

Appendix B

2D vibrational eigenenergies for
 FHF^- , FDF^- , OHF^- , and ODF^-

Table B.1: Twenty-six ($\Psi_0 - \Psi_{25}$) lowest 2D vibrational eigenfunctions and eigenenergies of FHF⁻ and FDF⁻ (QCISD), and of OHF⁻ and ODF⁻ (UMP4). The states and corresponding energies are labelled according to symmetric and asymmetric stretching quanta, ν_{sas} and E_{sas} , respectively. All energies are given in cm⁻¹.

	FHF ⁻		FDF ⁻		OHF ⁻		ODF ⁻	
	E_{sas}	ν_{sas}	E_{sas}	ν_{sas}	E_{sas}	ν_{sas}	E_{sas}	ν_{sas}
Ψ_0	1019	ν_{00}	792	ν_{00}	1125	ν_{00}	847	ν_{00}
Ψ_1	1612	ν_{10}	1390	ν_{10}	1621	ν_{10}	1311	ν_{10}
Ψ_2	2196	ν_{20}	1794	ν_{01}	2071	ν_{20}	1735	ν_{20}
Ψ_3	2467	ν_{01}	1977	ν_{20}	2492	ν_{30}	2058	ν_{01}
Ψ_4	2774	ν_{30}	2338	ν_{11}	2804	ν_{01}	2182	ν_{30}
Ψ_5	2996	ν_{11}	2547	ν_{30}	2899	ν_{40}	2529	ν_{40}
Ψ_6	3324	ν_{40}	2863	ν_{21}	3289	ν_{50}	2712	ν_{11}
Ψ_7	3512	ν_{21}	2957	ν_{02}	3418	ν_{11}	2952	ν_{50}
Ψ_8	3865	ν_{50}	3088	ν_{40}	3669	ν_{60}	3106	ν_{02}
Ψ_9	4011	ν_{31}	3372	ν_{31}	4006	ν_{21}	3288	ν_{21}
Ψ_{10}	4165	ν_{02}	3505	ν_{12}	4131	ν_{70}	3405	ν_{60}
Ψ_{11}	4390	ν_{60}	3619	ν_{50}	4347	ν_{02}	3608	ν_{31}
Ψ_{12}	4531	ν_{41}	3875	ν_{41}	4541	ν_{80}	3820	ν_{70}
Ψ_{13}	4713	ν_{12}	4036	ν_{60}	4629	ν_{31}	3911	ν_{12}
Ψ_{14}	4912	ν_{70}	4154	ν_{03}	4886	ν_{12}	4098	ν_{41}
Ψ_{15}	5045	ν_{51}	4179	ν_{70}	4982	ν_{90}	4300	ν_{80}
Ψ_{16}	5265	ν_{22}	4359	ν_{51}	5166	ν_{41}	4341	ν_{03}
Ψ_{17}	5446	ν_{80}	4553	ν_{80}	5405	ν_{22}	4433	ν_{22}
Ψ_{18}	5573	ν_{61}	4689	ν_{42}	5441	ν_{100}	4600	ν_{51}
Ψ_{19}	5830	ν_{32}	4709	ν_{13}	5675	ν_{51}	4776	ν_{90}
Ψ_{20}	5927	ν_{03}	4851	ν_{61}	5899	ν_{32}	4891	ν_{13}
Ψ_{21}	5991	ν_{90}	5071	ν_{90}	5922	ν_{110}	4947	ν_{32}
Ψ_{22}	6108	ν_{71}	5232	ν_{23}	6005	ν_{03}	5121	ν_{61}
Ψ_{23}	6383	ν_{42}	5239	ν_{52}	6163	ν_{42}	5271	ν_{100}
Ψ_{24}	6460	ν_{13}	5362	ν_{71}	6381	ν_{61}	5413	ν_{23}
Ψ_{25}	6551	ν_{100}	5453	ν_{04}	6406	ν_{71}	5470	ν_{52}