

CHAPTER - 3

CALCULATIONS OF RKR_V POTENTIAL ENERGY CURVES
FOR
NON-POLAR DIATOMIC MOLECULES USING GMR FUNCTION

3.1 THE RKR^V PROCEDURE

The calculation of potential energy curves for the bound states of diatomic molecules using analytical functions is found inadequate when accurate potential energy curves are required. In this case the RKR^V method¹ is commonly used. In this method the experimentally known vibrational energy levels of a molecule are employed to calculate points on P.E. curve corresponding to the classical turning points of the nuclear motion. This determines very accurately pair of points on the P.E. curve up to the highest vibrational energy levels known experimentally. Though RKR^V is a WKB method, the results near the minimum agree with the curve calculated by Dunham procedure which is known to be accurate in this region. However, by this method the P.E. curve can be constructed in the region for which sufficient spectroscopic data exist.

There are many modified versions of the method available as we have described in Sec. 1.2.1. Though the method is laborious its great advantage is that it makes use of the experimental levels without reference to any empirical function for representing the potential energy curve. Further the ready availability of microcomputers and programmable calculators enables one to carry out the laborious calculations rapidly and more efficiently. The method is very useful to test validity of a given empirical function in evaluating the accurate dissociation energy values for maximum number of diatomic molecules.

The usual procedure to test a given potential function is the curve fitting in which r_{\min} and r_{\max} values obtained by RKR data are substituted in an expression for the potential function and the potential energy is calculated in wavenumbers (cm^{-1}) for a given value of dissociation energy (D_e) of the molecule. The values of D_e are varied until the best fit to the true potential curve is achieved i.e. the calculated values of potential energy should be comparable to the experimental $G(v)$ values in RKR data. In order to determine the best fit among the empirical potential curve and the true curve, the following criteria¹⁰ are usually used :

- i) the near equality of U_{\min} and U_{\max} with U_{RKR} for a large number of vibrational levels.
- ii) the minimum average % deviation of U values as a function of $G(v)$ values.
- iii) the minimum average % deviation of U values as a function of dissociation energy.
- iv) the best agreement between the average deviation of U_{\min} and U_{\max} to that of U_{RKR} values.
- v) the maximum value of correlation coefficient representing the best fit.

Validity of D_e values estimated by the curve fitting method depends upon the extent to which a given empirical function fits the true potential energy curve. It is well known that the more the number of parameters in the potential function, the greater is its ability to reproduce RKR curves.

However, usually a three parameter potential function is preferred in view of limited number of molecular data for diatomic molecules. The best fit should be achieved at least for lower vibrational levels. For higher levels one needs the knowledge of the rotational constant B_e . The calculated potential energy values are normally expressed in wavenumbers (i.e. cm^{-1}) instead of electron volts because even a 0.01 eV energy corresponds to about 80.6 cm^{-1} .

3.2 RKR CURVES FOR GMR FUNCTION

In the present work we have chosen the modified RKR method due to Reddy and Reddy¹ because by this procedure one can evaluate the true turning points directly by means of experimentally $G(v)$ values for various vibrational levels only. The knowledge of two r_{\min} and two r_{\max} values from RKR method is not required. As a consequence this method is seen to be more rapid than any other method available at present to our knowledge. We have chosen GMR function⁶ as the empirical function to calculate potential energy curves for a number of diatomic molecules by varying the respective dissociation energies and to estimate D_e values giving the best fits. For a comparative study, Morse and Rydberg functions have also been utilised in this connection.

The necessary molecular data is taken from Huber and Herzberg⁷ and the same have been listed in Table 3.1. In order to carry out rapid and accurate computations of potential energy curves

and the average % deviations, we have developed suitable computer programs in BASIC as given in Tables 3.2-3.4. Our calculated results have been presented in two ways. For the first nine molecules mentioned in Table 3.1, we have given the graphical illustrations of RKR potential energy curves corresponding to respective D_e values giving the best fits. In the case of remaining six molecules in Table 3.1 however, we have presented our RKR results in Tables 3.5-3.10.

3.3 RESULTS AND DISCUSSION

a) Graphical Illustration of RKR Curves

Figs. 3.1 and 3.2 include RKR potential energy curves for the AgCl and AgH molecules in their ground state ($X^1\Sigma^+$). By the linear Birge-Sponer extrapolation method the dissociation energy for AgCl is found to be 3.1 eV in agreement with thermochemical results. In the present work we have varied D_e value in the range 3 to 3.45 eV in the step of 0.15 eV. We find that the best curve fitting is observed for a D_e value of 3.15 eV. This is quite close to the thermochemical value. Further the corresponding P.E. curves with the GMR function closely follows the RKR curves for Morse and Rydberg potential.

The excited state P.E. curves for AgH molecule is reported to be anomalous having a hump in the right limb. For the ground state the convergence of vibrational levels in AgH is found to be approximately linear at lower v'' values. Its rate increases at higher v'' values. The extrapolation has given a value of 2.3 eV to the

dissociation energy of AgH molecule. However, in our work the GMR P.E. curve for $X^1\Sigma^+$ state leads to a value of 2 eV for the dissociation energy resulting from the curve fitting. The GMR curve is in close agreement with Morse and Rydberg curves in the L.H.S. limbs, while there is increasing asymptotic variation in the right limb.

In Fig. 3.3 we have given the RKR V P.E. curve for AlSe molecule in the state $2\Sigma^-$. The vibrational analysis of AlSe molecules in the region 3900-4610 A^0 has been reported for the first time by Singh et al³ both in emission and absorption. The higher resolution studies of emission spectrum of AlSe in the region 3700-4700 A^0 were carried out by Lavendy et al⁴. Rao et al⁵ have calculated a dissociation value 2.257 eV by the curve fitting method using Lippincott potential function. This estimated value is lower than the thermochemical value of 3.46 eV given by Huber and Herzberg. This discrepancy has been attributed by Rao et al⁵ to the strong ionic binding in the ground state of AlSe molecule. The RKR V P.E. curve for the present work using GMR function gives a best fit for the value of 2.25 eV which is in good agreement with the value reported by Rao et al⁵.

The RKR V curves for Br_2 molecules are illustrated in Fig. 3.4. Employing GMR function the dissociation energy was varied from 1.8 eV to 2.2 eV by small step. The best curve fitting is found to be at 2 eV which is in good agreement with the experimentally

observed value of 1.991 eV. The GMR curve closely follows the curves due to Morse and Rydberg in the L.H.S. and R.H.S limbs at low lying vibrational levels. However, towards asymptote, it lies somewhat below the other curves.

Diatomic chromium fluoride CrF is an example of molecules involving transition metals in the middle of the periodic table. It gives rise to complex spectrum due to transitions in the electronic state having high multiplicities. Dubov and Shenyavaskaya⁸ have recently re-examined the CrF molecule in emission as well as in absorption and reported the molecular constants of $A^6\Sigma-X^6\Sigma$ transition as listed in Table 3.1 of this thesis. We have constructed the RKR curves of CrF molecule using this molecular data and have reported these in Fig. 3.5. The dissociation energy values were varied from 3 to 4 eV in the expression for GMR function and the best curve fitting was found to be at 3.7 eV. This value is in excellent agreement with one obtained by Bhartiya and Behere⁹ using the correlation coefficient method due to Rao et al¹⁰. The GMR curve satisfactorily follows the other two curves for $r < r_e$. It however, shows a little shift on higher r side in the R.H.S. limb.

The CrO molecule is astrophysically important and its spectra have been observed in the β -Pegasi Stars¹. Reddy and Reddy¹ have constructed the RKR curve for this molecule in the ground state ($X^5\Pi$). They have found that the Hulbert-Hirschfelder function fits the curve best when $D_e = 4.311$ eV. In the present work we have constructed the RKR curve by employing the GMR function (Fig. 3.6)

and for the best fit have obtained the dissociation energy value of 2.8 eV which is comparatively lower. The GMR function seems to be unsuitable to give the best fit of dissociation energy of CrO molecule. However, our value of 2.8 eV is in agreement with that predicted by the Lippincott function.¹ The GMR curve reproduces satisfactorily the other RKR curves given in Fig. 3.6.

In Fig. 3.7 we have given the RKR curves for CN molecule in its ground state ($X^2\Sigma^+$). The dissociation energy value of 8.5 eV gives the best fit using the GMR function.

The GMR curve closely follows the other RKR curves both for $r < r_e$ and $> r_e$ when we consider low lying vibrational states. The GMR curve shows a deviation in the asymptote part and it lies below the Morse and Rydberg asymptote. The RKR curves for N_2 molecule in its ground state are depicted in Fig. 3.8. The best fit with GMR function is obtained at value of 10.3 eV for dissociation energy which is slightly higher than the experimental value of 9.901 eV. The GMR curve is in satisfactorily good agreement with the Morse and Rydberg RKR curves.

The PN molecule being astrophysically important we constructed its RKR curves both for ground state ($X^1\Sigma^+$) and excited states ($A^1\Pi$ and $A^2\Pi$). In Fig. 3.9 we have reported the curves only for $A^1\Pi$ state. The calculations of remaining curves are presented in tabular form to be discussed in the next section. The best fit yields a value of 6.2 eV for the dissociation energy.

b) **Tabular Presentation of RKR_V Curves**

The calculated turning points of RKR_V and different sets of potential energy (U) values corresponding to these points obtained by employing GMR, Morse and Rydberg empirical functions for the last six molecules in Table 3.1 have been presented in Tables 3.5-3.10. In determining the best fit among potential curves we have adopted the criterion (i) given in Sec.3.1

Comparing the potential energy values in all the Tables we find that our GMR function evaluates U_{\min} and U_{\max} in very good agreement with the corresponding Morse energy values for almost all the vibrational levels of a given molecule. Further these values satisfactorily reproduce the respective experimental $G(v)$ values for nearly all the vibrational levels. However, in this connection the Rydberg function is found to be more accurate than the GMR or Morse function. The potential energy curve calculations presented in this work are mostly for excited states of the molecules under consideration. For each molecule the dissociation energy value has been selected on the basis of best fit between the RKR_V and empirical curves. Therefore the reported values of dissociation energies for excited states of different molecules may be treated as accurate ones. Further these values are found to be less than the corresponding experimental values for the ground states of respective molecules. For example in the case of AlSe ($A^2 \Sigma^+$), $N_2(A^3 \Sigma^+)$, $P_2(1 \Sigma_u)$ and $PN^+(A^2 \Pi)$ molecules, the dissociation energy values are reported to be 1.2 (3.4), 3.7(9.759), 3.3 (5.033) and 5.4(5.00)eV

respectively. The bracketed values correspond to the respective ground states of the molecules. Only $C_2(A^3\Pi_u)$ molecule is found to be an exception to these observations. In this case we have obtained D_e value of 6.25 eV which is slightly higher than the value of 6.21 eV observed experimentally for ground state. In Table 3.9 we have presented the RKR calculations for the ground state ($X^1\Sigma^+$) of PN molecule. By the best fit procedure we have calculated a value of 6.3 eV for the dissociation energy in very good agreement with the experimental value of 6.36 eV.

3.4 SUMMARY

In the beginning of this chapter the importance of the RKR method has been briefly outlined by giving its features. Next the actual RKR procedure is described by giving the usual criteria which are followed to determine the best fit among the empirical and true curves. We have chosen our GMR function as an empirical function to obtain potential energy curves for different molecules by following the modified RKR method given by Reddy and Reddy¹. Suitable computer programs for rapid and accurate computations of the potential curves have been reported. The calculations of the RKR curves using GMR, Morse and Rydberg functions have been presented both graphically and in tabular forms. Among the different diatomic molecules chosen for this study, there are some molecules like AgCl, AgH and Br_2 which are partly ionic and partly covalent in nature. The dissociation energy values for these molecules along with others have been determined by the best fit procedure. In general the D_e

values so fixed for the ground states of the respective molecules are in reasonably good agreement with the corresponding experimental values. In particular the reproducibility of the potential energy curves for AgCl, AgH and Br₂ molecules by using GMR function as an empirical potential shows that this function can be successfully applied to molecules with less ionicity and partial covalency. Lastly the potential energy curve calculations for the excited states of some molecules have also been worked out.

† TABLE 3.1
MOLECULAR DATA USED IN THE CALCULATIONS

Molecule	State	μ (a.m.u.)	ω (cm^{-1})	$\omega_e x_e$ (cm^{-1})	B_e (cm^{-1})	α_e (cm^{-1})	r_e (Å)	D_e (D_0^0) (eV)
AgCl	X $1^1\Sigma^+$	26.3497888	343.49	1.17	0.12298388	0.0005954	2.280792	3.22
AgH	X $1^1\Sigma^+$	0.99841289	1759.9	34.06	6.449	0.201	1.618	2.28
AlSe	X $2^2\Sigma^+$	20.1712814	472.6	2.81	0.1793	0.0011	2.158	3.4
Br ₂	X $1^1\Sigma_g^+$	39.459166	325.321	1.0774	0.082107	0.0003187	2.2810	1.9707
CrF ^{**}	X $6^6\Sigma_g$	13.9103739	662.3	3.4	0.379	0.002596	1.785	-
CrO [*]	X $5^5\Pi$	12.2290254	898.5	6.72	0.526648	0.004434	1.6179	4.4
CN	X $2^2\Sigma^+$	6.46219329	2068.59	13.087	1.8997	0.01736	1.1718	7.7
N ₂	X $1^1\Sigma_g^+$	7.00153720	2358.57	14.324	1.99824	0.017318	1.09768	9.759
PN	A $1^1\Pi$	9.6433616	1103.09	7.222	0.7307	0.00663	1.5467	6.3
AlSe	X $2^2\Sigma^+$	20.1712816	391.72	1.56	0.1569	0.0008	2.307	3.4
C ₂	A $3^3\Pi_u$	6.000000	1641.35	11.67	1.6324	0.01661	1.3119	6.21
N ₂	A $3^3\Sigma_u^+$	7.00153720	1460.64	13.87	1.4546	0.0180	1.2866	9.759
P ₂	C $1^1\Sigma_u^+$	15.4868817	473.93	2.340	0.24211	0.00175	2.1204	5.033
PN	X $1^1\Sigma^+$	9.6433616	1337.24	6.983	0.7864854	0.0055364	1.490866	6.3
PN(ionic)	A $2^2\Pi$	9.6433616	1106.09	7.222	0.7307	0.00663	1.5467	5.0

* Ref.(1) , † Ref.(7) , ** Ref.(8)

TABLE 3.2
 COMPUTER PROGRAM FOR RKRVM POTENTIAL ENERGY
 CURVES (REDDY & REDDY) METHOD

```

10 REM"File RKRVM"
20 PRINT "U","RN","RM"
30 REM RKRVM P.E. CURVES: Reddy & Reddy Method
40 REM"U=Dissociation E.,RN=r-min, RM=r-max
50 REM"Br2 Molecule
60 W= 325.32
70 WX=1.0774
80 B=.0821
90 A=.0003187
100 RE=2.281
110 U3=1118.45
120 U4=1433.12
130 INPUT U
140 P=(B/W)^.5
150 K=WX/W
160 M=A/B
170 B3=3.75-12.15*M
180 B4=2.917-7.35*M
190 H1=1-3*M
200 H2=1-(7/3)*M
210 B1=(3.75/H1)-(B3/H1^2)+135*P^2
220 B2=(2.917/H2)-(B4/H2^2)+82*P^2
230 G1=18*P^2+(1/H1)
240 G2=14*P^2+(1/H2)
250 X=P*(.501+5*K+43.1*K^2)
260 BG=(B1/(2*G1^.5))-(B2/(2*G2^.5))
270 G=(G1^.5)-(G2^.5)
280 R1=(BG*K+G+X)*RE
290 R2=(BG*K+G-X)*RE
300 M1=LOG((W-(4*WX*U4)^.5)/(W-(4*WX*U3)^.5))/(R1)
310 M2=LOG((W+(4*WX*U4)^.5)/(W+(4*WX*U3)^.5))/(R2)
320 PK=P*(3.74166+10.9132*K+49.273*K^2)
330 R3=((B2*K/(2*G2^.5))+G2^.5+PK)*RE
340 R4=((B2*K/(2*G2^.5))+G2^.5-PK)*RE
350 C1=LOG(W-(4*WX*U3)^.5)-M1*R3
360 C2=LOG(W+(4*WX*U3)^.5)-M2*R4
370 RM=(LOG(W-(4*WX*U)^.5)-C1)/M1
380 RN=(LOG(W+(4*WX*U)^.5)-C2)/M2
390 PRINT U, RN, RM
400 END

```

TABLE 3.3
 COMPUTER PROGRAM FOR POTENTIAL ENERGY
 CURVES ON GMR FUNCTION

```

10 REM"File:Dienergy
20 REM"Dissociation Energy of CN Molecule--GMR Function
30 REM"Programming by Shri.V.M.Patil"
40 W=2068.59
50 M=6.46219329#
60 RE=1.1718
70 INPUT U, RN, RM
80 K=.058883*M*((W)^2)
90 FOR D=7.6 TO 7.8 STEP .05
100 D1=((K*(RE)^2)/(2*D))*6.241307E-05
110 B=(D1)^.5
120 XM=(RM-RE)/RE
130 XN=(RN-RE)/RE
140 UM1=D*(1-EXP(-B*XM))^2*8065.47
150 UN1=D*(1-EXP(-B*XN))^2*8065.47
160 UM=UM1+(D*((1+B*XM)*(XM^3)*EXP(-2*B*XM))-
  D*(XM^3)*EXP(-B*XM))*8065.47
170 UN=UN1+(D*((1+B*XN)*(XN^3)*EXP(-2*B*XN))-
  D*(XN^3)*EXP(-B*XN))*8065.47
180 EUM=((UM-U)/U)*100
190 EUN=((UN-U)/U)*100
200 PRINT "D=";D;"eV"
210 PRINT"rn=";RN, "Un=";UN, "EUn=";EUN
220 PRINT "rm=";RM, "Um=";UM, "EUm=";EUM
230 PRINT "Un1=";UN1; "Um1=";UM1
240 PRINT D1, K
250 NEXT D
260 END

```

TABLE 3.4

COMPUTER PROGRAM FOR POTENTIAL ENERGY
CURVES ON MORSE RYDBERG FUNCTIONS

```

10 REM"File:MR-pot
20 REM"Dissociation Energy of CN Molecule--Morse Rydberg Function"
30 REM"Programming by Shri.V.M.Patil"
40 W=2068.59
50 M=6.46219329#
60 RE=1.1718
70 INPUT U,RN,RM
80 REM"U=exptl.Dissociation E.,RN=r-min,RM-r-max"
90 REM"UM1=U-max.,UN1=U_min.,EUM1=% in U-max.,EUN1=% in U-min."
100 K=.058883*M*((W)^2)
110 PRINT "K=";K;"dyne/cm"
120 FOR D=7.6 TO 7.8 STEP .05
130 D1=((K*(RE)^2)/(2*D))*6.241807E-05
140 B=(D1)^.5
150 B2=B*1.4142
160 XM=(RM-RE)/RE
170 XN=(RN-RE)/RE
180 UM1=D*(1-EXP(-B*XM))^2*8065.47
190 UN1=D*(1-EXP(-B*XN))^2*8065.47
200 UM2=(-D*((1+B2*XM)*EXP(-B2*XM))+D)*8065.47
210 UN2=(-D*((1+B2*XN)*EXP(-B2*XN))+D)*8065.47
220 EUM1=((UM1-U)/U)*100
230 EUN1=((UN1-U)/U)*100
240 EUM2=((UM2-U)/U)*100
250 EUN2=((UN2-U)/U)*100
260 PRINT "D=";D;"eV"
270 PRINT "rn=";RN,"Un1=";UN1,"EUn1=";EUN1
280 PRINT "rm=";RM,"Um1=";UM1,"EUm1=";EUM1
290 PRINT "rn=";RN,"Un2=";UN2,"EUn2=";EUN2
300 PRINT "rm=";RM,"Um2=";UM2,"EUm2=";EUM2
310 NEXT D
320 END

```

TABLE 3.5

POTENTIAL ENERGY CURVE CALCULATIONS FOR AISE ($A^2 \Sigma^+$)

G (v) @ (cm^{-1})	RKR Reddy & Reddy		GMR		Morse		Rydberg	
	r_{\min}^A	r_{\max}^A	D_e	D_e	D_e	D_e	D_e	D_e
	\AA	\AA	eV cm^{-1}	eV cm^{-1}	eV cm^{-1}	eV cm^{-1}	eV cm^{-1}	eV cm^{-1}
			U_{\min}	U_{\max}	U_{\min}	U_{\max}	U_{\min}	U_{\max}
195.46	2.2462	2.3733	193.86	175.04	193.86	175.04	192.30	176.39
583.78	2.2029	2.4283	626.94	521.39	626.91	521.42	617.91	528.36
968.21	2.1746	2.4683	1080.03	849.02	1079.91	849.13	1059.70	863.52
1348.22	2.1526	2.5022	1544.64	1160.15	1544.36	1160.41	1509.98	1183.33
1719.71	2.1345	2.5322	2012.10	1453.58	2011.56	1454.07	1960.72	1486.09
2092.96	2.1185	2.5603	2493.21	1738.77	2492.32	1739.56	2422.52	1781.27
2456.65	2.1045	2.5863	2971.99	2008.17	2970.65	2009.31	2880.21	2086.86
2813.87	2.0920	2.6109	3451.05	2265.14	3449.17	2266.77	3336.47	2328.19
3164.1	2.0806	2.6342	2928.67	2510.20	3926.13	2512.37	3789.78	2583.65
3506.82	2.0703	2.6564	4403.14	2743.76	4399.84	2746.55	4238.65	2827.54
3841.51	2.0608	2.6778	4873.012	2966.14	4868.85	2969.61	4681.84	3060.12

@ Ref. (5)

TABLE 3.6
 POTENTIAL ENERGY CURVE CALCULATIONS FOR $C_2(A^3\Pi_u)$

$G(v)$ (cm^{-1})	RKR Reddy and Reddy		GMR		Morse		Rydberg	
	r_{min} A^0	r_{max} A^0	U_{min} cm^{-1}	D_e e	U_{min} cm^{-1}	D_e e	U_{min} cm^{-1}	D_e e
817	1.2568	1.3742	819.93	6.25	819.90	6.25	813.84	819.77
2435	1.2203	1.4249	2458.27	6.25	2457.79	6.25	2403.62	2433.70
4030	1.1970	1.4627	4084.22	6.25	4082.60	6.25	3955.86	4019.30
5601	1.1790	1.4953	5693.48	6.25	5689.91	6.25	5473.39	5576.37
7149	1.1642	1.5250	7285.79	6.25	7279.38	6.25	6958.99	7106.13

@ Ref. (11)

TABLE 3.7
 POTENTIAL ENERGY CURVE CALCULATIONS FOR $N_2(A^3\Sigma_u^+)$

G(v) cm ⁻¹	RKR (Reddy & Reddy)		GMR		Morse		Rydberg
	r _{min} (A ⁰)	r _{max} (A ⁰)	U _{min} (cm ⁻¹)	U _{max} (cm ⁻¹)	D _e (3.7 eV)	D _e (3.7 eV)	D _e (3.7 eV)
			U _{min} (cm ⁻¹)	U _{max} (cm ⁻¹)	U _{min} (cm ⁻¹)	U _{max} (cm ⁻¹)	U _{min} (cm ⁻¹) U _{max} (cm ⁻¹)
726.7	1.2336	1.3487	721.63	721.40	721.60	721.43	715.23 727.82
2159.6	1.1982	1.3995	2215.21	2087.56	2214.79	2088.13	2180.82 2119.76
3564.9	1.1758	1.4378	3710.60	3396.26	3709.16	3398.33	3636.00 3463.77
4942.3	1.1587	1.4713	5195.85	4655.77	5192.65	4650.63	5072.15 4765.18
6291.9	1.1446	1.5021	6666.17	5969.99	6660.42	5879.15	6486.23 6026.32
7613.7	1.1327	1.5312	8118.82	7041.3	8109.70	7056.46	7876.69 7248.50
8907.2	1.1222	1.5592	9550.73	8170.90	9537.44	8193.94	9241.46 8432.17
10172.4	1.1129	1.5865	10960.69	9260.24	10942.42	9293.13	10580.04 9578.11
11409.1	1.1045	1.6132	12347.12	10310.16	12323.09	10354.92	11891.52 10686.61
12616.8	1.0969	1.6396	13708.19	11321.3	13677.66	11380.14	13174.65 11757.82

TABLE 3.8

POTENTIAL ENERGY CURVE. CALCULATIONS FOR $P_2(\Sigma_u^{1,+})$

G(v) (cm^{-1})	RKR (Reddy and Reddy)		GMR		Morse		Rydberg	
	$r_{\min}(\text{A}^{\circ})$	$r_{\max}(\text{A}^{\circ})$	$D_e = 3.3 \text{ eV}$	$U_{\min}(\text{cm}^{-1})$	$U_{\max}(\text{cm}^{-1})$	$D_e = (3.3 \text{ eV})$	$U_{\min}(\text{cm}^{-1})$	$U_{\max}(\text{cm}^{-1})$
236.9	2.0556	2.1907	237.01	230.63	237.01	230.64	235.73	231.87
708.7	2.013	2.2491	690.30	714.48	690.25	714.55	683.94	721.28
1179.1	1.9853	2.2922	1137.05	1202.58	1136.88	1202.86	1123.58	1217.52
1633.2	1.9643	2.3282	1565.61	1676.50	1565.25	1677.15	1543.82	1701.27
2086.6	1.9466	2.3610	1991.59	2151.53	1990.94	2152.78	1960.28	2187.82
2534.6	1.9313	2.3914	2410.98	2622.95	2409.97	2624.37	2369.22	2671.46
2983.7	1.9175	2.4201	2830.18	3095.26	2828.70	3098.55	2776.99	3158.86
3424.7	1.9053	2.4480	3240.77	3560.60	3228.72	3565.40	3175.50	3639.70
3862.6	1.8940	2.4748	3647.58	4023.42	3644.86	4030.10	3569.52	4119.18
4295.8	1.8837	2.5006	4049.21	4481.87	4045.73	4490.84	3957.77	4595.36
4725	1.8741	22.5260	4446.43	4936.59	4442.08	4948.27	4341.05	5068.83

* Ref. (12)

TABLE 3.9
POTENTIAL ENERGY CURVE CALCULATIONS FOR $\text{PN}(\text{X } ^1\Sigma^+)$

* G(v) (cm^{-1})	RKR (Reddy and Reddy)		GMR		Morse		Rydberg	
	$r_{\min}(\text{A}^0)$	$r_{\max}(\text{A}^0)$	$D_e(6.3 \text{ eV})$	$U_{\min}(\text{cm}^{-1})$	$U_{\max}(\text{cm}^{-1})$	$D_e(6.3 \text{ eV})$	$U_{\min}(\text{cm}^{-1})$	$U_{\max}(\text{cm}^{-1})$
666.76	1.4426	1.5450	666.07	661.95	666.65	661.33	662.26	665.68
1981.95	1.4099	1.5877	2023.72	1932.36	2023.54	1932.59	2000.67	1954.20
3299.37	1.3884	1.6195	3403.52	3185.42	3402.87	3186.26	3353.23	3231.98
4595.05	1.3718	1.6465	4773.51	4403.47	4772.05	4405.44	4689.93	4479.65
5877.02	1.3580	1.6709	6139.09	5596.51	6136.45	5600.24	6017.11	5706.37
7145.32	1.3461	1.6936	7498.65	6766.03	7494.40	6772.23	7333.83	6913.00
8399.97	1.3355	1.7150	8850.94	7912.99	8844.65	7922.46	8639.37	8100.05
9640.99	1.3260	1.7355	10195.23	9038.15	10186.46	9051.77	9933.41	9267.92
10868.44	1.3173	1.7553	11530.63	10142.05	11518.93	10160.75	11215.41	10416.85
12082.33	1.3094	1.7746	12856.76	11225.27	12841.67	11250.04	12485.25	11547.22
13282.69	1.3020	1.7934	14173.22	12288.24	14154.29	12320.13	13742.79	12659.23

* Ref. (13)

TABLE 3.10
 POTENTIAL ENERGY CURVE CALCULATIONS FOR $\text{PN}(\text{A } 2\Pi)$

G(v) (cm^{-1})	RKRv		GMR		Morse		Rydberg	
	$r_{\min}(\text{A}^0)$	$r_{\max}(\text{A}^0)$	$U_{\min}(\text{cm}^{-1})$	$U_{\max}(\text{cm}^{-1})$	$D_e = 5.4 \text{ eV}$	$U_{\min}(\text{cm}^{-1})$	$U_{\max}(\text{cm}^{-1})$	$D_e = 5.4 \text{ eV}$
549.74	1.4933	1.6061	555.64	548.13	555.14	548.14	551.56	551.66
1638.39	1.4586	1.6549	1623.99	1654.29	1623.82	1654.54	1606.05	1673.02
2712.59	1.4363	1.6911	2671.54	2749.36	2670.98	2750.97	2633.66	2789.87
3773.35	1.4190	1.7224	3702.52	3831.80	3701.29	3834.01	3648.62	3899.08
4817.66	1.4048	1.7505	4715.27	4897.82	4713.08	4902.06	4626.17	4995.93
5848.53	1.3925	1.7772	5713.33	5949.98	5709.87	5957.14	5594.32	6082.53
6864.96	1.3817	1.8023	6696.23	6986.97	6691.19	6998.03	6544.97	7157.16
7866.94	1.3719	1.8266	7664.09	8008.55	7657.16	8024.63	7478.49	8219.13
8854.48	1.3631	1.8501	8617.22	9014.56	8608.10	9036.84	8395.71	9268.55
9827.57	1.3551	1.8731	9555.70	10004.89	9544.08	10034.67	9296.65	10304.59
10786.22	1.3476	1.8956	10479.84	10979.29	10465.41	11017.92	10181.85	11326.96

* Ref. (13)

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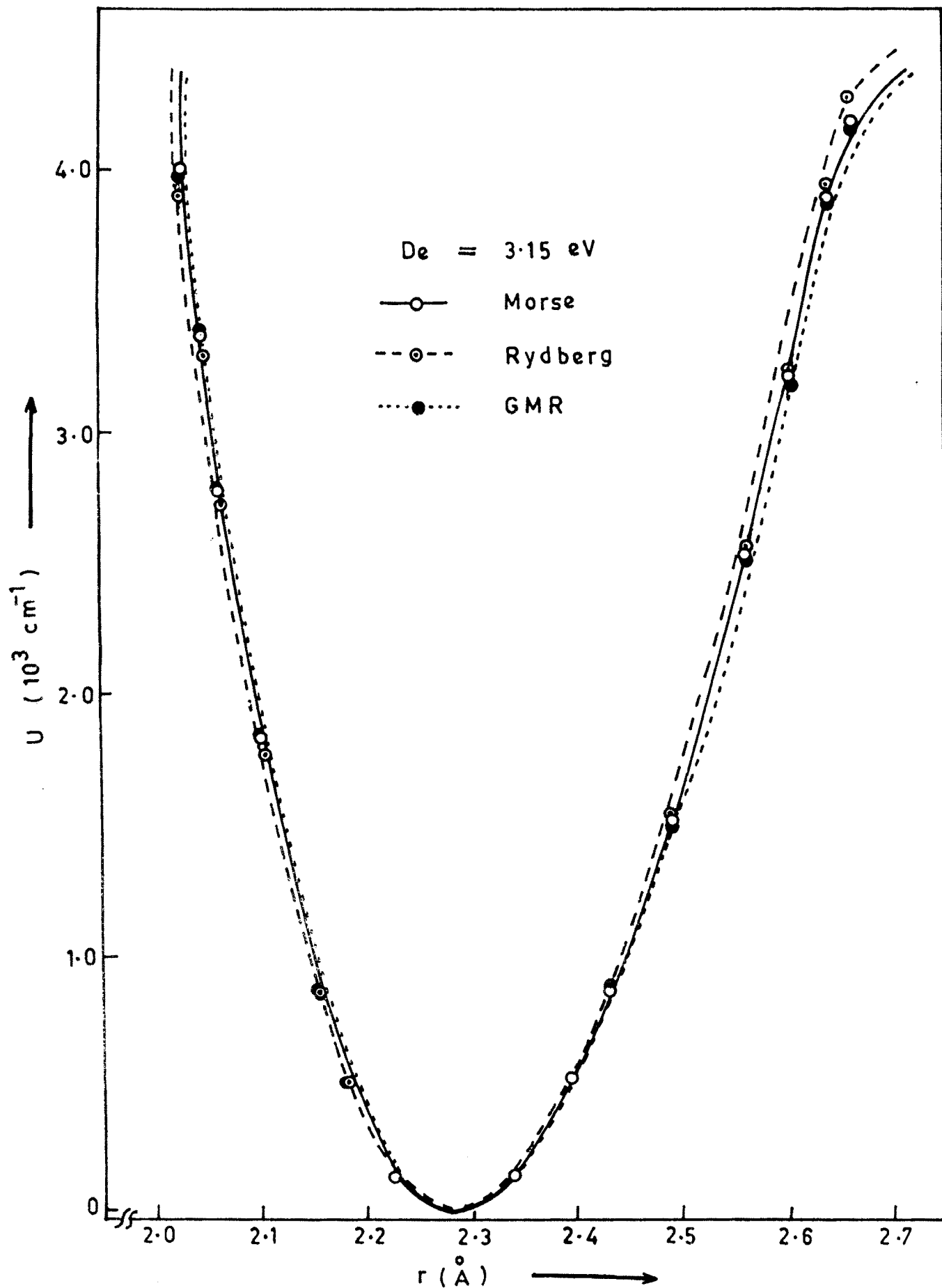


FIG. 3-1 — RKR POTENTIAL ENERGY CURVES FOR $\text{AgCl} (X^1 \Sigma^+)$.

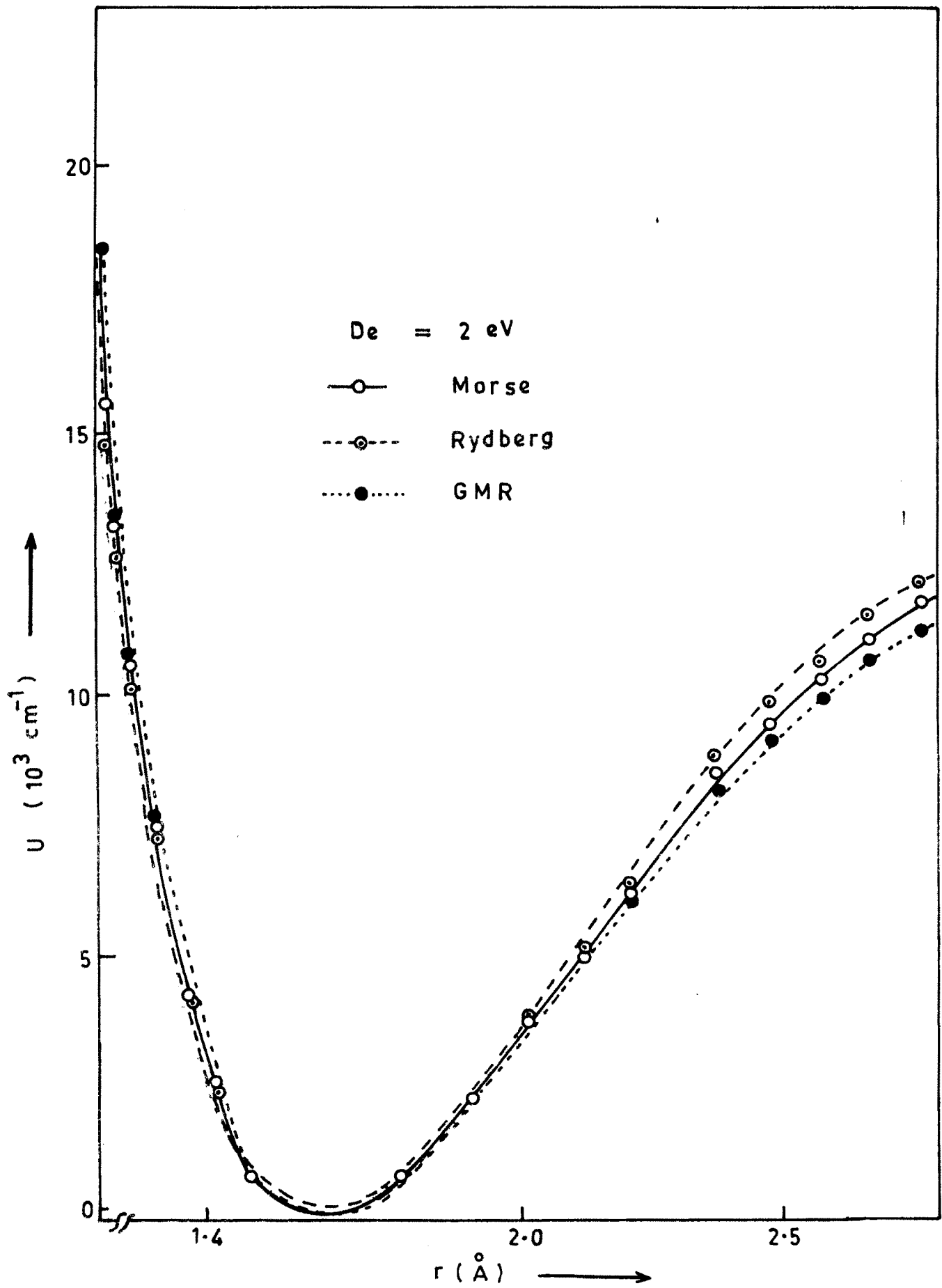


FIG. 3-2 - RKR V POTENTIAL ENERGY CURVES FOR $\text{AgH} (X^1\Sigma^+)$.

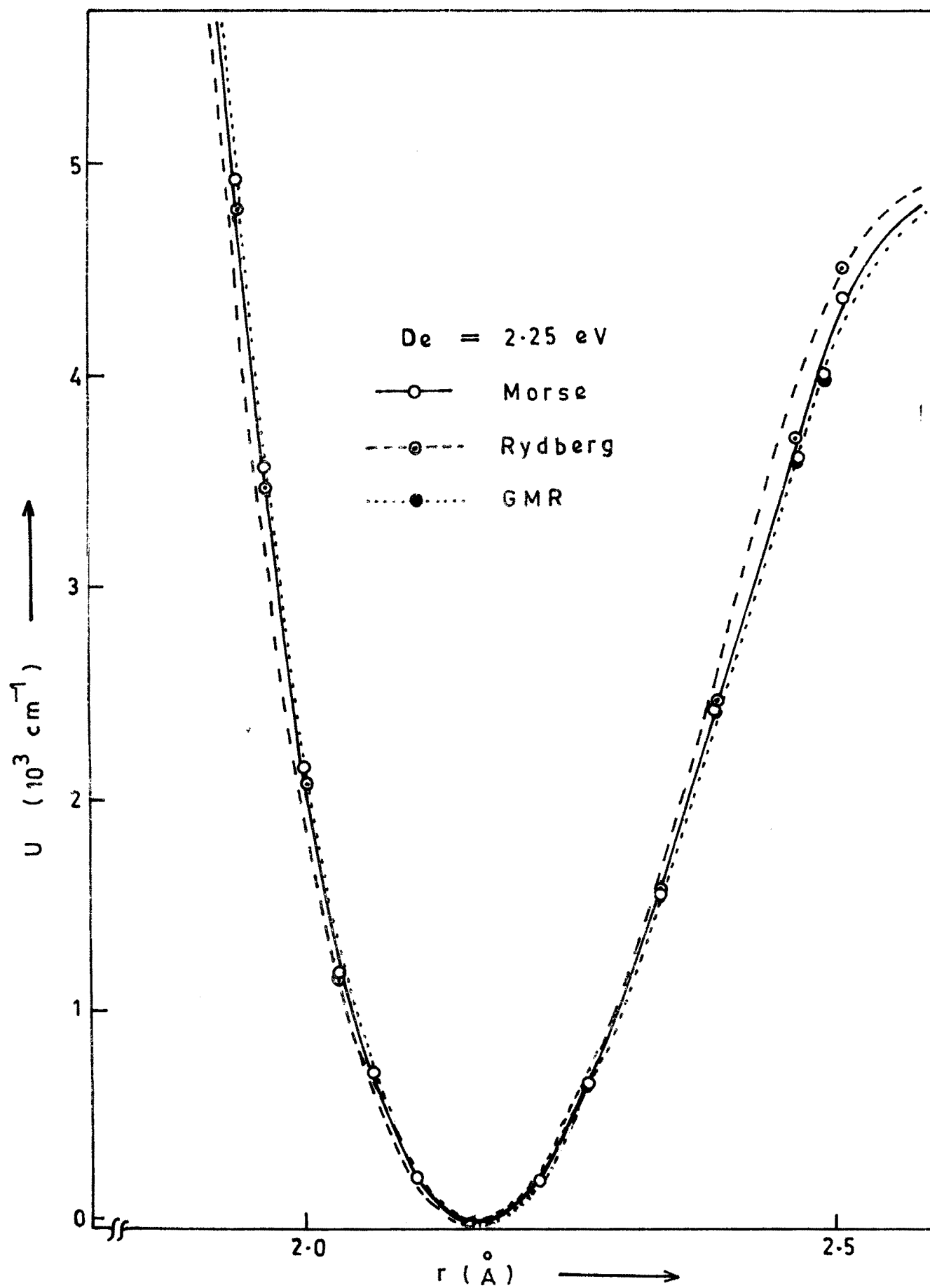


FIG. 3-3 — RKR V POTENTIAL ENERGY CURVES FOR $\text{AlSe}(X^2\Sigma)$.

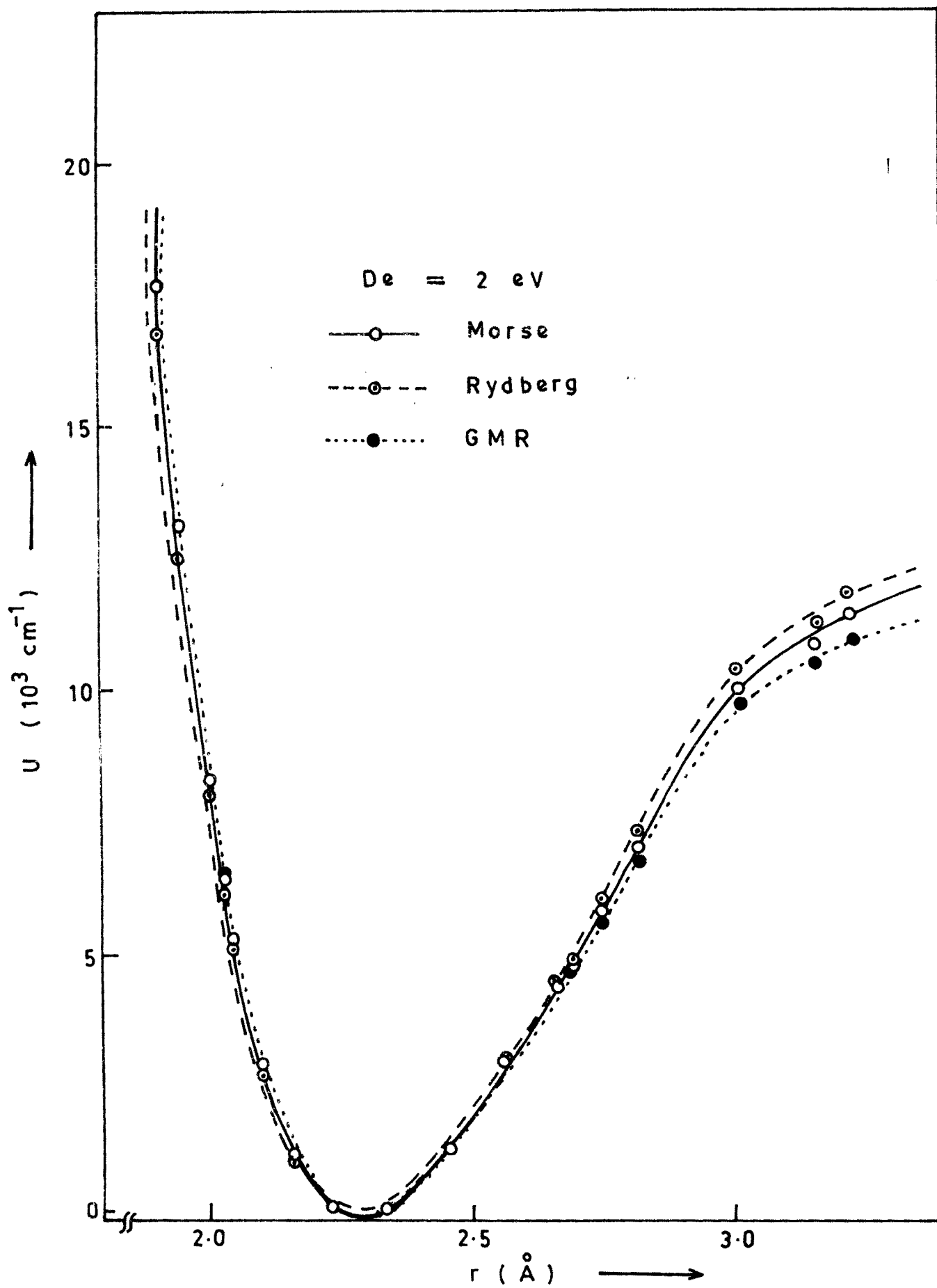


FIG. 3.4 — RKR V POTENTIAL ENERGY CURVES FOR Br_2 ($X^1\Sigma_g^+$)

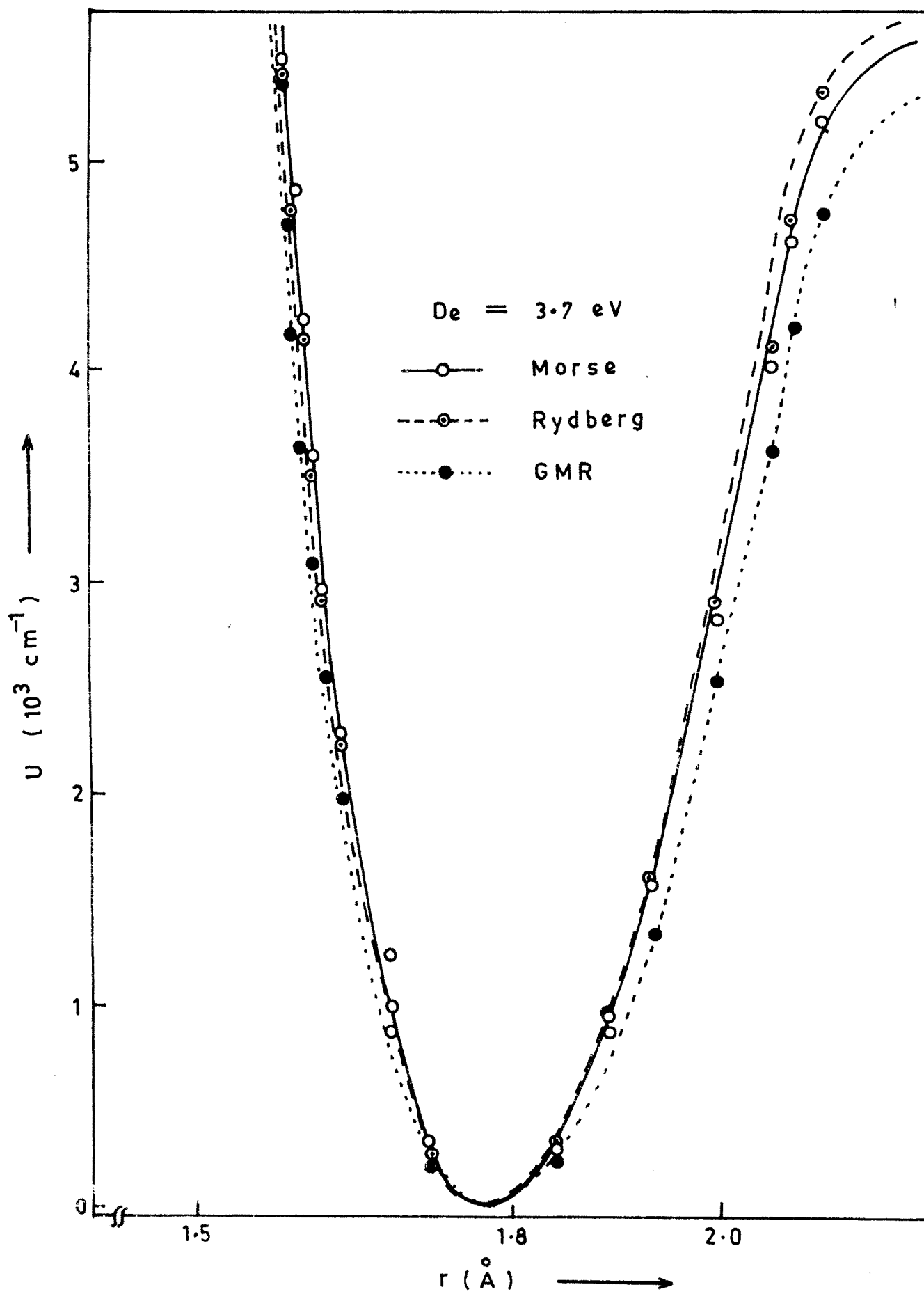


FIG. 3.5 — RKR POTENTIAL ENERGY CURVES FOR $\text{CrF} (X^6\Sigma)$.

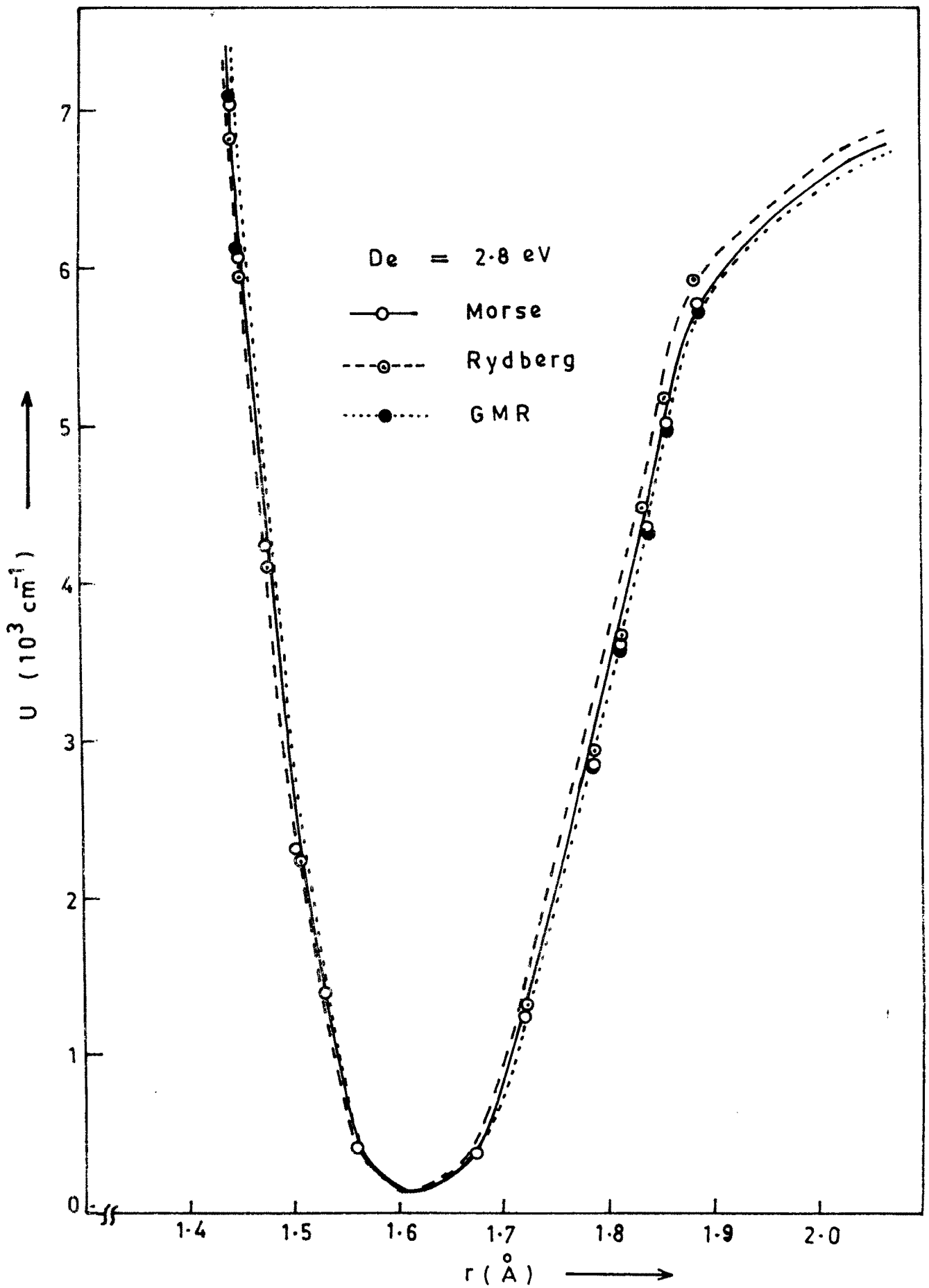


FIG. 3-6 — RKR V POTENTIAL ENERGY CURVES FOR $\text{CrO}(X^5\Pi)$

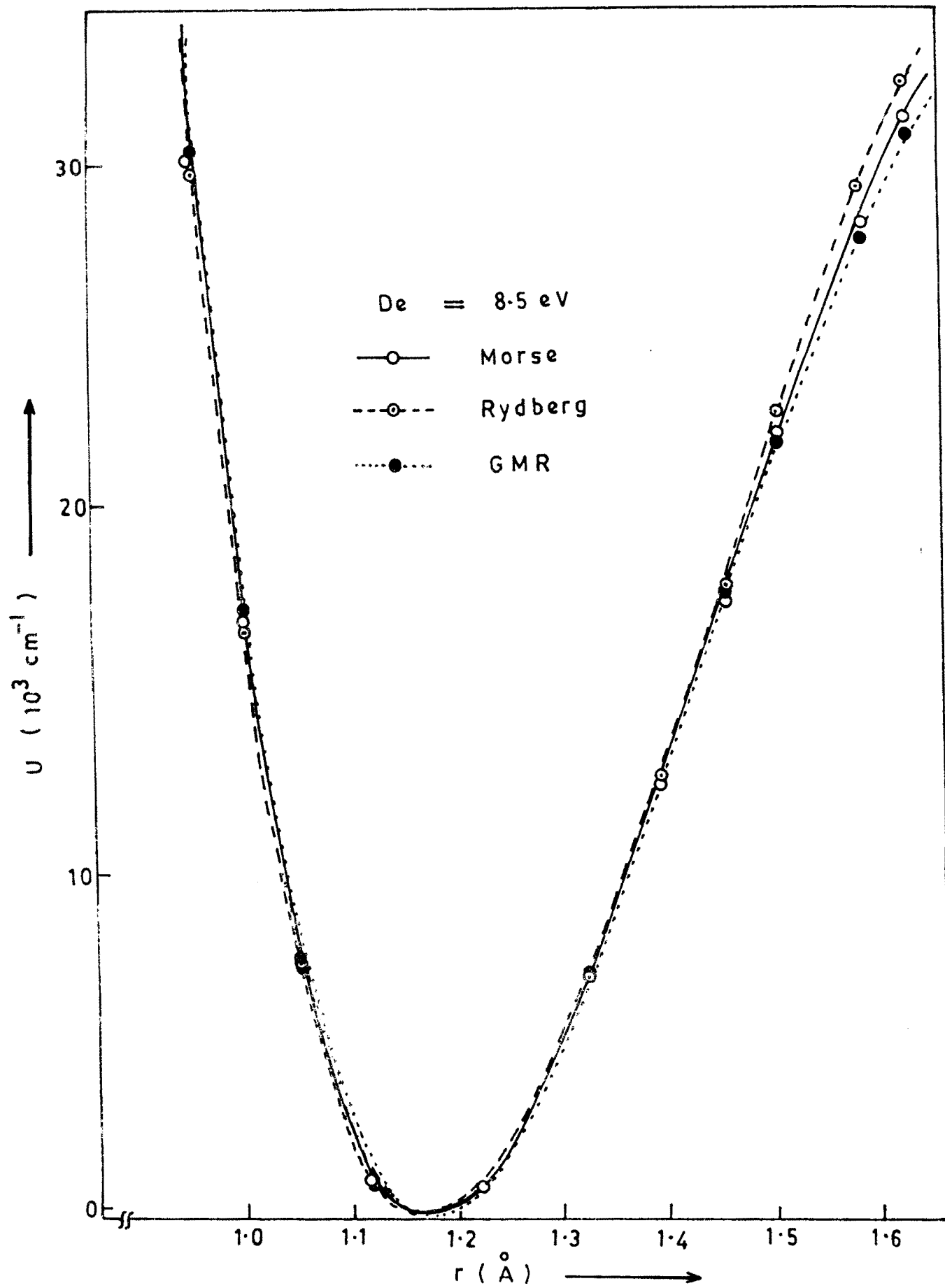


FIG. 3.7 — RKR V POTENTIAL ENERGY CURVES FOR $\text{CN} (X^2\Sigma^+)$

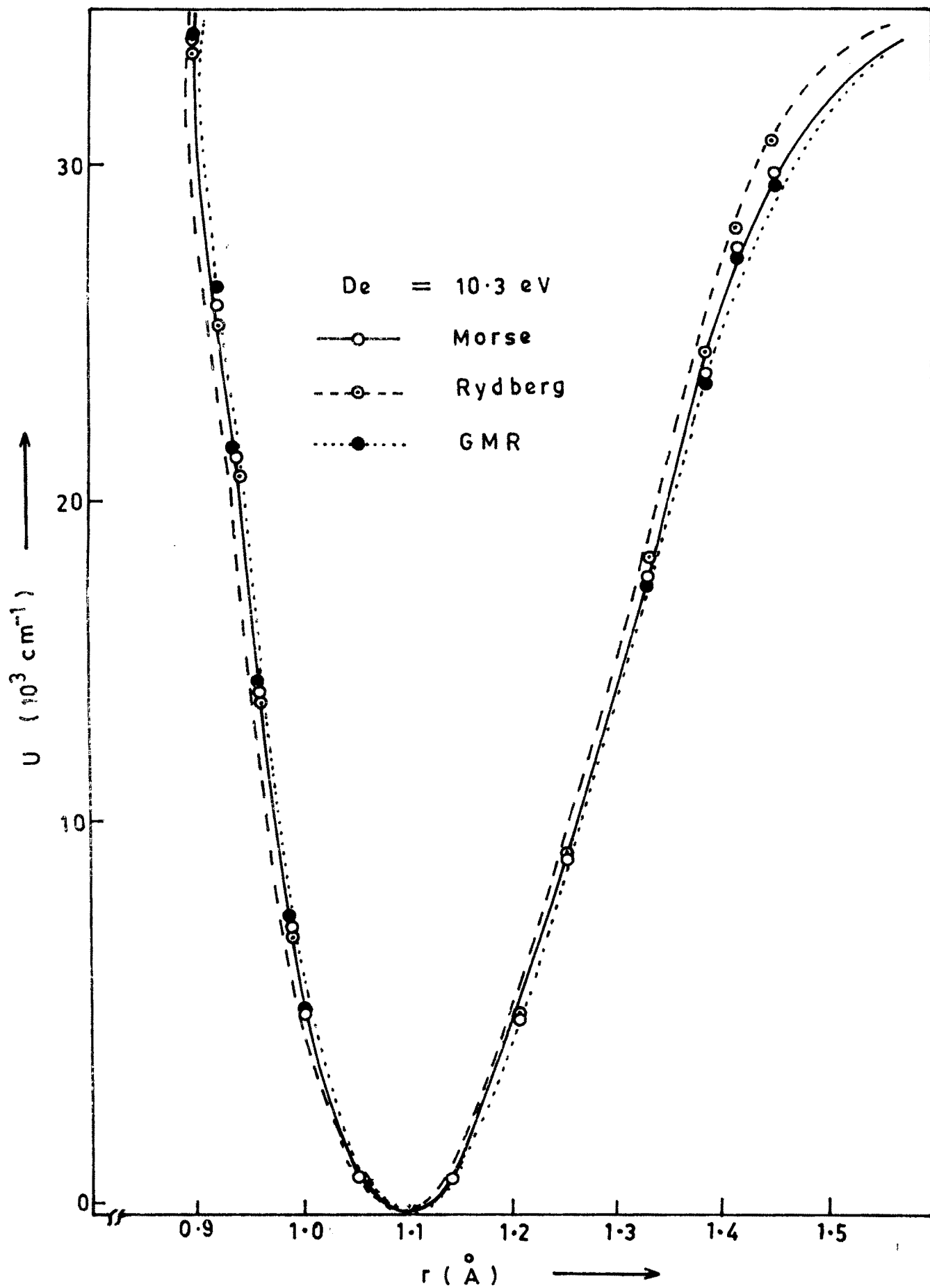


FIG. 3-8 — RKR POTENTIAL ENERGY CURVES FOR N₂



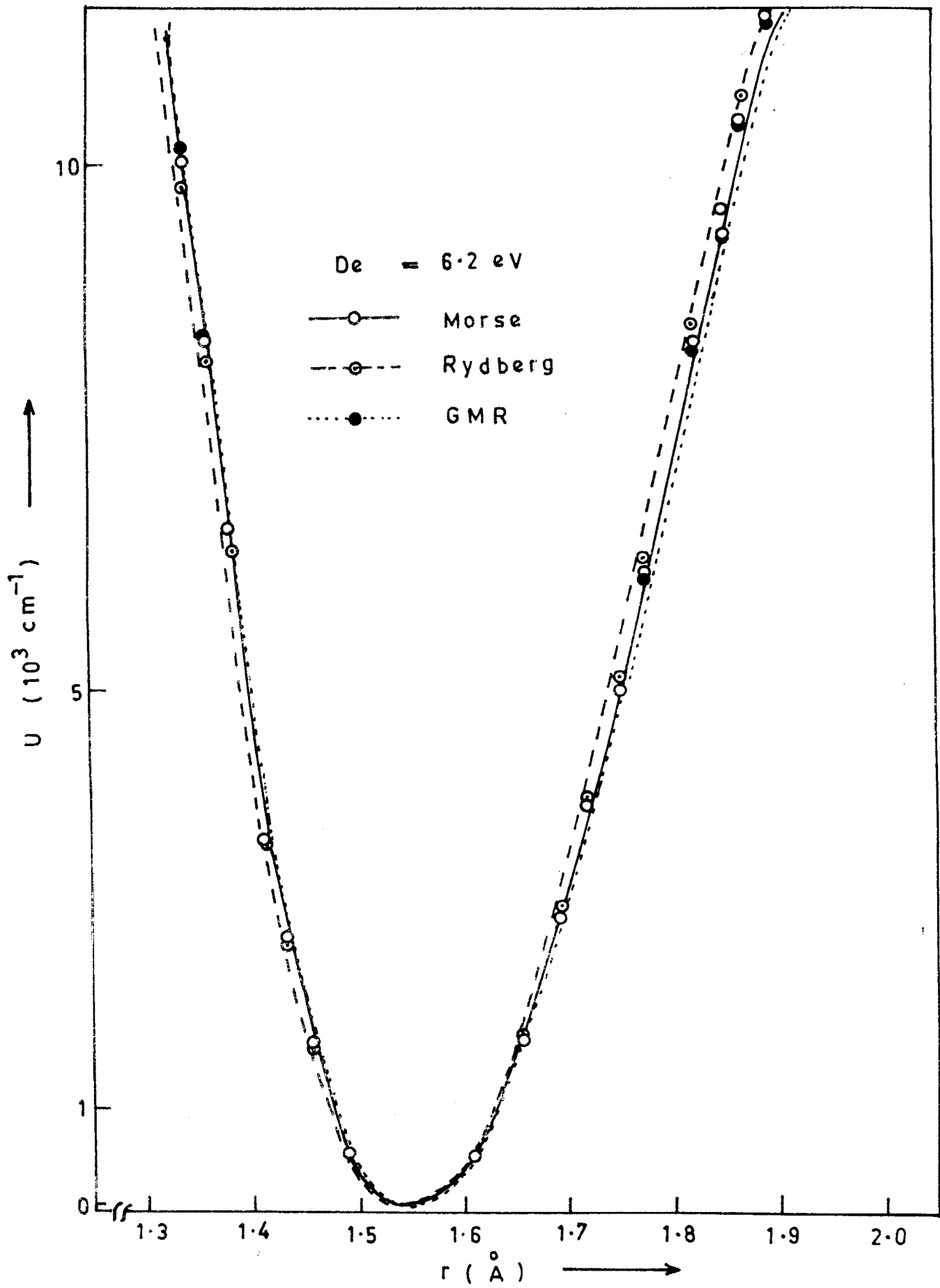


FIG. 3-9 — RKR V POTENTIAL ENERGY CURVES FOR PN ($A^1\Pi$).