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Boron-boron, carbon-carbon and nitrogen-nitrogen bonding in N-heterocyclic carbenes and their diazaboryl and triazole analogues; Wanzlick equilibria revisited

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Molecule partitioning scheme in functional SAPT0 calculations

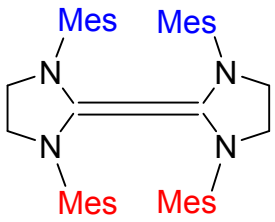

Figure S1. Functional SAPT0 partitioning scheme used throughout the study, taking dimer of **2** as an example. For each dimer the intramolecular interaction energy estimation consisted of two independent calculations. In the first one the interaction energy was calculated between the two side groups in blue, with the remainder of the molecule (in red and black) acting as the linker. Second calculations included interaction energy between the two side groups in red, with the remainder of the molecule (in blue and black) acting as the linker.

Calculated structural and energetic parameters and partial charges

Table S1. The comparison of calculated structural and energetic parameters of **1-6** and their dimers at the M06-2X level of theory.

parameter	**1**	**2**	**2 dim**	**3**	**3 dim**	**4**	**4 dim**	**5**	**5 dim**	**6**	**6 dim**
X1-X1' bond length [Å]	-	-	1.36	-	1.34	-	1.35	-	1.35	-	1.35
X1-X1' bond order (NBO)	2	-	2	-	2	-	2	-	2	-	2
more stable form[a]	dim	-	mon	-	dim	-	dim	-	mon	-	mon
ΔG DFT (kcal/mol)[b]	-	-	6.6	-	-1.3	-	-3.8	-	22.2	-	22.8
ΔG CCSD(T)(kcal/mol)[b]	-	-	8.0	-	-3.5	-	-4.2	-	21.9	-	24.2
HOMO-LUMO gap (eV)	2.91	7.96	5.93	9.53	7.83	9.31	7.79	9.31	6.65	9.35	6.62
Natural charges											
X1	-0.14	0.24	0.28	0.22	0.27	0.22	0.26	0.13	0.25	0.13	0.25
Imidazole	-0.34	-0.41	-0.35	-0.45	-0.40	-0.46	-0.42	-0.50	-0.43	-0.51	-0.44
R2	0.24	0.21	0.20	0.22	0.20	0.23	0.21	0.25	0.21	0.25	0.22
R3	0.24	0.21	0.16	0.22	0.20	0.23	0.21	0.25	0.21	0.25	0.22
X1'	-0.14	-	0.28	-	0.27	-	0.26	-	0.25	-	0.25
Imidazole'	-0.34	-	-0.36	-	-0.40	-	-0.42	-	-0.43	-	-0.44
R2'	0.24	-	0.20	-	0.20	-	0.21	-	0.21	-	0.22
R3'	0.24	-	0.16	-	0.20	-	0.21	-	0.21	-	0.22
Mulliken partial charges											
X1	-0.25	0.19	0.41	0.18	0.31	0.17	0.30	0.12	0.33	0.11	0.32

Imidazole	-0.15	-0.44	-0.35	-0.39	-0.32	-0.39	-0.33	-0.45	-0.35	-0.44	-0.35
R2	0.20	0.22	0.19	0.20	0.16	0.19	0.16	0.22	0.18	0.22	0.17
R3	0.20	0.22	0.16	0.20	0.16	0.19	0.16	0.22	0.18	0.22	0.18
X1’	-0.25	-	0.40	-	0.31	-	0.31	-	0.33	-	0.31
Imidazole’	-0.15	-	-0.35	-	-0.32	-	-0.32	-	-0.35	-	-0.35
R2’	0.20	-	0.19	-	0.16	-	0.16	-	0.18	-	0.18
R3’	0.20	-	0.16	-	0.16	-	0.16	-	0.18	-	0.17

[a] dim - dimer, mon – monomer

Table S2. The comparison of calculated structural and energetic parameters of **1-6** and their dimers at the M06 level of theory.

parameter	**1**	**2**	**2 dim**	**3**	**3 dim**	**4**	**4 dim**	**5**	**5 dim**	**6**	**6 dim**
X1-X1’ bond length [Å]	-	-	1.37	-	1.3	-	1.35	-	1.35	-	1.35
X1-X1’ bond order (NBO)	2	-	2	-	2	-	2	-	2	-	2
HOMO-LUMO gap (eV)	2.91	5.92	4.11	7.18	5.86	7.00	5.85	6.93	4.74	6.98	4.72
					Natural charges						
X1	-0.14	0.24	0.29	0.23	0.27	0.22	0.26	0.14	0.25	0.14	0.25
Imidazole	-0.34	-0.42	-0.36	-0.44	-0.40	-0.46	-0.42	-0.50	-0.42	-0.50	-0.44
R2	0.24	0.21	0.20	0.22	0.20	0.23	0.15	0.25	0.21	0.25	0.22
R3	0.24	0.21	0.16	0.22	0.20	0.23	0.15	0.25	0.21	0.25	0.22
X1’	-0.14	-	0.28	-	0.27	-	0.26	-	0.25	-	0.25
Imidazole’	-0.34	-	-0.36	-	-0.40	-	-0.42	-	-0.42	-	-0.44
R2’	0.24	-	0.20	-	0.20	-	0.15	-	0.21	-	0.22
R3’	0.24	-	0.16	-	0.20	-	0.15	-	0.21	-	0.22
					Mulliken partial charges						
X1	-0.25	0.17	0.44	0.16	0.33	0.15	0.33	0.11	0.35	0.10	0.34
Imidazole	-0.15	-0.37	-0.37	-0.34	-0.30	-0.36	-0.30	-0.40	-0.32	-0.40	-0.33
R2	0.20	0.21	0.20	0.17	0.15	0.18	0.15	0.20	0.16	0.20	0.17
R3	0.20	0.21	0.17	0.17	0.15	0.18	0.15	0.20	0.16	0.20	0.16
X1’	-0.25	-	0.43	-	0.33	-	0.33	-	0.35	-	0.34
Imidazole’	-0.15	-	-0.37	-	-0.30	-	-0.30	-	-0.32	-	-0.33
R2’	0.20	-	0.20	-	0.15	-	0.15	-	0.16	-	0.17
R3’	0.20	-	0.17	-	0.15	-	0.15	-	0.16	-	0.16

Table S3. The comparison of calculated structural and energetic parameters of **7-9, 16** and **17** and their dimers at the M06-2X level of theory.

parameter	7	7 dim	8	8 dim	9	9 dim	16	16 dim	17	17 dim
X1-X1' bond length [Å]	-	1.35	-	1.35	-	1.35	-	1.38	-	1.37
X1-X1' bond order (NBO)	-	2	-	2	-	2	-	2	-	2
more stable form[a]	-	dim	-	dim	-	dim	-	mon	-	mon
ΔG DFT (kcal/mol)	-	-5.4	-	-5.9	-	-0.6	-	54.8	-	33.6
ΔG CCSD(T)(kcal/mol)	-	-4.4	-	-2.9	-	0.7	-	55.9	-	37.7
HOMO-LUMO gap	7.89	6.28	7.27	5.33	7.71	5.80	5.01	3.81	6.20	4.76
				Natural charges						
X1	0.22	0.30	0.22	0.27	0.22	0.27	0.24	0.29	0.24	0.29
imidazole	-0.42	-0.34	-0.41	-0.36	-0.42	-0.37	-0.42	-0.36	-0.42	-0.36
R2	0.21	0.19	0.20	0.18	0.20	0.17	0.21	0.20	0.21	0.20
R3	0.20	0.18	0.21	0.18	0.22	0.19	0.21	0.16	0.21	0.16
X1'	-	0.26	-	0.27	-	0.27	-	0.28	-	0.28
imidazole'	-	-0.38	-	-0.36	-	-0.37	-	-0.36	-	-0.36
R2'	-	0.19	-	0.18	-	0.17	-	0.20	-	0.20
R3'	-	0.16	-	0.18	-	0.19	-	0.16	-	0.16
				Mulliken partial charges						
X1	0.19	0.35	0.19	0.37	0.18	0.37	0.17	0.44	0.17	0.44
imidazole	-0.39	-0.32	-0.38	-0.32	-0.40	-0.33	-0.42	-0.37	-0.42	-0.37
R2	0.22	0.16	0.22	0.16	0.21	0.16	0.21	0.20	0.21	0.20
R3	0.17	0.14	0.16	0.16	0.19	0.17	0.21	0.17	0.21	0.17
X1'	-	0.34	-	0.37	-	0.37	-	0.43	-	0.43
imidazole'	-	-0.32	-	-0.32	-	-0.33	-	-0.37	-	-0.37
R2'	-	0.16	-	0.18	-	0.16	-	0.20	-	0.20
R3'	-	0.14	-	0.16	-	0.17	-	0.17	-	0.17

[a] dim - dimer, mon – monomer

Table S4. The comparison of calculated structural and energetic parameters of **7-9, 16** and **17** and their dimers at the M06 level of theory.

parameter	7	7 dim	8	8 dim	9	9 dim	16	16 dim	17	17 dim
X1-X1' bond length [Å]	-	1.35	-	1.35	-	1.36	-	1.40	-	1.38
X1-X1' bond order (NBO)	-	2	-	2	-	2	-	2	-	2
HOMO-LUMO gap	5.81	4.42	5.15	3.43	5.66	4.03	3.33	2.37	4.54	3.16
				Natural charges						
X1	0.22	0.30	0.22	0.27	0.22	0.27	0.24	0.29	0.24	0.29
imidazole	-0.42	-0.37	-0.42	-0.36	-0.43	-0.36	-0.42	-0.36	-0.42	-0.36

R2	0.21	0.19	0.21	0.18	0.21	0.17	0.21	0.20	0.21	0.20
R3	0.21	0.18	0.21	0.18	0.22	0.19	0.21	0.16	0.21	0.16
X1’	-	0.26	-	0.27	-	0.27	-	0.28	-	0.28
imidazole’	-	-0.37	-	-0.36	-	-0.36	-	-0.36	-	-0.36
R2’	-	0.16	-	0.18	-	0.17	-	0.20	-	0.20
R3’	-	0.18	-	0.18	-	0.19	-	0.16	-	0.16
				Mulliken partial charges						
X1	0.17	0.39	0.17	0.40	0.16	0.41	0.17	0.44	0.17	0.44
imidazole	-0.37	-0.30	-0.37	-0.33	-0.38	-0.34	-0.42	-0.37	-0.42	-0.37
R2	0.21	0.17	0.22	0.18	0.21	0.17	0.21	0.20	0.21	0.20
R3	0.16	0.13	0.15	0.15	0.17	0.17	0.21	0.17	0.21	0.17
X1’	-	0.36	-	0.40	-	0.40	-	0.43	-	0.43
imidazole’	-	-0.30	-	-0.34	-	-0.34	-	-0.37	-	-0.37
R2’	-	0.18	-	0.19	-	0.17	-	0.20	-	0.20
R3’	-	0.15	-	0.15	-	0.17	-	0.17	-	0.17

Table S5. The comparison of calculated structural and energetic parameters of systems **10** and **11** and their dimers at the M06-2X level of theory.

parameter	**10**	**10A**	**10B**	**10C**	**11**	**11A**	**11B**	**11C**
X1-X1’ bond length [Å]	-	1.61	1.72	1.67	-	1.67	1.670	1.68
X1-X1’ bond order (NBO)	-	1	1	1	-	1	1	1
more stable form[a]	-	mon	-	-	-	mon	-	-
ΔG DFT (kcal/mol)[b]	-	11.7	-	-	-	24.6	-	-
ΔG CCSD(T)(kcal/mol)	-	29.0	-	-	-	40.5	-	-
HOMO-LUMO gap	4.21	2.80	7.45	2.40	4.24	1.60	7.08	2.86
				Natural charges				
X1	0.21	0.32	0.69	0.67	0.13	0.47	0.59	0.57
imidazole	-1.10	-0.77	-0.37	-0.50	-1.15	-0.62	-0.41	-0.52
R2	0.05	-0.11	0.19	-0.75	0.07	-0.21	0.20	-0.74
R3	0.05	-0.11	0.18	-0.81	0.07	-0.17	0.21	-0.74
X1’	-	0.32	0.69	0.67	-	0.47	0.59	0.57
imidazole’	-	-0.77	-0.37	-0.49	-	-0.62	-0.41	-0.52
R2’	-	-0.12	0.19	-0.74	-	-0.22	0.20	-0.75
R3’	-	-0.12	0.18	-0.70	-	-0.17	0.21	-0.74
				Mulliken partial charges				
X1	-0.07	0.30	0.41	0.41	-0.11	0.32	0.36	0.34
imidazole	-0.92	-0.60	-0.32	-0.46	-0.96	-0.54	-0.36	-0.53
R2	-0.04	-0.20	0.16	-0.75	-0.02	-0.24	0.18	-0.73
R3	-0.05	-0.20	0.16	-0.81	-0.02	-0.21	0.18	-0.73
X1’	-	0.29	0.40	0.39	-	0.31	0.35	0.34
imidazole’	-	-0.60	-0.32	-0.50	-	-0.55	-0.37	-0.53

R2'	-	-0.20	0.16	-0.76	-	-0.25	0.19	-0.75
R3'	-	-0.20	0.16	-0.72	-	-0.21	0.18	-0.72

[a] dim - dimer, mon – monomer [b] – in the 6-31G** basis set

Table S6. The comparison of calculated structural and energetic parameters of systems **10** and **11** and their dimers at the M06 level of theory.

parameter	**10**	**10A**	**10B**	**10C**	**11**	**11A**	**11B**	**11C**
X1-X1' bond length [Å]	-	1.63	1.71	1.670	-	1.67	1.69	1.68
X1-X1' bond order (NBO)	-	1	1	1	-	1	1	1
HOMO-LUMO gap	2.57	1.67	5.68	0.63	2.62	0.90	5.31	1.70
				Natural charges				
X1	0.23	0.39	0.68	0.59	0.17	0.51	0.61	0.57
imidazole	-1.08	-0.72	-0.37	-0.60	-1.12	-0.61	-0.42	-0.55
R2	0.05	-0.13	0.19	-0.63	0.06	-0.23	0.20	-0.73
R3	0.04	-0.15	0.18	-0.77	0.06	-0.16	0.21	-0.71
X1'	-	0.40	0.68	0.58	-	0.51	0.61	0.57
imidazole'	-	-0.73	-0.37	-0.61	-	-0.61	-0.42	-0.57
R2'	-	-0.13	0.19	-0.64	-	-0.23	0.20	-0.73
R3'	-	-0.14	0.18	-0.75	-	-0.16	0.21	-0.70
				Mulliken partial charges				
X1	-0.08	0.35	0.41	0.37	-0.11	0.33	0.36	0.34
imidazole	-0.88	-0.56	-0.32	-0.55	-0.77	-0.52	-0.35	-0.53
R2	-0.05	-0.21	0.16	-0.67	-0.18	-0.26	0.17	-0.74
R3	-0.07	-0.23	0.16	-0.78	-0.04	-0.21	0.17	-0.73
X1'	-	0.35	0.41	0.39	-	0.33	0.36	0.34
imidazole'	-	-0.57	-0.31	-0.56	-	-0.52	-0.35	-0.53
R2'	-	-0.21	0.15	-0.68	-	-0.27	0.18	-0.74
R3'	-	-0.22	0.16	-0.76	-	-0.21	0.17	-0.73

Table S7. The comparison of calculated structural and energetic parameters of systems **12** and **13** and their dimers at the M06-2X level of theory.

parameter	**12**	**12A**	**12B**	**12C**	**13**	**13A**	**13B**	**13C**
X1-X1' bond length [Å]	-	1.589	1.689	1.674	-	1.593	1.677	1.763
X1-X1' bond order (NBO)	-	2	1	1	-	2	1	1
more stable form[a]	-	mon	-	-	-	mon	-	-

ΔG DFT (kcal/mol)[b]	-	21.6	-	-	-	37.6	-	-
ΔG CCSD(T)(kcal/mol)	-	36.0	-	-	-	55.6	-	-
HOMO-LUMO gap	6.46	4.67	8.38	2.54	6.09	4.18	8.01	4.69
				Natural charges				
X1	0.14	0.12	0.67	0.07	0.06	0.15	0.57	0.60
imidazole	-1.23	-1.16	-0.40	-1.75	-1.27	-1.15	-0.45	-2.03
R2	0.11	0.08	0.20	-0.08	0.14	0.09	0.22	0.01
R3	0.11	0.08	0.20	-0.18	0.14	0.07	0.22	0.02
X1’	-	0.12	0.67	0.07	-	0.12	0.57	0.59
imidazole’	-	-1.16	-0.40	-1.75	-	-1.18	-0.45	-2.03
R2’	-	0.08	0.20	-0.08	-	0.08	0.22	0.01
R3’	-	0.08	0.20	-0.18	-	0.06	0.22	0.02
				Mulliken partial charges				
X1	-0.20	0.11	0.37	0.04	-0.25	0.09	0.32	0.23
imidazole	-1.02	-0.92	-0.29	-1.45	-1.07	-0.92	-0.35	-1.67
R2	0.01	-0.04	0.15	-0.22	0.04	-0.03	0.17	-0.16
R3	0.01	-0.04	0.15	-0.33	0.04	-0.04	0.17	-0.16
X1’	-	0.11	0.37	0.04	-	0.09	0.32	0.22
imidazole’	-	-0.92	-0.29	-1.45	-	-0.92	-0.35	-1.68
R2’	-	-0.04	0.15	-0.22	-	-0.03	0.17	-0.17
R3’	-	-0.04	0.15	-0.33	-	-0.06	0.17	-0.16

[a] dim - dimer, mon – monomer [b] – in the 6-31G** basis set

Table S8. The comparison of calculated structural and energetic parameters of systems **12** and **13** and their dimers at the M06 level of theory.

parameter	**12**	**12A**	**12B**	**12C**	**13**	**13A**	**13B**	**13C**
X1-X1’ bond length [Å]	-	1.59	1.69	1.67	-	1.59	1.68	1.76
X1-X1’ bond order (NBO)	-	2	1	1	-	2	1	1
HOMO-LUMO gap	4.61	3.00	6.35	1.35	4.18	2.51	6.08	2.88
				Natural charges				
X1	0.15	0.16	0.66	0.18	0.09	0.18	0.59	0.60
imidazole	-1.22	-1.13	-0.39	-1.66	-1.26	-1.14	-0.44	-1.98
R2	0.11	0.06	0.20	-0.13	0.13	0.08	0.22	-0.02
R3	0.11	0.06	0.20	-0.22	0.13	0.05	0.22	0.00
X1’	-	0.16	0.66	0.18	-	0.16	0.59	0.59
imidazole’	-	-1.13	-0.39	-1.66	-	-1.12	-0.44	-1.99
R2’	-	0.06	0.20	-0.13	-	0.07	0.22	-0.01
R3’	-	0.06	0.20	-0.22	-	0.05	0.22	0.00

Mulliken partial charges

X1	-0.21	0.14	0.36	0.09	-0.24	0.13	0.32	0.23
imidazole	-0.98	-0.87	-0.25	-1.37	-1.02	-0.88	-0.30	-1.60
R2	-0.01	-0.06	0.13	-0.27	0.01	-0.04	0.15	-0.21
R3	-0.01	-0.06	0.13	-0.36	0.01	-0.07	0.15	0.19
X1’	-	0.14	0.36	0.09	-	0.10	0.32	0.21
imidazole’	-	-0.87	-0.25	-1.37	-	-0.86	-0.30	-1.60
R2’	-	-0.06	0.13	-0.27	-	-0.06	0.15	-0.20
R3’	-	-0.06	0.13	-0.36	-	-0.08	0.15	-0.20

Geometries in xyz format

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130
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 B2 4.1595 12.1489 3.9926
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 N2_1 8.0532 12.7190 4.1784
 C3_1 9.3198 12.2280 3.8915
 H3_1 10.2067 12.7945 4.1380
 C4_1 9.1619 11.0283 3.2996
 H4_1 9.8812 10.3077 2.9360
 N5_1 7.7970 10.7879 3.2069
 C1_2 2.6895 12.2861 4.1056
 N2_2 1.8937 13.3505 3.7194
 C3_2 0.5574 13.0920 3.9945
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H36 9.0149 7.9597 2.4337
H37 9.6553 8.0624 4.0875
H38 10.0916 9.2947 2.8943
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H40 15.0409 7.6048 7.7001
H41 14.4078 6.5008 6.4686
H42 15.0537 8.0860 5.9882
43
M7
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H2B 5.3277 4.1290 1.5729
C3 3.5392 2.9989 1.0216
H3A 2.9518 3.7442 1.5693
H3B 3.0218 2.7868 0.0729
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C5 1.9814 1.6358 3.5127
C6 0.8700 0.9948 4.0560
H6 0.4127 1.4046 4.9583
C7 0.3419 -0.1621 3.4892
C8 0.9605 -0.6841 2.3547
H8 0.5673 -1.5973 1.9054
C9 2.0689 -0.0731 1.7734
C10 2.5403 2.8636 4.1690
H10A 2.1310 3.7852 3.7314
H10B 3.6311 2.9128 4.0659
H10C 2.2915 2.8810 5.2353
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H11B -0.9229 -1.8803 3.8092
H11C -1.7942 -0.3470 3.7247
C12 2.7208 -0.6596 0.5589
H12A 2.7699 0.0679 -0.2622
H12B 2.1712 -1.5367 0.2028
H12C 3.7552 -0.9504 0.7757
C13 7.1197 2.0803 1.0820
H13A 7.5269 2.4686 0.1364
H13B 7.4042 1.0243 1.1603
C14 7.6763 2.8669 2.2453
C15 8.6366 3.8572 2.0602
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C18 7.6873 3.3344 4.6168
H18 7.3121 3.1281 5.6170
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N2 3.6981 1.7499 1.7950
86
D7 dim
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C4 4.5537 -0.9091 0.5977
C5 3.4294 -0.1439 0.9476
C6 2.1672 -0.5876 0.5557
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C9 4.4060 -2.0805 -0.1603
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H10C 4.0773 0.9384 2.7028
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H12B 5.3163 -3.8290 -1.0178
H12C 6.1536 -3.1691 0.4122
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C45 6.3223 -3.4564 4.1773
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H47 5.5823 -4.1487 4.5928
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C75 2.0307 -3.4383 3.0611
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C37 1.7212 -5.4719 1.8081
H38 1.0644 -6.2321 1.3907
C39 3.0964 -5.5580 1.6286
H40 3.5211 -6.3859 1.0642
C41 3.9375 -4.5861 2.1628
H42 5.0128 -4.6386 2.0018
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C46 6.8996 -2.4692 5.1845
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H48 7.7433 -2.8679 5.7557
C47 8.7492 -1.1691 4.1969
C48 9.3858 -0.5454 5.2895
C49 10.7546 -0.3056 5.2406
H50 11.2305 0.1978 6.0840
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C52 10.8757 -1.2807 3.0727
H53 11.4605 -1.5813 2.2013
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H57 8.3735 -0.9554 7.1637
H58 7.6482 0.3368 6.2189
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H61 13.4090 -0.5234 3.0948
H62 13.5473 -1.0174 4.7871
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H64 8.2002 -3.0381 2.1454
H65 9.7545 -2.7806 1.3379
H66 8.4459 -1.5933 1.1869
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C72 6.9459 1.6244 3.5009
H74 6.8832 0.9585 4.3718
H75 5.9655 2.1403 3.4244
C76 8.0253 2.6480 3.7248
C77 7.7032 3.9008 4.2437
C78 8.6974 4.8343 4.5168
H77 8.4298 5.8079 4.9223
C79 10.0292 4.5251 4.2647
H79 10.8088 5.2542 4.4750
C80 10.3572 3.2800 3.7362
H81 11.3970 3.0283 3.5328
C82 9.3631 2.3485 3.4655
H83 9.6157 1.3720 3.0547
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43
M8
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H3A 5.3930 3.5587 8.9969
H3B 6.3960 3.3842 10.4563
C4 4.5218 4.5009 10.7758
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H4B 4.3864 5.4057 10.1724
C5 2.1481 4.4336 11.6045
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H10 0.5261 4.5869 14.5764
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C12 1.7067 5.6706 9.4436
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H12B 0.8218 6.0649 8.9326
H12C 2.0424 4.7720 8.9138
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H13B -1.5291 5.9048 14.3433
H13C -1.9041 6.7360 12.8225
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H14B 2.4930 2.1257 13.2892
H14C 2.3183 3.1111 14.7654
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H15B 6.0966 0.7631 10.2340
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C17 5.9173 0.7098 7.5114
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C19 4.3491 0.6501 5.6875
H19 4.1509 0.5804 4.6201
C20 3.3010 0.7769 6.5944
H20 2.2720 0.8085 6.2434
C21 3.5738 0.8622 7.9497
H21 2.7693 0.9805 8.6776
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N2 4.6133 2.2168 10.4400
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86
D8 dim
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H3B 6.5823 2.0484 0.9125
C4 8.0136 1.1059 2.8281
C5 9.2697 1.6941 3.0618
C6 9.4887 2.3721 4.2574
H6 10.4726 2.8079 4.4424
C7 8.4937 2.4945 5.2246
C8 7.2445 1.9492 4.9482
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C9 6.9738 1.2637 3.7622
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H10B 10.2062 2.3243 1.2206
H10C 10.4064 0.6087 1.5895
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H11A 14.2841 -1.1801 3.5874
H11B 7.8541 3.5268 7.0101
H11C 9.4551 4.0146 6.4207
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H12A 5.2607 0.7735 2.5041
H12B 4.8668 1.3146 4.1471
H12C 5.5096 -0.3127 3.8641
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H47 5.7775 -3.0862 4.4256
C71 4.7766 -2.4980 2.1771
H72 4.7090 -1.6106 1.5354
H73 4.3321 -2.1934 3.1446
C74 3.9361 -3.5864 1.5646
C75 2.5526 -3.4485 1.4254
I35 1.5493 -1.7065 2.1483
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H78 0.7043 -4.2697 0.6938
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H80 1.7792 -6.3135 -0.2069
C81 3.7566 -5.7231 0.4199
H82 4.2441 -6.6094 0.0192
C83 4.5174 -4.7467 1.0502
H84 5.5987 -4.8550 1.1351
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H49 8.4657 -4.1369 3.4214
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C49 10.2530 -1.2821 4.1412
C50 11.6226 -1.0841 3.9886
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C56 9.5907 -0.9429 5.4423
H57 10.2081 -0.2490 6.0244
H58 9.4382 -1.8394 6.0602
H59 8.6067 -0.4888 5.2817
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H63 14.2147 -1.8259 1.9359
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C82 2.4894 -2.3717 -2.6603
H81 1.5425 -2.5101 -3.1775
C84 2.6653 -1.3172 -1.7748
H83 1.8524 -0.6203 -1.5818
C85 3.8781 -1.1568 -1.1169
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47
M9
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H20B 3.2408 12.8096 15.5319
H20C 4.4730 13.6532 14.5555
O1 4.1256 11.6412 14.1556

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H2B 1.9198 11.4571 11.4316
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H3A 1.2959 10.8708 9.1645
H3B 2.6748 11.8970 8.7136
C4 3.2628 9.4300 7.5756
C5 2.4884 8.3837 7.0588
C6 2.6432 8.0446 5.7171
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H8 5.0168 10.2750 4.8009
C9 4.1820 10.1159 6.7717
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H11C 2.7903 7.8841 3.0431
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H12C 4.5128 12.1735 7.3647
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H13B 3.0838 9.7731 13.1681
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N2 3.1226 9.8157 8.9369
94
D9 dim
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H3B 6.6991 2.5053 1.5359
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C6 9.7751 2.5374 4.7341
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C9 7.1608 1.6262 4.3791
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H10B 10.3085 2.5111 1.6661
H10C 10.3886 0.7733 1.9763
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H11B 8.4062 3.7570 7.5986
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H29 10.8671 6.0582 8.0795
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H41 10.6915 3.8402 -0.8408
C42 13.6040 8.2653 1.7326
H43 14.4003 8.0698 1.0051
H44 14.0190 8.1688 2.7447
H45 13.2608 9.3024 1.6325
O46 11.3023 10.1315 2.5666
C47 11.3590 11.1158 5.6150
C48 11.3698 12.3243 4.6972
O49 11.2475 11.2927 6.8392
H50 10.5779 13.0117 5.0162
H51 12.3229 12.8527 4.8297
H52 11.2551 12.0547 3.6432
104
D17 dimer
N1 12.3383 5.6180 6.1020
N2 11.8149 5.2499 3.9217

C3 12.0235 6.2752 4.8859
C4 12.2758 4.1840 5.9340
C5 11.9512 3.9562 4.5849
C6 12.3047 6.0326 7.4621
C7 13.4617 5.8481 8.2363
C8 13.4059 6.0947 9.6057
H9 14.3167 5.9729 10.1973
C10 12.2324 6.4952 10.2346
C11 11.0813 6.6033 9.4616
H12 10.1369 6.8818 9.9368
C13 11.0923 6.3580 8.0913
C14 14.7349 5.3508 7.6270
H15 15.5814 5.5091 8.3069
H16 14.9532 5.8559 6.6800
H17 14.6403 4.2801 7.4092
C18 12.2154 6.8383 11.6943
H19 12.9534 6.2537 12.2584
H20 11.2273 6.6616 12.1394
H21 12.4530 7.9014 11.8516
C22 9.8160 6.4021 7.3195
H23 8.9554 6.4953 7.9929
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H25 9.8091 7.2551 6.6316
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C27 13.8765 5.6032 2.5774
C28 14.5110 5.5503 1.3366
H29 15.5807 5.7690 1.2857
C30 13.8258 5.2208 0.1718
C31 12.4706 4.9391 0.2744
H32 11.9055 4.6762 -0.6240
C33 11.7912 4.9762 1.4924
C34 14.6999 5.9282 3.7883
H35 15.7679 5.9032 3.5387
H36 14.5203 5.2028 4.5917
H37 14.4644 6.9230 4.1932
C38 14.5180 5.2196 -1.1597
H39 14.1015 4.4567 -1.8302
H40 15.5935 5.0269 -1.0550
H41 14.4116 6.1888 -1.6688
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H43 9.8044 5.2091 0.7303
H44 9.8755 4.7684 2.4586
H45 10.2423 3.5484 1.2490
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N47 11.5307 8.2295 3.4049
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C51 12.1586 9.1343 6.6868
C52 10.8971 9.7315 6.8592
C53 10.4980 10.1214 8.1395
H54 9.4975 10.5439 8.2706
C55 11.3419 10.0103 9.2388
C56 12.6334 9.5412 9.0222
H57 13.3336 9.4874 9.8602
C58 13.0616 9.1120 7.7682
C59 9.9908 10.0679 5.7114
H60 8.9461 10.1325 6.0460
H61 10.0486 9.3576 4.8866
H62 10.2715 11.0398 5.2836
C63 10.8629 10.3462 10.6203
H64 11.6809 10.7171 11.2516
H65 10.4462 9.4603 11.1252
H66 10.0738 11.1094 10.6033
C67 14.4896 8.7145 7.5778
H68 14.9376 8.3650 8.5171
H69 15.0237 9.5915 7.1927
H70 14.5845 7.9430 6.8102
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C72 9.2450 7.4400 2.7647
C73 8.2958 7.3188 1.7501
H74 7.2940 6.9767 2.0223
C75 8.5801 7.5868 0.4179
C76 9.8887 7.9385 0.1087
H77 10.1703 8.0885 -0.9371
C78 10.8788 8.0691 1.0787
C79 8.8219 7.0269 4.1404
H80 7.8129 6.5973 4.1079
H81 8.8043 7.8551 4.8557
H82 9.5026 6.2668 4.5397
C83 7.5518 7.3841 -0.6557
H84 7.6975 8.0793 -1.4927
H85 6.5336 7.5269 -0.2715
H86 7.5984 6.3665 -1.0718
C87 12.2746 8.3341 0.5980
H88 12.4424 7.8086 -0.3521
H89 13.0184 7.9755 1.3172
H90 12.4443 9.4063 0.4650
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O92 12.4498 3.4235 6.8928
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O94 14.3317 11.0804 5.7936
C95 11.8293 2.6786 3.9836
O96 11.5555 2.4384 2.7926
C97 13.6851 11.9749 3.6918
H98 14.4291 12.7156 4.0065
H99 13.9240 11.5867 2.6960
H100 12.7025 12.4515 3.5870
C101 12.0897 1.4804 4.8948
H102 12.0417 0.5857 4.2638
H103 13.0594 1.5432 5.4001
H104 11.3503 1.4135 5.7012