The Supplementary Material
Interaction–induced electric properties and cooperative effects in model systems

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TABLE I: Geometrical parameters of the HCHO$\cdots$(HF)$_n$ complexes. Interatomic distances in Å.

n	r(C–H)	r(C=O)	r(O$\cdots$H)	r(H–F)	r(F$\cdots$H)	r(H–F)	r(F$\cdots$H)	r(H–F)	r(F$\cdots$H)	r(H–F)	r(F$\cdots$H)	r(H–F)	r(F$\cdots$H)	r(H–F)	r(F$\cdots$H)	r(H–F)
1	1.0978	1.2206	1.8766	0.9258												
2	1.0968	1.2212	1.7690	0.9307	1.7792	0.9260										
3	1.0964	1.2215	1.7298	0.9332	1.6822	0.9307	1.7722	0.9263								
4	1.0962	1.2216	1.7132	0.9345	1.6474	0.9330	1.6743	0.9312	1.7676	0.9266						
5	1.0961	1.2217	1.7044	0.9352	1.6356	0.9341	1.6392	0.9335	1.6693	0.9316	1.7650	0.9267				
6	1.0960	1.2218	1.6993	0.9356	1.6246	0.9348	1.6242	0.9347	1.6338	0.9339	1.6661	0.9318	1.7634	0.9268		
7	1.0960	1.2218	1.6967	0.9358	1.6204	0.9352	1.6162	0.9354	1.6173	0.9353	1.6309	0.9343	1.6639	0.9318	1.7627	0.9267
8	1.0960	1.2218	1.6950	0.9360	1.6178	0.9354	1.6115	0.9358	1.6088	0.9360	1.6148	0.9356	1.6279	0.9344	1.6630	0.9318
															1.7620	0.9268
9	1.0960	1.2219	1.6937	0.9361	1.6159	0.9355	1.6085	0.9361	1.6042	0.9364	1.6062	0.9362	1.6116	0.9358	1.6266	0.9345
													1.6627	0.9319	1.7613	0.9268

TABLE II: Finite field CCSD(T) electric dipole moment $\mu(0)$, polarizability $\alpha_{zz}(0)$ and hyperpolarizability $\beta_{zzz}(0)$ of HF molecule obtained using different values of static electric field strength F. All values in au.

	HF											
	$\mu(0)$				$\alpha_{zz}(0)$				$\beta_{zzz}(0)$			
F	ds	fs	dl	fl	ds	fs	dl	fl	ds	fs	dl	fl
0.0010	0.706575	0.707317	0.706718	0.706424	6.4380	6.4487	6.4298	6.4405	−9.921	−9.820	−10.019	−9.599
0.0020	0.706575	0.707317	0.706718	0.706424	6.4380	6.4487	6.4298	6.4405	−9.926	−9.824	−10.023	−9.600
0.0030	0.706575	0.707317	0.706718	0.706424	6.4380	6.4487	6.4298	6.4405	−9.930	−9.828	−10.027	−9.603
0.0035	0.706575	0.707317	0.706718	0.706424	6.4380	6.4487	6.4298	6.4405	−9.933	−9.831	−10.030	−9.606
0.0040	0.706575	0.707317	0.706718	0.706424	6.4380	6.4487	6.4298	6.4405	−9.936	−9.834	−10.033	−9.608
0.0045	0.706575	0.707317	0.706718	0.706424	6.4380	6.4487	6.4298	6.4405	−9.940	−9.837	−10.037	−9.611
0.0050	0.706575	0.707317	0.706719	0.706424	6.4380	6.4487	6.4298	6.4405	−9.945	−9.841	−10.041	−9.614
0.0055	0.706575	0.707317	0.706719	0.706425	6.4380	6.4487	6.4298	6.4405	−9.949	−9.845	−10.045	−9.618
0.0060	0.706575	0.707317	0.706719	0.706425	6.4380	6.4487	6.4298	6.4405	−9.954	−9.850	−10.050	−9.622
0.0080	0.706576	0.707318	0.706719	0.706425	6.4380	6.4487	6.4298	6.4405	−9.980	−9.873	−10.075	−9.641
0.0100	0.706576	0.707318	0.706720	0.706425	6.4380	6.4487	6.4298	6.4405	−10.013	−9.903	−10.107	−9.667
0.0160	0.706583	0.707325	0.706726	0.706431	6.4379	6.4485	6.4296	6.4403	−10.161	−10.039	−10.252	−9.784
0.0200	0.706596	0.707336	0.706739	0.706441	6.4376	6.4481	6.4293	6.4399	−10.306	−10.175	−10.395	−9.900

TABLE III: Finite field CCSD(T) electric dipole moment $\mu(0)$, polarizability $\alpha_{zz}(0)$ and hyperpolarizability $\beta_{zzz}(0)$ of HCHO molecule obtained using different values of static electric field strength F. All values in au.

	HCHO											
	$\mu(0)$				$\alpha_{zz}(0)$				$\beta_{zzz}(0)$			
F	ds	fs	dl	fl	ds	fs	dl	fl	ds	fs	dl	fl
0.0010	0.944735	0.953481	0.943900	0.954157	22.5836	22.5740	22.5694	22.5571	−30.760	−31.649	−31.314	−30.014
0.0020	0.944735	0.953481	0.943900	0.954157	22.5836	22.5740	22.5694	22.5573	−30.810	−31.668	−31.269	−30.263
0.0030	0.944735	0.953482	0.943900	0.954157	22.5835	22.5740	22.5694	22.5573	−30.898	−31.755	−31.365	−30.321
0.0035	0.944735	0.953482	0.943900	0.954157	22.5835	22.5740	22.5694	22.5573	−30.956	−31.813	−31.419	−30.378
0.0040	0.944735	0.953482	0.943901	0.954157	22.5835	22.5739	22.5694	22.5573	−31.023	−31.879	−31.486	−30.429
0.0045	0.944736	0.953482	0.943901	0.954158	22.5835	22.5739	22.5694	22.5573	−31.099	−31.956	−31.559	−30.504
0.0050	0.944736	0.953483	0.943901	0.954158	22.5835	22.5739	22.5693	22.5573	−31.185	−32.042	−31.642	−30.576
0.0055	0.944737	0.953484	0.943902	0.954159	22.5835	22.5739	22.5693	22.5572	−31.281	−32.139	−31.735	−30.664
0.0060	0.944738	0.953484	0.943903	0.954160	22.5834	22.5738	22.5692	22.5571	−31.386	−32.245	−31.837	−30.758
0.0080	0.944745	0.953492	0.943910	0.954166	22.5831	22.5735	22.5689	22.5568	−31.916	−32.782	−32.348	−31.239
0.0100	0.944760	0.953507	0.943925	0.954180	22.5824	22.5727	22.5682	22.5559	−32.634	−33.520	−33.044	−31.903
0.0160	0.944934	0.953699	0.944095	0.954358	22.5751	22.5633	22.5598	22.5451	−36.349	−37.638	−36.694	−35.748
0.0200	0.945322	0.954217	0.944488	0.954923	22.5593	22.5388	22.5413	22.5124	−41.064	−44.163	−41.493	−43.039

TABLE IV: Counterpoise corrected and uncorrected finite field induced static electric dipole moment of the HCHO···HF complex. All results in au.

Method	apc1	apc2	ds	fs	dl	fl	aVDZ	aVTZ	aVQZ	aV5Z	daVDZ	daVTZ
BSSE corrected results												
HF SCF	0.3266	0.3304	0.3292	0.3316	0.3301	0.3317	0.3298	0.3317	0.3317	0.3317	0.3302	0.3316
MP2	0.3190	0.3223	0.3225	0.3250	0.3231	0.3249	0.3220	0.3239	0.3241	0.3241	0.3230	0.3240
CCSD	0.3218	0.3251	0.3251	0.3278	0.3257	0.3276	0.3248	0.3267	0.3269	—	0.3257	0.3267
CCSD(T)	0.3221	0.3254	0.3255	0.3282	0.3260	0.3280	0.3250	0.3270	0.3272	—	0.3262	0.3271
BSSE uncorrected results												
HF SCF	0.3262	0.3303	0.3295	0.3312	0.3307	0.3318	0.3249	0.3311	0.3317	0.3317	0.3279	0.3314
MP2	0.3184	0.3229	0.3220	0.3248	0.3234	0.3257	0.3184	0.3240	0.3244	0.3244	0.3209	0.3240
CCSD	0.3211	0.3258	0.3249	0.3280	0.3260	0.3286	0.3210	0.3265	0.3271	—	0.3237	0.3267
CCSD(T)	0.3210	0.3262	0.3251	0.3282	0.3263	0.3289	0.3215	0.3269	0.3274	—	0.3241	0.3271

TABLE V: Counterpoise corrected and uncorrected finite field induced static electric dipole moment of the HCHO···$(HF)_2$ complex. All results in au.

Method	apc1	apc2	ds	fs	dl	fl	aVDZ	aVTZ	aVQZ	aV5Z	daVDZ	daVTZ
BSSE corrected results												
HF SCF	0.6475	0.6521	0.6501	0.6540	0.6515	0.6544	0.6501	0.6544	0.6546	0.6546	0.6514	0.6544
MP2	0.6499	0.6537	0.6541	0.6585	0.6549	0.6584	0.6522	0.6566	0.6566	0.6565	0.6546	0.6570
CCSD	0.6505	0.6542	0.6547	0.6591	0.6554	0.6587	0.6532	0.6568	0.6568	—	0.6554	0.6570
CCSD(T)	0.6526	0.6569	0.6575	0.6621	0.6581	0.6617	0.6554	0.6596	0.6597	—	0.6580	0.6599
BSSE uncorrected results												
HF SCF	0.6499	0.6518	0.6510	0.6537	0.6524	0.6549	0.6438	0.6530	0.6543	0.6546	0.6482	0.6540
MP2	0.6509	0.6547	0.6539	0.6578	0.6556	0.6602	0.6487	0.6564	0.6570	0.6570	0.6518	0.6568
CCSD	0.6519	0.6553	0.6551	0.6592	0.6562	0.6609	0.6495	0.6564	0.6569	—	0.6528	0.6570
CCSD(T)	0.6533	0.6584	0.6576	0.6619	0.6589	0.6637	0.6521	0.6592	0.6599	—	0.6554	0.6598

TABLE VI: Counterpoise corrected and uncorrected finite field zz–component of the induced static electric polarizability of the HCHO$\cdots$HF complex. All results in au.

Method	apc1	apc2	ds	fs	dl	fl	aVDZ	aVTZ	aVQZ	aV5Z	daVDZ	daVTZ
BSSE corrected results												
HF SCF	1.886	1.883	1.890	1.890	1.892	1.892	1.873	1.894	1.896	1.896	1.887	1.897
MP2	2.496	2.534	2.532	2.557	2.542	2.563	2.502	2.557	2.557	2.552	2.520	2.564
CCSD	2.376	2.391	2.404	2.425	2.411	2.426	2.378	2.415	2.405	—	2.401	2.421
CCSD(T)	2.428	2.466	2.471	2.500	2.480	2.503	2.434	2.491	2.485	—	2.461	2.499
BSSE uncorrected results												
HF SCF	1.992	1.882	1.873	1.898	1.903	1.893	1.956	1.924	1.907	1.898	1.928	1.901
MP2	2.635	2.544	2.516	2.559	2.559	2.560	2.619	2.607	2.575	2.561	2.558	2.566
CCSD	2.501	2.396	2.387	2.417	2.423	2.417	2.486	2.455	2.419	—	2.434	2.422
CCSD(T)	2.562	2.472	2.456	2.494	2.493	2.495	2.550	2.535	2.501	—	2.496	2.500

TABLE VII: Counterpoise corrected and uncorrected finite field zz–component of the induced static electric polarizability of the HCHO$\cdots$(HF)$_2$ complex. All results in au.

Method	apc1	apc2	ds	fs	dl	fl	aVDZ	aVTZ	aVQZ	aV5Z	daVDZ	daVTZ
BSSE corrected results												
HF SCF	3.380	3.344	3.359	3.355	3.360	3.357	3.328	3.361	3.363	3.364	3.355	3.368
MP2	4.563	4.589	4.585	4.628	4.598	4.635	4.533	4.628	4.624	4.625	4.570	4.640
CCSD	4.368	4.352	4.373	4.409	4.381	4.408	4.336	4.391	4.368	—	4.379	4.404
CCSD(T)	4.487	4.518	4.528	4.578	4.539	4.580	4.466	4.562	4.545	—	4.517	4.577
BSSE uncorrected results												
HF SCF	3.574	3.331	3.335	3.364	3.378	3.358	3.482	3.416	3.379	3.368	3.431	3.382
MP2	4.827	4.590	4.566	4.628	4.626	4.627	4.742	4.711	4.653	4.638	4.633	4.654
CCSD	4.606	4.344	4.352	4.393	4.399	4.390	4.531	4.460	4.388	—	4.435	4.414
CCSD(T)	4.743	4.512	4.509	4.564	4.560	4.563	4.672	4.636	4.567	—	4.575	4.587

TABLE VIII: Counterpoise corrected and uncorrected finite field *zzz*–component of the induced static electric first hyperpolarizability of the HCHO···HF complex. All results in au.

Method	apc1	apc2	ds	fs	dl	fl	aVDZ	aVTZ	aVQZ	aV5Z	daVDZ	daVTZ
BSSE corrected results												
HF SCF	3.86	3.83	3.65	3.68	3.75	3.68	2.86	3.13	3.51	3.61	3.93	3.75
MP2	11.92	12.22	11.74	12.15	12.02	12.12	9.90	10.97	11.68	11.97	12.19	12.24
CCSD	11.51	11.45	11.22	11.49	11.43	11.42	9.58	10.34	10.82	—	11.70	11.44
CCSD(T)	13.37	13.61	13.35	13.70	13.60	13.64	11.24	12.38	12.98	—	13.62	13.65
BSSE uncorrected results												
HF SCF	3.68	3.65	3.47	4.54	4.86	3.64	5.81	4.54	4.00	4.00	3.40	3.48
MP2	12.11	11.84	12.10	13.31	13.63	12.07	13.64	12.81	12.48	12.43	11.10	11.88
CCSD	11.58	11.08	11.53	12.41	12.77	11.41	13.25	11.99	11.53	—	10.70	11.11
CCSD(T)	13.46	13.18	13.75	14.71	15.05	13.65	15.14	14.15	13.76	—	12.57	13.31

TABLE IX: Counterpoise corrected and uncorrected finite field *zzz*–component of the induced static electric first hyperpolarizability of the HCHO···$(HF)_2$ complex. All results in au.

Method	apc1	apc2	ds	fs	dl	fl	aVDZ	aVTZ	aVQZ	aV5Z	daVDZ	daVTZ
BSSE corrected results												
HF SCF	12.44	12.61	12.39	12.37	12.38	12.35	11.33	11.73	12.15	12.24	12.37	12.41
MP2	26.49	26.90	26.54	26.77	26.60	26.74	24.01	25.30	26.09	26.24	26.60	26.82
CCSD	25.89	25.68	25.69	25.76	25.70	25.67	23.57	24.26	24.53	—	25.93	25.57
CCSD(T)	29.32	29.66	29.68	29.83	29.73	29.76	26.80	28.10	28.52	—	29.52	29.63
BSSE uncorrected results												
HF SCF	11.14	12.30	12.34	13.41	13.84	12.27	15.55	14.33	13.09	12.83	10.70	12.13
MP2	25.26	26.36	27.34	28.30	28.75	26.68	29.56	28.93	27.64	27.12	23.84	26.39
CCSD	24.60	25.20	26.35	27.00	27.51	25.64	29.03	27.49	25.89	—	23.42	25.19
CCSD(T)	27.96	29.09	30.51	31.19	31.69	29.76	32.60	31.60	30.01	—	26.90	29.23

TABLE X: Counterpoise corrected and uncorrected interaction energy of the HCHO···HF complex. All results in kcal mol^{-1}.

Method	apc1	apc2	ds	fs	dl	fl	aVDZ	aVTZ	aVQZ	aV5Z	daVDZ	daVTZ
BSSE corrected results												
HF SCF	−5.73	−6.17	−5.98	−6.21	−6.04	−6.21	−6.00	−6.15	−6.18	−6.18	−6.01	−6.16
MP2	−5.27	−5.96	−5.70	−5.99	−5.73	−6.02	−5.60	−5.99	−6.15	−6.20	−5.64	−6.01
CCSD	−5.28	−5.99	−5.70	−6.02	−5.73	−6.05	−5.58	−6.02	−6.19	—	−5.62	−6.04
CCSD(T)	−5.33	−6.05	−5.76	−6.10	−5.80	−6.13	−5.64	−6.10	−6.28	—	−5.70	−6.13
BSSE uncorrected results												
HF SCF	−6.63	−6.40	−6.19	−6.77	−6.32	−6.45	−6.26	−6.26	−6.22	−6.18	−6.52	−6.30
MP2	−6.86	−6.96	−7.15	−9.98	−6.87	−8.57	−6.41	−6.51	−6.47	−6.37	−6.88	−6.65
CCSD	−6.89	−6.95	−7.02	−9.91	−6.80	−8.46	−6.38	−6.52	−6.46	—	−6.87	−6.66
CCSD(T)	−7.07	−7.07	−7.18	−10.16	−6.92	−8.66	−6.54	−6.62	−6.56	—	−7.08	−6.77

TABLE XI: Counterpoise corrected and uncorrected interaction energy of the HCHO$\cdots$(HF)$_2$ complex. All results in kcal mol^{-1}.

Method	apc1	apc2	ds	fs	dl	fl	aVDZ	aVTZ	aVQZ	aV5Z	daVDZ	daVTZ
BSSE corrected results												
HF SCF	−10.92	−11.88	−11.46	−11.92	−11.57	−11.93	−11.43	−11.79	−11.88	−11.89	−11.44	−11.83
MP2	−9.95	−11.53	−10.92	−11.58	−11.00	−11.64	−10.62	−11.55	−11.94	−12.06	−10.70	−11.62
CCSD	−9.95	−11.60	−10.93	−11.65	−11.02	−11.72	−10.58	−11.62	−12.04	—	−10.68	−11.69
CCSD(T)	−10.08	−11.74	−11.06	−11.82	−11.16	−11.90	−10.71	−11.79	−12.23	—	−10.83	−11.87
BSSE uncorrected results												
HF SCF	−13.44	−12.35	−12.01	−12.87	−12.11	−12.46	−12.12	−12.00	−11.97	−11.90	−12.97	−12.20
MP2	−13.79	−13.61	−13.96	−19.11	−13.80	−17.37	−12.45	−12.61	−12.59	−12.41	−13.89	−13.07
CCSD	−13.83	−13.61	−13.74	−19.06	−13.63	−17.17	−12.39	−12.65	−12.58	—	−13.89	−13.13
CCSD(T)	−14.21	−13.86	−14.05	−19.55	−13.90	−17.59	−12.74	−12.88	−12.80	—	−14.37	−13.36

TABLE XII: Counterpoise corrected (C) and uncorrected (UC) induced electric dipole properties of the HCHO$\cdots$(HF)$_n$ complexes obtained in the ds basis set. All results in au.

n		$\Delta\mu_z$		$\Delta\alpha_{zz}$		$\Delta\beta_{zzz}$	
		C	UC	C	UC	C	UC
1	HF SCF	0.3292	0.3295	1.890	1.873	3.65	3.47
	MP2	0.3225	0.3220	2.532	2.516	11.74	12.10
	CCSD	0.3251	0.3249	2.404	2.387	11.22	11.53
	CCSD(T)	0.3255	0.3251	2.471	2.456	13.35	13.75
2	HF SCF	0.6501	0.6510	3.359	3.335	12.39	12.34
	MP2	0.6541	0.6539	4.585	4.566	26.54	27.34
	CCSD	0.6547	0.6551	4.373	4.352	25.69	26.35
	CCSD(T)	0.6575	0.6576	4.528	4.509	29.68	30.51
3	HF SCF	0.9743	0.9758	4.725	4.696	22.29	22.28
	MP2	0.9945	0.9947	6.501	6.480	41.68	42.80
	CCSD	0.9921	0.9932	6.226	6.202	40.52	41.44
	CCSD(T)	0.9981	0.9988	6.474	6.454	46.14	47.28
4	HF SCF	1.3031	1.3052	6.068	6.034	32.72	32.70
	MP2	1.3420	1.3426	8.379	8.358	57.15	58.53
	CCSD	1.3361	1.3380	8.050	8.024	55.66	56.78
	CCSD(T)	1.3458	1.3472	8.393	8.372	62.81	64.21
5	HF SCF	1.6365	1.6393	7.407	7.368	43.44	43.42
	MP2	1.6954	1.6964	10.252	10.230	72.86	74.49
	CCSD	1.6859	1.6886	9.871	9.843	71.02	72.35
	CCSD(T)	1.6995	1.7016	10.312	10.290	79.66	81.32
6	HF SCF	1.9739	1.9774	8.750	8.706	54.35	54.31
	MP2	2.0536	2.0549	12.129	12.107	88.76	90.62
7	HF SCF	2.3142	2.3183	10.096	10.048	65.42	65.37
	MP2	2.4150	2.4167	14.012	13.990	104.84	106.96
8	HF SCF	2.6571	2.6618	11.448	11.395	76.58	76.53
	MP2	2.7795	2.7815	15.902	15.880	121.04	123.43
9	HF SCF	3.0022	3.0075	12.803	12.746	87.81	87.74
	MP2	3.1464	3.1488	17.798	17.776	137.33	139.95

TABLE XIII: Counterpoise corrected (C) and uncorrected (UC) induced electric dipole properties of the HCHO$\cdots$(HF)$_n$ complexes obtained in the dl basis set. All results in au.

n		$\Delta\mu_z$		$\Delta\alpha_{zz}$		$\Delta\beta_{zzz}$	
		C	UC	C	UC	C	UC
1	HF SCF	0.3301	0.3307	1.892	1.903	3.75	4.86
	MP2	0.3231	0.3234	2.542	2.559	12.02	13.63
	CCSD	0.3257	0.3260	2.411	2.423	11.43	12.77
	CCSD(T)	0.3260	0.3263	2.480	2.493	13.60	15.05
2	HF SCF	0.6515	0.6524	3.360	3.378	12.38	13.84
	MP2	0.6549	0.6556	4.598	4.626	26.60	28.75
	CCSD	0.6554	0.6562	4.381	4.399	25.70	27.51
	CCSD(T)	0.6581	0.6589	4.539	4.560	29.73	31.69
3	HF SCF	0.9760	0.9771	4.728	4.745	22.30	23.66
	MP2	0.9955	0.9964	6.516	6.548	41.77	43.99
4	HF SCF	1.3052	1.3067	6.070	6.098	32.62	34.62
	MP2	1.3432	1.3447	8.397	8.442	57.12	60.16
5	HF SCF	1.6390	1.6409	7.410	7.434	43.45	45.29
	MP2	1.6968	1.6988	10.271	10.317	72.94	75.99
6	HF SCF	1.9769	1.9792	8.752	8.783	54.26	56.68
	MP2	2.0552	2.0577	12.150	12.206	88.71	92.54
7	HF SCF	2.3175	2.3202	10.099	10.131	65.39	67.67
	MP2	2.4168	2.4199	14.035	14.095	104.86	108.73
8	HF SCF	2.6609	2.6640	11.450	11.487	76.48	79.19
	MP2	2.7816	2.7852	15.926	15.995	120.96	125.46
9	HF SCF	3.0063	3.0099	12.805	12.845	87.75	90.48
	MP2	3.1487	3.1528	17.823	17.898	137.29	141.99

TABLE XIV: Counterpoise corrected (C) and uncorrected (UC) induced electric dipole properties of the HCHO$\cdots$(HF)$_n$ complexes obtained in the fl basis set. All results in au.

n		$\Delta\mu_z$		$\Delta\alpha_{zz}$		$\Delta\beta_{zzz}$	
		C	UC	C	UC	C	UC
1	HF SCF	0.3317	0.3318	1.892	1.893	3.68	3.64
	MP2	0.3249	0.3257	2.563	2.560	12.12	12.07
	CCSD	0.3276	0.3286	2.426	2.417	11.42	11.41
	CCSD(T)	0.3280	0.3289	2.503	2.495	13.64	13.65
2	HF SCF	0.6544	0.6549	3.357	3.358	12.35	12.27
	MP2	0.6584	0.6602	4.635	4.627	26.74	26.68
	CCSD	0.6587	0.6609	4.408	4.390	25.67	25.64
	CCSD(T)	0.6617	0.6637	4.580	4.563	29.76	29.76
3	HF SCF	0.9804	0.9811	4.721	4.725	22.20	22.11
	MP2	1.0007	1.0033	6.570	6.560	41.76	41.71
4	HF SCF	1.3110	1.3120	6.060	6.066	32.61	32.54
	MP2	1.3501	1.3536	8.468	8.456	57.14	57.15
5	HF SCF	1.6462	1.6474	7.397	7.401	43.32	43.16
	MP2	1.7054	1.7096	10.359	10.343	72.76	72.69
6	HF SCF	1.9855	1.9869	8.736	8.744	54.21	54.08
	MP2	2.0655	2.0705	12.256	12.239	88.56	88.56
7	HF SCF	2.3276	2.3292	10.080	10.087	65.24	65.10
	MP2	2.4288	2.4346	14.158	14.136	104.55	104.55
8	HF SCF	2.6724	2.6742	11.428	11.438	76.39	76.23
	MP2	2.7953	2.8019	16.067	16.042	120.66	120.68

TABLE XV: Counterpoise corrected (C) and non-corrected (UC) interaction energies of the HCHO$\cdots$(HF)$_n$ complexes. All results in kcal mol^{-1}.

n		ds		dl		fl	
		C	UC	C	UC	C	UC
1	HF SCF	−5.98	−6.19	−6.04	−6.32	−6.21	−6.45
	MP2	−5.70	−7.15	−5.73	−6.87	−6.02	−8.57
	CCSD	−5.70	−7.02	−5.73	−6.80	−6.05	−8.46
	CCSD(T)	−5.76	−7.18	−5.80	−6.92	−6.13	−8.66
2	HF SCF	−11.46	−12.01	−11.57	−12.11	−11.93	−12.46
	MP2	−10.92	−13.96	−11.00	−13.80	−11.64	−17.37
	CCSD	−10.93	−13.74	−11.02	−13.63	−11.72	−17.17
	CCSD(T)	−11.06	−14.05	−11.16	−13.90	−11.90	−17.59
3	HF SCF	−16.86	−17.76	−17.00	−17.83	−17.59	−18.34
	MP2	−16.13	−20.81	−16.25	−20.73	−17.29	−26.09
	CCSD	−16.11	−20.46				
	CCSD(T)	−16.32	−20.94				
4	HF SCF	−22.26	−23.53	−22.45	−23.54	−23.26	−24.26
	MP2	−21.38	−27.73	−21.55	−27.72	−23.01	−34.62
	CCSD	−21.33	−27.23				
	CCSD(T)	−21.62	−27.88				
5	HF SCF	−27.71	−29.33	−27.93	−29.31	−28.98	−30.16
	MP2	−26.69	−34.70	−26.89	−34.81	−28.78	−43.38
	CCSD	−26.59	−34.04				
	CCSD(T)	−26.96	−34.88				
6	HF SCF	−33.18	−35.13	−33.45	−35.09	−34.72	−36.11
	MP2	−32.02	−41.59	−32.29	−41.91	−34.60	−52.23
7	HF SCF	−38.68	−40.99	−38.99	−40.90	−40.50	−42.11
	MP2	−37.39	−48.65	−37.71	−49.06	−40.46	−61.27
8	HF SCF	−44.18	−46.83	−44.54	−46.72	−46.30	−48.14
	MP2	−42.77	−55.58	−43.15	−56.23	−46.34	−70.34
9	HF SCF	−49.72	−52.72	−50.12	−52.57	—	—
	MP2	−48.17	−62.68	−48.61	−63.42	—	—

TABLE XVI: Counterpoise corrected and uncorrected finite field two– and many–body contributions to the induced static dipole moment of the HCHO$\cdots$(HF)$_2$ complex. All results in au.

Method	ds		fs		dl		fl		aVQZ		daVTZ	
	2–body	Many–body	2–body	Many–body	2–body	Many–body	2–body	Many–body	2–body	Many–body	2–body	Many–body
						BSSE corrected results						
HF SCF	0.6120	0.0381	0.6158	0.0382	0.6133	0.0382	0.6162	0.0382	0.6163	0.0383	0.6161	0.0383
MP2	0.6097	0.0444	0.6138	0.0447	0.6105	0.0444	0.6136	0.0448	0.6120	0.0446	0.6121	0.0449
CCSD	0.6113	0.0434	0.6154	0.0437	0.6119	0.0435	0.6150	0.0437	0.6134	0.0434	0.6134	0.0436
CCSD(T)	0.6130	0.0445	0.6172	0.0449	0.6135	0.0446	0.6168	0.0449	0.6151	0.0446	0.6151	0.0448
						BSSE uncorrected results						
HF SCF	0.6126	0.0384	0.6150	0.0387	0.6143	0.0381	0.6169	0.0380	0.6159	0.0384	0.6154	0.0386
MP2	0.6094	0.0445	0.6128	0.0450	0.6109	0.0447	0.6161	0.0441	0.6122	0.0448	0.6119	0.0449
CCSD	0.6116	0.0435	0.6153	0.0439	0.6126	0.0436	0.6180	0.0429	0.6134	0.0435	0.6132	0.0438
CCSD(T)	0.6130	0.0446	0.6168	0.0451	0.6141	0.0448	0.6197	0.0440	0.6151	0.0448	0.6149	0.0449

TABLE XVII: Counterpoise corrected and uncorrected finite field two– and many–body contributions to the induced static dipole polarizability of the HCHO$\cdots$(HF)$_2$ complex. All results in au.

Method	ds		fs		dl		fl		aVQZ		daVTZ	
	2–body	Many–body	2–body	Many–body	2–body	Many–body	2–body	Many–body	2–body	Many–body	2–body	Many–body
						BSSE corrected results						
HF SCF	3.096	0.263	3.095	0.260	3.098	0.262	3.097	0.260	3.102	0.261	3.106	0.262
MP2	4.175	0.410	4.217	0.411	4.188	0.410	4.223	0.412	4.212	0.412	4.227	0.413
CCSD	3.981	0.392	4.015	0.394	3.989	0.392	4.014	0.394	3.978	0.390	4.009	0.395
CCSD(T)	4.109	0.419	4.156	0.422	4.119	0.419	4.156	0.424	4.126	0.419	4.154	0.423
						BSSE uncorrected results						
HF SCF	3.062	0.273	3.111	0.253	3.114	0.264	3.098	0.260	3.120	0.259	3.124	0.258
MP2	4.137	0.429	4.227	0.402	4.215	0.411	4.213	0.414	4.240	0.413	4.239	0.415
CCSD	3.943	0.409	4.008	0.385	4.007	0.392	3.995	0.395	3.997	0.391	4.019	0.395
CCSD(T)	4.072	0.437	4.151	0.413	4.139	0.421	4.139	0.424	4.146	0.421	4.163	0.424

TABLE XVIII: Counterpoise corrected and uncorrected finite field two– and many–body contributions to the induced static first hyperpolarizability of the HCHO$\cdots$(HF)$_2$ complex. All results in au.

Method	ds		fs		dl		fl		aVQZ		daVTZ	
	2–body	Many–body	2–body	Many–body	2–body	Many–body	2–body	Many–body	2–body	Many–body	2–body	Many–body
						BSSE corrected results						
HF SCF	7.49	4.90	7.46	4.91	7.49	4.89	7.43	4.92	7.23	4.92	7.47	4.94
MP2	18.33	8.21	18.50	8.27	18.40	8.20	18.44	8.30	17.87	8.22	18.51	8.31
CCSD	17.27	8.42	17.29	8.47	17.29	8.41	17.20	8.47	16.17	8.36	17.13	8.44
CCSD(T)	20.00	9.68	20.06	9.77	20.05	9.68	19.99	9.77	18.87	9.65	19.90	9.73
						BSSE uncorrected results						
HF SCF	6.98	5.36	9.05	4.36	9.61	4.23	7.25	5.02	8.06	5.03	6.96	5.17
MP2	18.56	8.78	20.84	7.46	21.55	7.20	18.26	8.42	19.24	8.40	17.75	8.64
CCSD	17.45	8.90	19.19	7.81	19.92	7.59	17.09	8.55	17.46	8.43	16.45	8.74
CCSD(T)	20.31	10.20	22.12	9.07	22.89	8.80	19.90	9.86	20.28	9.73	19.17	10.06

TABLE XIX: Counterpoise corrected and uncorrected finite field two– and many–body contributions to the interaction energy of the HCHO$\cdots$(HF)$_2$ complex. All results in kcal mol^{-1}.

Method	ds		fs		dl		fl		aVQZ		daVTZ	
	2–body	Many–body	2–body	Many–body	2–body	Many–body	2–body	Many–body	2–body	Many–body	2–body	Many–body
BSSE corrected results												
HF SCF	−9.75	−1.71	−10.20	−1.72	−9.86	−1.71	−10.21	−1.72	−10.15	−1.73	−10.11	−1.72
MP2	−9.33	−1.59	−9.98	−1.60	−9.40	−1.60	−10.04	−1.60	−10.34	−1.60	−10.02	−1.60
CCSD	−9.30	−1.63	−10.01	−1.64	−9.40	−1.62	−10.08	−1.64	−10.40	−1.64	−10.06	−1.63
CCSD(T)	−9.44	−1.62	−10.19	−1.63	−9.54	−1.62	−10.26	−1.64	−10.59	−1.64	−10.24	−1.63
BSSE uncorrected results												
HF SCF	−10.23	−1.78	−11.35	−1.52	−10.60	−1.51	−10.70	−1.76	−10.26	−1.71	−10.48	−1.72
MP2	−12.44	−1.52	−18.01	−1.10	−12.12	−1.68	−16.07	−1.30	−10.97	−1.62	−11.47	−1.60
CCSD	−12.15	−1.59	−17.91	−1.15	−11.95	−1.68	−15.79	−1.38	−10.94	−1.64	−11.50	−1.63
CCSD(T)	−12.49	−1.56	−18.43	−1.12	−12.21	−1.69	−16.25	−1.34	−11.16	−1.64	−11.74	−1.62

TABLE XX: Counterpoise corrected and uncorrected finite field two– and many–body contributions to the induced static induced electric dipole properties [au] and interaction energies [kcal mol^{-1}] of the HCHO$\cdots$(HF)$_3$ and HCHO$\cdots$(HF)$_4$ complexes. Results of calculations with LPol-ds basis set.

n	Method	$\Delta\mu(0)$		$\Delta\alpha_{zz}(0)$		$\Delta\beta_{zzz}(0)$		$\Delta E(0)$	
		2–body	Many–body	2–body	Many–body	2–body	Many–body	2–body	Many–body
					BSSE corrected results				
3	HF SCF	0.8946	0.0797	4.206	0.519	10.93	11.36	−12.93	−3.93
	MP2	0.8999	0.0946	5.696	0.805	22.97	18.71	−12.40	−3.73
	CCSD	0.8997	0.0924	5.449	0.777	21.63	18.89	−12.34	−3.77
	CCSD(T)	0.9031	0.0950	5.641	0.833	24.62	21.52	−12.55	−3.77
4	HF SCF	1.1805	0.1226	5.296	0.772	14.24	18.48	−15.85	−6.41
	MP2	1.1947	0.1473	7.191	1.188	26.93	30.22	−15.23	−6.15
	CCSD	1.1923	0.1438	6.896	1.154	25.40	30.26	−15.12	−6.21
	CCSD(T)	1.1976	0.1482	7.155	1.238	28.54	34.27	−15.41	−6.21
					BSSE uncorrected results				
3	HF SCF	0.8955	0.0803	4.156	0.540	10.14	12.14	−13.69	−4.07
	MP2	0.9000	0.0947	5.636	0.844	23.12	19.68	−17.22	−3.59
	CCSD	0.9008	0.0924	5.391	0.811	21.69	19.75	−16.75	−3.71
	CCSD(T)	0.9037	0.0951	5.584	0.870	24.86	22.42	−17.28	−3.66
4	HF SCF	1.1817	0.1235	5.230	0.804	13.17	19.53	−16.90	−6.63
	MP2	1.1951	0.1475	7.110	1.248	27.03	31.50	−21.77	−5.96
	CCSD	1.1942	0.1438	6.818	1.206	25.37	31.41	−21.12	−6.11
	CCSD(T)	1.1990	0.1482	7.078	1.294	28.74	35.47	−21.84	−6.04

TABLE XXI: The estimation of the two– and many–body contributions in the HCHO$\cdots$(HF)$_n$ complexes. Counterpoise corrected and uncorrected interaction induced dipole moments. All results in au.

n	HF SCF/ds		HF SCF/dl		MP2/ds		MP2/dl	
	2–body	Many–Body	2–body	Many–Body	2–body	Many–Body	2–body	Many–Body
				BSSE corrected results				
2	0.6120	0.0381	0.6133	0.0382	0.6097	0.0444	0.6105	0.0444
3	0.8946	0.0797	0.8962	0.0798	0.8999	0.0946	0.9007	0.0948
4	1.1805	0.1226	1.1824	0.1228	1.1947	0.1473	1.1956	0.1476
5	1.4699	0.1666	1.4722	0.1668	1.4935	0.2019	1.4946	0.2022
6	1.7624	0.2115	1.7651	0.2118	1.7957	0.2579	1.7970	0.2582
7	2.0569	0.2573	—	—	2.1001	0.3149	—	—
8	2.3510	0.3061	—	—	2.4043	0.3752	—	—
9	2.6516	0.3506	—	—	2.7146	0.4318	—	—
				BSSE uncorrected results				
2	0.6126	0.0384	0.6143	0.0381	0.6094	0.0445	0.6109	0.0447
3	0.8955	0.0803	0.8977	0.0794	0.9000	0.0947	0.9015	0.0949
4	1.1817	0.1235	1.1844	0.1223	1.1951	0.1475	1.1965	0.1482
5	1.4716	0.1677	1.4746	0.1663	1.4944	0.2020	1.4956	0.2032
6	1.7645	0.2129	1.7679	0.2113	1.7970	0.2579	1.7981	0.2596
7	2.0594	0.2589	2.0632	0.2570	2.1018	0.3149	2.1028	0.3171
8	2.3564	0.3054	2.3606	0.3034	2.4088	0.3727	2.4096	0.3756
9	2.6550	0.3525	2.6595	0.3504	2.7175	0.4313	2.7181	0.4347

TABLE XXII: The estimation of the two– and many–body contributions in the HCHO$\cdots$(HF)$_n$ complexes. Counterpoise corrected and uncorrected interaction induced dipole polarizability. All results in au.

n	HF SCF/ds		HF SCF/dl		MP2/ds		MP2/dl	
	2–body	Many–Body	2–body	Many–Body	2–body	Many–Body	2–body	Many–Body
				BSSE corrected results				
2	3.096	0.263	3.098	0.262	4.175	0.410	4.188	0.410
3	4.206	0.519	4.209	0.519	5.696	0.805	5.711	0.805
4	5.296	0.772	5.300	0.770	7.191	1.188	7.208	1.189
5	6.383	1.024	6.388	1.022	8.684	1.568	8.703	1.568
6	7.472	1.278	7.477	1.275	10.181	1.948	10.202	1.948
7	8.563	1.533	—	—	11.681	2.331	—	—
8	9.626	1.822	—	—	13.153	2.749	—	—
9	10.752	2.051	—	—	14.694	3.104	—	—
				BSSE uncorrected results				
2	3.062	0.273	3.114	0.264	4.137	0.429	4.215	0.411
3	4.156	0.540	4.227	0.518	5.636	0.844	5.745	0.803
4	5.230	0.804	5.321	0.777	7.110	1.248	7.250	1.192
5	6.301	1.067	6.412	1.022	8.581	1.649	8.753	1.564
6	7.373	1.333	7.505	1.278	10.055	2.052	10.259	1.947
7	8.447	1.601	8.599	1.532	11.533	2.457	11.769	2.326
8	9.524	1.871	9.696	1.791	13.016	2.864	13.283	2.712
9	10.603	2.143	10.796	2.049	14.502	3.274	14.801	3.097

TABLE XXIII: The estimation of the two– and many–body contributions in the HCHO$\cdots$(HF)$_n$ complexes. Counterpoise corrected and uncorrected interaction induced dipole first hyperpolarizability. All results in au.

n	HF SCF/ds		HF SCF/dl		MP2/ds		MP2/dl	
	2–body	Many–Body	2–body	Many–Body	2–body	Many–Body	2–body	Many–Body
				BSSE corrected results				
2	7.49	4.90	7.49	4.89	18.33	8.21	18.40	8.20
3	10.93	11.36	10.94	11.36	22.97	18.71	23.05	18.72
4	14.24	18.48	14.16	18.46	26.93	30.22	26.89	30.23
5	17.43	26.01	17.45	26.00	30.52	42.34	30.54	42.40
6	20.54	33.81	20.48	33.78	33.86	54.90	33.78	54.93
7	23.60	41.82	—	—	37.06	67.78	—	—
8	26.75	49.83	—	—	40.24	80.80	—	—
9	29.49	58.32	—	—	43.06	94.27	—	—
				BSSE uncorrected results				
2	6.98	5.36	9.61	4.23	18.56	8.78	21.55	7.20
3	10.14	12.14	13.60	10.06	23.12	19.68	27.05	16.94
4	13.17	19.53	17.37	17.25	27.03	31.50	31.77	28.39
5	16.09	27.33	21.00	24.29	30.56	43.93	36.08	39.91
6	18.92	35.39	24.54	32.14	33.87	56.75	40.17	52.37
7	21.72	43.65	28.05	39.62	37.02	69.94	44.11	64.62
8	24.45	52.08	31.49	47.70	40.07	83.36	47.92	77.54
9	27.16	60.58	34.91	55.57	43.04	96.91	51.67	90.32

TABLE XXIV: The estimation of the two– and many–body contributions in the HCHO$\cdots$(HF)$_n$ complexes. Counterpoise corrected and uncorrected interaction energies. All results in kcal mol^{-1}.

n	HF SCF/ds		HF SCF/dl		MP2/ds		MP2/dl	
	2–body	Many–Body	2–body	Many–Body	2–body	Many–Body	2–body	Many–Body
				BSSE corrected results				
2	−9.75	−1.71	−9.86	−1.71	−9.33	−1.59	−9.40	−1.60
3	−12.93	−3.93	−13.07	−3.93	−12.40	−3.73	−12.52	−3.73
4	−15.85	−6.41	−16.03	−6.42	−15.23	−6.15	−15.39	−6.16
5	−18.64	−9.07	−18.84	−9.09	−17.92	−8.77	−18.13	−8.76
6	−21.33	−11.85	−21.58	−11.87	−20.52	−11.50	−20.78	−11.51
7	−23.97	−14.71	—	—	−23.07	−14.32	−−	−−
8	−26.62	−17.56	—	—	−25.40	−17.37	−−	−−
9	−29.15	−20.57	—	—	−28.15	−20.02	−−	−−
				BSSE uncorrected results				
2	−10.23	−1.78	−10.60	−1.51	−12.44	−1.52	−12.12	−1.68
3	−13.69	−4.07	−14.24	−3.59	−17.22	−3.59	−16.78	−3.95
4	−16.90	−6.63	−17.62	−5.92	−21.77	−5.96	−21.20	−6.52
5	−19.97	−9.36	−20.87	−8.44	−26.22	−8.48	−25.49	−9.32
6	−22.96	−12.17	−24.02	−11.07	−30.59	−11.00	−29.70	−12.21
7	−25.89	−15.10	−27.12	−13.78	−34.91	−13.74	−33.85	−15.21
8	−28.78	−18.05	−30.17	−16.55	−39.19	−16.39	−37.96	−18.27
9	−31.63	−21.09	−33.18	−19.39	−43.44	−19.24	−42.04	−21.38