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POTENTIAL ENERGY CURVE OF N_2 REVISITED. Supplementary Material (4 tables).

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Description

56-reference RMR-CCSD and RMR-CCSD(T) potentials for N_2 obtained with cc-pVDZ, cc-pVTZ and cc-pVQZ basis sets, vibrational energies of the bound states of the N_2 isotopomers obtained using the morphed (r_{12})-MR-ACPF potential energy curve, and the tables of the parameters of the morphed RMR-CCSD and RMR-CCSD(T) potential curves.

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Table A-1. Ab initio PECs for N_2 as obtained with 56-reference RMRCCSD and RMRCCSD(T) and cc-pVDZ, cc-pVTZ and cc-pVQZ basis sets (1.45 a.u. $\leq R \leq$ 2 a.u.).

	RMR-CCSD			RMR-CCSD(T)		
R	cc-pVDZ	cc-pVTZ	cc-pVQZ	cc-pVDZ	cc-pVTZ	cc-pVQZ
1.4500	-108.4500398	-108.6378082	-108.6838996	-108.4528154	-108.6447544	-108.6928172
1.4585	-108.4814986	-108.6666423	-108.7121601	-108.4842860	-108.6736106	-108.7211025
1.4670	-108.5119855	-108.6945557	-108.7395175	-108.5147847	-108.7015460	-108.7484845
1.4755	-108.5415269	-108.7215740	-108.7659968	-108.5443378	-108.7285862	-108.7749880
1.4840	-108.5701481	-108.7477220	-108.7916224	-108.5729708	-108.7547559	-108.8006375
1.4925	-108.5978740	-108.7730237	-108.8164177	-108.6007085	-108.7800792	-108.8254563
1.5000	-108.6216138	-108.7946646	-108.8376248	-108.6244588	-108.8017391	-108.8466840
1.5165	-108.6715330	-108.8400968	-108.8821435	-108.6744008	-108.8472127	-108.8912469
1.5330	-108.7184124	-108.8826646	-108.9238514	-108.7213031	-108.8898217	-108.9329980
1.5495	-108.7624086	-108.9225204	-108.9628976	-108.7653222	-108.9297182	-108.9720862
1.5660	-108.8036701	-108.9598084	-108.9994232	-108.8066068	-108.9670467	-109.0086527
1.5825	-108.8423379	-108.9946653	-109.0335620	-108.8452977	-109.0019438	-109.0428314
1.6000	-108.8806636	-109.0291223	-109.0673027	-108.8836481	-109.0364434	-109.0766135
1.6165	-108.9144002	-109.0595421	-109.0969153	-108.9174081	-109.0667312	-109.1062643
1.6330	-108.9459308	-109.0877518	-109.1245083	-108.9489622	-109.0949622	-109.1338949
1.6495	-108.9753693	-109.1140161	-109.1501894	-108.9784244	-109.1212471	-109.1596128
1.6660	-109.0028237	-109.1384391	-109.1740604	-109.0059027	-109.1456901	-109.1835202
1.6825	-109.0283968	-109.1611195	-109.1962180	-109.0315000	-109.1683898	-109.2057138
1.7000	-109.0535729	-109.1833744	-109.2179483	-109.0567020	-109.1906648	-109.2274818
1.7170	-109.0762133	-109.2033175	-109.2374089	-109.0793678	-109.2106267	-109.2469791
1.7340	-109.0971608	-109.2217012	-109.2553355	-109.1003410	-109.2290291	-109.2649421
1.7500	-109.1154114	-109.2376569	-109.2708824	-109.1186161	-109.2450020	-109.2805234
1.7670	-109.1333291	-109.2532571	-109.2860697	-109.1365601	-109.2606205	-109.2957474
1.7840	-109.1498094	-109.2675400	-109.2999605	-109.1530670	-109.2749218	-109.3096751
1.8000	-109.1640776	-109.2798456	-109.3119146	-109.1673605	-109.2872448	-109.3216643
1.8170	-109.1779882	-109.2917784	-109.3234920	-109.1812984	-109.2991967	-109.3332795
1.8340	-109.1906812	-109.3026000	-109.3339752	-109.1940189	-109.3100378	-109.3438010
1.8500	-109.2015758	-109.3118260	-109.3428981	-109.2049398	-109.3192831	-109.3527605
1.8670	-109.2120950	-109.3206665	-109.3514315	-109.2154871	-109.3281452	-109.3613336
1.8840	-109.2215858	-109.3285709	-109.3590439	-109.2250062	-109.3360728	-109.3689864
1.9000	-109.2296308	-109.3352031	-109.3654145	-109.2330781	-109.3427285	-109.3753959
1.9170	-109.2372885	-109.3414404	-109.3713875	-109.2407646	-109.3489931	-109.3814110
1.9340	-109.2440805	-109.3468906	-109.3765872	-109.2475856	-109.3544735	-109.3866539
1.9500	-109.2497270	-109.3513420	-109.3808153	-109.2532595	-109.3589566	-109.3909236
1.9670	-109.2549792	-109.3553917	-109.3846410	-109.2585409	-109.3630444	-109.3947946
1.9840	-109.2595060	-109.3587808	-109.3878200	-109.2630968	-109.3664767	-109.3980200
2.0000	-109.2631422	-109.3608654	-109.3902558	-109.2667604	-109.3692383	-109.4005005

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Table A-1. (Continued) (2.01 a.u. $\leq R \leq$ 2.875 a.u.)

	RMR-CCSD			RMR-CCSD(T)		
R	cc-pVDZ	cc-pVTZ	cc-pVQZ	cc-pVDZ	cc-pVTZ	cc-pVQZ
2.0100	-109.2651231	-109.3622417	-109.3915184	-109.2687583	-109.3706450	-109.4017915
2.0200	-109.2668893	-109.3634239	-109.3925897	-109.2705414	-109.3718578	-109.4028917
2.0300	-109.2684484	-109.3644192	-109.3934768	-109.2721174	-109.3728839	-109.4038081
2.0400	-109.2698080	-109.3652343	-109.3941864	-109.2734938	-109.3737300	-109.4045474
2.0500	-109.2709755	-109.3658759	-109.3947250	-109.2746779	-109.3744029	-109.4051162
2.0600	-109.2719580	-109.3663505	-109.3950990	-109.2756767	-109.3749089	-109.4055208
2.0700	-109.2727622	-109.3666643	-109.3953146	-109.2764973	-109.3752543	-109.4057674
2.0800	-109.2733950	-109.3668233	-109.3953777	-109.2771461	-109.3754451	-109.4058619
2.0900	-109.2738627	-109.3668335	-109.3952941	-109.2776296	-109.3754872	-109.4058102
2.1000	-109.2741716	-109.3667004	-109.3950693	-109.2779540	-109.3753862	-109.4056177
2.1100	-109.2743278	-109.3664297	-109.3947089	-109.2781255	-109.3751477	-109.4052900
2.1500	-109.2735410	-109.3640749	-109.3920138	-109.2773963	-109.3729225	-109.4027299
2.1750	-109.2720120	-109.3616692	-109.3894088	-109.2759000	-109.3705982	-109.4002126
2.2000	-109.2697787	-109.3586303	-109.3861794	-109.2736963	-109.3676403	-109.3970732
2.2250	-109.2669126	-109.3550231	-109.3823894	-109.2708561	-109.3641134	-109.3933755
2.2500	-109.2634793	-109.3509078	-109.3780979	-109.2674452	-109.3600771	-109.3891783
2.2750	-109.2595400	-109.3463404	-109.3733594	-109.2635240	-109.3555865	-109.3845358
2.3000	-109.2551505	-109.3413723	-109.3682246	-109.2591485	-109.3506926	-109.3794984
2.3250	-109.2503627	-109.3360515	-109.3627401	-109.2543706	-109.3454423	-109.3741125
2.3500	-109.2452243	-109.3304224	-109.3569491	-109.2492380	-109.3398789	-109.3684206
2.3750	-109.2397793	-109.3245258	-109.3508917	-109.2437948	-109.3340426	-109.3624624
2.4000	-109.2340680	-109.3183997	-109.3446047	-109.2380819	-109.3279701	-109.3562740
2.4250	-109.2281278	-109.3120792	-109.3381225	-109.2321368	-109.3216955	-109.3498891
2.4500	-109.2219929	-109.3055965	-109.3314766	-109.2259943	-109.3152501	-109.3433382
2.4750	-109.2156949	-109.2989813	-109.3246963	-109.2196863	-109.3086626	-109.3366498
2.5000	-109.2092628	-109.2922606	-109.3178086	-109.2132423	-109.3019596	-109.3298497
2.5250	-109.2027234	-109.2854593	-109.3108388	-109.2066894	-109.2951656	-109.3229617
2.5500	-109.1961012	-109.2786001	-109.3038099	-109.2000526	-109.2883032	-109.3160077
2.5750	-109.1894188	-109.2717032	-109.2967433	-109.1933548	-109.2813928	-109.3090075
2.6000	-109.1826970	-109.2647871	-109.2896591	-109.1866169	-109.2744537	-109.3019795
2.6250	-109.1759548	-109.2578683	-109.2825752	-109.1798583	-109.2675033	-109.2949402
2.6500	-109.1692098	-109.2509618	-109.2755086	-109.1730967	-109.2605576	-109.2879051
2.6750	-109.1624779	-109.2440808	-109.2684744	-109.1663483	-109.2536312	-109.2808881
2.7000	-109.1557738	-109.2372376	-109.2614864	-109.1596277	-109.2467376	-109.2739019
2.7250	-109.1491110	-109.2304429	-109.2545569	-109.1529485	-109.2398891	-109.2669585
2.7500	-109.1425017	-109.2237066	-109.2476969	-109.1463231	-109.2330967	-109.2600688
2.7750	-109.1359570	-109.2170378	-109.2409157	-109.1397626	-109.2263704	-109.2532428
2.8000	-109.1294870	-109.2104445	-109.2342213	-109.1332770	-109.2197194	-109.2464896
2.8250	-109.1231010	-109.2039342	-109.2276208	-109.1268758	-109.2131518	-109.2398180
2.8500	-109.1168073	-109.1975138	-109.2211196	-109.1205672	-109.2066753	-109.2332355
2.8750	-109.1106134	-109.1911894	-109.2147227	-109.1143588	-109.2002964	-109.2267494

Table A-1. (Continued) (2.9 a.u. $\leq R \leq$ 5.5 a.u.)

	RMR-CCSD			RMR-CCSD(T)		
R	cc-pVDZ	cc-pVTZ	cc-pVQZ	cc-pVDZ	cc-pVTZ	cc-pVQZ
2.9000	-109.1045262	-109.1849667	-109.2084342	-109.1082573	-109.1940209	-109.2203661
2.9250	-109.0985517	-109.1788511	-109.2022576	-109.1022690	-109.1878547	-109.2140914
2.9500	-109.0926953	-109.1728472	-109.1961963	-109.0963991	-109.1818024	-109.2079307
2.9750	-109.0869619	-109.1669592	-109.1902530	-109.0906526	-109.1758684	-109.2018884
3.0000	-109.0813557	-109.1611912	-109.1844303	-109.0850336	-109.1700568	-109.1959687
3.0250	-109.0758810	-109.1555464	-109.1787310	-109.0795464	-109.1643707	-109.1901755
3.0500	-109.0705406	-109.1500282	-109.1731572	-109.0741940	-109.1588135	-109.1845116
3.0750	-109.0653377	-109.1446390	-109.1677112	-109.0689794	-109.1533877	-109.1789800
3.1000	-109.0602746	-109.1393817	-109.1623957	-109.0639050	-109.1480959	-109.1735836
3.1250	-109.0553534	-109.1342580	-109.1572111	-109.0589729	-109.1429400	-109.1683231
3.1500	-109.0505759	-109.1292698	-109.1521608	-109.0541847	-109.1379216	-109.1632021
3.1750	-109.0459432	-109.1244187	-109.1472451	-109.0495420	-109.1330424	-109.1582207
3.2000	-109.0414564	-109.1197057	-109.1424658	-109.0450454	-109.1283033	-109.1533806
3.2250	-109.0371159	-109.1151320	-109.1378239	-109.0406956	-109.1237053	-109.1486827
3.2500	-109.0329225	-109.1106979	-109.1333199	-109.0364932	-109.1192489	-109.1441274
3.2750	-109.0288753	-109.1064039	-109.1289544	-109.0324375	-109.1149344	-109.1397151
3.3000	-109.0249742	-109.1022500	-109.1247281	-109.0285283	-109.1107618	-109.1354461
3.3250	-109.0212185	-109.0982363	-109.1206399	-109.0247650	-109.1067311	-109.1313195
3.3500	-109.0176069	-109.0943617	-109.1166905	-109.0211460	-109.1028412	-109.1273355
3.3750	-109.0141380	-109.0906256	-109.1128788	-109.0176704	-109.0990914	-109.1234930
3.4000	-109.0108101	-109.0870268	-109.1092051	-109.0143360	-109.0954806	-109.1197920
3.4250	-109.0076209	-109.0835640	-109.1056660	-109.0111409	-109.0920073	-109.1162290
3.4500	-109.0045686	-109.0802353	-109.1022613	-109.0080830	-109.0886697	-109.1128037
3.4750	-109.0016497	-109.0770388	-109.0989892	-109.0051590	-109.0854658	-109.1095140
3.5000	-108.9988618	-109.0739723	-109.0958473	-109.0023664	-109.0823933	-109.1063575
3.5250	-108.9962016	-109.0710331	-109.0928334	-108.9997019	-109.0794495	-109.1033320
3.5500	-108.9936652	-109.0682185	-109.0899457	-108.9971615	-109.0766317	-109.1004352
3.6000	-108.9889508	-109.0629516	-109.0845336	-108.9924405	-109.0713625	-109.0950126
3.6500	-108.9846886	-109.0581440	-109.0795867	-108.9881729	-109.0665573	-109.0900646
3.7000	-108.9808452	-109.0537670	-109.0750774	-108.9843255	-109.0621873	-109.0855626
3.7500	-108.9773870	-109.0497907	-109.0709743	-108.9808644	-109.0582220	-109.0814742
3.8000	-108.9742812	-109.0461835	-109.0672456	-108.9777567	-109.0546295	-109.0777668
3.9000	-108.9690083	-109.0399487	-109.0607918	-108.9724836	-109.0484334	-109.0713719
4.0000	-108.9647933	-109.0348256	-109.0554807	-108.9682692	-109.0433589	-109.0661362
4.2500	-108.9577412	-109.0259546	-109.0460987	-108.9612289	-109.0346283	-109.0569805
4.5000	-108.9540360	-109.0209401	-109.0406199	-108.9575419	-109.0297631	-109.0517409
4.7500	-108.9521688	-109.0183746	-109.0376878	-108.9556981	-109.0273427	-109.0490380
5.0000	-108.9512226	-109.0171439	-109.0362137	-108.9547820	-109.0262612	-109.0477953
5.2500	-108.9507236	-109.0165600	-109.0354821	-108.9543219	-109.0258574	-109.0473419
5.5000	-108.9504429	-109.0161865	-109.0348900	-108.9540913	-109.0257388	-109.0471447

Table A-2. Vibrational energies (in cm^{-1}) of $^{14}N^{14}N$, $^{14}N^{15}N$ and $^{15}N^{15}N$ generated from the *Fit 1* potential of Table 1.

v	$^{14}N^{14}N$	$^{14}N^{15}N$	$^{15}N^{15}N$	v	$^{14}N^{14}N$	$^{14}N^{15}N$	$^{15}N^{15}N$
0	1175.72	1156.07	1136.08	32	61082.98	60333.90	59560.95
1	3505.62	3447.40	3388.16	33	62430.40	61678.50	60901.75
2	5806.85	5711.01	5613.47	34	63740.77	62987.78	62208.89
3	8079.41	7946.91	7812.01	35	65013.04	64260.84	63481.59
4	10323.29	10155.08	9983.79	36	66245.81	65496.59	64718.95
5	12538.34	12335.39	12128.68	37	67437.09	66693.47	65919.79
6	14724.50	14487.77	14246.58	38	68584.41	67849.38	67082.46
7	16881.82	16612.27	16337.58	39	69685.97	68961.99	68204.76
8	19010.21	18708.81	18401.58	40	70741.06	70030.10	69284.73
9	21109.66	20777.38	20438.57	41	71747.80	71052.97	70321.61
10	23180.11	22817.91	22448.51	42	72703.48	72028.15	71314.31
11	25221.48	24830.35	24431.32	43	73606.47	72953.56	72260.24
12	27233.71	26814.63	26386.97	44	74453.81	73827.34	73157.85
13	29216.70	28770.65	28315.34	45	75243.21	74646.68	74004.88
14	31170.34	30698.34	30216.38	46	75971.56	75409.36	74799.01
15	33094.53	32597.57	32089.96	47	76636.23	76112.46	75537.78
16	34989.11	34468.23	33935.98	48	77234.32	76753.35	76218.68
17	36853.96	36310.17	35754.32	49	77763.50	77329.49	76839.00
18	38688.87	38123.23	37544.82	50	78222.50	77838.67	77396.49
19	40493.69	39907.25	39307.33	51	78611.72	78279.89	77889.17
20	42268.17	41662.02	41041.66	52	78934.26	78653.91	78316.17
21	44012.12	43387.34	42747.63	53	79196.17	78964.03	78678.42
22	45725.25	45082.96	44425.02	54	79405.34	79216.27	78979.33
23	47407.29	46748.63	46073.57	55	79569.33	79418.20	79224.73
24	49057.93	48384.07	47693.06	56	79693.60	79576.90	79421.83
25	50676.83	49988.96	49283.17	57	79779.29	79697.43	79577.32
26	52263.60	51562.95	50843.60	58	79821.79	79780.55	79695.96
27	53817.83	53105.67	52374.01	59	79840.01	79821.86	79778.58
28	55339.06	54616.69	53874.01	60	79844.79	79839.87	79820.51
29	56826.79	56095.56	55343.18	61		79844.75	79839.20
30	58280.44	57541.77	56781.08	62			79844.63
31	59699.40	58954.76	58187.19				

Table A-3. Morphing the RMR-CCSD potentials with D_e=79845 cm^{-1}.

Parameter	VDZ	VQZ	T-VDZ	T-VTZ	T-VQZ	T-CBS
R_e, Å	**1.097620**	**1.097659**	**1.097650**	**1.097694**	**1.097707**	**1.097681**
ρ_{ij}, Å	**0.801416**	**0.743307**	**0.778465**	**0.727295**	**0.734060**	**0.700906**
α	**0.860374**	**0.990914**	**0.948541**	**1.032025**	**1.043202**	**0.822340**
β	**0.812198**	**1.015705**	**0.923515**	**0.967979**	**1.034609**	**0.678316**
γ, Å^{-1}	0.0	-0.0163[c]	-0.011[c]	-0.08[c]	**0.012702**	**0.390070**
St.dev.[b]	0.209	0.167	0.152	0.727	0.125	0.074

[a] Values of the fitted parameters are typed in boldface. [b] Standard deviation of the fit. [c] Fixed after a preliminary determination.

Table A-4. Morphing the RMR-CCSD potentials with relaxed D_e.

Parameter	VDZ	VQZ	T-VDZ	T-VTZ	T-VQZ	T-CBS
R_e, Å	**1.097708**	**1.097695**	**1.097685**	**1.097691**	**1.097685**	**1.097687**
ρ_{ij}, Å	**0.738105**	**0.642194**	**0.700572**	**0.773128**	**0.879163**	**0.771853**
D_e, cm^{-1}	**80548.09**	**88038.44**	**83418.89**	**77520.95**	**76437.33**	**76489.79**
α	**0.926447**	**1.114024**	**0.961831**	**1.004189**	**1.012167**	**0.965827**
β	**0.809267**	**1.057881**	**0.866294**	**0.986524**	**1.050094**	**0.952430**
γ, Å^{-1}	**0.161294**	**0.112381**	**0.155102**	0.0	-0.14[c]	**0.218337**
St.dev.[b]	0.106	0.069	0.011	0.086	0.021	0.049

[a] Values of the fitted parameters are typed in boldface. [b] Standard deviation of the fit. [c] Fixed after a preliminary determination.