

MP2 geometries of formic acid tetramers

Alfred Karpfen,
Institute for Theoretical Chemistry, University of Vienna,
Währinger Straße 17, A-1090 Vienna, Austria

and

Ajit J. Thakkar
Department of Chemistry, University of New Brunswick,
Fredericton, New Brunswick, Canada E3B 6E2

June 14, 2006

This report contains tables of the coordinates, in Å, of the MP2 geometries of 12 formic acid tetramers as reported in the J. Chem. Phys. 124, 224313 (2006) article: “Does the most stable formic acid tetramer have π -stacking or C–H \cdots O interactions?” Two sets of geometries are given, one for the aug-cc-pVDZ basis set and the other for the cc-pVTZ basis set.

AS1 [MP2/aug-cc-pVDZ]

C	2.247595	-0.373210	0.805828
O	1.601985	0.421864	1.490858
O	2.284719	-0.411028	-0.521570
H	2.879127	-1.155661	1.253296
H	1.695778	0.314426	-0.884986
O	0.689061	1.505859	-1.490853
C	0.015435	2.277351	-0.805829
O	-0.015435	2.320457	0.521565
H	-0.648212	3.032746	-1.253306
H	0.599305	1.616750	0.885007
C	-2.247595	0.373210	0.805828
O	-1.601985	-0.421864	1.490858
O	-2.284719	0.411028	-0.521570
H	-2.879127	1.155661	1.253296
H	-1.695778	-0.314426	-0.884986
O	-0.689061	-1.505859	-1.490853
C	-0.015435	-2.277351	-0.805829
O	0.015435	-2.320457	0.521565
H	0.648212	-3.032746	-1.253306
H	-0.599305	-1.616750	0.885007

AS2 [MP2/aug-cc-pVDZ]

C	1.754552	1.468328	0.759993
C	-1.754552	1.468328	-0.759993
O	1.595532	1.486954	-0.464694
O	-1.595532	1.486954	0.464694
O	0.797140	1.475281	1.672149
O	-0.797140	1.475281	-1.672149
H	-0.094780	1.490316	1.216497
H	0.094780	1.490316	-1.216497
H	2.754242	1.443233	1.219628
H	-2.754242	1.443233	-1.219628
C	1.754552	-1.468328	-0.759993
C	-1.754552	-1.468328	0.759993
O	1.595532	-1.486954	0.464694
O	-1.595532	-1.486954	-0.464694
O	0.797140	-1.475281	-1.672149
O	-0.797140	-1.475281	1.672149
H	-0.094780	-1.490316	-1.216497
H	0.094780	-1.490316	1.216497
H	2.754242	-1.443233	-1.219628
H	-2.754242	-1.443233	1.219628

AS3 [MP2/aug-cc-pVDZ]

C	-0.123546	1.905828	1.459248
C	0.123546	-1.905828	1.459248
O	-1.132388	1.198564	1.460411
O	1.132388	-1.198564	1.460411
O	1.132388	1.475835	1.503677
O	-1.132388	-1.475835	1.503677
H	1.131870	0.473502	1.514566
H	-1.131870	-0.473502	1.514566
H	-0.177213	3.004456	1.421536
H	0.177213	-3.004456	1.421536
C	1.358384	1.347735	-1.477161
C	-1.358384	-1.347735	-1.477161
O	0.161268	1.652147	-1.462487
O	-0.161268	-1.652147	-1.462487
O	1.852508	0.121183	-1.485696
O	-1.852508	-0.121183	-1.485696
H	1.099967	-0.539363	-1.471175
H	-1.099967	0.539363	-1.471175
H	2.154795	2.107316	-1.484685
H	-2.154795	-2.107316	-1.484685

SS1 [MP2/aug-cc-pVDZ]

C	0.398449	2.582543	1.172455
O	0.312782	2.843930	-0.030273
O	-0.220405	1.600672	1.808813
H	-0.744838	1.061744	1.150809
H	1.023069	3.178572	1.855534
C	-0.398449	-2.582543	1.172455
O	-0.312782	-2.843930	-0.030273
O	0.220405	-1.600672	1.808813
H	0.744838	-1.061744	1.150809
H	-1.023069	-3.178572	1.855534
C	-1.580965	0.326213	-1.188569
O	-1.580965	0.103383	0.025358
O	-0.984613	1.344461	-1.791614
H	-0.527771	1.916466	-1.102046
H	-2.094228	-0.332565	-1.905887
C	1.580965	-0.326213	-1.188569
O	1.580965	-0.103383	0.025358
O	0.984613	-1.344461	-1.791614
H	0.527771	-1.916466	-1.102046
H	2.094228	0.332565	-1.905887

SS2 [MP2/aug-cc-pVDZ]

C	-0.838892	-1.891422	0.462949
O	-0.573136	-0.934847	1.198117
O	-1.680794	-1.886647	-0.556569
H	-2.096117	-0.979206	-0.641510
H	-0.376922	-2.880530	0.601901
C	2.598211	-1.460508	0.019145
O	2.862655	-0.506479	0.751367
O	1.730266	-1.463987	-0.986054
H	1.308803	-0.555864	-1.060625
H	3.082473	-2.442931	0.138534
C	-2.598211	1.460508	-0.019145
O	-2.862655	0.506479	-0.751367
O	-1.730266	1.463987	0.986054
H	-1.308803	0.555864	1.060625
H	-3.082473	2.442931	-0.138534
C	0.838992	1.891422	-0.462949
O	0.573136	0.934847	-1.198117
O	1.680794	1.886647	0.556569
H	2.096117	0.979206	0.641510
H	0.376922	2.880530	-0.601901

B1 [MP2/aug-cc-pVDZ]

C	-1.473535	0.858460	1.766590
O	-2.043538	0.346225	0.804119
O	-0.346225	1.558032	1.735328
H	-0.034764	1.657035	0.791840
H	-1.866814	0.778184	2.791921
C	-0.858460	-1.473535	-1.766590
O	-0.346225	-2.043538	-0.804119
O	-1.558032	-0.346225	-1.735328
H	-1.657035	-0.034764	-0.791840
H	-0.778184	-1.866814	-2.791921
C	0.858460	1.473535	-1.766590
O	0.346225	2.043538	-0.804119
O	1.558032	0.346225	-1.735328
H	1.657035	0.034764	-0.791840
H	0.778184	1.866814	-2.791921
C	1.473535	-0.858460	1.766590
O	2.043538	-0.346225	0.804119
O	0.346225	-1.558032	1.735328
H	0.034764	-1.657035	0.791840
H	1.866814	-0.778184	2.791921

B2 [MP2/aug-cc-pVDZ]

C	-0.480934	1.660737	1.794680
O	-1.307269	0.829032	1.411934
O	0.480934	2.209498	1.073639
H	0.512324	1.807280	0.159249
H	-0.473261	2.040694	2.828471
C	-1.660737	-0.480934	-1.794680
O	-0.829032	-1.307269	-1.411934
O	-2.209498	0.480934	-1.073639
H	-1.807280	0.512324	-0.159249
H	-2.040694	-0.473261	-2.828471
C	1.660737	0.480934	-1.794680
O	0.829032	1.307269	-1.411934
O	2.209498	-0.480934	-1.073639
H	1.807280	-0.512324	-0.159249
H	2.040694	0.473261	-2.828471
C	0.480934	-1.660737	1.794680
O	1.307269	-0.829032	1.411934
O	-0.480934	-2.209498	1.073639
H	-0.512324	-1.807280	0.159249
H	0.473261	-2.040694	2.828471

PA1 [MP2/aug-cc-pVDZ]

C	1.098475	1.385216	0.000000
O	1.681820	0.293429	0.000000
O	1.681820	2.573036	0.000000
H	2.675969	2.455954	0.000000
H	0.000766	1.451793	0.000000
C	-1.098475	-1.385216	0.000000
O	-1.681820	-0.293429	0.000000
O	-1.681820	-2.573036	0.000000
H	-2.675969	-2.455954	0.000000
H	-0.000766	-1.451793	0.000000
C	4.927198	1.188029	0.000000
O	4.352305	2.278755	0.000000
O	4.346244	-0.003904	0.000000
H	3.352019	0.117210	0.000000
H	6.025376	1.104336	0.000000
C	-4.927198	-1.188029	0.000000
O	-4.352305	-2.278755	0.000000
O	-4.346244	0.003904	0.000000
H	-3.352019	-0.117210	0.000000
H	-6.025376	-1.104336	0.000000

PA2 [MP2/aug-cc-pVDZ]			
C	-4.924407	-1.231297	0.000000
O	-4.386102	-2.340535	0.000000
O	-4.304020	-0.059345	0.000000
H	-3.314872	-0.213601	0.000000
H	-6.019125	-1.111077	0.000000
C	4.927956	1.426358	0.000000
O	4.315297	0.355531	0.000000
O	4.391235	2.637368	0.000000
H	3.392315	2.555612	0.000000
H	6.028432	1.469861	0.000000
C	-1.105401	-1.560547	0.000000
O	-1.648584	-0.448785	0.000000
O	-1.729581	-2.727043	0.000000
H	-2.719348	-2.575381	0.000000
H	-0.011185	-1.669425	0.000000
C	1.098485	1.366531	0.000000
O	1.721238	2.430563	0.000000
O	1.643356	0.150727	0.000000
H	2.641263	0.237311	0.000000
H	0.000000	1.312585	0.000000

PA3 [MP2/aug-cc-pVDZ]

C	1.013593	1.610638	0.000000
O	1.598491	2.695770	0.000000
O	1.598491	0.414541	0.000000
H	2.593431	0.534584	0.000000
H	-0.082481	1.522449	0.000000
C	-4.837153	-1.797474	0.000000
O	-4.258767	-0.707713	0.000000
O	-4.262279	-2.990841	0.000000
H	-3.266784	-2.877492	0.000000
H	-5.935638	-1.875782	0.000000
C	4.837153	1.797474	0.000000
O	4.258767	0.707713	0.000000
O	4.262279	2.990841	0.000000
H	3.266784	2.877492	0.000000
H	5.935638	1.875782	0.000000
C	-1.013593	-1.610638	0.000000
O	-1.598491	-2.695770	0.000000
O	-1.598491	-0.414541	0.000000
H	-2.593431	-0.534584	0.000000
H	0.082481	-1.522449	0.000000

CE [MP2/aug-cc-pVDZ]

C	3.586765	-1.290115	0.000000
O	3.277904	-0.101750	0.000000
O	2.751785	-2.323723	0.000000
H	1.805483	-1.998139	0.000000
H	4.635931	-1.627133	0.000000
C	0.335619	1.867074	0.000000
O	-0.450027	2.816663	0.000000
O	1.647961	2.067062	0.000000
H	2.123416	1.203245	0.000000
H	0.000000	0.815270	0.000000
C	-0.650964	-2.539471	0.000000
O	0.179450	-1.625649	0.000000
O	-1.962693	-2.385045	0.000000
H	-2.183368	-1.408453	0.000000
H	-0.368602	-3.605068	0.000000
C	-3.258735	1.092057	0.000000
O	-2.381495	0.221160	0.000000
O	-3.028997	2.387056	0.000000
H	-2.024454	2.538382	0.000000
H	-4.335623	0.858428	0.000000

CZ [MP2/aug-cc-pVDZ]			
C	1.074256	3.048638	0.000000
C	-3.048638	1.074256	0.000000
C	-1.074256	-3.048638	0.000000
C	3.048638	-1.074256	0.000000
O	0.078708	2.330835	0.000000
O	-2.330835	0.078708	0.000000
O	-0.078708	-2.330835	0.000000
O	2.330835	-0.078708	0.000000
H	1.033963	4.150820	0.000000
H	-4.150820	1.033963	0.000000
H	-1.033963	-4.150820	0.000000
H	4.150820	-1.033963	0.000000
O	2.330835	2.616688	0.000000
O	-2.616688	2.330835	0.000000
O	-2.330835	-2.616688	0.000000
O	2.616688	-2.330835	0.000000
H	2.336005	1.621059	0.000000
H	-1.621059	2.336005	0.000000
H	-2.336005	-1.621059	0.000000
H	1.621059	-2.336005	0.000000

AS1 [MP2/cc-pVTZ]

C	1.532668	1.707900	0.806578
C	1.532668	-1.707900	-0.806578
O	1.579788	0.695913	1.488582
O	1.579788	-0.695913	-1.488582
O	1.529414	1.761941	-0.507031
O	1.529414	-1.761941	0.507031
H	1.567710	0.833035	-0.875761
H	1.567710	-0.833035	0.875761
H	1.487726	2.702474	1.251566
H	1.487726	-2.702474	-1.251566
C	-1.532668	1.707900	-0.806578
C	-1.532668	-1.707900	0.806578
O	-1.579788	0.695913	-1.488582
O	-1.579788	-0.695913	1.488582
O	-1.529414	1.761941	0.507031
O	-1.529414	-1.761941	-0.507031
H	-1.567710	0.833035	0.875761
H	-1.567710	-0.833035	-0.875761
H	-1.487726	2.702474	-1.251566
H	-1.487726	-2.702474	1.251566

AS2 [MP2/cc-pVTZ]

C	-1.512608	1.723639	0.776653
C	-1.512608	-1.723639	-0.776653
O	-1.535556	1.591611	-0.439811
O	-1.535556	-1.591611	0.439811
O	-1.530797	0.760611	1.663924
O	-1.530797	-0.760611	-1.663924
H	-1.551355	-0.123076	1.197583
H	-1.551355	0.123076	-1.197583
H	-1.472868	2.706198	1.248130
H	-1.472868	-2.706198	-1.248130
C	1.512608	-1.723639	0.776653
C	1.512608	1.723639	-0.776653
O	1.535556	-1.591611	-0.439811
O	1.535556	1.591611	0.439811
O	1.530797	-0.760611	1.663924
O	1.530797	0.760611	-1.663924
H	1.551355	0.123076	1.197583
H	1.551355	-0.123076	-1.197583
H	1.472868	-2.706198	1.248130
H	1.472868	2.706198	-1.248130

AS3 [MP2/cc-pVTZ]

C	-0.114691	1.884542	1.510366
C	0.114691	-1.884542	1.510366
O	-1.124445	1.198824	1.545713
O	1.124445	-1.198824	1.545713
O	1.124445	1.446854	1.535659
O	-1.124445	-1.446854	1.535659
H	1.120019	0.447521	1.571671
H	-1.120019	-0.447521	1.571671
H	-0.157724	2.972713	1.453709
H	0.157724	-2.972713	1.453709
C	1.363342	1.311725	-1.527457
C	-1.363342	-1.311725	-1.527457
O	0.184542	1.640998	-1.519414
O	-0.184542	-1.640998	-1.519414
O	1.828331	0.087730	-1.545007
O	-1.828331	-0.087730	-1.545007
H	1.066032	-0.558379	-1.539182
H	-1.066032	0.558379	-1.539182
H	2.166814	2.049034	-1.519265
H	-2.166814	-2.049034	-1.519265

SS1 [MP2/cc-pVTZ]

C	0.432102	2.592993	1.129676
O	0.364223	2.827237	-0.068485
O	-0.220247	1.661654	1.781618
H	-0.765786	1.129265	1.138769
H	1.071475	3.176252	1.793528
C	-0.432102	-2.592993	1.129676
O	-0.364223	-2.827237	-0.068485
O	0.220247	-1.661654	1.781618
H	0.765786	-1.129265	1.138769
H	-1.071475	-3.176252	1.793528
C	-1.634735	0.394909	-1.143046
O	-1.634735	0.191705	0.063327
O	-1.012058	1.366914	-1.765908
H	-0.519923	1.933202	-1.099891
H	-2.175474	-0.250692	-1.836590
C	1.634735	-0.394909	-1.143046
O	1.634735	-0.191705	0.063327
O	1.012058	-1.366914	-1.765908
H	0.519923	-1.933202	-1.099891
H	2.175474	0.250692	-1.836590

SS2 [MP2/cc-pVTZ]

C	-1.029506	-1.941884	0.423296
O	-0.685913	-0.983355	1.102344
O	-1.979975	-1.961297	-0.475978
H	-2.399266	-1.056999	-0.547712
H	-0.545789	-2.914747	0.517785
C	2.729500	-1.394132	0.030904
O	3.109271	-0.426571	0.671607
O	1.778425	-1.410082	-0.873121
H	1.380672	-0.494548	-0.957656
H	3.177874	-2.381020	0.160111
C	-2.729500	1.394132	-0.030904
O	-3.109271	0.426571	-0.671607
O	-1.778425	1.410082	0.873121
H	-1.380672	0.494548	0.957656
H	-3.177874	2.381020	-0.160111
C	1.029506	1.941884	-0.423296
O	0.685913	0.983355	-1.102344
O	1.979975	1.961297	0.475978
H	2.399266	1.056999	0.547712
H	0.545789	2.914747	-0.517785

B1 [MP2/cc-pVTZ]

C	-1.564541	0.760671	1.744979
O	-2.066034	0.174057	0.801596
O	-0.525580	1.564541	1.709624
H	-0.210908	1.678477	0.772968
H	-1.954554	0.663040	2.759327
C	-0.760671	-1.564541	-1.744979
O	-0.174057	-2.066034	-0.801596
O	-1.564541	-0.525580	-1.709624
H	-1.678477	-0.210908	-0.772968
H	-0.663040	-1.954554	-2.759327
C	0.760671	1.564541	-1.744979
O	0.174057	2.066034	-0.801596
O	1.564541	0.525580	-1.709624
H	1.678477	0.210908	-0.772968
H	0.663040	1.954554	-2.759327
C	1.564541	-0.760671	1.744979
O	2.066034	-0.174057	0.801596
O	0.525580	-1.564541	1.709624
H	0.210908	-1.678477	0.772968
H	1.954554	-0.663040	2.759327

B2 [MP2/cc-pVTZ]

C	-1.776880	1.277523	1.209898
O	-1.358650	1.597795	0.107724
O	-1.113115	0.663372	2.156586
H	-0.200059	0.415597	1.847006
H	-2.802267	1.488783	1.518596
C	1.776770	1.209729	-1.277809
O	1.358322	0.107619	-1.598016
O	1.113256	2.156503	-0.663521
H	0.200198	1.847052	-0.415595
H	2.802175	1.518265	-1.489221
C	1.777245	-1.209627	1.277355
O	1.358848	-0.107520	1.597635
O	1.113612	-2.156429	0.663236
H	0.200484	-1.847012	0.415531
H	2.802712	-1.518129	1.488517
C	-1.777137	-1.277669	-1.209415
O	-1.358532	-1.597868	-0.107362
O	-1.113743	-0.663432	-2.156307
H	-0.200622	-0.415547	-1.847004
H	-2.802592	-1.489063	-1.517797

PA1 [MP2/cc-pVTZ]

C	1.102567	1.388903	0.000000
O	1.679543	0.306259	0.000000
O	1.676957	2.565696	0.000000
H	2.669639	2.455292	0.000000
H	0.014764	1.450710	0.000000
C	-1.102567	-1.388903	0.000000
O	-1.679543	-0.306259	0.000000
O	-1.676957	-2.565696	0.000000
H	-2.669639	-2.455292	0.000000
H	-0.014764	-1.450710	0.000000
C	4.888162	1.216786	0.000000
O	4.318203	2.297478	0.000000
O	4.318203	0.035010	0.000000
H	3.325499	0.148215	0.000000
H	5.976547	1.139206	0.000000
C	-4.888162	-1.216786	0.000000
O	-4.318203	-2.297478	0.000000
O	-4.318203	-0.035010	0.000000
H	-3.325499	-0.148215	0.000000
H	-5.976547	-1.139206	0.000000

PA2 [MP2/cc-pVTZ]

C	-4.869989	-1.244222	0.000000
O	-4.348478	-2.348911	0.000000
O	-4.247691	-0.088804	0.000000
H	-3.261801	-0.246469	0.000000
H	-5.953828	-1.117981	0.000000
C	4.873544	1.422413	0.000000
O	4.263328	0.363209	0.000000
O	4.350193	2.624207	0.000000
H	3.352598	2.552606	0.000000
H	5.964254	1.457372	0.000000
C	-1.095088	-1.584197	0.000000
O	-1.620552	-0.476629	0.000000
O	-1.722575	-2.733653	0.000000
H	-2.709146	-2.577986	0.000000
H	-0.011827	-1.700588	0.000000
C	1.088777	1.406667	0.000000
O	1.709500	2.459149	0.000000
O	1.618882	0.200245	0.000000
H	2.615418	0.275796	0.000000
H	0.000000	1.362784	0.000000

PA3 [MP2/cc-pVTZ]

C	1.021320	1.624481	0.000000
O	1.598069	2.701528	0.000000
O	1.598069	0.440454	0.000000
H	2.591838	0.554748	0.000000
H	-0.064972	1.539806	0.000000
C	-4.799800	-1.791353	0.000000
O	-4.229341	-0.710018	0.000000
O	-4.232416	-2.972847	0.000000
H	-3.238416	-2.864524	0.000000
H	-5.888323	-1.866407	0.000000
C	4.799800	1.791353	0.000000
O	4.229341	0.710018	0.000000
O	4.232416	2.972847	0.000000
H	3.238416	2.864524	0.000000
H	5.888323	1.866407	0.000000
C	-1.021320	-1.624481	0.000000
O	-1.598069	-2.701528	0.000000
O	-1.598069	-0.440454	0.000000
H	-2.591838	-0.554748	0.000000
H	0.064972	-1.539806	0.000000

CE [MP2/cc-pVTZ]

C	3.601647	-1.030987	0.000000
O	3.171601	0.106549	0.000000
O	2.890558	-2.136919	0.000000
H	1.918637	-1.916064	0.000000
H	4.671422	-1.250632	0.000000
C	0.237870	1.922437	0.000000
O	-0.623838	2.787452	0.000000
O	1.515841	2.229871	0.000000
H	2.055144	1.410458	0.000000
H	0.000000	0.855205	0.000000
C	-0.502266	-2.605017	0.000000
O	0.285484	-1.669608	0.000000
O	-1.806090	-2.503465	0.000000
H	-2.064314	-1.539237	0.000000
H	-0.180015	-3.648597	0.000000
C	-3.269200	0.862757	0.000000
O	-2.343732	0.060469	0.000000
O	-3.133279	2.157662	0.000000
H	-2.144548	2.381869	0.000000
H	-4.316987	0.555780	0.000000

CZ [MP2/cc-pVTZ]

C	1.067073	3.019644	0.000000
C	-3.019644	1.067073	0.000000
C	-1.067073	-3.019644	0.000000
C	3.019644	-1.067073	0.000000
O	0.078730	2.310981	0.000000
O	-2.310981	0.078730	0.000000
O	-0.078730	-2.310981	0.000000
O	2.310981	-0.078730	0.000000
H	1.027060	4.111511	0.000000
H	-4.111511	1.027060	0.000000
H	-1.027060	-4.111511	0.000000
H	4.111511	-1.027060	0.000000
O	2.310981	2.591798	0.000000
O	-2.591798	2.310981	0.000000
O	-2.310981	-2.591798	0.000000
O	2.591798	-2.310981	0.000000
H	2.315456	1.599515	0.000000
H	-1.599515	2.315456	0.000000
H	-2.315456	-1.599515	0.000000
H	1.599515	-2.315456	0.000000