

Supplementary Materials

Organometallic acids with azaborine, oxaborine, azaborole and oxaborole scaffolds

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Table S1. The NICS values for the azaboroles & oxaboroles and their conjugated bases in ppm.

Compound	NICS(0) _{iso}	NICS(0) _{zz}	NICS(1) _{iso}	NICS(1) _{zz}
1a	-3.21	12.52	-4.42	-9.85
1b	-2.32	14.30	-3.17	-8.40
(1-H) ⁻	-10.18	-9.74	-7.51	-26.60
2a	-3.04	12.09	-3.62	-8.23
(2a-H) ⁻	-8.20	-10.57	-7.57	-26.81
2b	-3.14	13.96	-2.68	-6.50
(2b-H) ⁻	-5.49	2.38	-5.66	-14.91
2c	-2.59	16.01	-3.10	-6.27
(2c-H) ⁻	-7.51	-2.42	-4.70	-19.50
3a	-2.92	11.13	-4.66	-10.01
3b	-1.87	14.69	-3.38	-7.94
(3-H) ⁻	-8.24	-5.84	-6.57	-22.60
4a	-1.72	8.44	-3.72	-9.16
(4a-H) ⁻	-5.13	-9.23	-7.17	-24.84
4b	-5.23	6.70	-4.04	-8.01
(4b-H) ⁻	-8.62	-1.38	-6.09	-13.78
4c	-2.58	14.24	-3.42	-6.90
(4c-H) ⁻	-5.36	3.35	-3.80	-13.65
5a	-4.68	13.36	-3.89	-7.91
5b	-2.18	18.31	-1.99	-4.27
(5-H) ⁻	-10.58	-4.44	-6.04	-21.37
6a	-5.36	11.97	-3.14	-4.88
(6-H) ⁻	-9.90	-4.10	-6.68	-18.98
6b	-3.88	18.19	-1.30	-1.13
(6b-H) ⁻	-7.05	9.54	-3.80	-7.07
6c	-4.91	17.64	-2.25	-2.65
(6c-H) ⁻	-8.67	5.35	-2.73	-11.09
7a	-3.74	13.52	-3.99	-7.72
7b	-1.59	19.55	-2.26	-4.05
(7-H) ⁻	-8.08	0.75	-4.98	-17.38
8a	-2.60	14.55	-2.55	-4.53
(8a-H) ⁻	4.27	4.50	-2.29	-11.50
8b	-3.79	17.71	-2.26	-1.84
(8b-H) ⁻	-8.80	9.53	-4.70	-6.60
8c	-3.43	19.37	-2.35	-3.10
(8c-H) ⁻	-5.61	12.59	-2.08	-6.76
9a	-3.71	12.86	-4.57	-9.52
9b	-2.71	15.24	-3.24	-7.79
(9-H) ⁻	-11.22	-8.64	-8.06	-25.94
10a	-4.19	12.30	-4.03	-7.48
(10a-H) ⁻	-11.49	-8.32	-7.95	-23.85
10b	-3.46	16.35	-2.67	-4.94
(10b-H) ⁻	-7.59	2.81	-6.43	-15.36
10c	-3.34	17.15	-3.18	-5.36
(10c-H) ⁻	-9.79	-1.41	-6.25	-19.29
11a	-3.37	11.90	-4.68	-9.55
11b	-2.15	15.68	-3.39	-7.22
(11-H) ⁻	-9.18	-4.95	-7.14	-22.36
12a	-2.68	10.41	-3.71	-8.01
(12a-H) ⁻	-8.49	-6.34	-7.01	-21.39
12b	-3.94	13.11	-3.40	-5.02
(12b-H) ⁻	-8.48	1.93	-6.21	-12.73
12c	-2.85	16.29	-3.38	-5.61
(12c-H) ⁻	-6.93	4.43	-4.91	-13.86

Table S2. The NICS values for the azaborines & oxaborines and their conjugated bases in ppm.

Compound	NICS(0) _{iso}	NICS(0) _{zz}	NICS(1) _{iso}	NICS(1) _{zz}
13a	1.71	12.05	-2.92	-5.77
13b	2.97	12.57	-2.10	-5.25
(13-H) ⁻	-5.64	-11.99	-8.04	-25.32
14	2.28	16.32	-1.48	-1.48
(14-H) ⁻	-2.99	-2.97	-5.03	-16.74
15	2.84	17.65	-1.35	-0.77
(15-H) ⁻	-1.16	1.32	-3.87	-13.09
16	2.14	18.63	-0.75	0.71
(16-H) ⁻	-1.51	5.40	-3.17	-8.97
17	2.63	20.41	-0.87	0.82
(17-H) ⁻	0.06	11.01	-2.34	-5.08
18a	0.90	11.98	-2.61	-4.26
18b	2.85	14.28	-1.24	-2.24
(18-H) ⁻	-6.87	-11.09	-7.80	-23.24
19	0.10	15.71	-1.46	-0.19
(19-H) ⁻	-4.70	0.77	-4.19	-11.82
20	0.58	16.74	-1.61	-0.14
(20-H) ⁻	-2.70	5.29	-3.11	-8.73
21	-1.49	16.60	-1.28	1.36
(21-H) ⁻	-5.05	8.58	-2.82	-4.24
22	-0.85	18.02	-1.60	0.43
(22-H) ⁻	-3.44	12.94	-2.51	-2.53
23a	1.08	11.14	-3.25	-6.18
23b	2.37	12.27	-2.30	-5.37
(23-H) ⁻	-6.71	-12.06	-8.56	-25.36
24	1.32	15.91	-1.84	-1.68
(24-H) ⁻	-4.84	-3.90	-6.22	-17.70
25	1.94	17.36	-1.68	-0.90
(25-H) ⁻	-2.88	0.25	-5.04	-14.22
26	0.83	18.37	-1.24	0.75
(26-H) ⁻	-3.59	4.48	-4.45	-10.05
27	1.41	20.16	-1.32	0.85
(27-H) ⁻	-1.46	10.57	-3.22	-5.79

Table S3. The NICS values for the enolic derivatives of azaboroles and oxaboroles in ppm.

Compound	NICS (0) _{iso}	NICS(0) _{zz}	NICS(1) _{iso}	NICS(1) _{zz}
28a	-2.01	15.08	-3.90	-7.80
(28a-H)	-6.61	2.58	-6.40	-18.54
28b	-2.33	14.92	-3.03	-7.11
(28b-H)	-7.81	-0.30	-6.17	-19.02
28c	-2.26	14.93	-3.98	-8.08
(28c-H)	-7.28	0.69	-6.92	-19.87
28d	-1.92	15.43	-2.97	-7.01
(28d-H)	-7.21	1.21	-5.97	-18.17
29a	-2.60	16.49	-3.09	-5.55
(29a-H)	-5.93	5.88	-4.58	-13.75
29b	-1.85	17.16	-2.83	-5.21
(29b-H)	-5.01	8.05	-4.24	-12.36
30a	-2.87	12.25	-4.85	-10.04
(30a-H)	-6.01	2.60	-6.28	-17.56
30b	-2.26	14.37	-3.52	-7.58
(30b-H)	-6.28	3.07	-5.49	-16.28
30c	-2.77	12.03	-4.86	-9.99
(30c-H)	-6.52	1.30	-6.67	-18.47
30d	-1.88	14.44	-3.55	-7.56
(30d-H)	-5.91	3.70	-5.54	-15.71
31a	-2.73	14.36	-3.67	-6.95
(31a-H)	-4.63	8.32	-3.99	-10.76
31b	-2.47	15.02	-3.55	-6.78
(31b-H)	-4.08	9.36	-3.89	-10.07
32a	-3.55	15.29	-3.56	-6.09
(32a-H)	-7.63	5.25	-5.63	-14.79
32b	-3.74	15.57	-2.69	-5.16
(32b-H)	-8.08	4.03	-4.84	-14.35
32c	-3.84	15.10	-3.70	-6.29
(32c-H)	-8.23	4.06	-5.97	-15.93
32d	-2.15	18.09	-1.96	-3.37
(32d-H)	-7.57	5.26	-4.68	-13.39
33a	-5.68	16.03	-2.63	-2.84
(33a-H)	-7.83	10.45	-3.13	-7.34
33b	-4.35	17.82	-2.11	-1.85
(33b-H)	-6.95	12.15	-2.89	-6.19
34a	-3.64	14.68	-4.17	-7.47
(34a-H)	-6.39	7.02	-5.28	-13.42
34b	-3.22	16.44	-3.01	-5.29
(34b-H)	-6.39	7.73	-4.32	-11.85
34c	-3.54	14.45	-4.26	-7.48
(34c-H)	-6.72	6.58	-5.43	-14.05
34d	-1.94	17.94	-2.58	-4.18
(34d-H)	-6.06	8.57	-4.31	-11.26
35a	-4.09	18.18	-2.76	-3.26
(35a-H)	-5.26	15.15	-2.65	-5.08

Table S3- continued.

Compound	NICS(0) _{iso}	NICS(0) _{zz}	NICS(1) _{iso}	NICS(1) _{zz}
35b	-3.48	19.07	-2.56	-3.04
(35b-H)	-4.97	15.70	-2.57	-4.76
36a	-3.10	14.44	-4.27	-8.43
(36a-H)	-8.10	1.71	-7.17	-19.34
36b	-4.60	11.60	-4.23	-9.85
(36b-H)	-9.15	-0.94	-6.81	-19.90
36c	-3.63	13.95	-4.60	-8.80
(36c-H)	-8.75	0.15	-7.57	-20.47
36d	-3.01	14.19	-3.52	-7.85
(36d-H)	-8.60	0.21	-6.69	-19.06
37a	-5.10	13.86	-4.16	-7.51
(37a-H)	-8.31	4.40	-5.77	-15.9
37b	-3.64	16.06	-3.51	-5.97
(37b-H)	-7.51	6.64	-5.50	-13.79
38a	-3.85	11.66	-5.26	-10.56
(38a-H)	-7.30	1.90	-7.01	-18.19
38b	-4.10	11.94	-4.48	-9.51
(38b-H)	-7.63	2.01	-6.24	-17.28
38c	-3.80	11.59	-5.29	-10.40
(38c-H)	-7.76	1.03	-7.23	-19.02
38d	-2.75	13.81	-3.89	-8.08
(38d-H)	-7.06	2.96	-6.11	-16.51
39a	-3.76	14.76	-4.00	-6.78
(39a-H)	-6.19	8.33	-4.80	-11.27
39b	-3.55	15.55	-3.92	-6.58
(39b-H)	-5.74	9.34	-4.74	-10.63

Table S4. The NICS values for the enolic derivatives of azaborines and oxaborines in ppm.

Compound	NICS(0) _{iso}	NICS(0) _{zz}	NICS(1) _{iso}	NICS(1) _{zz}
40	0.88	10.01	-3.71	-7.41
(40-H) ⁻	-3.92	-4.34	-7.20	-19.78
41a	1.26	13.84	-2.25	-3.29
(41a-H) ⁻	-1.97	3.34	-4.43	-12.06
41b	1.38	13.88	-2.30	-3.28
(41b-H) ⁻	-1.82	3.53	-4.46	-11.91
42a	1.63	14.71	-2.13	-2.78
(42a-H) ⁻	-0.77	6.15	-3.67	-9.67
42b	1.85	14.90	-2.18	-2.65
(42b-H) ⁻	-0.54	6.48	-3.69	-9.41
43	1.24	16.03	-1.53	-0.81
(43-H) ⁻	-1.06	9.29	-2.86	-5.97
44	1.46	17.52	-1.63	-0.59
(44-H) ⁻	-0.26	12.68	-2.53	-3.76
45	0.21	10.28	-3.24	-5.76
(45-H) ⁻	-4.69	-2.89	-6.70	-17.22
46a	-1.34	12.56	-2.44	-2.23
(46a-H) ⁻	-3.62	6.03	-3.70	-7.77
46b	-0.31	14.50	-1.89	-0.87
(46b-H) ⁻	-3.36	6.65	-3.65	-7.39
47a	-0.57	14.38	-2.22	-1.63
(47a-H) ⁻	-2.24	9.33	-2.98	-5.77
47b	0.33	16.02	-1.89	-0.68
(47b-H) ⁻	-1.93	10.04	-3.01	-5.43
48	-2.68	14.54	-1.87	0.55
(48-H) ⁻	-4.45	10.70	-2.58	-2.07
49	-1.94	16.54	-2.04	0.11
(49-H) ⁻	-3.38	14.00	-2.52	-1.33
50	-0.10	8.38	-4.19	-8.56
(50-H) ⁻	-5.17	-5.52	-7.84	-20.73
51a	-1.18	9.94	-3.68	-6.39
(51a-H) ⁻	-4.01	1.10	-5.65	-13.85
51b	0.01	12.55	-2.99	-4.34
(51b-H) ⁻	-3.75	1.72	-5.65	-13.54
52a	-0.35	11.71	-3.25	-5.09
(52a-H) ⁻	-2.53	4.29	-4.74	-11.16
52b	0.73	14.02	-2.73	-3.43
(52b-H) ⁻	-2.23	4.92	-4.74	-10.91
53	-1.05	13.92	-2.62	-2.35
(53-H) ⁻	-3.19	7.73	-4.02	-7.32
54	-0.35	16.59	-2.35	-1.25
(54-H) ⁻	-1.80	12.25	-3.21	-4.33