

SUPPORTING INFORMATION

Evaluation of Mesoionic Compound Aromaticity Using the HOMHED Index

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Table S1. Bond lengths^a (Å) of compounds **1–25**.

Heterocycle						Exocyclic
Compound	O1-N2	N2-N3	N3-C4	C4-C5	C5-O1	C5-O6
1	1.376	1.315	1.341	1.404	1.415	1.219
2	1.381	1.316	1.343	1.408	1.423	1.217
3	1.370	1.306	1.362	1.429	1.420	1.207
4	1.378	1.311	1.334	1.407	1.415	1.211
5	1.380	1.315	1.344	1.414	1.416	1.218
6	1.381	1.320	1.328	1.413	1.430	1.200
7	1.375	1.308	1.331	1.397	1.405	1.214
8	1.367	1.297	1.363	1.424	1.412	1.208
9	1.377	1.311	1.346	1.419	1.405	1.210
10	1.399	1.304	1.353	1.424	1.395	1.196
Compound	N1-N2	N2-N3	N3-C4	C4-C5	C5-N1	C5-O6
11	1.347	1.295	1.366	1.416	1.427	1.218
Compound	O1-N2	N2-N3	N3-C4	C4-C5	C5-O1	C5-N6
12	1.382	1.301	1.347	1.400	1.379	1.313
13	1.378	1.312	1.348	1.388	1.382	1.312
14	1.383	1.301	1.349	1.409	1.391	1.296
Compound	N1-N2	N2-N3	N3-N4	N4-C5	C5-N1	C5-N6
15	1.342	1.294	1.335	1.378	1.403	1.299
16	1.333	1.293	1.341	1.355	1.389	1.324
17	1.340	1.294	1.340	1.384	1.410	1.287
Compound	S1-C2	C2-N3	N3-N4	N4-C5	C5-S1	C5-S6
18	1.703	1.320	1.379	1.317	1.769	1.678
Compound	N1-C2	C2-S3	S3-C4	C4-C5	C5-N1	C4-S6
19	1.330	1.709	1.748	1.376	1.406	1.706
20	1.341	1.705	1.737	1.391	1.400	1.713
Compound	N1-N2	N2-N3	N3-C4	C4-C5	C5-N1	C5-B6
21	1.332	1.321	1.364	1.394	1.370	1.606
22	1.328	1.315	1.358	1.393	1.365	1.610
23	1.334	1.323	1.367	1.390	1.376	1.605
24	1.339	1.325	1.366	1.396	1.369	1.600
Compound	N1-C2	C2-N3	N3-N4	N4-C5	C5-N1	C2-O6
25	1.485	1.349	1.395	1.305	1.333	1.231

^aBond lengths (Å) obtained experimentally from X-ray data.

Table S2. HOMHED, HOMHED⁺ and difference of these values for **1-25**.

Compound	HOMHED	HOMHED ⁺	Difference
1	0.653	0.653	0.00
2	0.607	0.607	0.00
3	0.61	0.614	0.01
4	0.647	0.646	0.00
5	0.634	0.634	0.00
6	0.569	0.568	0.00
7	0.696	0.695	0.00
8	0.65	0.654	0.01
9	0.678	0.679	0.00
10	0.659	0.661	0.00
11	0.814	0.855	0.05
12	0.768	0.769	0.00
13	0.771	0.772	0.00
14	0.722	0.724	0.00
15	0.872	0.902	0.03
16	0.925	0.941	0.02
17	0.845	0.881	0.04
18	0.761	0.76	0.00
19	0.812	0.834	0.03
20	0.856	0.875	0.02
21	0.963	0.974	0.01
22	0.976	0.984	0.01
23	0.951	0.965	0.01
24	0.955	0.966	0.01
25	0.494	0.586	0.19

Table S3. I^{AS}, I^{BS} indices of **1-25**.

Compound	I ^{AS}	I ^{BS}	Compound	I ^{AS}	I ^{BS}
1	0.458	0.542	14	0.618	0.382
2	0.390	0.610	15	0.830	0.170
3	0.397	0.603	16	0.885	0.115
4	0.456	0.544	17	0.789	0.211
5	0.445	0.555	18	0.591	0.409
6	0.352	0.648	19	0.680	0.320
7	0.533	0.467	20	0.752	0.248
8	0.460	0.540	21	0.943	0.057
9	0.527	0.473	22	0.963	0.037
10	0.571	0.429	23	0.924	0.076
11	0.705	0.295	24	0.939	0.061
12	0.694	0.306	25	0.208	0.792
13	0.680	0.320			