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Supporting Information for "Extensions and applications of the A24 data set of accurate interaction energies"

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Table 1: Single-point CCSDT(Q)/aug-cc-pVDZ correlation energies in the A24 data set (in atomic units)

	system	Dimer	Monomer A	Monomer B
1	water $\cdots$ ammonia	-0.457323932	-0.234060847	-0.221348787
2	water dimer	-0.468831905	-0.233753103	-0.233905720
3	HCN dimer	-0.638287213	-0.318831990	-0.319061836
4	HF dimer	-0.463033043	-0.231325562	-0.231365590
5	ammonia dimer	-0.443876811	-0.220962757	-0.220962757
6	HF $\cdots$ methane	-0.429570901	-0.196673725	-0.231390794
7	ammonia $\cdots$ methane	-0.418463634	-0.220947219	-0.196489756
8	water $\cdots$ methane	-0.430752511	-0.196455430	-0.233442073
9	formaldehyde dimer	-0.725982242	-0.362235975	-0.361985602
10	water $\cdots$ ethene	-0.563072718	-0.327404718	-0.233734470
11	formaldehyde $\cdots$ ethene	-0.690657711	-0.327128022	-0.361561079
12	ethyne dimer	-0.589243158	-0.294267936	-0.293786647
13	ammonia $\cdots$ ethene	-0.549837074	-0.327190412	-0.220885323
14	ethene dimer	-0.656877484	-0.327271549	-0.326792741
15	methane $\cdots$ ethene	-0.524607640	-0.326917670	-0.196469671
16	borane $\cdots$ methane	-0.322211253	-0.196745412	-0.121985128
17	methane $\cdots$ ethane	-0.560214873	-0.196682450	-0.361325642
18	methane $\cdots$ ethane	—	—	—
19	methane dimer	-0.394510404	-0.196543417	-0.196543417
20	Ar $\cdots$ methane	-0.366689662	-0.196356042	-0.169393043
21	Ar $\cdots$ ethene	-0.496784661	-0.326514437	-0.169291789
22	ethene $\cdots$ ethyne	-0.624262876	-0.326891373	-0.293701065
23	ethene dimer	-0.658210404	-0.326959446	-0.326959446
24	ethyne dimer	-0.590600277	-0.293652757	-0.293652757

Table 2: Single-point CCSDT(Q)/aug-cc-pVTZ correlation energies in a subset of the A24 data set (in atomic units)

	system	Dimer	Monomer A	Monomer B
2	water dimer	-0.598373504	-0.298367230	-0.298153066
4	HF dimer	-0.608225480	-0.303628018	-0.303672425
5	ammonia dimer	-0.559481770	-0.278499762	-0.278499762
19	methane dimer	-0.496874422	-0.247648158	-0.247648158

Table 3: Single-point fixed-node diffuse Monte Carlo energies and their respective statistical errors in a subset of the A24 data set (in atomic units)

			Dimer		Monomer A		Monomer B	
	system	Jastrow	energy	stat. err.	energy	stat. err.	energy	stat. err.
2	water dimer	3B	-34.531821790	2.909e-5	-17.261805340	2.084e-5	-17.261861870	2.097e-5
4	HF dimer	3B	-49.828061510	4.159e-5	-24.910306270	2.855e-5	-24.910296720	2.794e-5
4	HF dimer	3B pol.	-49.828133729	2.598e-5	-24.910323310	1.860e-5	-24.910400240	1.703e-5
5	ammonia dimer	3B	-23.530814260	3.469e-5	-11.762822850	1.835e-5	-11.762822850	1.835e-5
19	methane dimer	3B	-16.189631180	2.585e-5	-8.094385307	1.774e-5	-8.094385307	1.774e-5