

8-Dec-23									
John W. Keller, University of Alaska Fairbanks									
Department of Chemistry and Biochemistry									
jwkeller@alaska.edu									
This is a spreadsheet to create a jmol dipole command given									
the cartesian coordinates of the dipole as calculated by ORCA v 5									
See the Jmol documentation for dipole command at			https://chemapps.stolaf.edu/jmol/docs/						
		x	y	z					
enter the dipole coor here		0.00	0.00	0.00	+end				
negative of ORCA dipole xyz		-0.65	0.39	-0.58	-end				
x 8 (or webmo x2.5)	8	0.00	0.00	0.00	+end				
		-5.20	3.12	-4.64	-end				
middle	/2	-2.60	1.56	-2.32					
move middl to origin		2.60	-1.56	2.32	+end				
		-2.60	1.56	-2.32	-end				
cartesian center (from below)		0.55	0.14	0.09					
move dipole to cartisian center		3.15	-1.42	2.41	+end				
		-2.05	1.70	-2.23	-end				
	molecule cartesian center								
	C	0.064	0.016	0.048					
	N	1.470	0.020	0.020					
	H	1.839	0.966	0.031					
	H	1.846	-0.503	0.806					
	F	-0.483	0.677	1.134					
	H	-0.327	-1.003	0.047					
	Cl	-0.583	0.836	-1.433					
	ave	0.547	0.144	0.093					
dipole dip width 0.2 {		3.15	-1.42	2.41	{ {	-2.05	1.70	-2.23	};
jmol dipole command		dipole dip width 0.2 {3.15 -1.42 2.413} { -2.05 1.7 -2.227};							