Effective Inclusion of Mechanical and Electrical Anharmonicity in Excited Electronic States: the VPT2-TDDFT Route

Franco Egidi,[†,‡] David B. Williams-Young,[¶,†] Alberto Baiardi,[‡,†] Julien Bloino,[§] Giovanni Scalmani,[‖] Michael J. Frisch,[‖] Xiaosong Li,[*,¶] and Vincenzo Barone[*,‡]

†*These authors contributed equally to this work*

‡*Scuola Normale Superiore, Piazza dei Cavalieri 7, 56126 Pisa, Italy*

¶*University of Washington, Department of Chemistry, University of Washington, Seattle, WA, 98195*

§*Consiglio Nazionale delle Ricerche, Istituto di Chimica dei Composti OrganoMetallici (ICCOM-CNR), UOS di Pisa, Area della Ricerca CNR, Via G. Moruzzi 1, Pisa 56124, Italy*

‖*Gaussian Inc. 340 Quinnipiac St Bldg 40, Wallingford, CT 06492, USA*

E-mail: xsli@uw.edu; vincenzo.barone@sns.it

Table 1: Ground and excited state optimized geometries of imidazole, B3LYP/aug-cc-pVTZ level of theory. Coordinates are in Ångstroms.

	Ground state S_0			Excited state S_1		
Atom	X	Y	Z	X	Y	Z
C	-1.089076	0.282714	0.000000	-1.050570	-0.612180	0.019555
H	-2.097430	0.661527	0.000000	-1.687812	-0.930590	0.866125
C	0.635169	-0.982619	0.000000	1.174356	-0.266475	0.073650
H	1.196260	-1.901156	0.000000	2.220947	-0.507819	0.008412
C	1.116431	0.296913	0.000000	0.583325	0.983225	0.110961
H	2.113497	0.697930	0.000000	1.045184	1.949781	0.013710
N	-0.739829	-0.979889	0.000000	0.179638	-1.141640	-0.139945
N	0.000000	1.101785	0.000000	-0.797142	0.774234	-0.178832
H	-0.008665	2.106381	0.000000	-1.498456	1.433048	0.118189

Table 2: Ground and excited state optimized geometries of phenyl radical, B3LYP/SNSD level of theory. Coordinates are in Ångstroms.

	Ground state D_0			Excited state D_1		
Atom	X	Y	Z	X	Y	Z
C	0.000000	0.000000	-1.323637	0.000000	0.000000	-1.342249
H	0.000000	0.000000	-2.409746	0.000000	0.000000	-2.429528
C	0.000000	1.213646	-0.632208	0.000000	1.227614	-0.643781
H	0.000000	2.153825	-1.178148	0.000000	2.160154	-1.203784
C	0.000000	-1.213646	-0.632208	0.000000	-1.227614	-0.643781
H	0.000000	-2.153825	-1.178148	0.000000	-2.160154	-1.203784
C	0.000000	1.226316	0.772027	0.000000	1.213274	0.734025
H	0.000000	2.162200	1.323720	0.000000	2.168876	1.257235
C	0.000000	-1.226316	0.772027	0.000000	-1.213274	0.734025
H	0.000000	-2.162200	1.323720	0.000000	-2.168876	1.257235
C	0.000000	0.000000	1.397099	0.000000	0.000000	1.548865

Table 3: Ground and excited state optimized geometries of anisole, B3LYP/6-311+G(d,p) level of theory. Coordinates are in Ångstroms.

	Ground state S_0			Excited state S_1		
Atom	X	Y	Z	X	Y	Z
C	1.808791	-1.072718	0.000000	-1.917550	-0.974211	0.000000
C	1.371851	0.244512	0.000000	-0.531048	-1.301876	0.000000
C	0.000000	0.527572	0.000000	0.411330	-0.233821	0.000000
C	-0.925649	-0.519303	0.000000	0.035261	1.136568	0.000000
C	-0.469452	-1.840366	0.000000	-1.357512	1.442230	0.000000
C	0.890805	-2.126902	0.000000	-2.302263	0.384867	0.000000
H	2.873234	-1.279841	0.000000	-2.667350	-1.753353	0.000000
H	2.071242	1.071952	0.000000	-0.166773	-2.319354	0.000000
H	-1.989546	-0.323889	0.000000	0.773755	1.924168	0.000000
H	-1.194431	-2.646919	0.000000	-1.690692	2.470915	0.000000
H	1.235238	-3.154165	0.000000	-3.358549	0.631508	0.000000
O	-0.331452	1.852768	0.000000	1.698050	-0.640423	0.000000
C	-1.706220	2.210251	0.000000	2.769289	0.305536	0.000000
H	-2.217215	1.836811	0.894258	2.729094	0.930817	0.895073
H	-1.730446	3.298821	0.000000	3.681157	-0.287186	0.000000
H	-2.217215	1.836811	-0.894258	2.729094	0.930817	-0.895073

Table 4: Ground and excited state optimized geometries of anthranilic acid, B3LYP/SNSD level of theory. Coordinates are in Ångstroms.

	Ground state S_0			Excited state S_1		
Atom	X	Y	Z	X	Y	Z
C	-1.941158	0.902021	0.004880	0.801382	-2.012740	0.000000
C	-0.529172	0.985850	-0.007165	-0.243012	-1.082539	0.000000
C	0.212758	-0.231353	-0.006584	0.000000	0.345122	0.000000
C	-0.476193	-1.461384	-0.004857	1.343267	0.736622	0.000000
C	-1.858519	-1.520858	0.002597	2.407282	-0.220749	0.000000
C	-2.586922	-0.320564	0.009641	2.160106	-1.582152	0.000000
H	-2.517558	1.824090	0.005604	0.557717	-3.072351	0.000000
H	0.107218	-2.375116	-0.006565	1.583439	1.793151	0.000000
H	-2.369480	-2.478042	0.004763	3.429737	0.146753	0.000000
H	-3.673631	-0.346032	0.018125	2.967545	-2.305054	0.000000
C	1.678638	-0.202025	0.002862	-1.105955	1.289111	0.000000
O	2.377347	0.805601	0.023760	-2.335818	1.023902	0.000000
O	2.259261	-1.430624	-0.009308	-0.704398	2.599767	0.000000
H	3.215683	-1.271425	0.001651	-1.522596	3.118038	0.000000
N	0.076910	2.206828	-0.038292	-1.546817	-1.476735	0.000000
H	1.085670	2.249155	0.038490	-2.249599	-0.712524	0.000000
H	-0.475728	3.039634	0.082120	-1.795213	-2.456278	0.000000