Supplementary Material (ESI) for Physical Chemistry Chemical Physics

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Quantifying the Anisotropy of Intermolecular Potential Energy Surfaces: a Critical Assessment of Available N_2-N_2 Potentials

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TABLE S1. Isotropic component of interaction energy (in cm^{-1}) obtained from available analytical N_2-N_2 potentials[1-6].

R/au	AWJ	AWJ-scaled	CVPHD	ABCCP	KMS	GBCBCP	CPBGB
4.5	27013.2	26864.0	28448.8	19264.2	29742.2	16617.2	30957.5
4.75	17216.3	16561.0	17514.2	12119.4	17852.2	11049.2	16934.0
5	10845.7	10067.4	10637.5	7551.5	10639.6	7201.2	9341.6
5.5	4129.1	3523.2	3723.1	2805.1	3654.2	2841.8	2831.1
6	1450.0	1093.4	1160.9	933.1	1151.4	975.1	786.4
6.5	433.3	248.9	270.3	229.8	287.9	242.4	146.3
7	75.3	-12.7	-6.9	-10.2	12.2	-11.4	-38.6
7.5	-34.0	-73.5	-72.9	-74.2	-60.2	-78.5	-77.1
8	-55.7	-72.7	-73.5	-76.8	-67.1	-80.8	-72.1
8.5	-50.6	-57.6	-58.7	-62.1	-56.3	-65.6	-57.4
9	-39.7	-42.5	-43.5	-46.0	-43.3	-48.9	-43.1
10	-21.7	-22.1	-22.8	-27.6	-23.9	-25.5	-23.3
12	-6.7	-6.7	-7.0	-7.2	-7.7	-7.6	-7.3

TABLE S2. Angular spreadness of interaction energy (in cm^{-1}) obtained from available analytical N_2-N_2 potentials[1-6].

R	AWJ	AWJ-scaled	CVPHD	ABCCP	KMS	GBCBCP	CPBGB
4.5	24350.5	24405.3	25574.3	14942.8	32797.4	13726.4	10880.7
4.75	15728.5	15316.4	16016.4	9086.9	19848.7	9285.7	6264.3
5	10094.1	9542.2	9957.7	5530.0	11999.8	6295.3	3676.2
5.5	4075.9	3618.1	3760.3	2050.6	4366.1	2808.0	1322.1
6	1598.9	1323.5	1370.1	759.4	1573.3	1186.8	493.6
6.5	605.8	462.2	476.6	279.3	557.9	468.4	187.6
7	219.5	151.4	155.5	101.2	193.1	169.6	72.4
7.5	75.1	46.1	47.1	36.2	65.9	55.6	30.4
8	24.9	16.3	16.4	14.0	25.3	20.4	16.6
8.5	10.7	10.7	10.7	7.7	14.7	14.0	11.9
9	7.5	8.4	8.4	5.9	11.0	11.4	9.2
10	4.5	4.7	4.7	3.8	6.5	6.5	5.5
12	1.5	1.5	1.5	1.5	2.4	2.0	2.1

TABLE S3. Angular skewness of interaction energy obtained from available analytical N_2-N_2 potentials[1-6].

R	AWJ	AWJ-scaled	CVPHD	ABCCP	KMS	GBCBCP	CPBGB
4.5	2.50	2.48	2.48	1.56	3.04	4.62	1.07
4.75	2.48	2.48	2.47	1.56	3.02	3.63	1.11
5	2.48	2.48	2.48	1.56	3.01	3.04	1.15
5.5	2.50	2.53	2.52	1.57	3.00	2.62	1.29
6	2.57	2.64	2.63	1.61	3.04	2.67	1.51
6.5	2.71	2.86	2.85	1.71	3.18	2.93	1.86
7	2.99	3.32	3.29	1.92	3.47	3.42	2.29
7.5	3.49	3.98	3.97	2.24	3.78	4.03	2.19
8	3.84	2.27	2.33	2.03	2.61	2.00	0.86
8.5	1.46	-0.02	-0.01	0.48	0.32	-0.15	0.08
9	-0.07	-0.15	-0.15	-0.07	-0.15	-0.19	-0.05
10	-0.16	-0.15	-0.15	-0.07	-0.18	-0.19	-0.06
12	-0.18	-0.18	-0.18	-0.07	-0.19	-0.18	-0.08

TABLE S4. Angular peakedness of interaction energy obtained from available analytical N_2-N_2 potentials[1-6].

R	AWJ	AWJ-scaled	CVPHD	ABCCP	KMS	GBCBCP	CPBGB
4.5	11.03	10.91	10.86	5.22	14.78	42.08	3.94
4.75	10.89	10.83	10.78	5.22	14.62	26.92	4.06
5	10.82	10.83	10.78	5.23	14.49	18.52	4.21
5.5	10.89	11.06	11.00	5.29	14.38	12.47	4.64
6	11.27	11.71	11.63	5.44	14.62	12.08	5.39
6.5	12.13	13.13	13.02	5.79	15.51	13.61	6.70
7	13.91	16.27	16.09	6.59	17.56	17.07	8.71
7.5	17.52	22.09	21.94	8.14	20.41	22.81	9.08
8	21.56	13.60	13.98	8.48	14.79	12.48	4.41
8.5	8.87	2.22	2.23	3.73	3.46	2.05	2.10
9	2.12	1.93	1.93	2.05	1.93	1.96	1.86
10	1.91	1.92	1.92	1.90	1.88	1.92	1.87
12	1.87	1.87	1.87	1.88	1.87	1.89	1.86

TABLE S5. Isotropic component of interaction energy (in cm^{-1}) of N_2-N_2 at different levels of *ab initio* calculations.

R/au	MP2			CCSD(T)		
	aDZ	**aTZ**	**aTZ+b**	**aDZ**	**aTZ**	**aTZ+b**
4.50	19112.6	17991.3	17825.9	19634.6	18493.8	
4.75	12951.0	12123.1		13431.6		
5.00	8513.1	7913.6	7805.1	8905.2	8294.9	
5.50	3397.9	3101.4	3029.9	3626.2		
6.00	1197.9	1057.7	1012.1	1326.9	1181.8	
6.50	333.1	265.8		407.4		
7.00	28.1	-6.3	-22.3	72.6	36.9	
7.50	-59.9	-79.1	-88.2	-32.0	-51.7	-61.1
8.00	-71.9	-83.2	-88.4	-53.6	-65.0	-70.5
8.50	-61.6	-68.4	-71.5	-49.2	-55.8	-59.1
9.00	-47.7	-51.8		-39.0	-42.8	
10.00	-26.4	-27.8	-28.5	-21.7		
12.00	-8.4	-8.7		-6.8	-7.0	

TABLE S6. Angular spreadness of interaction energy (in cm^{-1}) of N_2-N_2 at different levels of *ab initio* calculations.

R/au	MP2			CCSD(T)		
	aDZ	**aTZ**	**aTZ+b**	**aDZ**	**aTZ**	**aTZ+b**
4.50	12798.2	12352.3	12316.3	12693.1	12209.9	
4.75	9919.6	9566.4		9993.1		
5.00	7124.6	6846.5	6827.3	7233.5	6938.3	
5.50	3280.2	3124.1	3111.9	3346.5		
6.00	1383.3	1308.1	1298.9	1416.4	1332.4	
6.50	546.0	513.8		562.1		
7.00	201.6	189.2	185.8	209.5	194.2	
7.50	69.8	65.7	64.0	73.5	67.8	65.8
8.00	25.4	24.7	24.4	26.4	24.8	24.3
8.50	14.2	14.7	15.0	13.4	13.7	14.0
9.00	10.8	11.4		9.8	10.3	
10.00	6.4	6.6	6.8	5.7		
12.00	2.2	2.3		2.0	2.0	

TABLE S7. Angular skewness of interaction energy of N_2-N_2 at different levels of *ab initio* calculations.

R/au	MP2			CCSD(T)		
	aDZ	**aTZ**	**aTZ+b**	**aDZ**	**aTZ**	**aTZ+b**
4.50	1.66	1.67	1.68	1.59	1.61	
4.75	2.17	2.22		2.14		
5.00	2.36	2.42	2.42	2.34	2.41	
5.50	2.52	2.58	2.59	2.48		
6.00	2.66	2.72	2.73	2.61	2.67	
6.50	2.88	2.94		2.80		
7.00	3.27	3.32	3.37	3.14	3.21	
7.50	3.78	3.80	3.83	3.62	3.68	3.73
8.00	2.99	2.62	2.37	3.27	2.93	2.69
8.50	0.31	0.13	0.04	0.72	0.34	0.18
9.00	-0.17	-0.17		-0.14	-0.17	
10.00	-0.15	-0.15	-0.14	-0.18		
12.00	-0.17	-0.17		-0.18	-0.19	

TABLE S8. Angular peakedness of interaction energy of N_2-N_2 at different levels of *ab initio* calculations.

R/au	MP2			CCSD(T)		
	aDZ	**aTZ**	**aTZ+b**	**aDZ**	**aTZ**	**aTZ+b**
4.50	6.41	6.48	6.49	6.10	6.17	
4.75	9.63	9.92		9.48		
5.00	10.64	11.03	11.06	10.53	10.97	
5.50	11.29	11.74	11.78	11.06		
6.00	11.97	12.41	12.50	11.63	12.09	
6.50	13.30	13.73		12.77		
7.00	15.87	16.32	16.68	14.95	15.48	
7.50	20.09	20.35	20.75	18.61	19.21	19.73
8.00	17.26	15.09	13.81	18.21	16.47	15.31
8.50	3.53	2.80	2.50	5.14	3.56	2.97
9.00	1.92	1.90		1.99	1.90	
10.00	1.90	1.90	1.89	1.88		
12.00	1.86	1.86		1.85	1.85	

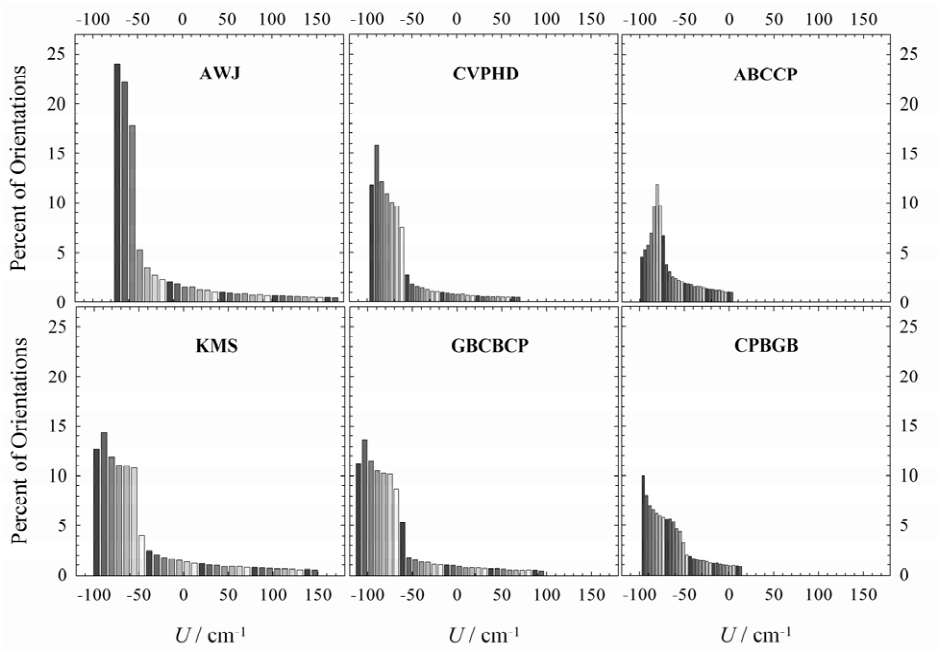

Figure S1. Distribution of interaction energy over a uniform random sample of angular space for analytical N_2-N_2 potentials[1-6] at $R = 8$ au.

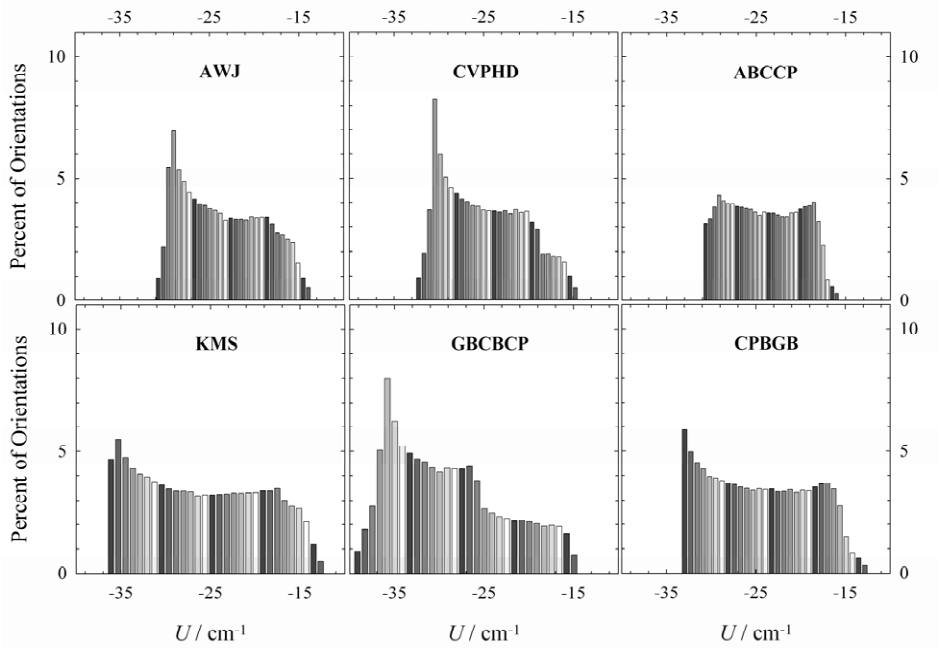

Figure S2. Distribution of interaction energy over a uniform random sample of angular space for analytical N_2-N_2 potentials[1-6] at $R = 8$ au.

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