

Supplement of

Comparative measurements of ambient atmospheric concentrations of ice nucleating particles using multiple immersion freezing methods and a continuous flow diffusion chamber

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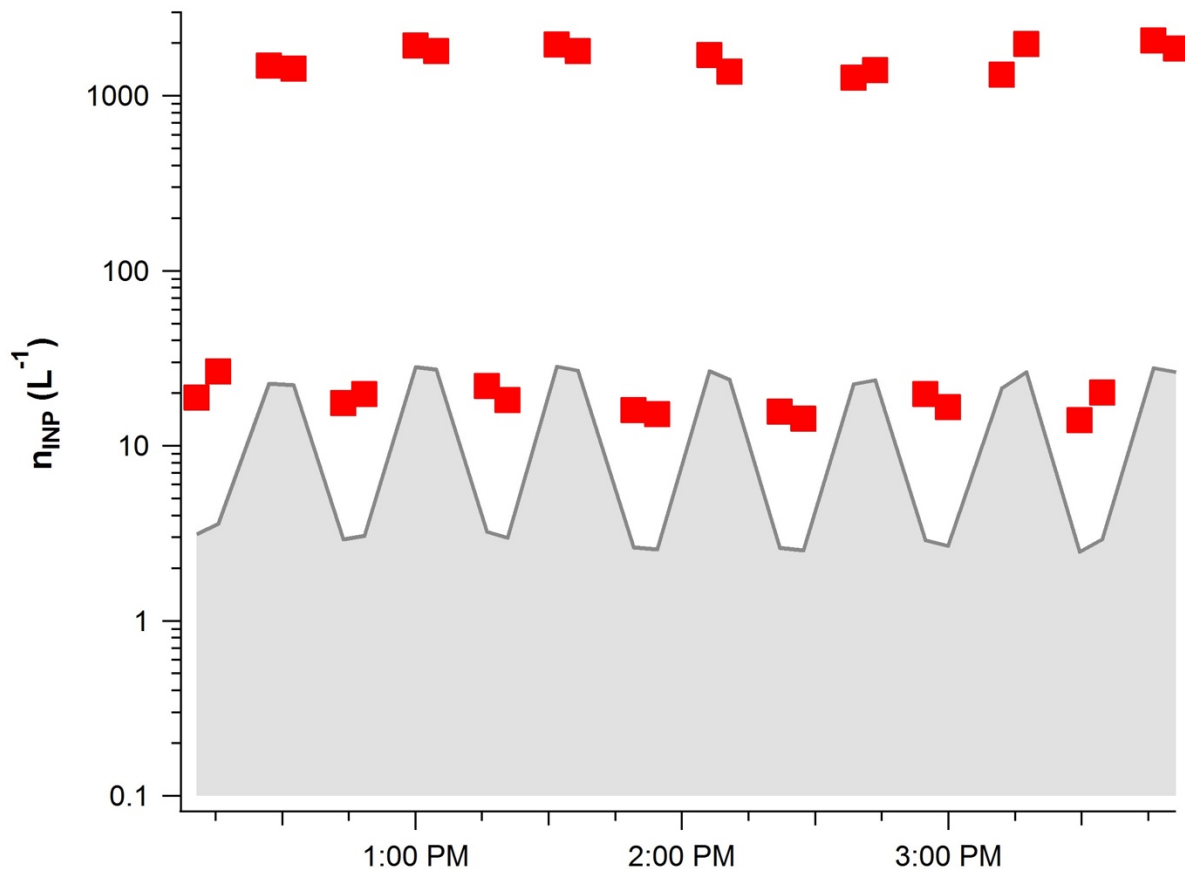


Figure S1. Aerosol Concentrator calibration check at -30°C at CSU on May 19, 2016. This is a typical experimental sampling period at one temperature, alternating off (lower points) and on (higher points) the aerosol concentrator to derive the CF factor, which is ~90 in this case. The shaded lower region is the limit of significance for INP concentrations, as described in the manuscript.

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Table S1. Data for Figures 3 and 4. INP concentrations and confidence limits (CL+; CL-) are in units L⁻¹, and Temp is in °C. Concentrator (Y: On; N: Off; B: both on and off for integrated period). IS_pore-size and CS_pore-size or BioSampler (Bio) use are indicated.

Date	Site	Temp	CFDC	CFDC_CL-	CFDC_CL+	Concentrator	IS_0.2um	IS_CL-	IS_CL+	IS_3um	IS_CL-	IS_CL+
29-Sep-10	NoCO Ag	-19.9	1.40	0.30	0.20	N	5.40	2.50	4.50			
4-Oct-10	NoCO Ag	-20.0	13.20	0.20	0.20	N	20.00	10.00	18.80			
8-Oct-10	NoCO Ag	-20.1	1.10	0.40	0.40	N	5.30	2.50	3.75			
3-Nov-10	NoCO Ag	-20.0	5.90	1.00	1.00	N	53.00	22.00	31.00			
6-Sep-13	CSU ATChem	-18.2	0.34	0.11	0.11	Y	2.20	1.20	2.00	1.90	0.92	1.80
12-Sep-13	CSU ATChem	-16.0	0.23	0.09	0.09	Y	0.29	0.16	0.32	0.52	0.25	0.41
12-Nov-13	CSU ATChem	-30.5	98.00	13.00	12.00	N						
13-Nov-13	CSU ATChem	-21.8	12.50	2.50	3.00	N	81.00	26.00	32.00	42.00	17.70	22.00
14-Nov-13	CSU ATChem	-26.8	21.50	4.50	4.50	N	105.00	41.00	53.00			
18-May-16	CSU ATChem	-20.0	0.25	0.02	0.02	Y	0.55	0.27	0.46			
19-May-16	CSU ATChem	-30.0	20.00	0.20	0.20	Y						
11-May-16	CRC (all STP)	-21.0	0.82	0.81	2.56	N	0.29	0.12	0.18			
11-May-16	CRC (all STP)	-25.0	1.25	1.4	1.24	N	8.50	3.20	3.77			
12-May-16	CRC (all STP)	-16.0	0.12	1.80	0.11	N	0.02	0.01	0.02			
12-May-16	CRC (all STP)	-21.0	0.51	1.40	0.51	N	0.38	0.19	0.31			
12-May-16	CRC (all STP)	-24.5	1.30	0.88	0.88	N	3.40	1.50	3.00			
12-May-16	CRC (all STP)	-28.5	5.20	1.30	1.30	N						
26-Jan-15	BBY	-17.5	0.84	0.74	0.74	B	0.07	0.04	0.12			
26-Jan-15	BBY	-21.0	0.99	0.81	0.81	Y	0.12	0.07	0.14			
26-Jan-15	BBY	-23.0	0.25	0.24	0.50	Y	0.45	0.20	0.27			
26-Jan-15	BBY	-24.0	1.64	0.90	0.90	Y	0.78	0.33	0.40			
26-Jan-15	BBY	-25.0	1.02	0.50	0.50	Y	4.20	2.17	3.70			
2-Feb-15	BBY	-20.0	0.17	0.16	0.21	Y	0.05	0.03	0.02			
2-Feb-15	BBY	-21.0	0.21	0.20	0.65	N	0.06	0.02	0.03			
2-Feb-15	BBY	-22.0	0.46	0.44	0.55	Y	0.09	0.04	0.05			
2-Feb-15	BBY	-24.0	0.59	0.58	0.76	B	1.10	0.46	0.65			
2-Feb-15	BBY	-25.0	1.19	0.54	0.54	B	2.74	1.07	1.29			
30-Apr-14	SGP	-21.2	0.84	0.82	0.82	B	0.40	0.21	0.35			
30-Apr-14	SGP	-27.2	10.59	4.75	4.75	B	47.64	19.80	21.60			
4-May-14	SGP	-21.6	2.75	2.40	2.40	B	1.19	0.87	2.92			
4-May-14	SGP	-24.9	21.05	8.96	8.96	B	27.89	11.61	13.66			
4-May-14	SGP	-15.0	0.28	0.13	0.13	Y	0.08	0.03	0.03			
5-May-14	SGP	-19.9	2.98	2.11	2.11	B	0.44	0.22	0.36			
5-May-14	SGP	-22.4	4.85	2.99	2.99	B	3.03	2.02	5.43			
5-May-14	SGP	-24.4	13.55	6.36	6.36	N	40.74	16.75	20.16			
5-May-14	SGP	-26.1	27.80	11.65	11.65	B	79.55	39.21	42.74			
5-Jun-14	SGP	-19.7	0.08	0.07	0.27	B	0.30	0.17	0.33			
7-Jun-14	SGP	-17.1	0.19	0.18	1.12	B	0.22	0.13	0.27			
7-Jun-14	SGP	-21.3	0.32	0.17	0.17	Y	0.43	0.21	0.35			
7-Jun-14	SGP	-25.1	0.61	0.27	0.27	Y	4.05	2.03	2.23			
8-Jun-14	SGP	-15.0	0.08	0.07	0.11	Y	0.18	0.11	0.26			
8-Jun-14	SGP	-21.8	0.89	0.88	1.15	Y	1.30	0.50	0.65			
30-Apr-14	SGP	-17.2	0.29	0.19	0.19	Y	0.14	0.08	0.18			
14-Oct-14	Kansas-harvest	-18.7	1.63	0.66	0.66	Y	1.10	0.49	0.75			
14-Oct-14	Kansas-harvest	-24.3	6.43	2.58	2.58	Y	69.00	26.40	31.90			
14-Oct-14	Kansas-harvest	-29.2	12.06	5.12	5.12	Y						
15-Oct-14	Kansas-harvest	-17.2	3.00	1.84	1.84	Y	0.57	0.31	0.63			
15-Oct-14	Kansas-harvest	-22.6	1.74	0.91	0.91	Y	21.00	10.10	16.50			
15-Oct-14	Kansas-harvest	-27.1	7.29	2.93	2.93	Y						
10/15/2014-10/16/2014	Kansas	-18.2	0.26	0.12	0.12	Y	1.20	0.62	1.13			
10/15/2014-10/16/2014	Kansas	-21.6	0.29	0.14	0.14	Y	4.70	1.99	2.49			
10/15/2014-10/16/2014	Kansas	-25.0	2.12	1.94	1.94	Y	77.03	30.88	39.60			
14-Oct-14	Kansas	-17.7	0.49	0.48	1.00	Y	0.19	0.11	0.23			
14-Oct-14	Kansas	-20.9	0.97	0.97	0.98	Y	2.10	1.32	3.14			
14-Oct-14	Kansas	-24.8	4.54	3.59	3.59	Y	55.00	25.90	27.70			
14-Oct-14	Kansas	-30.7	7.84	4.35	4.35	Y						
17-Aug-11	MEFO	-25.0	3.92	1.22	1.22	Y						
17-Aug-11	MEFO	-25.0	4.26	2.48	2.48	Y						
18-Aug-11	MEFO	-20.3	0.43	0.30	0.30	Y						

Table S1. (continued)

Date	Site	Temp	IS-Biosamp	IS_CL-	IS_CL+CS_0.2um	CS_CL-	CS_CL+CS_3um	CS_CL-	CS_CL+		
29-Sep-10	NoCO Ag	-19.9									
4-Oct-10	NoCO Ag	-20.0									
8-Oct-10	NoCO Ag	-20.1									
3-Nov-10	NoCO Ag	-20.0									
6-Sep-13	CSU ATChem	-18.2	0.80	0.35	0.55	2.02	1.25	3.26	1.20	0.88	2.86
12-Sep-13	CSU ATChem	-16.0	0.26	0.17	0.46						
12-Nov-13	CSU ATChem	-30.5				624.06	443.30	1250.50	752.79	548.80	1348.50
13-Nov-13	CSU ATChem	-21.8	40.00	19.00	21.00	42.90	27.30	75.30	42.40	29.70	98.90
14-Nov-13	CSU ATChem	-26.8	105.00	40.50	52.30						
18-May-16	CSU ATChem	-20.0									
19-May-16	CSU ATChem	-30.0									
11-May-16	CRC (all STP)	-21.0									
11-May-16	CRC (all STP)	-25.0									
12-May-16	CRC (all STP)	-16.0									
12-May-16	CRC (all STP)	-21.0									
12-May-16	CRC (all STP)	-24.5									
12-May-16	CRC (all STP)	-28.5									
26-Jan-15	BBY	-17.5									
26-Jan-15	BBY	-21.0									
26-Jan-15	BBY	-23.0									
26-Jan-15	BBY	-24.0									
26-Jan-15	BBY	-25.0									
2-Feb-15	BBY	-20.0									
2-Feb-15	BBY	-21.0									
2-Feb-15	BBY	-22.0									
2-Feb-15	BBY	-24.0									
2-Feb-15	BBY	-25.0									
30-Apr-14	SGP	-21.2									
30-Apr-14	SGP	-27.2									
4-May-14	SGP	-21.6									
4-May-14	SGP	-24.9									
4-May-14	SGP	-15.0									
5-May-14	SGP	-19.9									
5-May-14	SGP	-22.4									
5-May-14	SGP	-24.4									
5-May-14	SGP	-26.1									
5-Jun-14	SGP	-19.7									
7-Jun-14	SGP	-17.1									
7-Jun-14	SGP	-21.3									
7-Jun-14	SGP	-25.1									
8-Jun-14	SGP	-15.0									
8-Jun-14	SGP	-21.8									
30-Apr-14	SGP	-17.2									
14-Oct-14	Kansas-harvest	-18.7									
14-Oct-14	Kansas-harvest	-24.3									
14-Oct-14	Kansas-harvest	-29.2									
15-Oct-14	Kansas-harvest	-17.2									
15-Oct-14	Kansas-harvest	-22.6									
15-Oct-14	Kansas-harvest	-27.1									
10/15/2014-10/16/2014	Kansas	-18.2									
10/15/2014-10/16/2014	Kansas	-21.6									
10/15/2014-10/16/2014	Kansas	-25.0									
14-Oct-14	Kansas	-17.7									
14-Oct-14	Kansas	-20.9									
14-Oct-14	Kansas	-24.8									
14-Oct-14	Kansas	-30.7									
17-Aug-11	MEFO	-25.0									
17-Aug-11	MEFO	-25.0									
18-Aug-11	MEFO	-20.3									

Table S1. (continued)

Date	Site	Temp	CS_Biosamp	CS_CL-	CS_CL+	DFT_all	DFT_CLDFT_size	DFT_CL	CRAFT	CRAFT_CL-	CRAFT_CL+
29-Sep-10	NoCO	Ag -19.9									
4-Oct-10	NoCO	Ag -20.0									
8-Oct-10	NoCO	Ag -20.1									
3-Nov-10	NoCO	Ag -20.0									
6-Sep-13	CSU ATChem	-18.2	1.98	1.12	2.60						
12-Sep-13	CSU ATChem	-16.0									
12-Nov-13	CSU ATChem	-30.5	1281.00	884.00	2389.00						
13-Nov-13	CSU ATChem	-21.8	69.60	45.80	134.30	4.59	3.49	4.12	3.47		
14-Nov-13	CSU ATChem	-26.8	238.00	168.70	579.00	28.10	11.10	25.20	11.10		
18-May-16	CSU ATChem	-20.0							0.46	0.34	1.17
19-May-16	CSU ATChem	-30.0							188.2	59.4	68
11-May-16	CRC (all STP)	-21.0							0.5	0.34	1.17
11-May-16	CRC (all STP)	-25.0							7	4.7	13
12-May-16	CRC (all STP)	-16.0							0.03	0.013	0.021
12-May-16	CRC (all STP)	-21.0							0.7	0.5	1.3
12-May-16	CRC (all STP)	-24.5							4.7	1.8	2.7
12-May-16	CRC (all STP)	-28.5							54	20	29
26-Jan-15	BBY	-17.5	0.24	0.12	0.24						
26-Jan-15	BBY	-21.0	0.72	0.46	1.28						
26-Jan-15	BBY	-23.0	2.22	1.35	3.45						
26-Jan-15	BBY	-24.0	5.76	3.66	10.06						
26-Jan-15	BBY	-25.0	14.56	8.92	23.02						
2-Feb-15	BBY	-20.0	0.14	0.09	0.36						
2-Feb-15	BBY	-21.0	0.53	0.3	0.72						
2-Feb-15	BBY	-22.0	0.99	0.58	1.42						
2-Feb-15	BBY	-24.0	2.39	1.57	4.57						
2-Feb-15	BBY	-25.0	7.66	4.96	14.04						
30-Apr-14	SGP	-21.2									
30-Apr-14	SGP	-27.2									
4-May-14	SGP	-21.6									
4-May-14	SGP	-24.9									
4-May-14	SGP	-15.0									
5-May-14	SGP	-19.9									
5-May-14	SGP	-22.4									
5-May-14	SGP	-24.4									
5-May-14	SGP	-26.1									
5-Jun-14	SGP	-19.7									
7-Jun-14	SGP	-17.1									
7-Jun-14	SGP	-21.3									
7-Jun-14	SGP	-25.1									
8-Jun-14	SGP	-15.0									
8-Jun-14	SGP	-21.8									
30-Apr-14	SGP	-17.2									
14-Oct-14	Kansas-harvest	-18.7				0.70	0.50	0.50	0.30		
14-Oct-14	Kansas-harvest	-24.3				8.90	2.90	4.10	1.40		
14-Oct-14	Kansas-harvest	-29.2				68.50	23.50	32.30	11.00		
15-Oct-14	Kansas-harvest	-17.2				1.40	1.00	0.25	0.24		
15-Oct-14	Kansas-harvest	-22.6				2.10	1.40	0.34	0.32		
15-Oct-14	Kansas-harvest	-27.1				23.30	6.60	10.70	2.90		
10/15/2014-10/16/2014	Kansas	-18.2				0.26	0.24				
10/15/2014-10/16/2014	Kansas	-21.6				1.40	0.80	0.35	0.20		
10/15/2014-10/16/2014	Kansas	-25.0				5.40	2.00	2.40	0.80		
14-Oct-14	Kansas	-17.7				0.90	0.50	0.80	0.50		
14-Oct-14	Kansas	-20.9				1.30	0.80	1.10	0.70		
14-Oct-14	Kansas	-24.8				4.50	1.90	2.40	0.90		
14-Oct-14	Kansas	-30.7				60.80	28.10	16.00	4.50		
17-Aug-11	MEFO	-25.0						8.60	5.35		
17-Aug-11	MEFO	-25.0						0.8	0.40		
18-Aug-11	MEFO	-20.3						0.1	0.04		

Table S2. Data for Figure 5. Instrument name column data and positive (+) and negative (-) confidence intervals are INP concentrations in L⁻¹, and T is in °C. “Bio” indicates use of the BioSampler, while all other samples used 0.2 μm pore size filters for collections.

Location	Date	T	CS	CS+	CS-	IS	IS+	IS-	LOG(CS/IS)
BBY	1/26/15	-17.5	0.240	0.240	0.120	0.070	0.118	0.044	0.535
		-21.0	0.720	1.280	0.460	0.116	0.141	0.068	0.794
		-23.0	2.220	3.450	1.350	0.450	0.270	0.197	0.693
		-24.0	5.760	10.060	3.660	0.780	0.403	0.329	0.868
		-25.0	14.560	23.020	8.920	4.200	3.702	2.171	0.540
BBY	2/2/15	-20.0	0.140	0.360	0.090	0.050	0.021	0.031	0.448
		-21.0	0.530	0.720	0.300	0.060	0.034	0.025	0.945
		-22.0	0.990	1.420	0.580	0.093	0.045	0.035	1.028
		-24.0	2.390	4.570	1.570	1.098	0.654	0.457	0.338
		-25.0	7.660	14.040	4.960	2.736	1.290	1.074	0.447
Kansas	14-Oct-14	T MOUDI-DFT	DFT+	DFT-	IS	IS+	IS-	LOG(DFT/IS)	
		-15.0	0.210	0.200	0.200	0.078	0.191	0.057	0.428
		-16.0	0.210	0.200	0.200	0.078	0.191	0.057	0.428
		-17.0	0.550	0.460	0.460	0.078	0.191	0.057	0.846
		-18.0	0.900	0.500	0.500	0.210	0.257	0.123	0.631
		-19.0	1.040	0.500	0.500	0.624	0.418	0.284	0.222
		-20.0	1.110	0.640	0.640	1.613	0.823	0.690	-0.162
		-20.5	1.190	0.700	0.700	2.237	1.153	1.019	-0.274
		-20.0	1.100	0.640	0.640	1.772	3.220	1.179	-0.207
		-20.5	1.190	0.700	0.700	2.404	3.527	1.486	-0.305
		-21.0	1.750	0.890	0.890	2.404	3.527	1.486	-0.138
		-21.5	1.840	0.920	0.920	3.738	4.103	2.062	-0.308
		-22.0	2.260	1.100	1.100	4.608	4.533	2.430	-0.309
		-22.5	2.690	1.230	1.230	7.012	5.417	3.313	-0.416
		-23.0	3.300	1.380	1.380	13.069	7.461	5.358	-0.598
-23.5	4.450	1.930	1.930	20.369	9.943	7.839	-0.661		
-24.0	4.590	1.940	1.940	36.865	16.591	14.488	-0.905		
-24.5	6.560	2.850	2.850	61.823	31.151	29.048	-0.974		
Kansas	10/1514-10/16/14	T MOUDI-DFT	DFT+	DFT-	IS	IS+	IS-	LOG(DFT/IS)	
		-8.0	0.070	0.067	0.067	0.059	0.056	0.031	0.074
		-9.0	0.100	0.100	0.100	0.104	0.074	0.049	0.000
		-10.0	0.100	0.100	0.100	0.132	0.084	0.059	-0.114
		-11.0	0.150	0.140	0.140	0.186	0.105	0.080	-0.103
		-12.0	0.150	0.150	0.150	0.186	0.105	0.080	-0.094
		-13.0	0.170	0.150	0.150	0.235	0.125	0.099	-0.141
		-14.0	0.170	0.150	0.150	0.266	0.138	0.113	-0.195
		-15.0	0.170	0.150	0.150	0.353	0.179	0.154	-0.317
		-16.0	0.200	0.180	0.180	0.422	0.217	0.192	-0.324
		-17.0	0.250	0.220	0.220	0.539	0.293	0.268	-0.334
		-18.0	0.270	0.250	0.250	1.170	1.126	0.622	-0.637
		-19.0	0.620	0.420	0.420	1.376	1.207	0.704	-0.346
		-20.0	0.760	0.460	0.460	1.829	1.381	0.877	-0.381
		-21.0	1.160	0.660	0.660	3.728	2.096	1.592	-0.507
-22.0	1.570	0.800	0.800	10.640	5.867	5.343	-0.831		
-23.0	2.260	1.100	1.100	23.274	19.293	11.364	-1.013		
-24.0	3.140	1.200	1.200	53.948	29.684	21.755	-1.235		
-25.0	5.610	2.100	2.100	77.026	39.603	30.877	-1.138		
-26.0	7.570	2.600	2.600	179.101	87.033	78.307	-1.376		
Kansas harvest soy	14-Oct-14	T MOUDI-DFT	DFT+	DFT-	IS	IS+	IS-	LOG(DFT/IS)	
		-16.0	0.230	0.230	0.230	0.265	0.117	0.103	-0.061
		-17.0	0.520	0.300	0.300	0.301	0.135	0.121	0.237
		-18.0	0.720	0.400	0.400	0.732	0.659	0.370	-0.007
		-19.0	0.720	0.550	0.550	1.196	0.822	0.533	-0.220
		-20.0	0.820	0.630	0.630	2.960	1.411	1.122	-0.558
		-21.0	1.040	0.670	0.670	6.797	9.973	4.202	-0.815
		-22.0	2.180	1.010	1.010	8.648	10.799	5.028	-0.598
		-23.0	4.140	1.560	1.560	35.281	20.186	14.416	-0.931
		-24.0	8.430	2.880	2.880	76.000	34.812	28.865	-0.955
-25.0	12.850	3.820	3.820	180.000	223.096	104.167	-1.146		
-26.0	25.000	7.150	7.150	220.000	239.811	120.883	-0.944		

Table S2. (continued)

Kansas harvest sorghum	15-Oct-14	T	MOUDI-DFT	DFT+	DFT-	IS	IS+	IS-	LOG(DFT/IS)		
		-9.0	0.350	0.340	0.340	0.104	0.059	0.042	0.528		
		-10.0	1.140	0.854	0.854	0.174	0.083	0.066	0.816		
		-11.0	1.140	0.854	0.854	0.228	0.103	0.086	0.700		
		-12.0	1.140	0.854	0.854	0.415	0.192	0.175	0.439		
		-13.0	1.260	0.908	0.908	0.415	0.192	0.175	0.482		
		-14.0	1.260	0.908	0.908	0.519	0.259	0.242	0.385		
		-13.0	1.260	0.908	0.908	0.295	0.536	0.196	0.631		
		-14.0	1.260	0.908	0.908	0.400	0.587	0.247	0.498		
		-15.0	1.260	0.908	0.908	0.509	0.635	0.296	0.394		
		-16.0	1.260	0.908	0.908	0.509	0.635	0.296	0.394		
		-17.0	1.260	0.908	0.908	0.622	0.683	0.343	0.307		
		-18.0	1.580	1.136	1.136	0.989	0.822	0.482	0.203		
		-19.0	1.580	1.136	1.136	2.698	1.392	1.053	-0.232		
		-20.0	1.910	1.358	1.358	3.483	1.660	1.320	-0.261		
		-21.0	2.020	1.402	1.402	5.900	10.714	3.923	-0.466		
		-22.0	2.160	1.447	1.447	10.000	12.707	5.917	-0.666		
		-23.0	2.490	1.503	1.503	57.000	29.303	22.305	-1.360		
		-24.0	4.030	1.689	1.689	86.000	211.495	62.475	-1.329		
		-25.0	8.790	2.870	2.870	180.000	259.082	110.061	-1.311		
		-26.0	14.550	4.683	4.683	330.000	323.840	174.819	-1.356		
		CRC	11-May-16	T	CRAFT	CRAFT+	CRAFT-	IS	IS+	IS-	LOG(CRAFT/IS)
				-13.0	0.005	0.012	0.003	0.002	0.009	0.002	0.333
				-14.0	0.007	0.013	0.005	0.002	0.009	0.002	0.514
				-15.0	0.015	0.016	0.008	0.009	0.013	0.006	0.197
				-16.0	0.023	0.019	0.011	0.009	0.013	0.006	0.389
-17.0	0.041			0.025	0.016	0.020	0.018	0.010	0.297		
-18.0	0.099			0.041	0.033	0.035	0.023	0.016	0.454		
-19.0	0.188			0.068	0.059	0.070	0.037	0.030	0.429		
-20.0	0.432			0.192	0.184	0.167	0.139	0.081	0.413		
-21.0	0.463			1.175	0.337	0.291	0.181	0.124	0.202		
-22.0	1.195			1.529	0.691	0.858	1.072	0.499	0.144		
-23.0	2.822			2.111	1.273	3.195	1.547	0.974	-0.054		
-24.0	6.213			3.087	2.249	4.954	2.484	1.911	0.098		
-25.0	11.118			4.422	3.584	8.454	3.769	3.197	0.119		
-26.0	20.121	7.230	6.392	13.677	6.481	5.872	0.168				
CRC	12-May-16	T	CRAFT	CRAFT+	CRAFT-	IS	IS+	IS-	LOG(CRAFT/IS)		
		-13.0	0.002	0.010	0.002	0.002	0.007	0.001	0.126		
		-14.0	0.007	0.013	0.005	0.007	0.011	0.005	-0.022		
		-15.0	0.023	0.019	0.011	0.009	0.012	0.006	0.387		
		-16.0	0.028	0.021	0.013	0.022	0.016	0.010	0.113		
		-17.0	0.041	0.025	0.016	0.032	0.020	0.014	0.110		
		-18.0	0.066	0.032	0.024	0.063	0.033	0.027	0.019		
		-19.0	0.094	0.040	0.031	0.128	0.070	0.064	-0.135		
		-20.0	0.188	0.068	0.059	0.189	0.230	0.110	-0.001		
		-21.0	0.702	1.304	0.466	0.380	0.308	0.188	0.267		
		-22.0	1.451	1.633	0.795	0.888	0.499	0.379	0.213		
		-23.0	2.254	1.925	1.087	1.422	0.738	0.615	0.200		
		-24.0	3.738	2.392	1.554	1.628	0.853	0.725	0.361		
		-25.0	6.216	3.089	2.251	5.309	5.128	2.818	0.069		
-26.0	10.524	4.258	3.420	9.371	6.669	4.358	0.050				
-27.0	20.132	7.234	6.396	25.182	14.644	11.668	-0.097				

Table S2. (continued)

CSU	18-May-16	T	CRAFT	CRAFT+	CRAFT-	IS	IS+	IS-	LOG(CRAFT/IS)
		-8.0	0.002	0.010	0.002	0.025	0.022	0.013	-1.160
		-9.0	0.007	0.013	0.005	0.098	0.051	0.042	-1.261
		-10.0	0.012	0.015	0.007	0.156	0.080	0.071	-1.229
		-11.0	0.017	0.017	0.009	0.156	0.080	0.071	-1.073
		-12.0	0.034	0.023	0.015	0.168	0.298	0.112	-0.804
		-13.0	0.047	0.027	0.018	0.168	0.298	0.112	-0.663
		-14.0	0.058	0.030	0.021	0.229	0.329	0.142	-0.708
		-15.0	0.079	0.036	0.027	0.229	0.329	0.142	-0.574
		-16.0	0.118	0.046	0.038	0.361	0.387	0.201	-0.601
		-17.0	0.156	0.057	0.049	0.352	0.399	0.201	-0.466
		-18.0	0.278	0.103	0.095	0.428	0.431	0.233	-0.301
		-19.0	0.229	1.027	0.189	0.509	0.464	0.266	-0.461
		-20.0	0.463	1.175	0.337	0.509	0.464	0.266	-0.155
		-21.0	0.702	1.304	0.466	0.509	0.483	0.272	0.025
		-22.0	1.196	1.530	0.691	0.812	0.604	0.393	0.054
		-23.0	3.120	2.205	1.367	1.379	0.831	0.620	0.241
		-24.0	6.620	3.199	2.360	3.575	2.168	1.916	0.154
		-25.0	11.124	4.425	3.586	7.224	8.657	4.245	0.074
		-26.0	16.595	6.047	5.209	15.970	13.469	8.353	-0.097
-27.0	43.230	19.237	18.398	27.586	19.757	14.032	0.081		
CSU	19-May-16	T	CRAFT	CRAFT+	CRAFT-	IS	IS+	IS-	LOG(CRAFT/IS)
		-11.0	0.020	0.018	0.010	0.005	0.012	0.004	0.598
		-12.0	0.031	0.022	0.014	0.005	0.012	0.004	0.796
		-13.0	0.058	0.030	0.021	0.010	0.015	0.007	0.745
		-14.0	0.124	0.048	0.040	0.031	0.023	0.015	0.604
		-15.0	0.188	0.068	0.059	0.045	0.029	0.020	0.623
		-16.0	0.229	1.027	0.189	0.080	0.042	0.034	0.459
		-17.0	0.463	1.175	0.337	0.099	0.052	0.043	0.669
		-18.0	0.946	1.421	0.582	0.139	0.073	0.064	0.833
		-19.0	0.946	1.421	0.582	0.256	0.335	0.154	0.567
		-20.0	1.980	1.830	0.992	0.256	0.335	0.154	0.888
		-21.0	2.824	2.112	1.274	0.312	0.376	0.183	0.956
		-22.0	3.425	2.298	1.460	0.551	0.477	0.284	0.794
-23.0	6.216	3.089	2.251	1.648	0.926	0.733	0.577		
-24.0	8.895	3.813	2.975	2.474	1.464	1.234	0.556		
-25.0	11.956	15.297	6.913	8.335	7.987	4.439	0.157		
-26.0	25.355	20.192	11.808	9.895	9.339	5.303	0.409		
CSU	6-Sep-13	T	CS	CS+	CS-	IS	IS+	IS-	LOG(CS/IS)
		-15	0.584	0.584	0.292	0.567	0.331	0.245	-0.013
		-16	0.806	1.122	0.469	0.621	0.351	0.266	-0.113
		-17	1.163	1.876	0.718	1.545	1.732	0.874	0.123
		-18	2.017	3.257	1.246	2.236	2.014	1.156	0.045
		-19	2.697	4.820	1.729	3.411	2.462	1.604	0.102
		-21	11.097	17.508	6.792	8.567	4.478	3.620	-0.112
		-22	21.839	44.909	14.693	15.670	17.416	8.835	-0.144
-23	33.488	76.010	23.246	26.778	21.857	13.276	-0.097		
CSU	12-Nov-13	T	CS-Bio	CS+	CS-	IS-Bio	IS+	IS-	LOG(CS/IS)
		-12.0	0.954	0.954	0.477	0.364	0.163	0.146	0.418
		-13.0	1.258	1.833	0.746	0.514	0.754	0.318	0.389
		-14.0	1.693	2.318	0.978	0.653	0.816	0.380	0.413
		-15.0	2.712	3.340	1.497	0.653	0.816	0.380	0.618
		-16.0	3.781	7.196	2.479	2.299	1.405	0.969	0.216
		-17.0	7.550	11.301	4.526	3.277	1.726	1.290	0.362
		-18.0	12.922	19.174	7.720	4.631	2.187	1.751	0.446
		-19.0	20.698	29.290	12.128	4.631	2.187	1.751	0.650
		-20.0	24.259	33.646	14.096	10.126	4.632	4.196	0.379
		-21.0	39.027	64.816	24.360	19.965	21.915	11.014	0.291
-22.0	75.870	115.796	45.837	27.063	24.670	13.769	0.448		
-23.0	138.679	189.600	80.095	51.655	33.204	22.303	0.429		
-24.0	181.408	208.552	97.018	195.255	86.523	75.622	-0.032		

Table S2. (continued)

CSU	12-Nov-13	T	MOUDI-DFT	DFT+	DFT-	IS-Bio	IS+	IS-	LOG(DFT/IS)
		-10.0	0.118	0.116	0.116	0.179	0.085	0.068	-0.180
		-11.0	0.200	0.198	0.198	0.320	0.142	0.124	-0.203
		-12.0	0.508	0.423	0.423	0.364	0.163	0.146	0.145
		-13.0	0.710	0.622	0.622	0.514	0.754	0.318	0.141
		-14.0	0.891	0.801	0.801	0.653	0.816	0.380	0.134
		-15.0	1.314	1.193	1.193	0.653	0.816	0.380	0.303
		-16.0	1.987	1.836	1.836	2.299	1.405	0.969	-0.063
		-17.0	2.838	2.579	2.579	3.277	1.726	1.290	-0.062
		-18.0	4.643	4.381	4.381	4.631	2.187	1.751	0.001
CSU	13-Nov-13	T	CS-Bio	CS+	CS-	IS-Bio	IS+	IS-	LOG(CS/IS)
		-12.0	0.499	0.682	0.288	0.163	0.075	0.069	0.486
		-13.0	1.010	1.873	0.656	0.330	0.255	0.156	0.486
		-14.0	2.686	4.921	1.737	0.459	0.299	0.200	0.767
		-15.0	6.192	9.914	3.811	1.763	2.587	1.090	0.546
		-16.0	10.297	14.612	6.040	1.953	2.674	1.177	0.722
		-17.0	16.744	23.844	9.837	5.625	4.066	2.569	0.474
		-18.0	27.020	49.350	17.460	9.487	5.346	3.849	0.455
		-19.0	40.174	73.178	25.936	11.494	6.006	4.509	0.543
		-20.0	55.401	116.584	37.555	23.015	10.228	8.731	0.382
		-21.0	69.563	134.262	45.822	35.055	16.064	14.567	0.298
		-22.0	108.495	225.122	73.212	26.920	29.928	14.679	0.605
		-23.0	301.880	301.880	150.940	28.820	30.662	15.413	1.020
CSU	14-Nov-13	T	CS-Bio	CS+	CS-	IS-Bio	IS+	IS-	LOG(CS/IS)
		-18.0	4.175	5.715	2.412	1.490	2.092	0.906	0.447
		-19.0	5.571	9.910	3.566	2.771	2.618	1.433	0.303
		-21.0	12.507	13.803	6.562	8.134	4.437	3.252	0.187
		-22.0	21.512	55.815	15.528	9.997	5.055	3.869	0.333
		-23.0	33.414	64.636	22.027	17.330	7.734	6.548	0.285
		-24.0	64.863	97.105	38.887	26.450	12.001	10.815	0.390
CSU	14-Nov-13	T	MOUDI-DFT	DFT+	DFT-	IS-Bio	IS+	IS-	LOG(DFT/IS)
		-18.0	0.470	0.269	0.269	1.490	2.092	0.906	-0.501
		-19.0	0.770	0.400	0.400	2.771	2.618	1.433	-0.556
		-20.0	1.300	0.577	0.577	5.233	3.483	2.297	-0.605
		-21.0	2.167	0.786	0.786	8.134	4.437	3.252	-0.574
		-22.0	3.961	1.354	1.354	9.997	5.055	3.869	-0.402
		-23.0	6.533	2.124	2.124	17.330	7.734	6.548	-0.424
-24.0	11.187	3.750	3.750	26.450	12.001	10.815	-0.374		
-25.0	19.657	7.929	7.929	53.411	35.189	23.335	-0.434		
-26.0	23.834	10.783	10.783	102.554	51.415	39.561	-0.634		
-27.0	28.450	11.128	11.128	167.467	75.003	63.149	-0.770		