

Natural Cluster Unit (NCU) Analysis:

NCU thr.	Unit formula	Unit charge	Atom list
1.000	1. H	0.495	H1
	2. O	-0.957	O2
	3. H	0.452	H3
	4. O	-0.941	O4
	5. H	0.475	H5
	6. H	0.475	H6
0.890	1. H	0.495	H1
	2. HO	-0.504	O2, H3
	3. O	-0.941	O4
	4. H	0.475	H5
	5. H	0.475	H6
0.880	1. H	0.495	H1
	2. HO	-0.504	O2, H3
	3. H2O	0.009	O4, H5, H6
0.860	1. H2O	-0.009	H1, O2, H3
	2. H2O	0.009	O4, H5, H6
0.120	1. H4O2	0.000	H1, O2, H3, O4, H5, H6