Supporting Information for "Embracing local suppression and enhancement of dynamic correlation effects in a CASΠDFT method for efficient description of excited states"

Katarzyna Pernal[1] and Oleg V. Gritsenko[1,2]

[1]*Institute of Physics, Lodz University of Technology, ul. Wolczanska 219, 90-924 Lodz, Poland*

[2]*Section Theoretical Chemistry, VU University, NL-1081 HV Amsterdam, The Netherlands*

TABLE S1: Total energies (in Hartree) calculated with CASSCF, CAS+LYP and CASΠDFT methods.

molecule	state	CASSCF	CASSCF+LYP	CASΠDFT
pyridine	1^1A_1	-246.85890	-248.26526	-248.20257
	1^1B_1	-246.66802	-248.07409	-248.03809
	1^1B_2	-246.67299	-248.07994	-248.02506
	1^1A_2	-246.64057	-248.04630	-248.00308
	2^1A_1	-246.56610	-247.97142	-247.96703
pyrazine	1^1A_g	-262.86001	-264.28643	-264.21870
	1^1B_{3u}	-262.68240	-264.10868	-264.09041
	1^1A_u	-262.63971	-264.06581	-264.02510
	1^1B_{2u}	-262.67698	-264.10395	-264.04545
	1^1B_{2g}	-262.64660	-264.07297	-264.04466
	1^1B_{1g}	-262.59564	-264.02194	-263.97686
	1^1B_{1u}	-262.55030	-263.97530	-263.97589
pyrimidine	1^1A_1	-262.88551	-264.31258	-264.23885
	1^1B_1	-262.69432	-264.12111	-264.08482
	1^1A_2	-262.67152	-264.09810	-264.05991
	1^1B_2	-262.68920	-264.11679	-264.06163
	2^1A_1	-262.59632	-264.02306	-263.99036
pyridazine	1^1A_1	-262.84747	-264.27222	-264.19517
	1^1B_1	-262.69228	-264.11727	-264.07657
	1^1A_2	-262.67311	-264.09814	-264.03943
	2^1A_1	-262.66210	-264.08711	-264.02992
	2^1A_2	-262.62207	-264.04758	-263.99661
	2^1B_1	-262.58574	-264.01120	-263.95104
	1^1B_2	-262.55685	-263.98195	-263.93949