

NATURAL COULOMB ELECTROSTATICS (NCE):

Lewis(L) and non-Lewis(NL) contributions to NPA atomic charge and Coulomb potential energy

atomic charge

atom	unit	L	NL	total
H 1	1	0.50493	-0.00966	0.49527
O 2	1	-0.95998	0.00335	-0.95663
H 3	1	0.45505	-0.00268	0.45237

Total unit	1	0.00000	-0.00900	-0.00900

O 4	2	-0.95504	0.01380	-0.94125
H 5	2	0.47752	-0.00240	0.47512
H 6	2	0.47752	-0.00240	0.47512

Total unit	2	0.00000	0.00900	0.00900

Total species		0.00000	0.00000	0.00000

NCE Potential Energy (au)

	unit	unit	L	NL	total
within	1		-0.42570	0.00624	-0.41946
within	2		-0.42263	0.00894	-0.41369

	Total		-0.84833	0.01518	-0.83316

between	1	2	-0.01516	0.00092	-0.01424

	Total		-0.86350	0.01610	-0.84740