

**XCC2 – a new coupled cluster model for second-order
polarization propagator.
Supporting Information**

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TABLE I: Components of dipole polarizabilities for 24 molecules used to generate the statistical data presented in the paper. All values in a.u. Missing polarizabilities correspond to unconverged first-order excitation operators

method	$\omega = 0.0$			$\omega = 0.1$			$\omega = 0.2$		
	α_{xx}	α_{yy}	α_{zz}	α_{xx}	α_{yy}	α_{zz}	α_{xx}	α_{yy}	α_{zz}
3-pentanone									
XCCSD	76.679	67.280	54.577	79.829	69.862	56.257	93.085	80.034	62.411
XCC2	76.320	65.448	53.512	79.637	68.061	55.202	100.538	78.824	61.478
TD-CCSD	75.782	65.850	53.708	78.875	68.357	55.357	91.812	78.204	61.395
TD-CC2	79.880	69.043	55.330	83.474	71.896	57.098	108.229	83.925	63.697
propionamide									
XCCSD	61.539	54.077	41.273	64.811	56.436	42.740	81.759	67.820	49.478
XCC2	60.369	52.765	40.385	63.769	55.242	41.865	110.157	82.153	49.171
TD-CCSD	60.213	52.993	40.542	63.332	55.319	41.974	79.446	66.430	48.522
TD-CC2	64.116	56.298	41.994	67.935	59.114	43.580	137.261	83.156	51.584
2-aminopropane									
XCCSD	55.429	53.606	46.869	59.260	55.957	48.610	-	65.902	55.710
XCC2	54.814	53.194	46.050	58.970	55.657	47.817	-	67.780	55.357
TD-CCSD	54.451	52.763	46.079	58.141	55.057	47.779	43.194	65.328	54.690
TD-CC2	57.821	55.540	47.925	62.573	58.205	49.817	53.294	71.591	58.084
2-methylpropane									
XCCSD	55.283	55.283	48.832	57.427	57.427	50.587	65.738	65.739	57.302
XCC2	54.984	54.984	48.065	57.187	57.187	49.837	65.908	65.908	56.696
TD-CCSD	54.612	54.611	48.095	56.723	56.722	49.819	64.900	64.898	56.408
TD-CC2	56.871	56.870	49.714	59.182	59.180	51.566	68.358	68.356	58.757
2-nitropropane									
XCCSD	62.774	58.172	51.137	65.959	61.243	52.790	87.005	86.036	58.780
XCC2	60.642	54.688	50.717	63.620	57.362	52.415	80.428	74.951	58.629
TD-CCSD	62.206	55.892	50.515	65.548	58.550	52.145	89.728	77.747	58.048
TD-CC2	64.857	58.457	52.463	68.362	61.311	54.246	90.379	79.092	60.784

TABLE I: ... continued.

propanoic acid									
XCCSD	55.450	49.557	37.737	57.795	51.580	38.864	65.114	56.669	43.190
XCC2	54.843	47.890	36.987	57.347	49.914	38.122	70.191	58.642	42.438
TD-CCSD	54.292	48.573	37.096	56.570	50.528	38.200	66.378	58.711	42.359
TD-CC2	58.067	51.113	38.420	60.877	53.340	39.622	75.604	63.303	44.213
<i>N</i> -methylacetamide									
XCCSD	62.180	54.895	39.989	65.698	57.504	41.248	84.717	72.014	46.292
XCC2	60.298	54.130	39.182	63.877	56.924	40.463	97.286	113.932	46.041
TD-CCSD	61.232	53.362	39.312	64.695	55.816	40.544	83.331	69.350	45.471
TD-CC2	65.253	56.770	40.683	69.372	59.879	42.044	106.786	136.380	48.002
<i>N</i> -methylformamide									
XCCSD	49.143	40.441	30.407	52.393	42.085	31.479	70.857	49.749	36.810
XCC2	47.097	39.768	29.827	50.326	41.584	30.919	73.238	56.337	37.029
TD-CCSD	47.624	39.791	29.889	50.722	41.398	30.935	68.319	48.800	36.119
TD-CC2	51.094	42.429	30.976	54.870	44.497	32.142	85.742	61.860	38.930
acetaldehyde									
XCCSD	36.958	30.716	24.230	38.776	32.093	24.975	46.972	38.534	27.748
XCC2	35.811	30.231	23.958	37.690	31.740	24.721	48.175	40.599	27.696
TD-CCSD	36.208	30.142	23.903	37.973	31.475	24.635	45.897	37.670	27.353
TD-CC2	38.467	32.031	24.671	40.601	33.720	25.475	53.264	43.864	28.664
acetone									
XCCSD	47.572	46.281	34.649	49.732	48.410	35.708	58.778	59.871	39.593
XCC2	46.016	46.012	34.121	48.347	48.187	35.193	74.639	57.773	39.225
TD-CCSD	46.560	45.621	34.149	48.656	47.695	35.188	57.414	58.754	38.998
TD-CC2	48.974	48.456	35.216	51.376	51.067	36.343	62.158	82.997	40.629

TABLE I: ... continued.

pentanol									
XCCSD	83.432	66.469	61.807	86.580	68.908	63.992	98.364	78.424	72.666
XCC2	83.085	65.576	60.500	86.343	68.079	62.707	98.799	78.081	71.766
TD-CCSD	82.590	65.291	60.731	85.693	67.678	62.867	97.295	76.991	71.327
TD-CC2	86.703	68.105	62.992	90.154	70.744	65.339	103.401	81.327	75.149
trifluoroethane									
XCCSD	32.104	31.477	31.477	32.958	32.245	32.245	35.989	34.916	34.916
XCC2	31.592	30.716	30.716	32.465	31.495	31.495	35.601	34.226	34.226
TD-CCSD	31.586	30.847	30.847	32.423	31.597	31.597	35.391	34.209	34.209
TD-CC2	33.285	32.466	32.466	34.226	33.301	33.301	37.617	36.232	36.232
fluorobenzene									
XCCSD	85.447	83.486	45.266	91.608	89.929	47.232	127.625	-	56.709
XCC2	85.874	84.387	45.521	92.692	91.525	47.620	135.899	-	58.178
TD-CCSD	83.131	81.420	44.628	89.048	87.630	46.570	123.526	116.217	55.924
TD-CC2	87.916	85.388	45.671	94.788	92.453	47.738	138.096	123.261	58.072
chloroethane									
XCCSD	49.953	39.743	37.080	52.101	41.232	38.418	60.497	47.088	43.681
XCC2	49.247	39.034	36.213	51.404	40.521	37.532	59.918	46.413	42.747
TD-CCSD	49.345	39.210	36.612	51.462	40.674	37.932	59.731	46.431	43.131
TD-CC2	51.095	40.330	37.450	53.353	41.882	38.830	62.282	48.051	44.307
chloroformamide									
XCCSD	52.312	47.144	30.490	55.290	49.814	31.572	70.198	63.118	36.151
XCC2	51.317	44.664	29.623	54.588	47.346	30.694	75.291	61.608	35.363
TD-CCSD	51.635	45.159	29.987	54.506	47.721	31.044	68.595	60.684	35.514
TD-CC2	56.007	47.709	30.771	59.837	50.666	31.911	85.334	66.189	36.944

TABLE I: ... continued.

benzene									
XCCSD	83.668	83.668	45.723	90.058	90.058	47.914	127.742	127.740	58.725
XCC2	84.715	84.715	46.190	91.765	91.765	48.534	136.380	136.379	60.552
TD-CCSD	81.664	81.659	45.103	87.834	87.829	47.263	124.121	124.106	57.914
TD-CC2	85.538	85.534	46.042	92.504	92.499	48.339	136.238	136.220	60.058
cyanomethane									
XCCSD	39.569	24.302	24.302	41.276	25.094	25.094	47.741	28.014	28.014
XCC2	37.863	24.171	24.171	39.532	24.969	24.969	45.902	27.914	27.914
TD-CCSD	38.992	24.098	24.098	40.673	24.883	24.883	47.037	27.775	27.775
TD-CC2	39.885	24.551	24.551	41.656	25.363	25.363	48.424	28.361	28.361
nitrobenzene									
XCCSD	116.459	103.960	51.752	128.004	111.862	53.613	355.281	-	61.145
XCC2	118.354	99.857	51.615	131.377	107.764	53.573	-	-	61.740
TD-CCSD	113.784	100.436	50.982	124.997	107.960	52.816	345.691	152.266	60.236
TD-CC2	121.174	104.765	52.120	134.158	113.016	54.086	718.332	159.628	62.185
phenol									
XCCSD	96.128	87.411	48.266	104.025	94.437	50.411	-	-	-
XCC2	96.642	88.040	48.398	105.409	95.824	50.685	173.525	-	63.312
TD-CCSD	93.412	85.170	47.510	100.979	91.926	49.621	151.898	116.817	60.798
TD-CC2	99.520	89.351	48.791	108.520	97.079	51.072	178.939	124.125	62.858
toluene									
XCCSD	104.739	92.881	55.236	112.915	99.517	57.602	162.714	138.543	69.033
XCC2	106.257	93.531	55.304	115.274	100.846	57.810	174.783	147.462	70.555
TD-CCSD	102.470	90.599	54.414	110.383	96.994	56.743	158.436	134.496	67.996
TD-CC2	107.821	94.834	55.664	116.817	102.091	58.153	175.769	147.775	70.748

TABLE I: ... continued.

cyanoethane									
XCCSD	52.507	37.496	34.704	54.761	38.775	35.833	63.384	43.523	40.010
XCC2	50.828	37.250	34.355	53.053	38.546	35.490	61.636	43.386	39.705
TD-CCSD	51.839	37.069	34.333	54.060	38.332	35.449	62.556	43.018	39.578
TD-CC2	53.277	38.085	35.098	55.630	39.418	36.261	64.715	44.394	40.582
cyclopentane									
XCCSD	62.774	62.275	54.994	65.123	64.594	56.922	74.060	73.406	64.256
XCC2	62.060	62.605	54.040	64.460	65.038	55.990	73.756	74.473	63.500
TD-CCSD	61.908	61.403	54.134	64.216	63.681	56.028	72.992	72.332	63.226
TD-CC2	64.772	64.221	55.986	67.324	66.739	58.026	77.251	76.522	65.898
cyanopropane									
XCCSD	69.456	47.876	44.905	72.458	49.506	46.372	83.890	55.582	51.824
XCC2	67.875	47.424	44.316	70.878	49.074	45.791	82.422	55.269	51.299
TD-CCSD	68.649	47.263	44.349	71.611	48.868	45.797	82.890	54.852	51.176
TD-CC2	71.000	48.645	45.434	74.172	50.348	46.953	86.386	56.749	52.632
<i>o</i> -dichlorobenzene									
XCCSD	128.351	111.224	61.224	138.962	119.336	63.561	-	174.839	74.929
XCC2	129.496	111.527	60.250	141.299	120.499	62.658	-	192.157	75.159
TD-CCSD	125.195	108.577	60.313	135.428	116.396	62.619	202.878	169.715	73.861
TD-CC2	132.585	113.942	61.392	144.557	123.001	63.848	233.178	195.483	76.666