Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Assessment of Binding Energies of Atmospheric Relevant Clusters

Jonas Elm[†], Merete Bilde[‡] and Kurt V. Mikkelsen[†]

[†] *Department of Chemistry, H. C. Ørsted Institute, University of Copenhagen, DK-2100 Copenhagen Ø, Denmark*

[‡] *Department of Chemistry, Aarhus University, Langelandsgade 140, DK-8000 Århus C, Denmark*

E-mail: elm@chem.ku.dk

Abbrevations:

w = water

a = ammonia

dma = dimethylamine

sa = sulfuric acid

sa^- = bisulfate ion

Complete List of Extracted Structures

Herb CPL 2011	Herb JPC 2013	Loukonen ACP 2010	Ortega ACP 2012	Kupianinen ACP 2012
(1sa)(1a)	($1sa^-$)(1w)	(1sa)(1w)	(1sa)(1a)	(1sa)(1a)$^+$
(1sa)(1w)	(1sa)($1sa^-$)	(1sa)(2w)	(1sa)(2a)	(1sa)(2a)$^+$
(1sa)(2w)	(1sa)($1sa^-$)(1w)	(1sa)(3w)	(1sa)(3a)	(1sa)(3a)$^+$
(1sa)(3w)	(1sa)($1sa^-$)(2w)	(1sa)(4w)	(1sa)(4a)	(1sa)(1dma)$^+$
(2sa)	(1sa)($1sa^-$)(1a)(1w)	(1sa)(5w)	(2sa)(1a)	(1sa)(1dma)(1a)$^+$
(2sa)(2a)	(1sa)($1sa^-$)(1a)(2w)	(1sa)(1a)	(2sa)(2a)	(1sa)(1dma)(2a)$^+$
(2sa)(3a)	(1sa)($1sa^-$)(1a)(3w)	(1sa)(1a)(1w)	(2sa)(3a)	(1sa)(2dma)$^+$
(2sa)(1w)	(2sa)($1sa^-$)	(1sa)(1a)(2w)	(2sa)(4a)	(1sa)(2dma)(1a)$^+$
(2sa)(2w)	(2sa)($1sa^-$)(1a)	(1sa)(1a)(3w)	(3sa)(1a)	(2sa)(1a)$^+$
(2sa)(3w)	(2sa)($1sa^-$)(1w)	(1sa)(1a)(4w)	(3sa)(2a)	(2sa)(2a)$^+$
(2sa)(1a)(1w)	(2sa)($1sa^-$)(2w)	(1sa)(1a)(5w)	(3sa)(3a)	(2sa)(3a)$^+$
(2sa)(1a)(2w)	(2sa)($1sa^-$)(3w)	(1sa)(1dma)	(1sa)(1dma)	(2sa)(4a)$^+$
(2sa)(1a)(3w)	(2sa)($1sa^-$)(1a)(1w)	(1sa)(1dma)(1w)	(1sa)(2dma)	(2sa)(1dma)(1a)$^+$
(2sa)(2a)(1w)	(2sa)($1sa^-$)(1a)(2w)	(1sa)(1dma)(2w)	(1sa)(3dma)	(2sa)(1dma)(2a)$^+$
(2sa)(2a)(2w)		(1sa)(1dma)(3w)	(2sa)(1dma)	(2sa)(1dma)(3a)$^+$
(2sa)(2a)(3w)		(1sa)(1dma)(4w)	(2sa)(2dma)	(2sa)(1dma)$^+$
(3sa)		(1sa)(1dma)(5w)	(3sa)(1dma)	(2sa)(2dma)$^+$
(3sa)(1a)		(2sa)		(2sa)(2dma)(1a)$^+$
(3sa)(2a)		(2sa)(1w)		
(3sa)(3a)		(2sa)(2w)		
(3sa)(1w)		(2sa)(3w)		
(3sa)(2w)		(2sa)(4w)		
(3sa)(1a)(1w)		(2sa)(5w)		
		(2sa)(1a)		
		(2sa)(1a)(1w)		
		(2sa)(1a)(2w)		
		(2sa)(1a)(3w)		
		(2sa)(1a)(4w)		
		(2sa)(1a)(5w)		
		(2sa)(1dma)		
		(2sa)(1dma)(1w)		
		(2sa)(1dma)(2w)		
		(2sa)(1dma)(3w)		
		(2sa)(1dma)(4w)		
		(2sa)(1dma)(5w)		

Table 1: List of extracted structures from five different studies.

Coupled Cluster Calculated Absolute- and Binding Energies

Geometries extracted from Reference:
Herb, J.; Nadykto, A. B.; Yu, F. Chem. Phys. Lett. 2011, 518, 7-14.

Cluster	E_{abs} L-F12	$E_{binding}$ L-F12	E_{abs} F12	$E_{binding}$ F12	Ratio
1w	-76.3687		-76.36		
1a	-56.4996		-56.4962		
1sa	-699.6199		-699.5935		
(1sa)(1a)	-756.1437	-15.15	-756.1151	-15.95	1.05
(1sa)(1w)	-776.0066	-11.32	-775.9764	-12.48	1.10
(1sa)(2w)	-852.3921	-21.84	-852.3575	-23.81	1.09
(1sa)(3w)	-928.7782	-32.80	-928.7400	-36.07	1.10
(2sa)	-1399.2649	-15.71	-1399.2154	-17.83	1.13
(2sa)(2a)	-1512.3365	-61.10	-	-	-
(2sa)(3a)	-1568.8552	-73.06	-	-	-
(2sa)(1w)	-1475.6152	-4.19	-	-	-
(2sa)(2w)	-1552.0017	-15.40	-	-	-
(2sa)(3w)	-1628.4321	-54.10	-	-	-
(2sa)(1a)(1w)	-1532.1955	-54.78	-	-	-
(2sa)(1a)(2w)	-1608.5803	-64.90	-	-	-
(2sa)(1a)(3w)	-1684.9657	-75.45	-	-	-
(2sa)(2a)(1w)	-1588.7274	-75.06	-	-	-
(2sa)(2a)(2w)	-1665.1103	-84.00	-	-	-
(2sa)(2a)(3w)	-1741.4900	-90.92	-	-	-
(3sa)	-2098.9100	-31.52	-	-	-
(3sa)(1a)	-2155.4513	-57.62	-	-	-
(3sa)(2a)	-2211.9970	-86.56	-	-	-
(3sa)(3a)	-2268.5302	-107.59	-	-	-
(3sa)(1w)	-2175.2982	-43.74	-	-	-
(3sa)(2w)	-2251.6898	-58.16	-	-	-
(3sa)(1a)(1w)	-2231.8468	-74.50	-	-	-

Table 2: List of extracted structures from five different studies. LF12 and F12 refer to the DF-LCCSD(T)-F12a/VDZ-F12 and CCSD(T)-F12a/VDZ-F12, respectively. The Ratio is calculated as F12/LF12.

Coupled Cluster Calculated Absolute- and Binding Energies

Geometries extracted from Reference:
Herb, J.; Xu, Y.; Yu, F.; Nadykto, A. B. J. Phys. Chem. A 2013, 117, 133-152.

Cluster	E_{abs} L-F12	$E_{binding}$ L-F12	E_{abs} F12	$E_{binding}$ F12	Ratio
1w	-76.3687		-76.3630		
1a	-56.4996		-56.4962		
1sa	-699.6199		-699.5935		
$1sa^-$	-699.1106		-699.0836		
$(1sa^-)(1w)$	-775.5027	-14.70	-775.4724	-16.13	1.10
$(1sa)(1sa^-)$	-1398.7996	-43.33	-1398.7510	-46.37	1.07
$(1sa)(1sa^-)(1w)$	-1475.1844	-53.45	-1475.1311	-57.03	1.07
$(1sa)(1sa^-)(2w)$	-1551.5645	-60.63	-1551.5072	-65.29	1.08
$(1sa)(1sa^-)(1a)(1w)$	-1531.6987	-62.65	-1531.6429	-66.91	1.07
$(1sa)(1sa^-)(1a)(2w)$	-1608.0897	-76.69	-	-	-
$(1sa)(1sa^-)(1a)(3w)$	-1684.4792	-89.75	-	-	-
$(2sa)(1sa^-)$	-2098.4651	-71.93	-	-	-
$(2sa)(1sa^-)(1a)$	-2154.9964	-91.76	-	-	-
$(2sa)(1sa^-)(1w)$	-2174.8521	-83.41	-	-	-
$(2sa)(1sa^-)(2w)$	-2251.2405	-95.79	-	-	-
$(2sa)(1sa^-)(3w)$	-2327.6219	-103.78	-	-	-
$(2sa)(1sa^-)(1a)(1w)$	-2231.3829	-102.94	-	-	-
$(2sa)(1sa^-)(1a)(2w)$	-2307.7666	-112.41	-	-	-

Table 3: List of extracted structures from five different studies. LF12 and F12 refer to the DF-LCCSD(T)-F12a/VDZ-F12 and CCSD(T)-F12a/VDZ-F12, respectively. The Ratio is calculated as F12/LF12.

Coupled Cluster Calculated Absolute- and Binding Energies

Geometries extracted from Reference:
Loukonen, V.; Kurtén, T.; Ortega, I. K.; Vehkamäki, H.; Pàdua, A. A. H.; Sellegri, K.; Kulmala, M. Atmos. Chem. Phys. 2010, 10, 4961-4974.

Cluster	E_{abs} L-F12	$E_{binding}$ L-F12	E_{abs} F12	$E_{binding}$ F12	Ratio
1dma	-134.9805		-134.9734		
1sa	-699.5992		-699.5739		
1w	-76.3683		-76.3627		
1a	-56.4990		-56.4956		
(1sa)(1w)	-775.9844	-10.58	-775.9552	-11.73	1.11
(1sa)(2w)	-852.3698	-21.32	-852.3358	-22.97	1.08
(1sa)(3w)	-928.7555	-32.24	-928.7187	-35.64	1.11
(1sa)(4w)	-1005.1407	-42.81	-1005.0982	-46.20	1.08
(1sa)(5w)	-1081.5223	-51.14	-1081.4743	-54.62	1.07
(1sa)(1a)	-756.1223	-15.07	-756.0947	-15.82	1.05
(1sa)(1a)(1w)	-832.5052	-24.25	-832.4741	-26.32	1.09
(1sa)(1a)(2w)	-908.8921	-35.87	-908.8562	-38.51	1.07
(1sa)(1a)(3w)	-985.2817	-49.23	-985.2412	-52.51	1.07
(1sa)(1a)(4w)	-1061.6631	-57.45	-1061.6195	-62.32	1.09
(1sa)(1a)(5w)	-1138.0500	-69.11	-1138.0018	-74.62	1.08
(1sa)(1dma)	-834.6130	-20.84	-834.5824	-22.05	1.06
(1sa)(1dma)(1w)	-911.0040	-35.09	-910.9692	-37.13	1.06
(1sa)(1dma)(2w)	-987.3860	-43.69	-987.3473	-46.85	1.07
(1sa)(1dma)(3w)	-1063.7710	-54.15	-1063.7280	-58.14	1.07
(1sa)(1dma)(4w)	-1140.1558	-64.50	-	-	-
(1sa)(1dma)(5w)	-1216.5344	-71.00	-	-	-
(2sa)	-1399.2251	-16.69	-	-	-
(2sa)(1w)	-1475.6117	-28.16	-	-	-
(2sa)(2w)	-1552.0013	-41.53	-	-	-
(2sa)(3w)	-1628.3859	-51.73	-	-	-
(2sa)(4w)	-1704.7719	-62.85	-	-	-
(2sa)(5w)	-1781.1610	-75.89	-	-	-
(2sa)(1a)	-1455.7635	-41.38	-	-	-
(2sa)(1a)(1w)	-1532.1505	-53.15	-	-	-
(2sa)(1a)(2w)	-1608.5308	-60.62	-	-	-
(2sa)(1a)(3w)	-1684.9217	-74.80	-	-	-
(2sa)(1a)(4w)	-1761.3037	-83.44	-	-	-
(2sa)(1a)(5w)	-1837.6883	-93.66	-	-	-
(2sa)(1dma)	-1534.2629	-52.65	-	-	-
(2sa)(1dma)(1w)	-1610.6462	-62.06	-	-	-
(2sa)(1dma)(2w)	-1687.0242	-68.14	-	-	-
(2sa)(1dma)(3w)	-1763.4179	-84.07	-	-	-
(2sa)(1dma)(4w)	-1839.8038	-95.09	-	-	-
(2sa)(1dma)(5w)	-1916.1856	-103.55	-	-	-

Table 4: List of extracted structures from five different studies. LF12 and F12 refer to the DF-LCCSD(T)-F12a/VDZ-F12 and CCSD(T)-F12a/VDZ-F12, respectively. The Ratio is calculated as F12/LF12.

Coupled Cluster Calculated Absolute- and Binding Energies

Geometries extracted from Reference:
Ortega, I. K.; Kupiainen, O.; Kurtén, T.; Olenius, T.; Wilkman, O.; McGrath, M. J.; Loukonen, V.; Vehkamäki, H. Atmos. Chem. Phys. 2012, 12, 225-235.

Cluster	E_{abs} L-F12	$E_{binding}$ L-F12	E_{abs} F12	$E_{binding}$ F12	Ratio
1a	-56.4998		-56.4963		
1sa	-699.6209		-699.5944		
1dma	-134.9833		-134.9762		
(1sa)(1a)	-756.1223	-0.99	-	-	-
(1sa)(2a)	-812.6659	-28.52	-812.6362	-30.90	1.08
(1sa)(3a)	-869.1845	-40.30	-869.1517	-42.91	1.06
(1sa)(4a)	-925.7006	-50.55	-925.6662	-54.37	1.08
(2sa)(1a)	-1455.8085	-41.94	-1455.7574	-45.37	1.08
(2sa)(2a)	-1512.3392	-61.35	-	-	-
(2sa)(3a)	-1568.8634	-76.66	-	-	-
(2sa)(4a)	-1625.3826	-88.86	-	-	-
(3sa)(1a)	-2155.4598	-60.97	-	-	-
(3sa)(2a)	-2211.9999	-86.28	-	-	-
(3sa)(3a)	-2268.5398	-111.48	-	-	-
(1sa)(1dma)	-834.6416	-23.43	-834.6094	-24.34	1.04
(1sa)(2dma)	-969.6467	-37.10	-969.6092	-39.18	1.06
(1sa)(3dma)	-1104.6531	-51.56	-	-	-
(2sa)(1dma)	-1534.3105	-53.54	-	-	-
(2sa)(2dma)	-1669.3357	-79.77	-	-	-
(3sa)(1dma)	-2233.9647	-74.37	-	-	-

Table 5: List of extracted structures from five different studies. LF12 and F12 refer to the DF-LCCSD(T)-F12a/VDZ-F12 and CCSD(T)-F12a/VDZ-F12, respectively. The Ratio is calculated as F12/LF12.

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Coupled Cluster Calculated Absolute- and Binding Energies

Geometries extracted from Reference:
Kupiainen, O.; Ortega, I. K.; Kurtén, T.; Vehkamäki, H. Atmos. Chem. Phys. 2012, 12, 3591-3599.

Cluster	E_{abs} L-F12	$E_{binding}$ L-F12	E_{abs} F12	$E_{binding}$ F12	Ratio
$1a^+$	-56.8377		-56.8342		
$1dma^+$	-135.3512		-135.3440		
1sa	-699.6209		-699.5944		
1a	-56.4998		-56.4963		
1dma	-134.9833		-134.9762		
$(1sa)(1a)^+$	-756.4906	-20.00	-756.4618	-20.83	1.04
$(1sa)(2a)^+$	-813.0442	-53.82	-813.0126	-55.04	1.02
$(1sa)(3a)^+$	-869.5723	-71.58	-869.5387	-73.72	1.03
$(1sa)(1dma)^+$	-835.0002	-17.58	-834.9680	-18.62	1.06
$(1sa)(1dma)(1a)^+$	-891.5487	-48.17	-891.5140	-49.81	1.03
$(1sa)(1dma)(2a)^+$	-948.0754	-65.05	-948.0389	-67.76	1.04
$(1sa)(2dma)^+$	-970.0512	-60.06	-	-	-
$(1sa)(2dma)(1a)^+$	-1026.5764	-76.03	-	-	-
$(2sa)(1a)^+$	-1456.1485	-43.21	-1456.0973	-46.60	1.08
$(2sa)(2a)^+$	-1512.7031	-77.63	-	-	-
$(2sa)(3a)^+$	-1569.2542	-109.80	-	-	-
$(2sa)(4a)^+$	-1625.7798	-126.02	-	-	-
$(2sa)(1dma)(1a)^+$	-1591.2072	-90.52	-	-	-
$(2sa)(1dma)(2a)^+$	-1647.7586	-122.88	-	-	-
$(2sa)(1dma)(3a)^+$	-1704.2794	-136.09	-	-	-
$(2sa)(1dma)^+$	-1534.6545	-38.53	-	-	-
$(2sa)(2dma)^+$	-1669.7111	-84.49	-	-	-
$(2sa)(2dma)(1a)^+$	-1726.2613	-116.15	-	-	-

Table 6: List of extracted structures from five different studies. LF12 and F12 refer to the DF-LCCSD(T)-F12a/VDZ-F12 and CCSD(T)-F12a/VDZ-F12, respectively. The Ratio is calculated as F12/LF12.

Best Estimate of Coupled Cluster Binding Energy

The best estimate of the binding energy is calculated from the average of the above 38 F12/L-F12 ratios:

	F12/LF12 ratios
1	1.05
2	1.10
3	1.09
4	1.10
5	1.13
6	1.10
7	1.07
8	1.07
9	1.08
10	1.07
11	1.11
12	1.08
13	1.11
14	1.08
15	1.07
16	1.05
17	1.09
18	1.07
19	1.07
20	1.08
21	1.08
22	1.06
23	1.06
24	1.07
25	1.07
26	1.08
27	1.06
28	1.08
29	1.08
30	1.04
31	1.06
32	1.04
33	1.02
34	1.03
35	1.06
36	1.03
37	1.04
38	1.08
Average	**1.07**

DFT Binding energies

Geometries extracted from Reference:
Herb, J.; Nadykto, A. B.; Yu, F. Chem. Phys. Lett. 2011, 518, 7-14.

Cluster	s*L-F12	M06-2X	PW91	CAM	PBE0	B3LYP	wB97XD	LC-PW91
(1sa)(1a)	-16.23	-17.50	-17.69	-16.73	-17.02	-14.98	-16.56	-20.15
(1sa)(1w)	-12.13	-13.97	-13.30	-13.25	-12.88	-11.37	-12.68	-15.86
(1sa)(2w)	-23.40	-26.53	-27.14	-26.24	-25.47	-22.93	-25.23	-30.67
(1sa)(3w)	-35.14	-40.00	-39.95	-39.02	-37.87	-33.82	-37.64	-45.98
(2sa)	-16.84	-19.17	-17.15	-18.60	-17.66	-15.76	-18.34	-22.28
(2sa)(2a)	-65.47	-64.38	-65.07	-64.47	-63.88	-57.53	-66.10	-75.16
(2sa)(3a)	-78.28	-78.92	-79.84	-78.07	-77.78	-69.24	-79.82	-92.38
(2sa)(1w)	-4.49	-9.88	-8.77	-9.61	-6.48	-6.72	-8.82	-9.58
(2sa)(2w)	-16.50	-21.27	-21.49	-22.21	-18.91	-18.44	-21.06	-22.72
(2sa)(3w)	-57.97	-65.44	-63.30	-62.37	-60.55	-53.40	-62.33	-74.37
(2sa)(1a)(1w)	-58.70	-60.39	-58.50	-59.86	-58.10	-52.87	-61.00	-68.85
(2sa)(1a)(2w)	-69.54	-73.13	-71.15	-71.96	-69.94	-63.15	-72.70	-83.61
(2sa)(1a)(3w)	-80.85	-85.59	-84.67	-84.66	-82.28	-74.40	-85.26	-98.09
(2sa)(2a)(1w)	-80.43	-78.84	-80.36	-79.77	-78.64	-71.77	-81.56	-90.62
(2sa)(2a)(2w)	-90.00	-89.79	-91.50	-90.66	-89.09	-80.89	-91.82	-103.86
(2sa)(2a)(3w)	-97.42	-99.15	-98.20	-97.22	-95.63	-85.78	-98.81	-112.80
(3sa)	-33.77	-39.22	-34.27	-36.72	-34.84	-30.57	-37.01	-44.61
(3sa)(1a)	-61.74	-64.32	-61.59	-64.25	-61.97	-56.09	-64.73	-74.60
(3sa)(2a)	-92.75	-90.91	-90.75	-92.25	-90.15	-82.53	-94.28	-105.01
(3sa)(3a)	-115.28	-111.30	-112.52	-113.34	-111.48	-101.98	-116.62	-128.73
(3sa)(1w)	-46.87	-54.38	-50.96	-52.55	-50.40	-43.91	-51.51	-64.30
(3sa)(2w)	-62.32	-69.94	-68.83	-68.52	-66.19	-57.89	-67.13	-83.51
(3sa)(1a)(1w)	-79.82	-81.96	-78.62	-81.35	-78.64	-72.09	-83.29	-91.99

Table 7: Binding Energies of the seven tested DFT functionals compared to the scaled DF-LCCSD(T)-F12a/VDZ-F12 (s*L-F12) results.

DFT Binding energies

Geometries extracted from Reference:
Herb, J.; Xu, Y.; Yu, F.; Nadykto, A. B. J. Phys. Chem. A 2013, 117, 133-152.

Cluster	s*L-F12	M06-2X	PW91	CAM	PBE0	B3LYP	wB97XD	LC-PW91
$(1sa^-)(1w)$	-15.75	-18.00	-15.98	-15.74	-15.68	-13.69	-16.06	-18.65
$(1sa)(1sa^-)$	-46.43	-48.72	-45.48	-46.31	-45.48	-42.80	-46.27	-51.25
$(1sa)(1sa^-)(1w)$	-57.28	-59.76	-55.33	-56.38	-55.16	-51.72	-56.63	-61.99
$(1sa)(1sa^-)(2w)$	-64.97	-69.44	-64.12	-64.11	-62.82	-58.02	-66.13	-70.85
$(1sa)(1sa^-)(1a)(1w)$	-67.13	-70.82	-66.45	-67.90	-66.91	-60.96	-68.11	-77.94
$(1sa)(1sa^-)(1a)(2w)$	-82.17	-83.57	-83.46	-83.02	-81.76	-74.91	-83.82	-93.74
$(1sa)(1sa^-)(1a)(3w)$	-96.17	-98.34	-97.27	-96.28	-94.65	-86.86	-98.59	-107.70
$(2sa)(1sa^-)$	-77.07	-81.59	-74.64	-78.41	-76.57	-70.64	-78.63	-89.59
$(2sa)(1sa^-)(1a)$	-98.32	-101.94	-95.80	-98.50	-96.76	-88.57	-100.84	-113.00
$(2sa)(1sa^-)(1w)$	-89.37	-95.00	-88.86	-91.35	-89.19	-82.22	-91.88	-103.85
$(2sa)(1sa^-)(2w)$	-102.64	-111.20	-104.03	-105.56	-103.45	-93.88	-105.93	-122.43
$(2sa)(1sa^-)(3w)$	-111.20	-119.82	-114.24	-114.95	-112.46	-102.02	-114.85	-132.92
$(2sa)(1sa^-)(1a)(1w)$	-110.30	-113.92	-107.11	-110.09	-107.62	-99.02	-113.16	-124.55
$(2sa)(1sa^-)(1a)(2w)$	-120.45	-124.56	-118.27	-120.76	-117.82	-108.42	-123.78	-136.27

Table 8: Binding Energies of the seven tested DFT functionals compared to the scaled DF-LCCSD(T)-F12a/VDZ-F12 (s*L-F12) results.

DFT Binding energies

Geometries extracted from Reference:
Loukonen, V.; Kurtén, T.; Ortega, I. K.; Vehkamäki, H.; Pàdua, A. A. H.; Sellegri, K.; Kulmala, M. Atmos. Chem. Phys. 2010, 10, 4961-4974.

Cluster	s*L-F12	M06-2X	PW91	CAM	PBE0	B3LYP	wB97XD	LC-PW91
(1sa)(1w)	-11.33	-13.26	-12.50	-12.70	-12.21	-10.42	-11.85	-16.05
(1sa)(2w)	-22.85	-26.03	-26.12	-25.98	-24.90	-22.11	-24.51	-31.35
(1sa)(3w)	-34.54	-40.39	-38.65	-38.66	-36.77	-32.41	-38.21	-46.40
(1sa)(4w)	-45.87	-53.53	-53.86	-50.68	-49.90	-42.60	-49.27	-63.13
(1sa)(5w)	-54.80	-61.22	-65.01	-62.56	-60.60	-53.60	-58.34	-75.51
(1sa)(1a)	-16.15	-17.26	-16.86	-16.27	-16.47	-14.27	-16.18	-19.88
(1sa)(1a)(1w)	-25.98	-29.45	-27.97	-27.25	-26.90	-22.93	-27.26	-33.85
(1sa)(1a)(2w)	-38.43	-39.37	-43.45	-40.99	-39.97	-35.88	-40.59	-48.08
(1sa)(1a)(3w)	-52.75	-54.47	-57.96	-56.49	-55.18	-49.34	-55.10	-66.62
(1sa)(1a)(4w)	-61.56	-66.05	-69.35	-66.93	-64.98	-57.72	-65.61	-79.79
(1sa)(1a)(5w)	-74.05	-77.34	-81.99	-79.09	-77.18	-69.18	-78.17	-91.71
(1sa)(1dma)	-22.33	-21.01	-21.56	-20.65	-20.31	-17.78	-21.54	-25.41
(1sa)(1dma)(1w)	-37.60	-37.57	-36.77	-36.70	-35.64	-31.93	-37.79	-43.48
(1sa)(1dma)(2w)	-46.82	-47.74	-48.11	-46.58	-44.85	-40.44	-48.35	-54.07
(1sa)(1dma)(3w)	-58.02	-60.65	-61.23	-60.44	-58.28	-52.15	-60.43	-71.62
(1sa)(1dma)(4w)	-69.11	-73.42	-71.18	-70.59	-67.80	-59.81	-72.01	-84.19
(1sa)(1dma)(5w)	-76.07	-85.21	-82.91	-80.50	-77.72	-67.23	-81.30	-99.01
(2sa)	-17.88	-20.36	-17.43	-19.65	-18.70	-16.23	-19.09	-24.53
(2sa)(1w)	-30.17	-35.94	-31.64	-33.91	-32.45	-27.70	-32.83	-42.92
(2sa)(2w)	-44.50	-51.47	-47.32	-48.60	-46.88	-40.11	-47.65	-61.09
(2sa)(3w)	-55.43	-62.60	-60.56	-61.18	-59.06	-51.53	-59.21	-74.99
(2sa)(4w)	-67.34	-76.20	-73.02	-73.63	-70.96	-61.58	-70.96	-90.95
(2sa)(5w)	-81.32	-91.32	-91.79	-89.23	-87.09	-75.77	-86.67	-108.86
(2sa)(1a)	-44.34	-46.94	-43.02	-44.87	-44.05	-38.18	-45.27	-55.52
(2sa)(1a)(1w)	-56.95	-59.24	-56.32	-58.28	-56.65	-50.20	-58.91	-69.68
(2sa)(1a)(2w)	-64.96	-67.77	-66.22	-67.42	-65.45	-58.07	-67.27	-80.24
(2sa)(1a)(3w)	-80.15	-87.75	-85.67	-83.88	-82.32	-71.42	-84.63	-102.38
(2sa)(1a)(4w)	-89.40	-94.81	-97.33	-94.68	-92.92	-81.85	-93.89	-113.00
(2sa)(1a)(5w)	-100.36	-108.88	-110.73	-107.13	-104.53	-91.80	-107.18	-128.18
(2sa)(1dma)	-56.42	-56.94	-51.45	-54.60	-52.79	-47.44	-56.46	-64.52
(2sa)(1dma)(1w)	-66.50	-69.36	-62.41	-64.34	-62.27	-55.32	-67.07	-76.34
(2sa)(1dma)(2w)	-73.01	-77.77	-71.85	-73.12	-70.46	-62.15	-75.16	-87.92
(2sa)(1dma)(3w)	-90.09	-96.25	-91.23	-90.44	-88.04	-77.39	-92.63	-108.73
(2sa)(1dma)(4w)	-101.89	-107.67	-106.04	-104.05	-101.51	-90.13	-106.41	-122.10
(2sa)(1dma)(5w)	-110.96	-117.78	-113.82	-113.04	-109.36	-97.13	-115.41	-132.27

Table 9: Binding Energies of the seven tested DFT functionals compared to the scaled DF-LCCSD(T)-F12a/VDZ-F12 (s*L-F12) results.

DFT Binding energies

Geometries extracted from Reference:
Ortega, I. K.; Kupiainen, O.; Kurtén, T.; Olenius, T.; Wilkman, O.; McGrath, M. J.; Loukonen, V.; Vehkamäki, H. Atmos. Chem. Phys. 2012, 12, 225-235.

Cluster	s*L-F12	M06-2X	PW91	CAM	PBE0	B3LYP	wB97XD	LC-PW91
(1sa)(1a)	-1.06	-2.40	-10.92	-2.22	-2.76	-3.73	-1.60	0.90
(1sa)(2a)	-30.56	-32.98	-32.59	-31.64	-31.74	-28.34	-31.82	-37.09
(1sa)(3a)	-43.19	-42.42	-45.22	-43.04	-43.19	-38.74	-44.90	-49.36
(1sa)(4a)	-54.17	-54.65	-57.16	-54.57	-54.62	-48.50	-56.62	-63.57
(2sa)(1a)	-44.94	-46.28	-44.01	-45.57	-44.36	-39.98	-46.35	-53.52
(2sa)(2a)	-65.74	-64.47	-64.25	-64.35	-63.26	-57.24	-66.28	-74.53
(2sa)(3a)	-82.15	-81.08	-79.89	-79.47	-78.36	-70.86	-82.92	-91.23
(2sa)(4a)	-95.21	-93.79	-93.74	-92.43	-91.49	-82.99	-96.91	-105.00
(3sa)(1a)	-65.33	-67.45	-62.41	-65.94	-63.37	-57.65	-67.07	-75.85
(3sa)(2a)	-92.44	-92.92	-88.93	-90.97	-88.80	-80.71	-94.57	-104.37
(3sa)(3a)	-119.45	-116.77	-112.55	-114.66	-112.29	-102.24	-119.59	-130.68
(1sa)(1dma)	-25.11	-22.69	-23.41	-23.63	-22.74	-21.08	-24.32	-27.29
(1sa)(2dma)	-39.75	-38.00	-37.90	-37.38	-36.58	-32.87	-39.47	-44.08
(1sa)(3dma)	-55.25	-54.29	-51.22	-50.10	-49.28	-43.67	-56.50	-58.42
(2sa)(1dma)	-57.37	-56.94	-52.73	-55.70	-53.35	-49.68	-57.82	-62.70
(2sa)(2dma)	-85.47	-79.55	-76.10	-78.50	-75.65	-71.18	-83.74	-85.80
(3sa)(1dma)	-79.68	-81.15	-72.95	-77.64	-74.09	-68.54	-81.84	-87.07

Table 10: Binding Energies of the seven tested DFT functionals compared to the scaled DF-LCCSD(T)-F12a/VDZ-F12 (s*L-F12) results.

DFT Binding energies

Geometries extracted from Reference:
Kupiainen, O.; Ortega, I. K.; Kurtén, T.; Vehkamäki, H. Atmos. Chem. Phys. 2012, 12, 3591-3599.

Cluster	s*L-F12	M06-2X	PW91	CAM	PBE0	B3LYP	wB97XD	LC-PW91
$(1sa)(1a)^+$	-21.43	-21.43	-21.45	-22.01	-21.53	-20.84	-21.63	-23.22
$(1sa)(2a)^+$	-57.66	-55.42	-55.92	-55.50	-55.29	-51.91	-55.63	-61.11
$(1sa)(3a)^+$	-76.70	-75.31	-77.23	-75.10	-75.42	-69.96	-75.04	-84.17
$(1sa)(1dma)^+$	-18.84	-18.56	-18.01	-18.27	-18.09	-16.92	-19.15	-19.62
$(1sa)(1dma)(1a)^+$	-51.62	-49.10	-49.32	-48.93	-48.75	-45.10	-50.13	-54.81
$(1sa)(1dma)(2a)^+$	-69.70	-67.90	-69.35	-67.48	-67.77	-62.07	-68.71	-76.73
$(1sa)(2dma)^+$	-64.36	-60.12	-59.58	-60.27	-58.86	-56.55	-61.94	-64.40
$(1sa)(2dma)(1a)^+$	-81.46	-78.23	-77.56	-76.98	-76.06	-71.22	-79.52	-85.04
$(2sa)(1a)^+$	-46.30	-48.69	-44.38	-47.37	-45.56	-42.86	-47.58	-51.68
$(2sa)(2a)^+$	-83.19	-82.25	-80.96	-82.57	-81.09	-76.23	-83.21	-90.64
$(2sa)(3a)^+$	-117.65	-113.81	-111.44	-112.28	-111.05	-103.86	-115.74	-123.04
$(2sa)(4a)^+$	-135.03	-132.60	-131.22	-130.46	-129.69	-120.48	-133.84	-144.59
$(2sa)(1dma)(1a)^+$	-97.00	-94.48	-91.35	-94.08	-91.55	-87.41	-96.03	-101.14
$(2sa)(1dma)(2a)^+$	-131.67	-125.74	-122.61	-124.23	-122.16	-115.61	-129.18	-133.94
$(2sa)(1dma)(3a)^+$	-145.83	-139.92	-139.79	-139.87	-137.89	-129.04	-143.59	-154.41
$(2sa)(1dma)^+$	-41.28	-43.09	-38.75	-41.53	-39.90	-36.95	-42.74	-46.00
$(2sa)(2dma)^+$	-90.53	-87.71	-83.91	-86.54	-84.11	-79.54	-89.90	-94.01
$(2sa)(2dma)(1a)^+$	-124.45	-117.97	-114.15	-115.79	-113.79	-106.70	-122.61	-125.94

Table 11: Binding Energies of the seven tested DFT functionals compared to the scaled DF-LCCSD(T)-F12a/VDZ-F12 (s*L-F12) results.