ADDITIONS AND CORRECTIONS

2006, Volume 110A

A. J. C. Varandas and S. P. J. Rodrigues: New Double Many-Body Expansion Potential Energy Surface for Ground-State HCN from a Multiproperty Fit to Accurate ab Initio Energies and Rovibrational Calculations

Page 485. In eq 2, $\chi_n(r_i)$ are the usual damping functions, with R_0 taken as the average of the AB and AC diatomic valuesfor each A-BC channel. In addition to $n = 7$ terms, the $C_8{}^4$ ones have also been neglected.

TABLE 5: Numerical Values of the Extended Hartree−Fock Energy (Eq 13) in Atomic Units

$\gamma_i^\alpha = 1.0$ ($i = 1, 2, 3$; $\alpha = 1, 2, 3$)

$R^1_{1,\mathrm{ref}} = 2.179$	$R^1_{2,\mathrm{ref}} = 2.013$	$R^1_{3,\mathrm{ref}} = 4.192$
$R^2_{1,\mathrm{ref}} = 2.209$	$R^2_{2,\mathrm{ref}} = 4.087$	$R^2_{3,\mathrm{ref}} = 1.878$
$R^3_{1,\mathrm{ref}} = 2.2439$	$R^2_{2,\mathrm{ref}} = 2.2365$	$R^2_{3,\mathrm{ref}} = 2.6252$
$C_1 = 0.10610383\mathrm{E}{+02}$	$C_2 = -0.19340384\mathrm{E}{+01}$	$C_3 = 0.45079700\mathrm{E}{+01}$
$C_4 = -0.84619326\mathrm{E}{+00}$	$C_5 = 0.63942964\mathrm{E}{-01}$	$C_6 = -0.11095907\mathrm{E}{-01}$
$C_7 = 0.15199860\mathrm{E}{+01}$	$C_8 = 0.33462808\mathrm{E}{+00}$	$C_9 = 0.54814834\mathrm{E}{+00}$
$C_{10} = 0.17923807\mathrm{E}{+00}$	$C_{11} = -0.10580572\mathrm{E}{-01}$	$C_{12} = 0.30540079\mathrm{E}{+01}$
$C_{13} = -0.10680413\mathrm{E}{+01}$	$C_{14} = 0.13085298\mathrm{E}{+01}$	$C_{15} = -0.71036643\mathrm{E}{+00}$
$C_{16} = -0.35589832\mathrm{E}{-01}$	$C_{17} = -0.17994167\mathrm{E}{-02}$	$C_{18} = 0.13956473\mathrm{E}{+00}$
$C_{19} = -0.12637979\mathrm{E}{+00}$	$C_{20} = -0.87964970\mathrm{E}{-01}$	$C_{21} = 0.19498599\mathrm{E}{-01}$
$C_{22} = -0.25118989\mathrm{E}{+01}$	$C_{23} = 0.24163953\mathrm{E}{+00}$	$C_{24} = -0.10251614\mathrm{E}{+01}$
$C_{25} = 0.11462454\mathrm{E}{+00}$	$C_{26} = 0.56345921\mathrm{E}{-01}$	$C_{27} = -0.12090187\mathrm{E}{+01}$
$C_{28} = 0.40219081\mathrm{E}{+00}$	$C_{29} = -0.65139622\mathrm{E}{+00}$	$C_{30} = 0.16207674\mathrm{E}{+00}$
$C_{31} = -0.59897087\mathrm{E}{+00}$	$C_{32} = 0.48146049\mathrm{E}{+00}$	$C_{33} = -0.57764857\mathrm{E}{+00}$
$C_{34} = -0.91645637\mathrm{E}{-01}$	$C_{35} = 0.52397000\mathrm{E}{+00}$	$C_{36} = -0.13553368\mathrm{E}{+00}$
$C_{37} = 0.11713043\mathrm{E}{+00}$	$C_{38} = -0.60895252\mathrm{E}{+00}$	$C_{39} = 0.20460885\mathrm{E}{-01}$
$C_{40} = -0.41369282\mathrm{E}{+00}$	$C_{41} = 0.51298070\mathrm{E}{+00}$	$C_{42} = -0.29124304\mathrm{E}{+00}$
$C_{43} = 0.16735091\mathrm{E}{+00}$	$C_{44} = 0.31931820\mathrm{E}{+00}$	$C_{45} = -0.19230240\mathrm{E}{+00}$
$C_{46} = -0.28994934\mathrm{E}{-02}$	$C_{47} = -0.37904051\mathrm{E}{+00}$	$C_{48} = 0.11845177\mathrm{E}{+00}$
$C_{49} = -0.86521615\mathrm{E}{-02}$	$C_{50} = -0.34143449\mathrm{E}{+00}$	$C_{51} = -0.25233214\mathrm{E}{+00}$
$C_{52} = -0.30043971\mathrm{E}{+00}$	$C_{53} = 0.23392596\mathrm{E}{-01}$	$C_{54} = -0.13045230\mathrm{E}{+00}$
$C_{55} = 0.24562120\mathrm{E}{+00}$	$C_{56} = 0.17996557\mathrm{E}{-01}$	$C_{57} = -0.61128899\mathrm{E}{+01}$
$C_{58} = 0.15149154\mathrm{E}{+00}$	$C_{59} = -0.19003976\mathrm{E}{+01}$	$C_{60} = 0.99316782\mathrm{E}{-01}$
$C_{61} = 0.63927148\mathrm{E}{-01}$	$C_{62} = -0.36013834\mathrm{E}{-01}$	$C_{63} = 0.11856847\mathrm{E}{+01}$
$C_{64} = 0.44466241\mathrm{E}{+00}$	$C_{65} = 0.99987876\mathrm{E}{+00}$	$C_{66} = 0.23429188\mathrm{E}{+00}$
$C_{67} = 0.90363327\mathrm{E}{-01}$	$C_{68} = -0.28952234\mathrm{E}{+01}$	$C_{69} = 0.30323044\mathrm{E}{-02}$
$C_{70} = -0.87238395\mathrm{E}{+00}$	$C_{71} = -0.68638072\mathrm{E}{-01}$	$C_{72} = 0.50256232\mathrm{E}{+00}$
$C_{73} = 0.15882123\mathrm{E}{+00}$	$C_{74} = 0.48747910\mathrm{E}{+00}$	$C_{75} = -0.19696705\mathrm{E}{+00}$
$C_{76} = 0.31833196\mathrm{E}{-01}$	$C_{77} = -0.69782464\mathrm{E}{-02}$	$C_{78} = 0.50285409\mathrm{E}{+01}$
$C_{79} = 0.12953787\mathrm{E}{+01}$	$C_{80} = 0.16726755\mathrm{E}{+01}$	$C_{81} = 0.92969131\mathrm{E}{-01}$
$C_{82} = -0.26764667\mathrm{E}{+00}$	$C_{83} = 0.15652166\mathrm{E}{+00}$	$C_{84} = 0.30100732\mathrm{E}{+00}$
$C_{85} = 0.76563091\mathrm{E}{-01}$	$C_{86} = 0.92258457\mathrm{E}{-01}$	$C_{87} = 0.20583422\mathrm{E}{+01}$
$C_{88} = 0.38994608\mathrm{E}{+00}$	$C_{89} = 0.51934641\mathrm{E}{+00}$	$C_{90} = 0.24338964\mathrm{E}{+00}$
$C_{91} = 0.16570251\mathrm{E}{+00}$	$C_{92} = 0.54893325\mathrm{E}{-01}$	$C_{93} = -0.94748868\mathrm{E}{+00}$
$C_{94} = -0.44480162\mathrm{E}{-01}$	$C_{95} = -0.18625756\mathrm{E}{+00}$	$C_{96} = -0.30683006\mathrm{E}{-02}$
$C_{97} = -0.14683392\mathrm{E}{+00}$	$C_{98} = -0.70366109\mathrm{E}{-01}$	$C_{99} = -0.18663426\mathrm{E}{+00}$
$C_{100} = -0.48321405\mathrm{E}{+00}$	$C_{101} = 0.16116635\mathrm{E}{+00}$	$C_{102} = -0.26353165\mathrm{E}{+00}$
$C_{103} = -0.22605742\mathrm{E}{+00}$	$C_{104} = -0.15924577\mathrm{E}{+00}$	$C_{105} = -0.22569460\mathrm{E}{+00}$
$C_{106} = 0.49843875\mathrm{E}{-01}$	$C_{107} = -0.17585547\mathrm{E}{-01}$	$C_{108} = -0.14272548\mathrm{E}{-01}$
$C_{109} = 0.29618814\mathrm{E}{-01}$	$C_{110} = -0.28029353\mathrm{E}{-01}$	$C_{111} = 0.55923590\mathrm{E}{-01}$
$C_{112} = 0.21473814\mathrm{E}{-01}$	$C_{113} = -0.19794019\mathrm{E}{+02}$	$C_{114} = -0.50902338\mathrm{E}{+01}$
$C_{115} = -0.85554180\mathrm{E}{+01}$	$C_{116} = -0.18957444\mathrm{E}{+01}$	$C_{117} = -0.19882871\mathrm{E}{+00}$
$C_{118} = 0.59072664\mathrm{E}{-01}$	$C_{119} = 0.89270055\mathrm{E}{+00}$	$C_{120} = -0.10170253\mathrm{E}{+01}$
$C_{121} = 0.44232389\mathrm{E}{+00}$	$C_{122} = -0.41911880\mathrm{E}{+00}$	$C_{123} = -0.78000529\mathrm{E}{-01}$
$C_{124} = -0.66800079\mathrm{E}{+01}$	$C_{125} = 0.96961018\mathrm{E}{-01}$	$C_{126} = -0.19985627\mathrm{E}{+01}$
$C_{127} = 0.19612037\mathrm{E}{+00}$	$C_{128} = 0.15463175\mathrm{E}{-01}$	$C_{129} = -0.56418645\mathrm{E}{+00}$
$C_{130} = 0.85452377\mathrm{E}{-01}$	$C_{131} = -0.70210567\mathrm{E}{-01}$	$C_{132} = -0.35224747\mathrm{E}{+00}$
$C_{133} = -0.88943653\mathrm{E}{-02}$	$C_{134} = 0.13303124\mathrm{E}{+01}$	$C_{135} = 0.48852797\mathrm{E}{+01}$
$C_{136} = 0.14242070\mathrm{E}{+01}$	$C_{137} = 0.13979380\mathrm{E}{+01}$	$C_{138} = 0.21762543\mathrm{E}{+00}$
$C_{139} = 0.13736614\mathrm{E}{+01}$	$C_{140} = 0.31961762\mathrm{E}{-01}$	$C_{141} = 0.11604787\mathrm{E}{+01}$
$C_{142} = -0.19595221\mathrm{E}{+00}$	$C_{143} = -0.88366935\mathrm{E}{+00}$	$C_{144} = 0.14435189\mathrm{E}{+01}$
$C_{145} = -0.21390063\mathrm{E}{+00}$	$C_{146} = -0.62564293\mathrm{E}{+00}$	$C_{147} = 0.53400304\mathrm{E}{+00}$
$C_{148} = -0.25046792\mathrm{E}{+00}$	$C_{149} = -0.43312630\mathrm{E}{+01}$	$C_{150} = 0.70645975\mathrm{E}{+00}$
$C_{151} = -0.11923902\mathrm{E}{+01}$	$C_{152} = 0.42006153\mathrm{E}{+00}$	$C_{153} = -0.37793442\mathrm{E}{+00}$
$C_{154} = -0.20340238\mathrm{E}{+01}$	$C_{155} = -0.38184706\mathrm{E}{+00}$	$C_{156} = -0.19185785\mathrm{E}{+00}$
$C_{157} = -0.78841100\mathrm{E}{+00}$	$C_{158} = 0.34216901\mathrm{E}{+00}$	$C_{159} = 0.74795225\mathrm{E}{+00}$
$C_{160} = 0.56923700\mathrm{E}{+00}$	$C_{161} = 0.51196399\mathrm{E}{+00}$	$C_{162} = 0.16941512\mathrm{E}{+00}$
$C_{163} = 0.27699812\mathrm{E}{+00}$	$C_{164} = 0.55072932\mathrm{E}{+00}$	$C_{165} = -0.19439041\mathrm{E}{+00}$
$C_{166} = 0.11101788\mathrm{E}{-01}$	$C_{167} = -0.26070196\mathrm{E}{+00}$	$C_{168} = 0.91524140\mathrm{E}{-01}$

TABLE 7: Stationary Points of Dmbe II Potential Energy Surface[a]

	R_1/a_0	R_2/a_0	R_3/a_0	E/E_h	ΔE	ω_1	ω_2	ω_3
HCN	2.179	2.013	4.192	−0.4992	313.3[b]	3446.71	727.98	2131.52
	(2.179)[c]	(2.013)[c]	(4.192)[c]		(313.07 ± 0.25)[d]	(3443.1)[e]	(727.0)[e]	(2127.4)[e]
HNC	2.209	4.087	1.878	−0.4750	15.19	3812.80	462.82	2057.37
	(2.209)[f]	(4.087)[f]	(1.878)[f]		(14.8 ± 1.0)[g]	(3813.4, 3816.6)[h]	(460.5, 468.2)[h]	(2059.1, 2059.9)[h]
CNH[†]	2.244	2.237	2.625	−0.4237	47.38	2924.61	1201.01i	2035.80
	(2.258)[i]	(2.241)[i]	(2.634)[i]		(48.4 ± 1.0)[g]			
TS2	5.161	3.129	2.032	−0.1208		3559.54	611.83i	299.32
TS3	5.794	3.710	2.084	−0.1189		2700.69	296.60	345.06i
TS4	6.023	2.719	3.304	−0.0677		2089.23i	644.68	664.75

[a] Harmonic frequencies are in cm^{-1} and ΔE in kcal mol^{-1}. Experimental and other theoretical values are presented in parentheses. [b] Atomization energy. [c] Experimental geometry (see ref 70). [d] Atomization energy best estimate (see ref 49). [e] Experimental harmonic frequencies (see ref 42). [f] Experimental geometry from ref 71. [g] Theoretical estimate (see ref 80). [h] Experimental harmonic frequencies (see refs 47 and 48). [i] Theoretical estimate (see ref 2).

In eq 7, the upper limit of the second summation should be 2:

$$C_n^{L,A-BC}(R) = D_M(1 + \sum_{i=1}^{3} a_i r^i) \exp(-\sum_{i=1}^{2} b_i r^i) + C_n^{AB} + C_n^{AC} \quad (7)$$

Equation 12 should read:

$$\theta_a = \mp \arctan\{2 \sin\theta(8C_5 \cos\theta + C_4 R)/ \{[256C_5^2 \sin^2\theta \cos^2\theta + 2C_4 C_5 R \cos\theta(36 - 25\sin^2\theta) + 361C_5^2 \sin^4\theta + 9C_4^2 R^2 + 144C_5^2 - (5C_4^2 R^2 + 456C_5^2)\sin^2\theta]^{1/2} \mp 3C_4 R \cos\theta \pm C_5(19\sin^2\theta - 12)\}\} \quad (12)$$

The analytic dependence of the NH quadrupole in the internuclear distance, as well as the carbon atom quadrupole, $Q_C = 1.430\ ea_0^2$, has been taken from ref 1.

Some data misassignment has been detected in the Fortran code, calling for an update of the HCN DMBE potential function. The new frequencies are within 1 cm^{-1} of the reported ones, with an identical rmsd (new Tables 1−4 are available as Supporting Information). The rmsd of the ab initio data in Table 6 is within the accuracy originally reported. All major topographical features of the potential function are identical. The new coefficients are shown in the new Table 5. Although keeping identical stationary points, these show slightly different attributes (new Table 7).

Acknowledgment. We thank Professor Alan Isaacson (Miami University) for carefully testing the potential and calling the authors' attention to some misprints.

Supporting Information Available: Corrected versions of Tables 1−4 from the original Article. This material is available free of charge via the Internet at http://pubs.acs.org.

References and Notes

(1) Rodrigues, S. P. J.; Varandas, A. J. C. *Phys. Chem. Chem. Phys.* **2000**, *2*, 435.

10.1021/jp073029z
Published on Web 05/10/2007