Supplementary material. New basis sets for the evaluation of interaction energies: An *ab initio* study of the He–He, Ne–Ne, Ar–Ar, He–Ne, He–Ar and Ne–Ar van der Waals complex intermolecular potentials and ro-vibrational spectra

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TABLE I: He_2 interaction energies. Symbol n denotes the number of basis functions, R is the interatomic distance. Interaction energy values in cm^{-1}, interatomic distances in Å. See the text for basis set notation.

R	daV5Z-33221	ds-3321	apc2-33221
n	255	55	91
1.750	1255.69903	1286.01673	1268.18198
1.900	617.13066	635.33893	624.55979
2.000	376.64173	389.16379	381.85392
2.150	171.76853	178.40691	174.70099
2.250	97.25913	101.36603	99.16674
2.400	36.39188	38.16754	37.31624
2.500	15.56415	16.45305	16.10384
2.600	3.68090	4.02646	3.97791
2.700	-2.74846	-2.71892	-2.60196
2.750	-4.63954	-4.70949	-4.54521
2.800	-5.91589	-6.05702	-5.86278
2.850	-6.72525	-6.91536	-6.70477
2.900	-7.18319	-7.40529	-7.18858
2.950	-7.37990	-7.62097	-7.40558
2.955	-7.38806	-7.63043	-7.41552
2.960	-7.39441	-7.63796	-7.42353
2.965	-7.39891	-7.64362	-7.42970
2.970	-7.40172	-7.64744	-7.43415
2.975	-7.40286	-7.64952	-7.43685
2.980	-7.40240	-7.64992	-7.43789
2.985	-7.40033	-7.64871	-7.43736
2.990	-7.39682	-7.64586	-7.43525
3.000	-7.38541	-7.63563	-7.42663

3.005	-7.37762	-7.62835	-7.42015
3.010	-7.36855	-7.61972	-7.41236
3.015	-7.35817	-7.60969	-7.40325
3.020	-7.34661	-7.59843	-7.39285
3.025	-7.33385	-7.58586	-7.38122
3.030	-7.31996	-7.57214	-7.36844
3.040	-7.28886	-7.54121	-7.33945
3.050	-7.25372	-7.50601	-7.30624
3.075	-7.14978	-7.40108	-7.20654
3.100	-7.02633	-7.27558	-7.08637
3.125	-6.88694	-7.13334	-6.94940
3.150	-6.73491	-6.97771	-6.79893
3.175	-6.57291	-6.81157	-6.63770
3.200	-6.40339	-6.63748	-6.46825
3.225	-6.22840	-6.45760	-6.29260
3.250	-6.04971	-6.27384	-6.11268
3.275	-5.86882	-6.08770	-5.93003
3.300	-5.68707	-5.90066	-5.74598
3.325	-5.50554	-5.71376	-5.56179
3.350	-5.32520	-5.52806	-5.37836
3.375	-5.14672	-5.34434	-5.19659
3.400	-4.97082	-5.16325	-5.01721
3.425	-4.79804	-4.98539	-4.84075
3.450	-4.62881	-4.81115	-4.66772
3.475	-4.46339	-4.64094	-4.49857
3.500	-4.30212	-4.47496	-4.33355
3.550	-3.99279	-4.15665	-4.01687
3.600	-3.70175	-3.85713	-3.71893
3.650	-3.42933	-3.57673	-3.44029
3.700	-3.17536	-3.31527	-3.18091

3.750	-2.93942	-3.07218	-2.94030
3.800	-2.72078	-2.84672	-2.71775
3.900	-2.33179	-2.44484	-2.32334
4.000	-2.00077	-2.10180	-1.98949
4.250	-1.37701	-1.45022	-1.36636
4.500	-0.96365	-1.01244	-0.95954
5.000	-0.49821	-0.50892	-0.51019

TABLE II: Ne_2 interaction energies. See caption of Table I for details.

R	daV5Z-33221	fl-321	apc2-332
n	371	170	114
2.250	755.27857	788.99290	783.21692
2.300	571.72919	598.88918	594.12344
2.350	428.39424	450.12429	446.31705
2.450	230.30937	243.98297	241.75624
2.500	163.52736	174.32034	172.66697
2.650	43.56986	48.87689	48.16803
2.750	5.03310	8.27343	7.84108
2.755	3.65992	6.81673	6.39523
2.800	-6.87509	-4.40418	-4.73606
2.825	-11.48140	-9.34562	-9.63336
2.850	-15.33568	-13.50568	-13.75307
2.900	-21.15367	-19.85600	-20.03411
2.925	-23.27452	-22.20677	-22.35608
2.950	-24.95977	-24.09972	-24.22401
2.975	-26.26694	-25.59375	-25.69668
3.000	-27.24681	-26.74088	-26.82605
3.050	-28.39852	-28.17323	-28.23229
3.065	-28.56914	-28.41516	-28.46849
3.075	-28.64458	-28.53510	-28.58512
3.085	-28.69168	-28.62423	-28.67131
3.090	-28.70515	-28.65783	-28.70359
3.095	-28.71213	-28.68443	-28.72894
3.100	-28.71297	-28.70425	-28.74756
3.105	-28.70768	-28.71749	-28.75971
3.110	-28.69662	-28.72440	-28.76553

3.115	-28.67991	-28.72508	-28.76529
3.120	-28.65772	-28.71979	-28.75914
3.125	-28.63031	-28.70873	-28.74727
3.130	-28.59781	-28.69209	-28.72984
3.140	-28.51823	-28.64271	-28.67912
3.150	-28.42030	-28.57309	-28.60839
3.165	-28.24180	-28.43355	-28.46759
3.175	-28.10344	-28.31892	-28.35235
3.190	-27.86968	-28.11755	-28.15036
3.210	-27.51426	-27.79971	-27.83226
3.230	-27.11578	-27.43281	-27.46556
3.250	-26.68092	-27.02404	-27.05740
3.275	-26.09534	-26.46394	-26.49860
3.300	-25.47255	-25.85955	-25.89594
3.325	-24.82166	-25.22075	-25.25918
3.350	-24.15026	-24.55598	-24.59674
3.375	-23.46502	-23.87265	-23.91595
3.400	-22.77163	-23.17711	-23.22316
3.450	-21.37898	-21.77092	-21.82267
3.500	-20.00292	-20.37280	-20.43030
3.575	-18.01498	-18.34498	-18.40999
3.650	-16.15616	-16.44730	-16.51694
3.750	-13.91436	-14.16487	-14.23482
3.850	-11.95272	-12.17757	-12.24284
4.000	-9.50527	-9.70754	-9.76743
4.150	-7.57337	-7.75338	-7.82374
4.300	-6.05919	-6.21155	-6.30902
4.500	-4.53810	-4.65578	-4.79633
4.750	-3.21396	-3.29767	-3.47457
5.000	-2.31552	-2.37869	-2.55993

5.250	-1.69893	-1.74621	-1.90190
5.500	-1.26624	-1.30282	-1.41570
6.000	-0.73458	-0.75438	-0.78998
6.500	-0.44606	-0.45771	-0.46145
7.000	-0.28187	-0.29085	-0.28835

TABLE III: Ar_2 interaction energies. See caption of Table I for details.

R	daV5Z-33221	fl-3321	apc2-33211
n	379	203	138
3.000	669.35366	703.55422	708.60312
3.150	267.74151	287.87072	289.50334
3.250	112.98833	126.72913	127.11591
3.300	58.50680	69.71346	69.70001
3.350	15.73969	24.77294	24.46923
3.400	-17.43136	-10.25853	-10.76881
3.450	-42.77144	-37.18611	-37.84190
3.500	-61.74842	-57.51151	-58.26926
3.550	-75.57978	-72.48038	-73.31047
3.600	-85.27250	-83.12518	-84.00708
3.650	-91.65737	-90.29864	-91.21807
3.700	-95.41741	-94.70425	-95.65077
3.750	-97.11281	-96.92015	-97.88661
3.755	-97.18721	-97.04036	-98.00857
3.760	-97.24607	-97.14393	-98.11378
3.765	-97.28968	-97.23126	-98.20267
3.770	-97.31847	-97.30274	-98.27576
3.775	-97.33296	-97.35884	-98.33328
3.780	-97.33327	-97.39977	-98.37577
3.785	-97.32001	-97.42613	-98.40360
3.790	-97.29339	-97.43813	-98.41705
3.795	-97.25380	-97.43627	-98.41653
3.800	-97.20158	-97.42082	-98.40248
3.805	-97.13719	-97.39215	-98.37516
3.810	-97.06075	-97.35067	-98.33493

3.820	-96.87331	-97.23036	-98.21720
3.830	-96.64203	-97.06257	-98.05189
3.840	-96.36918	-96.84981	-97.84153
3.850	-96.05711	-96.59449	-97.58865
3.860	-95.70795	-96.29899	-97.29543
3.870	-95.32389	-95.96546	-96.96422
3.880	-94.90713	-95.59595	-96.59717
3.890	-94.45927	-95.19278	-96.19628
3.900	-93.98248	-94.75773	-95.76352
3.910	-93.47839	-94.29273	-95.30089
3.925	-92.67498	-93.54296	-94.55470
3.950	-91.22287	-92.16820	-93.18592
3.975	-89.64957	-90.65790	-91.68193
4.000	-87.97566	-89.03427	-90.06471
4.050	-84.39857	-85.52393	-86.56744
4.075	-82.52652	-83.67084	-84.72061
4.100	-80.61674	-81.77184	-82.82733
4.150	-76.72873	-77.88485	-78.94937
4.200	-72.81135	-73.94717	-75.01542
4.250	-68.92362	-70.02397	-71.08867
4.300	-65.11038	-66.16502	-67.21724
4.350	-61.40448	-62.40741	-63.43730
4.400	-57.83023	-58.77774	-59.77523
4.450	-54.40302	-55.29428	-56.25001
4.500	-51.13353	-51.96878	-52.87442
5.000	-27.06190	-27.44833	-27.73187
5.250	-19.79415	-20.05656	-20.12690
5.500	-14.53330	-14.82466	-14.77415
5.750	-10.88945	-11.10243	-11.00483
6.000	-8.29645	-8.42276	-8.32428

6.500	-4.93539	-5.02182	-4.96449
7.000	-3.09306	-3.12495	-3.09745
7.500	-1.99829	-2.02015	-2.00538
8.000	-1.33188	-1.34817	-1.33972
9.000	-0.63951	-0.64789	-0.64438

TABLE IV: HeNe interaction energies. See caption of Table I for details.

R	daV5Z-33221	fs-331	apc2-3321
n	313	102	98
2.000	946.76033	982.39346	969.74356
2.150	439.22211	459.98968	452.17010
2.250	253.85717	268.10360	262.68991
2.350	139.94466	149.44978	145.95752
2.450	71.10188	77.14568	75.18108
2.500	48.03292	52.72667	51.38656
2.550	30.43692	33.99860	33.18902
2.600	17.13706	19.76347	19.38960
2.650	7.19798	9.06621	9.03467
2.700	-0.12244	1.14500	1.36724
2.750	-5.41174	-4.60789	-4.21227
2.800	-9.13394	-8.67726	-8.17738
2.850	-11.65470	-11.44894	-10.90124
2.875	-12.55689	-12.44656	-11.89195
2.900	-13.26125	-13.22932	-12.67692
2.925	-13.79411	-13.82558	-13.28304
2.950	-14.17863	-14.26047	-13.73406
2.975	-14.43542	-14.55626	-14.05088
3.000	-14.58240	-14.73259	-14.25205
3.005	-14.60009	-14.75506	-14.27988
3.010	-14.61414	-14.77358	-14.30386
3.015	-14.62469	-14.78831	-14.32410
3.020	-14.63182	-14.79933	-14.34074
3.025	-14.63564	-14.80675	-14.35386
3.030	-14.63628	-14.81067	-14.36360

3.035	-14.63387	-14.81129	-14.37004
3.040	-14.62847	-14.80861	-14.37333
3.045	-14.62013	-14.80284	-14.37350
3.050	-14.60909	-14.79397	-14.37069
3.075	-14.51500	-14.70779	-14.31521
3.100	-14.36422	-14.55990	-14.19852
3.125	-14.16612	-14.36069	-14.03040
3.150	-13.92902	-14.11922	-13.81946
3.175	-13.66010	-13.84345	-13.57328
3.200	-13.36563	-13.54031	-13.29832
3.225	-13.05106	-13.21591	-13.00040
3.250	-12.72108	-12.87555	-12.68449
3.275	-12.37980	-12.52368	-12.35497
3.300	-12.03070	-12.16443	-12.01560
3.325	-11.67686	-11.80100	-11.66964
3.350	-11.32081	-11.43630	-11.32160
3.375	-10.96471	-11.07278	-10.96877
3.400	-10.61048	-10.71238	-10.61825
3.425	-10.25963	-10.35672	-10.27018
3.450	-9.91347	-10.00708	-9.92594
3.475	-9.57307	-9.66452	-9.58674
3.500	-9.23929	-9.32978	-9.25358
3.550	-8.59432	-8.68599	-8.60854
3.600	-7.98251	-8.07844	-7.99553
3.650	-7.40595	-7.50812	-7.41717
3.750	-6.36108	-6.47760	-6.36830
3.850	-5.45634	-5.58618	-5.46031
4.000	-4.33642	-4.48277	-4.33827
4.150	-3.45712	-3.61806	-3.45975
4.300	-2.76975	-2.94366	-2.77455

4.500	-2.08018	-2.26529	-2.08712
4.750	-1.47801	-1.66397	-1.48332
5.000	-1.06904	-1.24598	-1.07062
5.250	-0.78631	-0.94991	-0.78629
5.500	-0.58740	-0.73377	-0.58824

TABLE V: HeAr interaction energies. See caption of Table I for details.

R	daV5Z-33221	ds-3321	apc2-33211
n	317	92	111
2.250	1771.89612	1861.35988	1822.78840
2.375	1036.90793	1097.37541	1071.58525
2.500	590.64442	630.83360	613.90403
2.625	323.49257	349.67069	338.81938
2.750	166.32979	182.95177	176.24199
2.875	75.95525	86.16190	82.22534
3.000	25.61493	31.60046	29.45453
3.100	2.90045	6.62607	5.40028
3.200	-10.11971	-7.94233	-8.57217
3.250	-14.14960	-12.54214	-12.96412
3.275	-15.69542	-14.33095	-14.66681
3.300	-16.97496	-15.82838	-16.08854
3.325	-18.01856	-17.06692	-17.26082
3.350	-18.85359	-18.07586	-18.21185
3.375	-19.50464	-18.88151	-18.96715
3.400	-19.99374	-19.50763	-19.54964
3.425	-20.34069	-19.97551	-19.97992
3.450	-20.56321	-20.30430	-20.27647
3.475	-20.67708	-20.51118	-20.45587
3.480	-20.68805	-20.53931	-20.47900
3.485	-20.69545	-20.56332	-20.49821
3.490	-20.69922	-20.58327	-20.51355
3.495	-20.69953	-20.59934	-20.52511
3.500	-20.69650	-20.61156	-20.53301
3.505	-20.69018	-20.62008	-20.53738

3.510	-20.68070	-20.62506	-20.53830
3.515	-20.66810	-20.62649	-20.53580
3.520	-20.65258	-20.62454	-20.53014
3.525	-20.63417	-20.61929	-20.52123
3.550	-20.50130	-20.54669	-20.43247
3.575	-20.30810	-20.40478	-20.27739
3.600	-20.06340	-20.20352	-20.06549
3.625	-19.77523	-19.95163	-19.80530
3.650	-19.45065	-19.65694	-19.50436
3.675	-19.09592	-19.32648	-19.16938
3.700	-18.71651	-18.96638	-18.80636
3.725	-18.31744	-18.58208	-18.42057
3.750	-17.90294	-18.17849	-18.01665
3.775	-17.47676	-17.75980	-17.59879
3.800	-17.04227	-17.32983	-17.17049
3.825	-16.60236	-16.89182	-16.73496
3.850	-16.15961	-16.44866	-16.29498
3.875	-15.71612	-16.00284	-15.85294
3.900	-15.27385	-15.55658	-15.41092
3.925	-14.83440	-15.11168	-14.97072
3.950	-14.39918	-14.66979	-14.53390
3.975	-13.96941	-14.23229	-14.10171
4.000	-13.54602	-13.80037	-13.67538
4.050	-12.72172	-12.95688	-12.84359
4.100	-11.93123	-12.14537	-12.04433
4.150	-11.17782	-11.36969	-11.28133
4.250	-9.78846	-9.93412	-9.87186
4.350	-8.55648	-8.65615	-8.62079
4.500	-6.98665	-7.02220	-7.02718
4.650	-5.71174	-5.69352	-5.73553

4.800	-4.68333	-4.62514	-4.69643
5.000	-3.61729	-3.52970	-3.62241
5.500	-1.96996	-1.89470	-1.97099
6.000	-1.13328	-1.09094	-1.13633
6.500	-0.68434	-0.65695	-0.68702

TABLE VI: NeAr interaction energies. See caption of Table I for details.

R	daV5Z-33221	ds-3321	apc2-3321
n	375	120	125
2.500	1376.60701	1469.25092	1437.07223
2.600	850.12447	915.28357	892.07184
2.750	384.27657	422.04339	407.82600
2.875	175.51204	199.11153	189.66752
3.000	59.97912	74.40350	68.23473
3.100	8.13560	17.56462	13.31722
3.200	-21.44680	-15.59736	-18.37310
3.250	-30.57170	-26.10791	-28.28681
3.275	-34.06591	-30.21068	-32.12182
3.300	-36.95536	-33.65687	-35.31957
3.325	-39.30925	-36.51988	-37.95228
3.350	-41.19078	-38.86547	-40.08500
3.375	-42.65597	-40.75280	-41.77610
3.400	-43.75534	-42.23486	-43.07771
3.425	-44.53406	-43.35928	-44.03684
3.450	-45.03242	-44.16868	-44.69553
3.475	-45.28637	-44.70132	-45.09135
3.480	-45.31093	-44.77770	-45.14198
3.485	-45.32711	-44.84466	-45.18372
3.490	-45.33534	-44.90242	-45.21684
3.495	-45.33575	-44.95124	-45.24151
3.500	-45.32856	-44.99140	-45.25804
3.505	-45.31392	-45.02303	-45.26658
3.510	-45.29252	-45.04647	-45.26741
3.515	-45.26405	-45.06189	-45.26074

3.520	-45.22894	-45.06951	-45.24678
3.525	-45.18724	-45.06955	-45.22573
3.550	-44.88807	-44.96320	-45.02140
3.575	-44.45424	-44.69689	-44.66914
3.600	-43.90550	-44.29246	-44.19038
3.625	-43.25981	-43.76954	-43.60432
3.650	-42.53368	-43.14555	-42.92788
3.675	-41.74056	-42.43606	-42.17624
3.700	-40.89317	-41.65499	-41.36280
3.725	-40.00250	-40.81480	-40.49939
3.750	-39.07792	-39.92645	-39.59652
3.775	-38.12845	-38.99981	-38.66335
3.800	-37.16109	-38.04362	-37.70791
3.825	-36.18239	-37.06571	-36.73738
3.850	-35.19800	-36.07294	-35.75784
3.875	-34.21287	-35.07143	-34.77466
3.900	-33.23092	-34.06668	-33.79244
3.925	-32.25641	-33.06344	-32.81512
3.950	-31.29179	-32.06588	-31.84610
3.975	-30.33978	-31.07765	-30.88829
4.000	-29.40288	-30.10202	-29.94407
4.050	-27.58105	-28.19880	-28.10419
4.100	-25.83647	-26.37337	-26.33858
4.150	-24.17656	-24.63726	-24.65499
4.200	-22.60472	-22.99734	-23.05772
4.250	-21.12230	-21.45685	-21.54872
4.300	-19.72877	-20.01584	-20.12786
4.350	-18.42228	-18.67216	-18.79383
4.500	-14.99409	-15.18189	-15.28531
4.650	-12.22406	-12.38662	-12.44162

4.800	-9.99562	-10.13896	-10.15595
5.000	-7.70887	-7.79271	-7.80050
5.500	-4.16234	-4.13003	-4.20513
6.000	-2.38518	-2.33420	-2.40786
6.500	-1.43466	-1.41166	-1.45479