

## POTENTIAL ENERGY CURVE OF N<sub>2</sub> IN ITS GROUND ELECTRONIC STATE

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*Dedicated to Professor Josef Paldus on the occasion of his 70th birthday.*

The potential energy curve of N<sub>2</sub> is constructed by morphing a very accurate (*r*<sub>12</sub>)-MR-ACPF *ab initio* potential within the framework of the reduced potential curve (RPC) approach of Jenč and Pliva. The actual morphing is performed by fitting the RPC parameters to highly accurate experimental ro-vibrational data. The resulting potential energy curve is in a close harmony with these data allowing thus for reliable prediction of the so-far unknown molecular states. The (*r*<sub>12</sub>)-MR-ACPF reduced potential is also used as a reference for fitting less accurate SR-CCSD and RMR-CCSD theoretical data of Li and Paldus (Li X., Paldus J.: *J. Chem. Phys.* **2000**, *113*, 9966). Though not fully quantitative, the fittings reveal high coincidence of the CCSD reduced potentials with their reference (*r*<sub>12</sub>)-MR-ACPF counterpart evidencing thus physical adequacy of the probed CCSD methods for rationalizing experimental data by means of the RPC approach.

**Keywords:** N<sub>2</sub> molecule; Coupled-cluster calculations; Reduced potential curve; Ro-vibrational states; *Ab initio* calculations, Nitrogen; (*r*<sub>12</sub>)-MR-ACPF.

A physically correct description of highly excited ro-vibrational molecular states requires knowledge of accurate potential energy functions defined over a wide range of vibrational displacements. Although conceptually simple, determination of such functions is an open and challenging problem both for experiment and theory. A straightforward RKR inverting of experimental data is strongly limited by scarcity of these data even in the case of very small molecular systems, and, theoretically evaluated potentials cannot meet accuracy requirements imposed by many important applications. Determination of the sought potential energy functions is also strongly hampered by the lack of flexible empirical potential function models. Consequently, complete and spectroscopically accurate potential energy func-

tions are available only for very few molecular systems (mostly diatomics, see e.g.<sup>1-3</sup> and references therein).

A very general and promising way of overcoming the above problems consists in taking a realistic *ab initio* potential and modifying it to fit the available experimental data (see e.g.<sup>3,4</sup>). Apparently, the main goal of this (morphing) procedure is to achieve adequate description of the experimental data by means of inexpensive *ab initio* procedures. The aim of the present paper is to investigate prospects of the coupled-cluster methods which can be used for routine applications. The actual investigation consists in evaluating the potential energy curve of N<sub>2</sub> within the framework of the reduced potential curve (RPC) method of Jenč and Plíva<sup>5-8</sup>. In this context, N<sub>2</sub> appears as an ideal model system: (i) breaking of its triple bond provides a challenging test for any computational quantum chemical method (see e.g.<sup>9-12</sup>), (ii) there is a highly accurate (*r*<sub>12</sub>)-MRACPF potential available in the literature<sup>13</sup> which provides excellent reference for the cheaper MR-CC calculations, (iii) the dissociation energy of N<sub>2</sub>, which is the most important energy scaling RPC parameter, is known with very high accuracy<sup>14,15</sup>, (iv) available experimental data cover fairly high vibrational excitations (*v* = 0–19) (lit.<sup>16-19</sup>) allowing thus for a direct accuracy checking for a sizable part of the morphed potentials.

## THEORETICAL

The calculations scheduled above were performed in a very similar way as in our previous studies on CN and NeH<sup>+</sup> (lit.<sup>20,21</sup>). The literature (pointwise calculated) *ab initio* energies were smoothed using the following potential energy function, *U*(*r*):

$$U(r) = \sum_i F_i \{1 - e^{-a_1 (r-r_e) - a_2 (r-r_e)^2 - a_4 (r-r_e)^4}\}^i, \quad (1)$$

where *r* is the internuclear distance (*r*<sub>e</sub> being its equilibrium value) and *a*<sub>1</sub>, *a*<sub>2</sub>, *a*<sub>4</sub>, and *F*<sub>*i*</sub> are fitting parameters. The parameters of the reference (*r*<sub>12</sub>)-ACPF potential acquire the following values: *F*<sub>2</sub> = 232552.0731, *F*<sub>3</sub> = -122316.4277, *F*<sub>5</sub> = -35098.7113, *F*<sub>8</sub> = -36379.8574, *F*<sub>10</sub> = 41217.7212 (all values in cm<sup>-1</sup>; *a*<sub>1</sub> = 1.577252 Å<sup>-1</sup>, *a*<sub>2</sub> = -0.043308 Å<sup>-2</sup>, *a*<sub>4</sub> = 0.255872 Å<sup>-4</sup>, *r*<sub>e</sub> = 1.097771 Å. The dissociation energy, *D*<sub>e</sub>, and harmonic force constant, *k*<sub>e</sub>, consistent with these parameters are 79974.8 and 1157051 cm<sup>-1</sup>, respectively. The corresponding theoretical ro-vibrational energies were found as eigenvalues of the radial Hamiltonian

$$H^{\text{rv}} = -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + U(r) + \frac{\hbar^2}{2\mu r^2} J(J+1) , \quad (2)$$

where  $\hbar$  is Planck's constant,  $\mu$  is the reduced mass and  $J$  is the rotational quantum number.

The reduced potential curve scheme of Jenč and Plíva was used in the the following (generalized) form (see lit.<sup>5-8</sup>)

$$u(\rho) = \frac{U}{D_e} , \quad (3)$$

$$\rho = \frac{r - \{1 - \alpha \exp[-\beta(1 + \gamma)r/\rho_{ij}]\}\rho_{ij}}{r_e - \{1 - \alpha \exp[-\beta(1 + \gamma)r/\rho_{ij}]\}\rho_{ij}} , \quad (4)$$

$$\rho_{ij} = \frac{r_e - (\kappa D_e/k_e)^{1/2}}{\{1 - \alpha \exp[-\beta(1 + \gamma)r/\rho_{ij}]\}\rho_{ij}} , \quad \kappa = 396 , \quad (5)$$

where  $\rho$ ,  $u$  and  $U$  are the reduced internuclear distance, the reduced energy and the true potential, respectively;  $D_e$ ,  $r_e$ , and  $k_e$  are the depth of the minimum of the potential curve, the equilibrium internuclear distance, and the harmonic force constant, respectively;  $\kappa$  is the universal force constant;  $\alpha$ ,  $\beta$  and  $\gamma$  are correction parameters (in the standard RPC formula,  $\alpha = \beta = 1$  and  $\gamma = 0$ ).

## RESULTS AND DISCUSSION

The accuracy of the ( $r_{12}$ )-MR-ACPF potential energy curve is probably beyond reach of any traditional CI method. Nevertheless, as we can see in Table I, the ( $r_{12}$ )-MR-ACPF vibrational energies are still in a sizable disharmony with their experimental values. The corresponding ( $r_{12}$ )-MR-ACPF reduced potential, however, is closely coinciding with its experimental counterpart. We can see in Table II that already variation of only one of the RPC parameters allows for a pleasing description of all of experimentally available ( $n = 0, \dots, 19$ ) vibrational energy terms. The quality of reproduction of experiment by theory is improved when varying more parameters, and, already three-parameter schemes allow for a quantitative reproduction of the experimental data (importantly, the morphed potentials closely reproduce also available rotational data). Increasing the number of fitted parameters leads also to a closer agreement with the  $n > 19$  data predicted by means of the stan-

standard Dunham expansion approach<sup>17</sup>. Nevertheless, the differences of the predicted Dunham and RPC data are not negligible, raising thus interesting questions concerning the predictive power of these schemes. Unfortunately, any critical answering of these questions is prohibited by the scarcity of the  $(r_{12})$ -MR-ACPF *ab initio* data. We can see in Fig. 1 that the avail-

TABLE I

The deviations ( $\Delta = G^{\text{theor}} - G^{\text{exp}}$ ) of the experimental and  $(r_{12})$ -MR-ACPF vibrational energy terms ( $G_n = E_n - E_0$ ) of  $\text{N}_2$ <sup>a</sup>

$n$	$G_n^{\text{exp}}$	$\Delta_n$	$\frac{1000\Delta}{G^{\text{exp}}}$	$n$	$G_n^{\text{exp}}$	$\Delta_n$	$\frac{1000\Delta}{G^{\text{exp}}}$
1	2329.95	-1.85	-0.79	10	22004.35	-18.82	-0.86
2	4631.19	-3.76	-0.81	11	24045.73	-20.52	-0.85
3	6903.78	-5.63	-0.81	12	26057.86	-22.25	-0.85
4	9147.61	-7.51	-0.82	13	28040.86	-23.80	-0.85
5	11362.55	-9.51	-0.84	14	29994.54	-25.25	-0.84
6	13548.74	-11.42	-0.84	15	31918.68	-26.70	-0.84
7	15706.08	-13.30	-0.85	16	33813.08	-28.23	-0.83
8	17834.49	-15.17	-0.85	17	35677.80	-29.63	-0.83
9	19933.99	-16.96	-0.85	18	37513.26	-30.31	-0.81

<sup>a</sup> The experimental term values taken from<sup>19</sup>.

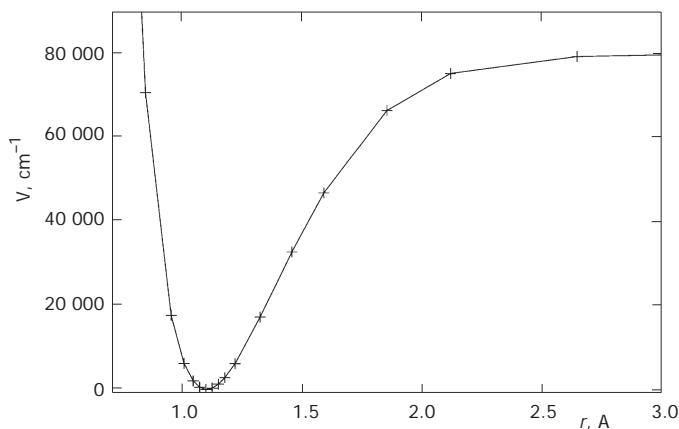


FIG. 1  
 $(r_{12})$ -MR-ACPF potential energy curve of  $\text{N}_2$  (see lit.<sup>13</sup>)

TABLE II  
The experimental vibrational term and band center values ( $G_{mn} = E_m - E_n$ ) fitted by means of the standard ( $r_{12}$ )-MR-ACPF reduced potential curve ( $\Delta = G^{\text{theor}} - G^{\text{exp}}$ )<sup>a</sup>

m	n	exp	$\Delta^1$	$\Delta^2$	$\Delta^3$	$\Delta^4$	$\Delta^5$	$\Delta^6$	$\Delta^7$	$\Delta^8$	$\Delta^9$	$\Delta^{10}$
0	1	2329.95	-0.07	0.07	0.07	0.16	0.19	0.02	0.02	0.02	0.02	0.02
0	2	4631.19	-0.20	0.06	0.06	0.24	0.28	0.00	0.00	0.00	0.00	0.00
0	3	6903.78	-0.29	0.07	0.07	0.32	0.37	0.04	0.04	0.04	0.04	0.04
0	4	9147.61	-0.40	0.05	0.04	0.36	0.40	0.07	0.07	0.07	0.07	0.07
0	5	11362.55	-0.61	-0.10	-0.12	0.25	0.28	-0.01	-0.01	-0.01	-0.01	-0.01
0	6	13548.74	-0.74	-0.18	-0.21	0.20	0.21	-0.01	-0.01	-0.01	-0.01	-0.02
0	7	15706.08	-0.84	-0.26	-0.29	0.13	0.13	0.00	0.00	0.00	0.00	0.00
0	8	17834.49	-0.93	-0.35	-0.39	0.04	0.02	-0.01	-0.01	-0.01	-0.01	-0.01
0	9	19933.99	-0.94	-0.38	-0.42	0.00	-0.04	0.03	0.03	0.03	0.03	0.04
0	10	22004.35	-1.02	-0.50	-0.55	-0.16	-0.22	-0.05	-0.05	-0.04	-0.05	-0.03
0	11	24045.73	-0.94	-0.50	-0.54	-0.21	-0.28	-0.02	-0.02	-0.02	-0.02	0.00
0	12	26057.86	-0.89	-0.55	-0.59	-0.33	-0.41	-0.08	-0.08	-0.08	-0.08	-0.07
0	13	28040.86	-0.65	-0.44	-0.47	-0.31	-0.39	-0.03	-0.03	-0.03	-0.03	-0.02
0	14	29994.54	-0.31	-0.26	-0.27	-0.25	-0.32	0.04	0.04	0.04	0.04	0.04
0	15	31918.68	0.02	-0.12	-0.11	-0.24	-0.29	0.01	0.01	0.01	0.01	-0.01
0	16	33813.08	0.28	-0.08	-0.04	-0.37	-0.38	-0.20	-0.20	-0.20	-0.20	-0.23
0	17	35677.80	0.67	0.05	0.13	-0.42	-0.37	-0.40	-0.40	-0.40	-0.40	-0.43
0	18	37513.26	1.78	0.86	0.99	0.19	0.30	-0.02	-0.02	-0.02	-0.02	-0.03
0	19	39318.48	2.80	1.55	1.74	0.64	0.85	0.12	0.12	0.12	0.12	0.14
0	20	41094.76 <sup>b</sup>	5.24	3.61	3.87	2.43	2.76	1.50	1.49	1.51	1.50	1.60
0	21	42839.82 <sup>b</sup>	7.04	4.98	5.34	3.51	4.00	2.07	2.05	2.08	2.07	2.28
0	22	44554.28 <sup>b</sup>	9.05	6.52	6.98	4.72	5.40	2.63	2.59	2.66	2.63	3.02
0	23	46237.78 <sup>b</sup>	11.19	8.15	8.73	5.98	6.90	3.10	3.04	3.14	3.10	3.75
0	24	47889.92 <sup>b</sup>	13.36	9.74	10.47	7.17	8.36	3.34	3.23	3.40	3.34	4.35

TABLE II  
(Continued)

m	n	exp	$\Delta^1$	$\Delta^2$	$\Delta^3$	$\Delta^4$	$\Delta^5$	$\Delta^6$	$\Delta^7$	$\Delta^8$	$\Delta^9$	$\Delta^{10}$
0	25	49510.19 <sup>b</sup>	15.38	11.13	12.03	8.11	9.64	3.15	2.98	3.24	3.15	4.65
0	26	51098.01 <sup>b</sup>	17.03	12.08	13.18	8.57	10.50	2.28	2.03	2.40	2.28	4.42
0	27	52652.68 <sup>b</sup>	18.01	12.30	13.63	8.26	10.64	0.39	0.04	0.57	0.39	3.36
1	2	2301.25	-0.12	0.00	0.00	0.09	0.10	-0.01	-0.01	-0.01	-0.01	-0.01
2	3	2272.56	-0.12	-0.02	-0.02	0.05	0.06	0.01	0.01	0.01	0.01	0.01
3	4	2243.82	-0.12	-0.03	-0.04	0.02	0.02	0.02	0.02	0.02	0.02	0.02
4	5	2215.05	-0.11	-0.04	-0.05	0.00	-0.01	0.03	0.03	0.03	0.03	0.03
5	6	2186.23	-0.10	-0.05	-0.06	-0.02	-0.04	0.03	0.03	0.03	0.03	0.03
6	7	2157.36	-0.08	-0.05	-0.06	-0.04	-0.06	0.03	0.03	0.03	0.03	0.03
7	8	2128.45	-0.05	-0.05	-0.05	-0.05	-0.07	0.03	0.03	0.03	0.03	0.04
0	1	2252.08 <sup>c</sup>	-0.11	0.03	0.03	0.12	0.14	-0.02	-0.02	-0.02	-0.02	-0.02
1	2	2225.33 <sup>c</sup>	-0.11	0.00	0.00	0.08	0.10	-0.01	-0.01	-0.01	-0.01	-0.01
2	3	2198.54 <sup>c</sup>	-0.12	-0.02	-0.02	0.05	0.06	0.01	0.01	0.01	0.01	0.00
3	4	2171.72 <sup>c</sup>	-0.12	-0.03	-0.04	0.03	0.02	0.02	0.02	0.02	0.02	0.01
4	5	2144.86 <sup>c</sup>	-0.11	-0.05	-0.05	0.00	-0.01	0.02	0.02	0.02	0.02	0.02
5	6	2117.96 <sup>c</sup>	-0.10	-0.06	-0.06	-0.02	-0.04	0.02	0.02	0.02	0.02	0.02
6	7	2091.03 <sup>c</sup>	-0.08	-0.06	-0.06	-0.04	-0.05	0.03	0.03	0.03	0.03	0.03
$r_e$ , Å		1.09760	1.09777	1.09777	1.09760	1.09777	1.09760	<b>1.09450</b>	1.09777	1.09777	1.09777	1.09760
$P_{ij}$		0.74349	0.74566	<b>0.74467</b>	0.74566	<b>0.74398</b>	<b>0.74642</b>	<b>0.73469</b>	<b>0.73453</b>	<b>0.73881</b>	<b>0.73796</b>	<b>0.75382</b>
$D_e$ , cm <sup>-1</sup>		79906	<b>79854</b>	79975	79906	<b>80059</b>	79906	<b>80540</b>	<b>80642</b>	<b>80505</b>	<b>80540</b>	79906
$\alpha$		1	1	1	1	1	1	1	1	<b>0.99497</b>	1	<b>0.92199</b>
$\beta$		1	1	1	1	1	1	1	1	1	<b>1.00444</b>	<b>0.92947</b>
$\gamma$		0	0	0	-0.0121	0	-0.0249	0	<b>0.00846</b>	0	0	0

<sup>a</sup> The term values taken from<sup>19</sup>, the band centers taken from<sup>18</sup>; values of the fitted parameters typed in boldface, the remaining parameters fixed at their experimental or ( $r_{12}$ )-MR-ACPF values. <sup>b</sup> Values predicted in<sup>17</sup>. <sup>c</sup>  $^{13}\text{N}_2$  data.

TABLE III  
The SR, 4R and 8R RMR CCSD cc-pVTZ term values ( $G_n = E_n - E_0$ ) fitted by means of the standard ( $r_{12}$ )-MR-ACPF RPC formula<sup>a</sup>

<i>n</i>	exp	$G^{\text{SR}}$	$\Delta_{\text{SR}}$	$G^{\text{4R}}$	$\Delta_{\text{4R}}$	$G^{\text{8R}}$	$\Delta_{\text{8R}}$
1	2329.95	2399.7	−0.3	2337.0	−0.2	2336.5	−0.8
2	4631.19	4773.7	−0.4	4646.1	−0.1	4644.9	−0.9
3	6903.78	7121.9	−0.4	6927.1	0.1	6924.7	−0.8
4	9147.61	9444.4	−0.4	9179.9	0.3	9176.1	−0.2
5	11362.55	11741.3	−0.3	11404.4	0.5	11398.6	0.4
6	13548.74	14012.5	−0.2	13600.8	0.8	13592.3	1.2
7	15706.08	16258.1	−0.1	15768.7	0.9	15757.0	2.0
8	17834.49	18478.2	0.1	17908.2	1.0	17892.3	2.6
9	19933.99	20672.7	0.1	20019.3	1.0	19998.3	3.1
10	22004.35	22841.8	0.2	22101.8	0.9	22074.7	3.2
11	24045.73	24985.6	0.3	24155.9	0.9	24121.4	3.1
12	26057.86	27103.9	0.2	26181.3	0.7	26138.2	2.6
13	28040.86	29197.0	0.2	28178.0	0.4	28125.2	1.8
14	29994.54	31264.8	0.1	30146.0	0.1	30082.1	0.7
15	31918.68	33307.5	0.1	32085.1	−0.3	32009.1	−0.4
16	33813.08	35325.0	0.0	33995.5	−0.6	33906.0	−1.6
17	35677.80	37317.5	0.0	35876.8	−1.0	35772.7	−2.7
18	37513.26	39284.9	−0.1	37729.1	−1.3	37609.3	−3.6
19	39318.48	41227.3	−0.1	39552.3	−1.5	39415.6	−4.2
20	41094.76	43144.8	−0.1	41346.3	−1.5	41191.5	−4.3
21	42839.82	45037.3	−0.1	43111.0	−1.3	42937.0	−3.7
22	44554.28	46905.0	0.0	44846.1	−0.9	44651.8	−2.4
23	46237.78	48747.7	0.0	46551.7	−0.1	46335.8	−0.2
24	47889.92	50565.5	0.0	48227.5	1.1	47988.6	2.8
25	49510.19	52358.4	0.0	49873.4	2.7	49610.2	7.1
<i>r</i> <sub>e</sub> , Å	1.09760	1.09620		1.10120		1.10110	
$\rho_{jj^*}$ , Å	0.74349	0.59659		0.72969		0.76460	
<i>D</i> <sub>e</sub> , cm <sup>−1</sup>	79906	109118		83303		78659	

<sup>a</sup> The term values derived from values given in Table VIII of lit.<sup>10</sup>;  $\Delta_n = G_n^{\text{theor}} - G_n^{\text{exp}}$ .

able energy points (represented by crosses) provide reasonable coverage of the studied potential only in its equilibrium region. Interpolating the points outside this region is thus loaded by inaccuracy, which cannot be determined accurately with the presently available information. Apparently, a more decisive comparison of the Dunham and RPC schemes would require evaluation of highly accurate *ab initio* points on a denser grid of the vibrational displacements.

Despite the doubts concerning the accuracy of its interpolated (high-energy) parts, the  $(r_{12})$ -MR-ACPF RPC potential is a perfect approximant of its true counterpart in the energy region which is decisive for describing all of the observed  $N_2$  spectral data. Therefore, the potential should be a very suitable tool for probing any quantum chemical method, including computationally inexpensive methods that are affordable for large molecular systems. A very promising class of such methods was recently developed within the framework of the coupled-cluster theory<sup>22</sup> by Paldus and Piecuch and their collaborators<sup>23,24</sup>. Obviously, the mentioned probing may be done in various ways. In this study  $(r_{12})$ -MR ACPF RPC is used as an empirical potential for fitting of the theoretical energy terms obtained by Li and Paldus using single-reference (SR) and reduced multireference (RMR) coupled-cluster CCSD methods with the correlation-consistent polarized valence-triple-zeta (cc-pVTZ) basis set<sup>10</sup>. The results of this dereducing procedure are collected in Table III. A brief inspection of the table reveals a rather surprising feature of the obtained fits: the single-reference vibrational energies are better reproduced than the multireference data and quality of reproduction of these data decreases (slightly) with increasing dimension of the reference space. In other words, the lower part of the single-reference RPC potential is found to be in a closer harmony with the reference RPC potential than the multireference RPC potentials. On the other hand, however, the fitted parameters converge to their experimental values with increasing dimension of the reference space. Apparently, the RMR way of accounting for higher-order clusters exhibits a slightly incorrect vibrational dependence which causes relatively tiny oscillations of the RMR reduced potentials around the true potential.

## CONCLUSIONS

The explicitly correlated  $(r_{12})$ -MR-ACPF approach has allowed for constructing a very accurate approximant of the true reduced potential energy curve of  $N_2$  in the framework of the Jenč and Pliva approach. The approximant allows for a quantitative reproduction of all of the observed ro-vibrational



data in terms of a few fitting parameters and for realistic predictions of the so-far unobserved molecular states. Moreover, it allows also for a critical probing of approximate coupled-cluster methods which are much more suitable for routine applications than computationally very demanding CI procedures.

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