Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPLEMENTARY INFORMATION

Relating nucleus independent chemical shifts with integrated current density strengths†

Slavko Radenković* and Slađana Đorđević

University of Kragujevac, Faculty of Science, P. O. Box 60, 34000 Kragujevac, Serbia

*Corresponding authors: slavkoradenkovic@kg.ac.rs

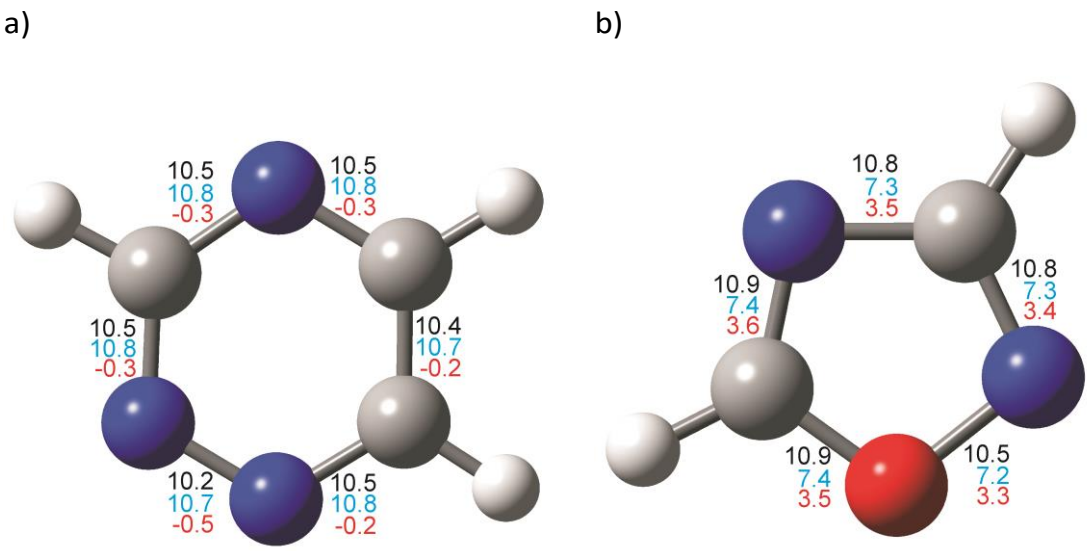

Fig. S1 Integrated bond current strengths in 1,2,4-triazine (a) and 2,4-diazafuran (b). J^{total} values are given in black, J^{π} in blue, and J^{σ} in red.

Table S1 Calculated $NICS_{iso}$ aromaticity indices for different hights above the ring plane of the studied molecules.

molecule	$NICS_{iso}(0)$	$NICS_{iso}(0.25)$	$NICS_{iso}(0.5)$	$NICS_{iso}(0.75)$	$NICS_{iso}(1)$	$NICS_{iso}(1.25)$	$NICS_{iso}(1.5)$	$NICS_{iso}(1.75)$
benzene	-8.13	-8.76	-9.94	-10.49	-10.01	-8.84	-7.43	-6.07
pyridine	-6.81	-7.67	-9.33	-10.28	-9.99	-8.86	-7.43	-6.04
1,2-diazine	-5.52	-6.26	-8.63	-10.17	-9.77	-9.17	-7.72	-5.88
1,3-diazine	-5.20	-6.59	-8.65	-9.91	-10.06	-8.68	-7.26	-6.16
1,4-diazine	-5.07	-6.35	-8.62	-10.08	-10.20	-9.02	-7.58	-6.28
1,2,3-triazine	-4.03	-5.30	-8.20	-10.15	-9.34	-9.35	-7.87	-5.56
1,2,4-triazine	-3.35	-4.82	-7.75	-9.77	-10.04	-9.09	-7.67	-6.23
1,3,5-triazine	-3.84	-5.30	-7.80	-9.36	-10.35	-8.29	-6.90	-6.38
1,2,3,4-tetrazine	-1.89	-3.75	-7.30	-9.81	-9.87	-9.42	-7.95	-6.09
1,2,3,5-tetrazine	-1.29	-3.62	-7.07	-9.45	-10.14	-8.95	-7.53	-6.38
1,2,4,5-tetrazine	-1.97	-3.14	-6.88	-9.55	-10.32	-9.29	-7.86	-6.45
pentazine	0.09	-2.02	-6.25	-9.30	-10.07	-9.27	-7.84	-6.35
hexazine	2.36	-0.11	-5.12	-8.86	-10.03	-9.38	-7.96	-6.43
furan	-11.97	-12.05	-11.87	-10.90	-9.28	-7.50	-5.91	-4.60
thiophene	-13.43	-13.51	-13.33	-12.38	-10.77	-8.95	-7.25	-5.80
pyrrole	-13.75	-13.73	-13.33	-12.11	-10.27	-8.30	-6.57	-5.15
2-azafuran	-12.35	-12.69	-12.96	-12.18	-10.47	-8.47	-6.64	-5.14
2-azathiophene	-13.66	-13.87	-13.92	-13.09	-11.45	-9.52	-7.69	-6.12
2-azapyrrole	-13.88	-14.12	-14.15	-13.13	-11.23	-9.10	-7.17	-5.58
3-azafuran	-12.15	-12.41	-12.53	-11.66	-9.97	-8.07	-6.35	-4.94
3-azathiophene	-13.53	-13.86	-14.14	-13.44	-11.80	-9.82	-7.93	-6.31
3-azapyrrole	-13.61	-13.80	-13.75	-12.71	-10.86	-8.82	-6.98	-5.47
2,3-diazafuran	-12.83	-13.39	-14.01	-13.36	-11.57	-9.40	-7.39	-5.72
2,3-diazathiophene	-13.66	-14.22	-14.96	-14.59	-13.04	-10.95	-8.86	-7.02
2,3-diazapyrrole	-13.93	-14.40	-14.84	-14.06	-12.17	-9.94	-7.86	-6.12
2,4-diazafuran	-13.14	-13.58	-13.95	-13.09	-11.19	-9.00	-7.03	-5.43
2,4-diazathiophene	-14.62	-14.97	-15.23	-14.40	-12.56	-10.38	-8.32	-6.58
2,4-diazapyrrole	-14.05	-14.44	-14.72	-13.77	-11.80	-9.55	-7.51	-5.84
2,5-diazafuran	-13.30	-13.89	-14.56	-13.90	-12.03	-9.75	-7.63	-5.87
2,5-diazathiophene	-14.86	-15.17	-15.39	-14.59	-12.81	-10.65	-8.57	-6.79
2,5-diazapyrrole	-14.51	-14.98	-15.41	-14.55	-12.57	-10.23	-8.05	-6.24
3,4-diazafuran	-12.39	-12.81	-13.19	-12.42	-10.66	-8.64	-6.80	-5.28
3,4-diazathiophene	-14.41	-14.89	-15.42	-14.77	-12.99	-10.78	-8.66	-6.85
3,4-diazapyrrole	-13.40	-13.81	-14.18	-13.37	-11.53	-9.39	-7.42	-5.80
2,3,4-triazafuran	-13.78	-14.43	-14.97	-13.87	-11.59	-9.13	-7.01	-5.34
2,3,4-triazathiophene	-15.41	-16.07	-16.78	-15.99	-13.89	-11.37	-9.02	-7.05
2,3,4-triazapyrrole	-14.26	-15.16	-16.18	-15.36	-13.06	-10.42	-8.08	-6.19
2,3,5-triazafuran	-15.12	-15.88	-16.59	-15.51	-13.05	-10.32	-7.92	-6.03
2,3,5-triazathiophene	-15.33	-16.01	-16.81	-16.17	-14.16	-11.65	-9.27	-7.27
2,3,5-triazapyrrole	-14.41	-15.36	-16.48	-15.72	-13.42	-10.72	-8.31	-6.37
tetraazafuran	-18.21	-18.85	-19.13	-17.43	-14.43	-11.31	-8.64	-6.54
tetraazathiophene	-18.60	-19.33	-20.06	-19.06	-16.55	-13.52	-10.68	-8.28
tetraazapyrrole	-16.56	-17.67	-18.90	-17.92	-15.22	-12.14	-9.38	-7.15

Table S2 Calculated $NICS_{zz}$ aromaticity indices for different hights above the ring plane of the studied molecules.

molecule	$NICS_{zz}(0)$	$NICS_{zz}(0.25)$	$NICS_{zz}(0.5)$	$NICS_{zz}(0.75)$	$NICS_{zz}(1)$	$NICS_{zz}(1.25)$	$NICS_{zz}(1.5)$	$NICS_{zz}(1.75)$
benzene	-16.08	-18.70	-24.25	-28.64	-29.78	-28.06	-24.78	-21.03
pyridine	-14.85	-17.66	-23.57	-28.12	-29.17	-27.28	-23.87	-20.08
1,2-diazine	-12.73	-16.41	-22.89	-27.78	-28.02	-26.85	-23.32	-18.96
1,3-diazine	-14.42	-15.76	-22.09	-26.91	-29.09	-26.10	-22.69	-19.43
1,4-diazine	-13.30	-17.40	-23.61	-28.22	-28.86	-26.93	-23.31	-19.48
1,2,3-triazine	-9.35	-15.07	-22.15	-27.38	-26.21	-26.34	-22.70	-17.64
1,2,4-triazine	-11.48	-14.82	-21.73	-26.89	-28.01	-25.93	-22.36	-18.54
1,3,5-triazine	-11.64	-12.64	-19.52	-24.81	-28.48	-24.47	-21.20	-18.83
1,2,3,4-tetrazine	-8.19	-13.00	-20.68	-26.36	-26.69	-25.49	-21.86	-17.56
1,2,3,5-tetrazine	-9.08	-11.89	-19.53	-25.27	-27.50	-24.75	-21.27	-17.98
1,2,4,5-tetrazine	-9.26	-12.79	-20.46	-26.18	-27.61	-25.42	-21.81	-18.03
pentazine	-5.37	-9.54	-18.13	-24.56	-26.24	-24.32	-20.81	-17.09
hexazine	-0.05	-4.82	-14.65	-22.16	-24.48	-22.91	-19.63	-16.09
furan	-10.26	-14.09	-21.62	-26.59	-27.07	-24.51	-20.79	-17.07
thiophene	-13.81	-17.46	-24.97	-30.52	-31.69	-29.42	-25.53	-21.33
pyrrole	-14.04	-18.03	-25.84	-30.91	-31.17	-28.14	-23.86	-19.58
2-azafuran	-14.24	-17.98	-25.04	-29.17	-28.73	-25.43	-21.22	-17.21
2-azathiophene	-17.10	-20.57	-27.54	-32.30	-32.65	-29.75	-25.44	-21.03
2-azapyrrole	-16.70	-20.66	-28.20	-32.66	-32.22	-28.62	-23.96	-19.47
3-azafuran	-13.22	-16.95	-24.09	-28.44	-28.25	-25.15	-21.06	-17.11
3-azathiophene	-17.04	-20.59	-27.72	-32.58	-32.97	-30.06	-25.74	-21.28
3-azapyrrole	-16.20	-20.14	-27.68	-32.21	-31.87	-28.35	-23.75	-19.31
2,3-diazafuran	-19.98	-23.46	-29.73	-32.72	-31.13	-26.93	-22.10	-17.69
2,3-diazathiophene	-22.82	-26.16	-32.59	-36.35	-35.57	-31.68	-26.65	-21.77
2,3-diazapyrrole	-21.31	-25.12	-32.08	-35.58	-34.12	-29.70	-24.49	-19.67
2,4-diazafuran	-18.61	-22.04	-28.31	-31.48	-30.21	-26.29	-21.66	-17.39
2,4-diazathiophene	-22.17	-25.34	-31.48	-35.15	-34.49	-30.82	-26.00	-21.28
2,4-diazapyrrole	-19.59	-23.38	-30.41	-34.18	-33.07	-28.97	-23.98	-19.31
2,5-diazafuran	-20.67	-24.10	-30.24	-33.04	-31.31	-27.02	-22.14	-17.71
2,5-diazathiophene	-23.59	-26.63	-32.49	-35.87	-34.98	-31.12	-26.17	-21.37
2,5-diazapyrrole	-21.47	-25.24	-32.14	-35.63	-34.18	-29.77	-24.56	-19.73
3,4-diazafuran	-17.03	-20.54	-27.07	-30.57	-29.56	-25.84	-21.35	-17.17
3,4-diazathiophene	-23.11	-26.34	-32.54	-36.12	-35.29	-31.43	-26.47	-21.64
3,4-diazapyrrole	-19.31	-23.12	-30.22	-34.04	-32.94	-28.83	-23.85	-19.20
2,3,4-triazafuran	-22.48	-26.03	-32.10	-34.31	-31.82	-26.93	-21.72	-17.16
2,3,4-triazathiophene	-28.44	-31.51	-37.02	-39.38	-37.24	-32.36	-26.75	-21.58
2,3,4-triazapyrrole	-24.70	-29.28	-37.11	-40.11	-37.27	-31.50	-25.34	-19.96
2,3,5-triazafuran	-29.73	-32.99	-38.18	-39.17	-35.44	-29.54	-23.58	-18.50
2,3,5-triazathiophene	-32.32	-35.24	-40.36	-42.17	-39.38	-33.88	-27.78	-22.25
2,3,5-triazapyrrole	-27.50	-31.93	-39.40	-41.94	-38.65	-32.49	-26.03	-20.44
tetraazafuran	-39.34	-41.78	-44.97	-43.76	-38.31	-31.28	-24.64	-19.14
tetraazathiophene	-43.91	-46.10	-49.31	-48.75	-43.88	-36.85	-29.73	-23.56
tetraazapyrrole	-36.55	-40.62	-46.83	-47.46	-42.32	-34.78	-27.43	-21.29

Table S3 Calculated $NICS_{\pi,iso}$ aromaticity indices for different hights above the ring plane of the studied molecules.

molecule	$NICS_{\pi,iso}(0)$	$NICS_{\pi,iso}(0.25)$	$NICS_{\pi,iso}(0.5)$	$NICS_{\pi,iso}(0.75)$	$NICS_{\pi,iso}(1)$	$NICS_{\pi,iso}(1.25)$	$NICS_{\pi,iso}(1.5)$	$NICS_{\pi,iso}(1.75)$
benzene	-24.76	-23.47	-20.07	-15.72	-11.51	-8.08	-5.56	-3.80
pyridine	-25.07	-23.65	-19.99	-15.40	-11.07	-7.65	-5.17	-3.49
1,2-diazine	-25.24	-23.69	-19.73	-14.87	-10.43	-7.02	-4.65	-3.07
1,3-diazine	-25.17	-23.68	-19.83	-15.06	-10.69	-7.27	-4.88	-3.26
1,4-diazine	-25.09	-23.62	-19.84	-15.15	-10.79	-7.39	-4.95	-3.30
1,2,3-triazine	-25.07	-23.38	-19.14	-14.05	-9.54	-6.19	-3.95	-2.51
1,2,4-triazine	-25.05	-23.49	-19.50	-14.61	-10.20	-6.82	-4.50	-2.95
1,3,5-triazine	-25.50	-23.95	-19.96	-15.06	-10.58	-7.14	-4.73	-3.12
1,2,3,4-tetrazine	-25.22	-23.55	-19.36	-14.29	-9.77	-6.40	-4.12	-2.64
1,2,3,5-tetrazine	-25.22	-23.62	-19.51	-14.52	-10.04	-6.65	-4.35	-2.83
1,2,4,5-tetrazine	-25.18	-23.59	-19.54	-14.61	-10.16	-6.80	-4.45	-2.90
pentazine	-25.34	-23.69	-19.48	-14.38	-9.85	-6.46	-4.18	-2.68
hexazine	-25.42	-23.77	-19.56	-14.49	-9.98	-6.59	-4.27	-2.74
furan	-23.62	-21.37	-16.14	-10.67	-6.47	-3.74	-2.10	-1.16
thiophene	-25.24	-23.20	-18.29	-12.83	-8.31	-5.24	-3.30	-2.09
pyrrole	-25.16	-23.00	-17.83	-12.24	-7.78	-4.76	-2.88	-1.76
2-azafuran	-24.02	-21.75	-16.44	-10.85	-6.55	-3.78	-2.12	-1.17
2-azathiophene	-25.38	-23.29	-18.21	-12.59	-8.04	-4.99	-3.07	-1.90
2-azapyrrole	-25.72	-23.49	-18.18	-12.41	-7.82	-4.73	-2.85	-1.72
3-azafuran	-23.61	-21.29	-15.88	-10.26	-6.03	-3.35	-1.81	-0.96
3-azathiophene	-25.74	-23.61	-18.48	-12.80	-8.19	-5.09	-3.15	-1.97
3-azapyrrole	-25.56	-23.26	-17.83	-12.02	-7.45	-4.44	-2.64	-1.58
2,3-diazafuran	-24.43	-22.07	-16.57	-10.83	-6.49	-3.73	-2.10	-1.18
2,3-diazathiophene	-26.11	-23.93	-18.71	-12.97	-8.34	-5.23	-3.27	-2.05
2,3-diazapyrrole	-26.17	-23.82	-18.30	-12.38	-7.74	-4.69	-2.84	-1.71
2,4-diazafuran	-24.10	-21.72	-16.18	-10.38	-6.03	-3.31	-1.76	-0.89
2,4-diazathiophene	-25.80	-23.57	-18.24	-12.41	-7.75	-4.67	-2.81	-1.70
2,4-diazapyrrole	-25.84	-23.49	-17.93	-11.97	-7.33	-4.31	-2.51	-1.47
2,5-diazafuran	-24.49	-22.20	-16.78	-11.05	-6.67	-3.84	-2.17	-1.18
2,5-diazathiophene	-25.74	-23.55	-18.31	-12.55	-7.94	-4.87	-2.98	-1.81
2,5-diazapyrrole	-25.89	-23.69	-18.30	-12.44	-7.82	-4.75	-2.86	-1.71
3,4-diazafuran	-23.61	-21.21	-15.66	-9.92	-5.66	-3.05	-1.60	-0.80
3,4-diazathiophene	-26.15	-23.93	-18.60	-12.75	-8.07	-4.96	-3.05	-1.88
3,4-diazapyrrole	-25.6	-23.23	-17.68	-11.74	-7.14	-4.17	-2.42	-1.41
2,3,4-triazafuran	-24.52	-21.68	-15.27	-8.99	-4.65	-2.18	-0.94	-0.31
2,3,4-triazathiophene	-26.38	-23.87	-18.00	-11.79	-7.08	-4.12	-2.40	-1.38
2,3,4-triazapyrrole	-27.81	-24.92	-18.28	-11.54	-6.64	-3.68	-2.03	-1.12
2,3,5-triazafuran	-25.88	-23.04	-16.63	-10.23	-5.66	-2.96	-1.50	-0.72
2,3,5-triazathiophene	-27.10	-24.57	-18.63	-12.32	-7.48	-4.37	-2.55	-1.54
2,3,5-triazapyrrole	-28.50	-25.59	-18.90	-12.08	-7.10	-4.03	-2.31	-1.32
tetraazafuran	-25.28	-22.38	-15.85	-9.44	-5.04	-2.54	-1.21	-0.53
tetraazathiophene	-27.22	-24.63	-18.57	-12.24	-7.48	-4.46	-2.64	-1.54
tetraazapyrrole	-18.27	-17.11	-13.88	-9.79	-6.28	-3.88	-2.38	-1.44

Table S4 Calculated $NICS_{\pi,zz}$ aromaticity indices for different hights above the ring plane of the studied molecules.

molecule	$NICS_{\pi,zz}(0)$	$NICS_{\pi,zz}(0.25)$	$NICS_{\pi,zz}(0.5)$	$NICS_{\pi,zz}(0.75)$	$NICS_{\pi,zz}(1)$	$NICS_{\pi,zz}(1.25)$	$NICS_{\pi,zz}(1.5)$	$NICS_{\pi,zz}(1.75)$
benzene	-36.63	-36.53	-35.70	-33.40	-29.61	-25.10	-20.56	-16.52
pyridine	-36.46	-36.32	-35.38	-32.90	-28.96	-24.33	-19.76	-15.76
1,2-diazine	-35.59	-35.39	-34.33	-31.72	-27.71	-23.08	-18.61	-14.73
1,3-diazine	-36.99	-36.84	-35.79	-33.08	-28.88	-24.01	-19.33	-15.28
1,4-diazine	-36.75	-36.51	-35.46	-32.82	-28.72	-23.95	-19.34	-15.32
1,2,3-triazine	-34.03	-33.81	-32.65	-29.99	-25.99	-21.48	-17.20	-13.53
1,2,4-triazine	-36.55	-36.30	-35.13	-32.30	-28.02	-23.16	-18.52	-14.56
1,3,5-triazine	-37.04	-36.72	-35.52	-32.70	-28.41	-23.52	-18.85	-14.84
1,2,3,4-tetrazine	-36.09	-35.82	-34.54	-31.59	-27.20	-22.32	-17.73	-13.85
1,2,3,5-tetrazine	-37.50	-37.26	-35.98	-32.90	-28.30	-23.18	-18.39	-14.35
1,2,4,5-tetrazine	-37.17	-36.80	-35.45	-32.47	-28.00	-23.01	-18.31	-14.33
pentazine	-37.59	-37.27	-35.84	-32.60	-27.88	-22.71	-17.92	-13.93
hexazine	-38.40	-38.07	-36.49	-32.99	-28.03	-22.68	-17.79	-13.76
furan	-19.58	-18.03	-25.90	-23.91	-20.71	-17.03	-13.56	-10.61
thiophene	-20.97	-26.84	-29.86	-28.52	-25.36	-21.43	-17.45	-13.92
pyrrole	-19.91	-31.94	-31.77	-29.42	-25.47	-20.94	-16.66	-13.03
2-azafuran	-21.49	-24.90	-25.31	-23.46	-20.30	-16.68	-13.25	-10.34
2-azathiophene	-30.21	-28.78	-28.93	-27.41	-24.26	-20.40	-16.54	-13.13
2-azapyrrole	-32.42	-31.73	-31.26	-28.85	-24.87	-20.34	-16.11	-12.55
3-azafuran	-19.23	-26.45	-25.51	-23.29	-19.98	-16.32	-12.91	-10.05
3-azathiophene	-21.04	-29.91	-29.98	-28.14	-24.78	-20.76	-16.80	-13.33
3-azapyrrole	-20.38	-31.90	-31.10	-28.56	-24.53	-20.02	-15.81	-12.29
2,3-diazafuran	-27.79	-27.40	-26.32	-23.95	-20.46	-16.63	-13.10	-10.15
2,3-diazathiophene	-31.07	-30.92	-30.24	-28.18	-24.67	-20.54	-16.54	-13.05
2,3-diazapyrrole	-32.69	-32.54	-31.57	-28.83	-24.62	-19.98	-15.70	-12.15
2,4-diazafuran	-26.31	-25.66	-24.77	-22.59	-19.36	-15.78	-12.46	-9.67
2,4-diazathiophene	-29.47	-29.06	-28.51	-26.64	-23.36	-19.49	-15.71	-12.42
2,4-diazapyrrole	-31.51	-31.27	-30.37	-27.76	-23.74	-19.28	-15.17	-11.73
2,5-diazafuran	-27.51	-26.57	-25.45	-23.37	-20.15	-16.48	-13.02	-10.11
2,5-diazathiophene	-30.05	-29.70	-28.92	-27.02	-23.75	-19.83	-15.98	-12.62
2,5-diazapyrrole	-32.72	-32.44	-31.46	-28.80	-24.65	-20.02	-15.75	-12.19
3,4-diazafuran	-18.90	-25.62	-24.59	-22.32	-19.05	-15.48	-12.20	-9.46
3,4-diazathiophene	-30.34	-30.31	-29.67	-27.60	-24.13	-20.10	-16.19	-12.78
3,4-diazapyrrole	-31.33	-31.24	-30.30	-27.66	-23.61	-19.15	-15.04	-11.65
2,3,4-triazafuran	-24.61	-24.26	-23.02	-20.66	-17.45	-14.03	-10.93	-8.40
2,3,4-triazathiophene	-28.71	-28.54	-27.64	-25.48	-22.08	-18.24	-14.57	-11.43
2,3,4-triazapyrrole	-33.81	-33.73	-32.54	-29.22	-24.39	-19.31	-14.83	-11.27
2,3,5-triazafuran	-28.31	-27.89	-26.57	-23.88	-20.09	-16.03	-12.38	-9.44
2,3,5-triazathiophene	-31.59	-31.54	-30.74	-28.36	-24.47	-20.09	-15.91	-12.32
2,3,5-triazapyrrole	-36.09	-36.03	-34.81	-31.25	-26.03	-20.52	-15.70	-11.88
tetraazafuran	-26.27	-25.87	-24.46	-21.78	-18.19	-14.46	-11.17	-8.50
tetraazathiophene	-30.96	-30.85	-29.91	-27.38	-23.46	-19.17	-15.12	-11.74
tetraazapyrrole	-20.89	-22.34	-24.28	-23.63	-20.49	-16.45	-12.67	-9.59

Table S5 Statistical data pertaining to the approximation of the form: $\mathrm{NICS}_{ZZ}(z) \approx a \cdot J^{\pi} + b$. The unit for constant *a* is ppm/(nA T^{-1}), and for constant *b* is ppm.

z	*a*±Δ*a*	*b*±Δ*b*	R	S	F	P
0.00	3.55±0.87	-51.49±8.16	0.5357	7.576	16.50	$2.1 \cdot 10^{-4}$
0.25	3.55±0.85	-55.01±7.89	0.5486	7.327	17.65	$1.4 \cdot 10^{-4}$
0.50	3.23±0.76	-58.68±7.08	0.5534	6.578	18.10	$1.2 \cdot 10^{-4}$
0.75	2.38±0.62	-54.67±5.81	0.5122	5.393	14.58	$4.5 \cdot 10^{-4}$
1.00	1.36±0.47	-44.63±4.42	0.4095	4.106	8.26	$6.4 \cdot 10^{-3}$
1.25	0.56±0.35	-33.59±3.28	0.2415	3.042	2.54	$1.2 \cdot 10^{-1}$
1.50	0.07±0.26	-24.41±2.46	0.0388	2.284	0.06	$8.0 \cdot 10^{-1}$
1.75	-0.19±0.20	-17.63±1.90	0.1408	1.766	0.83	$3.7 \cdot 10^{-1}$

Table S6 Correlation coefficients (R) between different NICS indices and integrated bond current strengths for the six membered rings (in total 13 data-points).

	$\mathrm{NICS}_{iso}(0)$	$\mathrm{NICS}_{iso}(1)$	$\mathrm{NICS}_{zz}(0)$	$\mathrm{NICS}_{zz}(1)$	J^{total}	$J^{\mathrm{total}}_{\mathrm{dia}}$	$J^{\mathrm{total}}_{\mathrm{para}}$	J^{π}	J^{σ}	$J^{\sigma}_{\mathrm{dia}}$	$J^{\sigma}_{\mathrm{para}}$
$\mathrm{NICS}_{iso}(0)$	1.0000										
$\mathrm{NICS}_{iso}(1)$	-0.1384	1.0000									
$\mathrm{NICS}_{zz}(0)$	0.9598	0.0442	1.0000								
$\mathrm{NICS}_{zz}(1)$	0.8812	0.3080	0.9606	1.0000							
J^{total}	-0.9610	-0.0968	-0.9757	-0.9650	1.0000						
$J^{\mathrm{total}}_{\mathrm{dia}}$	-0.8181	-0.1769	-0.8591	-0.8526	0.8084	1.0000					
$J^{\mathrm{total}}_{\mathrm{para}}$	-0.1649	0.1391	-0.1204	-0.1143	0.2424	-0.3751	1.0000				
J^{π}	-0.6107	-0.5062	-0.6351	-0.7832	0.7606	0.5833	0.2363	1.0000			
J^{σ}	-0.9682	0.1286	-0.9753	-0.8858	0.9439	0.7791	0.2024	0.5036	1.0000		
$J^{\sigma}_{\mathrm{dia}}$	-0.6963	-0.0419	-0.7400	-0.6859	0.6325	0.9501	-0.5700	0.3078	0.6851	1.0000	
$J^{\sigma}_{\mathrm{para}}$	-0.1353	0.1993	-0.0844	-0.0579	0.1945	-0.4168	0.9934	0.1437	0.1858	-0.5885	1.0000

Table S7 Correlation coefficients (R) between different NICS indices and integrated bond current strengths for the five-membered rings (in total 30 data-points).

	$\mathrm{NICS}_{iso}(0)$	$\mathrm{NICS}_{iso}(1)$	$\mathrm{NICS}_{zz}(0)$	$\mathrm{NICS}_{zz}(1)$	J^{total}	$J^{\mathrm{total}}_{\mathrm{dia}}$	$J^{\mathrm{total}}_{\mathrm{para}}$	J^{π}	J^{σ}	$J^{\sigma}_{\mathrm{dia}}$	$J^{\sigma}_{\mathrm{para}}$
$\mathrm{NICS}_{iso}(0)$	1.0000										
$\mathrm{NICS}_{iso}(1)$	0.9039	1.0000									
$\mathrm{NICS}_{zz}(0)$	0.9319	0.9619	1.0000								
$\mathrm{NICS}_{zz}(1)$	0.8910	0.9693	0.9209	1.0000							
J^{total}	-0.8831	-0.9378	-0.8592	-0.9710	1.0000						
$J^{\mathrm{total}}_{\mathrm{dia}}$	-0.7425	-0.8321	-0.7314	-0.8934	0.9202	1.0000					
$J^{\mathrm{total}}_{\mathrm{para}}$	-0.4898	-0.4167	-0.4553	-0.3557	0.3659	-0.0275	1.0000				
J^{π}	0.0091	-0.0306	0.1716	-0.1844	0.3096	0.4223	-0.2136	1.0000			
J^{σ}	-0.8772	-0.9054	-0.9595	-0.8379	0.7850	0.6328	0.5002	-0.3461	1.0000		
$J^{\sigma}_{\mathrm{dia}}$	-0.8056	-0.8487	-0.8762	-0.8195	0.7752	0.8090	0.0563	-0.1338	0.8521	1.0000	
$J^{\sigma}_{\mathrm{para}}$	-0.5159	-0.5083	-0.5712	-0.4228	0.3857	0.0534	0.8582	-0.4609	0.6809	0.1967	1.0000

Table S8 Statistical data pertaining to the approximation of the form: $\mathrm{NICS}_{\mathrm{iso}}(z) \approx a \cdot J^{\mathrm{total}} + b$; correlation coefficient (R), standard error (S), Fisher's F-value (F) and probability (P).

z	*a±Δa*	*b±Δb*	R	S	F	P
0.00	-2.60±0.32	19.49±3.78	0.7850	3.369	65.83	$4.6 \cdot 10^{-10}$
0.25	-2.43±0.28	16.82±3.30	0.8060	2.940	76.02	$7.0 \cdot 10^{-11}$
0.50	-1.99±0.19	10.39±2.26	0.8509	2.016	107.61	$5.0 \cdot 10^{-13}$
0.75	-1.42±0.11	3.75±1.32	0.8924	1.179	160.41	$9.3 \cdot 10^{-16}$
1.00	-0.93±0.07	-0.62±0.85	0.8973	0.754	169.49	$3.7 \cdot 10^{-16}$
1.25	-0.60±0.06	-2.61±0.74	0.8338	0.655	93.49	$3.9 \cdot 10^{-12}$
1.50	-0.40±0.06	-3.13±0.68	0.7309	0.607	47.02	$2.6 \cdot 10^{-8}$
1.75	-0.27±0.05	-2.99±0.60	0.6342	0.535	25.59	$5.0 \cdot 10^{-6}$

Table S9 Statistical data pertaining to the approximation of the form: $\mathrm{NICS}_{\pi,\mathrm{iso}}(z) \approx a \cdot J^{\pi} + b$. The notation is the same as in Table S8.

z	*a±Δa*	*b±Δb*	R	S	F	P
0.00	-0.28±0.17	-22.63±1.56	0.2567	1.451	2.89	$9.7 \cdot 10^{-2}$
0.25	-0.54±0.13	-18.16±1.23	0.5394	1.143	16.82	$1.9 \cdot 10^{-4}$
0.50	-1.03±0.07	-8.59±0.62	0.9233	0.579	237.08	$1.2 \cdot 10^{-18}$
0.75	-1.31±0.04	-0.40±0.41	0.9781	0.378	903.81	$1.5 \cdot 10^{-29}$
1.00	-1.28±0.05	3.84±0.48	0.9693	0.441	637.58	$1.3 \cdot 10^{-26}$
1.25	-1.08±0.05	4.96±0.45	0.9606	0.422	489.71	$2.1 \cdot 10^{-24}$
1.50	-0.83±0.04	4.61±0.37	0.9568	0.342	443.94	$1.3 \cdot 10^{-23}$
1.75	-0.62±0.03	3.83±0.28	0.9561	0.257	436.56	$1.8 \cdot 10^{-23}$

Table S10 Statistical data pertaining to the approximation of the form $\mathrm{NICS}_{\mathrm{iso}}(z) \approx a \cdot J_{\mathrm{para}}^{\mathrm{total}} + b \cdot J_{\mathrm{dia}}^{\mathrm{total}} + c$. The notation is the same as in Table S8.

Z	*a±Δa*	*b±Δb*	*c±Δc*	R	S	F	P
0.00	-4.48±0.49	-1.71±0.33	-4.47±6.17	0.8633	2.779	58.54	$1.3 \cdot 10^{-12}$
0.25	-4.11±0.43	-1.64±0.28	-4.49±5.33	0.8787	2.401	67.75	$1.4 \cdot 10^{-13}$
0.50	-3.15±0.29	-1.44±0.19	-4.35±3.64	0.9068	1.638	92.54	$9.9 \cdot 10^{-16}$
0.75	-2.00±0.18	-1.14±0.12	-3.69±2.27	0.9222	1.023	113.79	$3.1 \cdot 10^{-17}$
1.00	-1.09±0.13	-0.86±0.09	-2.60±1.66	0.9023	0.746	87.59	$2.4 \cdot 10^{-15}$
1.25	-0.52±0.12	-0.64±0.08	-1.52±1.46	0.8371	0.657	46.82	$3.3 \cdot 10^{-11}$
1.50	-0.21±0.10	-0.48±0.07	-0.78±1.29	0.7622	0.583	27.73	$2.8 \cdot 10^{-8}$
1.75	-0.06±0.09	-0.37±0.06	-0.35±1.10	0.7066	0.496	19.94	$9.8 \cdot 10^{-7}$

Table S11 Statistical data pertaining to the approximation of the form: $\mathrm{NICS}_{\mathrm{iso}}(z) \approx a \cdot J^{\pi} + b \cdot J^{\sigma} + c$. The notation is the same as in Table S8.

Z	*a±Δa*	*b±Δb*	*c±Δc*	R	S	F	P
0.00	0.01±0.34	-2.12±0.19	-5.82±3.50	0.9364	1.933	142.33	$6.5 \cdot 10^{-19}$
0.25	-0.05±0.26	-2.00±0.15	-6.30±2.73	0.9542	1.505	203.24	$1.1 \cdot 10^{-21}$
0.50	-0.23±0.13	-1.66±0.07	-6.68±1.37	0.9810	0.753	511.95	$3.2 \cdot 10^{-29}$
0.75	-0.43±0.10	-1.24±0.05	-5.79±0.99	0.9783	0.548	446.01	$4.5 \cdot 10^{-28}$
1.00	-0.58±0.12	-0.87±0.07	-4.05±1.20	0.9239	0.662	116.63	$2.0 \cdot 10^{-17}$
1.25	-0.63±0.12	-0.61±0.07	-2.37±1.20	0.8340	0.663	45.71	$4.7 \cdot 10^{-11}$
1.50	-0.60±0.10	-0.43±0.06	-1.19±1.04	0.7693	0.575	29.00	$1.6 \cdot 10^{-8}$
1.75	-0.53±0.08	-0.31±0.05	-0.48±0.84	0.7490	0.464	25.56	$7.1 \cdot 10^{-8}$

Table S12 Statistical data pertaining to the approximation of the form: $\mathrm{NICS}_{\mathrm{iso}}(z) \approx a \cdot J^{\pi} + b \cdot J_{\mathrm{para}}^{\sigma} + c\mathrm{J}_{\mathrm{dia}}^{\sigma} + d$. The notation is the same as in Table S8.

z	*a±Δa*	*b±Δb*	*c±Δc*	*d±Δd*	R	S	F	P
0.00	-0.11±0.37	-2.39±0.36	-1.95±0.27	-7.74±4.10	0.9377	1.937	94.72	$5.9 \cdot 10^{-19}$
0.25	-0.14±0.29	-2.20±0.28	-1.87±0.21	-7.73±3.20	0.9550	1.510	134.86	$1.2 \cdot 10^{-20}$
0.50	-0.26±0.14	-1.73±0.14	-1.62±0.10	-7.18±1.61	0.9812	0.759	335.99	$6.8 \cdot 10^{-28}$
0.75	-0.42±0.10	-1.22±0.10	-1.25±0.08	-5.65±1.17	0.9783	0.554	290.34	$1.0 \cdot 10^{-26}$
1.00	-0.55±0.13	-0.81±0.12	-0.90±0.09	-3.63±1.41	0.9246	0.668	76.57	$2.1 \cdot 10^{-16}$
1.25	-0.59±0.13	-0.54±0.12	-0.65±0.09	-1.90±1.41	0.8360	0.668	30.18	$2.9 \cdot 10^{-10}$
1.50	-0.57±0.11	-0.37±0.11	-0.47±0.08	-0.77±1.23	0.7723	0.579	19.21	$8.3 \cdot 10^{-8}$
1.75	-0.50±0.90	-0.27±0.09	-0.34±0.06	-0.14±0.99	0.7521	0.468	16.93	$3.4 \cdot 10^{-7}$

Table S13 Statistical data pertaining to the approximation of the form: $NICS_{zz}(z) \approx a \cdot J^{\text{total}}_{\text{para}} + b \cdot J^{\text{total}}_{\text{dia}} + c$. The units for constants *a* and *b* are ppm/(nA T^{-1}), and for constant *c* is ppm.

Z	*a±Δa*	*b±Δb*	*c±Δc*	R	S	F	P
0.00	-6.04±0.62	-4.50±0.41	26.54±7.75	0.9231	3.492	115.29	$2.5 \cdot 10^{-17}$
0.25	-5.95±0.61	-4.35±0.41	20.93±7.64	0.9217	3.442	112.89	$3.6 \cdot 10^{-17}$
0.50	-5.40±0.56	-3.89±0.37	9.30±6.94	0.9202	3.129	110.60	$5.0 \cdot 10^{-17}$
0.75	-4.23±0.40	-3.21±0.27	-0.06±5.05	0.9338	2.275	136.22	$1.4 \cdot 10^{-18}$
1.00	-2.89±0.21	-2.52±0.14	-4.34±2.66	0.9647	1.200	268.30	$6.7 \cdot 10^{-24}$
1.25	-1.78±0.09	-1.93±0.06	-5.15±1.14	0.9867	0.515	738.89	$2.6 \cdot 10^{-32}$
1.50	-1.04±0.11	-1.47±0.07	-4.53±1.35	0.9647	0.610	267.98	$6.8 \cdot 10^{-24}$
1.75	-0.58±0.14	-1.12±0.09	-3.60±1.75	0.9000	0.787	85.22	$3.8 \cdot 10^{-15}$

Table S14 Statistical data pertaining to the approximation of the form: $NICS_{zz}(z) \approx a \cdot J^{\pi} + b \cdot J^{\sigma}_{\text{para}} + c]^{\sigma}_{\text{dia}} + d$. The units for constants *a, b* and *c* are ppm/(nA T^{-1}), and for constant *d* is ppm.

z	*a±Δa*	*b±Δb*	*c±Δc*	*d±Δd*	R	S	F	P
0.00	-2.09±0.44	-3.66±0.43	-5.07±0.32	21.61±4.95	0.9672	2.337	188.42	$3.0 \cdot 10^{-23}$
0.25	-1.94±0.42	-3.61±0.41	-4.87±0.31	15.43±4.74	0.9685	2.238	196.58	$1.4 \cdot 10^{-23}$
0.50	-1.76±0.39	-3.37±0.38	-4.29±0.28	3.53±4.39	0.9667	2.073	185.27	$4.1 \cdot 10^{-23}$
0.75	-1.80±0.31	-2.93±0.30	-3.44±0.23	-4.44±3.50	0.9665	1.651	184.62	$4.4 \cdot 10^{-23}$
1.00	-1.93±0.19	-2.39±0.19	-2.60±0.14	-6.53±2.15	0.9754	1.017	254.76	$1.2 \cdot 10^{-25}$
1.25	-1.96±0.10	-1.88±0.10	-1.91±0.07	-5.47±1.11	0.9866	0.524	476.42	$9.4 \cdot 10^{-31}$
1.50	-1.84±0.08	-1.46±0.08	-1.40±0.06	-3.70±0.91	0.9831	0.429	374.63	$8.8 \cdot 10^{-29}$
1.75	-1.64±0.10	-1.13±0.09	-1.03±0.07	-2.24±1.09	0.9600	0.512	152.71	$1.4 \cdot 10^{-21}$

Table S15 Cartesian coordinates (in au) of the optimized structures obtained at the B3LYP/def2-TZVPP level of theory.

benzene

C	1.20468300	0.69553400	0.00000000
C	0.00000400	1.39100000	0.00000000
C	-1.20468300	0.69547600	0.00000000
C	-1.20468300	-0.69553400	0.00000000
C	-0.00000400	-1.39100000	0.00000000
C	1.20468300	-0.69547600	0.00000000
H	2.14193700	1.23662700	0.00000000
H	0.00004400	2.47323100	0.00000000
H	-2.14192800	1.23658500	0.00000000
H	-2.14193700	-1.23662700	0.00000000
H	-0.00004400	-2.47323100	0.00000000
H	2.14192800	-1.23658500	0.00000000

1,2-diazine

C	-1.31876400	-0.07436900	-0.00012300
C	-0.69488400	1.17085400	0.00010900
C	0.68312200	1.17737100	0.00023400
C	1.31948100	-0.06112100	0.00009400
N	0.66973800	-1.22205000	-0.00012900
H	-1.27595200	2.08303100	0.00015700
H	-2.39831600	-0.16331100	-0.00020500
H	1.25502000	2.09547700	0.00042600
H	2.39969100	-0.13990300	0.00019200
N	-0.65747700	-1.22819300	-0.00022100

1,4-diazine

C	-1.13034500	0.69566800	0.00012400
C	-1.13038400	-0.69561300	0.00017400
C	1.13039500	-0.69559600	-0.00010600
C	1.13033500	0.69568300	-0.00020500
N	-0.00001100	1.39943800	-0.00008100
H	-2.06083200	1.25165500	0.00022800
H	-2.06079300	-1.25215600	0.00036200
H	2.06081400	-1.25212400	-0.00020400
H	2.06081100	1.25168800	-0.00035600
N	0.00001100	-1.39942600	0.00008800

1,2,4-triazine

C	-1.24671000	0.30302000	-0.00021500
C	0.88821600	0.97298400	0.00011300
C	1.24987500	-0.37226400	0.00019600
N	0.33710300	-1.33639500	0.00008300
H	-2.30414700	0.53800700	-0.00032700
H	1.63135200	1.76296000	0.00020000
H	2.28405900	-0.69174800	0.00035500
N	-0.94415400	-0.99249800	-0.00011000
N	-0.38717100	1.32437100	-0.00008600

1,2,3,4-tetrazine

N	-1.17820900	0.65486100	-0.00013400
N	-1.17816700	-0.65503000	-0.00018300

pyridine

C	-1.13993400	-0.71932500	-0.00021600
C	-1.19359000	0.67002300	-0.00012300
C	0.00030100	1.37890700	0.00009900
C	1.19388200	0.66952200	0.00021200
C	1.13962100	-0.71980100	0.00012100
N	-0.00030700	-1.41215400	-0.00009200
H	0.00050700	2.46106300	0.00016900
H	-2.05393300	-1.30305400	-0.00037300
H	-2.14826700	1.17799800	-0.00024300
H	2.14879800	1.17705300	0.00034800
H	2.05336100	-1.30392900	0.00018300

1,3-diazine

C	1.30719200	-0.00930800	-0.00015200
C	-0.62955700	-1.17616300	0.00001400
C	-1.34952800	0.00975100	0.00017100
C	-0.61178500	1.18524900	0.00008000
N	0.72103900	1.18611400	-0.00012400
H	-1.13014700	-2.13840400	0.00026800
H	2.39156300	-0.01792400	-0.00027000
H	-2.43030200	0.01806600	0.00036400
H	-1.09856500	2.15442600	0.00013700
N	0.70317800	-1.19659100	-0.00004300

1,2,3-triazine

C	-0.47188700	-1.22343300	0.00006400
C	-1.33808400	-0.14677300	0.00016100
C	-0.72786100	1.09137500	0.00004900
N	0.60084800	1.22325600	-0.00011400
H	-0.81919600	-2.24929700	0.00020300
H	-2.41250000	-0.26560000	0.00032100
H	-1.28831800	2.01801200	0.00009700
N	1.36766400	0.15121800	-0.00018200
N	0.85248800	-1.06449100	-0.00002800

1,3,5-triazine

C	1.13588700	0.61511800	-0.00023000
C	-0.03518600	-1.29093800	0.00018300
C	-1.10068600	0.67605300	0.00009300
N	0.03723700	1.36615500	-0.00015100
H	-0.06472600	-2.37509300	0.00018100
H	2.08969400	1.13138400	-0.00042500
H	-2.02493600	1.24353200	0.00012800
N	1.16484600	-0.71540600	-0.00010000
N	-1.20210100	-0.65092300	0.00022900

1,2,3,5-tetrazine

N	1.14109100	-0.70814000	-0.00014800
N	-0.00515500	-1.35919200	-0.00009900

N	-0.04809500	1.35397500	-0.00019500
N	-0.04785600	-1.35401800	0.00014200
C	1.09642300	0.69361400	0.00009700
H	2.00407000	1.28480600	0.00021200
C	1.09656400	-0.69342000	0.00022800
H	2.00429700	-1.28447900	0.00042700

1,2,4,5-tetrazine

C	-1.26221200	0.00001300	0.00033000
H	-2.34411300	0.00001800	-0.00003800
C	1.26168700	-0.00001200	-0.00018300
H	2.34357600	-0.00001900	-0.00022600
N	-0.65812400	1.18836300	0.00023100
N	0.65841000	1.18843000	0.00004100
N	-0.65814600	-1.18835300	-0.00010800
N	0.65838700	-1.18844100	-0.00025100

hexazine (D_{6h})

N	0.65788600	-1.13771000	-0.00005900
N	-0.65666900	-1.13843700	0.00057400
N	0.65658600	1.13846000	0.00023500
N	-0.65797900	1.13768100	-0.00032700
N	-1.31440100	-0.00075000	-0.00010400
N	1.31457600	0.00075600	-0.00031800

furan

C	-0.19872774	0.00523013	0.00260149
C	1.18085426	0.00523013	0.00260149
C	1.59558826	1.39259713	0.00260149
C	0.44152226	2.14869613	0.00251249
O	-0.67797974	1.31590713	0.00237949
H	-0.97237374	-0.75597487	0.00259049
H	1.84537226	-0.85346587	0.00270649
H	2.62217526	1.74609513	0.00259749
H	0.21206626	3.20955813	0.00246249

pyrrole

C	0.00047216	-0.87602303	-0.01156045
C	1.40222216	-0.87602303	-0.01156045
C	1.82622016	0.49477297	-0.01156045
C	0.66916316	1.28622597	-0.01166445
N	-0.43925484	0.44448497	-0.01156945
H	-1.37958284	0.73518597	-0.01178645
H	-0.70111584	-1.70925603	-0.01146245
H	2.04659516	-1.74872903	-0.01153545
H	2.85078316	0.85126497	-0.01158545
H	0.56024116	2.36999797	-0.01181145

2-azathiophene

C	1.15756073	-0.30857741	0.00000000
C	1.68293573	1.02369259	0.00000000
C	0.67647573	1.96374559	0.00081000
S	-0.83416027	1.24658859	0.00080200
H	1.78921073	-1.19871941	-0.00025400
H	2.75214473	1.24311659	-0.00057200
H	0.81588373	3.04298159	0.00145700
N	-1.14615600	-0.70017600	0.00003200
N	0.00493800	1.36281300	0.00009900
C	1.10643700	0.62556400	-0.00005700
H	2.06505300	1.13098800	-0.00008700
C	-1.10164200	0.63380800	0.00017500
H	-2.05685600	1.14564400	0.00018900

pentazine

C	-1.25233900	-0.00003100	0.00016200
H	-2.33525700	-0.00005300	0.00032700
N	-0.63586600	1.17552900	0.00021800
N	0.67763300	1.15118700	0.00003600
N	-0.63581500	-1.17555700	-0.00009200
N	0.67769300	-1.15115200	-0.00027000
N	1.32339800	0.00002700	-0.00007700

hexazine (D_2)

N	1.12282000	0.64657100	-0.17650700
N	1.13461500	-0.62583300	0.17841000
N	-1.13462700	0.62592700	0.17802700
N	-1.12273300	-0.64666400	-0.17674000
N	0.01238900	-1.27716800	-0.00156900
N	-0.01246300	1.27716800	-0.00162200

thiophene

C	-0.21966527	-0.30857741	0.00000000
C	1.15756073	-0.30857741	0.00000000
C	1.68293573	1.02369259	0.00000000
C	0.67647573	1.96374559	0.00081000
S	-0.83416027	1.24658859	0.00080200
H	-0.85434027	-1.19253041	-0.00051100
H	1.78921073	-1.19871941	-0.00025400
H	2.75214473	1.24311659	-0.00057200
H	0.81588373	3.04298159	0.00145700

2-azafuran

C	1.18085426	0.00523013	0.00260149
C	1.59558826	1.39259713	0.00260149
C	0.44152226	2.14869613	0.00251249
O	-0.67797974	1.31590713	0.00237949
H	1.84537226	-0.85346587	0.00270649
H	2.62217526	1.74609513	0.00259749
H	0.21206626	3.20955813	0.00246249
N	-0.19872774	0.00523013	0.00260149

2-azapyrrole

C	1.40222216	-0.87602303	-0.01156045
C	1.82622016	0.49477297	-0.01156045
C	0.66916316	1.28622597	-0.01166445
N	-0.43925484	0.44448497	-0.01156945
H	-1.37958284	0.73518597	-0.01178645
H	2.04659516	-1.74872903	-0.01153545
H	2.85078316	0.85126497	-0.01158545

N	-0.21966527	-0.30857741	0.00000000

3-azafuran

C	-0.19872774	0.00523013	0.00260149
C	1.59558826	1.39259713	0.00260149
C	0.44152226	2.14869613	0.00251249
O	-0.67797974	1.31590713	0.00237949
H	-0.97237374	-0.75597487	0.00259049
H	2.62217526	1.74609513	0.00259749
H	0.21206626	3.20955813	0.00246249
N	1.18085426	0.00523013	0.00260149

3-azapyrrole

C	0.00047216	-0.87602303	-0.01156045
C	1.82622016	0.49477297	-0.01156045
C	0.66916316	1.28622597	-0.01166445
N	-0.43925484	0.44448497	-0.01156945
H	-1.37958284	0.73518597	-0.01178645
H	-0.70111584	-1.70925603	-0.01146245
H	2.85078316	0.85126497	-0.01158545
H	0.56024116	2.36999797	-0.01181145
N	1.40222216	-0.87602303	-0.01156045

2,3-diazathiophene

C	1.68293573	1.02369259	0.00000000
C	0.67647573	1.96374559	0.00081000
S	-0.83416027	1.24658859	0.00080200
H	2.75214473	1.24311659	-0.00057200
H	0.81588373	3.04298159	0.00145700
N	-0.21966527	-0.30857741	0.00000000
N	1.15756073	-0.30857741	0.00000000

2,4-diazafuran

C	1.18085426	0.00523013	0.00260149
C	0.44152226	2.14869613	0.00251249
O	-0.67797974	1.31590713	0.00237949
H	1.84537226	-0.85346587	0.00270649
H	0.21206626	3.20955813	0.00246249
N	-0.19872774	0.00523013	0.00260149
N	1.59558826	1.39259713	0.00260149

2,4-diazapyrrole

C	1.40222216	-0.87602303	-0.01156045
C	0.66916316	1.28622597	-0.01166445
N	-0.43925484	0.44448497	-0.01156945
H	-1.37958284	0.73518597	-0.01178645
H	2.04659516	-1.74872903	-0.01153545
H	0.56024116	2.36999797	-0.01181145
N	0.00047216	-0.87602303	-0.01156045
N	1.82622016	0.49477297	-0.01156045

2,5-diazathiophene

C	1.15756073	-0.30857741	0.00000000
C	1.68293573	1.02369259	0.00000000
S	-0.83416027	1.24658859	0.00080200
H	0.56024116	2.36999797	-0.01181145
N	0.00047216	-0.87602303	-0.01156045

3-azathiophene

C	-0.21966527	-0.30857741	0.00000000
C	1.68293573	1.02369259	0.00000000
C	0.67647573	1.96374559	0.00081000
S	-0.83416027	1.24658859	0.00080200
H	-0.85434027	-1.19253041	-0.00051100
H	2.75214473	1.24311659	-0.00057200
H	0.81588373	3.04298159	0.00145700
N	1.15756073	-0.30857741	0.00000000

2,3-diazafuran

C	1.59558826	1.39259713	0.00260149
C	0.44152226	2.14869613	0.00251249
O	-0.67797974	1.31590713	0.00237949
H	2.62217526	1.74609513	0.00259749
H	0.21206626	3.20955813	0.00246249
N	-0.19872774	0.00523013	0.00260149
N	1.18085426	0.00523013	0.00260149

2,3-diazapyrrole

C	1.82622016	0.49477297	-0.01156045
C	0.66916316	1.28622597	-0.01166445
N	-0.43925484	0.44448497	-0.01156945
H	-1.37958284	0.73518597	-0.01178645
H	2.85078316	0.85126497	-0.01158545
H	0.56024116	2.36999797	-0.01181145
N	0.00047216	-0.87602303	-0.01156045
N	1.40222216	-0.87602303	-0.01156045

2,4-diazathiophene

C	1.15756073	-0.30857741	0.00000000
C	0.67647573	1.96374559	0.00081000
S	-0.83416027	1.24658859	0.00080200
H	1.78921073	-1.19871941	-0.00025400
H	0.81588373	3.04298159	0.00145700
N	-0.21966527	-0.30857741	0.00000000
N	1.68293573	1.02369259	0.00000000

2,5-diazafuran

C	1.18085426	0.00523013	0.00260149
C	1.59558826	1.39259713	0.00260149
O	-0.67797974	1.31590713	0.00237949
H	1.84537226	-0.85346587	0.00270649
H	2.62217526	1.74609513	0.00259749
N	-0.19872774	0.00523013	0.00260149
N	0.44152226	2.14869613	0.00251249

2,5-diazapyrrole

C	1.40222216	-0.87602303	-0.01156045
C	1.82622016	0.49477297	-0.01156045
N	-0.43925484	0.44448497	-0.01156945

H	1.78921073	-1.19871941	-0.00025400
H	2.75214473	1.24311659	-0.00057200
N	-0.21966527	-0.30857741	0.00000000
N	0.67647573	1.96374559	0.00081000

3,4-diazafuran

C	-0.19872774	0.00523013	0.00260149
C	0.44152226	2.14869613	0.00251249
O	-0.67797974	1.31590713	0.00237949
H	-0.97237374	-0.75597487	0.00259049
H	0.21206626	3.20955813	0.00246249
N	1.59558826	1.39259713	0.00260149
N	1.18085426	0.00523013	0.00260149

3,4-diazapyrrole

C	0.00047216	-0.87602303	-0.01156045
C	0.66916316	1.28622597	-0.01166445
N	-0.43925484	0.44448497	-0.01156945
H	-1.37958284	0.73518597	-0.01178645
H	-0.70111584	-1.70925603	-0.01146245
H	0.56024116	2.36999797	-0.01181145
N	1.82622016	0.49477297	-0.01156045
N	1.40222216	-0.87602303	-0.01156045

2,3,4-triazathiophene

C	0.06642700	1.16664900	0.00000400
S	-1.13825000	-0.02641500	-0.00000800
H	-0.11683900	2.22927700	0.00004100
N	0.06987300	-1.22250100	0.00002500
N	1.22233800	-0.69547300	-0.00001800
N	1.26925700	0.65989800	0.00000100

2,3,5-triazafuran

C	-1.00357200	0.42329500	-0.00075900
O	0.55996200	-0.96427300	-0.00058400
H	-1.98067400	0.87156500	-0.00038000
N	1.11570300	0.32379400	0.00021200
N	0.17281600	1.14286200	0.00030000
N	-0.78531800	-0.85196400	0.00086000

2,3,5-triazapyrrole

C	1.06049900	-0.30546000	-0.00008700
N	-0.97795900	-0.33100800	0.00014000
H	-1.93570000	-0.64499400	0.00015100
H	2.09284400	-0.60616700	-0.00007100
N	-0.65458000	0.94984800	-0.00027800
N	0.64955200	0.98285900	0.00016000
N	0.05154000	-1.16113900	0.00004100

tetraazathiophene

S	1.09454100	0.00000000	-0.00000100
N	-0.04329400	1.20324800	0.00004900
N	-1.20760800	0.68585000	-0.00008200
N	-1.20760900	-0.68584800	0.00007900
N	-0.04329600	-1.20324900	-0.00004300
H	-1.37958284	0.73518597	-0.01178645
H	2.04659516	-1.74872903	-0.01153545
H	2.85078316	0.85126497	-0.01158545
N	0.66916316	1.28622597	-0.01166445
N	0.00047216	-0.87602303	-0.01156045

3,4-diazathiophene

C	-0.21966527	-0.30857741	0.00000000
C	0.67647573	1.96374559	0.00081000
S	-0.83416027	1.24658859	0.00080200
H	-0.85434027	-1.19253041	-0.00051100
H	0.81588373	3.04298159	0.00145700
N	1.68293573	1.02369259	0.00000000
N	1.15756073	-0.30857741	0.00000000

2,3,4-triazafuran

C	1.05377900	0.11581200	0.00003400
O	0.42662700	-1.04109500	0.00007100
H	2.13053700	0.12706100	0.00006900
N	-0.97116200	-0.65408300	0.00002700
N	-0.99308900	0.58268600	-0.00010200
N	0.26907600	1.14380200	-0.00004500

2,3,4-triazapyrrole

C	0.96652500	0.50473400	0.00016200
N	0.67644000	-0.80579000	-0.00002300
H	1.27548800	-1.61431000	-0.00002200
H	1.96056800	0.91543200	0.00023800
N	-0.66329600	-0.94674900	0.00019900
N	-1.14666800	0.24264800	-0.00019500
N	-0.15722000	1.17710200	-0.00015100

2,3,5-triazathiophene

C	1.18778200	-0.60203900	-0.00030300
S	-1.09752400	-0.04503800	-0.00016700
H	2.12344900	-1.13969000	0.00033900
N	-0.01917300	1.23302000	0.00039500
N	1.17921400	0.76519500	-0.00018400
N	0.02713800	-1.21642400	0.00038200

tetraazafuran

O	-0.00024600	-1.09640700	0.00001400
N	-1.10011900	-0.27391600	-0.00011400
N	-0.70337000	0.90078500	0.00002000
N	0.70373500	0.90050100	0.00016100
N	1.10003500	-0.27433300	-0.00008300

tetraazapyrrole

N	1.01545200	0.00000500	-0.00029800
H	2.02430000	0.00001200	-0.00019400
N	0.28366800	1.09727100	0.00046900
N	-0.93599700	0.67502300	-0.00017700
N	-0.93598900	-0.67503300	-0.00059000
N	0.28368000	-1.09726800	0.00062400

Table S16 Complete ref.[61]

61. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Farkas, J. B. Foresman, J. V Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09, Revision B.01, Gaussian Inc., Wallingford CT, 2009.