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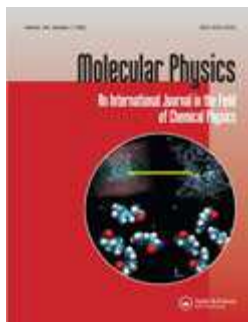
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**Comparison between predissociation mechanisms in two isoelectronic molecules CO and N<sub>2</sub>**

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## Comparison between predissociation mechanisms in two isoelectronic molecules: CO and N<sub>2</sub>

H. LEFEBVRE-BRION<sup>†</sup> and B. R. LEWIS<sup>‡</sup>

<sup>†</sup>Laboratoire de Photophysique Moléculaire, Bât. 213, Université Paris-Sud, 91405 Orsay Cedex, France

<sup>‡</sup>Research School of Physical Sciences and Engineering, The Australian National University, Canberra, ACT 0200, Australia

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A correspondence between the observed electronic states of N<sub>2</sub> and CO is presented, in order to compare the perturbations and predissociations of these two isoelectronic molecules. The homogeneous perturbations between the <sup>1</sup>Σ<sup>+</sup> (or <sup>1</sup>Σ<sub>u</sub><sup>+</sup>) and the <sup>1</sup>Π (or <sup>1</sup>Π<sub>u</sub>) states are reviewed, and comparisons are made between the indirect predissociations of the <sup>1</sup>Π states due to the <sup>3</sup>Π states in both N<sub>2</sub> and CO.

### 1 Introduction

Christian Jungen has made important contributions to knowledge of the Rydberg states of the two molecules, N<sub>2</sub> [1–3] and CO [4]. The present study is restricted to problems related to the comparison between the lowest Rydberg states of these two molecules. N<sub>2</sub> and CO are isoelectronic. Consequently, their properties should present similarities. Using the single-configuration approximation, it is possible to relate the electronic states of N<sub>2</sub> and CO, as shown for the states of relevance here in Table 1.

N<sub>2</sub> is known for the strong homogeneous perturbations between Rydberg and valence states for both <sup>1</sup>Π<sub>u</sub> and <sup>1</sup>Σ<sub>u</sub><sup>+</sup> symmetry. These have been studied intensively by Stahel *et al.* [5] and, more recently, by Spelsberg and Meyer [6]. For example, the *b'* <sup>1</sup>Σ<sub>u</sub><sup>+</sup> valence state of N<sub>2</sub> interacts electrostatically with the <sup>1</sup>Σ<sub>u</sub><sup>+</sup> Rydberg states having an *X* <sup>2</sup>Σ<sub>g</sub><sup>+</sup> core. These lowest states in energy are *c'* <sup>1</sup>Σ<sub>u</sub><sup>+</sup> and *e'* <sup>1</sup>Σ<sub>u</sub><sup>+</sup>.

In CO, the first <sup>1</sup>Σ<sup>+</sup> valence state is *D'* <sup>1</sup>Σ<sup>+</sup>. This state introduces not only perturbations in the <sup>1</sup>Σ<sup>+</sup> Rydberg states, but also strong predissociations. The first <sup>1</sup>Σ<sup>+</sup> Rydberg state in CO, *B* <sup>1</sup>Σ<sup>+</sup>, exhibits perturbations which do not appear in the corresponding state in N<sub>2</sub>, since *B* <sup>1</sup>Σ<sup>+</sup> corresponds in N<sub>2</sub> to a *gerade* state, *a''* <sup>1</sup>Σ<sub>g</sub><sup>+</sup>. The other <sup>1</sup>Σ<sup>+</sup> Rydberg states of CO are *C* <sup>1</sup>Σ<sup>+</sup> and *K* <sup>1</sup>Σ<sup>+</sup>. We will discuss the corresponding predissociations in Section 2.

The first <sup>1</sup>Π Rydberg state of CO is the *E* <sup>1</sup>Π state, the analogue of the *c* <sup>1</sup>Π<sub>u</sub> Rydberg state of N<sub>2</sub> (see Table 1). The second Rydberg state of this series, converging to the *X* <sup>2</sup>Σ<sup>+</sup> state of CO<sup>+</sup>, is *L* <sup>1</sup>Π, corresponding to the *e* <sup>1</sup>Π<sub>u</sub> state of N<sub>2</sub>. Furthermore, the first Rydberg state of N<sub>2</sub> with an *A* <sup>2</sup>Π<sub>u</sub> ion core, the *o* <sup>1</sup>Π<sub>u</sub> state, has a corresponding state in CO, the *W* <sup>1</sup>Π state.

The *b* <sup>1</sup>Π<sub>u</sub> valence state of N<sub>2</sub>, with the 2σ<sub>u</sub><sup>2</sup>3σ<sub>g</sub><sup>2</sup>1π<sub>u</sub><sup>3</sup>3sσ<sub>g</sub> configuration, has no corresponding <sup>1</sup>Π state observed in CO. This may be explained because the 4σ orbital of CO has an ionization potential relatively high compared with the 2σ<sub>u</sub> orbital of N<sub>2</sub>. The *B* <sup>2</sup>Σ<sub>u</sub><sup>+</sup> excited state of N<sub>2</sub><sup>+</sup> lies around 25 000 cm<sup>-1</sup> above the *X* <sup>2</sup>Σ<sub>g</sub><sup>+</sup> ground state. On the other hand, the *B* <sup>2</sup>Σ<sup>+</sup> state of CO<sup>+</sup> lies around 46 000 cm<sup>-1</sup> above the *X* <sup>2</sup>Σ<sup>+</sup> ground state. In fact, the *b* <sup>1</sup>Π<sub>u</sub> valence state of N<sub>2</sub> corresponds mainly to a mixing of two configurations, the 2σ<sub>u</sub>3σ<sub>g</sub><sup>2</sup>1π<sub>u</sub><sup>4</sup>1π<sub>g</sub> valence-hole configuration discussed above at smaller internuclear distances, but also the 2σ<sub>u</sub><sup>2</sup>3σ<sub>g</sub>1π<sub>u</sub><sup>3</sup>1π<sub>g</sub><sup>2</sup> configuration at larger internuclear distances. This latter configuration corresponds in CO to the 4σ<sup>2</sup>5σ1π<sup>3</sup>2π<sup>2</sup> configuration, which gives rise to a bound state that happens to interact with a repulsive state (4σ<sup>2</sup>5σ<sup>2</sup>6σ1π<sup>3</sup> configuration) to form the outer minimum of the calculated double-minimum <sup>3</sup>Π-state potential-energy curve [7]. The inner minimum in this <sup>3</sup>Π potential has Rydberg character corresponding to the *W* <sup>1</sup>Π state.

The <sup>3</sup>Π<sub>u</sub> states of N<sub>2</sub> play a major role in the predissociation of the <sup>1</sup>Π<sub>u</sub> states [8]. The *C* <sup>3</sup>Π<sub>u</sub> valence

Table 1. Comparison between the lowest Rydberg states, and their interacting valence states, in N<sub>2</sub> and CO. Values between parentheses are uncertain. For the more perturbed states,  $T_0$  and  $R_0$  are given (between square brackets), rather than  $T_e$  and  $R_e$ .

N <sub>2</sub>					CO				
State	Configuration	$T_e$ (cm <sup>-1</sup> )	$R_e$ (Å)	Ref.	State	Configuration	$T_e$ (cm <sup>-1</sup> )	$R_e$ (Å)	Ref.
$X^1\Sigma_g^+$	$2\sigma_u^2 3\sigma_g^2 1\pi_u^4$	0.0	1.09768	[10]	$X^1\Sigma^+$	$4\sigma^2 5\sigma^2 1\pi^4$	0.0	1.12832	[10]
$C^3\Pi_u$	$2\sigma_u 3\sigma_g^2 1\pi_u^4 1\pi_g$	[88977.9]	[1.1527]	[12]	$b^3\Sigma^+$	$4\sigma^2 5\sigma 1\pi^4 3s\sigma$	[83833.0]	[1.1695]	[19]
$E^3\Sigma_g^+$	$2\sigma_u^2 3\sigma_g 1\pi_u^4 3s\sigma_g$	(95858)	[1.118]	[10]	$k^3\Pi$	$4\sigma^2 5\sigma 1\pi^3 2\pi^2$	[90334.0]	[1.383]	[20]
$C'^3\Pi_u$	$2\sigma_u^2 3\sigma_g 1\pi_u^3 1\pi_g^2$	[97562.3]	[1.515]	[10]	$B^1\Sigma^+$	$4\sigma^2 5\sigma 1\pi^4 3s\sigma$	[86916.2]	[1.1234]	[21]
$a''^1\Sigma_g^+$	$2\sigma_u^2 3\sigma_g 1\pi_u^4 3s\sigma_g$	98938.	1.114	[11]	$D'^1\Sigma^+$	$4\sigma^2 5\sigma^2 1\pi^3 2\pi$	[88677.4]	1.583	[28]
$b^1\Pi_u$	$2\sigma_u 3\sigma_g^2 1\pi_u^4 1\pi_g$	[100816.8]	[1.290]	[13]	$j^3\Sigma^+$	$4\sigma^2 5\sigma 1\pi^4 3p\sigma$	[90833.2]	[1.1263]	[29]
$b'^1\Sigma_u^+$	$2\sigma_u^2 3\sigma_g^2 1\pi_u^3 1\pi_g$	[103670.8]	[1.445]	[12]	$c^3\Pi$	$4\sigma^2 5\sigma 1\pi^4 3p\pi$	[92076.9]	[1.1203]	[30]
$D^3\Sigma_u^+$	$2\sigma_u^2 3\sigma_g 1\pi_u^4 3p\sigma_u$	[104746.]	[1.108]	[10]	$E^1\Pi$	$4\sigma^2 5\sigma 1\pi^4 3p\pi$	[92929.9]	[1.1221]	[22]
$G^3\Pi_u$	$2\sigma_u^2 3\sigma_g 1\pi_u^4 3p\pi_u$	[103316.0]	[1.155]	[15]	$C^1\Sigma^+$	$4\sigma^2 5\sigma 1\pi^4 3p\sigma$	[91919.0]	[1.1248]	[23]
$c^1\Pi_u$	$2\sigma_u^2 3\sigma_g 1\pi_u^4 3p\pi_u$	[104138.5]	[1.264]	[14]	$W^1\Pi$	$4\sigma^2 5\sigma^2 1\pi^3 3s\sigma$	[102806.4]	[1.2548]	[24]
$c'^1\Sigma_u^+$	$2\sigma_u^2 3\sigma_g 1\pi_u^4 3p\sigma_u$	[104323.3]	[1.117]	[14]	$G^1\Pi$	$4\sigma^2 5\sigma 1\pi^4 3d\pi$	[101032.3]	[1.119]	[24]
$F^3\Pi_u$	$2\sigma_u^2 3\sigma_g^2 1\pi_u^3 3s\sigma_g$	[104727.4]	[1.155]	[16]	$C'^1\Sigma^+$	$4\sigma^2 5\sigma^2 1\pi^2 2\pi^2$	[102207.]	[1.7]	[31]
$o^1\Pi_u$	$2\sigma_u^2 3\sigma_g^2 1\pi_u^3 3s\sigma_g$	[105682.8]	[1.195]	[5]	$L^1\Pi$	$4\sigma^2 5\sigma 1\pi^4 4p\pi$	[103271.8]	[1.1201]	[27]
$k^1\Pi_g$	$2\sigma_u^2 3\sigma_g 1\pi_u^4 3d\pi_g$	[113630.9]	[1.109]	[17]	$K^1\Sigma^+$	$4\sigma^2 5\sigma 1\pi^4 4p\sigma$	[103054.1]	[1.1325]	[24]
$e^1\Pi_u$	$2\sigma_u^2 3\sigma_g 1\pi_u^4 4p\pi_u$	[115569.3]	[1.118]	[18]					
$e'^1\Sigma_u^+$	$2\sigma_u^2 3\sigma_g 1\pi_u^4 4p\sigma_u$	[115849.8]	[1.338]	[5]					

state, isoconfigurational with  $b^1\Pi_u$ , also has no equivalent state observed in CO, but the  $C'^3\Pi_u$  valence state has an analogous state in CO,  $k^3\Pi$ , identified for the first time by Baker *et al.* [9]. We will discuss later the indirect predissociations in CO due to this state. In N<sub>2</sub>, the triplet Rydberg states corresponding to the isoconfigurational singlet Rydberg states are the  $G^3\Pi_u$  state, associated with the  $c^1\Pi_u$  state, and the  $F^3\Pi_u$  state, associated with the  $o^1\Pi_u$  state. In CO, the  $c^3\Pi$  state is associated with the  $E^1\Pi$  state. The  $^3\Pi$  state associated with the  $W^1\Pi$  state seems not to have been observed yet. Some bands, first assigned to a  $V^3\Pi$  state [24], have later revealed no spin structure [25] and have since been reassigned, either to a valence state  $W'^1\Pi$  [25], or to higher vibrational levels of the  $E^1\Pi$  state [26].

## 2 Homogeneous interactions between the $^1\Sigma^+$ states

The lowest  $^1\Sigma^+$  Rydberg and valence potential-energy curves of CO are shown in Fig. 1, in a diabatic (crossing) representation, after Fig. 1 of Ref. [31]. The  $B^1\Sigma^+$  state, the first member of the  $n\sigma$  Rydberg series in CO, exhibits strong perturbations, manifested in the lowest vibrational levels as an energy shift. In addition, the  $v = 2$  level of the  $B$  state is strongly predissociated. This has been interpreted as due to the Rydberg-valence electrostatic interaction with the  $D'^1\Sigma^+$  valence state [32]. The corresponding close-coupling model reproduces reasonably well both the level shifts of the two first vibrational levels and the full-width-at-half-maximum (FWHM) predissociation width of the  $v = 2$  vibrational level of the  $B$  state [32]. The other Rydberg states,  $3p\sigma C^1\Sigma^+$  and  $4p\sigma K^1\Sigma^+$ , are also predissociated and it is the electrostatic interaction between these states and the  $D'^1\Sigma^+$  valence state which can be compared with the analogous interactions in N<sub>2</sub>, as explained in Section 1, but these states have not been introduced into the model of Tchang-Brillet *et al.* [32]. Other authors have utilized the potential-energy curves obtained for the  $B$  and  $D'$  states in Ref. [32] to calculate the predissociation widths of the upper levels of the  $B$  state [33–35]. However, their results are in disagreement with experiment (see Table 2), not only for the  $B$  state, but also for the other members of the  $n\sigma$  series [36]. In the case of the widths of the  $v = 2$  and 3 vibrational levels of the  $B^1\Sigma^+$  state, the *ab initio* calculations of Li *et al.* [41] are significantly lower than the experimental values, in worse agreement than the results of the close-coupling studies. On the other hand, their values for the widths of the vibrational levels of the  $C^1\Sigma^+$  state [41] are much larger than the

Table 2. Predissociation widths for vibrational levels of the  $B^1\Sigma^+$  state of CO, in  $\text{cm}^{-1}$  FWHM.

$v$	Calc. [35]	Calc. [41]	Exp.	Ref.(exp.)
0	0.00	0.0	0.0003 <sup>a</sup>	[40]
1	0.0004	0.0	0.0002 <sup>a</sup>	[40]
2	0.8947	0.1	0.7–2.	[37]
3	90.86	23.	90.	[37]
4	801.3		350.	[38]
5	1854.		450.	[38]
6	2149.		7.	[39]
7	9.387			
8	1191.			
9	622.3		50.–70.	[31]
10	0.2884			

<sup>a</sup> From the total (dissociative + radiative) decay rate.

Table 3. Predissociation widths for vibrational levels of the  $C^1\Sigma^+$  state of CO, in  $\text{cm}^{-1}$  FWHM.

$v$	Calc. [41]	Exp.	Ref.(exp.)
0	$<10^{-4}$	0.003 <sup>a</sup>	[42]
1	0.05	0.008 <sup>a</sup>	[42]
2	1.1		
3	4.9	2.3	[32]
4	8.9	$<5.0$	[32]

<sup>a</sup> From the total (dissociative + radiative) decay rate.

experimental values [42] (see Table 3).

To explain the homogeneous perturbations of the other, higher-lying  $^1\Sigma^+$  Rydberg states of CO, it is necessary to invoke a second  $^1\Sigma^+$  valence state predicted by Cooper and Kirby [43],  $C'^1\Sigma^+$ , the high vibrational levels of which have been observed recently [31]. This state is described mainly by the configuration  $4\sigma^2 5\sigma^2 1\pi^2 2\pi^2$ , corresponding in  $\text{N}_2$  to a non-observed  $^1\Sigma_g^+$  state ( $2\sigma_u^2 3\sigma_g^2 1\pi_u^2 1\pi_g^2$  configuration). This fact, and the important mixing of these states with the  $3s\sigma$  and  $4s\sigma^1\Sigma^+$  Rydberg states of CO, make difficult the comparison with  $\text{N}_2$ .

### 3 Homogeneous interactions between the $^1\Pi$ states

In  $\text{N}_2$ , there are strong homogeneous perturbations between the  $^1\Pi_u$  valence and Rydberg states [5]. In CO, the  $^1\Pi$  Rydberg states with an  $X^2\Sigma^+$  ion core ( $3p\pi E^1\Pi$ ,  $4p\pi L^1\Pi$ ), and with an  $A^2\Pi$  ion core ( $3s\sigma W^1\Pi$ ), are well determined, corresponding to the  $c^1\Pi_u [X^2\Sigma_g^+]3p\pi_u$ ,  $e^1\Pi_u [X^2\Sigma_g^+]4p\pi_u$ , and  $o^1\Pi_u [A^2\Pi_u]3s\sigma_g$  Rydberg states of  $\text{N}_2$ , respectively. The  $^1\Pi$  valence states of CO, corresponding to the  $b^1\Pi_u$  valence state of  $\text{N}_2$ , are not very well known. From the calculations of Cooper and Kirby [7], the  $W^1\Pi$ -state adiabatic potential has a second minimum at about 1.87 Å, corresponding to the  $4\sigma^2 5\sigma 1\pi^3 2\pi^2$  valence configuration, i.e., isoconfigurational with the  $k^3\Pi$  state. Numerous vibronic levels of  $^1\Pi$  states have been observed, e.g., by Ogawa and Ogawa [44], Casey [45], and Eidelsberg *et al.* [39]. From the above, it is clear that the diabatic singlet valence state, corresponding to the  $k^3\Pi$  state, must interact strongly with the  $[X^2\Sigma^+]3p\pi$ ,  $[X^2\Sigma^+]4p\pi$ , and  $[A^2\Pi]3s\sigma^1\Pi$  Rydberg states. We propose to name this diabatic state  $E'^1\Pi$ . A global deperturbation of all these states, using coupled equations, is currently planned, following previous successes in the case of  $\text{N}_2$  [5, 6, 8]. New, high-level *ab initio* calculations for the  $^1\Pi$  states of CO would be of significant benefit in setting up the diabatic potential-energy-curve basis for this deperturbation.

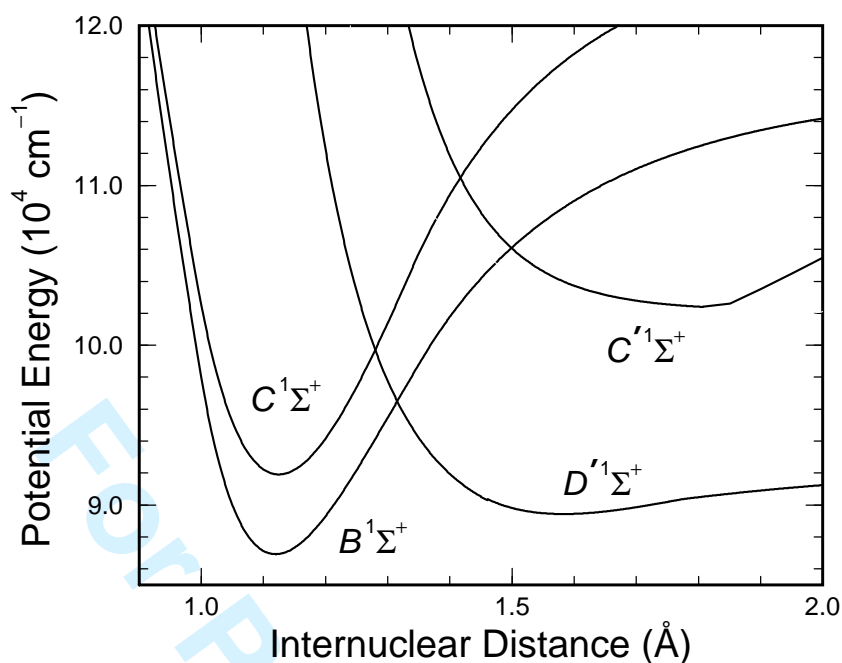


Figure 1. Diabatic potential-energy curves for the lowest excited Rydberg and valence  $^1\Sigma^+$  states of CO. The energy scale is referenced to the minimum in the ground-state potential-energy curve.

#### 4 Homogeneous Interactions between the $^3\Pi$ states

The homogeneous perturbations in CO between the  $c^3\Pi$  Rydberg state and the  $k^3\Pi$  valence state have been studied by Baker and Launay [46]. A deperturbation performed on many vibrational levels of these two states has given for the electronic interaction parameter:  $H_e(c^3\Pi \sim k^3\Pi) \approx 320 \text{ cm}^{-1}$  [46]. This differs strongly from the corresponding interaction in N<sub>2</sub>:  $H_e(G^3\Pi_u \sim C'^3\Pi_u) \approx 1400 \text{ cm}^{-1}$  [47]. However, comparison between the  $^3\Pi$  states of CO and N<sub>2</sub> is difficult because the  $^3\Pi$  valence states are described by a configuration ( $4\sigma^2 5\sigma 1\pi^3 2\pi^2$  for CO and  $2\sigma_u^2 3\sigma_g 1\pi_u^3 1\pi_g^2$  for N<sub>2</sub>) which gives rise to four separate  $^3\Pi$  states with strong mutual interactions. The  $^3\Pi_u$  states of N<sub>2</sub> have been calculated previously [48–50] and a new calculation of these states is in progress [51]. The  $^3\Pi$  states of CO have been calculated by Hall *et al.* [52, 53] and have been reported in Fig. 1 of Hill *et al.* [54], where the  $2^3\Pi$  state corresponds to the  $k^3\Pi$  state, with a calculated  $T_e = 96\,500 \text{ cm}^{-1}$  [53], somewhat higher than the experimental value in Table 1, and  $R_e = 1.377 \text{ \AA}$  [53], in good agreement with experiment. Figures 2 and 3 compare the  $\Pi$  states of N<sub>2</sub> and CO. Figure 2 is derived from the work of Refs. [8] and [47], including diabatic potential-energy curves for the  $c$ ,  $o$  and  $b^1\Pi_u$  states and the  $C$ ,  $C'$ ,  $F$  and  $G^3\Pi_u$  states of N<sub>2</sub>. Figure 3 has been built from experimental and calculated data [7], employing also Fig. 1 of [30] and Fig. 6 of [29]. Tentative potential curves for the  $E$  and  $W^1\Pi$  states, and the  $k$  and  $c^3\Pi$  states of CO are included, together with a schematic diabatic curve for the  $E'^1\Pi$  valence state. Also shown in Fig. 3, unlabelled, is the  $^3\Pi$  state associated with the  $W^1\Pi$  state, which, while not yet observed, certainly exists, and would be expected to play a role in the perturbation and predissociation of the  $^1\Pi$  states.

#### 5 Indirect predissociations in the $^1\Pi$ states

Accidental predissociations in the  $E^1\Pi$  Rydberg state of CO were observed by Simmons and Tilford [55], and later by Amiot *et al.* [56]. These have been interpreted by Baker *et al.* [9] as due to the mixing of the  $E^1\Pi$  state with the  $k^3\Pi$  triplet valence state, itself predissociated. Rather than ‘accidental’ predissociation, we prefer the term ‘indirect’ predissociation, which is more general [57]. A careful study of these predisso-

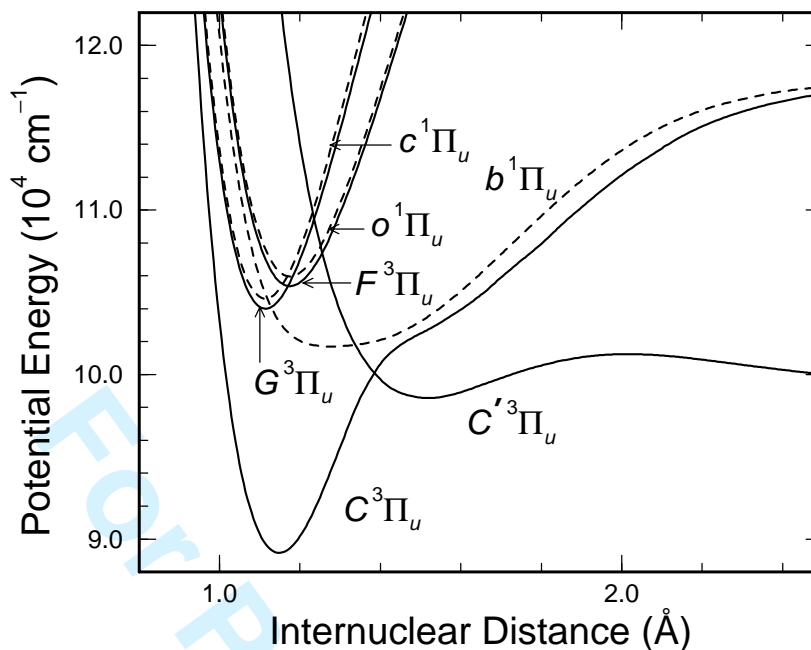


Figure 2. Diabatic potential-energy curves for the lowest <sup>1</sup>Π<sub>u</sub> and <sup>3</sup>Π<sub>u</sub> electronic states of N<sub>2</sub>. The energy scale is referenced to the minimum in the ground-state potential-energy curve.

ciations has been performed by Cacciani *et al.* [58], Sun *et al.* [59], and Ubachs *et al.* [60]. The observed FWHM predissociation widths are  $\Gamma[E^1\Pi(v=1)] = 0.034 \text{ cm}^{-1}$  and  $\Gamma[k^3\Pi(v=6)] = 0.335 \text{ cm}^{-1}$  [60] (Note that a change from  $v$  to  $v+1$  must be made for the levels of  $k$  in all papers published before Ref. [20]). This predissociation has been interpreted as due to a spin-orbit interaction matrix element  $\langle v_E = 1 | v_k = 6 \rangle \langle E^1\Pi | \mathbf{H}_{so} | k^3\Pi \rangle = 1.88 \text{ cm}^{-1}$  [60]. As the configurations of the  $E^1\Pi$  and  $k^3\Pi$  states differ by two orbitals, this spin-orbit interaction is indirect. On p. 542 of Ref. [57], it has been assumed that the  $E^1\Pi$  Rydberg state spin-orbit interacts with the isoconfigurational  $c^3\Pi$  state, which in turn electrostatically interacts with the  $k^3\Pi$  valence state. However, this Rydberg spin-orbit mixing is too weak to explain the observed predissociation and we suggest another process by comparison with N<sub>2</sub>. The predissociation of the  $c^1\Pi_u$  Rydberg state of N<sub>2</sub>, in its lowest vibrational levels, is due primarily to the mixing of  $c$  with the valence state  $b^1\Pi_u$ , which spin-orbit couples to the isoconfigurational  $C^3\Pi_u$  state, itself predissociated by the  $C'^3\Pi_u$  state [8, 47]. In CO, we can assume that  $E^1\Pi$  is mixed with the  $E'^1\Pi$  valence state. It is this valence state which can be mixed by spin-orbit interaction with the  $k^3\Pi$  valence state. The  $k^3\Pi$  state is probably predissociated by a repulsive  $^3\Pi$  state, going to the  $C(^3P) + O(^3P)$  dissociation limit, as suggested by Baker *et al.* [9]. This state, III<sup>3</sup>Π, is represented in Fig. 3. Using a model with an assumed electronic interaction  $\langle k^3\Pi | \mathbf{H}_{el} | III^3\Pi \rangle = 200 \text{ cm}^{-1}$  and the close coupling method, we can reproduce the width of  $k(v=6)$ . The upper levels have larger widths (e.g.,  $\Gamma[k^3\Pi(v=7)] = 3 \text{ cm}^{-1}$ ), in agreement with the observation of Mazeau *et al.* [61], by electron impact spectroscopy, of strongly predissociated <sup>3</sup>Π levels.

## 6 Conclusions

Perturbations and predissociations have been, or are currently being, well studied in N<sub>2</sub>. However, in CO, the homogeneous perturbations between both the <sup>1</sup>Σ<sup>+</sup> and <sup>1</sup>Π states are not completely understood. There exists a strong parallel between the indirect predissociations observed in the <sup>1</sup>Π (or <sup>1</sup>Π<sub>u</sub>) states of CO and N<sub>2</sub>. New *ab initio* calculations are necessary, in the case of CO, to contribute to an understanding of the homogeneous perturbations and indirect predissociations. The close coupling method will be then well

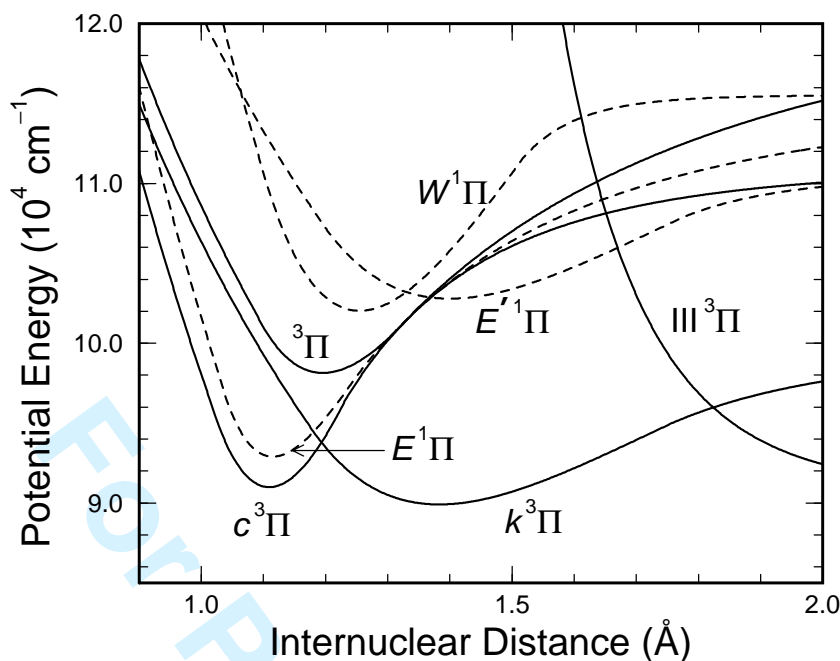


Figure 3. Schematic potential-energy curves for some of the lowest <sup>1</sup>Π and <sup>3</sup>Π electronic states of CO. The energy scale is referenced to the minimum in the ground-state potential-energy curve.

suitable to calculation of the predissociation widths for the CO molecule.

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