

Molecular Orbital Coefficients: H₂O

				1	2	3	4	5
				(A1)	(A1)	(B2)	(A1)	(B1)
		ϵ	--	-20.23449	-1.26075	-0.62397	-0.44044	-0.38694
χ_1	1	0	1S	0.99412	-0.23325	0.00000	-0.09978	0.00000
χ_2			2S	0.02656	0.83540	0.00000	0.52057	0.00000
χ_3			2PX	0.00000	0.00000	0.00000	0.00000	1.00000
χ_4			2PY	0.00000	0.00000	0.59969	0.00000	0.00000
χ_5			2PZ	-0.00415	-0.12325	0.00000	0.79176	0.00000
χ_6	2	H	1S	-0.00597	0.15955	0.44236	-0.27316	0.00000
χ_7	3	H	1S	-0.00597	0.15955	-0.44236	-0.27316	0.00000