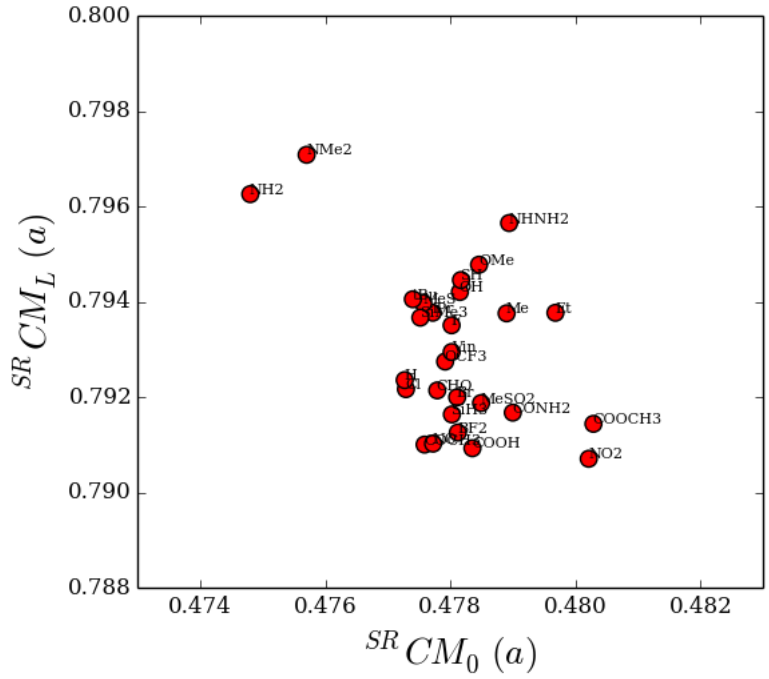
128


0.815
0.810
0.805
0.800
0.795
0.790
0.474
0.476
0.478
0.480
0.482
$^{SR}CM_q\ (ab)$
$^{SR}CM_0\ (a)$
NMe2
NH2
NHNH2
MeSO2
COOCH3
COOH
NO
NO2

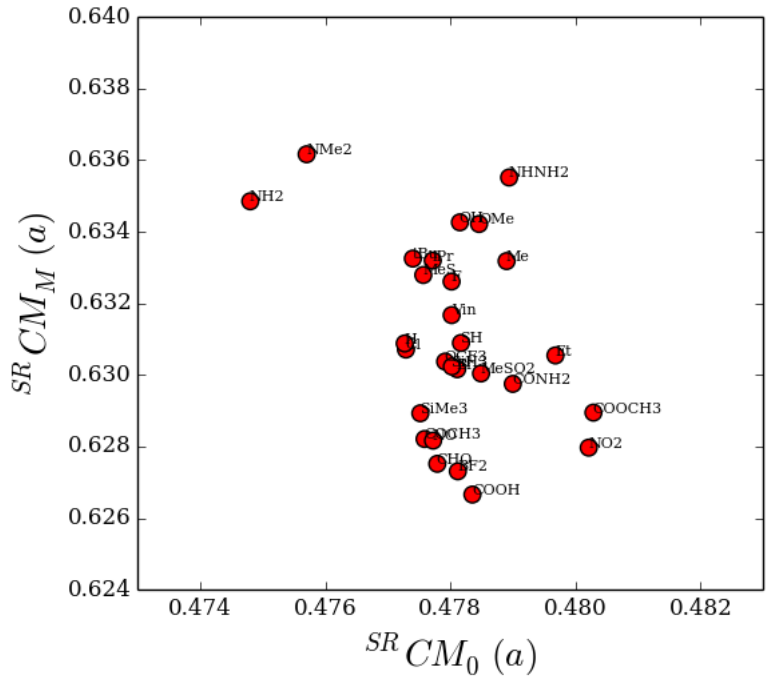
129


0.484
0.482
0.480
0.478
0.476
0.474
0.472
0.474
0.476
0.478
0.480
0.482
$^{SR}CM_0\ (a)$
$^{SR}CM_0\ (a)$
NMe2
NH2
COOCH3
Et

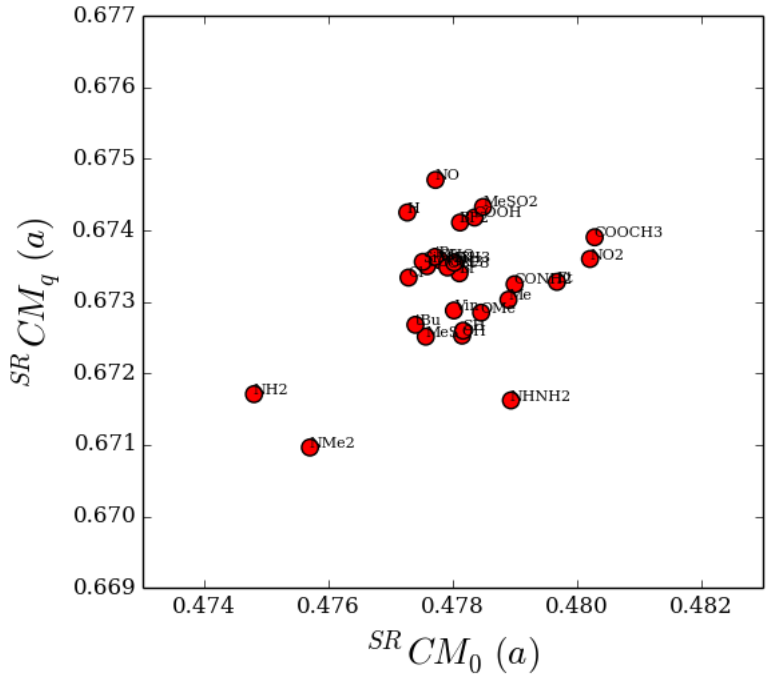
130


0.800
0.798
0.796
0.794
0.792
0.790
0.788
0.474
0.476
0.478
0.480
0.482
$^{SR}CM_L\ (a)$
$^{SR}CM_0\ (a)$
NMe2
NH2
NHNH2
Me
Et
CF3
CHO
MeSO2
CONH2
COOCH3
NO2
COOH

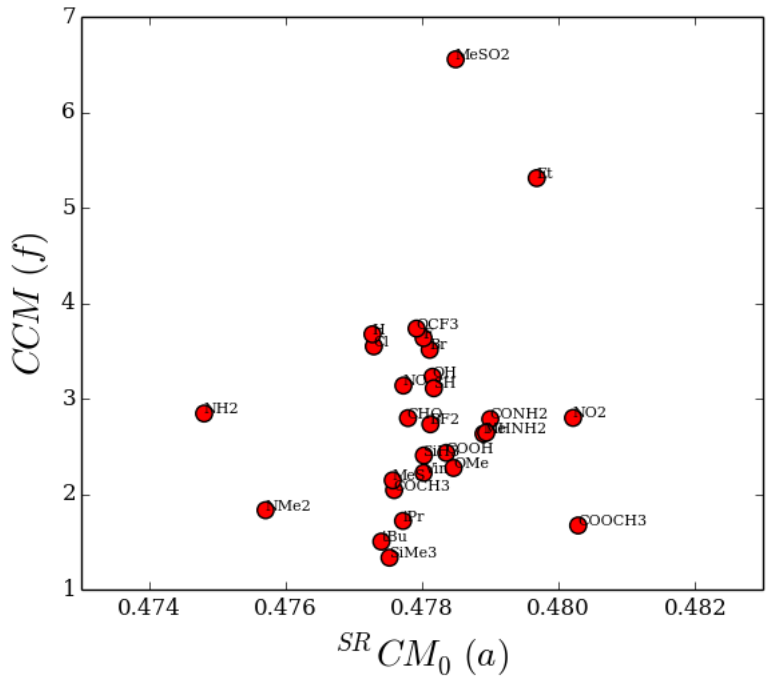
131


0.640
0.638
0.636
0.634
0.632
0.630
0.628
0.626
0.624
0.474
0.476
0.478
0.480
0.482
$^{SR}CM_M\ (a)$
$^{SR}CM_0\ (a)$
NMe2
NHNH2
NH2
OHOMe
Me
Vin
SH
Et
MeSO2
CONH2
SiMe3
COOCH3
NO2
F2
COOH

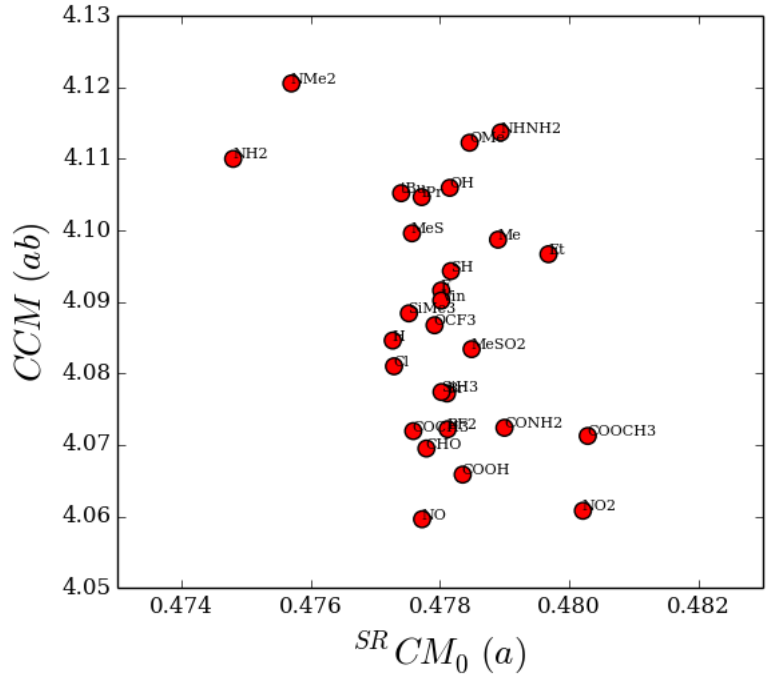
132


0.677
0.676
0.675
0.674
0.673
0.672
0.671
0.670
0.669
0.474
0.476
0.478
0.480
0.482
$^{SR}CM_q\ (a)$
$^{SR}CM_0\ (a)$
NO
MeSO2
COOH
COOCH3
NO2
CONH2
Me
NH2
NHNH2
NMe2

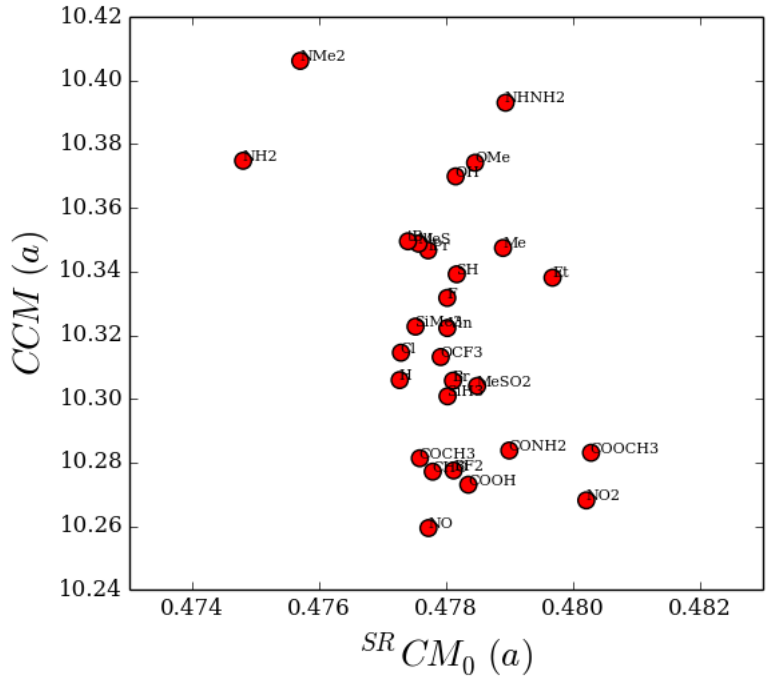
133


MeSO2
Et
OCF3
NH2
CONH2
NO2
NHNH2
SOOH
OMe
COCH3
NMe2
Pr
SOOCH3
tBu
SiMe3
CCM (f)
SR CM0 (a)

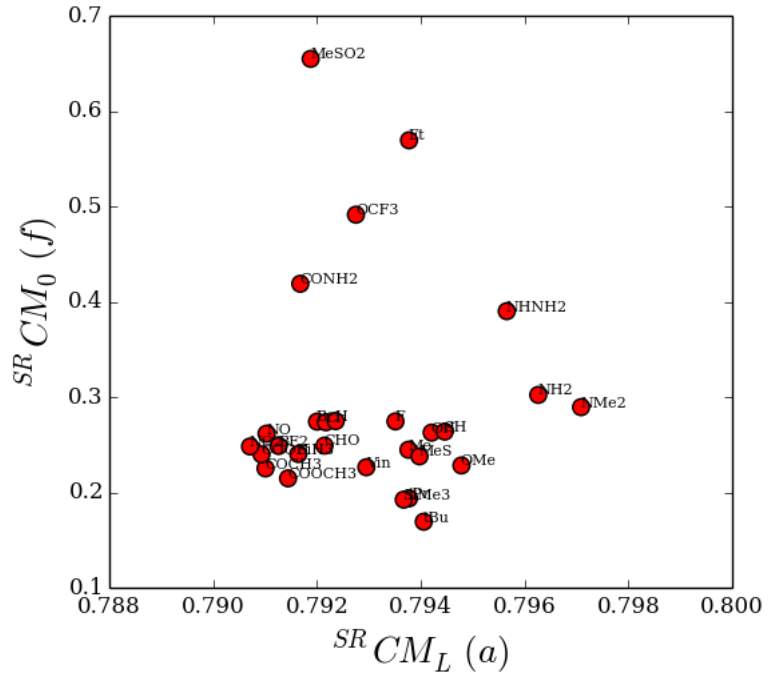
134


NMe2
NHNH2
NH2
OH
MeS
Me
Et
SH
SiMe3
OCF3
MeSO2
NH3
CONH2
SOOCH3
CHO
SOOH
NO2
NO
CCM (ab)
SR CM0 (a)

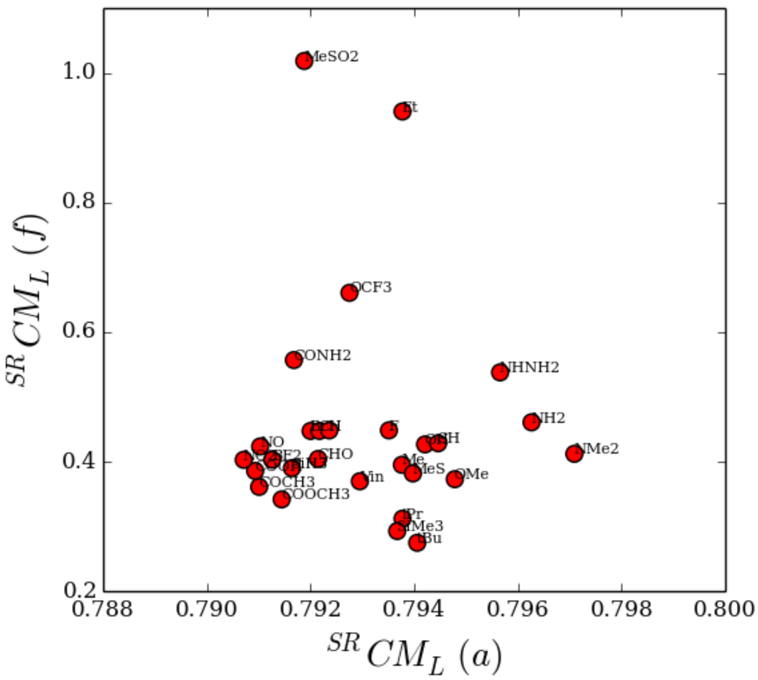
135


10.42
10.40
10.38
10.36
10.34
10.32
10.30
10.28
10.26
10.24
0.474
0.476
0.478
0.480
0.482
$CCM\ (a)$
$^{SR}CM_0\ (a)$
NMe2
NHNH2
NH2
OMe
Me
SH
Et
OCF3
MeSO2
SOCH3
CONH2
COOCH3
COOH
NO2
NO

136

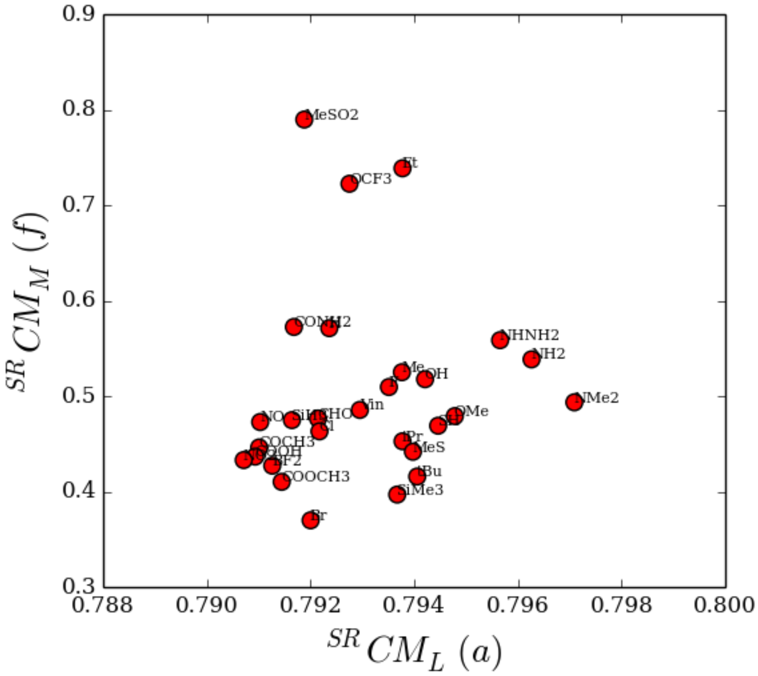

0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.788
0.790
0.792
0.794
0.796
0.798
0.800
$^{SR}CM_0\ (f)$
$^{SR}CM_L\ (a)$
MeSO2
Et
OCF3
CONH2
NHNH2
NH2
NMe2
SH
OMe
tBu

137



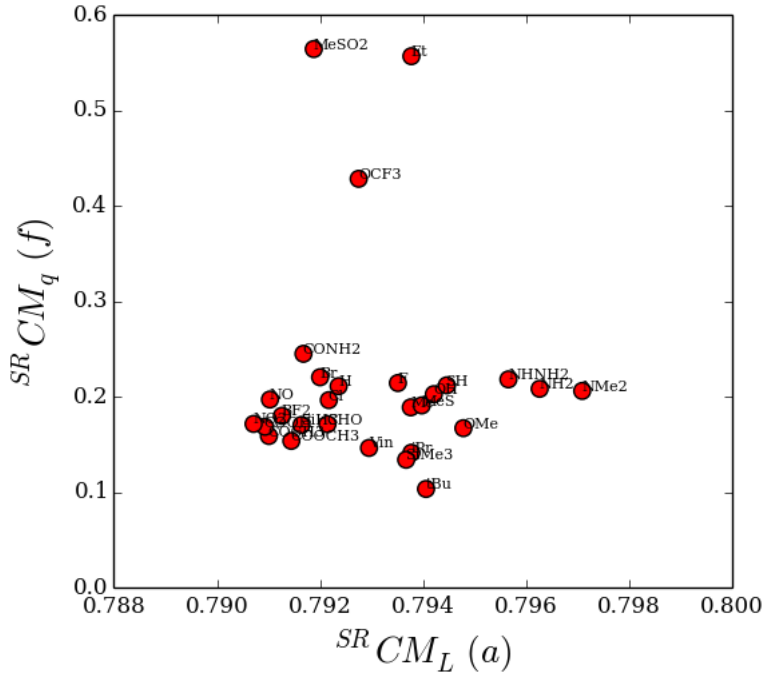
MeSO2
Et
OCF3
CONH2
NHNH2
NH2
NMe2
CHO
Vin
Me
MeS
OMe
COCH3
COOCH3
NO
SiMe3
tBu
$^{SR}CM_L\ (f)$
$^{SR}CM_L\ (a)$

138

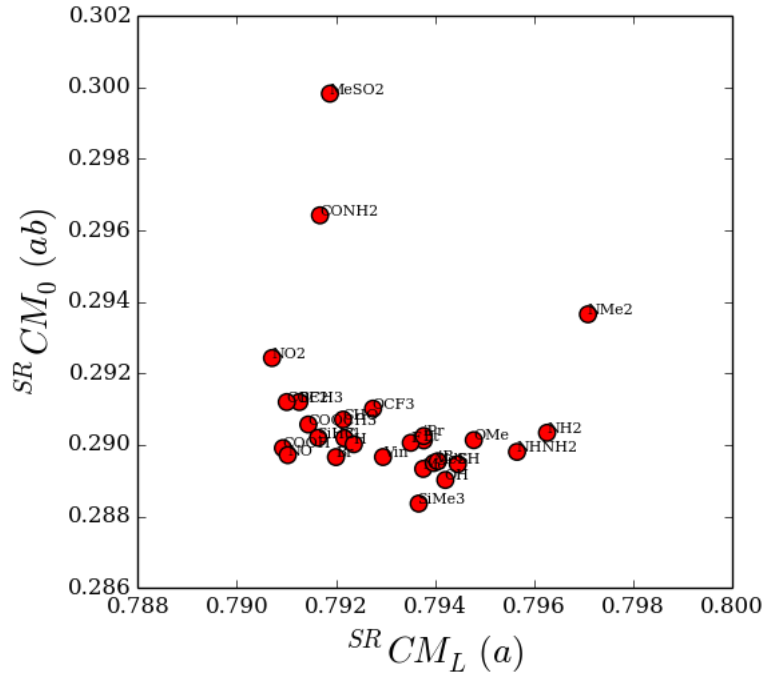


MeSO2
Et
OCF3
CONH2
NHNH2
NH2
NMe2
Me
OH
Vin
CHO
NO
OMe
Pr
MeS
COCH3
tBu
COOCH3
SiMe3
Br
$^{SR}CM_M\ (f)$
$^{SR}CM_L\ (a)$

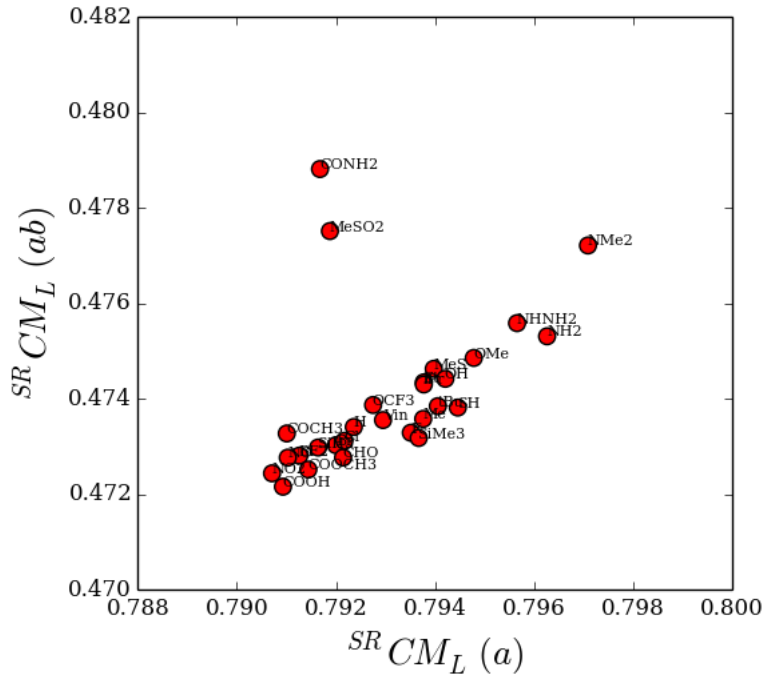
139


0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.788
0.790
0.792
0.794
0.796
0.798
0.800
$^{SR}CM_q\ (f)$
$^{SR}CM_L\ (a)$
MeSO2
OCF3
CONH2
NHNH2
NMe2
OMe
SiMe3
tBu

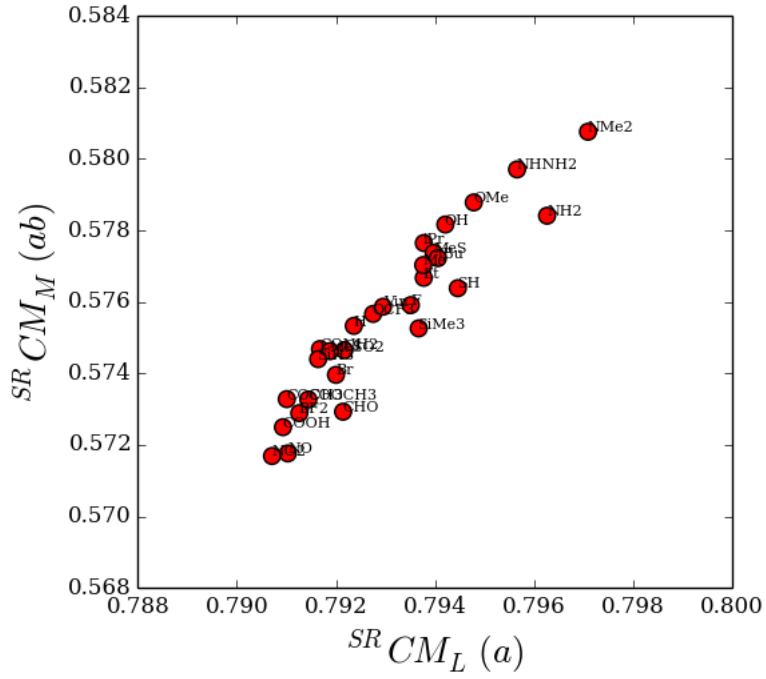
140


0.302
0.300
0.298
0.296
0.294
0.292
0.290
0.288
0.286
0.788
0.790
0.792
0.794
0.796
0.798
0.800
$^{SR}CM_0\ (ab)$
$^{SR}CM_L\ (a)$
MeSO2
CONH2
NMe2
NO2
OCF3
OMe
NHNH2
SiMe3

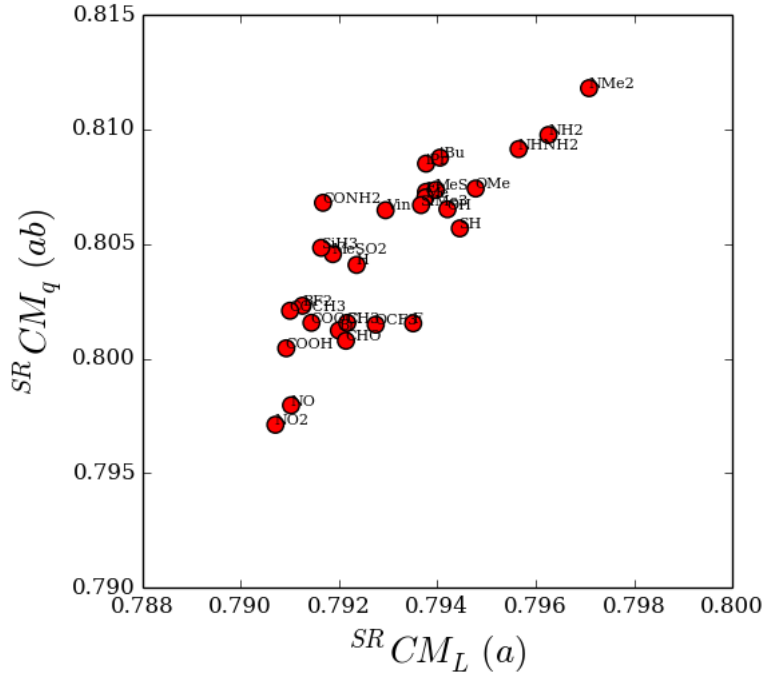
141


0.482
0.480
0.478
0.476
0.474
0.472
0.470
0.788
0.790
0.792
0.794
0.796
0.798
0.800
$^{SR}CM_L\ (ab)$
$^{SR}CM_L\ (a)$
CONH2
MeSO2
NMe2
NHNH2
NH2
OMe
OCF3
SiMe3
COOH

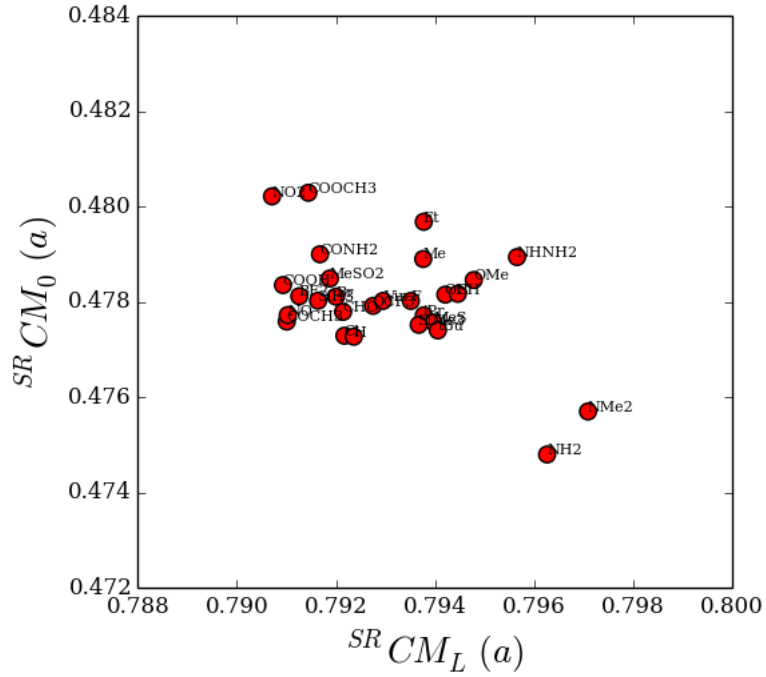
142


0.584
0.582
0.580
0.578
0.576
0.574
0.572
0.570
0.568
0.788
0.790
0.792
0.794
0.796
0.798
0.800
$^{SR}CM_M\ (ab)$
$^{SR}CM_L\ (a)$
NMe2
NHNH2
OMe
NH2
SiMe3
COOH

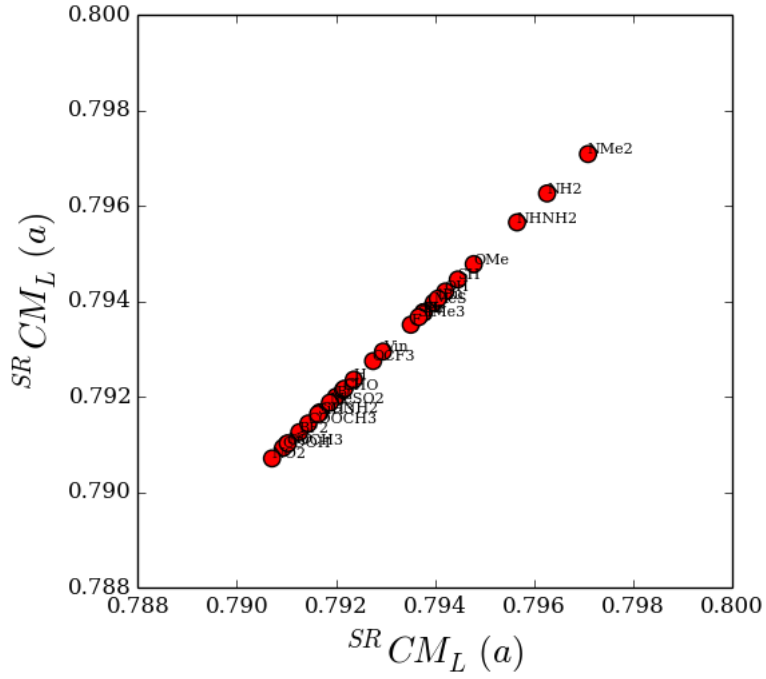
143


0.815
0.810
0.805
0.800
0.795
0.790
0.788
0.790
0.792
0.794
0.796
0.798
0.800
$^{SR}CM_q\ (ab)$
$^{SR}CM_L\ (a)$

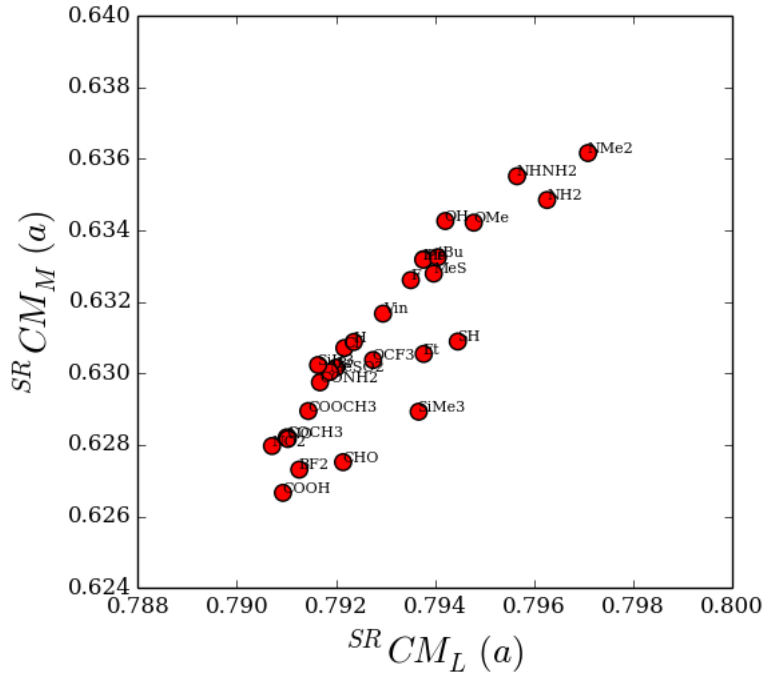
144


0.484
0.482
0.480
0.478
0.476
0.474
0.472
0.788
0.790
0.792
0.794
0.796
0.798
0.800
$^{SR}CM_0\ (a)$
$^{SR}CM_L\ (a)$

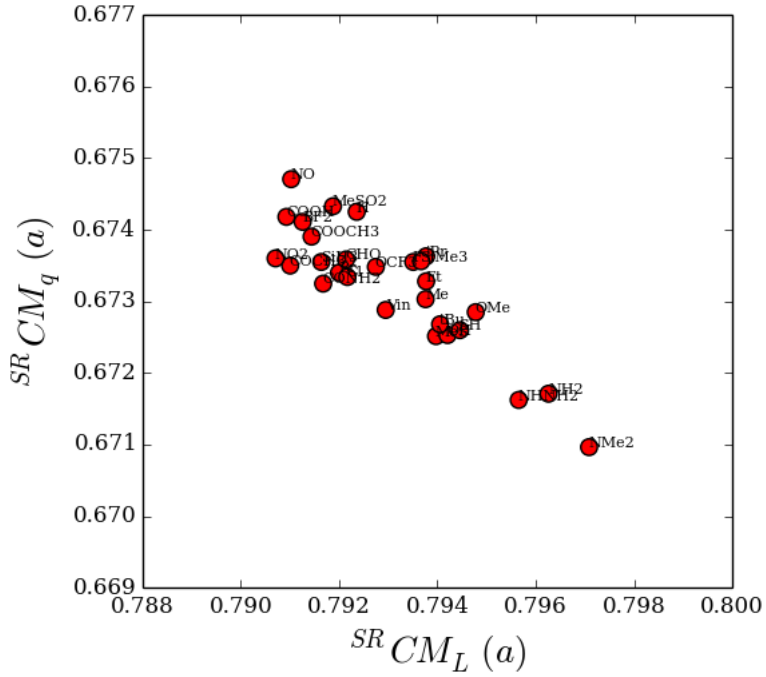
145


0.800
0.798
0.796
0.794
0.792
0.790
0.788
0.788
0.790
0.792
0.794
0.796
0.798
0.800
$^{SR}CM_L\ (a)$
$^{SR}CM_L\ (a)$
NMe2
NH2
NHNH2
OMe
Me3
Vin
F3
HO
SO2
OCH3

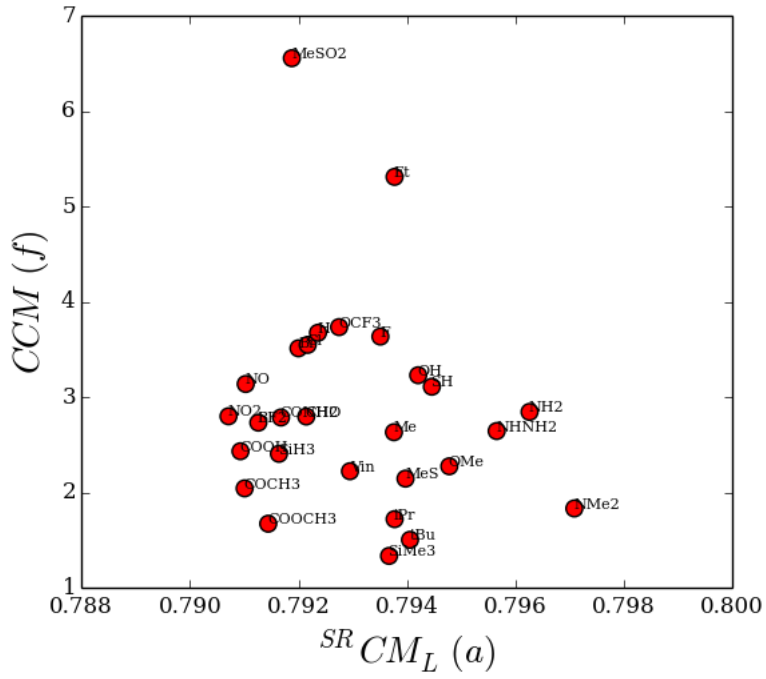
146


0.640
0.638
0.636
0.634
0.632
0.630
0.628
0.626
0.624
0.788
0.790
0.792
0.794
0.796
0.798
0.800
$^{SR}CM_M\ (a)$
$^{SR}CM_L\ (a)$
NMe2
NHNH2
NH2
OMe
Vin
SH
OCF3
SiMe3
F2
CHO
OOH

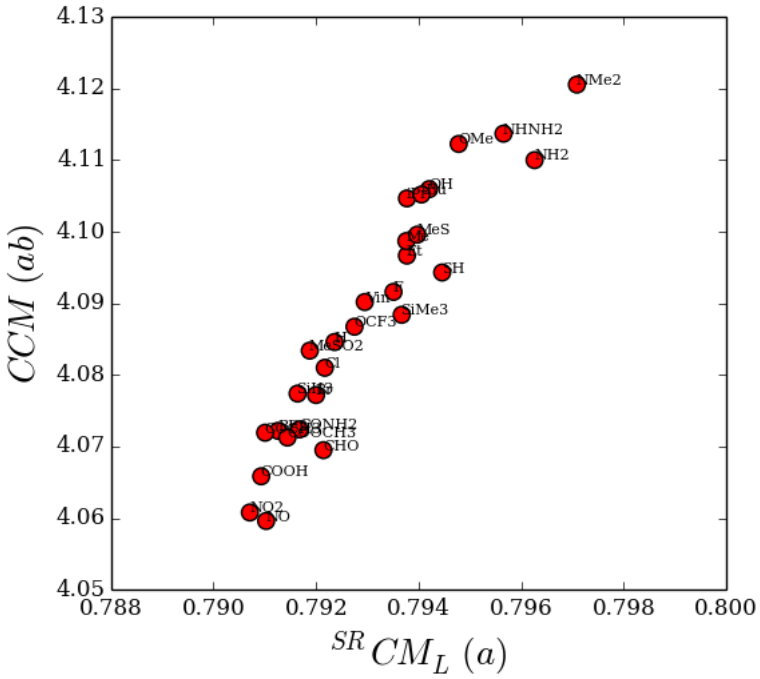
147


0.677
0.676
0.675
0.674
0.673
0.672
0.671
0.670
0.669
0.788
0.790
0.792
0.794
0.796
0.798
0.800
$^{SR}CM_q\ (a)$
$^{SR}CM_L\ (a)$
NO
MeSO2
SOOCH3
SMe3
Et
Me
Vin
OMe
NHNH2
NMe2

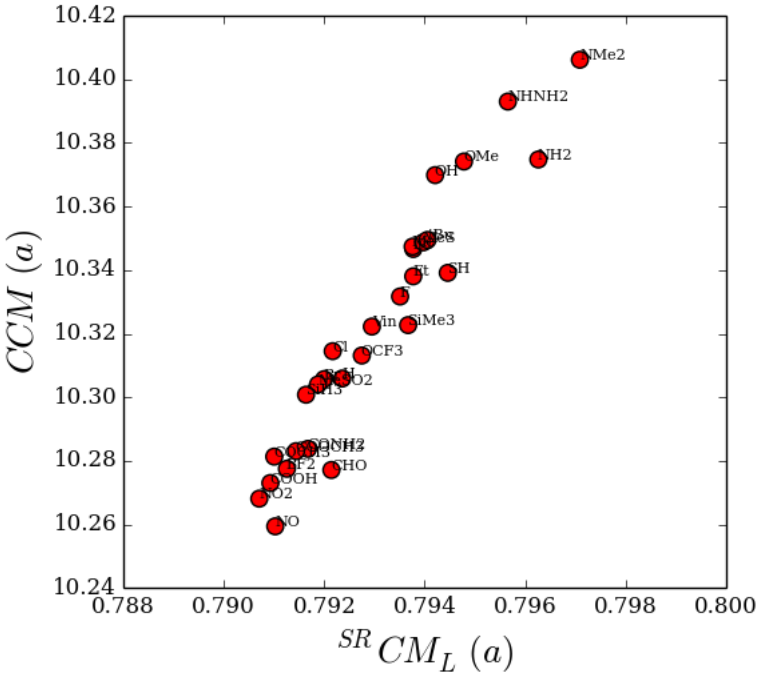
148


7
6
5
4
3
2
1
0.788
0.790
0.792
0.794
0.796
0.798
0.800
$CCM\ (f)$
$^{SR}CM_L\ (a)$
MeSO2
Et
NO
NHNH2
Me
Vin
MeS
OMe
NMe2
SOOCH3
SMe3

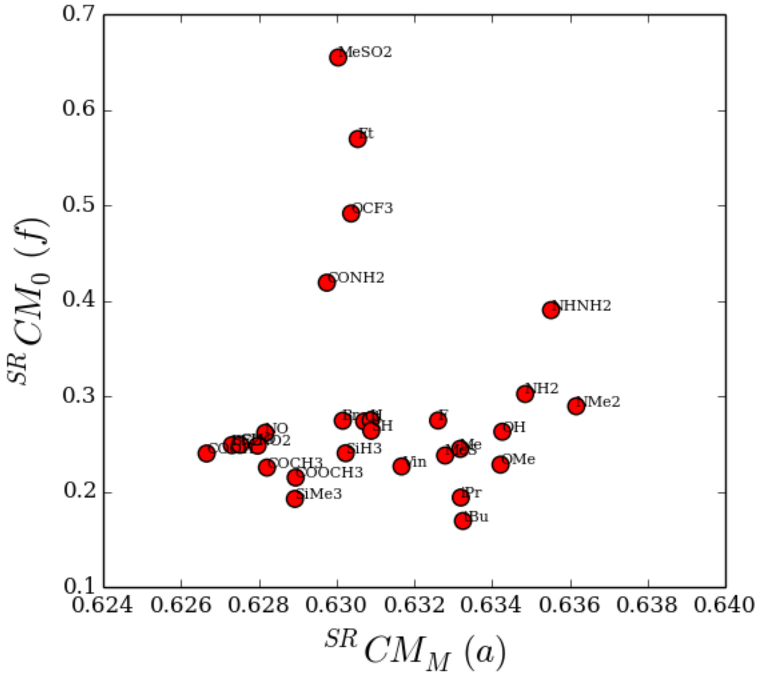
149


4.13
4.12
4.11
4.10
4.09
4.08
4.07
4.06
4.05
0.788
0.790
0.792
0.794
0.796
0.798
0.800
$CCM\ (ab)$
$^{SR}CM_L\ (a)$
NMe2
NHNH2
OMe
NH2
OH
SMe
Et
SH
Vin
SiMe3
OCF3
Cl
CHO
COOH

150

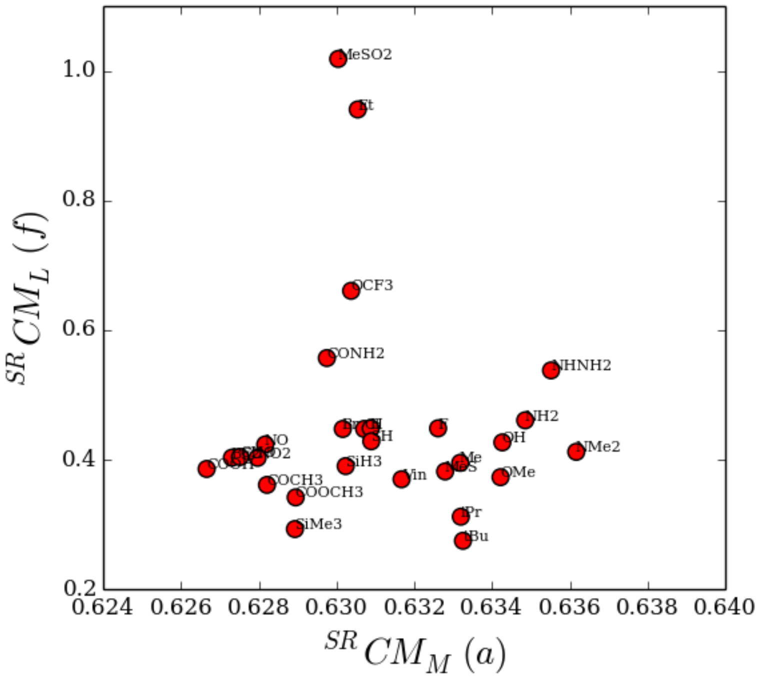

10.42
10.40
10.38
10.36
10.34
10.32
10.30
10.28
10.26
10.24
0.788
0.790
0.792
0.794
0.796
0.798
0.800
$CCM\ (a)$
$^{SR}CM_L\ (a)$
NMe2
NHNH2
OMe
NH2
OH
Et
SH
Vin
SiMe3
Cl
OCF3
CHO

151



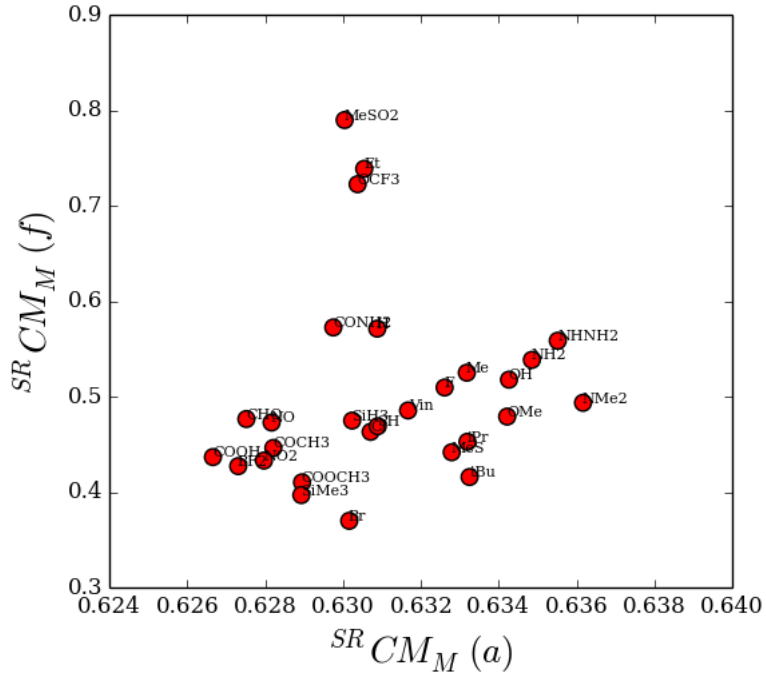
0.7
0.6
0.5
0.4
0.3
0.2
0.1
$^{SR}CM_0\ (f)$
0.624
0.626
0.628
0.630
0.632
0.634
0.636
0.638
0.640
$^{SR}CM_M\ (a)$
MeSO2
OCF3
CONH2
NHNH2
NH2
NMe2
OH
OMe
SiH3
COCH3
COOCH3
SiMe3
Vin

152

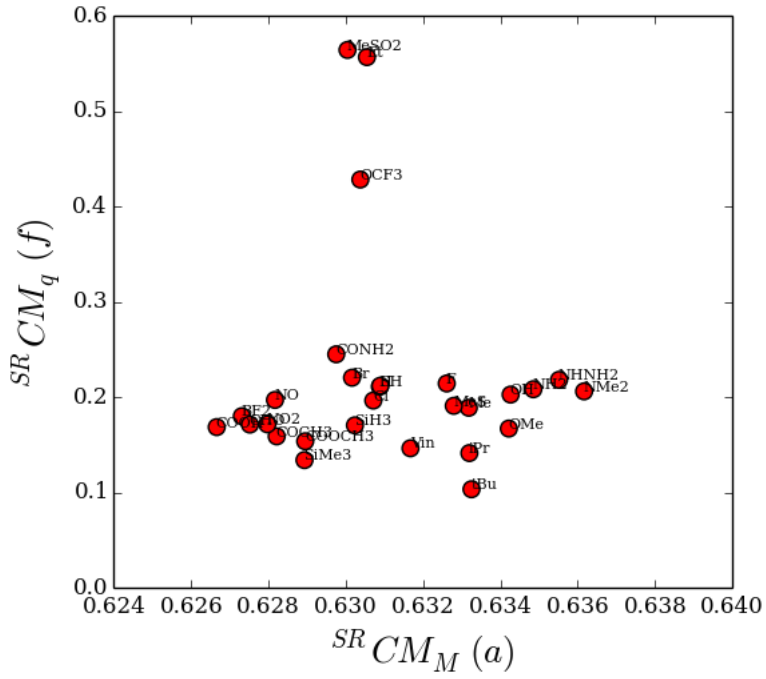


1.0
0.8
0.6
0.4
0.2
$^{SR}CM_L\ (f)$
0.624
0.626
0.628
0.630
0.632
0.634
0.636
0.638
0.640
$^{SR}CM_M\ (a)$
MeSO2
OCF3
CONH2
NHNH2
NH2
NMe2
OH
OMe
SiH3
COCH3
COOCH3
SiMe3
Vin

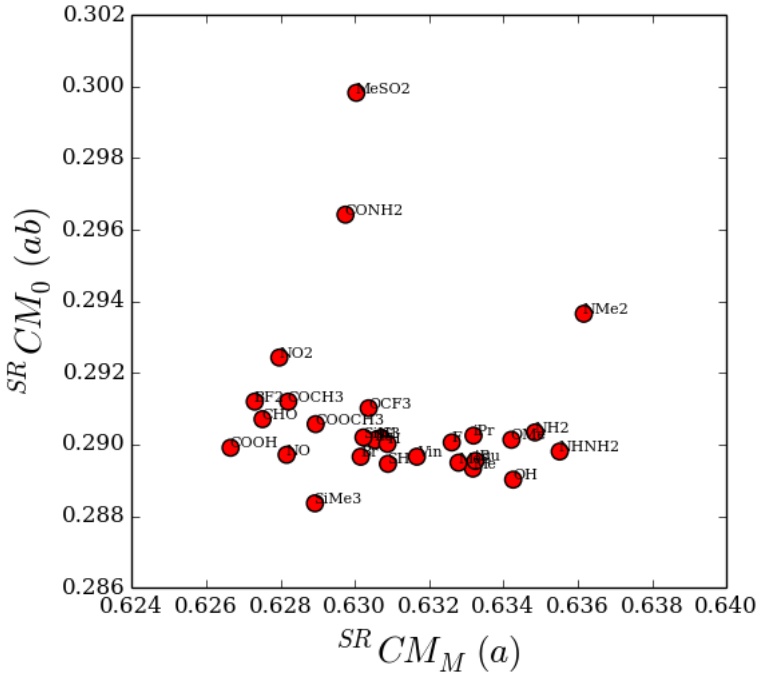
153


0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.624 0.626 0.628 0.630 0.632 0.634 0.636 0.638 0.640
$^{SR}CM_M\ (f)$
$^{SR}CM_M\ (a)$
MeSO2
Et
CF3
CONH2
NHNH2
NH2
Me
OH
Vin
NMe2
OMe
iPr
tBu
Br

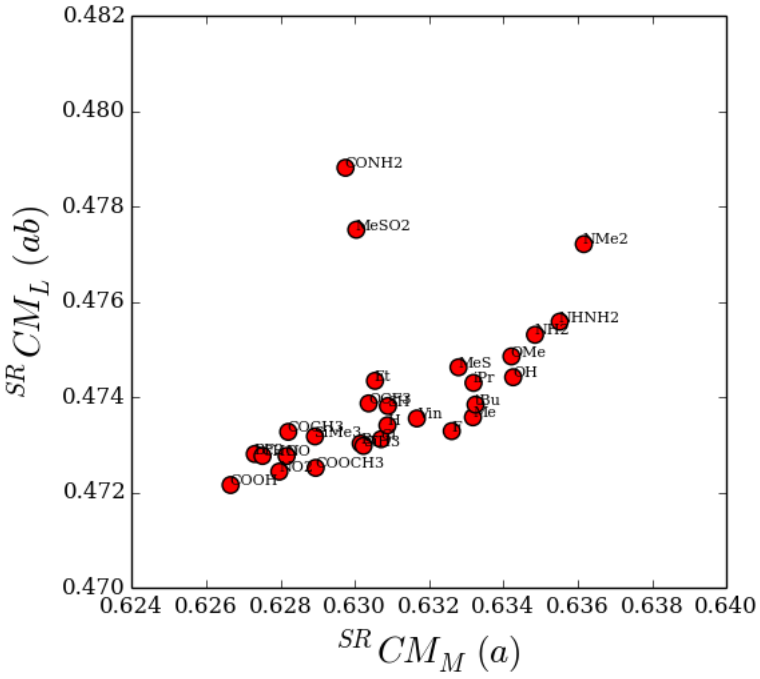
154


0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.624 0.626 0.628 0.630 0.632 0.634 0.636 0.638 0.640
$^{SR}CM_q\ (f)$
$^{SR}CM_M\ (a)$
MeSO2
CF3
CONH2
NHNH2
NMe2
OMe
Vin
iPr
tBu

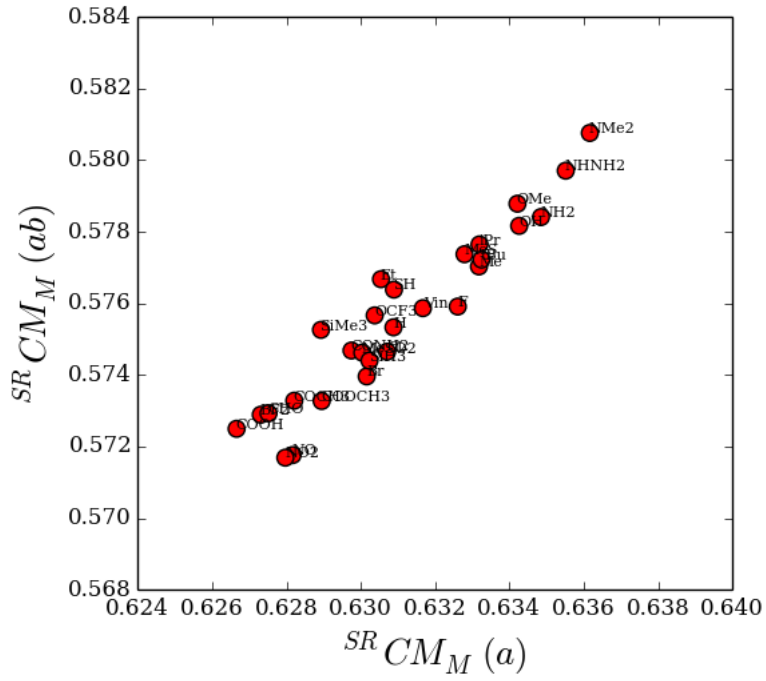
155


0.302
0.300
0.298
0.296
0.294
0.292
0.290
0.288
0.286
0.624 0.626 0.628 0.630 0.632 0.634 0.636 0.638 0.640
$^{SR}CM_0\ (ab)$
$^{SR}CM_M\ (a)$
MeSO2
SONH2
NMe2
NO2
SOCH3
OCF3
SOOCH3
NH2
NHNH2
SOOH
NO
Vin
OH
SiMe3

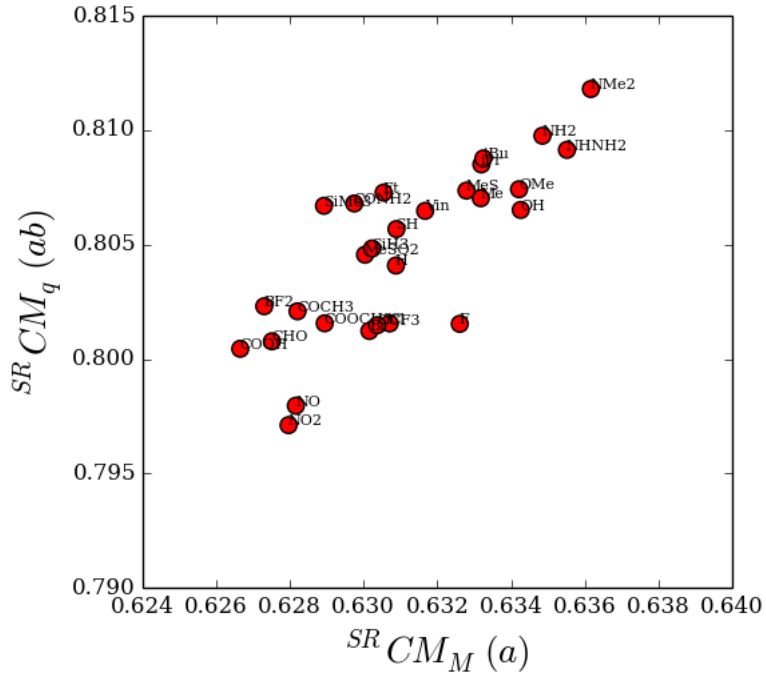
156


0.482
0.480
0.478
0.476
0.474
0.472
0.470
0.624 0.626 0.628 0.630 0.632 0.634 0.636 0.638 0.640
$^{SR}CM_L\ (ab)$
$^{SR}CM_M\ (a)$
SONH2
MeSO2
NMe2
NHNH2
OMe
OH
Vin
SOCH3
SiMe3
SOOCH3
SOOH

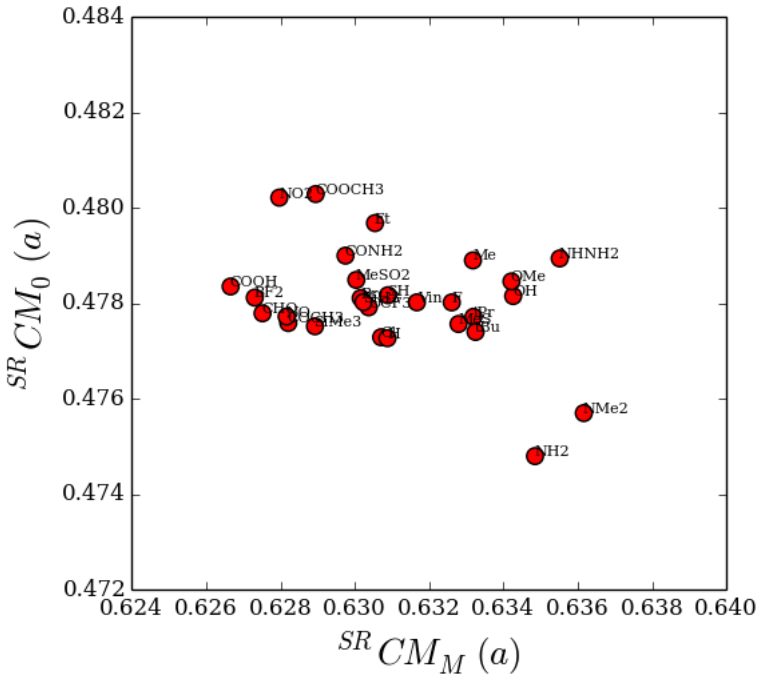
157


0.584
0.582
0.580
0.578
0.576
0.574
0.572
0.570
0.568
0.624 0.626 0.628 0.630 0.632 0.634 0.636 0.638 0.640
$^{SR}CM_M\ (ab)$
$^{SR}CM_M\ (a)$

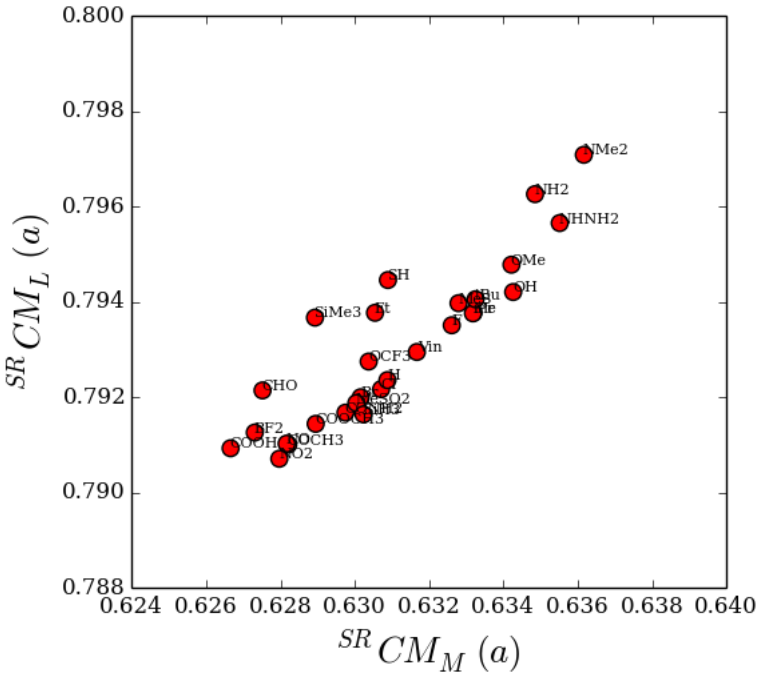
158


0.815
0.810
0.805
0.800
0.795
0.790
0.624 0.626 0.628 0.630 0.632 0.634 0.636 0.638 0.640
$^{SR}CM_q\ (ab)$
$^{SR}CM_M\ (a)$

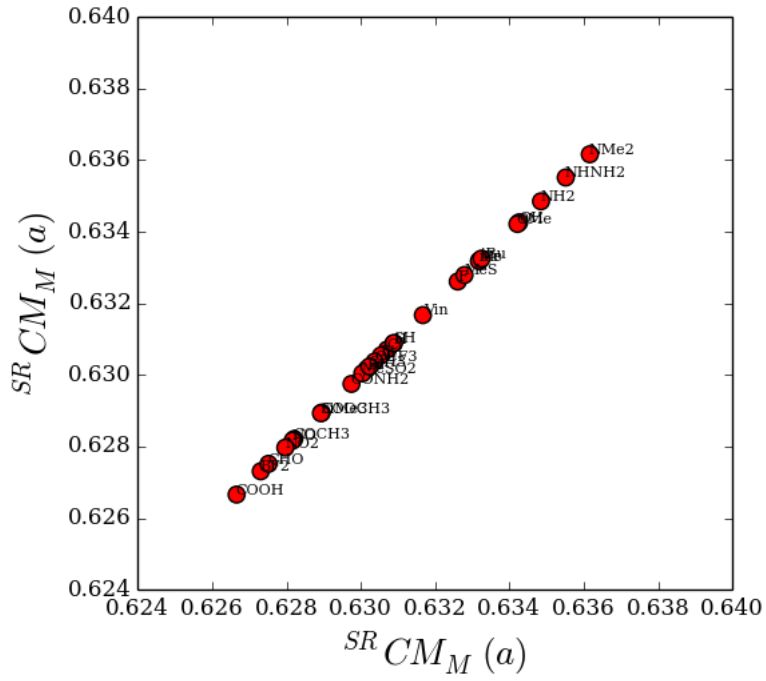
159


0.484
0.482
0.480
0.478
0.476
0.474
0.472
0.624 0.626 0.628 0.630 0.632 0.634 0.636 0.638 0.640
$^{SR}CM_0\ (a)$
$^{SR}CM_M\ (a)$
SOOCH3
CONH2
MeSO2
NHNH2
NMe2
NH2

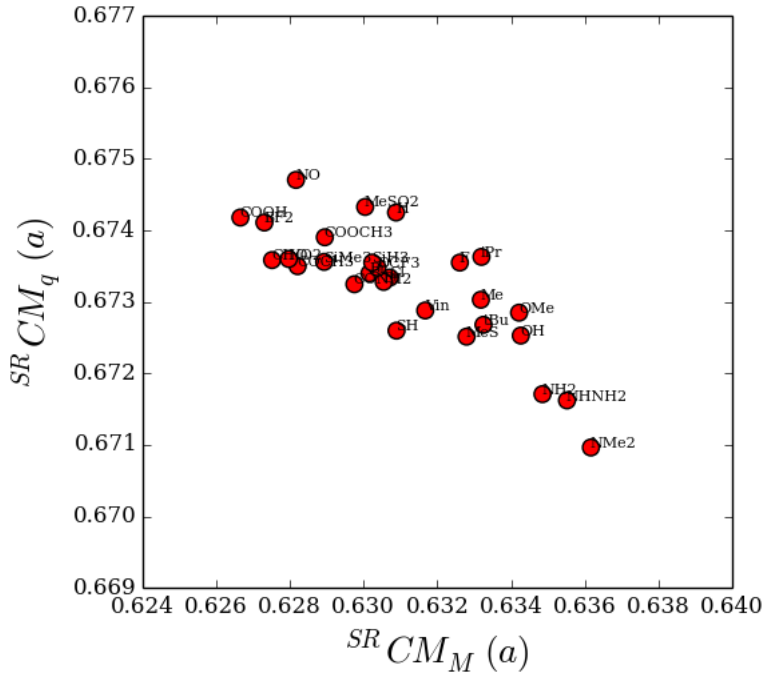
160


0.800
0.798
0.796
0.794
0.792
0.790
0.788
0.624 0.626 0.628 0.630 0.632 0.634 0.636 0.638 0.640
$^{SR}CM_L\ (a)$
$^{SR}CM_M\ (a)$
NMe2
NH2
NHNH2
OMe
OH
SiMe3
OCF3
Vin
CHO
NF2

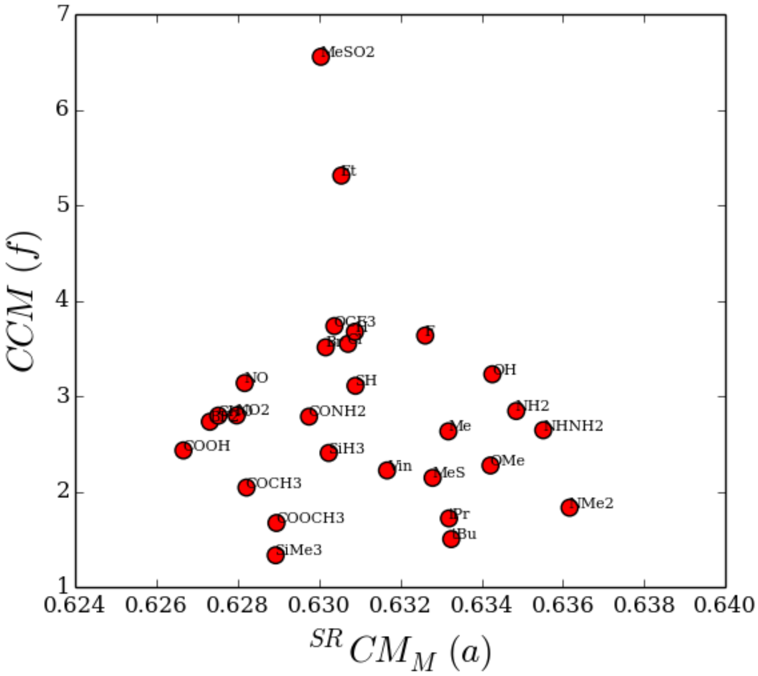
161


0.640
0.638
0.636
0.634
0.632
0.630
0.628
0.626
0.624
0.624 0.626 0.628 0.630 0.632 0.634 0.636 0.638 0.640
$^{SR}CM_M\ (a)$
$^{SR}CM_M\ (a)$

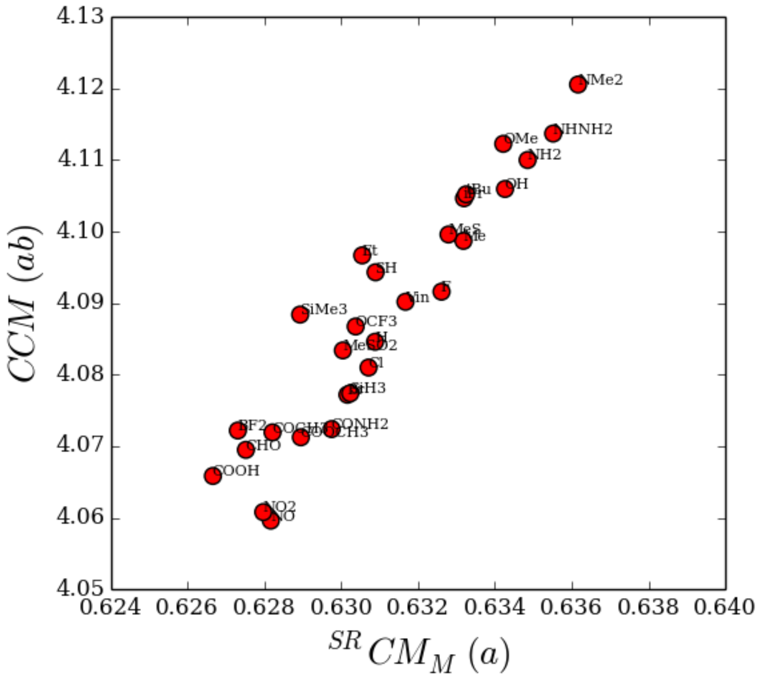
162


0.677
0.676
0.675
0.674
0.673
0.672
0.671
0.670
0.669
0.624 0.626 0.628 0.630 0.632 0.634 0.636 0.638 0.640
$^{SR}CM_q\ (a)$
$^{SR}CM_M\ (a)$

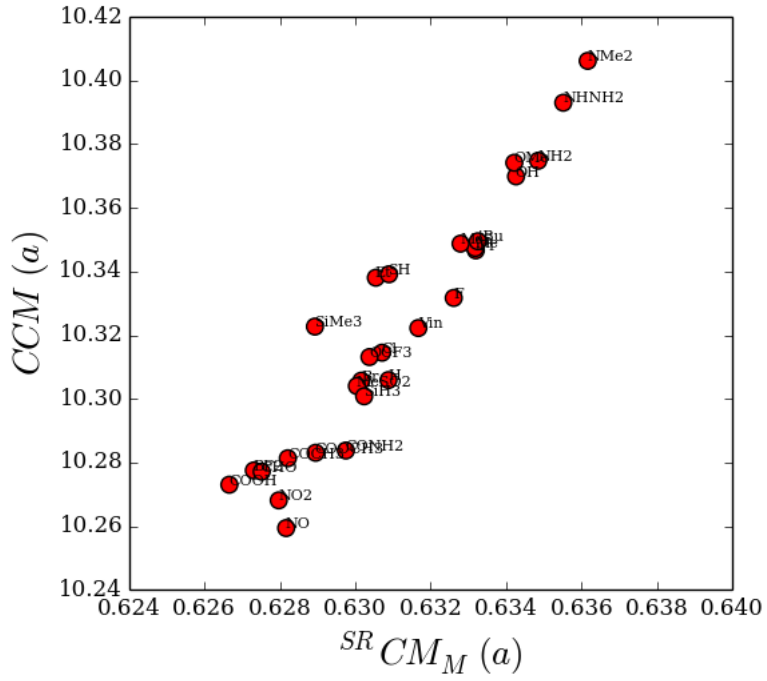
163


MeSO2
Et
OCF3
F
OH
NO
SH
NO2
CONH2
NH2
NHNH2
Me
COOH
SiH3
OMe
Vin
MeS
COCH3
NMe2
COOCH3
iPr
tBu
SiMe3
$CCM\ (f)$
$^{SR}CM_M\ (a)$

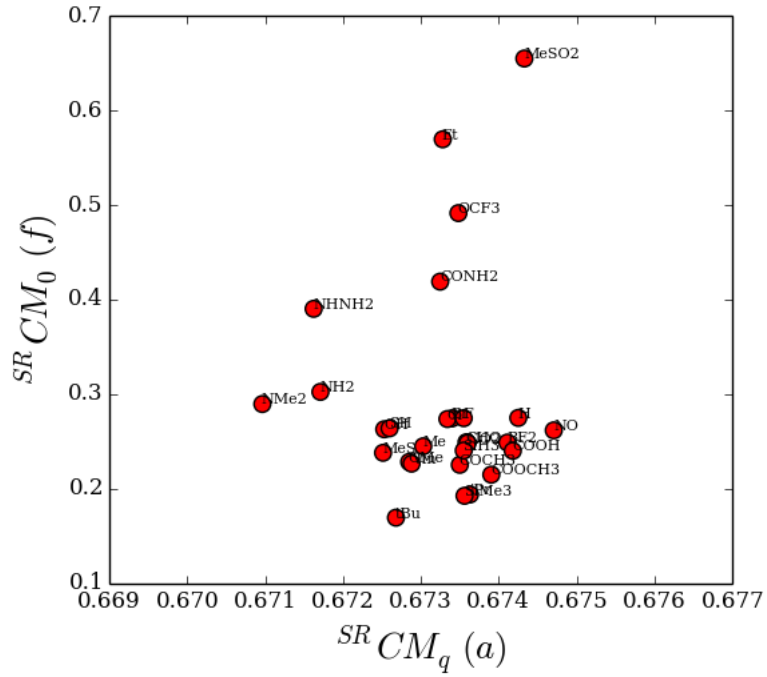
164


NMe2
NHNH2
OMe
NH2
OH
tBu
MeS
Me
Et
SH
F
Vin
SiMe3
OCF3
MeSO2
SiH3
CONH2
CHO
COOH
NO2
NO
$CCM\ (ab)$
$^{SR}CM_M\ (a)$

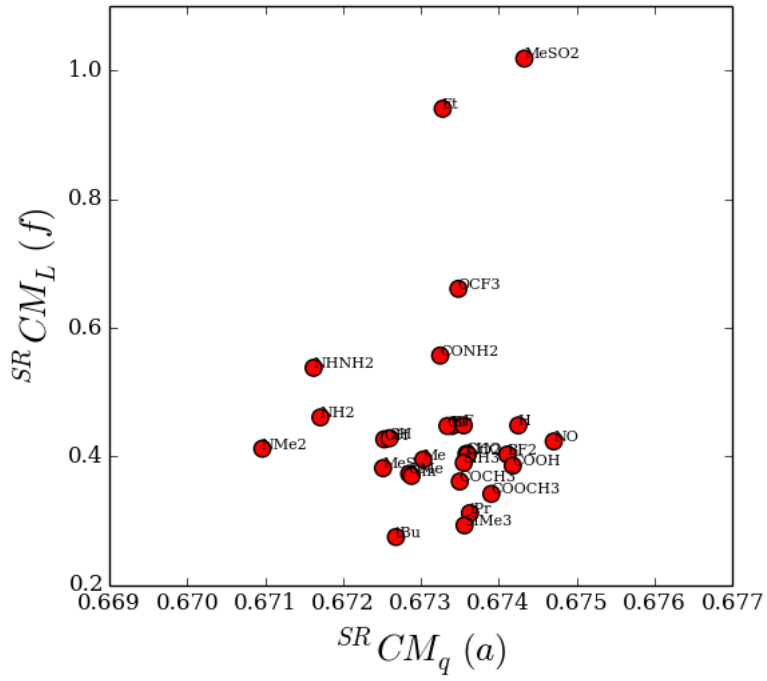
165


10.42
10.40
10.38
10.36
10.34
10.32
10.30
10.28
10.26
10.24
0.624 0.626 0.628 0.630 0.632 0.634 0.636 0.638 0.640
$CCM\ (a)$
$^{SR}CM_M\ (a)$
NMe2
NHNH2
SiMe3
Vin
NO2
NO
CONH2

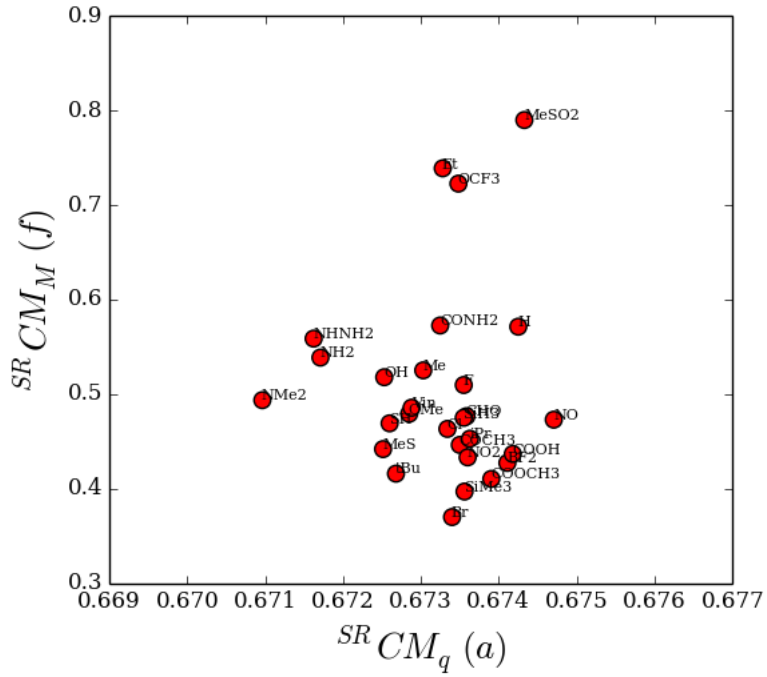
166


0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.669 0.670 0.671 0.672 0.673 0.674 0.675 0.676 0.677
$^{SR}CM_0\ (f)$
$^{SR}CM_q\ (a)$
MeSO2
Et
OCF3
CONH2
NHNH2
NMe2
NO
COOCH3
SiMe3
tBu

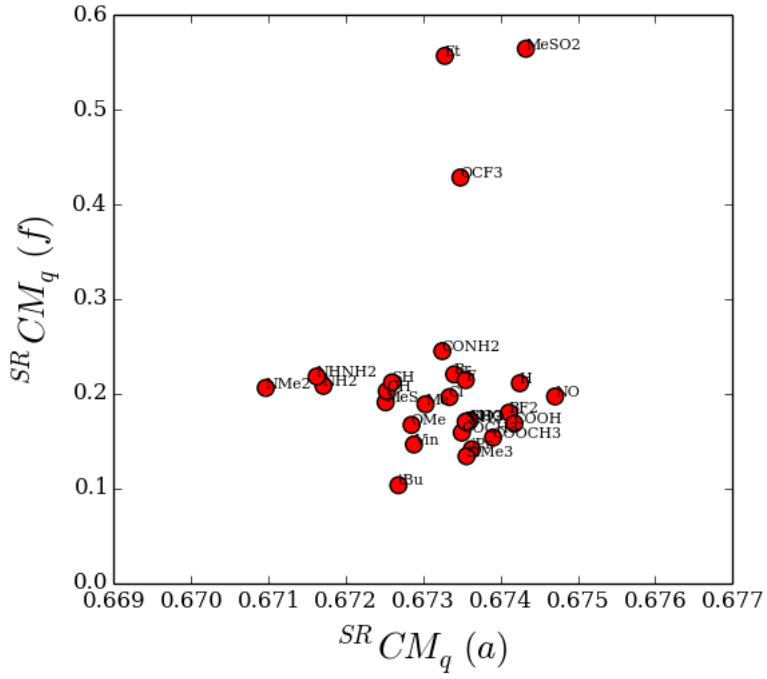
167


MeSO2
Et
OCF3
CONH2
NHNH2
NH2
NMe2
NO
COOH
COOCH3
NMe3
tBu
1.0
0.8
0.6
0.4
0.2
0.669 0.670 0.671 0.672 0.673 0.674 0.675 0.676 0.677
$^{SR}CM_L\ (f)$
$^{SR}CM_q\ (a)$

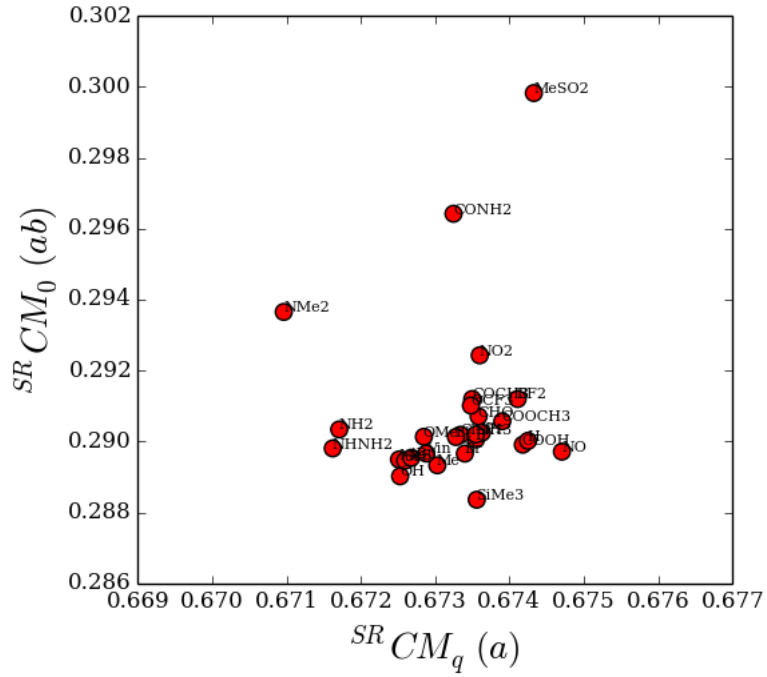
168


MeSO2
Et
OCF3
CONH2
NHNH2
NH2
NMe2
NO
COOH
COOCH3
NMe3
tBu
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.669 0.670 0.671 0.672 0.673 0.674 0.675 0.676 0.677
$^{SR}CM_M\ (f)$
$^{SR}CM_q\ (a)$

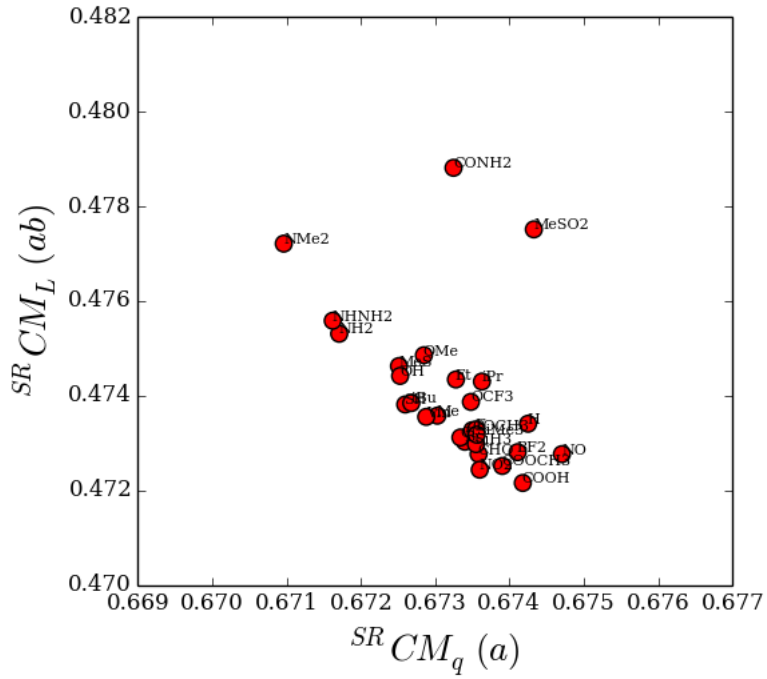
169


0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.669 0.670 0.671 0.672 0.673 0.674 0.675 0.676 0.677
$^{SR}CM_q\ (f)$
$^{SR}CM_q\ (a)$
MeSO2
OCF3
CONH2
NO
SiMe3
tBu

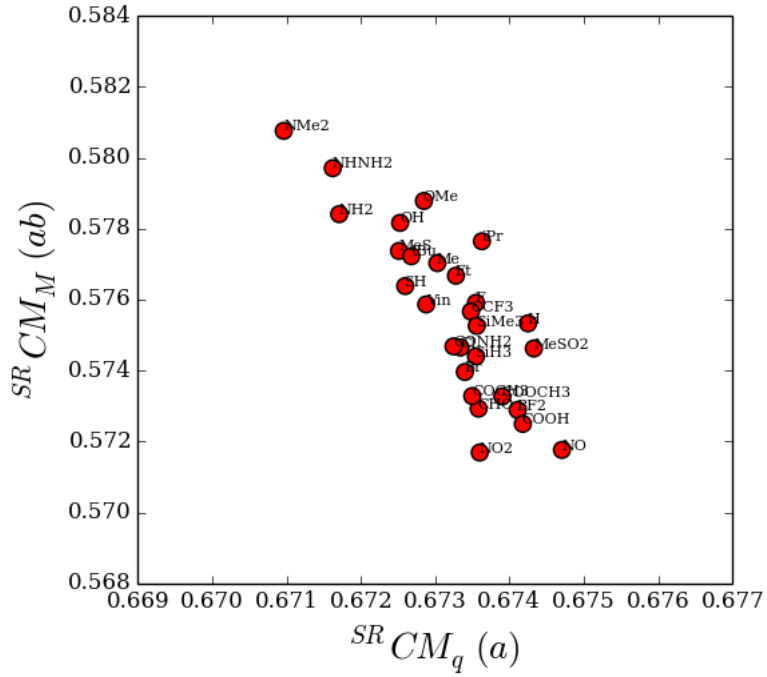
170


0.302
0.300
0.298
0.296
0.294
0.292
0.290
0.288
0.286
0.669 0.670 0.671 0.672 0.673 0.674 0.675 0.676 0.677
$^{SR}CM_0\ (ab)$
$^{SR}CM_q\ (a)$
MeSO2
CONH2
NMe2
NO2
SiMe3

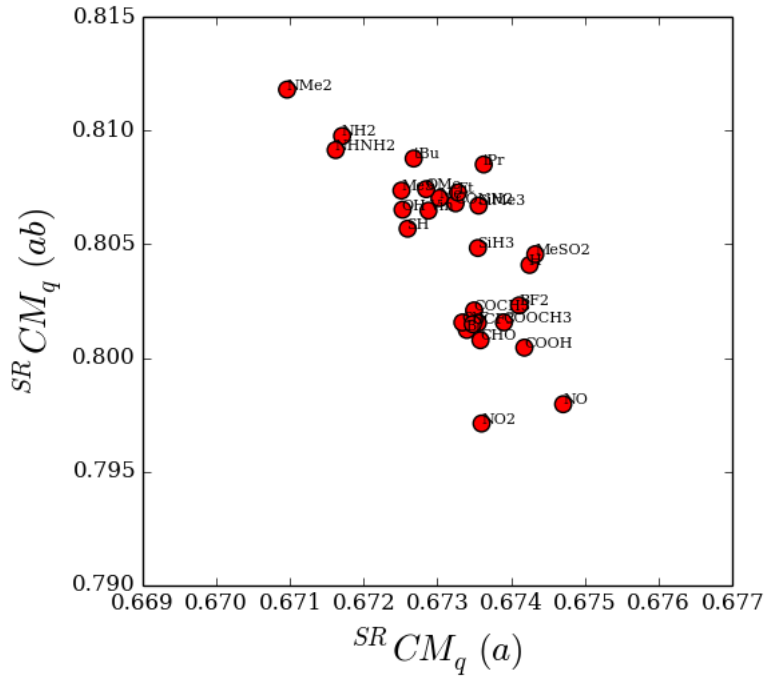
171


0.482
0.480
0.478
0.476
0.474
0.472
0.470
0.669 0.670 0.671 0.672 0.673 0.674 0.675 0.676 0.677
$^{SR}CM_L\ (ab)$
$^{SR}CM_q\ (a)$
CONH2
MeSO2
NMe2
NHNH2
NH2
OMe
OH
Et
iPr
NCF3
tBu
Me
NO
COOH

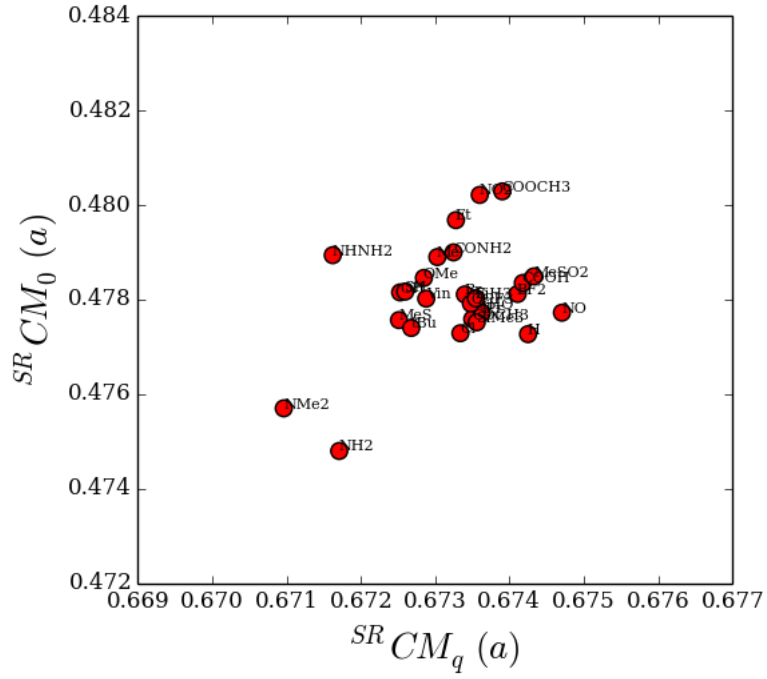
172


0.584
0.582
0.580
0.578
0.576
0.574
0.572
0.570
0.568
0.669 0.670 0.671 0.672 0.673 0.674 0.675 0.676 0.677
$^{SR}CM_M\ (ab)$
$^{SR}CM_q\ (a)$
NMe2
NHNH2
OMe
NH2
OH
iPr
Me
Et
NCF3
MeSO2
NO2
NO
COOH

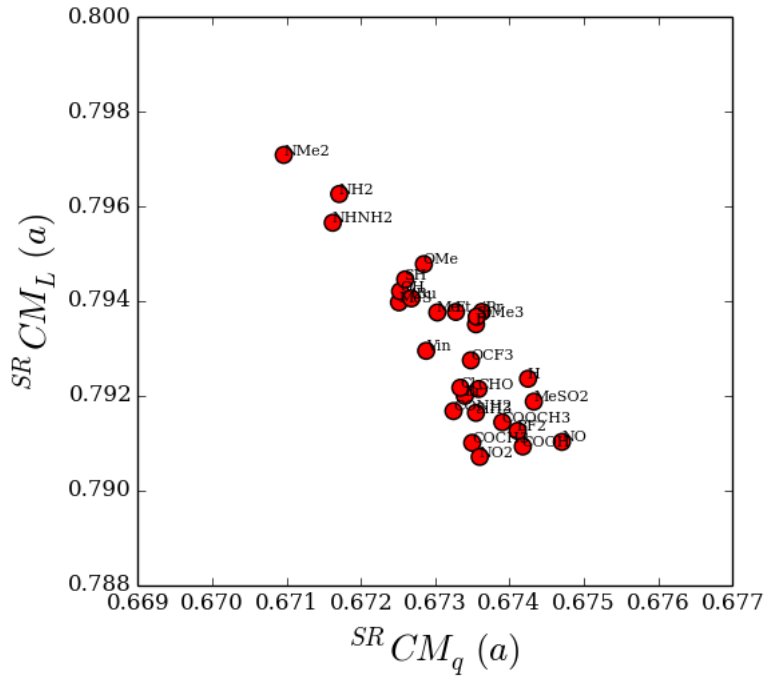
173


0.815
0.810
0.805
0.800
0.795
0.790
0.669 0.670 0.671 0.672 0.673 0.674 0.675 0.676 0.677
$^{SR}CM_q\ (ab)$
$^{SR}CM_q\ (a)$
NMe2
NH2
NHNH2
tBu
iPr
SiH3
MeSO2
CF2
COOH
NO
NO2

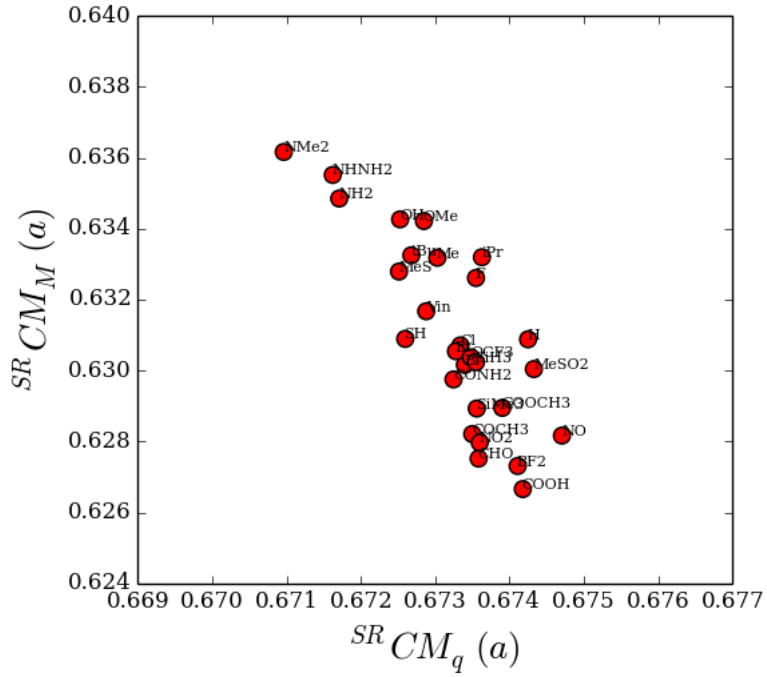
174


0.484
0.482
0.480
0.478
0.476
0.474
0.472
0.669 0.670 0.671 0.672 0.673 0.674 0.675 0.676 0.677
$^{SR}CM_0\ (a)$
$^{SR}CM_q\ (a)$
NHNH2
CONH2
OMe
MeSO2
CF2
NO
NMe2
NH2

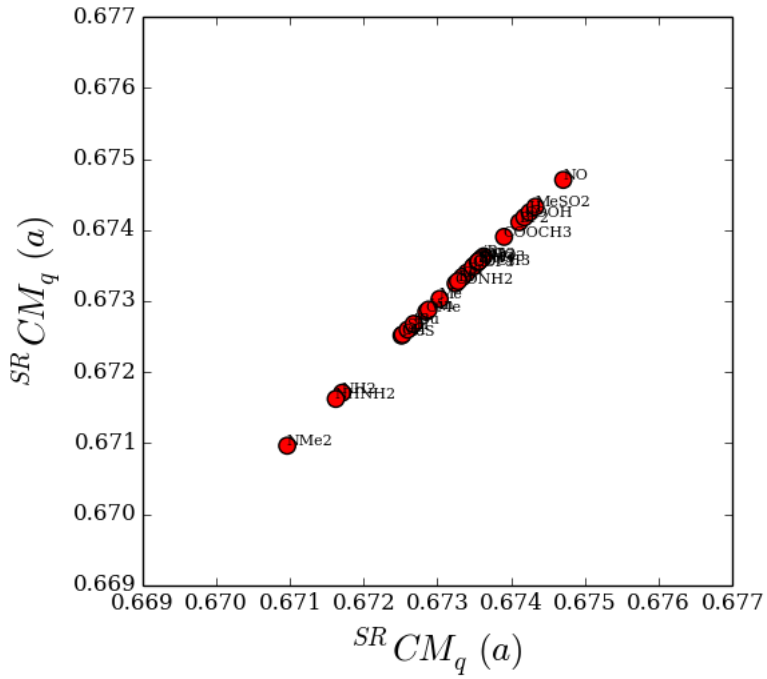
175


0.800
0.798
0.796
0.794
0.792
0.790
0.788
0.669 0.670 0.671 0.672 0.673 0.674 0.675 0.676 0.677
$^{SR}CM_L\ (a)$
$^{SR}CM_q\ (a)$
NMe2
NH2
NHNH2
OMe
Me3
Vin
OCF3
CHO
MeSO2
F2
NO
NO2

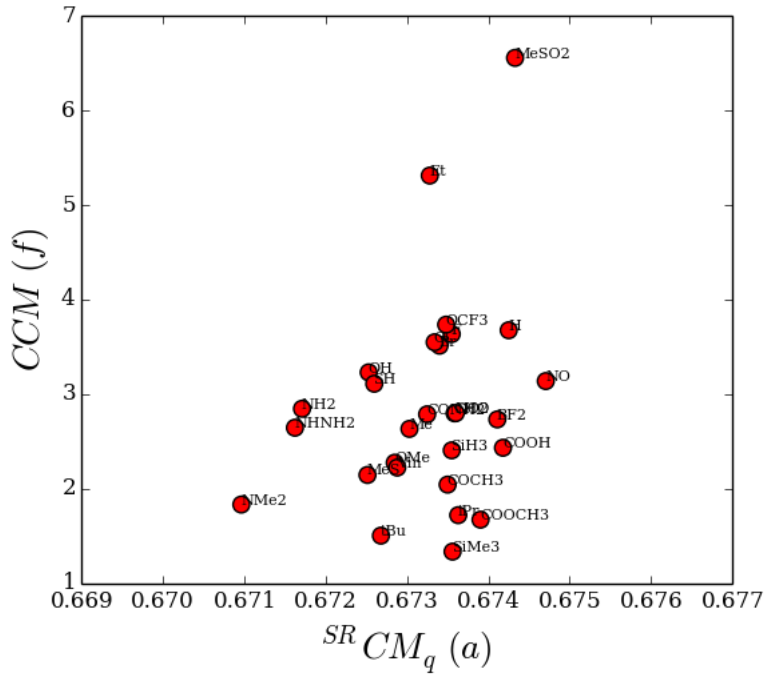
176


0.640
0.638
0.636
0.634
0.632
0.630
0.628
0.626
0.624
0.669 0.670 0.671 0.672 0.673 0.674 0.675 0.676 0.677
$^{SR}CM_M\ (a)$
$^{SR}CM_q\ (a)$
NMe2
NHNH2
NH2
OMe
Me
Pr
Vin
SH
MeSO2
NONH2
COOCH3
NO
CHO
F2
COOH

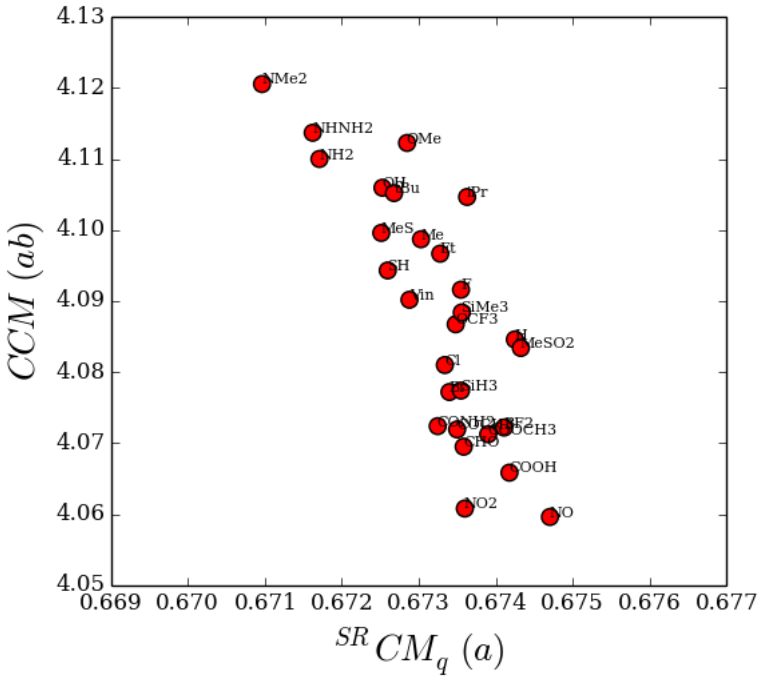
177


0.677
0.676
0.675
0.674
0.673
0.672
0.671
0.670
0.669
0.669 0.670 0.671 0.672 0.673 0.674 0.675 0.676 0.677
$^{SR}CM_q\ (a)$
$^{SR}CM_q\ (a)$

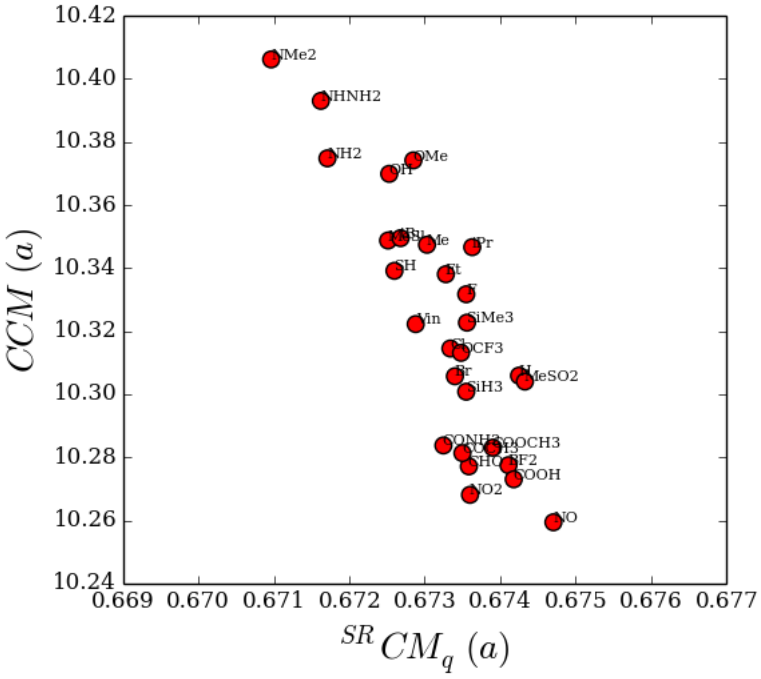
178


7
6
5
4
3
2
1
0.669 0.670 0.671 0.672 0.673 0.674 0.675 0.676 0.677
$CCM\ (f)$
$^{SR}CM_q\ (a)$

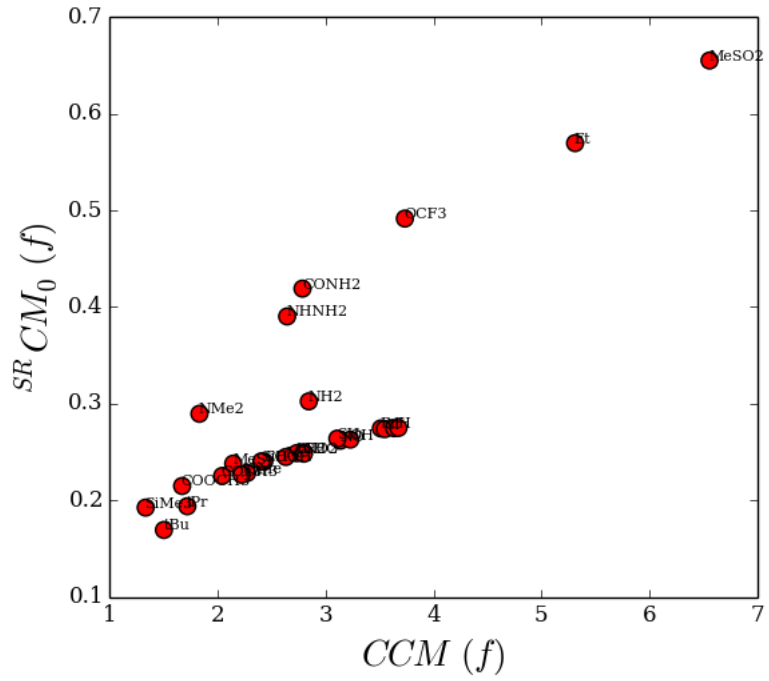
179


4.13
4.12
4.11
4.10
4.09
4.08
4.07
4.06
4.05
0.669 0.670 0.671 0.672 0.673 0.674 0.675 0.676 0.677
$CCM\ (ab)$
$^{SR}CM_q\ (a)$
NMe2
NHNH2
NH2
OMe
OH
tBu
iPr
MeS
Me
Et
SH
Vin
SiMe3
OCF3
MeSO2
SiH3
COOH
NO2
NO

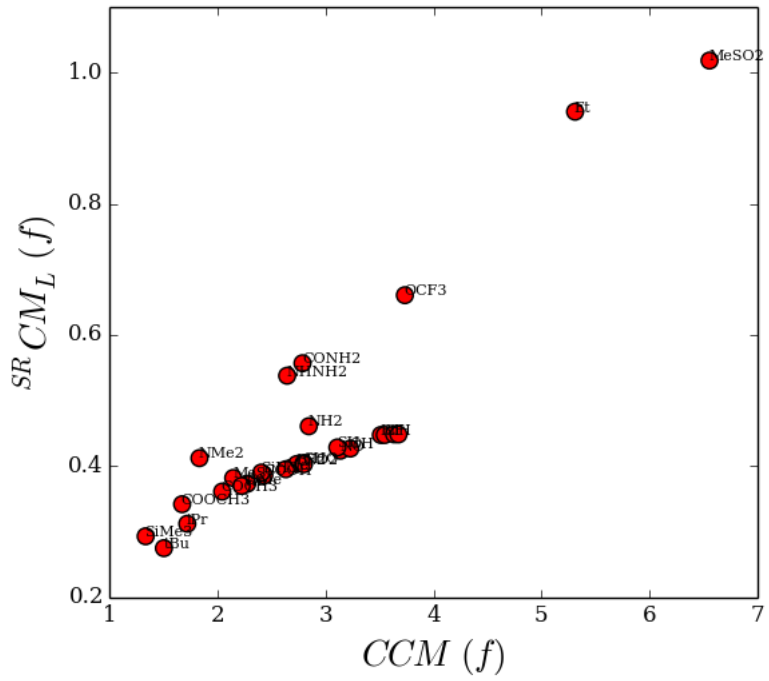
180


10.42
10.40
10.38
10.36
10.34
10.32
10.30
10.28
10.26
10.24
0.669 0.670 0.671 0.672 0.673 0.674 0.675 0.676 0.677
$CCM\ (a)$
$^{SR}CM_q\ (a)$
NMe2
NHNH2
NH2
OMe
OH
Me
iPr
SH
Et
Vin
SiMe3
OCF3
MeSO2
SiH3
COOH
NO2
NO

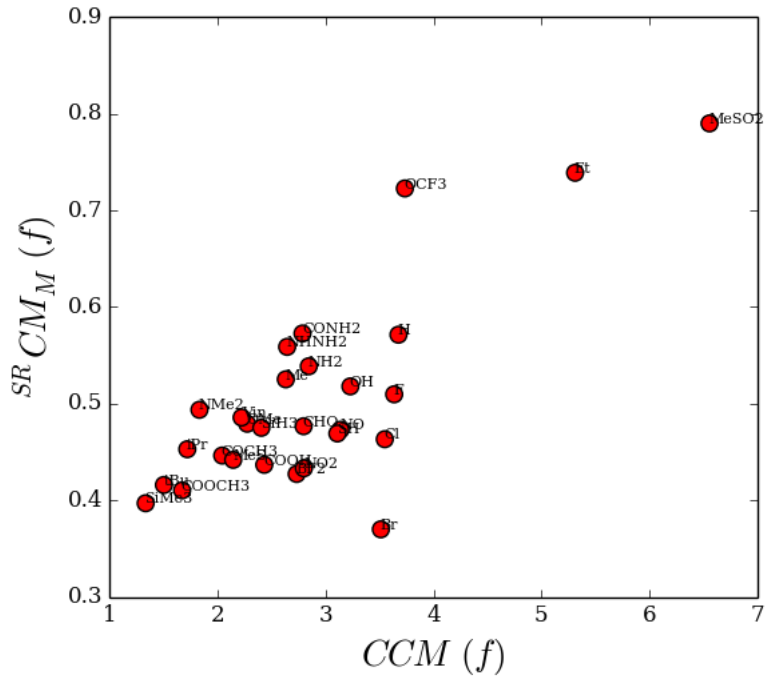
181


0.7
0.6
0.5
0.4
0.3
0.2
0.1
1
2
3
4
5
6
7
$^{SR}CM_0\ (f)$
$CCM\ (f)$
MeSO2
CF3
CONH2
NHNH2
NH2
NMe2
SiMe2Pr
tBu

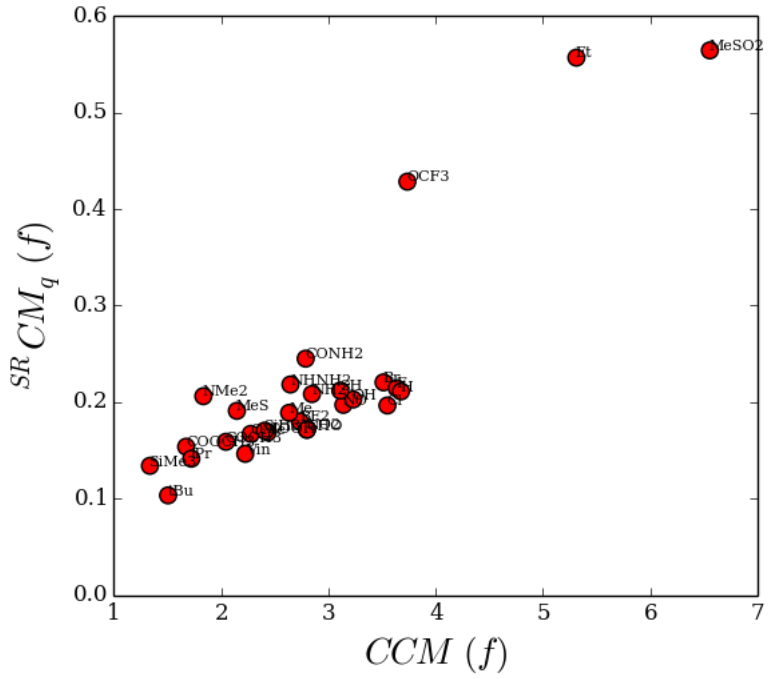
182


1.0
0.8
0.6
0.4
0.2
1
2
3
4
5
6
7
$^{SR}CM_L\ (f)$
$CCM\ (f)$
MeSO2
CF3
CONH2
NHNH2
NH2
NMe2
SiMe2Pr
tBu

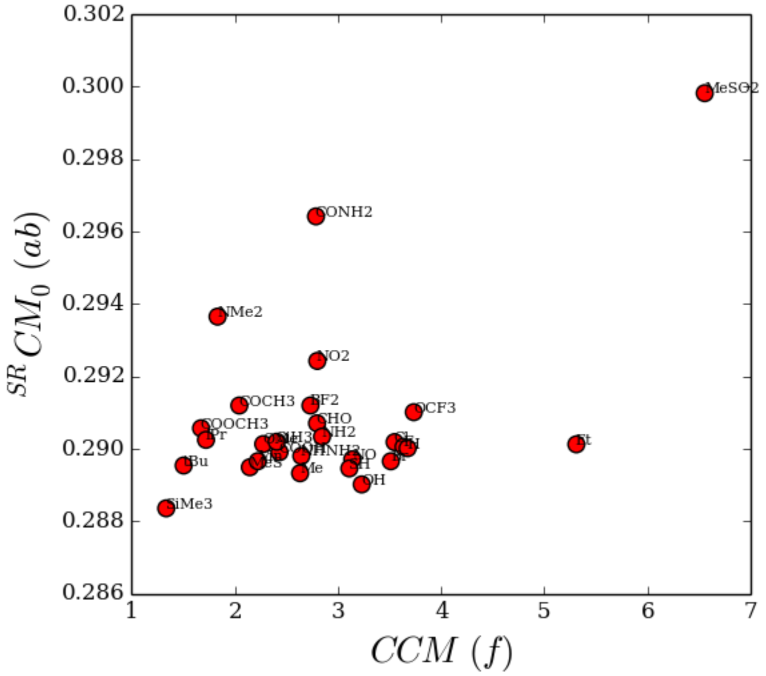
183


0.9
0.8
0.7
0.6
0.5
0.4
0.3
1
2
3
4
5
6
7
$SR\,CM_M\,(f)$
$CCM\,(f)$
MeSO2
Et
OCF3
CONH2
NHNH2
NH2
OH
NMe2
Cl
Br
tBu
SiMe3

184

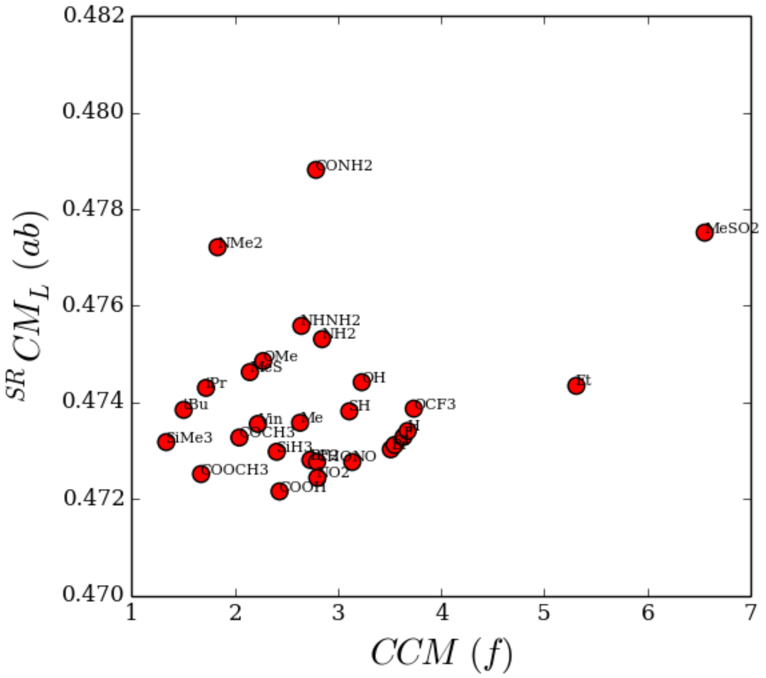

0.6
0.5
0.4
0.3
0.2
0.1
0.0
1
2
3
4
5
6
7
$SR\,CM_q\,(f)$
$CCM\,(f)$
MeSO2
Et
OCF3
CONH2
NHNH2
NMe2
MeS
tBu

185



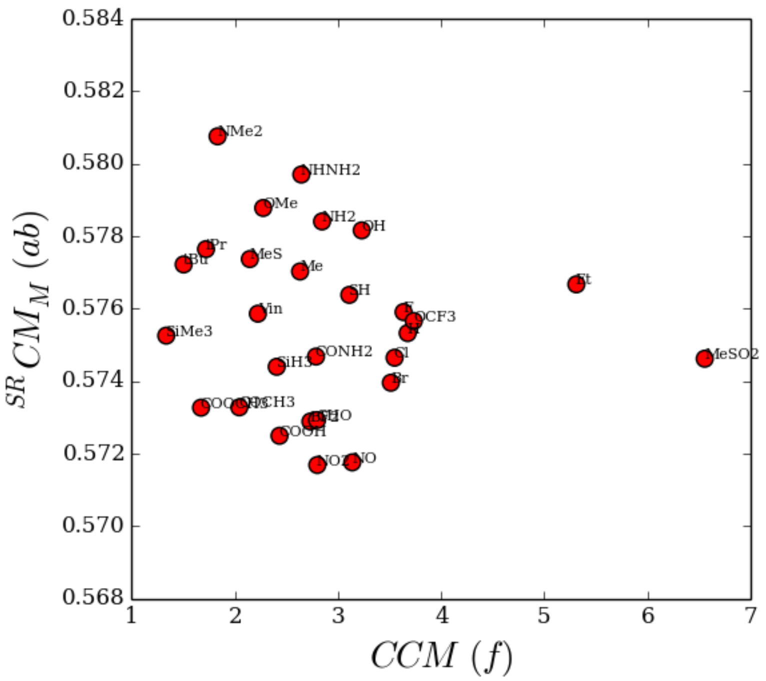
0.302
0.300
0.298
0.296
0.294
0.292
0.290
0.288
0.286
1
2
3
4
5
6
7
$^{SR}CM_0\ (ab)$
$CCM\ (f)$
MeSO2
CONH2
NMe2
NO2
COCH3
BF2
OCF3
CHO
COOCH3
NH2
iPr
Et
tBu
OH
SiMe3

186

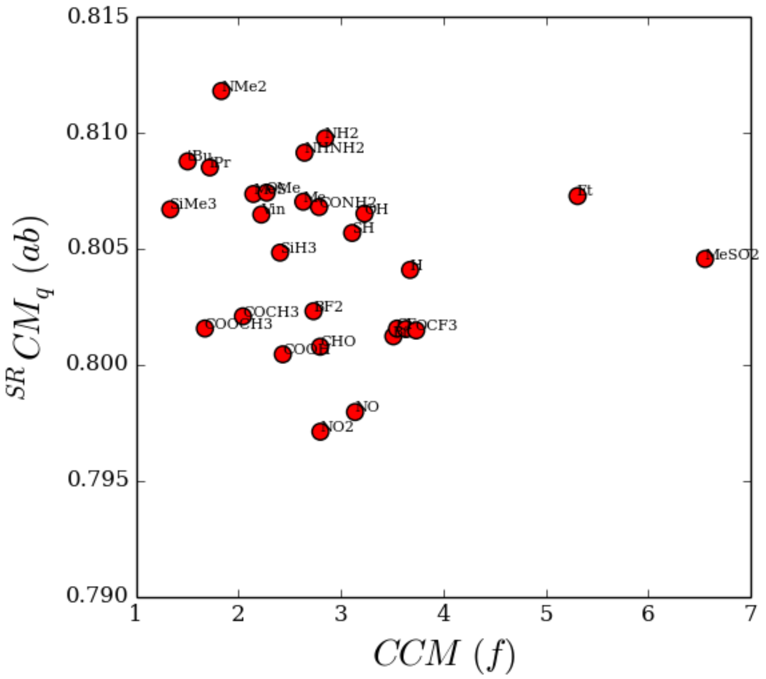


0.482
0.480
0.478
0.476
0.474
0.472
0.470
1
2
3
4
5
6
7
$^{SR}CM_L\ (ab)$
$CCM\ (f)$
CONH2
MeSO2
NMe2
NHNH2
NH2
OMe
OH
iPr
Et
tBu
SH
OCF3
Vin
Me
SiMe3
COCH3
SiH3
COOCH3
NO2
COOH

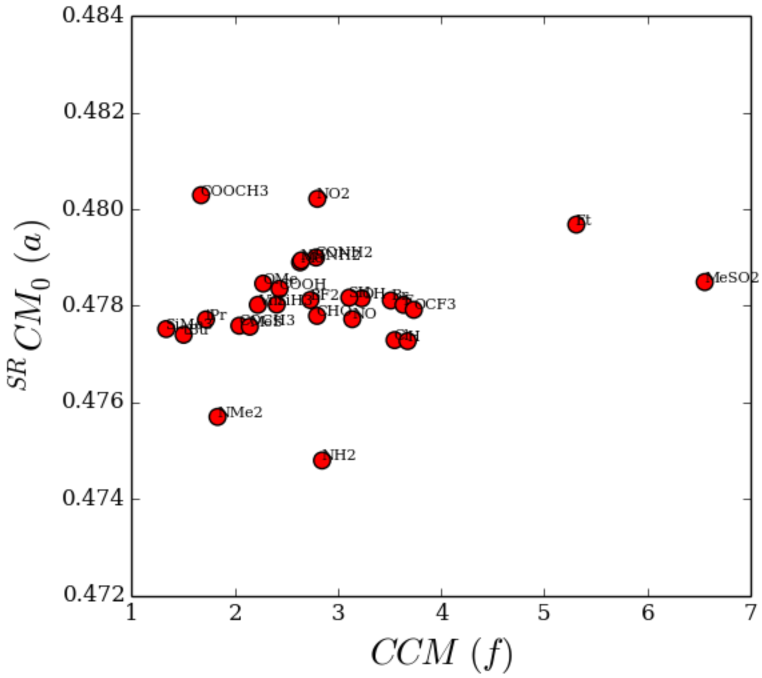
187


0.584
0.582
0.580
0.578
0.576
0.574
0.572
0.570
0.568
1
2
3
4
5
6
7
$^{SR}CM_M\ (ab)$
$CCM\ (f)$
NMe2
NHNH2
OMe
NH2
OH
iPr
tBu
MeS
Me
SH
Et
Vin
F
OCF3
SiMe3
CONH2
Cl
MeSO2
SiH3
Br
COCH3
CHO
COOH
NO2
NO

188

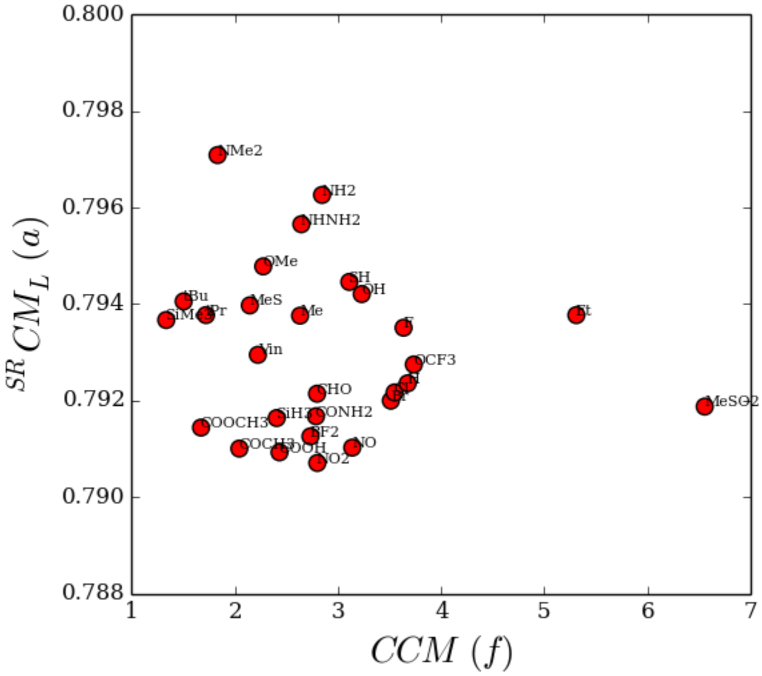

0.815
0.810
0.805
0.800
0.795
0.790
1
2
3
4
5
6
7
$^{SR}CM_q\ (ab)$
$CCM\ (f)$
NMe2
NH2
NHNH2
tBu
iPr
Et
SiMe3
Vin
CONH2
OH
SH
SiH3
H
MeSO2
COCH3
COOCH3
BF2
OCF3
CHO
COOH
NO
NO2

189



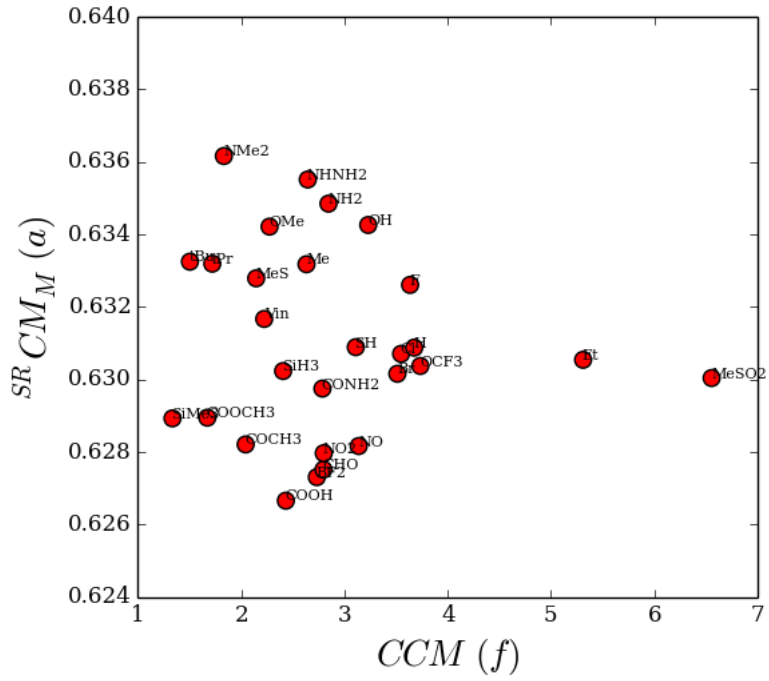
0.484
0.482
0.480
0.478
0.476
0.474
0.472
1
2
3
4
5
6
7
$^{SR}CM_0\ (a)$
$CCM\ (f)$
COOCH3
NO2
Et
MeSO2
CONH2
OCF3
iPr
NMe2
NH2

190

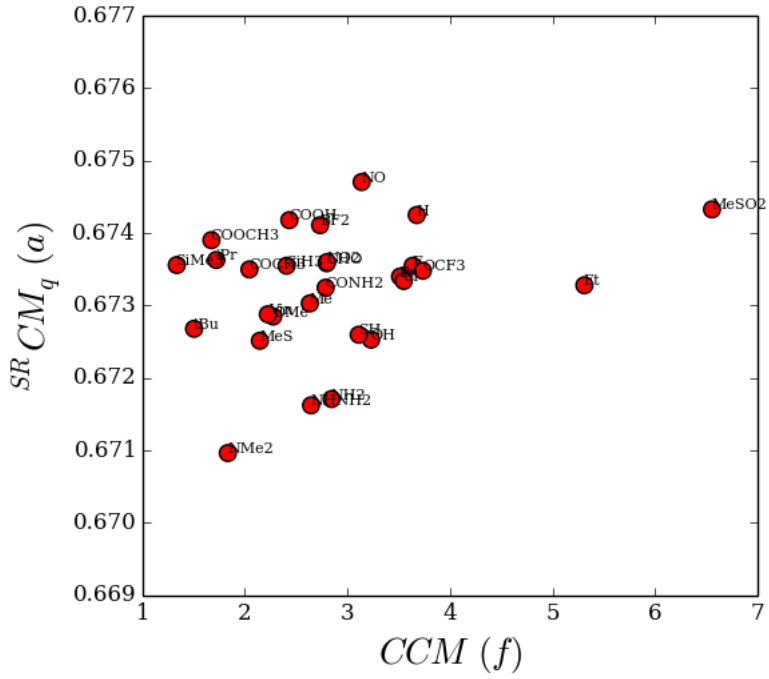


0.800
0.798
0.796
0.794
0.792
0.790
0.788
1
2
3
4
5
6
7
$^{SR}CM_L\ (a)$
$CCM\ (f)$
NMe2
NH2
NHNH2
OMe
SH
OH
tBu
MeS
Me
iPr
Et
F
Vin
OCF3
CHO
MeSO2
COOCH3
CONH2
SF2
NO
COCH3
COOH
NO2

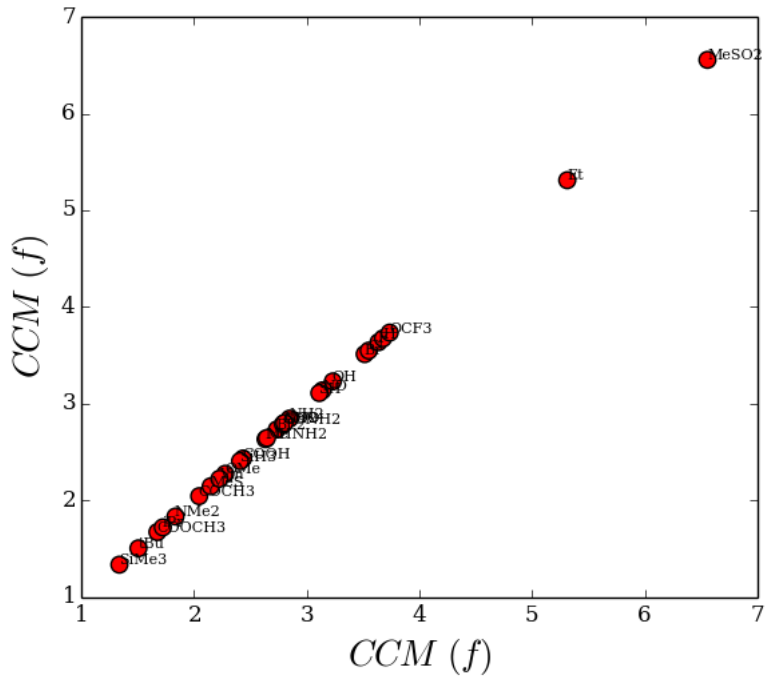
191


0.640
0.638
0.636
0.634
0.632
0.630
0.628
0.626
0.624
1
2
3
4
5
6
7
$^{SR}CM_M\ (a)$
$CCM\ (f)$
NMe2
NHNH2
NH2
OMe
OH
Me
MeS
Vin
SH
SiH3
CF3
Et
MeSO2
CONH2
SiMe3
COOCH3
COCH3
NO
CHO
COOH

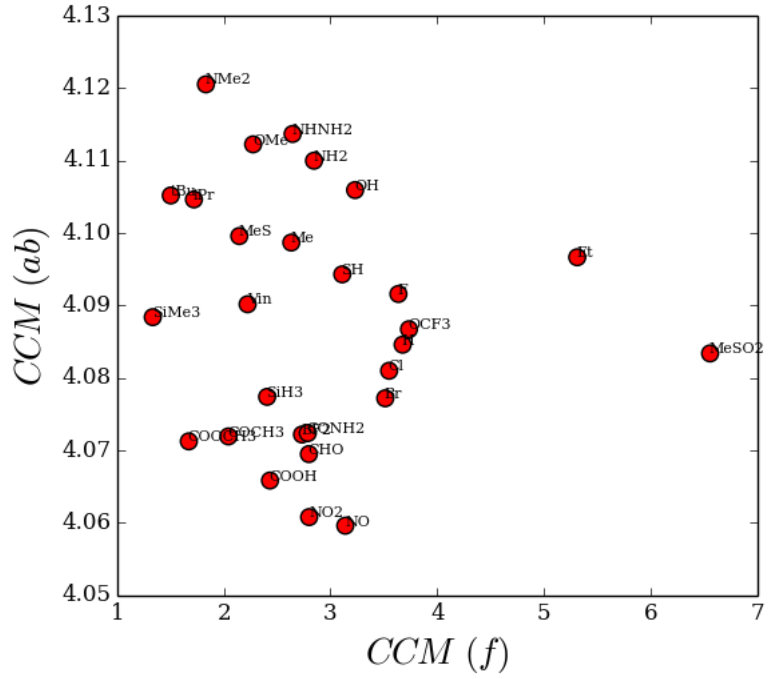
192


0.677
0.676
0.675
0.674
0.673
0.672
0.671
0.670
0.669
1
2
3
4
5
6
7
$^{SR}CM_q\ (a)$
$CCM\ (f)$
NO
MeSO2
COOH
COOCH3
CONH2
Et
tBu
MeS
SH
NMe2

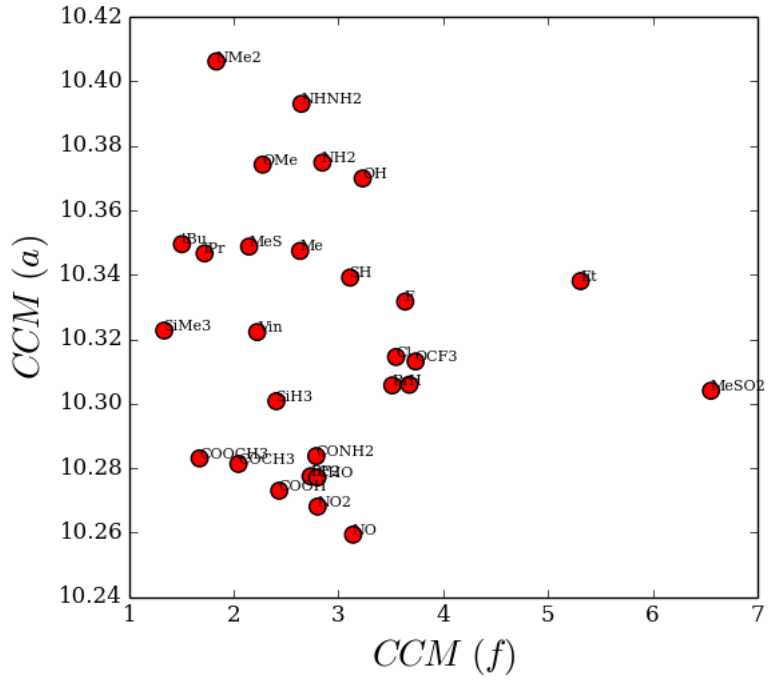
193


CCM (f)
CCM (f)
MeSO2
Et
OCF3
NMe2
SiMe3

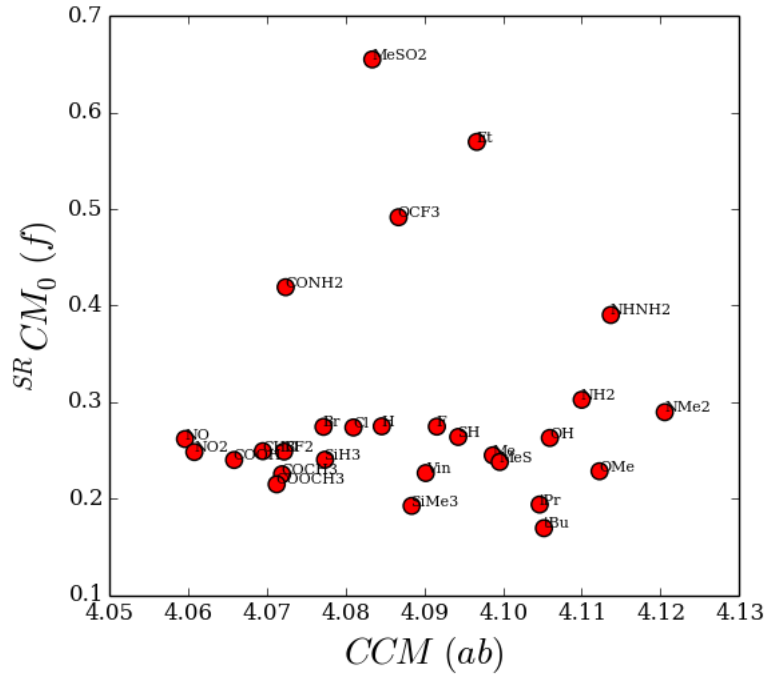
194


CCM (ab)
CCM (f)
NMe2
Et
MeSO2
SiMe3
OCF3
SiH3
CHO
COOH

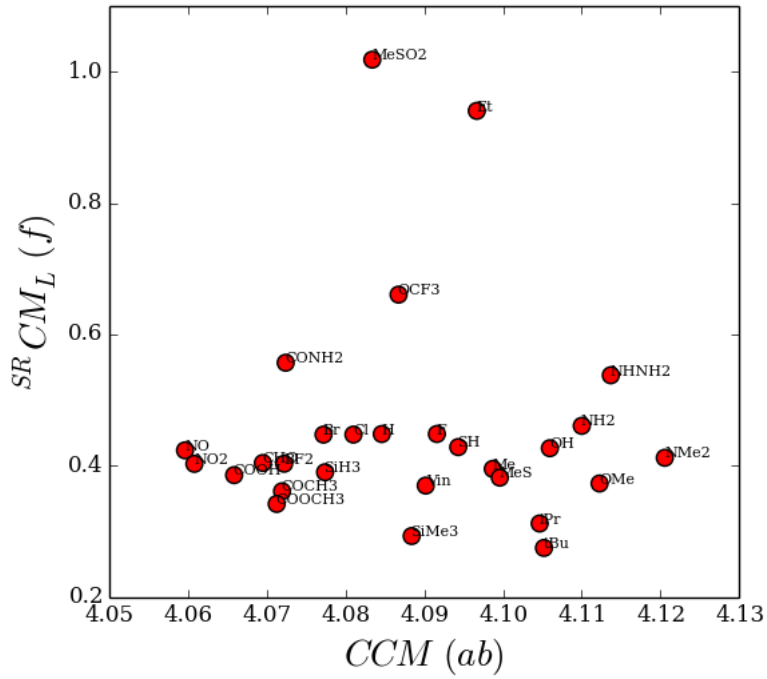
195


10.42
10.40
10.38
10.36
10.34
10.32
10.30
10.28
10.26
10.24
1
2
3
4
5
6
7
CCM (a)
CCM (f)
NMe2
NHNH2
OMe
NH2
OH
tBu
iPr
MeS
Me
SH
Et
F
SiMe3
Vin
Cl
OCF3
SiH3
MeSO2
COOCH3
CONH2
NO2
NO

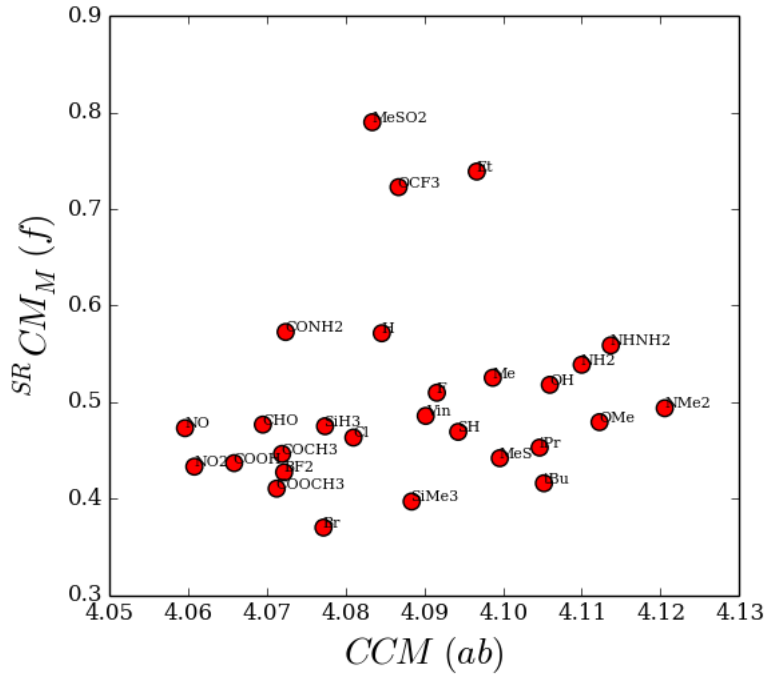
196


0.7
0.6
0.5
0.4
0.3
0.2
0.1
4.05
4.06
4.07
4.08
4.09
4.10
4.11
4.12
4.13
SR CM0 (f)
CCM (ab)
MeSO2
Et
OCF3
CONH2
NHNH2
NH2
NMe2
OH
SH
MeS
OMe
Vin
SiMe3
iPr
tBu
SiH3

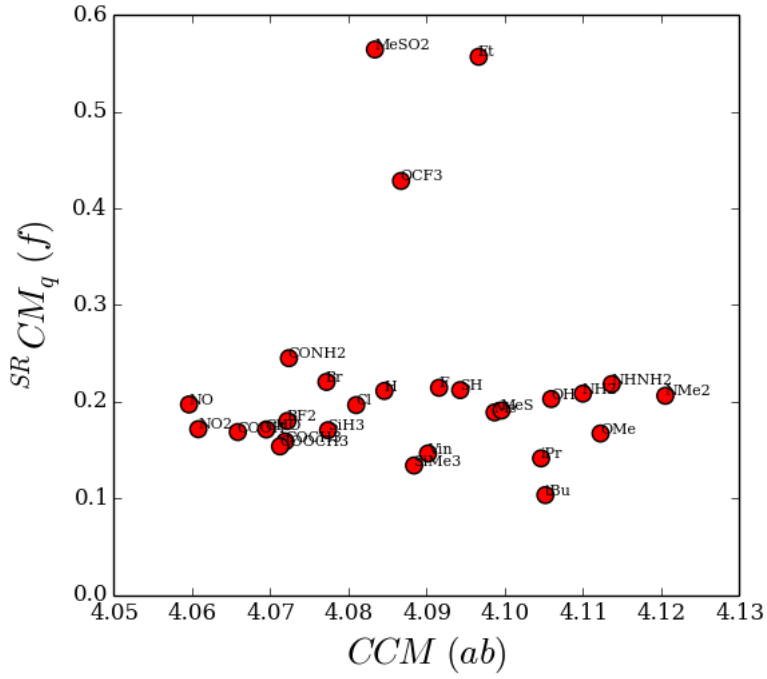
197


MeSO2
Et
OCF3
CONH2
NHNH2
NH2
OH
NMe2
SH
Me
MeS
OMe
Vin
SiMe3
iPr
tBu
$^{SR}CM_L\ (f)$
$CCM\ (ab)$

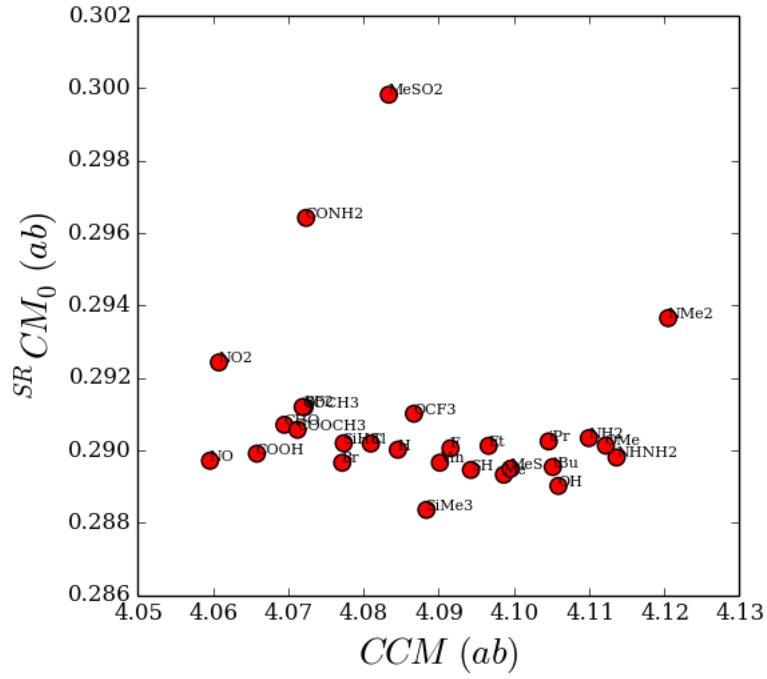
198


MeSO2
Et
OCF3
CONH2
NHNH2
NH2
Me
OH
NMe2
OMe
Vin
SH
iPr
MeS
tBu
SiMe3
Br
$^{SR}CM_M\ (f)$
$CCM\ (ab)$

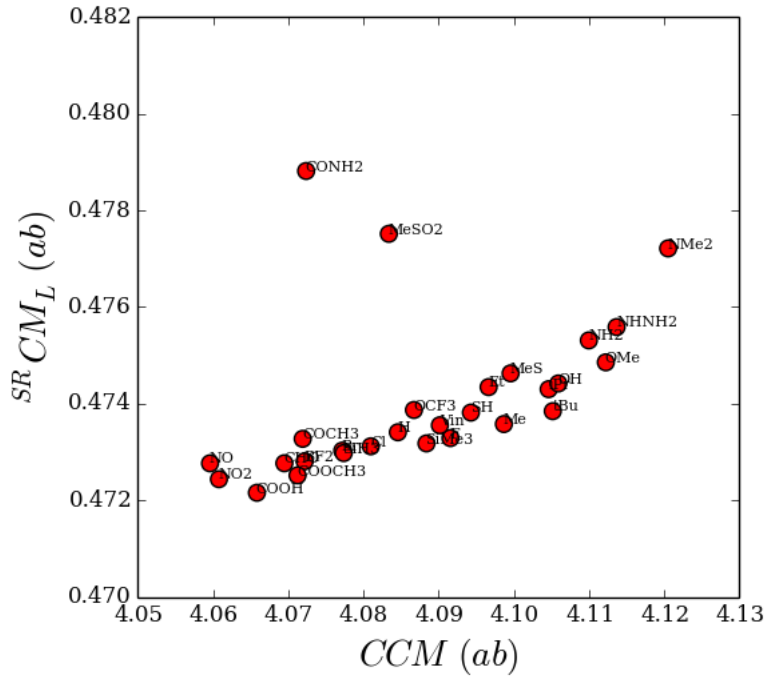
199


0.6
0.5
0.4
0.3
0.2
0.1
0.0
4.05
4.06
4.07
4.08
4.09
4.10
4.11
4.12
4.13
$^{SR}CM_q\ (f)$
$CCM\ (ab)$
MeSO2
Et
OCF3
CONH2
Br
SH
NHNH2
NMe2
NO
NO2
SiH3
OMe
iPr
SiMe3
tBu

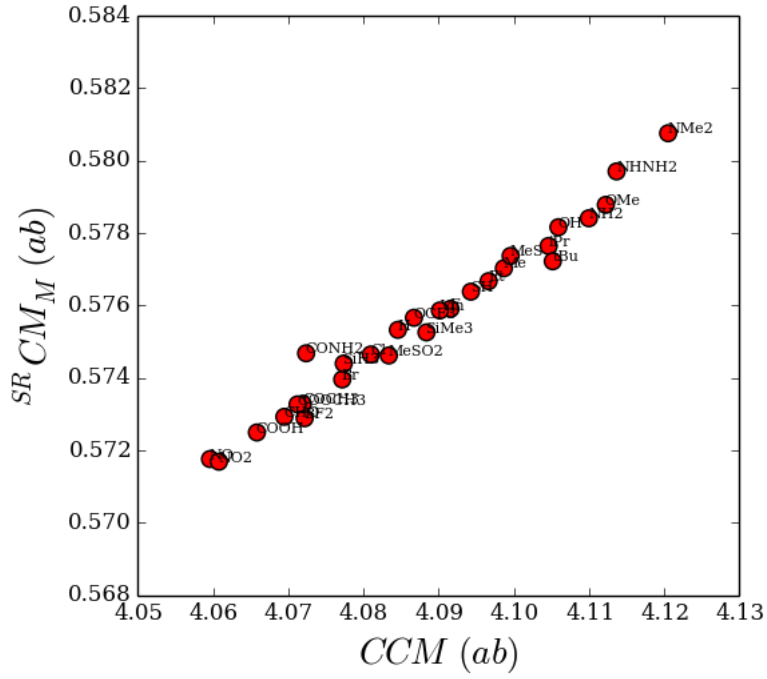
200


0.302
0.300
0.298
0.296
0.294
0.292
0.290
0.288
0.286
4.05
4.06
4.07
4.08
4.09
4.10
4.11
4.12
4.13
$^{SR}CM_0\ (ab)$
$CCM\ (ab)$
MeSO2
CONH2
NMe2
NO2
OCF3
NO
SiMe3
OH

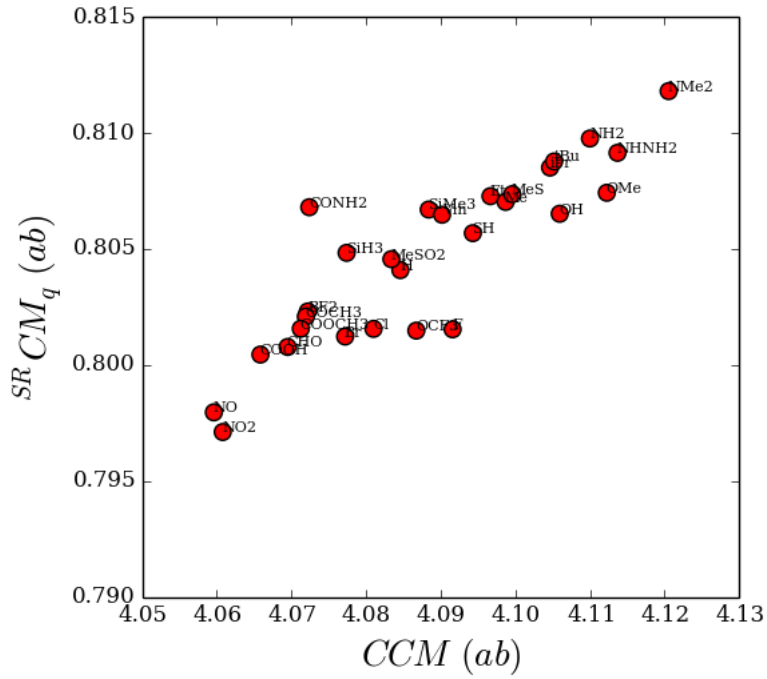
201


0.482
0.480
0.478
0.476
0.474
0.472
0.470
4.05
4.06
4.07
4.08
4.09
4.10
4.11
4.12
4.13
$^{SR}CM_L\ (ab)$
$CCM\ (ab)$
CONH2
MeSO2
NMe2
NHNH2
NH2
OMe
MeS
OH
OCF3
SH
tBu
Me
Vin
SiMe3
NO
NO2
COOH
COOCH3

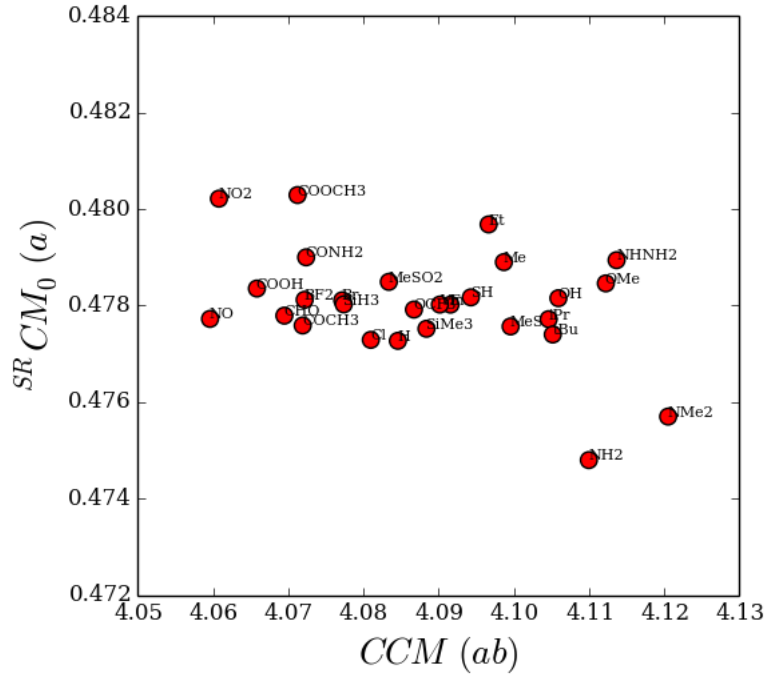
202


0.584
0.582
0.580
0.578
0.576
0.574
0.572
0.570
0.568
4.05
4.06
4.07
4.08
4.09
4.10
4.11
4.12
4.13
$^{SR}CM_M\ (ab)$
$CCM\ (ab)$
NMe2
NHNH2
OMe
NH2
OH
Pr
MeS
tBu
Me
SiMe3
CONH2
MeSO2
COOH
NO2

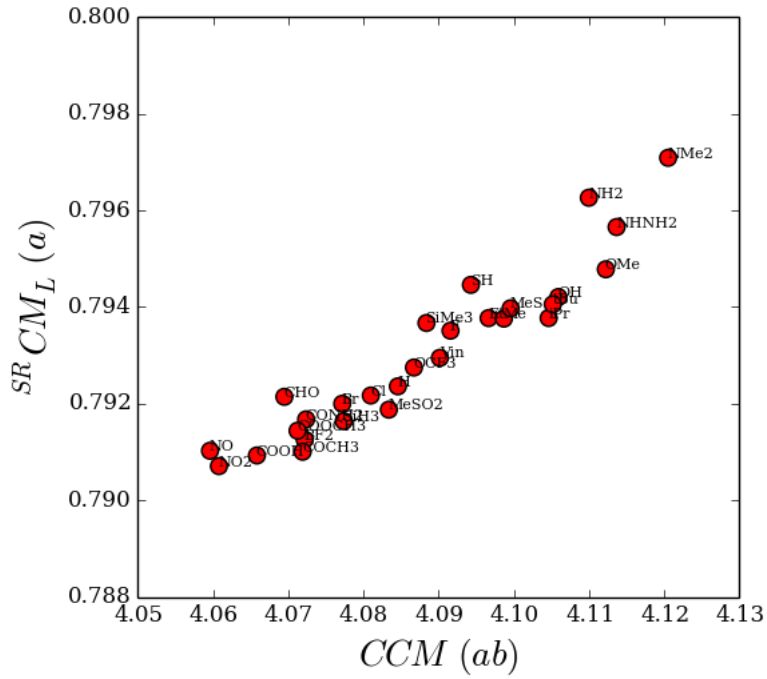
203


0.815
0.810
0.805
0.800
0.795
0.790
4.05
4.06
4.07
4.08
4.09
4.10
4.11
4.12
4.13
$^{SR}CM_q\ (ab)$
$CCM\ (ab)$
NMe2
NH2
NHNH2
OMe
OH
SH
SiH3
MeSO2
CONH2
NO
NO2

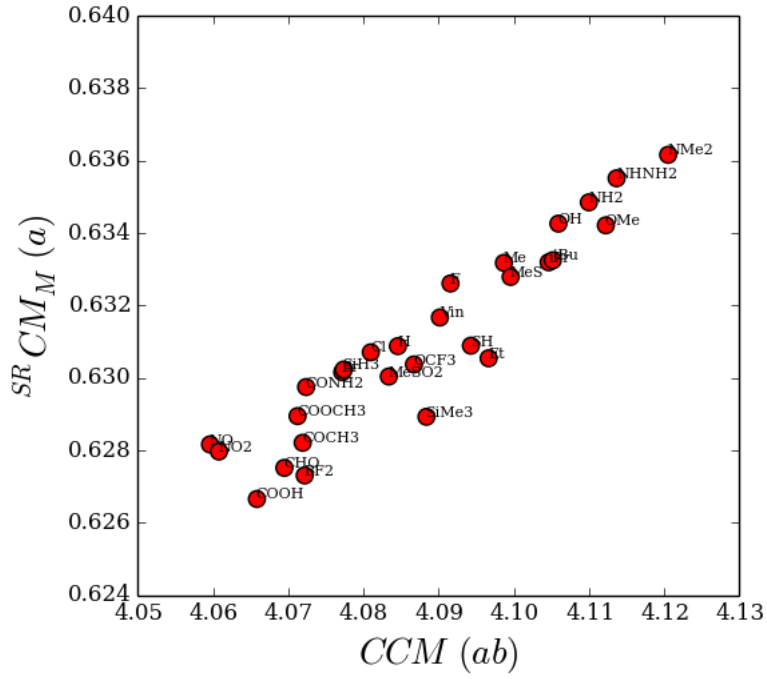
204


0.484
0.482
0.480
0.478
0.476
0.474
0.472
4.05
4.06
4.07
4.08
4.09
4.10
4.11
4.12
4.13
$^{SR}CM_0\ (a)$
$CCM\ (ab)$
NO2
COOCH3
Et
CONH2
Me
NHNH2
MeSO2
COOH
OMe
SH
OH
NO
SiMe3
NMe2
NH2

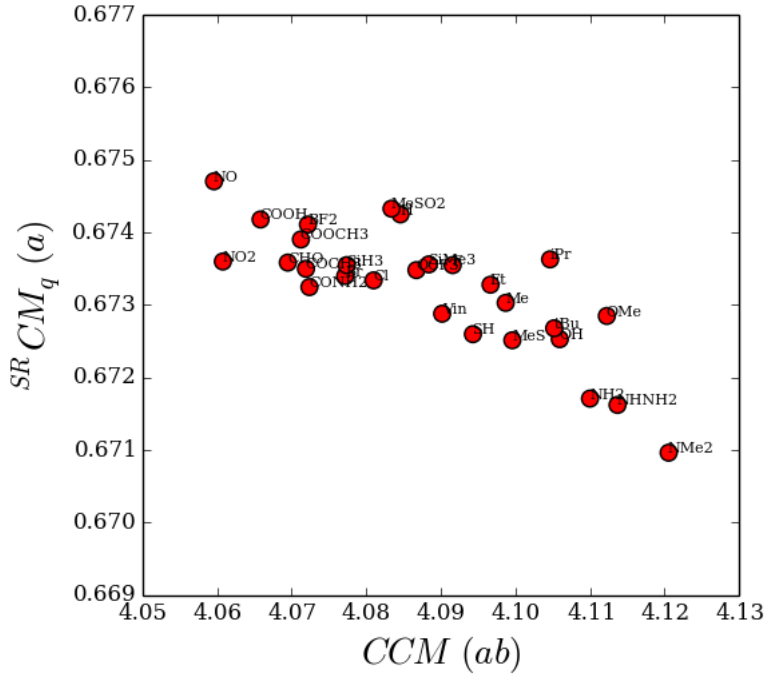
205


0.800
0.798
0.796
0.794
0.792
0.790
0.788
4.05
4.06
4.07
4.08
4.09
4.10
4.11
4.12
4.13
$^{SR}CM_L\ (a)$
$CCM\ (ab)$
NMe2
NH2
NHNH2
OMe
OH
SiMe3
Vin
CHO
MeSO2
NO2
SOOH
SOOCH3

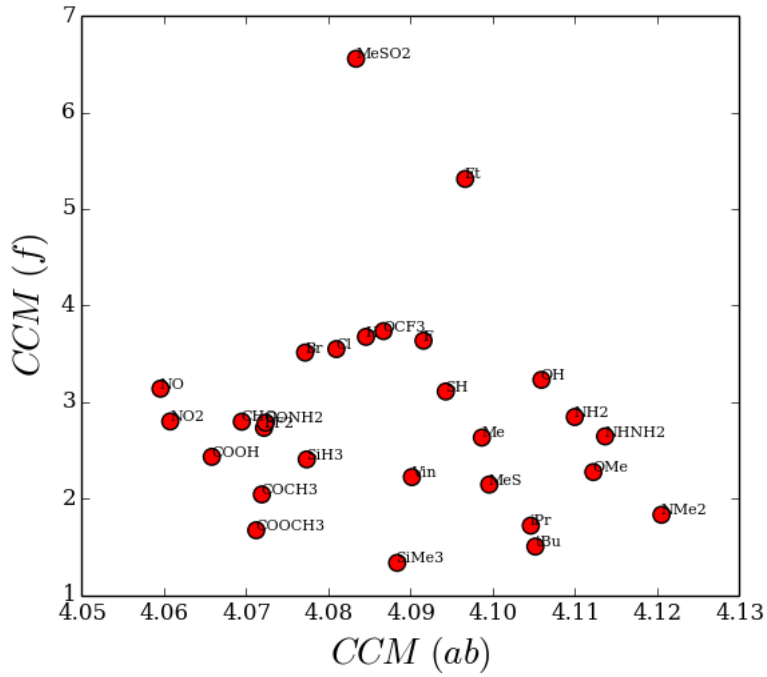
206


0.640
0.638
0.636
0.634
0.632
0.630
0.628
0.626
0.624
4.05
4.06
4.07
4.08
4.09
4.10
4.11
4.12
4.13
$^{SR}CM_M\ (a)$
$CCM\ (ab)$
NMe2
NHNH2
NH2
OH
OMe
Vin
SiMe3
SOOCH3
COCH3
CHO
SOOH

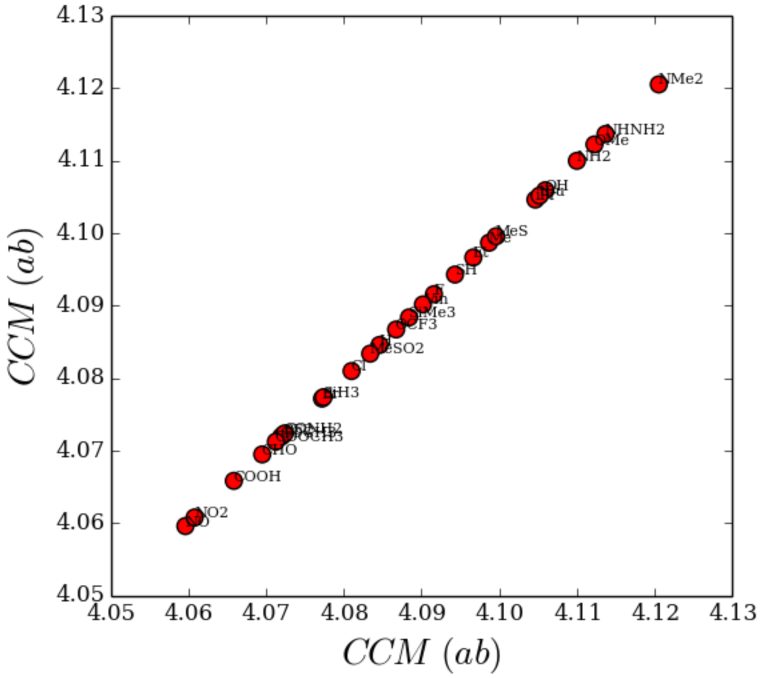
207


0.677
0.676
0.675
0.674
0.673
0.672
0.671
0.670
0.669
4.05
4.06
4.07
4.08
4.09
4.10
4.11
4.12
4.13
$^{SR}CM_q\ (a)$
$CCM\ (ab)$
NO
MeSO2
NO2
iPr
Et
Me
Vin
OMe
SH
MeS
NH2
NHNH2
NMe2

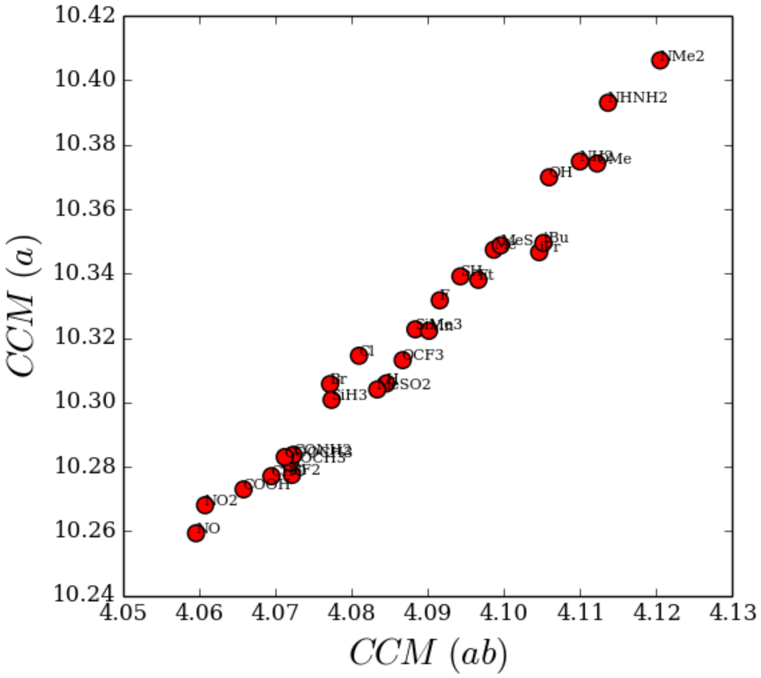
208


7
6
5
4
3
2
1
4.05
4.06
4.07
4.08
4.09
4.10
4.11
4.12
4.13
$CCM\ (f)$
$CCM\ (ab)$
MeSO2
Et
NO
NO2
OH
SH
NH2
NHNH2
Me
SiH3
Vin
OMe
MeS
COCH3
COOCH3
NMe2
iPr
tBu
SiMe3

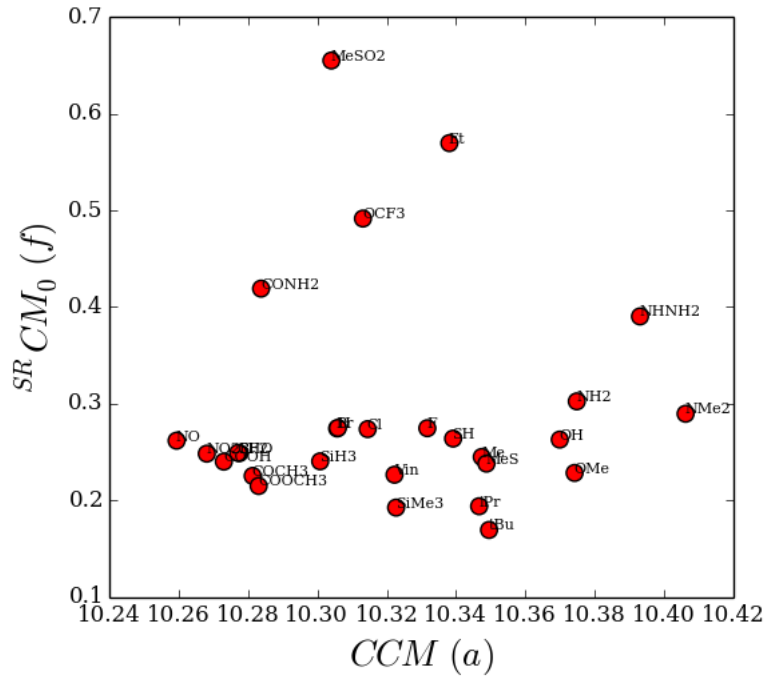
209


4.13
4.12
4.11
4.10
4.09
4.08
4.07
4.06
4.05
4.05 4.06 4.07 4.08 4.09 4.10 4.11 4.12 4.13
$CCM\ (ab)$
$CCM\ (ab)$
NMe2
NHNH2
OMe
NH2
OH
MeS
SH
NMe3
OCF3
MeSO2
SiH3
OCH3
CHO
COOH
NO2

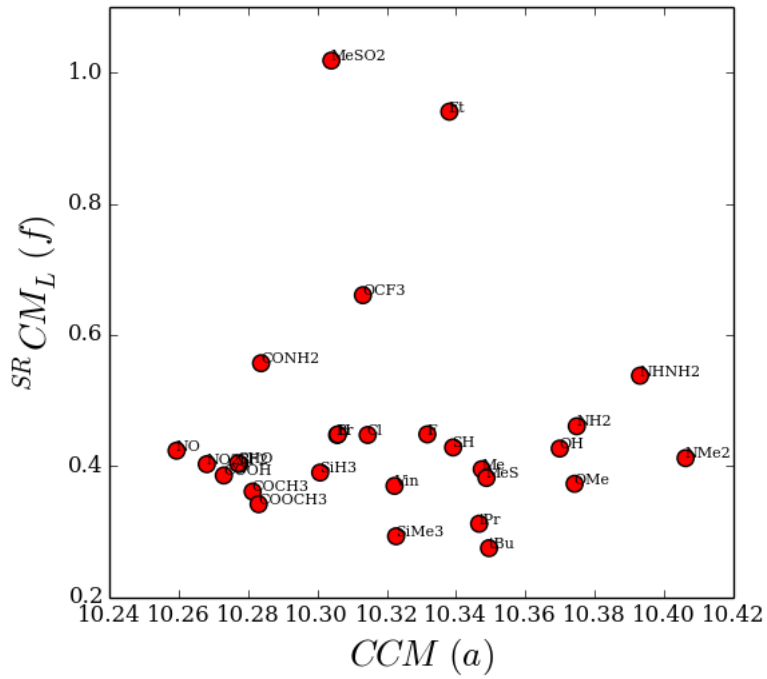
210


10.42
10.40
10.38
10.36
10.34
10.32
10.30
10.28
10.26
10.24
4.05 4.06 4.07 4.08 4.09 4.10 4.11 4.12 4.13
$CCM\ (ab)$
$CCM\ (a)$
NMe2
NHNH2
OMe
OH
MeS
tBu
SH
Et
F
Cl
OCF3
Br
SiH3
MeSO2
OCH3
COOH
NO2
NO

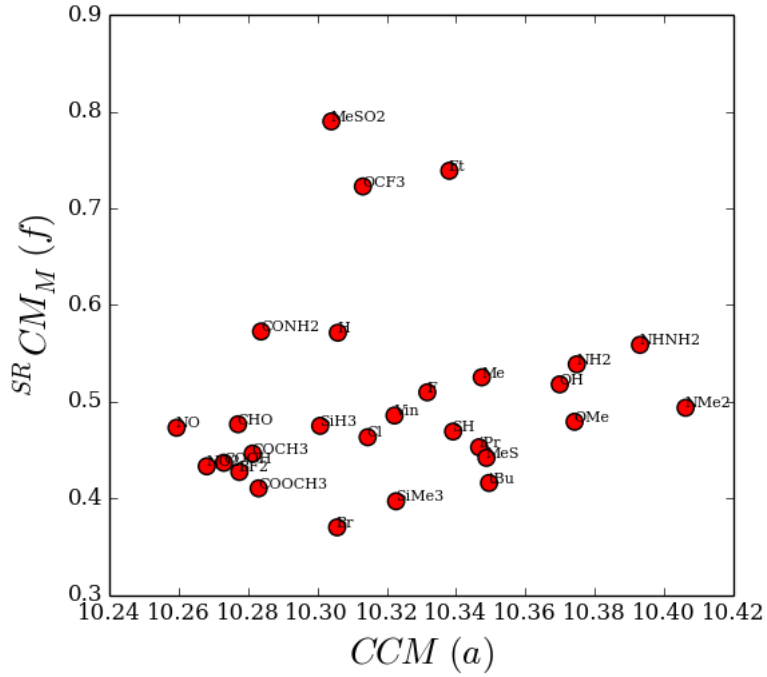
211


0.7
0.6
0.5
0.4
0.3
0.2
0.1
10.24 10.26 10.28 10.30 10.32 10.34 10.36 10.38 10.40 10.42
$CCM\ (a)$
$^{SR}CM_0\ (f)$
MeSO2
OCF3
CONH2
NHNH2
NH2
NMe2
OH
SiH3
Mn
SiMe3
OMe
iPr
tBu

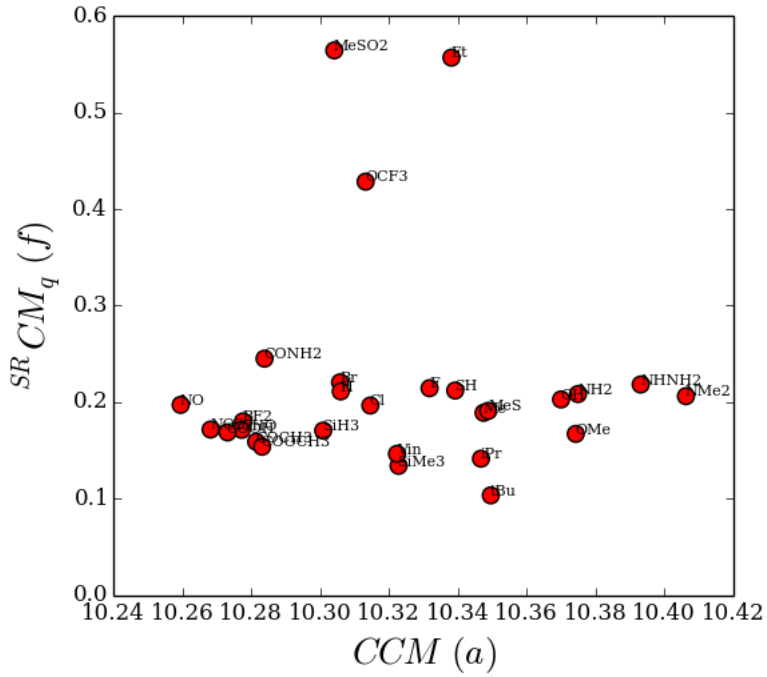
212


1.0
0.8
0.6
0.4
0.2
10.24 10.26 10.28 10.30 10.32 10.34 10.36 10.38 10.40 10.42
$CCM\ (a)$
$^{SR}CM_L\ (f)$
MeSO2
OCF3
CONH2
NHNH2
NH2
NMe2
OH
SiH3
Mn
SiMe3
OMe
iPr
tBu

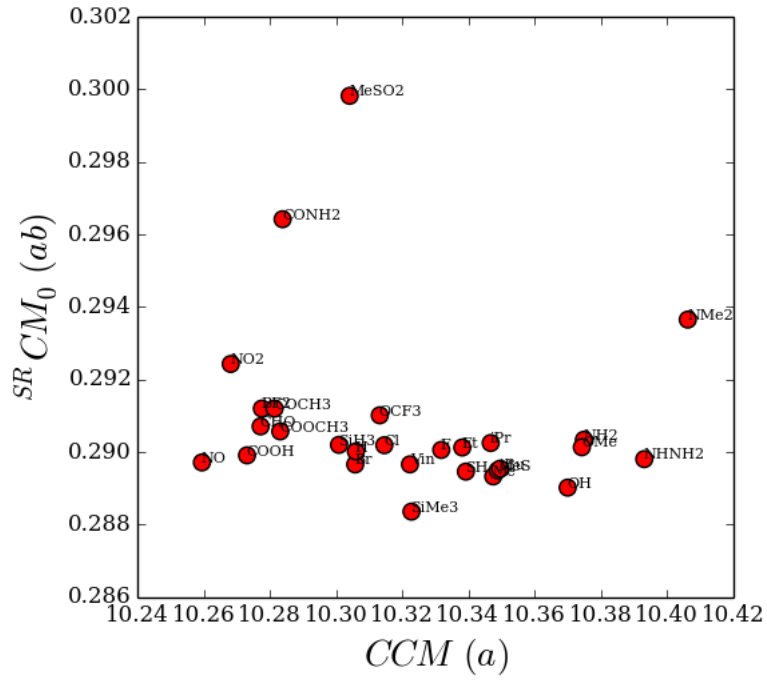
213


0.9
0.8
0.7
0.6
0.5
0.4
0.3
10.24 10.26 10.28 10.30 10.32 10.34 10.36 10.38 10.40 10.42
$^{SR}CM_M\ (f)$
$CCM\ (a)$
MeSO2
Et
OCF3
CONH2
NHNH2
NH2
Me
OH
NMe2
NO
CHO
SiH3
Cl
Vin
SH
OMe
iPr
SMe
NOOCH3
tBu
SiMe3
Br

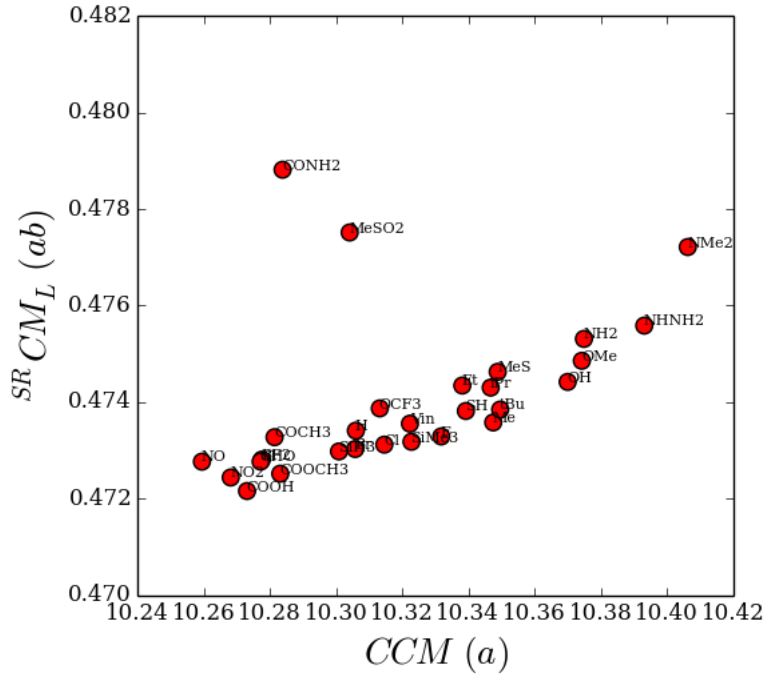
214


0.6
0.5
0.4
0.3
0.2
0.1
0.0
10.24 10.26 10.28 10.30 10.32 10.34 10.36 10.38 10.40 10.42
$^{SR}CM_q\ (f)$
$CCM\ (a)$
MeSO2
Et
OCF3
CONH2
Br
F
SH
NH2
NHNH2
NMe2
NO
Cl
SMe
SiH3
OMe
Vin
SiMe3
iPr
tBu

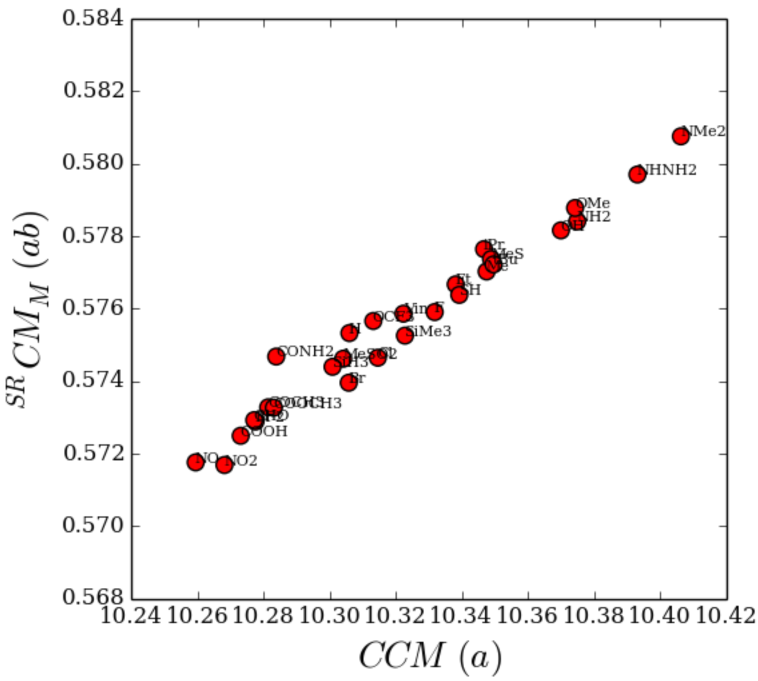
215


0.302
0.300
0.298
0.296
0.294
0.292
0.290
0.288
0.286
10.24 10.26 10.28 10.30 10.32 10.34 10.36 10.38 10.40 10.42
$^{SR}CM_0\ (ab)$
$CCM\ (a)$
MeSO2
CONH2
NMe2
NO2
OCF3
NHNH2
OH
SiMe3

216

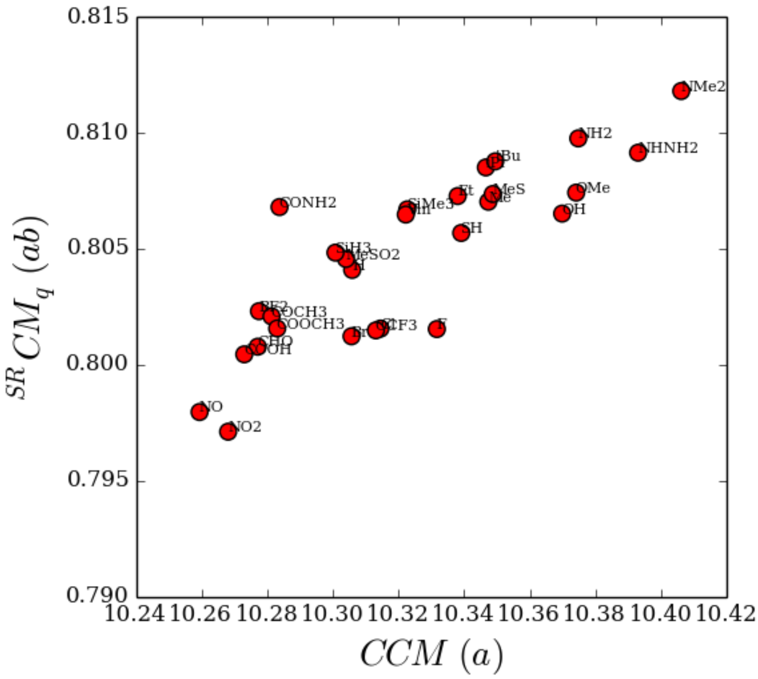

0.482
0.480
0.478
0.476
0.474
0.472
0.470
10.24 10.26 10.28 10.30 10.32 10.34 10.36 10.38 10.40 10.42
$^{SR}CM_L\ (ab)$
$CCM\ (a)$
CONH2
MeSO2
NMe2
NHNH2
NH2
OMe
OH
OCF3
COOCH3
NO2
COOH

217



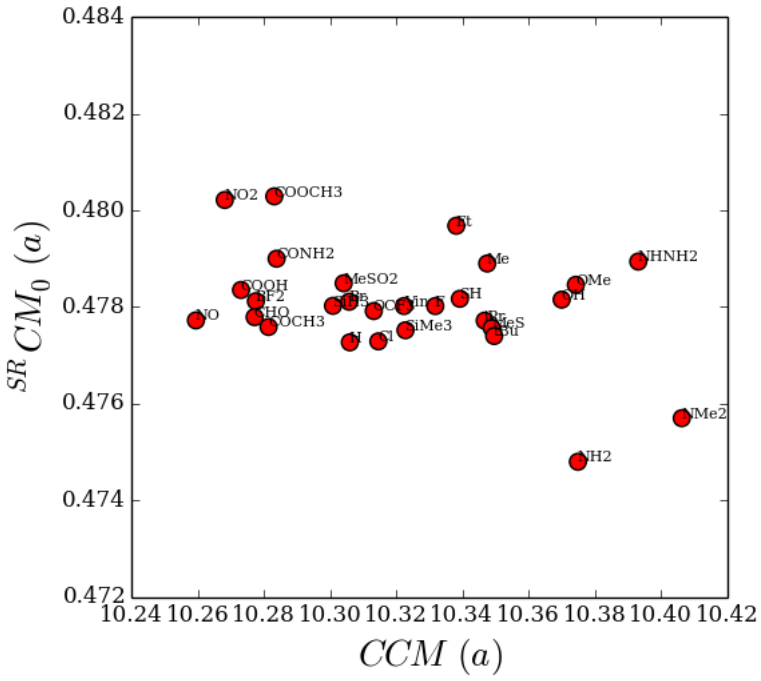
$^{SR}CM_M\ (ab)$
$CCM\ (a)$
NMe2
NHNH2
OMe
CONH2
NO2

218

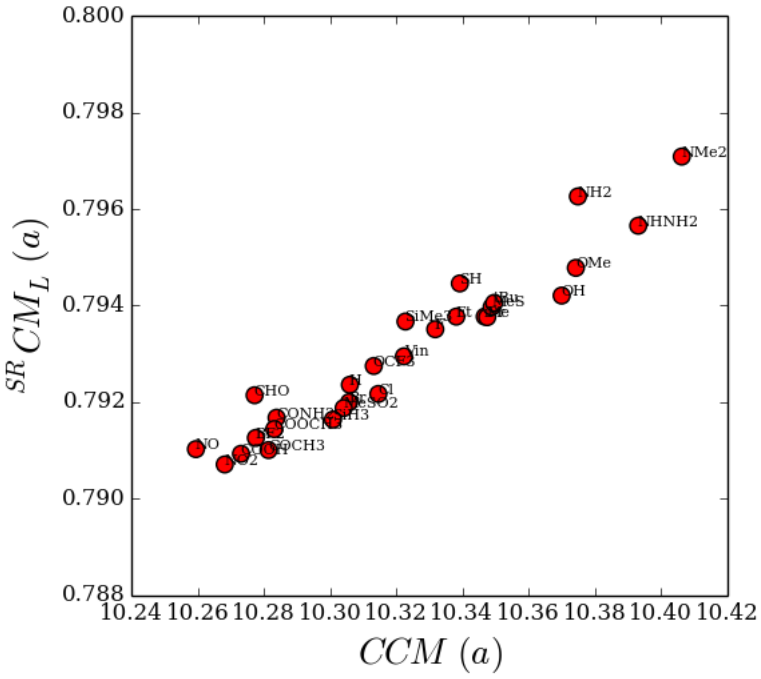


$^{SR}CM_q\ (ab)$
$CCM\ (a)$
NMe2
NH2
NHNH2
OMe
MeS
CONH2
MeSO2
SiH3
COOCH3
NO2
NO
SH
OH
Et
F

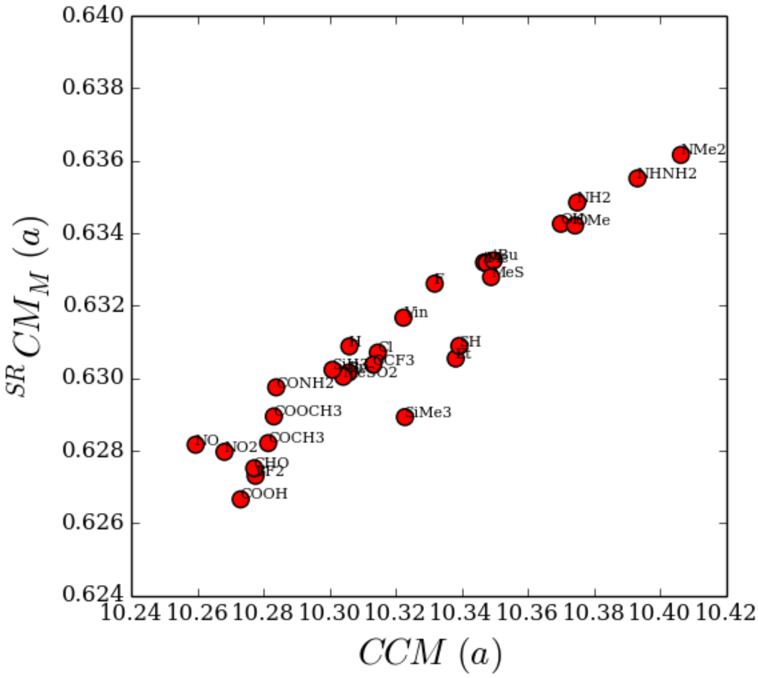
219


0.484
0.482
0.480
0.478
0.476
0.474
0.472
10.24 10.26 10.28 10.30 10.32 10.34 10.36 10.38 10.40 10.42
$^{SR}CM_0\ (a)$
$CCM\ (a)$
NO2
COOCH3
CONH2
COOH
CHO
NO
NHNH2
OMe
NMe2
NH2
SiMe3
SH

220

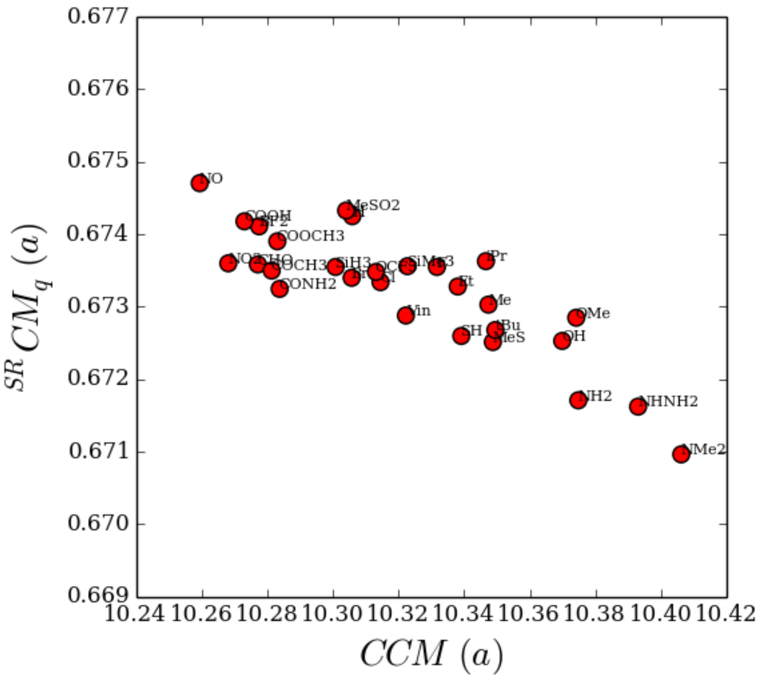

0.800
0.798
0.796
0.794
0.792
0.790
0.788
10.24 10.26 10.28 10.30 10.32 10.34 10.36 10.38 10.40 10.42
$^{SR}CM_L\ (a)$
$CCM\ (a)$
NMe2
NH2
NHNH2
OMe
SH
CHO
NO

221



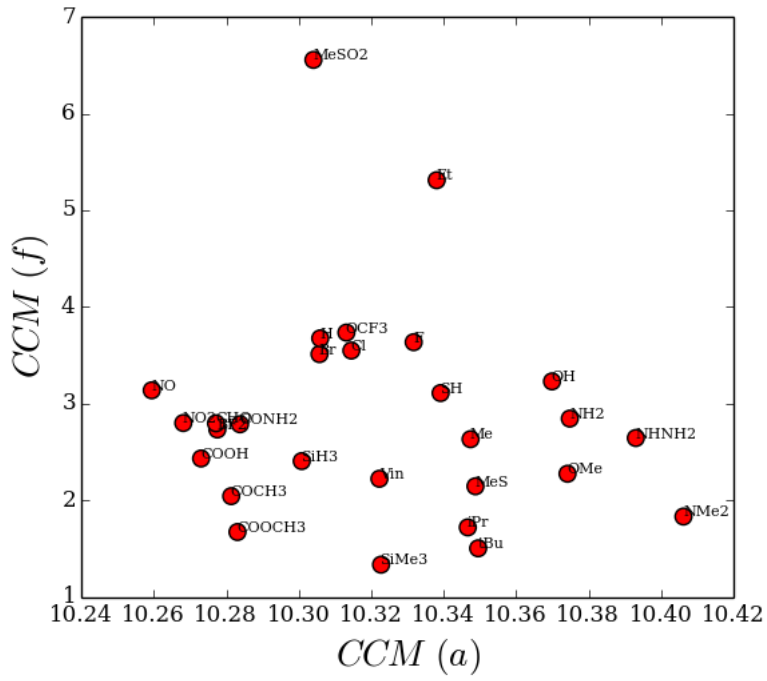
$^{SR}CM_M\ (a)$
$CCM\ (a)$
NMe2
NHNH2
NH2
OH
OMe
tBu
MeS
F
Vin
H
SH
Cl
Et
CF3
MeSO2
CONH2
SiMe3
COOCH3
COCH3
NO
NO2
CHO
CF2
COOH

222

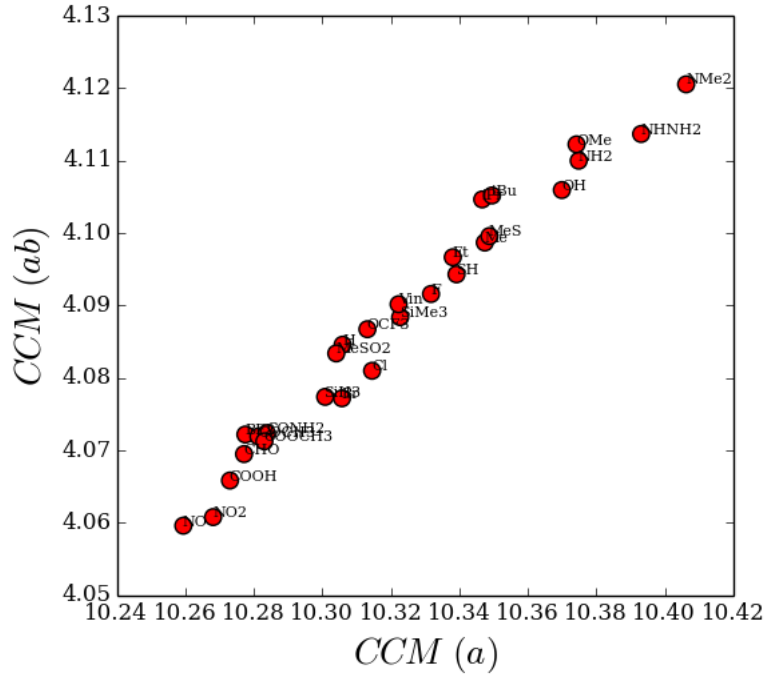


$^{SR}CM_q\ (a)$
$CCM\ (a)$
NO
MeSO2
COOH
CF2
COOCH3
NO2
CHO
COCH3
SiH3
CONH2
SiMe3
iPr
Et
Me
Vin
OMe
SH
tBu
MeS
OH
NH2
NHNH2
NMe2

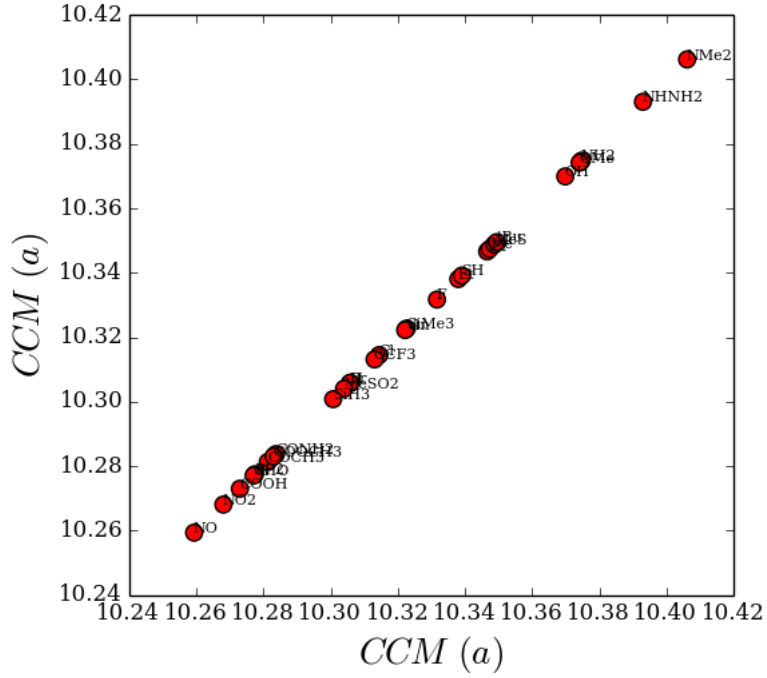
223


CCM (f)
CCM (a)
MeSO2
Et
OCF3
Br
Cl
F
NO
SH
OH
NH2
NHNH2
Me
SiH3
Vin
OMe
MeS
SOCH3
NMe2
SOOCH3
iPr
tBu
SiMe3
SOOH
NO2

224


CCM (ab)
CCM (a)
NMe2
NHNH2
OMe
NH2
OH
tBu
MeS
Et
SH
F
Vin
SiMe3
OCF3
MeSO2
Cl
SOOH
NO2

225


10.42
10.40
10.38
10.36
10.34
10.32
10.30
10.28
10.26
10.24
10.24 10.26 10.28 10.30 10.32 10.34 10.36 10.38 10.40 10.42
CCM (a)
CCM (a)
NMe2
NHNH2
SiMe3
CF3
SO2
OOH
O2
O

Spectral parameters of selected modes

TABLE S4. Spectral parameters of ν(CN) mode in CN-IND with energetics of the conformers. **% of population** was calculated at T=298.15K.

Substituent-Conformer	**Frequency** [cm^{-1}]	**IR intensity** [km/mol]	**dipole strength** [10^{-40} esu^2cm^2]	**rotational strength** [10^{-44} esu^2cm^2]	**Sum of electronic and thermal Free Energies** [Hartree]	**% of population**
BF_2	2341.1	16.61	28.31	-2.483	-664.044660	100.00
Br	2340.4	18.12	30.89	-2.647	-3013.509236	100.00
CHO-1	2341.3	16.73	28.50	-2.212	-553.275490	61.90
CHO-2	2341.6	16.45	28.03	-2.704	-553.275032	38.10
Cl	2340.3	17.77	30.29	-2.674	-899.571723	100.00
$COCH_3$-1	2340.8	17.78	30.30	-2.570	-592.574952	38.55
$COCH_3$-2	2340.3	18.07	30.80	-2.608	-592.575392	61.45
$CONH_2$-1	2340.5	18.01	30.70	-2.472	-608.652785	33.72
$CONH_2$-2	2340.3	18.23	31.07	-2.991	-608.653423	66.28
$COOCH_3$-1	2340.6	18.3	31.18	-2.488	-667.815360	43.65
$COOCH_3$-2	2340.3	18.42	31.39	-2.659	-667.815601	56.35
COOH-1	2341.1	17.11	29.16	-2.549	-628.538830	45.85
COOH-2	2340.9	17.28	29.44	-2.442	-628.538987	54.15

Et-1	2337.9	21.39	36.50	-3.746	-518.527153	42.61
Et-2	2337.7	21.20	36.18	-3.403	-518.525732	9.46
Et-3	2338.0	20.87	35.62	-2.341	-518.527264	47.93
F	2339.8	17.24	29.40	-2.907	-539.200550	100.00
H	2338.8	18.95	32.32	-3.162	-439.940965	100.00
iPr-1	2337.8	21.45	36.61	-3.323	-557.817476	52.36
iPr-2	2337.7	21.56	36.80	-2.646	-557.817387	47.64
Me	2337.9	20.65	35.24	-2.977	-479.237175	100.00
MeS-1	2337.9	21.35	36.43	-3.941	-877.442501	53.81
MeS-2	2338.2	21.75	37.11	-2.259	-877.442357	46.19
$MeSO_2$-1	2342.7	15.81	26.92	-2.646	-1027.836697	36.03
$MeSO_2$-2	2341.8	16.29	27.75	-1.662	-1027.837239	63.97
NH_2	2336.2	22.19	37.89	-3.591	-495.295515	100.00
$NHNH_2$-1	2335.8	23.26	39.73	-4.438	-550.604154	35.86
$NHNH_2$-2	2335.3	24.08	41.14	-3.018	-550.604703	64.14
NMe_2	2334.9	24.92	42.57	-4.122	-573.855889	100.00
NO-1	2342.5	15.33	26.12	-2.815	-569.259127	40.07
NO-2	2342.4	15.31	26.07	-2.002	-569.259507	59.93
NO_2	2343.0	14.50	24.69	-2.142	-644.479658	100.00

OCF_3-1	2340.5	17.26	29.42	-2.581	-852.256190	23.70
OCF_3-2	2340.4	16.84	28.71	-2.897	-852.256087	21.25
OCF_3-3	2341.2	16.07	27.38	-2.203	-852.256986	55.06
OH-1	2337.6	19.87	33.91	-3.446	-515.175261	57.80
OH-2	2337.9	19.72	33.64	-3.105	-515.174964	42.20
OMe-1	2337.4	21.33	36.41	-2.853	-554.449898	46.64
OMe-2	2337.1	20.91	35.69	-3.829	-554.450025	53.36
SH	2338.7	20.03	34.16	-3.103	-838.154955	48.89
SiH_3	2339.4	19.33	32.97	-2.676	-730.638443	100.00
$SiMe_3$	2338.2	21.64	36.93	-2.774	-848.551657	100.00
tBu-1	2337.6	21.89	37.35	-2.929	-597.104273	33.27
tBu-2	2337.6	21.88	37.34	-2.937	-597.104270	33.17
tBu-3	2337.6	21.87	37.33	-3.250	-597.104281	33.56
Vin-1	2338.6	21.18	36.14	-1.487	-517.319332	53.54
Vin-2	2338.6	20.97	35.77	-4.385	-517.319198	46.46

TABLE S5. Spectral parameters of ν(CH) mode in CN-IND with energetics of the conformers.

Substituent-Conformer	**Frequency** [cm^{-1}]	**IR intensity** [km/mol]	**dipole strength** [10^{-40} esu^2cm^2]	**rotational strength** [10^{-44} esu^2cm^2]	**Sum of electronic and thermal Free Energies** [Hartree]	**% of population**
BF_2	3010.8	0.55	0.73	1.061	-664.044660	100.00
Br	3010.8	0.24	0.32	0.680	-3013.509236	100.00
CHO-1	3010.2	0.50	0.66	1.056	-553.275490	61.90
CHO-2	3010.5	0.67	0.89	1.032	-553.275032	38.10
Cl	3010.7	0.24	0.32	0.655	-899.571723	100.00
$COCH_3$-1	3010.7	0.49	0.65	1.023	-592.574952	38.55
$COCH_3$-2	3010.1	0.41	0.54	1.118	-592.575392	61.45
$CONH_2$-1	3012.4	0.37	0.50	0.953	-608.652785	33.72
$CONH_2$-2	3009.6	0.36	0.48	1.083	-608.653423	66.28
$COOCH_3$-1	3010.8	0.44	0.58	1.047	-667.815360	43.65
$COOCH_3$-2	3010.3	0.41	0.55	1.086	-667.815601	56.35
COOH-1	3010.7	0.51	0.68	1.025	-628.538830	45.85
COOH-2	3010.5	0.49	0.64	1.054	-628.538987	54.15
Et-1	3010.3	0.33	0.44	0.801	-518.527153	42.61

Et-2	3010.2	0.38	0.50	0.845	-518.525732	9.46
Et-3	3010.4	0.34	0.45	0.796	-518.527264	47.93
F	3011.0	0.26	0.34	0.590	-539.200550	100.00
H	3011.1	0.31	0.41	1.007	-439.940965	100.00
iPr-1	3010.2	0.34	0.45	0.798	-557.817476	52.36
iPr-2	3010.4	0.35	0.47	0.750	-557.817387	47.64
Me	3010.2	0.35	0.47	0.803	-479.237175	100.00
MeS-1	3008.2	0.49	0.65	0.222	-877.442501	53.81
MeS-2	3008.8	0.39	0.52	0.036	-877.442357	46.19
$MeSO_2$-1	3009.7	0.66	0.87	1.037	-1027.836697	36.03
$MeSO_2$-2	3013.3	0.71	0.94	0.905	-1027.837239	63.97
NH_2	3005.9	1.18	1.57	-0.551	-495.295515	100.00
$NHNH_2$-1	3006.2	1.30	1.73	-0.407	-550.604154	35.86
$NHNH_2$-2	3006.6	1.19	1.58	-0.599	-550.604703	64.14
NMe_2-1	3004.5	1.91	2.54	-0.777	-573.855889	50.82
NMe_2-2	3004.6	1.62	2.15	-0.948	-573.855858	49.18
NO-1	3009.5	1.09	1.45	0.767	-569.259127	40.07
NO-2	3010.1	0.72	0.95	1.448	-569.259507	59.93
NO_2-1	3011.1	0.92	1.22	1.008	-644.479658	49.97

NO_2-2	3011.1	0.92	1.22	1.009	-644.479659	50.03
OCF_3-1	3011.3	0.24	0.32	0.552	-852.256190	23.70
OCF_3-2	3011.1	0.23	0.30	0.537	-852.256087	21.25
OCF_3-3	3011.9	0.32	0.42	0.801	-852.256986	55.06
OH-1	3008.6	0.55	0.73	0.183	-515.175261	57.80
OH-2	3009.0	0.48	0.64	0.107	-515.174964	42.20
OMe-1	3008.8	3.70	4.91	-8.624	-554.449898	46.64
OMe-2	3008.3	0.92	1.21	0.935	-554.450025	53.36
SH-1	3008.9	0.31	0.41	0.269	-838.154955	48.89
SH-2	3009.3	0.30	0.39	0.249	-838.154997	51.11
SiH_3-1	3010.8	0.29	0.39	0.968	-730.638443	49.97
SiH_3-2	3010.8	0.29	0.39	0.968	-730.638444	50.03
$SiMe_3$	3010.4	0.31	0.41	1.030	-848.551657	100.00
tBu-1	3010.4	0.35	0.47	0.825	-597.104273	33.27
tBu-2	3010.4	0.36	0.48	0.838	-597.104270	33.17
tBu-3	3010.4	0.35	0.47	0.863	-597.104281	33.56
Vin-1	3009.0	0.27	0.36	0.566	-517.319332	53.54
Vin-2	3009.0	0.27	0.36	0.713	-517.319198	46.46

Coordinates and energies of CN-IND

BF_2-CN-IND
Total energy (hartree): -664.144789
Sum of electronic and thermal Free Energies (hartree): -664.044660

C	1.512170	2.034827	0.008671
C	2.727423	1.497857	-0.215338
C	2.600711	0.006953	-0.515552
C	1.103967	-0.237843	-0.358783
C	0.372552	-1.413251	-0.475202
C	-1.017150	-1.345832	-0.310731
C	-1.668612	-0.124982	-0.035458
C	-0.905963	1.056029	0.084359
C	0.478197	0.994107	-0.073871
H	1.313296	3.083549	0.221851
H	3.684983	2.012380	-0.210883
H	0.860836	-2.366225	-0.679253
H	-1.609158	-2.256930	-0.395864
H	-1.399145	2.003553	0.301552
H	2.899260	-0.187291	-1.561117
C	3.438322	-0.843296	0.340255
N	4.107575	-1.517597	1.006942
B	-3.202587	-0.079880	0.137645
F	-3.850650	1.065448	0.400514
F	-3.964891	-1.178099	0.032463

Br-CN-IND
Total energy (hartree): -3013.600737
Sum of electronic and thermal Free Energies (hartree): -3013.509236

C	-1.861455	2.034365	-0.076026
C	-3.077299	1.503960	0.161631
C	-2.951532	0.024904	0.515379
C	-1.454171	-0.222562	0.375259
C	-0.714176	-1.386086	0.535857
C	0.679018	-1.328910	0.376663
C	1.289132	-0.109986	0.063591
C	0.558663	1.069712	-0.107007
C	-0.828465	0.997322	0.049245
H	-1.662611	3.074988	-0.325850
H	-4.034904	2.017889	0.133725
H	-1.192887	-2.336580	0.772012
H	1.282736	-2.226602	0.493672
H	1.057453	2.004586	-0.355079
H	-3.260732	-0.130368	1.564264
C	-3.785599	-0.852562	-0.316656
N	-4.452040	-1.549605	-0.962554

Br	3.195729	-0.055360	-0.143214

CHO-1-CN-IND

Total energy (hartree): -553.386724

Sum of electronic and thermal Free Energies (hartree): -553.275490

C	0.974809	2.037859	0.022432
C	2.225391	1.595433	-0.212556
C	2.211478	0.101294	-0.522732
C	0.739196	-0.258494	-0.357068
C	0.101788	-1.486203	-0.473437
C	-1.288242	-1.525848	-0.295815
C	-2.013727	-0.357491	-0.010941
C	-1.359845	0.882986	0.110544
C	0.021173	0.922944	-0.059562
H	0.698430	3.067022	0.243770
H	3.141100	2.181374	-0.211218
H	0.660083	-2.397654	-0.686414
H	-1.818582	-2.475823	-0.377629
H	-1.944590	1.773860	0.336950
H	2.516732	-0.062061	-1.571664
C	3.117527	-0.689243	0.320668
N	3.840130	-1.317325	0.976692
C	-3.484973	-0.448637	0.164710
H	-3.907242	-1.475591	0.057023
O	-4.211788	0.495318	0.406859

CHO-2-CN-IND

Total energy (hartree): -553.386220

Sum of electronic and thermal Free Energies (hartree): -553.275032

C	-1.271430	2.028217	-0.091761
C	-2.442456	1.423264	0.188019
C	-2.210253	-0.043360	0.538887
C	-0.705688	-0.197480	0.348081
C	0.104304	-1.321037	0.489686
C	1.479840	-1.178771	0.286225
C	2.027837	0.072340	-0.053340
C	1.203636	1.200397	-0.200503
C	-0.170676	1.059373	-0.000775
H	-1.147940	3.078526	-0.349436
H	-3.431321	1.874688	0.192764
H	-0.318973	-2.292733	0.744372
H	2.151605	-2.030486	0.384714
H	1.639447	2.164389	-0.468533
H	-2.467997	-0.215412	1.599144
C	-3.013700	-0.977192	-0.260780
N	-3.655832	-1.716912	-0.883214

C	3.490806	0.215379	-0.263855
H	3.825008	1.244663	-0.536500
O	4.298460	-0.686504	-0.157915

Cl-CN-IND

Total energy (hartree): -899.664910

Sum of electronic and thermal Free Energies (hartree): -899.571723

C	-1.177463	2.034751	-0.077010
C	-2.392451	1.514249	0.185779
C	-2.271836	0.033311	0.533327
C	-0.780044	-0.226448	0.360681
C	-0.046713	-1.396711	0.502839
C	1.342518	-1.351225	0.313425
C	1.955959	-0.137043	-0.010755
C	1.232712	1.049414	-0.162839
C	-0.150858	0.988750	0.023549
H	-0.975320	3.074269	-0.328817
H	-3.345928	2.036507	0.179794
H	-0.528582	-2.343371	0.747519
H	1.945320	-2.251532	0.414254
H	1.738665	1.977992	-0.420180
H	-2.560686	-0.122078	1.587975
C	-3.130678	-0.834747	-0.283328
N	-3.816336	-1.524545	-0.916794
Cl	3.703177	-0.102693	-0.239823

$COCH_3$-1-CN-IND

Total energy (hartree): -592.711713

Sum of electronic and thermal Free Energies (hartree): -592.574952

C	1.442930	2.039870	-0.018255
C	2.672302	1.532274	-0.234379
C	2.584035	0.034715	-0.514893
C	1.093933	-0.245557	-0.357691
C	0.387304	-1.438697	-0.461373
C	-1.001442	-1.404607	-0.300854
C	-1.676533	-0.197036	-0.040624
C	-0.950287	1.003074	0.067967
C	0.436708	0.971348	-0.088865
H	1.217914	3.086117	0.181411
H	3.616069	2.071708	-0.235262
H	0.896571	-2.383078	-0.654039
H	-1.592200	-2.315966	-0.373121
H	-1.454121	1.946108	0.272833
H	2.891177	-0.165810	-1.556759
C	3.441714	-0.780284	0.355351
N	4.127912	-1.425425	1.033580

C	-3.172339	-0.238196	0.115961
O	-3.778648	-1.292245	0.002651
C	-3.915454	1.050225	0.416700
H	-3.754564	1.790122	-0.380830
H	-4.983577	0.828262	0.497807
H	-3.560692	1.495705	1.357426

$COCH_3$-2-CN-IND

Total energy (hartree): -592.712179

Sum of electronic and thermal Free Energies (hartree): -592.575392

C	1.548419	2.025480	0.024287
C	2.748979	1.459582	-0.207745
C	2.584727	-0.025378	-0.520527
C	1.083127	-0.233169	-0.360119
C	0.318770	-1.385008	-0.480339
C	-1.069458	-1.283121	-0.307940
C	-1.679383	-0.048130	-0.023263
C	-0.891476	1.111950	0.100731
C	0.487593	1.012049	-0.063166
H	1.376544	3.076970	0.246550
H	3.719177	1.949978	-0.202252
H	0.777450	-2.350521	-0.693247
H	-1.674229	-2.183426	-0.397127
H	-1.381192	2.058009	0.325767
H	2.876378	-0.217219	-1.568456
C	3.403388	-0.904225	0.324888
N	4.056670	-1.603216	0.982024
C	-3.166879	0.081154	0.160071
O	-3.666663	1.171453	0.392313
C	-4.035356	-1.158079	0.052878
H	-3.739063	-1.909162	0.799333
H	-5.077959	-0.870597	0.217430
H	-3.935195	-1.621766	-0.939206

$CONH_2$-1-CN-IND

Total energy (hartree): -608.779655

Sum of electronic and thermal Free Energies (hartree): -608.652785

C	1.472841	2.026654	-0.139152
C	2.692199	1.483754	-0.324291
C	2.575869	-0.026043	-0.514486
C	1.080055	-0.267671	-0.345190
C	0.347729	-1.447221	-0.398234
C	-1.042682	-1.375966	-0.251073
C	-1.687525	-0.145541	-0.040749
C	-0.939236	1.043478	0.009529
C	0.446906	0.975008	-0.144227

H	1.268010	3.087229	-0.003469
H	3.645914	2.004467	-0.356168
H	0.835529	-2.410723	-0.546475
H	-1.653817	-2.275267	-0.301064
H	-1.427693	2.010226	0.130189
H	2.883278	-0.295460	-1.540433
C	3.415018	-0.801014	0.408993
N	4.086134	-1.414625	1.130272
C	-3.186636	-0.169442	0.098144
O	-3.863270	-1.088696	-0.347230
N	-3.760305	0.909162	0.727105
H	-4.753443	0.844904	0.903838
H	-3.219644	1.506460	1.334208

$CONH_2$-2-CN-IND

Total energy (hartree): -608.779990

Sum of electronic and thermal Free Energies (hartree): -608.653423

C	1.501292	2.027786	-0.089421
C	2.711279	1.472206	-0.296751
C	2.572856	-0.030336	-0.527493
C	1.076199	-0.255855	-0.346464
C	0.331566	-1.426191	-0.390138
C	-1.057701	-1.339077	-0.218556
C	-1.687059	-0.100076	-0.006316
C	-0.920886	1.075874	0.056264
C	0.459825	0.991481	-0.115336
H	1.310801	3.086381	0.076975
H	3.672280	1.979744	-0.322889
H	0.806978	-2.396223	-0.535386
H	-1.638095	-2.261028	-0.216656
H	-1.424944	2.021693	0.247014
H	2.862573	-0.272313	-1.565568
C	3.413150	-0.847380	0.357600
N	4.084050	-1.499007	1.044982
C	-3.173419	0.042683	0.194775
O	-3.660473	1.049253	0.697472
N	-3.955531	-1.015527	-0.192178
H	-4.955320	-0.884338	-0.130102
H	-3.612731	-1.732901	-0.811775

$COOCH_3$-1-CN-IND

Total energy (hartree): -667.956046

Sum of electronic and thermal Free Energies (hartree): -667.815360

C	1.745122	2.058457	-0.048614
C	3.001406	1.604956	-0.226469
C	2.989287	0.100824	-0.484761

C	1.510105	-0.246262	-0.357972
C	0.863539	-1.472076	-0.457456
C	-0.530019	-1.500754	-0.328797
C	-1.258251	-0.319701	-0.105453
C	-0.598619	0.917334	-0.000807
C	0.790622	0.943886	-0.125244
H	1.466707	3.095770	0.128238
H	3.919205	2.187377	-0.213851
H	1.419597	-2.394889	-0.622108
H	-1.074760	-2.440404	-0.398242
H	-1.166809	1.827744	0.175999
H	3.330293	-0.100940	-1.515751
C	3.862463	-0.660623	0.417994
N	4.561422	-1.263518	1.121644
C	-2.742982	-0.434669	0.017270
O	-3.360754	-1.476919	-0.073346
O	-3.339763	0.759061	0.242425
C	-4.774276	0.717536	0.371537
H	-5.228558	0.330231	-0.548340
H	-5.062566	0.076816	1.213433
H	-5.079312	1.752334	0.549109

$COOCH_3$-2-CN-IND

Total energy (hartree): -667.956200

Sum of electronic and thermal Free Energies (hartree): -667.815601

C	2.047273	1.996164	0.043181
C	3.222080	1.376074	-0.182534
C	2.990113	-0.096968	-0.507871
C	1.478601	-0.234699	-0.363194
C	0.661631	-1.349133	-0.501725
C	-0.721292	-1.186959	-0.343536
C	-1.267268	0.075499	-0.053727
C	-0.434273	1.198283	0.090012
C	0.941352	1.034398	-0.062003
H	1.923153	3.052916	0.272162
H	4.214223	1.819974	-0.164412
H	1.077636	-2.332928	-0.718808
H	-1.382218	-2.044457	-0.443805
H	-0.879452	2.164948	0.319072
H	3.282318	-0.295208	-1.554442
C	3.758904	-1.018654	0.338715
N	4.373923	-1.750581	0.996928
C	-2.737464	0.280853	0.116977
O	-3.253299	1.353739	0.362225
O	-3.446042	-0.861463	-0.031430
C	-4.872401	-0.728751	0.123639

H	-5.113515	-0.359317	1.127540
H	-5.273604	-0.032694	-0.622723
H	-5.274800	-1.734016	-0.027033

COOH-1-CN-IND

Total energy (hartree): -628.654413

Sum of electronic and thermal Free Energies (hartree): -628.538830

C	1.455188	2.036300	0.004994
C	2.676653	1.514005	-0.220161
C	2.567716	0.021162	-0.517785
C	1.074542	-0.241290	-0.358560
C	0.354765	-1.424592	-0.472594
C	-1.033959	-1.376176	-0.307282
C	-1.683287	-0.159904	-0.033775
C	-0.950519	1.033911	0.086444
C	0.434228	0.982583	-0.074663
H	1.243896	3.082829	0.216928
H	3.627742	2.040452	-0.217886
H	0.851533	-2.373041	-0.676311
H	-1.635064	-2.280023	-0.386586
H	-1.459637	1.970614	0.302486
H	2.867689	-0.170880	-1.563346
C	3.417414	-0.816579	0.338525
N	4.097029	-1.480391	1.005237
C	-3.164781	-0.186181	0.125045
O	-3.857792	-1.178089	0.030031
O	-3.693627	1.038553	0.393637
H	-4.651756	0.909641	0.477580

COOH-2-CN-IND

Total energy (hartree): -628.654584

Sum of electronic and thermal Free Energies (hartree): -628.538987

C	1.505487	2.034123	0.021843
C	2.713287	1.483840	-0.210137
C	2.568136	-0.003549	-0.519862
C	1.069509	-0.231465	-0.358313
C	0.321866	-1.395609	-0.477798
C	-1.066797	-1.317041	-0.307645
C	-1.684625	-0.086559	-0.024648
C	-0.922090	1.087744	0.100669
C	0.459092	1.006146	-0.063496
H	1.319658	3.083593	0.242432
H	3.676864	1.987075	-0.206069
H	0.795447	-2.354199	-0.689274
H	-1.675118	-2.214354	-0.393176
H	-1.423661	2.027571	0.324848

H	2.860593	-0.193523	-1.567924
C	3.399608	-0.869506	0.326231
N	4.063871	-1.556999	0.984397
C	-3.159550	0.024673	0.156692
O	-3.752115	1.056509	0.398480
O	-3.807201	-1.163483	0.023612
H	-4.749881	-0.978148	0.160425

Et-1-CN-IND

Total energy (hartree): -518.683180

Sum of electronic and thermal Free Energies (hartree): -518.527153

C	-1.191809	2.029706	-0.115288
C	-2.390815	1.545552	0.265452
C	-2.276010	0.063243	0.612166
C	-0.812814	-0.235745	0.304492
C	-0.096952	-1.422384	0.382428
C	1.267236	-1.401593	0.056531
C	1.916515	-0.219238	-0.339510
C	1.174135	0.971342	-0.419541
C	-0.185800	0.958850	-0.101076
H	-0.988811	3.062329	-0.394530
H	-3.326650	2.093131	0.344259
H	-0.577874	-2.356397	0.674384
H	1.838037	-2.330169	0.104192
H	1.658646	1.896080	-0.737576
H	-2.472432	-0.080993	1.689348
C	-3.228702	-0.784393	-0.117299
N	-3.988640	-1.456862	-0.681217
C	3.399460	-0.222662	-0.645342
H	3.683767	-1.200911	-1.059356
H	3.612485	0.524454	-1.423941
C	4.265263	0.074181	0.591936
H	5.332942	0.064731	0.331756
H	4.024344	1.060178	1.012806
H	4.097784	-0.675573	1.377486

Et-2-CN-IND

Total energy (hartree): -518.682039

Sum of electronic and thermal Free Energies (hartree): -518.525732

C	1.453207	2.007711	0.102010
C	2.606569	1.368471	-0.176800
C	2.330136	-0.088560	-0.540068
C	0.819591	-0.192815	-0.358709
C	-0.038259	-1.270671	-0.506628
C	-1.414320	-1.070195	-0.299901
C	-1.934052	0.186499	0.047854

C	-1.045500	1.268956	0.196925
C	0.320800	1.077128	-0.001222
H	1.364250	3.059833	0.367804
H	3.609193	1.788792	-0.172327
H	0.335756	-2.260978	-0.767873
H	-2.084020	-1.920709	-0.412281
H	-1.430051	2.252970	0.471687
H	2.597222	-0.262921	-1.597364
C	3.099205	-1.048617	0.263217
N	3.714644	-1.810854	0.886098
C	-3.418521	0.425352	0.273304
H	-3.545955	0.855909	1.279030
H	-3.748349	1.211765	-0.424079
C	-4.337481	-0.788995	0.128750
H	-5.378805	-0.497271	0.318882
H	-4.291913	-1.215483	-0.883080
H	-4.078083	-1.581515	0.844527

Et-3-CN-IND

Total energy (hartree): -518.683178

Sum of electronic and thermal Free Energies (hartree): -518.527264

C	1.238871	2.024733	0.147271
C	2.463592	1.486290	-0.016925
C	2.345371	0.026023	-0.445701
C	0.837441	-0.200613	-0.435501
C	0.091753	-1.337801	-0.714137
C	-1.307174	-1.247985	-0.662487
C	-1.961424	-0.046190	-0.340035
C	-1.190212	1.095064	-0.061029
C	0.203391	1.013192	-0.104576
H	1.036503	3.057223	0.427423
H	3.422806	1.981744	0.110622
H	0.572683	-2.284138	-0.963263
H	-1.903707	-2.134884	-0.881473
H	-1.680649	2.038082	0.186257
H	2.736825	-0.090530	-1.471792
C	3.097878	-0.899712	0.411547
N	3.701728	-1.633777	1.078037
C	-3.472407	0.007685	-0.257149
H	-3.818562	1.005666	-0.564117
H	-3.901793	-0.709525	-0.971702
C	-4.005888	-0.301645	1.152897
H	-5.103626	-0.253562	1.173035
H	-3.701246	-1.306326	1.476880
H	-3.618483	0.418443	1.886826

F-CN-IND

Total energy (hartree): -539.295927

Sum of electronic and thermal Free Energies (hartree): -539.200550

C	-0.747922	2.035557	-0.077439
C	-1.961209	1.528785	0.218503
C	-1.848542	0.045277	0.557108
C	-0.365345	-0.231806	0.341645
C	0.355949	-1.412952	0.460332
C	1.739645	-1.385531	0.231530
C	2.344603	-0.176001	-0.105270
C	1.647180	1.022465	-0.236015
C	0.268499	0.977570	-0.009808
H	-0.540886	3.073560	-0.331590
H	-2.908011	2.062619	0.241437
H	-0.133246	-2.352794	0.716275
H	2.347160	-2.285679	0.308480
H	2.171038	1.937755	-0.506212
H	-2.111844	-0.110567	1.618313
C	-2.740657	-0.807681	-0.239772
N	-3.452175	-1.485890	-0.857119
F	3.687534	-0.166416	-0.321306

H-CN-IND

Total energy (hartree): -440.045876

Sum of electronic and thermal Free Energies (hartree): -439.940965

C	-0.278688	2.029888	-0.085174
C	-1.497144	1.566587	0.257273
C	-1.423711	0.076969	0.581348
C	0.039364	-0.252184	0.302358
C	0.718144	-1.460990	0.384864
C	2.091920	-1.473766	0.097013
C	2.758792	-0.295015	-0.261820
C	2.071456	0.922070	-0.347976
C	0.702092	0.936328	-0.066758
H	-0.045254	3.062124	-0.341047
H	-2.422394	2.133604	0.322820
H	0.201906	-2.382497	0.655439
H	2.644822	-2.411744	0.151013
H	2.594539	1.835507	-0.631917
H	-1.645544	-0.079890	1.651829
C	-2.378104	-0.738468	-0.181496
N	-3.139889	-1.385320	-0.772127
H	3.826424	-0.328380	-0.481051

iPr-1-CN-IND

Total energy (hartree): -557.999806

Sum of electronic and thermal Free Energies (hartree): -557.817476

C	1.718988	2.007553	0.260592
C	2.891598	1.424013	-0.058004
C	2.655492	-0.003940	-0.543670
C	1.147027	-0.160829	-0.387729
C	0.318555	-1.247653	-0.636661
C	-1.059744	-1.099764	-0.429321
C	-1.617196	0.112334	0.018729
C	-0.763259	1.198814	0.266619
C	0.613424	1.059222	0.067683
H	1.599147	3.031163	0.611683
H	3.882788	1.867631	-0.007756
H	0.722939	-2.201760	-0.975999
H	-1.710569	-1.953155	-0.619914
H	-1.176400	2.145748	0.617761
H	2.934794	-0.082740	-1.609270
C	3.442158	-1.008353	0.184614
N	4.071783	-1.804467	0.748074
C	-3.117891	0.248010	0.239014
H	-3.295007	1.276973	0.588249
C	-3.625111	-0.703908	1.337485
H	-4.694285	-0.535432	1.528134
H	-3.498830	-1.755308	1.042913
H	-3.080056	-0.550013	2.278223
C	-3.910548	0.064301	-1.067880
H	-3.798309	-0.955575	-1.462167
H	-4.981608	0.240587	-0.895619
H	-3.568046	0.764352	-1.841585

iPr-2-CN-IND

Total energy (hartree): -557.999849

Sum of electronic and thermal Free Energies (hartree): -557.817387

C	1.402608	2.021681	0.155879
C	2.659173	1.603535	-0.094670
C	2.654107	0.135920	-0.515174
C	1.179292	-0.234995	-0.401390
C	0.529725	-1.440298	-0.621614
C	-0.865032	-1.484438	-0.466956
C	-1.609921	-0.351359	-0.100271
C	-0.932410	0.861301	0.122438
C	0.454406	0.913729	-0.024903
H	1.121523	3.031417	0.450771
H	3.572213	2.190556	-0.034885
H	1.080173	-2.339796	-0.898719
H	-1.386026	-2.428111	-0.634406
H	-1.482466	1.756860	0.412747

H	2.984981	0.050580	-1.565348
C	3.548784	-0.706996	0.289401
N	4.264535	-1.374649	0.913621
C	-3.121272	-0.444758	0.060059
H	-3.402388	-1.480799	-0.183247
C	-3.863566	0.476605	-0.924744
H	-4.950085	0.336002	-0.837696
H	-3.646322	1.535037	-0.721949
H	-3.572752	0.265183	-1.962350
C	-3.560047	-0.177983	1.511435
H	-3.331193	0.853983	1.813511
H	-4.643847	-0.325550	1.618925
H	-3.050627	-0.854478	2.210363

Me-CN-IND

Total energy (hartree): -479.366380

Sum of electronic and thermal Free Energies (hartree): -479.237175

C	0.785436	2.029998	0.077798
C	2.002600	1.527264	-0.209558
C	1.894969	0.043069	-0.550538
C	0.409780	-0.235616	-0.347096
C	-0.315008	-1.411161	-0.472440
C	-1.701151	-1.368884	-0.251436
C	-2.360533	-0.176807	0.088903
C	-1.609055	1.005681	0.215230
C	-0.230560	0.971249	0.001483
H	0.576058	3.067930	0.331657
H	2.948670	2.062699	-0.224510
H	0.171076	-2.353377	-0.727047
H	-2.280773	-2.288107	-0.344351
H	-2.103876	1.941051	0.482432
H	2.167263	-0.113687	-1.609298
C	2.781578	-0.808704	0.253703
N	3.489928	-1.484724	0.877353
C	-3.853241	-0.156748	0.324660
H	-4.087357	0.145867	1.356037
H	-4.351365	0.559510	-0.345011
H	-4.298088	-1.144873	0.154361

MeS-1-CN-IND

Total energy (hartree): -877.570634

Sum of electronic and thermal Free Energies (hartree): -877.442501

C	-1.769367	2.001767	-0.073754
C	-2.926119	1.360136	0.183872
C	-2.657100	-0.101824	0.531980
C	-1.145787	-0.206493	0.365929

C	-0.290351	-1.287837	0.507602
C	1.088421	-1.095775	0.320589
C	1.599557	0.172031	-0.003990
C	0.725947	1.267693	-0.151967
C	-0.640229	1.067215	0.030452
H	-1.674970	3.056864	-0.324967
H	-3.927923	1.782432	0.173701
H	-0.668092	-2.281247	0.751097
H	1.752977	-1.949112	0.429504
H	1.117313	2.252078	-0.409938
H	-2.938382	-0.287772	1.583742
C	-3.419105	-1.050269	-0.292068
N	-4.027705	-1.805055	-0.930492
S	3.334631	0.513703	-0.255455
C	4.135136	-1.109986	-0.025791
H	3.984731	-1.491059	0.991601
H	3.783444	-1.837120	-0.767751
H	5.204731	-0.928883	-0.183398

MeS-2-CN-IND

Total energy (hartree): -877.570554

Sum of electronic and thermal Free Energies (hartree): -877.442357

C	1.358557	2.033363	-0.045696
C	2.625900	1.618790	-0.241884
C	2.654826	0.116143	-0.507990
C	1.188187	-0.271799	-0.367078
C	0.562030	-1.509516	-0.465177
C	-0.827049	-1.574852	-0.317870
C	-1.588373	-0.413070	-0.076773
C	-0.953039	0.835174	0.025424
C	0.437048	0.890810	-0.117477
H	1.053066	3.061640	0.140945
H	3.525925	2.228570	-0.236454
H	1.131932	-2.421803	-0.642930
H	-1.329590	-2.539700	-0.387659
H	-1.517310	1.745343	0.214493
H	2.998405	-0.068444	-1.541370
C	3.559858	-0.618917	0.386133
N	4.283546	-1.203054	1.080888
S	-3.351137	-0.651777	0.082984
C	-3.984877	1.026830	0.413926
H	-3.572811	1.433230	1.345677
H	-3.785685	1.703930	-0.425772
H	-5.068977	0.909300	0.525880

$MeSO_2$-1-CN-IND

Total energy (hartree): -1027.970794

Sum of electronic and thermal Free Energies (hartree): -1027.836697

C	-2.093765	2.037860	-0.096116
C	-3.303922	1.511471	0.175859
C	-3.171442	0.037171	0.545005
C	-1.678645	-0.216777	0.369750
C	-0.949248	-1.390530	0.511131
C	0.438892	-1.342787	0.313941
C	1.044314	-0.125495	-0.012072
C	0.322973	1.061523	-0.174353
C	-1.059180	1.001435	0.018807
H	-1.898705	3.074237	-0.364790
H	-4.261640	2.025615	0.164003
H	-1.436164	-2.335843	0.750093
H	1.045016	-2.244378	0.383612
H	0.831064	1.978518	-0.468441
H	-3.447712	-0.103268	1.605305
C	-4.029208	-0.853266	-0.247427
N	-4.715388	-1.560124	-0.860823
S	2.844592	-0.086092	-0.253076
O	3.289402	-1.459134	-0.633531
O	3.162980	1.093121	-1.112121
C	3.501935	0.258054	1.406914
H	4.590362	0.290512	1.287093
H	3.113397	1.225490	1.740304
H	3.203350	-0.556408	2.074368

$MeSO_2$-2-CN-IND

Total energy (hartree): -1027.971341

Sum of electronic and thermal Free Energies (hartree): -1027.837239

C	2.108663	2.031402	0.108176
C	3.323798	1.489252	-0.103863
C	3.190018	0.019366	-0.489802
C	1.685903	-0.212456	-0.400686
C	0.945727	-1.366537	-0.624269
C	-0.450715	-1.297375	-0.511085
C	-1.052688	-0.080314	-0.177760
C	-0.323033	1.091481	0.045490
C	1.067035	1.010347	-0.065633
H	1.914260	3.069661	0.369904
H	4.286745	1.989452	-0.038843
H	1.428088	-2.309000	-0.882856
H	-1.070799	-2.171063	-0.704148
H	-0.836689	2.024370	0.272089
H	3.525586	-0.121838	-1.532470
C	3.982651	-0.887281	0.351034

N	4.613945	-1.605944	1.008211
S	-2.862996	-0.013682	-0.038255
O	-3.280904	1.406835	-0.232923
O	-3.430623	-1.105321	-0.883525
C	-3.187317	-0.443644	1.697807
H	-4.276833	-0.408826	1.806821
H	-2.804778	-1.452251	1.883425
H	-2.703307	0.302463	2.335819

NH_2-CN-IND

Total energy (hartree): -495.415180

Sum of electronic and thermal Free Energies (hartree): -495.295515

C	-0.768509	2.027849	-0.071869
C	-1.984556	1.525283	0.220708
C	-1.876929	0.039900	0.556781
C	-0.394177	-0.237656	0.345557
C	0.340044	-1.410969	0.463149
C	1.720643	-1.374710	0.237010
C	2.373493	-0.172023	-0.104160
C	1.622570	1.014060	-0.225311
C	0.246740	0.967595	-0.003641
H	-0.560166	3.066277	-0.324974
H	-2.929916	2.061961	0.240853
H	-0.140183	-2.356075	0.718538
H	2.303748	-2.293186	0.317113
H	2.114615	1.948753	-0.498348
H	-2.151838	-0.118142	1.614896
C	-2.769721	-0.804897	-0.249191
N	-3.482525	-1.477656	-0.871545
N	3.742075	-0.171288	-0.385268
H	4.213135	0.719080	-0.296301
H	4.276161	-0.932650	0.011711

$NHNH_2$-1-CN-IND

Total energy (hartree): -550.739226

Sum of electronic and thermal Free Energies (hartree): -550.604154

C	-1.380875	2.013061	-0.061345
C	-2.542781	1.398531	0.237359
C	-2.295529	-0.072669	0.562591
C	-0.794865	-0.211310	0.337738
C	0.047355	-1.309676	0.446707
C	1.419812	-1.150827	0.213601
C	1.948217	0.108502	-0.129369
C	1.091861	1.224023	-0.236210
C	-0.271594	1.050804	-0.008790
H	-1.271995	3.067852	-0.309202

H	-3.533595	1.845160	0.267861
H	-0.342036	-2.295730	0.702625
H	2.094069	-1.999641	0.289128
H	1.493845	2.202903	-0.504027
H	-2.545467	-0.262224	1.621673
C	-3.114432	-0.990366	-0.242158
N	-3.769607	-1.719935	-0.863892
N	3.307954	0.279527	-0.432092
H	3.621484	1.241805	-0.353679
N	4.213110	-0.691291	0.048600
H	4.632567	-0.411632	0.935693
H	4.947910	-0.827033	-0.639133

$NHNH_2$-2-CN-IND

Total energy (hartree): -550.739820

Sum of electronic and thermal Free Energies (hartree): -550.604703

C	1.030545	2.024960	-0.034782
C	2.295809	1.600867	-0.224831
C	2.313611	0.099894	-0.504321
C	0.842176	-0.274366	-0.379964
C	0.200578	-1.502295	-0.489597
C	-1.189851	-1.552885	-0.348663
C	-1.942847	-0.383740	-0.107707
C	-1.291271	0.857329	0.011733
C	0.097248	0.893023	-0.124312
H	0.732835	3.054344	0.158681
H	3.201239	2.202535	-0.207153
H	0.760070	-2.421129	-0.667423
H	-1.703412	-2.512506	-0.430337
H	-1.871936	1.755220	0.206737
H	2.670465	-0.078628	-1.534268
C	3.202663	-0.649148	0.394932
N	3.912611	-1.246500	1.093037
N	-3.341098	-0.491203	-0.046973
H	-3.663033	-1.428349	0.173835
N	-4.045948	0.553516	0.590828
H	-4.225643	0.343429	1.573168
H	-4.931505	0.692562	0.113596

NMe_2-CN-IND

Total energy (hartree): -574.027127

Sum of electronic and thermal Free Energies (hartree): -573.855889

C	1.549370	2.020214	-0.018825
C	2.766759	1.492116	-0.255153
C	2.649338	-0.004948	-0.533378
C	1.157798	-0.253890	-0.354264

C	0.402992	-1.414816	-0.451093
C	-0.982491	-1.352268	-0.268081
C	-1.641529	-0.127682	0.020549
C	-0.857165	1.051933	0.106191
C	0.522264	0.969813	-0.072516
H	1.347739	3.070826	0.185033
H	3.719159	2.016394	-0.269602
H	0.870189	-2.377380	-0.661933
H	-1.552170	-2.273508	-0.348916
H	-1.313222	2.016120	0.313765
H	2.954154	-0.210334	-1.575084
C	3.506647	-0.825659	0.334013
N	4.191809	-1.479943	1.005340
N	-3.012160	-0.088138	0.227867
C	-3.815228	-1.270343	-0.034885
H	-4.861433	-1.049111	0.196741
H	-3.755990	-1.598854	-1.088299
H	-3.503884	-2.110160	0.603268
C	-3.682781	1.195655	0.340177
H	-3.568202	1.814966	-0.567909
H	-4.750785	1.027303	0.507641
H	-3.298951	1.769555	1.196440

NO-1-CN-IND

Total energy (hartree): -569.357742

Sum of electronic and thermal Free Energies (hartree): -569.259127

C	-1.252888	2.032755	-0.098048
C	-2.420688	1.423920	0.186131
C	-2.182286	-0.040630	0.540988
C	-0.678443	-0.191000	0.345155
C	0.132245	-1.316930	0.486920
C	1.505797	-1.178349	0.280391
C	2.035690	0.078726	-0.061069
C	1.224046	1.212402	-0.211189
C	-0.148980	1.067545	-0.007709
H	-1.132259	3.082490	-0.358570
H	-3.411274	1.871478	0.192810
H	-0.293280	-2.287055	0.744140
H	2.183238	-2.025271	0.376273
H	1.683182	2.163109	-0.481681
H	-2.433298	-0.209058	1.603595
C	-2.984964	-0.982442	-0.249900
N	-3.625547	-1.729353	-0.865184
N	3.444161	0.311480	-0.288133
O	4.162028	-0.663320	-0.159171

NO-2-CN-IND

Total energy (hartree): -569.358216

Sum of electronic and thermal Free Energies (hartree): -569.259507

C	0.944780	2.039046	0.024929
C	2.194664	1.598247	-0.215594
C	2.182692	0.104530	-0.526946
C	0.712219	-0.259283	-0.355947
C	0.081542	-1.490826	-0.472027
C	-1.307313	-1.537503	-0.290807
C	-2.021299	-0.365448	-0.003801
C	-1.386691	0.883408	0.120709
C	-0.008043	0.923243	-0.054329
H	0.667700	3.067467	0.248416
H	3.109460	2.185635	-0.217204
H	0.644262	-2.398740	-0.687653
H	-1.858940	-2.474279	-0.366614
H	-1.978651	1.768059	0.350120
H	2.483041	-0.057968	-1.577469
C	3.093712	-0.684926	0.312106
N	3.820687	-1.310819	0.965227
N	-3.444836	-0.551729	0.154105
O	-4.076926	0.460592	0.398165

NO_2-CN-IND

Total energy (hartree): -644.582826

Sum of electronic and thermal Free Energies (hartree): -644.479659

C	1.445486	2.038778	0.019872
C	2.658451	1.501194	-0.214356
C	2.530444	0.012514	-0.522980
C	1.035639	-0.233316	-0.358179
C	0.303734	-1.408509	-0.475400
C	-1.085218	-1.352400	-0.303542
C	-1.688761	-0.123508	-0.022838
C	-0.970324	1.068974	0.105425
C	0.412344	0.997868	-0.062800
H	1.247131	3.085808	0.240195
H	3.616145	2.015515	-0.212707
H	0.788805	-2.360931	-0.686836
H	-1.702524	-2.243227	-0.382834
H	-1.489399	1.997137	0.329738
H	2.821420	-0.173628	-1.572206
C	3.373227	-0.844286	0.321109
N	4.045503	-1.524533	0.978344
N	-3.157268	-0.081509	0.150252
O	-3.777981	-1.134929	0.037058
O	-3.670689	1.007149	0.396269

OCF_3-1-CN-IND

Total energy (hartree): -852.361967

Sum of electronic and thermal Free Energies (hartree): -852.256190

C	1.842636	2.001335	-0.048201
C	3.136387	1.660553	-0.210414
C	3.260479	0.164790	-0.484269
C	1.815834	-0.309290	-0.385811
C	1.270211	-1.580942	-0.507076
C	-0.117100	-1.728582	-0.399961
C	-0.924838	-0.608595	-0.177434
C	-0.396039	0.678271	-0.048479
C	0.992607	0.807719	-0.152142
H	1.471396	3.008075	0.134660
H	3.998883	2.321422	-0.176567
H	1.897403	-2.456660	-0.672397
H	-0.586981	-2.706767	-0.484468
H	-1.023948	1.546447	0.127644
H	3.638949	0.008684	-1.510021
C	4.181921	-0.525860	0.427872
N	4.918098	-1.075321	1.137337
O	-2.291283	-0.915908	-0.101764
C	-3.223744	0.028443	0.149797
F	-3.265668	0.998448	-0.797058
F	-3.043798	0.648457	1.341111
F	-4.415228	-0.579543	0.172682

OCF_3-2-CN-IND

Total energy (hartree): -852.361797

Sum of electronic and thermal Free Energies (hartree): -852.256087

C	-2.518744	2.002175	-0.149137
C	-3.633837	1.294908	0.119937
C	-3.275237	-0.133468	0.520491
C	-1.758533	-0.145674	0.371979
C	-0.840081	-1.166703	0.559941
C	0.527800	-0.903196	0.381643
C	0.932382	0.384579	0.018697
C	0.019471	1.424876	-0.179389
C	-1.334731	1.145633	-0.002215
H	-2.488966	3.051800	-0.435662
H	-4.660597	1.650641	0.086131
H	-1.158231	-2.172184	0.834675
H	1.248296	-1.702037	0.526637
H	0.379611	2.411305	-0.466256
H	-3.553226	-0.300344	1.576215
C	-3.964648	-1.157426	-0.276097

N	-4.515808	-1.971014	-0.893741
O	2.265972	0.771510	-0.179144
C	3.287333	-0.110012	-0.100078
F	3.180921	-1.126349	-0.988456
F	3.411282	-0.669475	1.128568
F	4.415458	0.559344	-0.365338

OCF_3-3-CN-IND

Total energy (hartree): -852.362205

Sum of electronic and thermal Free Energies (hartree): -852.256986

C	2.157875	2.029315	0.131379
C	3.378980	1.461710	0.080105
C	3.270097	0.006453	-0.365119
C	1.763732	-0.187717	-0.497710
C	1.030767	-1.313573	-0.848827
C	-0.365479	-1.207814	-0.928104
C	-0.978102	0.015362	-0.653290
C	-0.259053	1.159163	-0.305253
C	1.130456	1.041139	-0.221749
H	1.951383	3.064475	0.396631
H	4.332783	1.934966	0.299358
H	1.517276	-2.266922	-1.053907
H	-0.978933	-2.063518	-1.202996
H	-0.776045	2.096532	-0.110282
H	3.751657	-0.114028	-1.351730
C	3.918207	-0.940791	0.551603
N	4.440022	-1.692646	1.265375
O	-2.375707	0.117262	-0.823450
C	-3.158367	-0.071891	0.264915
F	-2.919141	0.829800	1.248416
F	-3.003610	-1.298239	0.817491
F	-4.433614	0.058526	-0.120885

OH-1-CN-IND

Total energy (hartree): -515.282992

Sum of electronic and thermal Free Energies (hartree): -515.175261

C	-0.765229	2.031000	-0.077591
C	-1.977982	1.521899	0.216731
C	-1.862696	0.038410	0.557264
C	-0.378411	-0.233095	0.345430
C	0.354024	-1.405657	0.464059
C	1.737002	-1.365555	0.234958
C	2.365555	-0.158242	-0.106693
C	1.630762	1.029136	-0.232133
C	0.255437	0.976543	-0.007220
H	-0.561322	3.069546	-0.332729

H	-2.926147	2.053549	0.237040
H	-0.125054	-2.350857	0.720308
H	2.328400	-2.279155	0.319483
H	2.141693	1.952020	-0.502812
H	-2.132892	-0.117497	1.616767
C	-2.750468	-0.815839	-0.243768
N	-3.458194	-1.496458	-0.863148
O	3.714711	-0.077001	-0.336282
H	4.117018	-0.947996	-0.231979

OH-2-CN-IND

Total energy (hartree): -515.282679

Sum of electronic and thermal Free Energies (hartree): -515.174964

C	-0.749656	2.030842	-0.071642
C	-1.966613	1.530959	0.221833
C	-1.861922	0.045655	0.556766
C	-0.379818	-0.236762	0.344543
C	0.345637	-1.416723	0.462380
C	1.726439	-1.390757	0.236237
C	2.365114	-0.188112	-0.102794
C	1.640149	1.005705	-0.227365
C	0.261357	0.967182	-0.004073
H	-0.538109	3.068731	-0.323762
H	-2.910469	2.070074	0.243784
H	-0.142682	-2.357651	0.716967
H	2.325600	-2.296616	0.315427
H	2.143158	1.936776	-0.495209
H	-2.133211	-0.112293	1.615706
C	-2.756885	-0.797356	-0.248105
N	-3.471443	-1.467234	-0.871297
O	3.719860	-0.246274	-0.305066
H	4.054117	0.628019	-0.539988

OMe-1-CN-IND

Total energy (hartree): -554.583688

Sum of electronic and thermal Free Energies (hartree): -554.449898

C	0.997543	2.023942	-0.006047
C	2.262720	1.616763	-0.230772
C	2.289968	0.118952	-0.522621
C	0.826624	-0.274437	-0.364669
C	0.199495	-1.512454	-0.474725
C	-1.184572	-1.584272	-0.306173
C	-1.937533	-0.426467	-0.030907
C	-1.311045	0.824629	0.084434
C	0.077862	0.880442	-0.082344
H	0.692654	3.048041	0.203620

H	3.161117	2.228956	-0.229740
H	0.768608	-2.419715	-0.678695
H	-1.709301	-2.535660	-0.380527
H	-1.874215	1.728974	0.300573
H	2.619610	-0.047044	-1.563644
C	3.210796	-0.627325	0.345920
N	3.946867	-1.220453	1.019866
O	-3.281644	-0.626217	0.110623
C	-4.104199	0.498345	0.402897
H	-3.819919	0.962532	1.359862
H	-4.055211	1.248887	-0.401184
H	-5.124214	0.109234	0.475728

OMe-2-CN-IND

Total energy (hartree): -554.583814

Sum of electronic and thermal Free Energies (hartree): -554.450025

C	-1.392665	2.013270	-0.101886
C	-2.551151	1.386014	0.182176
C	-2.290846	-0.074101	0.544854
C	-0.783041	-0.194869	0.358092
C	0.065070	-1.280104	0.503103
C	1.444485	-1.107520	0.294183
C	1.953077	0.154367	-0.056286
C	1.092963	1.257483	-0.208136
C	-0.270241	1.070266	-0.002896
H	-1.292857	3.064120	-0.368394
H	-3.548938	1.817928	0.181536
H	-0.318047	-2.266294	0.766561
H	2.104577	-1.963674	0.405232
H	1.511859	2.224010	-0.484889
H	-2.561206	-0.244551	1.602017
C	-3.074269	-1.023481	-0.258073
N	-3.699747	-1.778985	-0.879231
O	3.276564	0.413476	-0.275884
C	4.207144	-0.657057	-0.150243
H	4.207022	-1.068457	0.870841
H	3.992171	-1.459606	-0.872301
H	5.187983	-0.223994	-0.368241

SH-CN-IND

Total energy (hartree): -838.255821

Sum of electronic and thermal Free Energies (hartree): -838.154997

C	-1.189280	2.031714	-0.069675
C	-2.405514	1.512644	0.190485
C	-2.287243	0.030064	0.533023
C	-0.795541	-0.229533	0.362378

C	-0.057144	-1.397103	0.502128
C	1.330225	-1.345877	0.313212
C	1.967114	-0.134822	-0.010153
C	1.219451	1.045027	-0.155482
C	-0.163340	0.984369	0.028918
H	-0.986705	3.072131	-0.318277
H	-3.358226	2.036363	0.184710
H	-0.535821	-2.346213	0.744233
H	1.920077	-2.256707	0.415748
H	1.705020	1.986970	-0.409347
H	-2.581662	-0.129361	1.585561
C	-3.145739	-0.831690	-0.291125
N	-3.831555	-1.516326	-0.930192
S	3.744582	-0.179186	-0.223617
H	3.906963	1.129315	-0.535667

SiH_3-CN-IND

Total energy (hartree): -730.753260

Sum of electronic and thermal Free Energies (hartree): -730.638444

C	1.231396	2.032764	0.078779
C	2.447892	1.512211	-0.176872
C	2.327248	0.031331	-0.526422
C	0.833335	-0.226997	-0.362513
C	0.101073	-1.395480	-0.510851
C	-1.290291	-1.337581	-0.327494
C	-1.947908	-0.134636	-0.002469
C	-1.181525	1.039915	0.147356
C	0.202522	0.989155	-0.028585
H	1.029988	3.072742	0.330133
H	3.402042	2.033061	-0.164595
H	0.585480	-2.341685	-0.753840
H	-1.869326	-2.255050	-0.440348
H	-1.660492	1.987324	0.402438
H	2.619946	-0.125346	-1.579792
C	3.180034	-0.839183	0.293671
N	3.862018	-1.529539	0.930632
Si	-3.825843	-0.101166	0.234951
H	-4.174091	0.335856	1.621580
H	-4.370538	-1.470555	-0.004459
H	-4.457989	0.857765	-0.722446

$SiMe_3$-CN-IND

Total energy (hartree): -848.745922

Sum of electronic and thermal Free Energies (hartree): -848.551657

C	2.194160	2.023382	0.068507
C	3.415761	1.500548	-0.156935

C	3.299563	0.020680	-0.513388
C	1.800777	-0.232933	-0.389992
C	1.065986	-1.396746	-0.561475
C	-0.329755	-1.331475	-0.414424
C	-0.997619	-0.130180	-0.102740
C	-0.223360	1.036738	0.070480
C	1.164929	0.983429	-0.068731
H	1.989835	3.063411	0.317568
H	4.370779	2.018485	-0.118213
H	1.551979	-2.344622	-0.795054
H	-0.903971	-2.248738	-0.546691
H	-0.700972	1.987317	0.317175
H	3.620995	-0.135023	-1.558444
C	4.127563	-0.853291	0.328277
N	4.790648	-1.546214	0.982338
Si	-2.891612	-0.055147	0.097213
C	-3.642777	-1.761298	-0.230487
H	-3.269605	-2.517715	0.474776
H	-4.735800	-1.718545	-0.117335
H	-3.431939	-2.115459	-1.249774
C	-3.592468	1.202201	-1.137108
H	-4.683320	1.294564	-1.028787
H	-3.159910	2.201867	-0.985289
H	-3.382241	0.904460	-2.174313
C	-3.305319	0.498785	1.862300
H	-2.880768	1.488368	2.085973
H	-4.393464	0.565386	2.009858
H	-2.908208	-0.207236	2.605497

tBu-1-CN-IND

Total energy (hartree): -597.314011

Sum of electronic and thermal Free Energies (hartree): -597.104273

C	1.829392	2.020287	0.070662
C	3.051961	1.505716	-0.168589
C	2.942347	0.025210	-0.526134
C	1.446780	-0.236682	-0.388339
C	0.708685	-1.397129	-0.551958
C	-0.686099	-1.338220	-0.388942
C	-1.352806	-0.143111	-0.067998
C	-0.578784	1.023279	0.097449
C	0.805667	0.973712	-0.057818
H	1.621399	3.058657	0.323811
H	4.003724	2.030148	-0.138559
H	1.188667	-2.346097	-0.792565
H	-1.249665	-2.258764	-0.517140
H	-1.054010	1.970003	0.351756

H	3.257476	-0.127115	-1.573538
C	3.783584	-0.843030	0.308627
N	4.456915	-1.531706	0.956750
C	-2.880205	-0.069214	0.113361
C	-3.201410	0.402175	1.550811
H	-2.786152	1.397023	1.755563
H	-4.289275	0.455741	1.699151
H	-2.788556	-0.294922	2.292445
C	-3.563318	-1.430415	-0.110038
H	-4.647540	-1.322805	0.027221
H	-3.394226	-1.810875	-1.126422
H	-3.213332	-2.186809	0.605283
C	-3.468525	0.938081	-0.901926
H	-3.251944	0.626767	-1.932855
H	-4.559695	1.000596	-0.785477
H	-3.058890	1.946431	-0.760940

tBu-2-CN-IND

Total energy (hartree): -597.314011

Sum of electronic and thermal Free Energies (hartree): -597.104270

C	1.829392	2.020286	0.070659
C	3.051961	1.505716	-0.168590
C	2.942347	0.025208	-0.526132
C	1.446780	-0.236683	-0.388337
C	0.708684	-1.397130	-0.551958
C	-0.686101	-1.338220	-0.388944
C	-1.352808	-0.143110	-0.068000
C	-0.578784	1.023278	0.097451
C	0.805667	0.973711	-0.057816
H	1.621399	3.058657	0.323804
H	4.003725	2.030147	-0.138563
H	1.188665	-2.346099	-0.792563
H	-1.249667	-2.258763	-0.517142
H	-1.054010	1.970002	0.351756
H	3.257477	-0.127115	-1.573536
C	3.783589	-0.843033	0.308623
N	4.456924	-1.531697	0.956752
C	-2.880208	-0.069213	0.113361
C	-3.468528	0.938082	-0.901926
H	-3.251949	0.626770	-1.932857
H	-4.559698	1.000597	-0.785478
H	-3.058896	1.946432	-0.760940
C	-3.201411	0.402175	1.550813
H	-4.289277	0.455740	1.699153
H	-2.788556	-0.294921	2.292446
H	-2.786155	1.397023	1.755565

C	-3.563319	-1.430416	-0.110037
H	-3.213333	-2.186808	0.605285
H	-4.647540	-1.322805	0.027220
H	-3.394227	-1.810878	-1.126421

tBu-3-CN-IND

Total energy (hartree): -597.314011

Sum of electronic and thermal Free Energies (hartree): -597.104281

C	1.829392	2.020289	0.070654
C	3.051961	1.505715	-0.168588
C	2.942344	0.025209	-0.526129
C	1.446778	-0.236679	-0.388333
C	0.708685	-1.397126	-0.551962
C	-0.686101	-1.338219	-0.388945
C	-1.352806	-0.143111	-0.067997
C	-0.578785	1.023281	0.097449
C	0.805666	0.973714	-0.057815
H	1.621401	3.058662	0.323794
H	4.003725	2.030147	-0.138562
H	1.188666	-2.346093	-0.792577
H	-1.249667	-2.258761	-0.517151
H	-1.054016	1.970003	0.351752
H	3.257479	-0.127122	-1.573532
C	3.783577	-0.843034	0.308634
N	4.456927	-1.531704	0.956743
C	-2.880206	-0.069214	0.113360
C	-3.563314	-1.430420	-0.110031
H	-3.213324	-2.186807	0.605295
H	-4.647535	-1.322811	0.027227
H	-3.394221	-1.810887	-1.126413
C	-3.468529	0.938076	-0.901929
H	-4.559699	1.000591	-0.785473
H	-3.058894	1.946426	-0.760949
H	-3.251956	0.626756	-1.932858
C	-3.201408	0.402179	1.550813
H	-2.786137	1.397022	1.755562
H	-4.289273	0.455760	1.699147
H	-2.788565	-0.294924	2.292445

Vin-1-CN-IND

Total energy (hartree): -517.453920

Sum of electronic and thermal Free Energies (hartree): -517.319332

C	0.981515	2.030092	0.008543
C	2.238542	1.601502	-0.219279
C	2.242211	0.104723	-0.519550
C	0.772632	-0.267426	-0.359531

C	0.133264	-1.493108	-0.471177
C	-1.257271	-1.536125	-0.298368
C	-2.011800	-0.379011	-0.019518
C	-1.341712	0.857563	0.094743
C	0.040063	0.904363	-0.071157
H	0.695181	3.058343	0.223204
H	3.147325	2.198176	-0.216944
H	0.689518	-2.407558	-0.678037
H	-1.773493	-2.493233	-0.379884
H	-1.895783	1.769196	0.314924
H	2.561366	-0.062481	-1.563635
C	3.152788	-0.664937	0.338884
N	3.880691	-1.275834	1.005575
C	-3.471187	-0.512578	0.145054
H	-3.850484	-1.532646	0.039305
C	-4.355020	0.463797	0.403620
H	-4.066391	1.508163	0.524106
H	-5.416233	0.239744	0.504352

Vin-2-CN-IND

Total energy (hartree): -517.453776

Sum of electronic and thermal Free Energies (hartree): -517.319198

C	-1.306305	2.018455	-0.090138
C	-2.477351	1.410501	0.184790
C	-2.241541	-0.056115	0.536334
C	-0.735729	-0.201857	0.352351
C	0.090940	-1.311322	0.494285
C	1.465878	-1.154463	0.292881
C	2.026451	0.095391	-0.047283
C	1.171470	1.205994	-0.190521
C	-0.202196	1.053391	0.005282
H	-1.186072	3.069462	-0.347373
H	-3.467592	1.859066	0.185117
H	-0.316528	-2.290123	0.748136
H	2.112702	-2.023656	0.401065
H	1.588759	2.178062	-0.456917
H	-2.509932	-0.230071	1.593576
C	-3.038144	-0.989768	-0.271109
N	-3.674702	-1.731393	-0.897460
C	3.473193	0.285909	-0.262948
H	3.763698	1.307658	-0.522943
C	4.441735	-0.638995	-0.176265
H	4.245846	-1.681167	0.076238
H	5.481632	-0.372206	-0.360629