Supporting Information

Hammett Neural Networks: Prediction of Frontier Orbital Energies of Tungsten-Benzylidyne Photoredox Complexes

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I. Derivation of Free-Energy Relation to Rate Constants

Hammett Equation:

$$\sigma\rho = \log\left(\frac{K}{K_0}\right)$$

Change in free energy between substituted and unsubstituted forms:

$$\Delta\Delta G^\circ = -RT\ln K + RT\ln K_0$$

Relating the equations:

$$-\frac{\Delta\Delta G^\circ}{2.303RT} = \log\left(\frac{K}{K_0}\right) = \sigma\rho$$

Note, the relation between substituent and reaction constants, σ and ρ, with temperature and solvent independent terms can be found elsewhere[1].

II. Redox-Active Orbital Visualization

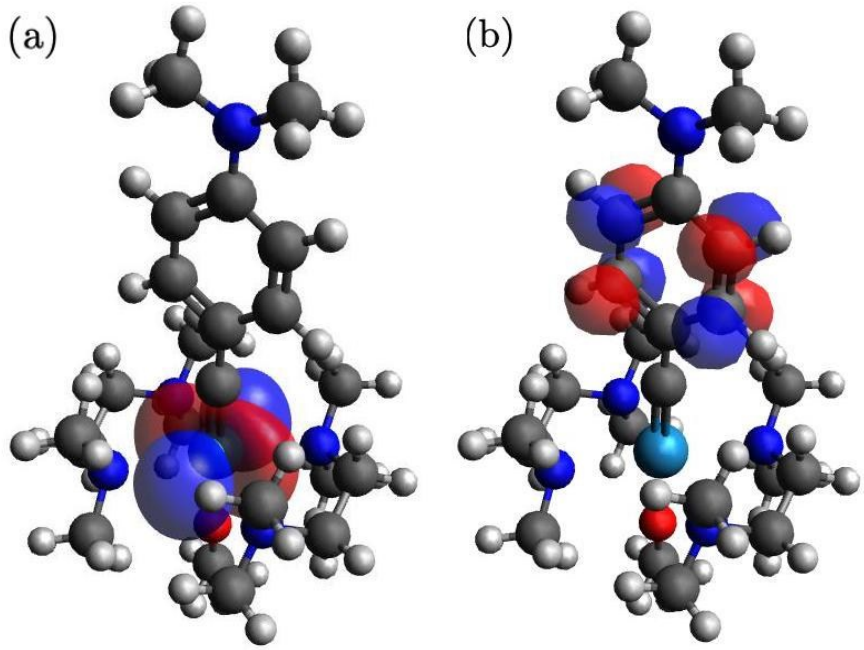

Figure S1(a-b). Visualizations of orbitals d_{xy} (**S1a**), which is usually the HOMO, and π^* (**S1b**), which is usually the LUMO, for molecule **513** in Avogadro 1.2.0.3.

III. Input Parameters

A. Atomic Coordinate HOMO and Atomic Coordinate HOMO-LUMO Gap Sets without labels (Sets **1A/1B)**

RLX	R Per	R Val	L_1 Per	L_1 Val	L_2 Per	L_2 Val	L_3 Per	L_3 Val	X Per	X Val
111	1	1	2	5	2	5	2	5	1	7
112	1	1	2	5	2	5	2	5	2	7
113	1	1	2	5	2	5	2	5	2	6
114	1	1	2	5	2	5	2	5	3	6
115	1	1	2	5	2	5	2	5	2	5
121	1	1	3	5	3	5	3	5	1	7
122	1	1	3	5	3	5	3	5	2	7
123	1	1	3	5	3	5	3	5	2	6
124	1	1	3	5	3	5	3	5	3	6
125	1	1	3	5	3	5	3	5	2	5
131	1	1	4	5	4	5	4	5	1	7
132	1	1	4	5	4	5	4	5	2	7
133	1	1	4	5	4	5	4	5	2	6
134	1	1	4	5	4	5	4	5	3	6
135	1	1	4	5	4	5	4	5	2	5
141	1	1	3	6	3	6	3	6	1	7
142	1	1	3	6	3	6	3	6	2	7
143	1	1	3	6	3	6	3	6	2	6
144	1	1	3	6	3	6	3	6	3	6
145	1	1	3	6	3	6	3	6	2	5
151	1	1	2	5	3	5	3	5	1	7
152	1	1	2	5	3	5	3	5	2	7
153	1	1	2	5	3	5	3	5	2	6
154	1	1	2	5	3	5	3	5	3	6
155	1	1	2	5	3	5	3	5	2	5
161	1	1	2	5	3	5	2	5	1	7
162	1	1	2	5	3	5	2	5	2	7
163	1	1	2	5	3	5	2	5	2	6
164	1	1	2	5	3	5	2	5	3	6
165	1	1	2	5	3	5	2	5	2	5
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215	2	4	2	5	2	5	2	5	2	5
221	2	4	3	5	3	5	3	5	1	7
222	2	4	3	5	3	5	3	5	2	7
223	2	4	3	5	3	5	3	5	2	6
224	2	4	3	5	3	5	3	5	3	6
225	2	4	3	5	3	5	3	5	2	5
231	2	4	4	5	4	5	4	5	1	7

232	2	4	4	5	4	5	4	5	2	7
233	2	4	4	5	4	5	4	5	2	6
234	2	4	4	5	4	5	4	5	3	6
235	2	4	4	5	4	5	4	5	2	5
241	2	4	3	6	3	6	3	6	1	7
242	2	4	3	6	3	6	3	6	2	7
243	2	4	3	6	3	6	3	6	2	6
244	2	4	3	6	3	6	3	6	3	6
245	2	4	3	6	3	6	3	6	2	5
251	2	4	2	5	3	5	3	5	1	7
252	2	4	2	5	3	5	3	5	2	7
253	2	4	2	5	3	5	3	5	2	6
254	2	4	2	5	3	5	3	5	3	6
255	2	4	2	5	3	5	3	5	2	5
261	2	4	2	5	3	5	2	5	1	7
262	2	4	2	5	3	5	2	5	2	7
263	2	4	2	5	3	5	2	5	2	6
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265	2	4	2	5	3	5	2	5	2	5
311	2	6	2	5	2	5	2	5	1	7
312	2	6	2	5	2	5	2	5	2	7
313	2	6	2	5	2	5	2	5	2	6
314	2	6	2	5	2	5	2	5	3	6
315	2	6	2	5	2	5	2	5	2	5
321	2	6	3	5	3	5	3	5	1	7
322	2	6	3	5	3	5	3	5	2	7
323	2	6	3	5	3	5	3	5	2	6
324	2	6	3	5	3	5	3	5	3	6
325	2	6	3	5	3	5	3	5	2	5
331	2	6	4	5	4	5	4	5	1	7
332	2	6	4	5	4	5	4	5	2	7
333	2	6	4	5	4	5	4	5	2	6
334	2	6	4	5	4	5	4	5	3	6
335	2	6	4	5	4	5	4	5	2	5
341	2	6	3	6	3	6	3	6	1	7
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343	2	6	3	6	3	6	3	6	2	6
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345	2	6	3	6	3	6	3	6	2	5
351	2	6	2	5	3	5	3	5	1	7
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355	2	6	2	5	3	5	3	5	2	5
361	2	6	2	5	3	5	2	5	1	7
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363	2	6	2	5	3	5	2	5	2	6
364	2	6	2	5	3	5	2	5	3	6
365	2	6	2	5	3	5	2	5	2	5

411	3	6	2	5	2	5	2	5	1	7
412	3	6	2	5	2	5	2	5	2	7
413	3	6	2	5	2	5	2	5	2	6
414	3	6	2	5	2	5	2	5	3	6
415	3	6	2	5	2	5	2	5	2	5
421	3	6	3	5	3	5	3	5	1	7
422	3	6	3	5	3	5	3	5	2	7
423	3	6	3	5	3	5	3	5	2	6
424	3	6	3	5	3	5	3	5	3	6
425	3	6	3	5	3	5	3	5	2	5
431	3	6	4	5	4	5	4	5	1	7
432	3	6	4	5	4	5	4	5	2	7
433	3	6	4	5	4	5	4	5	2	6
434	3	6	4	5	4	5	4	5	3	6
435	3	6	4	5	4	5	4	5	2	5
441	3	6	3	6	3	6	3	6	1	7
442	3	6	3	6	3	6	3	6	2	7
443	3	6	3	6	3	6	3	6	2	6
444	3	6	3	6	3	6	3	6	3	6
445	3	6	3	6	3	6	3	6	2	5
451	3	6	2	5	3	5	3	5	1	7
452	3	6	2	5	3	5	3	5	2	7
453	3	6	2	5	3	5	3	5	2	6
454	3	6	2	5	3	5	3	5	3	6
455	3	6	2	5	3	5	3	5	2	5
461	3	6	2	5	3	5	2	5	1	7
462	3	6	2	5	3	5	2	5	2	7
463	3	6	2	5	3	5	2	5	2	6
464	3	6	2	5	3	5	2	5	3	6
465	3	6	2	5	3	5	2	5	2	5
511	2	5	2	5	2	5	2	5	1	7
512	2	5	2	5	2	5	2	5	2	7
513	2	5	2	5	2	5	2	5	2	6
514	2	5	2	5	2	5	2	5	3	6
515	2	5	2	5	2	5	2	5	2	5
521	2	5	3	5	3	5	3	5	1	7
522	2	5	3	5	3	5	3	5	2	7
523	2	5	3	5	3	5	3	5	2	6
524	2	5	3	5	3	5	3	5	3	6
525	2	5	3	5	3	5	3	5	2	5
531	2	5	4	5	4	5	4	5	1	7
532	2	5	4	5	4	5	4	5	2	7
533	2	5	4	5	4	5	4	5	2	6
534	2	5	4	5	4	5	4	5	3	6
535	2	5	4	5	4	5	4	5	2	5
541	2	5	3	6	3	6	3	6	1	7
542	2	5	3	6	3	6	3	6	2	7
543	2	5	3	6	3	6	3	6	2	6
544	2	5	3	6	3	6	3	6	3	6

545	2	5	3	6	3	6	3	6	2	5
551	2	5	2	5	3	5	3	5	1	7
552	2	5	2	5	3	5	3	5	2	7
553	2	5	2	5	3	5	3	5	2	6
554	2	5	2	5	3	5	3	5	3	6
555	2	5	2	5	3	5	3	5	2	5
561	2	5	2	5	3	5	2	5	1	7
562	2	5	2	5	3	5	2	5	2	7
563	2	5	2	5	3	5	2	5	2	6
564	2	5	2	5	3	5	2	5	3	6
565	2	5	2	5	3	5	2	5	2	5

B. Hammett Constants HOMO and Hammett Constants HOMO-LUMO Gap Sets without labels (Sets **2A**/**2B)**

RLX	R σ_m	R σ_p	L_1 σ_m	L_1 σ_p	L_2 σ_m	L_2 σ_p	L_3 σ_m	L_3 σ_p	X σ_m	X σ_p
111	0	0	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	0.34	0.06
112	0	0	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	0.37	0.23
113	0	0	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	0.12	-0.27
114	0	0	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	0.15	0
115	0	0	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	-0.16	-0.83
121	0	0	0.10	0.13	0.10	0.13	0.10	0.13	0.34	0.06
122	0	0	0.10	0.13	0.10	0.13	0.10	0.13	0.37	0.23
123	0	0	0.10	0.13	0.10	0.13	0.10	0.13	0.12	-0.27
124	0	0	0.10	0.13	0.10	0.13	0.10	0.13	0.15	0
125	0	0	0.10	0.13	0.10	0.13	0.10	0.13	-0.16	-0.83
131	0	0	0.22	0	0.22	0	0.22	0	0.34	0.06
132	0	0	0.22	0	0.22	0	0.22	0	0.37	0.23
133	0	0	0.22	0	0.22	0	0.22	0	0.12	-0.27
134	0	0	0.22	0	0.22	0	0.22	0	0.15	0
135	0	0	0.22	0	0.22	0	0.22	0	-0.16	-0.83
141	0	0	0.18	0.03	0.18	0.03	0.18	0.03	0.34	0.06
142	0	0	0.18	0.03	0.18	0.03	0.18	0.03	0.37	0.23
143	0	0	0.18	0.03	0.18	0.03	0.18	0.03	0.12	-0.27
144	0	0	0.18	0.03	0.18	0.03	0.18	0.03	0.15	0
145	0	0	0.18	0.03	0.18	0.03	0.18	0.03	-0.16	-0.83
151	0	0	-0.23	-0.72	0.10	0.13	0.10	0.13	0.34	0.06
152	0	0	-0.23	-0.72	0.10	0.13	0.10	0.13	0.37	0.23
153	0	0	-0.23	-0.72	0.10	0.13	0.10	0.13	0.12	-0.27
154	0	0	-0.23	-0.72	0.10	0.13	0.10	0.13	0.15	0
155	0	0	-0.23	-0.72	0.10	0.13	0.10	0.13	-0.16	-0.83
161	0	0	-0.23	-0.72	0.10	0.13	-0.23	-0.72	0.34	0.06
162	0	0	-0.23	-0.72	0.10	0.13	-0.23	-0.72	0.37	0.23
163	0	0	-0.23	-0.72	0.10	0.13	-0.23	-0.72	0.12	-0.27
164	0	0	-0.23	-0.72	0.10	0.13	-0.23	-0.72	0.15	0
165	0	0	-0.23	-0.72	0.10	0.13	-0.23	-0.72	-0.16	-0.83
211	-0.07	-0.17	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	0.34	0.06
212	-0.07	-0.17	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	0.37	0.23
213	-0.07	-0.17	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	0.12	-0.27
214	-0.07	-0.17	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	0.15	0
215	-0.07	-0.17	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	-0.16	-0.83
221	-0.07	-0.17	0.10	0.13	0.10	0.13	0.10	0.13	0.34	0.06
222	-0.07	-0.17	0.10	0.13	0.10	0.13	0.10	0.13	0.37	0.23
223	-0.07	-0.17	0.10	0.13	0.10	0.13	0.10	0.13	0.12	-0.27
224	-0.07	-0.17	0.10	0.13	0.10	0.13	0.10	0.13	0.15	0
225	-0.07	-0.17	0.10	0.13	0.10	0.13	0.10	0.13	-0.16	-0.83
231	-0.07	-0.17	0.22	0	0.22	0	0.22	0	0.34	0.06
232	-0.07	-0.17	0.22	0	0.22	0	0.22	0	0.37	0.23
233	-0.07	-0.17	0.22	0	0.22	0	0.22	0	0.12	-0.27
234	-0.07	-0.17	0.22	0	0.22	0	0.22	0	0.15	0

235	-0.07	-0.17	0.22	0	0.22	0	0.22	0	-0.16	-0.83
241	-0.07	-0.17	0.18	0.03	0.18	0.03	0.18	0.03	0.34	0.06
242	-0.07	-0.17	0.18	0.03	0.18	0.03	0.18	0.03	0.37	0.23
243	-0.07	-0.17	0.18	0.03	0.18	0.03	0.18	0.03	0.12	-0.27
244	-0.07	-0.17	0.18	0.03	0.18	0.03	0.18	0.03	0.15	0
245	-0.07	-0.17	0.18	0.03	0.18	0.03	0.18	0.03	-0.16	-0.83
251	-0.07	-0.17	-0.23	-0.72	0.10	0.13	0.10	0.13	0.34	0.06
252	-0.07	-0.17	-0.23	-0.72	0.10	0.13	0.10	0.13	0.37	0.23
253	-0.07	-0.17	-0.23	-0.72	0.10	0.13	0.10	0.13	0.12	-0.27
254	-0.07	-0.17	-0.23	-0.72	0.10	0.13	0.10	0.13	0.15	0
255	-0.07	-0.17	-0.23	-0.72	0.10	0.13	0.10	0.13	-0.16	-0.83
261	-0.07	-0.17	-0.23	-0.72	0.10	0.13	-0.23	-0.72	0.34	0.06
262	-0.07	-0.17	-0.23	-0.72	0.10	0.13	-0.23	-0.72	0.37	0.23
263	-0.07	-0.17	-0.23	-0.72	0.10	0.13	-0.23	-0.72	0.12	-0.27
264	-0.07	-0.17	-0.23	-0.72	0.10	0.13	-0.23	-0.72	0.15	0
265	-0.07	-0.17	-0.23	-0.72	0.10	0.13	-0.23	-0.72	-0.16	-0.83
311	0.12	-0.27	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	0.34	0.06
312	0.12	-0.27	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	0.37	0.23
313	0.12	-0.27	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	0.12	-0.27
314	0.12	-0.27	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	0.15	0
315	0.12	-0.27	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	-0.16	-0.83
321	0.12	-0.27	0.10	0.13	0.10	0.13	0.10	0.13	0.34	0.06
322	0.12	-0.27	0.10	0.13	0.10	0.13	0.10	0.13	0.37	0.23
323	0.12	-0.27	0.10	0.13	0.10	0.13	0.10	0.13	0.12	-0.27
324	0.12	-0.27	0.10	0.13	0.10	0.13	0.10	0.13	0.15	0
325	0.12	-0.27	0.10	0.13	0.10	0.13	0.10	0.13	-0.16	-0.83
331	0.12	-0.27	0.22	0	0.22	0	0.22	0	0.34	0.06
332	0.12	-0.27	0.22	0	0.22	0	0.22	0	0.37	0.23
333	0.12	-0.27	0.22	0	0.22	0	0.22	0	0.12	-0.27
334	0.12	-0.27	0.22	0	0.22	0	0.22	0	0.15	0
335	0.12	-0.27	0.22	0	0.22	0	0.22	0	-0.16	-0.83
341	0.12	-0.27	0.18	0.03	0.18	0.03	0.18	0.03	0.34	0.06
342	0.12	-0.27	0.18	0.03	0.18	0.03	0.18	0.03	0.37	0.23
343	0.12	-0.27	0.18	0.03	0.18	0.03	0.18	0.03	0.12	-0.27
344	0.12	-0.27	0.18	0.03	0.18	0.03	0.18	0.03	0.15	0
345	0.12	-0.27	0.18	0.03	0.18	0.03	0.18	0.03	-0.16	-0.83
351	0.12	-0.27	-0.23	-0.72	0.10	0.13	0.10	0.13	0.34	0.06
352	0.12	-0.27	-0.23	-0.72	0.10	0.13	0.10	0.13	0.37	0.23
353	0.12	-0.27	-0.23	-0.72	0.10	0.13	0.10	0.13	0.12	-0.27
354	0.12	-0.27	-0.23	-0.72	0.10	0.13	0.10	0.13	0.15	0
355	0.12	-0.27	-0.23	-0.72	0.10	0.13	0.10	0.13	-0.16	-0.83
361	0.12	-0.27	-0.23	-0.72	0.10	0.13	-0.23	-0.72	0.34	0.06
362	0.12	-0.27	-0.23	-0.72	0.10	0.13	-0.23	-0.72	0.37	0.23
363	0.12	-0.27	-0.23	-0.72	0.10	0.13	-0.23	-0.72	0.12	-0.27
364	0.12	-0.27	-0.23	-0.72	0.10	0.13	-0.23	-0.72	0.15	0
365	0.12	-0.27	-0.23	-0.72	0.10	0.13	-0.23	-0.72	-0.16	-0.83
411	0.15	0	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	0.34	0.06
412	0.15	0	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	0.37	0.23
413	0.15	0	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	0.12	-0.27

414	0.15	0	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	0.15	0
415	0.15	0	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	-0.16	-0.83
421	0.15	0	0.10	0.13	0.10	0.13	0.10	0.13	0.34	0.06
422	0.15	0	0.10	0.13	0.10	0.13	0.10	0.13	0.37	0.23
423	0.15	0	0.10	0.13	0.10	0.13	0.10	0.13	0.12	-0.27
424	0.15	0	0.10	0.13	0.10	0.13	0.10	0.13	0.15	0
425	0.15	0	0.10	0.13	0.10	0.13	0.10	0.13	-0.16	-0.83
431	0.15	0	0.22	0	0.22	0	0.22	0	0.34	0.06
432	0.15	0	0.22	0	0.22	0	0.22	0	0.37	0.23
433	0.15	0	0.22	0	0.22	0	0.22	0	0.12	-0.27
434	0.15	0	0.22	0	0.22	0	0.22	0	0.15	0
435	0.15	0	0.22	0	0.22	0	0.22	0	-0.16	-0.83
441	0.15	0	0.18	0.03	0.18	0.03	0.18	0.03	0.34	0.06
442	0.15	0	0.18	0.03	0.18	0.03	0.18	0.03	0.37	0.23
443	0.15	0	0.18	0.03	0.18	0.03	0.18	0.03	0.12	-0.27
444	0.15	0	0.18	0.03	0.18	0.03	0.18	0.03	0.15	0
445	0.15	0	0.18	0.03	0.18	0.03	0.18	0.03	-0.16	-0.83
451	0.15	0	-0.23	-0.72	0.10	0.13	0.10	0.13	0.34	0.06
452	0.15	0	-0.23	-0.72	0.10	0.13	0.10	0.13	0.37	0.23
453	0.15	0	-0.23	-0.72	0.10	0.13	0.10	0.13	0.12	-0.27
454	0.15	0	-0.23	-0.72	0.10	0.13	0.10	0.13	0.15	0
455	0.15	0	-0.23	-0.72	0.10	0.13	0.10	0.13	-0.16	-0.83
461	0.15	0	-0.23	-0.72	0.10	0.13	-0.23	-0.72	0.34	0.06
462	0.15	0	-0.23	-0.72	0.10	0.13	-0.23	-0.72	0.37	0.23
463	0.15	0	-0.23	-0.72	0.10	0.13	-0.23	-0.72	0.12	-0.27
464	0.15	0	-0.23	-0.72	0.10	0.13	-0.23	-0.72	0.15	0
465	0.15	0	-0.23	-0.72	0.10	0.13	-0.23	-0.72	-0.16	-0.83
511	-0.16	-0.83	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	0.34	0.06
512	-0.16	-0.83	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	0.37	0.23
513	-0.16	-0.83	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	0.12	-0.27
514	-0.16	-0.83	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	0.15	0
515	-0.16	-0.83	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	-0.16	-0.83
521	-0.16	-0.83	0.10	0.13	0.10	0.13	0.10	0.13	0.34	0.06
522	-0.16	-0.83	0.10	0.13	0.10	0.13	0.10	0.13	0.37	0.23
523	-0.16	-0.83	0.10	0.13	0.10	0.13	0.10	0.13	0.12	-0.27
524	-0.16	-0.83	0.10	0.13	0.10	0.13	0.10	0.13	0.15	0
525	-0.16	-0.83	0.10	0.13	0.10	0.13	0.10	0.13	-0.16	-0.83
531	-0.16	-0.83	0.22	0	0.22	0	0.22	0	0.34	0.06
532	-0.16	-0.83	0.22	0	0.22	0	0.22	0	0.37	0.23
533	-0.16	-0.83	0.22	0	0.22	0	0.22	0	0.12	-0.27
534	-0.16	-0.83	0.22	0	0.22	0	0.22	0	0.15	0
535	-0.16	-0.83	0.22	0	0.22	0	0.22	0	-0.16	-0.83
541	-0.16	-0.83	0.18	0.03	0.18	0.03	0.18	0.03	0.34	0.06
542	-0.16	-0.83	0.18	0.03	0.18	0.03	0.18	0.03	0.37	0.23
543	-0.16	-0.83	0.18	0.03	0.18	0.03	0.18	0.03	0.12	-0.27
544	-0.16	-0.83	0.18	0.03	0.18	0.03	0.18	0.03	0.15	0
545	-0.16	-0.83	0.18	0.03	0.18	0.03	0.18	0.03	-0.16	-0.83
551	-0.16	-0.83	-0.23	-0.72	0.10	0.13	0.10	0.13	0.34	0.06
552	-0.16	-0.83	-0.23	-0.72	0.10	0.13	0.10	0.13	0.37	0.23

553	-0.16	-0.83	-0.23	-0.72	0.10	0.13	0.10	0.13	0.12	-0.27
554	-0.16	-0.83	-0.23	-0.72	0.10	0.13	0.10	0.13	0.15	0
555	-0.16	-0.83	-0.23	-0.72	0.10	0.13	0.10	0.13	-0.16	-0.83
561	-0.16	-0.83	-0.23	-0.72	0.10	0.13	-0.23	-0.72	0.34	0.06
562	-0.16	-0.83	-0.23	-0.72	0.10	0.13	-0.23	-0.72	0.37	0.23
563	-0.16	-0.83	-0.23	-0.72	0.10	0.13	-0.23	-0.72	0.12	-0.27
564	-0.16	-0.83	-0.23	-0.72	0.10	0.13	-0.23	-0.72	0.15	0
565	-0.16	-0.83	-0.23	-0.72	0.10	0.13	-0.23	-0.72	-0.16	-0.83

C. Hammett Constants HOMO and Hammett Constants HOMO-LUMO Gap Smaller Sets without labels (Sets **3A**/**3B**)

This set of 30 molecules was systematically selected such that each option at each site would appear an equal number of times and that each pair of options between sites are seen in at least one molecule.

RLX	**R** σ_m	**R** σ_p	**L$_1$** σ_m	**L$_1$** σ_p	**L$_2$** σ_m	**L$_2$** σ_p	**L$_3$** σ_m	**L$_3$** σ_p	**X** σ_m	**X** σ_p
111	0	0	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	0.34	0.06
122	0	0	0.10	0.13	0.10	0.13	0.10	0.13	0.37	0.23
133	0	0	0.22	0	0.22	0	0.22	0	0.12	-0.27
144	0	0	0.18	0.03	0.18	0.03	0.18	0.03	0.15	0
155	0	0	-0.23	-0.72	0.10	0.13	0.10	0.13	-0.16	-0.83
161	0	0	-0.23	-0.72	0.10	0.13	-0.23	-0.72	0.34	0.06
212	-0.07	-0.17	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	0.37	0.23
223	-0.07	-0.17	0.10	0.13	0.10	0.13	0.10	0.13	0.12	-0.27
234	-0.07	-0.17	0.22	0	0.22	0	0.22	0	0.15	0
245	-0.07	-0.17	0.18	0.03	0.18	0.03	0.18	0.03	-0.16	-0.83
251	-0.07	-0.17	-0.23	-0.72	0.10	0.13	0.10	0.13	0.34	0.06
262	-0.07	-0.17	-0.23	-0.72	0.10	0.13	-0.23	-0.72	0.37	0.23
313	0.12	-0.27	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	0.12	-0.27
324	0.12	-0.27	0.10	0.13	0.10	0.13	0.10	0.13	0.15	0
335	0.12	-0.27	0.22	0	0.22	0	0.22	0	-0.16	-0.83
341	0.12	-0.27	0.18	0.03	0.18	0.03	0.18	0.03	0.34	0.06
352	0.12	-0.27	-0.23	-0.72	0.10	0.13	0.10	0.13	0.37	0.23
363	0.12	-0.27	-0.23	-0.72	0.10	0.13	-0.23	-0.72	0.12	-0.27
414	0.15	0	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	0.15	0
425	0.15	0	0.10	0.13	0.10	0.13	0.10	0.13	-0.16	-0.83
431	0.15	0	0.22	0	0.22	0	0.22	0	0.34	0.06
442	0.15	0	0.18	0.03	0.18	0.03	0.18	0.03	0.37	0.23
453	0.15	0	-0.23	-0.72	0.10	0.13	0.10	0.13	0.12	-0.27
464	0.15	0	-0.23	-0.72	0.10	0.13	-0.23	-0.72	0.15	0
515	-0.16	-0.83	-0.23	-0.72	-0.23	-0.72	-0.23	-0.72	-0.16	-0.83
521	-0.16	-0.83	0.10	0.13	0.10	0.13	0.10	0.13	0.34	0.06
532	-0.16	-0.83	0.22	0	0.22	0	0.22	0	0.37	0.23
543	-0.16	-0.83	0.18	0.03	0.18	0.03	0.18	0.03	0.12	-0.27
554	-0.16	-0.83	-0.23	-0.72	0.10	0.13	0.10	0.13	0.15	0
565	-0.16	-0.83	-0.23	-0.72	0.10	0.13	-0.23	-0.72	-0.16	-0.83

D. Hammett Constants HOMO and Hammett Constants HOMO-LUMO Gap LASSO Regression Sets without labels (Sets **4A**/**4B**)

This data set is identical to sets **3A**/**3B**, but with the removal of certain Hammett parameters as suggested by the LASSO regression performed on set **3A**.

RLX	R σ_m	R σ_p	L_1 σ_p	L_2 σ_m	L_2 σ_p	L_3 σ_p	X σ_p
111	0	0	-0.72	-0.23	-0.72	-0.72	0.06
122	0	0	0.13	0.10	0.13	0.13	0.23
133	0	0	0	0.22	0	0	-0.27
144	0	0	0.03	0.18	0.03	0.03	0
155	0	0	-0.72	0.10	0.13	0.13	-0.83
161	0	0	-0.72	0.10	0.13	-0.72	0.06
212	-0.07	-0.17	-0.72	-0.23	-0.72	-0.72	0.23
223	-0.07	-0.17	0.13	0.10	0.13	0.13	-0.27
234	-0.07	-0.17	0	0.22	0	0	0
245	-0.07	-0.17	0.03	0.18	0.03	0.03	-0.83
251	-0.07	-0.17	-0.72	0.10	0.13	0.13	0.06
262	-0.07	-0.17	-0.72	0.10	0.13	-0.72	0.23
313	0.12	-0.27	-0.72	-0.23	-0.72	-0.72	-0.27
324	0.12	-0.27	0.13	0.10	0.13	0.13	0
335	0.12	-0.27	0	0.22	0	0	-0.83
341	0.12	-0.27	0.03	0.18	0.03	0.03	0.06
352	0.12	-0.27	-0.72	0.10	0.13	0.13	0.23
363	0.12	-0.27	-0.72	0.10	0.13	-0.72	-0.27
414	0.15	0	-0.72	-0.23	-0.72	-0.72	0
425	0.15	0	0.13	0.10	0.13	0.13	-0.83
431	0.15	0	0	0.22	0	0	0.06
442	0.15	0	0.03	0.18	0.03	0.03	0.23
453	0.15	0	-0.72	0.10	0.13	0.13	-0.27
464	0.15	0	-0.72	0.10	0.13	-0.72	0
515	-0.16	-0.83	-0.72	-0.23	-0.72	-0.72	-0.83
521	-0.16	-0.83	0.13	0.10	0.13	0.13	0.06
532	-0.16	-0.83	0	0.22	0	0	0.23
543	-0.16	-0.83	0.03	0.18	0.03	0.03	-0.27
554	-0.16	-0.83	-0.72	0.10	0.13	0.13	0
565	-0.16	-0.83	-0.72	0.10	0.13	-0.72	-0.83

E. Hammett Constants HOMO Stepwise Regression Set without labels (Set **5A**)

This data set is identical to set **3A**, but with the removal of certain Hammett parameters as suggested by the stepwise regression performed on set **3A**.

RLX	R σ_p	L_1 σ_m	L_1 σ_p	L_2 σ_m	L_3 σ_m	X σ_p
111	0	-0.23	-0.72	-0.23	-0.23	0.06
122	0	0.10	0.13	0.10	0.10	0.23
133	0	0.22	0	0.22	0.22	-0.27
144	0	0.18	0.03	0.18	0.18	0
155	0	-0.23	-0.72	0.10	0.10	-0.83
161	0	-0.23	-0.72	0.10	-0.23	0.06
212	-0.17	-0.23	-0.72	-0.23	-0.23	0.23
223	-0.17	0.10	0.13	0.10	0.10	-0.27
234	-0.17	0.22	0	0.22	0.22	0
245	-0.17	0.18	0.03	0.18	0.18	-0.83
251	-0.17	-0.23	-0.72	0.10	0.10	0.06
262	-0.17	-0.23	-0.72	0.10	-0.23	0.23
313	-0.27	-0.23	-0.72	-0.23	-0.23	-0.27
324	-0.27	0.10	0.13	0.10	0.10	0
335	-0.27	0.22	0	0.22	0.22	-0.83
341	-0.27	0.18	0.03	0.18	0.18	0.06
352	-0.27	-0.23	-0.72	0.10	0.10	0.23
363	-0.27	-0.23	-0.72	0.10	-0.23	-0.27
414	0	-0.23	-0.72	-0.23	-0.23	0
425	0	0.10	0.13	0.10	0.10	-0.83
431	0	0.22	0	0.22	0.22	0.06
442	0	0.18	0.03	0.18	0.18	0.23
453	0	-0.23	-0.72	0.10	0.10	-0.27
464	0	-0.23	-0.72	0.10	-0.23	0
515	-0.83	-0.23	-0.72	-0.23	-0.23	-0.83
521	-0.83	0.10	0.13	0.10	0.10	0.06
532	-0.83	0.22	0	0.22	0.22	0.23
543	-0.83	0.18	0.03	0.18	0.18	-0.27
554	-0.83	-0.23	-0.72	0.10	0.10	0
565	-0.83	-0.23	-0.72	0.10	-0.23	-0.83

F. Hammett Constants HOMO-LUMO Gap Stepwise Regression Set without labels (Set **5B**)

This data set is identical to set **3B**, but with the removal of certain Hammett parameters as suggested by the stepwise regression performed on set **3B**.

RLX	R σ_m	R σ_p	L_1 σ_p	L_2 σ_m	L_2 σ_p	X σ_m	X σ_p
111	0	0	-0.72	-0.23	-0.72	0.34	0.06
122	0	0	0.13	0.10	0.13	0.37	0.23
133	0	0	0	0.22	0	0.12	-0.27
144	0	0	0.03	0.18	0.03	0.15	0
155	0	0	-0.72	0.10	0.13	-0.16	-0.83
161	0	0	-0.72	0.10	0.13	0.34	0.06
212	-0.07	-0.17	-0.72	-0.23	-0.72	0.37	0.23
223	-0.07	-0.17	0.13	0.10	0.13	0.12	-0.27
234	-0.07	-0.17	0	0.22	0	0.15	0
245	-0.07	-0.17	0.03	0.18	0.03	-0.16	-0.83
251	-0.07	-0.17	-0.72	0.10	0.13	0.34	0.06
262	-0.07	-0.17	-0.72	0.10	0.13	0.37	0.23
313	0.12	-0.27	-0.72	-0.23	-0.72	0.12	-0.27
324	0.12	-0.27	0.13	0.10	0.13	0.15	0
335	0.12	-0.27	0	0.22	0	-0.16	-0.83
341	0.12	-0.27	0.03	0.18	0.03	0.34	0.06
352	0.12	-0.27	-0.72	0.10	0.13	0.37	0.23
363	0.12	-0.27	-0.72	0.10	0.13	0.12	-0.27
414	0.15	0	-0.72	-0.23	-0.72	0.15	0
425	0.15	0	0.13	0.10	0.13	-0.16	-0.83
431	0.15	0	0	0.22	0	0.34	0.06
442	0.15	0	0.03	0.18	0.03	0.37	0.23
453	0.15	0	-0.72	0.10	0.13	0.12	-0.27
464	0.15	0	-0.72	0.10	0.13	0.15	0
515	-0.16	-0.83	-0.72	-0.23	-0.72	-0.16	-0.83
521	-0.16	-0.83	0.13	0.10	0.13	0.34	0.06
532	-0.16	-0.83	0	0.22	0	0.37	0.23
543	-0.16	-0.83	0.03	0.18	0.03	0.12	-0.27
554	-0.16	-0.83	-0.72	0.10	0.13	0.15	0
565	-0.16	-0.83	-0.72	0.10	0.13	-0.16	-0.83

IV. Principal Component Analysis Results

Rotation Matrices

	PC1	PC2	PC3
R σ_m	0.01	-0.01	-0.71
R σ_p	0.01	-0.01	-0.71
L_1 σ_m	0.37	0.02	0.01
L_1 σ_p	0.37	0.02	0.01
L_2 σ_m	0.38	0.02	0.01
L_2 σ_p	0.31	0.01	0.00
L_3 σ_m	0.40	0.02	0.01
L_3 σ_p	0.38	0.02	0.01
X σ_m	0.01	-0.71	0.01
X σ_p	0.01	-0.71	0.01
$E_{DFT}(d_{xy})$	-0.42	0.05	0.04

	PC1	PC2	PC3
R σ_m	0.02	-0.04	0.69
R σ_p	0.03	-0.05	0.70
L_1 σ_m	-0.38	-0.02	0.04
L_1 σ_p	-0.37	-0.02	0.03
L_2 σ_m	-0.38	-0.02	0.03
L_2 σ_p	-0.31	-0.01	0.02
L_3 σ_m	-0.40	-0.03	0.05
L_3 σ_p	-0.38	-0.03	0.04
X σ_m	-0.02	0.70	0.05
X σ_p	-0.01	0.70	0.06
$E_{DFT}(\pi^*)$ - $E_{DFT}(d_{xy})$	-0.41	0.07	-0.12

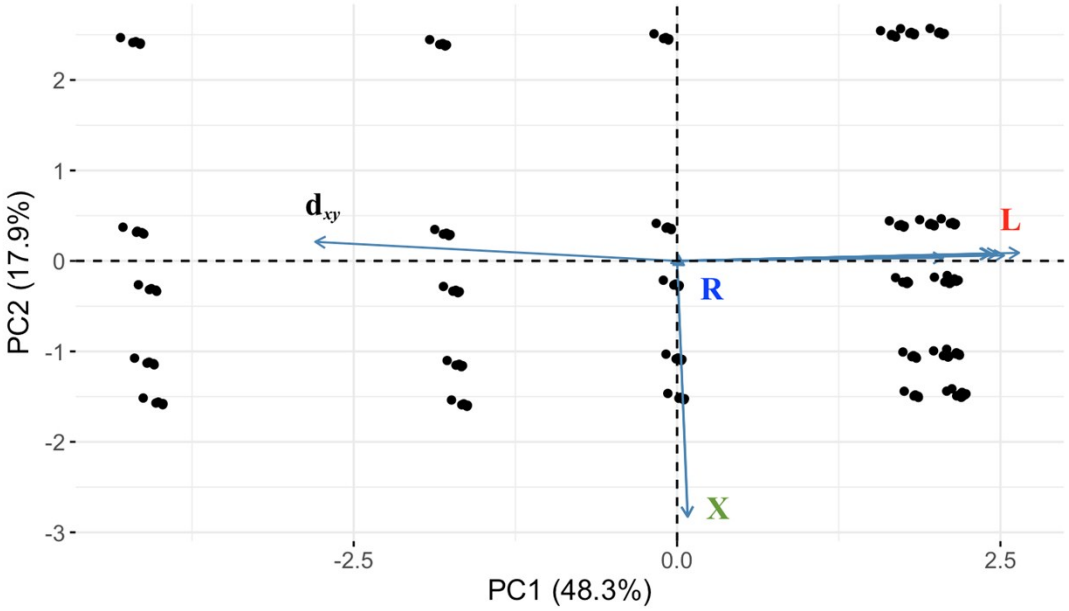


Figure S2. A biplot of the first two principal components for dataset **HCHO**. The vectors corresponding to the Hammett parameters at the L site point away from the vector of the d_{xy} energy label, showing anticorrelation between the two. The R vector is small because the third principal component dimension is not plotted. Black dots mark the 150 molecules in the input data.

V. DFT-Obtained and NN-Predicted Energies for All Candidates

Compound[a]	DFT $E(d_{xy})$[b,f,g]	ML $E(d_{xy})$[g]	DFT $E(\pi^*) - E(d_{xy})$[b,d,f,g]	ML $E(\pi^*) - E(d_{xy})$[g]
111	-2.52	-2.59(3)	2.47	2.45(3)
112	-2.60	-2.56(2)	2.31	2.34(3)
113	-2.44	-2.48(6)	2.47	2.37(5)
114	-2.56	-2.43(5)	2.18	2.20(6)
115	-2.47	-2.34(15)	2.25	2.28(14)
121	-4.05	-4.11(3)	3.47	3.47(3)
122	-4.06	-4.05(3)	3.30	3.35(3)
123	-3.97	-4.01(3)	3.46	3.37(4)
124	-3.99	-3.93(4)	3.17	3.19(4)
125	-3.92	-3.86(3)	3.03	3.22(3)
131	-3.95	-4.12(4)	3.38	3.46(2)
132	-4.01	-4.06(3)	3.24	3.34(3)
133	-3.95	-4.02(2)	3.43	3.36(2)
134	-3.96	-3.94(3)	3.10	3.18(4)
135	-3.88[c]	-3.86(3)	3.15[c]	3.23(4)
141	-4.08	-4.10(3)	3.46	3.45(2)
142	-4.20	-4.04(2)	3.41	3.33(2)
143	-3.96	-4.00(2)	3.42	3.36(2)
144	-4.12	-3.92(3)	3.34	3.18(3)
145	-3.81	-3.84(3)	3.23	3.22(3)
151	-3.53	-3.56(4)	3.03	3.02(2)
152	-3.54	-3.51(5)	2.88	2.90(4)
153	-3.45	-3.49(3)	3.01	2.94(2)
154	-3.52	-3.39(5)	2.74	2.75(5)
155	-3.48	-3.40(4)	2.84	2.86(3)
161	-3.36	-3.40(3)	2.99	2.97(3)
162	-3.40	-3.37(3)	2.83	2.86(4)
163	-3.27	-3.28(6)	2.97	2.89(5)
164	-3.34	-3.23(5)	2.72	2.71(6)
165	-3.28	-3.10(14)	2.80	2.81(15)
211	-2.49	-2.58(3)	2.50	2.50(4)
212	-2.57	-2.55(4)	2.34	2.40(3)
213	-2.40	-2.46(5)	2.49	2.42(4)
214	-2.53	-2.42(6)	2.22	2.25(5)
215	-2.43	-2.33(12)	2.29	2.33(11)
221	-4.03	-4.10(3)	3.52	3.53(3)

222	-4.04	-4.04(3)	3.36	3.41(3)
223	-3.94	-4.00(2)	3.51	3.43(3)
224	-3.99	-3.91(5)	3.19	3.25(4)
225	-3.90[c]	-3.84(4)	3.24[c]	3.28(3)
231	-3.93	-4.10(4)	3.43	3.51(2)
232	-3.98	-4.04(3)	3.28	3.40(3)
233	-3.93	-4.00(2)	3.47	3.42(2)
234	-3.93	-3.92(3)	3.14	3.24(3)
235	-3.85[c]	-3.84(3)	3.19[c]	3.29(3)
241	-4.05	-4.08(3)	3.50	3.51(3)
242	-4.18	-4.02(2)	3.46	3.39(3)
243	-3.94	-3.98(2)	3.46	3.42(3)
244	-4.09	-3.90(3)	3.39	3.23(3)
245	-3.79	-3.82(3)	3.27	3.28(2)
251	-3.50	-3.54(3)	3.07	3.08(2)
252	-3.51	-3.48(4)	2.92	2.96(4)
253	-3.43	-3.47(3)	3.05	3.00(2)
254	-3.49	-3.37(5)	2.78	2.81(5)
255	-3.46	-3.37(5)	2.89	2.91(3)
261	-3.33	-3.38(3)	3.03	3.02(4)
262	-3.37	-3.35(3)	2.87	2.92(3)
263	-3.24	-3.25(6)	3.00	2.95(5)
264	-3.32	-3.21(5)	2.75	2.77(5)
265	-3.25	-3.08(15)	2.83	2.86(13)
311	-2.46	-2.59(6)	2.68[e]	2.63(6)
312	-2.54	-2.56(7)	2.47	2.53(5)
313	-2.39	-2.47(4)	2.68[e]	2.55(4)
314	-2.50	-2.43(5)	2.35	2.39(4)
315	-2.40	-2.33(10)	2.41	2.45(10)
321	-4.01	-4.08(3)	3.67	3.64(3)
322	-4.02	-4.03(3)	3.50	3.52(2)
323	-3.91	-3.99(2)	3.65	3.54(3)
324	-3.94	-3.90(4)	3.32	3.37(3)
325	-3.89[c]	-3.84(3)	3.38[c]	3.39(4)
331	-3.92	-4.08(4)	3.58	3.62(3)
332	-3.96	-4.03(3)	3.43	3.51(2)
333	-3.90	-3.99(3)	3.56	3.53(3)
334	-3.93	-3.91(3)	3.27	3.35(3)
335	-3.83[c]	-3.84(3)	3.33[c]	3.39(4)
341	-4.02	-4.07(3)	3.65	3.62(3)
342	-4.15	-4.01(2)	3.60	3.51(2)

343	-3.92	-3.98(3)	3.58	3.52(3)
344	-4.06	-3.89(3)	3.44	3.35(3)
345	-3.77	-3.83(3)	3.41	3.38(4)
351	-3.47	-3.53(3)	3.20	3.19(2)
352	-3.49	-3.48(3)	3.06	3.08(3)
353	-3.40	-3.45(3)	3.18	3.11(3)
354	-3.47	-3.36(5)	2.90	2.93(5)
355	-3.43	-3.36(6)	3.02	3.01(5)
361	-3.29	-3.38(6)	3.15	3.14(5)
362	-3.34	-3.35(7)	3.01	3.03(4)
363	-3.20	-3.25(4)	3.13	3.06(4)
364	-3.28	-3.21(4)	2.87	2.89(4)
365	-3.21	-3.08(13)	2.94	2.97(12)
411	-2.52	-2.60(4)	2.47	2.51(4)
412	-2.59	-2.57(4)	2.32	2.41(4)
413	-2.45	-2.49(5)	2.47	2.43(5)
414	-2.56	-2.45(4)	2.22	2.27(5)
415	-2.46	-2.34(14)	2.26	2.34(14)
421	-4.04	-4.11(3)	3.49	3.51(3)
422	-4.05	-4.04(3)	3.32	3.40(2)
423	-3.95	-4.02(2)	3.47	3.42(3)
424	-3.97	-3.93(4)	3.17	3.24(3)
425	-3.92[c]	-3.87(2)	3.21[c]	3.26(3)
431	-3.94	-4.12(4)	3.40	3.51(2)
432	-3.99	-4.06(3)	3.25	3.39(2)
433	-3.93	-4.03(3)	3.44	3.41(3)
434	-3.93	-3.94(3)	3.11	3.23(3)
435	-3.86[c]	-3.87(3)	3.16[c]	3.27(4)
441	-4.06	-4.10(3)	3.25	3.50(3)
442	-4.18	-4.04(2)	3.47	3.39(2)
443	-3.95	-4.01(3)	3.42	3.41(3)
444	-4.09	-3.92(3)	3.42	3.23(3)
445	-3.80	-3.86(3)	3.31	3.26(4)
451	-3.51	-3.56(4)	3.04	3.07(3)
452	-3.53	-3.51(5)	2.89	2.95(4)
453	-3.44	-3.49(2)	3.02	2.99(2)
454	-3.50	-3.39(5)	2.75	2.80(5)
455	-3.46	-3.40(4)	2.86	2.90(4)
461	-3.34	-3.41(4)	2.99	3.02(4)
462	-3.38	-3.38(5)	2.84	2.92(5)
463	-3.24	-3.29(4)	2.97	2.94(4)

464	-3.32	-3.25(4)	2.72	2.77(5)
465	-3.25	-3.11(13)	2.79	2.86(14)
511	-2.37	-2.50(13)	2.72[e]	2.72(12)
512	-2.45	-2.47(15)	2.57	2.62(11)
513	-2.29	-2.39(9)	2.70[e]	2.63(9)
514	-2.43	-2.33(13)	2.45	2.48(10)
515	-2.31	-2.28(2)	2.49	2.54(3)
521	-3.96	-3.94(3)	3.78	3.72(3)
522	-3.96	-3.88(3)	3.61	3.61(3)
523	-3.86	-3.84(5)	3.72	3.63(5)
524	-3.90	-3.76(5)	3.43	3.46(5)
525	-3.82[c]	-3.70(11)	3.48[c]	3.49(11)
531	-3.86	-3.94(4)	3.69	3.69(3)
532	-3.91	-3.88(3)	3.55	3.59(3)
533	-3.84	-3.84(7)	3.66	3.60(5)
534	-3.89	-3.76(5)	3.39	3.44(4)
535	-3.78[c]	-3.71(12)	3.45[c]	3.48(11)
541	-3.96	-3.92(4)	3.75	3.70(3)
542	-4.08	-3.86(2)	3.71	3.59(3)
543	-3.86	-3.82(6)	3.68	3.60(5)
544	-3.99	-3.74(4)	3.54	3.44(4)
545	-3.71[c]	-3.68(12)	3.49[c]	3.47(11)
551	-3.41	-3.42(10)	3.29	3.29(7)
552	-3.41	-3.37(11)	3.15	3.18(8)
553	-3.34	-3.33(12)	3.25	3.20(8)
554	-3.40	-3.25(12)	2.99	3.03(9)
555	-3.37	-3.23(15)	3.11	3.11(12)
561	-3.24	-3.27(13)	3.26	3.23(10)
562	-3.27	-3.24(14)	3.11	3.13(9)
563	-3.15	-3.14(13)	3.22	3.15(10)
564	-3.22	-3.10(12)	2.95	2.98(9)
565	-3.15	-2.98(22)	3.01	3.05(13)

[a]All R groups are in the *para* position. [b]Unless otherwise specified, d_{xy} is the HOMO. [c]HOMO-1 used as d_{xy}. [d]Unless otherwise specified, π^* is the LUMO. [e]LUMO+1 used as π^*. [f]All DFT calculations reported include the THF dielectric continuum model. [g]All energies have unit eV.

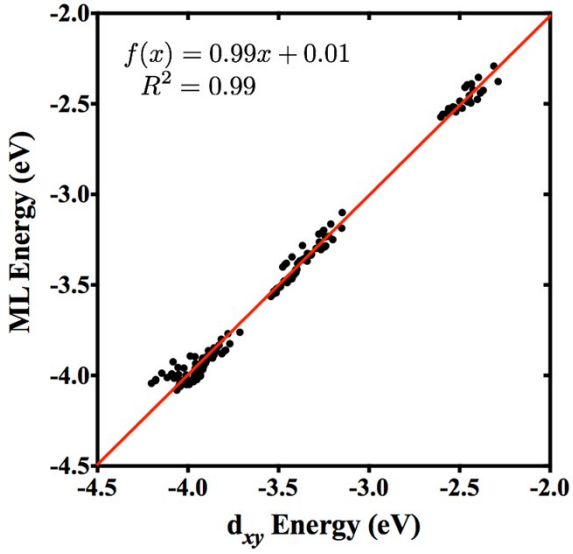
VI. DFT-Obtained Energies with Dispersion Corrections for Select Candidates

Compound	DFT $E_{disp}(d_{xy})$	$\Delta E_{disp}(d_{xy})$[a]	DFT $E_{disp}(\pi^*) - E_{disp}(d_{xy})$	$\Delta E_{disp}(d_{xy} - \pi^*)$[b]
121	-5.95	1.90	7.14	-3.67
231	-5.81	1.88	7.09	-3.66
242	-6.01	1.83	7.10	-3.64
334	-5.81	1.88	6.95	-3.68
362	-5.23	1.89	6.69	-3.68
424	-5.85	1.88	6.78	-3.61
455	-5.32	1.86	6.48	-3.62
513	-4.25	1.96	6.44	-3.74
515	-4.27	1.96	6.23	-3.74
543	-5.67	1.81	7.30	-3.62

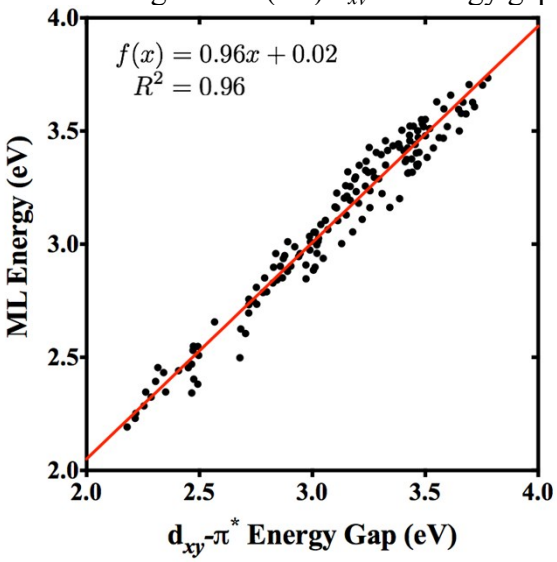
[a]$\Delta E_{disp}(d_{xy})$ is the difference between the non-dispersion-corrected d_{xy} energy and the dispersion-corrected d_{xy} energy. [b]$\Delta E_{disp}(d_{xy} - \pi^*)$ is the difference between the non-dispersion-corrected d_{xy} - π^* energy gap and the dispersion-corrected d_{xy} - π^* energy gap. All units are in eV.

VII. Predicted vs. DFT Energy Parity Plots

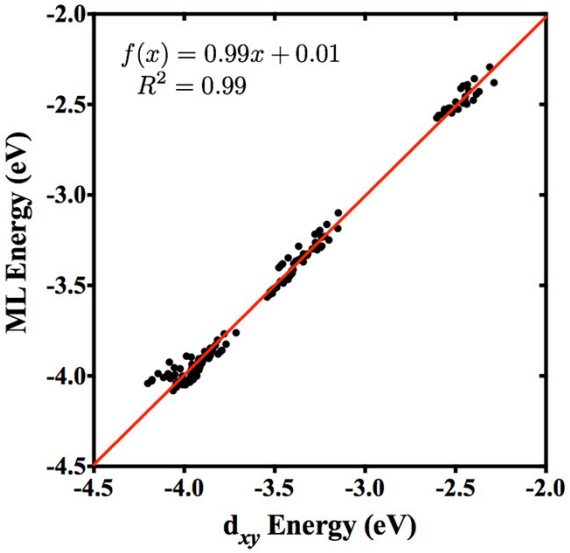
Linear Regression (3A) d_{xy} energy



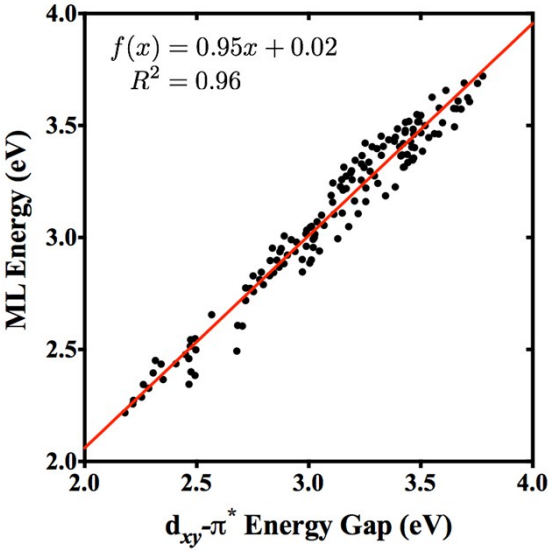
Linear Regression (3B) d_{xy}-π^* energy gap



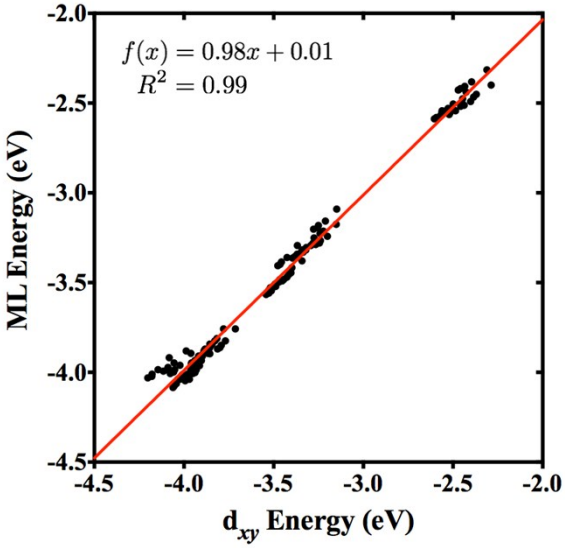
Ridge Regression (3A) d_{xy} energy



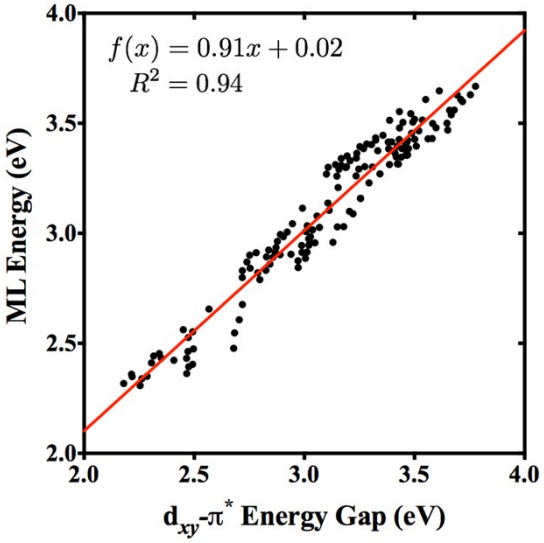
Ridge Regression (3B) d_{xy}-π^* energy gap



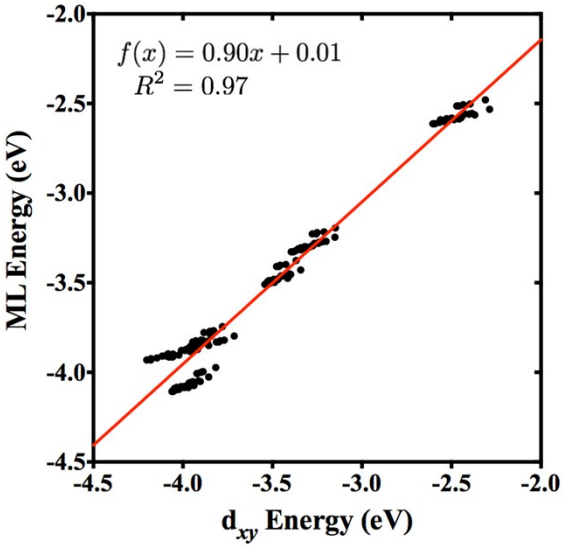
Ridge Regression with Cross Validation (3A) d_{xy} energy



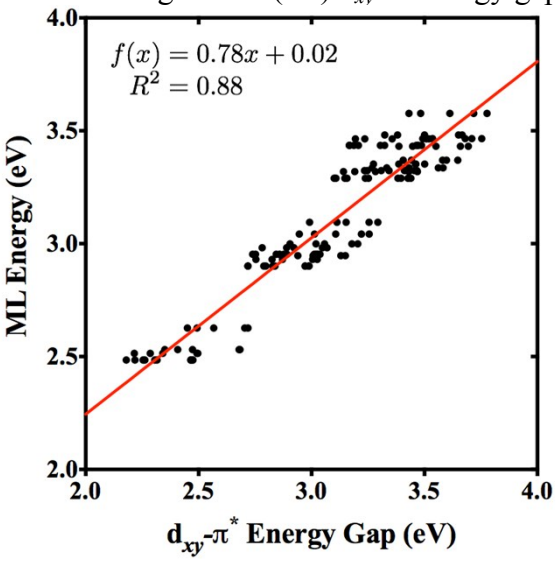
Ridge Regression with Cross Validation (3B) d_{xy}-π^* energy gap



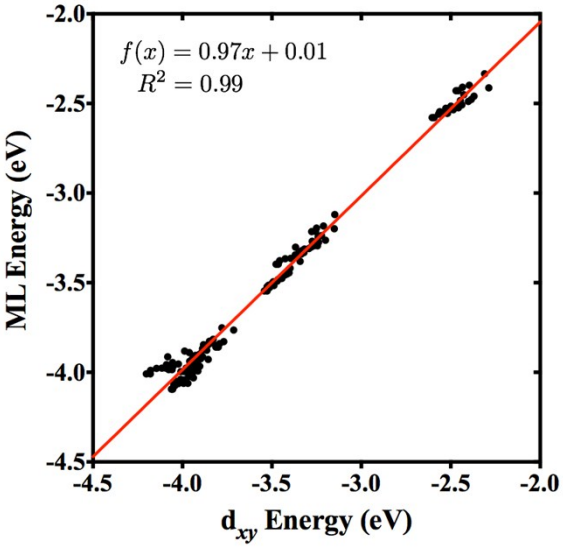
LASSO Regression (3A) d_{xy} energy



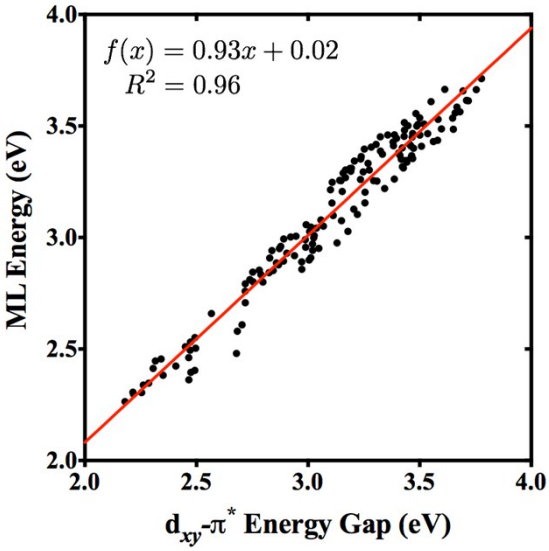
LASSO Regression (3B) d_{xy}-π^* energy gap



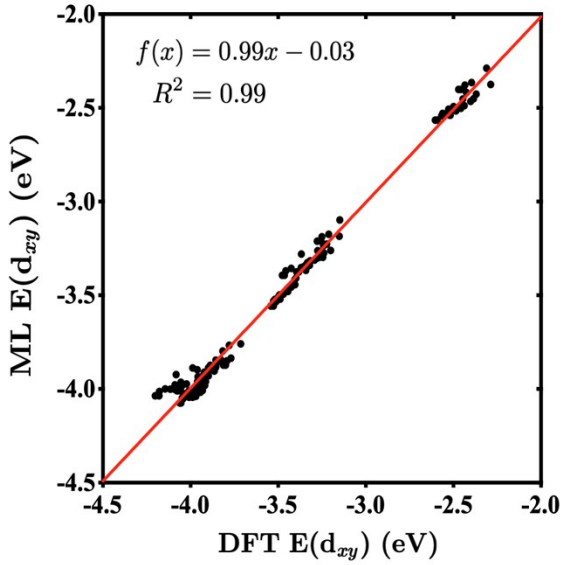
LASSO Regression with Cross Validation (3A) d_{xy} energy



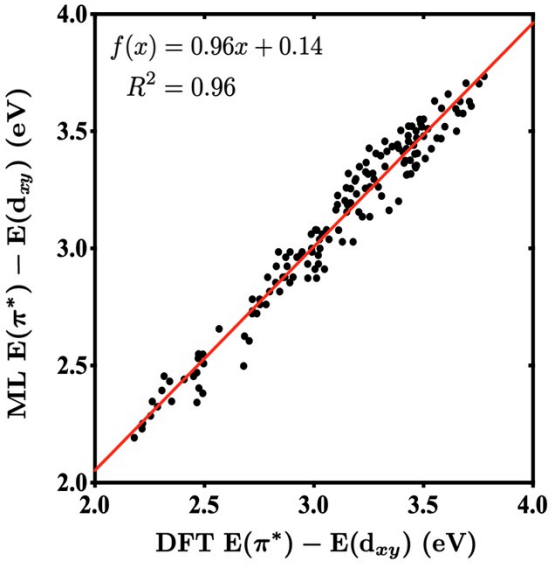
LASSO Regression with Cross Validation (3B) d_{xy}-π^* energy gap



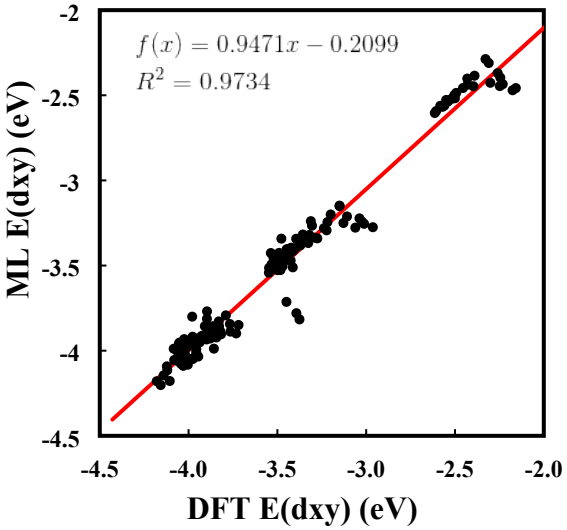
Stepwise Regression (3A) d_{xy} energy



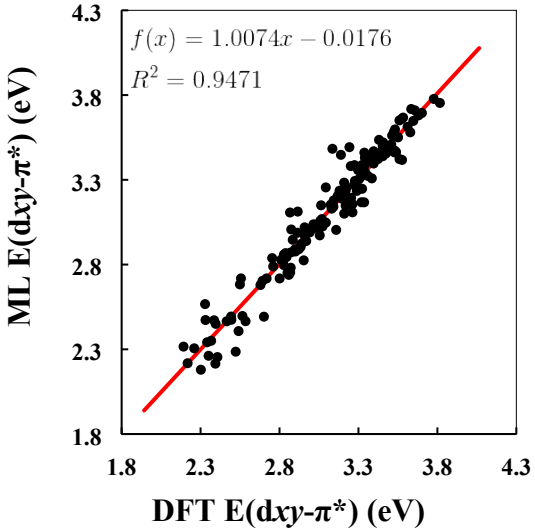
Stepwise Regression (3B) d_{xy}-π^* energy gap



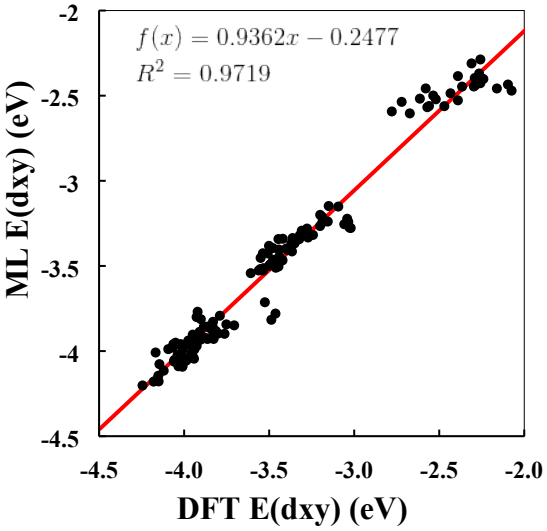
Gaussian Process (3A) d_{xy} energy



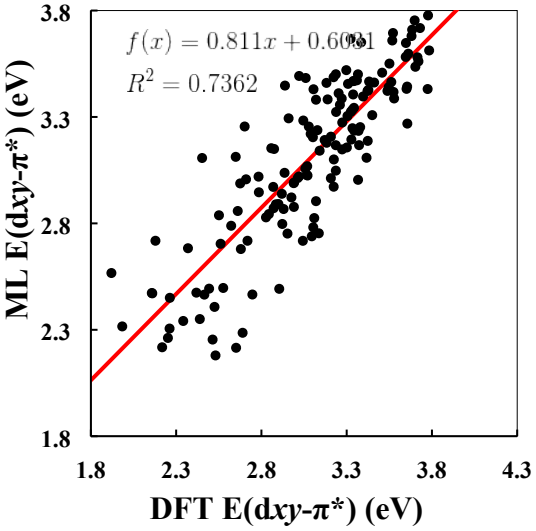
Gaussian Process (3B) d_{xy}-π^* energy gap



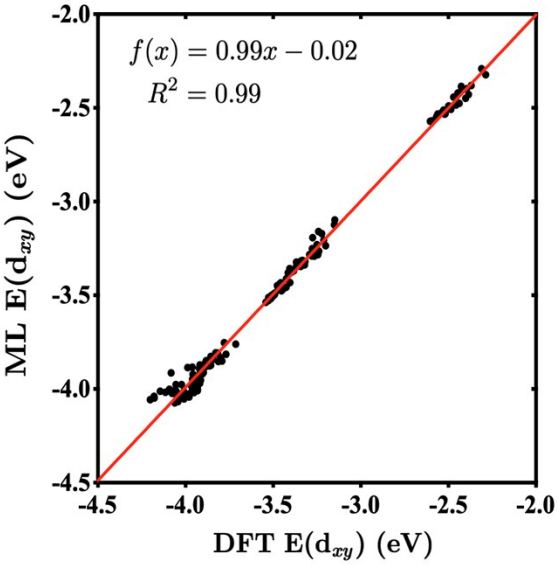
Gaussian Process (4A) d_{xy} energy



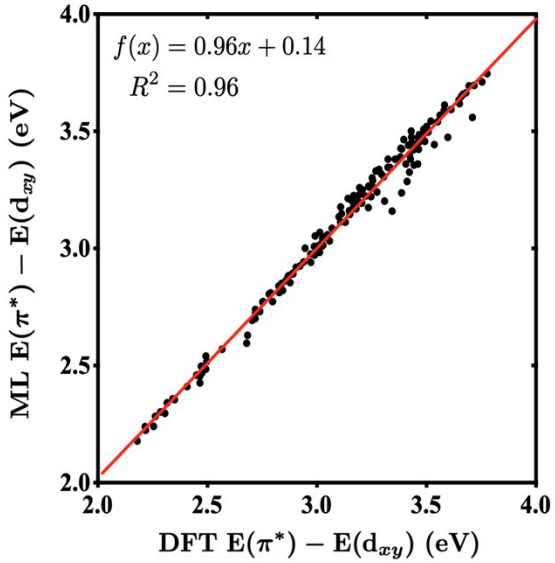
Gaussian Process (4B) d_{xy}-π^* energy gap



Set **2A** NN-predicted d_{xy} energy (120 molecules used for training)



Set **2B** NN-predicted d_{xy}-π^* energy gap (120 molecules used for training)



VIII. Catalyst Predictions for Regressive Models

This table presents the prediction results for each regressive method for datasets **3A/3B** and **4A/4B**, where **A** refers to the d_{xy} energy as the label, **B** refers to the d_{xy}-π^* energy gap as the label, **3** refers to using all Hammett parameters for input with a 30/120 train/test split that was hand selected to cover all ligands equally, and **4** has the same data split but only uses the parameters, R σ_m, R σ_p, L_1 σ_p, L_2 σ_m, L_2 σ_p, L_3 σ_p, and X σ_p , as selected by the LASSO cost function. Percentages refer to the DFT prediction being found in the top X% of that models predictions. The DFT predictions column below highlight the RLX code that corresponds to Table III.B. for convenience. Abreviations: Cross-Validation (CV); Neural Network (CV); Gaussian Process Regression (GPR). Point – by – point data and code available upon request.

Dataset	DFT Prediction	Linear	Ridge	LASSO	NN	Ridge CV	LASSO CV	GPR
3A	Top Reducing (513)	5%	5%	5%	5%	5%	5%	10%
	2nd Top Reducing (515)	Best	Best	Best	Best	Best	Best	10%
3B	Largest Gap (521)	Best	Best	Best	Best	Best	Best	5%
	2nd Largest Gap (541)	5%	5%	10%	5%	5%	5%	Best
4A	Top Reducing (513)	5%	5%	5%	5%	5%	5%	5%
4B	Largest Gap (541)	5%	5%	10%	5%	5%	5%	5%

IX. DFT Theoretical Coordinates

The first line indicates the number of atoms, the second line indicates the compound number. Only the coordinates of the top two reducing catalysts are shown.

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513

W	1.10998	-0.00000	-0.00533
C	-0.72360	-0.00001	-0.06701
N	1.41850	1.90298	-1.48443
N	1.17242	1.88603	1.49813
N	1.17244	-1.88603	1.49813
N	1.41852	-1.90298	-1.48442
C	1.76272	-3.05351	-0.61557
C	0.94073	-3.08294	0.65574
H	-0.12921	-3.11088	0.41117
H	1.17212	-4.01016	1.22053
H	2.83084	-2.97632	-0.36795
H	1.63100	-4.00915	-1.16287
C	1.76269	3.05352	-0.61558
C	0.94069	3.08293	0.65574
H	1.17208	4.01016	1.22052
H	-0.12925	3.11087	0.41117
H	1.63095	4.00916	-1.16288
H	2.83080	2.97634	-0.36796
C	0.18068	-2.19012	-2.23650
H	-0.08670	-1.31594	-2.84134
H	-0.65275	-2.37193	-1.55194
H	0.32193	-3.07085	-2.89726
C	2.51569	-1.73566	-2.45533
H	3.40706	-1.36594	-1.93573
H	2.22099	-1.00653	-3.21813
H	2.74265	-2.69371	-2.96587
C	0.10793	-1.83804	2.51814
H	-0.86090	-1.66780	2.03587
H	0.29912	-1.00922	3.20878
H	0.08318	-2.78113	3.10310
C	2.46868	-2.00496	2.19334
H	3.29239	-2.04168	1.47467
H	2.49030	-2.91012	2.83273
H	2.62312	-1.12135	2.82455
C	2.51568	1.73567	-2.45533
H	2.22099	1.00653	-3.21812
H	3.40705	1.36597	-1.93573
H	2.74261	2.69371	-2.96588
C	0.18066	2.19010	-2.23651

H	-0.08671	1.31592	-2.84134
H	0.32190	3.07083	-2.89727
H	-0.65277	2.37191	-1.55195
C	0.10792	1.83804	2.51814
H	0.29912	1.00923	3.20879
H	-0.86091	1.66777	2.03588
H	0.08315	2.78113	3.10309
C	2.46866	2.00498	2.19334
H	3.29237	2.04173	1.47466
H	2.62312	1.12136	2.82454
H	2.49026	2.91014	2.83273
C	-2.16672	-0.00001	-0.05099
C	-2.93915	1.19346	-0.03766
C	-2.93915	-1.19348	-0.03766
C	-4.33223	-1.20151	-0.01134
C	-5.07853	-0.00000	0.01577
C	-4.33222	1.20150	-0.01134
H	-2.41995	-2.15621	-0.05186
H	-4.84163	-2.16569	-0.00820
H	-4.84162	2.16568	-0.00820
C	4.59933	0.00004	0.22842
H	5.17259	-0.00003	-0.73195
H	4.98022	0.88750	0.79405
H	4.98025	-0.88732	0.79420
H	-2.41995	2.15619	-0.05185
N	-6.47710	-0.00000	0.07383
C	-7.18970	1.23962	-0.13280
H	-7.01793	1.68723	-1.13514
H	-8.26880	1.06378	-0.02167
H	-6.90496	1.99882	0.61597
C	-7.18970	-1.23962	-0.13281
H	-6.90497	-1.99883	0.61595
H	-8.26880	-1.06378	-0.02167
H	-7.01793	-1.68722	-1.13515
O	3.24570	-0.00000	0.04965

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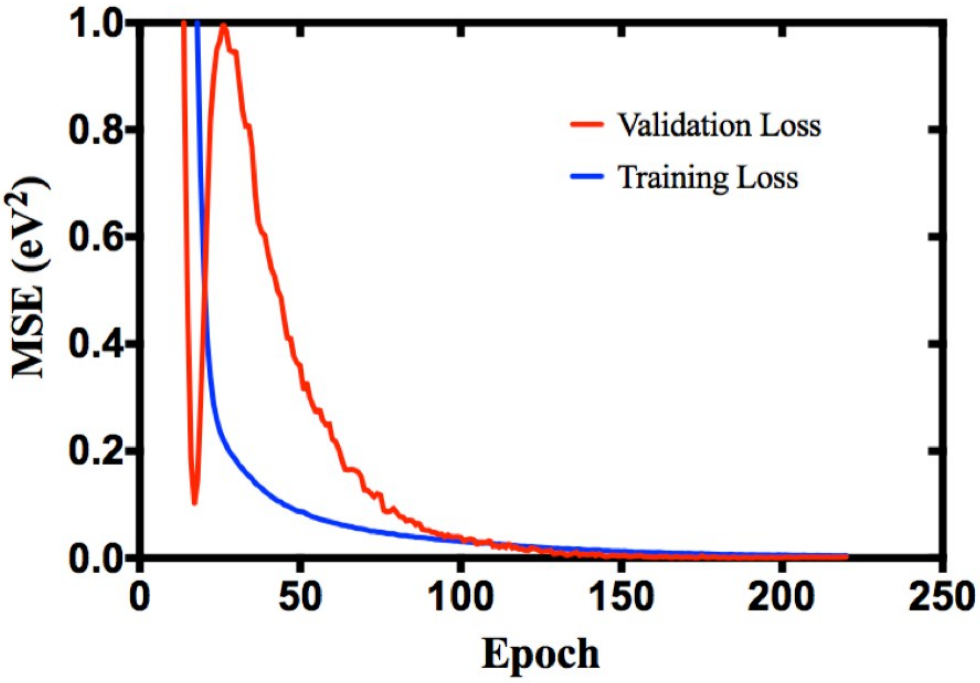
W	-1.10570	0.00000	0.00257
C	0.73429	-0.00001	0.05697
N	-1.23726	1.94018	1.54210
N	-0.98104	2.00398	-1.46839
N	-0.98106	-2.00396	-1.46841
N	-1.23726	-1.94019	1.54209
C	-1.33742	-3.15796	0.70320
C	-0.50552	-3.06895	-0.55781
H	0.53809	-2.85127	-0.30497
H	-0.52513	-4.05251	-1.07319
H	-2.39536	-3.29799	0.44127
H	-1.03383	-4.05324	1.28285
C	-1.33741	3.15795	0.70323
C	-0.50549	3.06895	-0.55778
H	-0.52510	4.05252	-1.07315
H	0.53811	2.85126	-0.30494
H	-1.03381	4.05323	1.28288
H	-2.39534	3.29799	0.44129
C	0.00019	-1.99521	2.34824
H	0.08116	-1.08526	2.95333
H	0.88241	-2.03635	1.70529
H	-0.01845	-2.87844	3.02024
C	-2.36875	-1.95891	2.48504
H	-3.31652	-1.93327	1.93971
H	-2.31570	-1.08451	3.14597
H	-2.34146	-2.87140	3.11452
C	0.02623	-1.82866	-2.53092
H	0.96884	-1.47964	-2.09578
H	-0.32684	-1.07753	-3.24764
H	0.19392	-2.78111	-3.07620
C	-2.23529	-2.44456	-2.10679
H	-3.05139	-2.48116	-1.37829
H	-2.10620	-3.44057	-2.57590
H	-2.51893	-1.73052	-2.88588
C	-2.36874	1.95890	2.48505
H	-2.31571	1.08449	3.14597
H	-3.31652	1.93325	1.93971
H	-2.34147	2.87138	3.11452
C	0.00020	1.99518	2.34826
H	0.08115	1.08523	2.95335
H	-0.01845	2.87841	3.02026
H	0.88242	2.03632	1.70531
C	0.02626	1.82868	-2.53091
H	-0.32682	1.07755	-3.24763

H	0.96886	1.47965	-2.09577
H	0.19395	2.78113	-3.07617
C	-2.23526	2.44459	-2.10677
H	-3.05137	2.48119	-1.37828
H	-2.51890	1.73057	-2.88588
H	-2.10616	3.44062	-2.57586
C	2.18354	-0.00001	0.02813
C	2.96051	1.19148	0.01516
C	2.96051	-1.19149	0.01517
C	4.35330	-1.20118	-0.00903
C	5.10045	-0.00001	-0.03392
C	4.35329	1.20117	-0.00904
H	2.44972	-2.15762	0.02595
H	4.86154	-2.16583	-0.01254
H	4.86153	2.16582	-0.01257
N	-3.41368	0.00001	-0.25542
C	-4.43869	-0.00001	0.75824
H	-4.03419	-0.00000	1.77751
H	-5.12591	0.88388	0.69256
H	-5.12587	-0.88393	0.69256
C	-4.11491	0.00002	-1.51462
H	-4.78969	-0.88429	-1.64522
H	-4.78969	0.88433	-1.64520
H	-3.43448	0.00003	-2.37708
H	2.44970	2.15760	0.02592
N	6.49489	-0.00000	-0.08583
C	7.21116	1.24332	0.08592
H	7.03744	1.71762	1.07466
H	8.28974	1.06090	-0.01596
H	6.93072	1.98279	-0.68445
C	7.21116	-1.24332	0.08590
H	6.93071	-1.98279	-0.68446
H	8.28975	-1.06090	-0.01601
H	7.03747	-1.71763	1.07465

X. Training and Validation Loss Graph



Validation loss and training loss curves are depicted for 220 epochs. The first few epochs are left out for the purpose of the scaling of the graph.

XI. Effect of α Hyperparameter on Ridge Regression Weights and MSE

	Linear	Ridge			
α	--	0	0.001	0.005	0.01
R σ_m	0.41	0.41	0.4	0.39	0.38
R σ_p	-0.39	-0.39	-0.39	-0.39	-0.39
L_1 σ_m	0.29	-5.28	0.29	0.29	0.29
L_1 σ_p	0.41	2.58	0.41	0.41	0.42
L_2 σ_m	0.31	8.57	0.31	0.31	0.31
L_2 σ_p	0.47	-2.74	0.47	0.47	0.47
L_3 σ_m	0.13	-2.56	0.13	0.13	0.13
L_3 σ_p	0.01	1.056	0.011	0.012	0.014
X σ_m	1.7	1.7	1.67	1.58	1.47
X σ_p	-0.75	-0.75	-0.73	-0.69	-0.64
MSE	0.017	0.017	0.017	0.017	0.017

References

1. Hammett, L. P., The Effect of Structure upon the Reactions of Organic Compounds. Benzene Derivatives. *J. Am. Chem. Soc.* **1937,** *59* (1), 96-103.