Supporting Information:

Equilibrium Structures of Pyrazine, s-Triazine, and s-Tetrazine

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Table S1. Computed Vibrational Contributions ΔX_{vib} (X=A,B,C; MHz) to the Ground-State Rotational Constants X_0 and Rotational g Tensors (dimensionless) of Selected Isotopologues of Pyrazine[a,b]

Isotopologue[c,d]	$-\Delta A_{vib}$	$-\Delta B_{vib}$	$-\Delta C_{vib}$	g_{aa}	g_{bb}	g_{cc}
12-1-14	52.44	39.31	23.66	–0.08830	–0.1330	+0.03192
13-1-14	48.18	37.57	22.25	–0.08289	–0.1300	+0.03060
12-1-15	52.11	36.92	22.79	–0.08830	–0.1271	+0.03117
13-1-15	47.86	35.32	21.45	–0.08289	–0.1244	+0.02991
12-2-14	37.44	39.20	19.76	–0.1239	–0.07250	+0.02793
13-2-14	35.74	36.45	18.64	–0.1213	–0.06881	+0.02691
12-2-15	35.37	38.93	19.14	–0.1187	–0.07250	+0.02735
13-2-15	33.79	36.18	18.06	–0.1163	–0.06881	+0.02637

[a] See footnote *a* in Table 4 of the main paper.

[b] The ΔX_{vib} values were computed at the CCSD(T)/VTZ level of theory at the associated optimized equilibrium geometry, and the g factors were calculated at the CCSD(T)/AVTZ level at the best estimated equilibrium geometry (see Table 5 of the main paper).

[c] The entries 12-1-14 and 12-2-14 stand for $^{12}C_4H_4{}^{14}N_2$ and $^{12}C_4D_4{}^{14}N_2$, respectively, with a completely analogous meaning of the other entries.

[d] When replacing all H by D atoms, the a- and b-axes are interchanged in the isotopic species listed here (in the parent species, the a-axis passes through both N atoms). This holds true for the best estimated equilibrium geometry (see Table 5 of the main paper). It also holds true for the equilibrium geometry optimized at the CCSD(T)/VTZ level of theory (see Table 5 of the main paper), except for the 12-2-15 ($^{12}C_4D_4{}^{15}N_2$) isotopologue. Nevertheless, in this exceptional case the corresponding entries for $-\Delta A_{vib}$ and $-\Delta B_{vib}$ were switched as if the a- and b-axes were interchanged, in order to make the whole table consistent with the situation at the best estimated geometry.

Table S2. Computed Vibrational Contributions ΔX_{vib} (X=A,B,C; MHz) to the Ground-State Rotational Constants X_0 and Rotational g Tensors (dimensionless) of Selected Isotopologues of s-Tetrazine[a,b]

Isotopologue[c,d]	$-\Delta A_{vib}$	$-\Delta B_{vib}$	$-\Delta C_{vib}$	g_{aa}	g_{bb}	g_{cc}
12-1-14	58.00	44.10	25.87	–0.1178	–0.1891	+0.00982
13-1-14	55.09	43.46	25.10	–0.1129	–0.1891	+0.00962
12-1-15	55.46	40.28	24.11	–0.1151	–0.1765	+0.00937
13-1-15	52.74	39.67	23.41	–0.1104	–0.1765	+0.00918
12-2-14	44.56	47.72	23.48	–0.1891	–0.1025	+0.00916
13-2-14	43.89	45.52	22.78	–0.1891	–0.09876	+0.00899
12-2-15	40.69	45.84	21.98	–0.1765	–0.1004	+0.00876
13-2-15	40.05	43.76	21.34	–0.1765	–0.09684	+0.00860

[a] See footnote *a* in Table 4 of the main paper.

[b] The ΔX_{vib} values were computed at the CCSD(T)/VTZ level of theory at the associated optimized equilibrium geometry, and the *g* factors were calculated at the CCSD(T)/AVTZ level at the best estimated equilibrium geometry (see Table 6 of the main paper).

[c] The entries 12-1-14 and 12-2-14 stand for $^{12}C_2H_2{}^{14}N_4$ and $^{12}C_2D_2{}^{14}N_4$, respectively, with a completely analogous meaning of the other entries.

[d] When replacing both H by D atoms, the a- and b-axes are interchanged in the isotopic species listed here (in the parent species, the a-axis passes through the midpoints of both N-N bonds). This holds true for both the best estimated equilibrium geometry and the equilibrium geometry optimized at the CCSD(T)/VTZ level of theory (see Table 6 of the main paper).

Table S3. Computed Equilibrium Geometries (pm, deg) of Water and Formaldehyde

		H_2O		H_2CO		
Method	Basis	r_e(OH)	θ_e(HOH)	r_e(CH)	r_e(CO)	θ_e(HCO)
CCSD(T)	VDZ	96.63	101.913	111.99	121.56	122.395
CCSD(T)	VTZ	95.94	103.582	110.33	120.96	121.907
CCSD(T)	VQZ	95.79	104.116	110.22	120.66	121.779
CCSD(T)	AVTZ	96.16	104.180	110.31	121.15	121.714
CCSD(T)	AWCVQZ	95.81	104.490	110.07	120.50	121.691
DKH2-CCSD(T)	AVTZ-DK	96.16	104.115	110.30	121.14	121.712
DKH2-CCSD(T)	AWCVQZ-DK	95.81	104.425	110.06	120.49	121.688
CCSDT	VDZ	96.64	101.908	112.02	121.57	122.404
CCSDT	VTZ	95.94	103.591	110.34	120.94	121.917
CCSDT	VQZ	95.79	104.125	110.23	120.64	121.789
CCSDT(Q)	VDZ	96.67	101.879	112.02	121.67	122.397
CCSDT(Q)	VTZ	95.97	103.553	110.34	121.06	121.906
CCSD(T)-F12b	CVTZ-F12	95.76	104.520	110.05	120.39	121.683
CCSD(T)-F12b	CVQZ-F12	95.74	104.573	110.03	120.37	121.677
Best estimate[a]		95.77	104.49	110.03	120.44	121.68 (116.64)[b]

[a] See text in the main paper. [b] θ_e(HCH) in parentheses.