Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Table S1. Fitted parameters for CKV data from eqns (5) and (6)

Set	E_r (eV)	Γ_p (eV)	Γ_d (eV)	$\delta_{bg,1}$	$\delta_{bg,2}$
A	3.48	0.000	0.170	0.000	-0.059
B	2.94	0.019	0.113	-0.189	-0.046
C	2.49	0.061	0.075	-0.160	-0.032
D	2.15	0.104	0.050	-0.136	-0.028
E	2.10	0.109	0.047	-0.134	-0.028
F	1.94	0.129	0.037	-0.128	-0.026

Table S2. Resonance Energy, E_r, in eV. Basis set designations are explained in the text.

	Method/Basis									
	CKV	Stabilization			CAP			RAC		
Set	(p + p)	(P)	(D)	(p + p)	(P)	(D)	(p + p)	(P)	(D)	(p + p)
A	3.48	-	3.47	3.47	-	3.48	3.47	-	3.48	3.47
B	2.94	3.00	2.93	2.93	3.00	2.93	2.93	2.99	2.94	2.93
C	2.49	2.55	2.50	2.48	2.55	2.50	2.48	2.53	2.51	2.48
D	2.15	2.19	2.18	2.13	2.20	2.18	2.14	2.17	2.18	2.13
E	2.10	2.15	2.14	2.08	2.15	2.14	2.10	2.12	2.14	2.08
F	1.94	1.97	1.99	1.91	1.98	1.99	1.93	1.95	1.99	1.91

Table S3. Total width, Γ, in eV. Basis set designations are explained in the text.

	Method/Basis						
	CKV	Stabilization		CAP		RAC	
Set	Sum[a]	Sum[a]	(p + p)	Sum[a]	(p + p)	Sum[a]	(p + p)
A	0.170	0.176	0.164	0.168	0.157	0.146	0.146
B	0.132	0.133	0.133	0.127	0.129	0.128	0.118
C	0.136	0.138	0.149	0.131	0.130	0.138	0.136
D	0.154	0.156	0.164	0.151	0.146	0.152	0.154
E	0.156	0.157	0.166	0.155	0.148	0.168	0.160
F	0.166	0.169	0.172	0.169	0.159	0.168	0.164

[a]"Sum" designates the sum of Γ_p and Γ_d for the indicated method.

Table S4. *p*-wave partial width, Γ_p, in eV.

Basis set designations are explained in the text.

	Method/Basis			
	CKV	Stab	CAP	RAC
Set	(p + p)	(P)	(P)	(P)
A	0.000	0.000	0.000	0.000
B	0.019	0.021	0.020	0.032
C	0.061	0.064	0.063	0.072
D	0.104	0.105	0.103	0.106
E	0.109	0.110	0.108	0.112
F	0.129	0.130	0.132	0.130

Table S5. *d*-wave partial width, Γ_d, in eV. Basis set designations are explained in the text.

	Method/Basis			
	CKV	Stab	CAP	RAC
Set	(p + p)	(D)	(D)	(D)
A	0.170	0.167	0.168	0.144
B	0.113	0.113	0.107	0.098
C	0.075	0.074	0.068	0.066
D	0.050	0.051	0.049	0.044
E	0.047	0.047	0.046	0.046
F	0.037	0.039	0.037	0.038

The real and imaginary parts of the orbitals from the CAP calculations are shown in Figure S1. The orbital associated with electron capture in set A (Figure S1a and S1b), the symmetric case, displays nodal and symmetry characteristics reminiscent of the π^* orbital of N_2, while that from the most asymmetric case (set F, Figure S1e and S1f) is heavily weighted on one site. The orbital from the intermediate case (set C, Figure S1c and S1d) has significant, but differing weights on both sites, similar to the π^* orbital in CO.

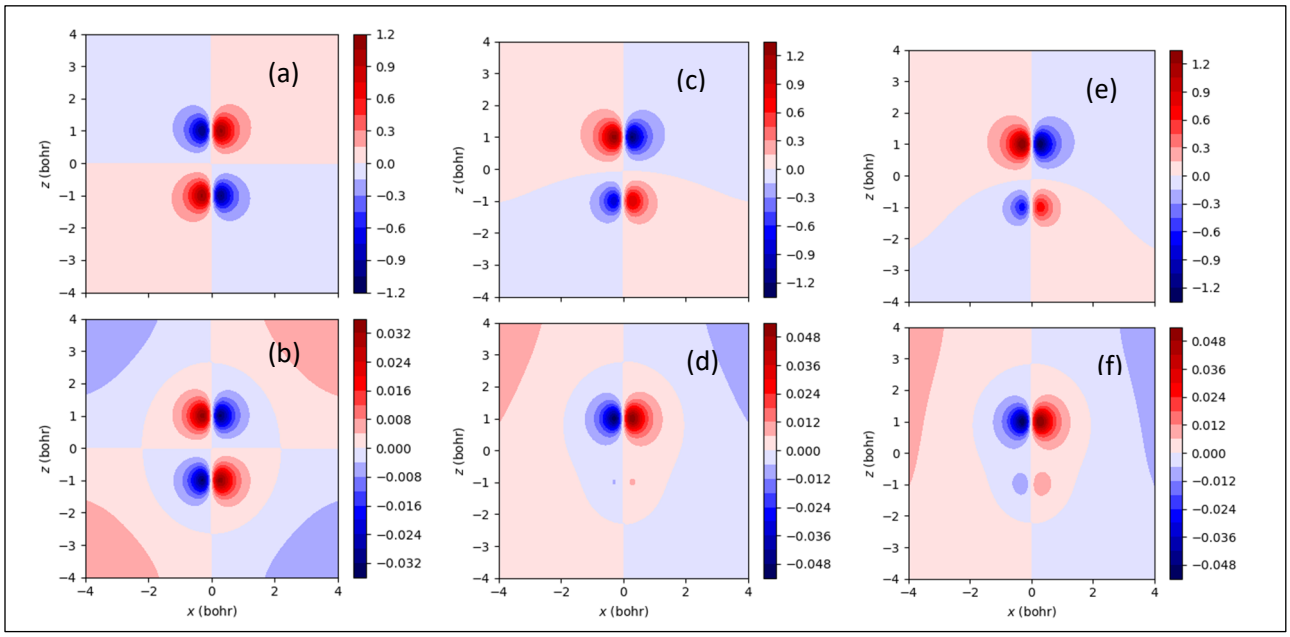

Figure S1. Complex orbitals from the CAP calculations for potential sets A [(a) and (b)], C [c) and (d)], and F [(e) and (f)]. The upper panels [(a), (c), and (e)] show the real parts, and the lower panels [(b), (d), and (f)] show cuts through imaginary parts of the complex orbitals. Note the different amplitudes (color scales) in the two panels. The maximum of the imaginary part is more than one order of magnitude smaller than the maximum of the real part.