

脯氨酸与 Ag 和 Ag⁺相互作用及性质

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Interaction and Properties of Proline-Ag and -Ag⁺ Complexes

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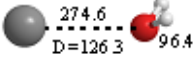
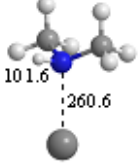
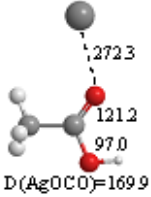
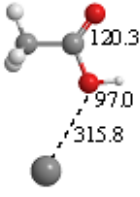
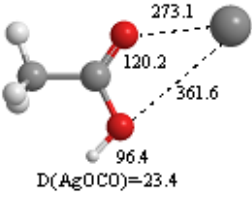
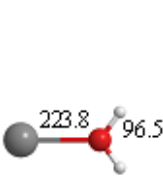
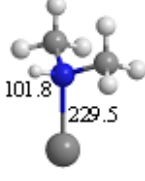
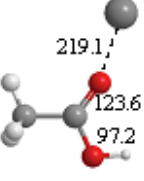
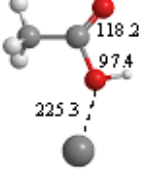
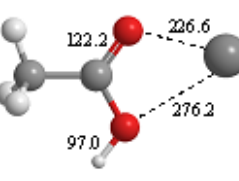
				
<p style="text-align: center;">Ag-H₂O</p>	<p style="text-align: center;">Ag-NH(CH₃)₂</p>	<p style="text-align: center;">Ag-CH₃COOH_c</p>		
				
<p style="text-align: center;">Ag-CH₃COOH_c</p>	<p style="text-align: center;">Ag-CH₃COOH_c</p>			
				
<p style="text-align: center;">Ag⁺-H₂O</p>	<p style="text-align: center;">Ag⁺-NH(CH₃)₂</p>	<p style="text-align: center;">Ag⁺-CH₃COOH_c</p>	<p style="text-align: center;">Ag⁺-CH₃COOH_c</p>	<p style="text-align: center;">Ag⁺-CH₃COOH_c</p>
<p style="text-align: center;">附图 1 X3LYP/LACV3P****方法优化的 Ag 和 Ag⁺与 H₂O、NH(CH₃)₂和 CH₃COOH_c 的几何结构 Supporting Fig. 1 The geometrical structures of Ag and Ag⁺ with H₂O, NH(CH₃)₂, and CH₃COOH_c at the level of X3LYP/LAV3P****.</p>				

表 s1 用 X3LYP/LACV3P**++方法计算的 Ag 和 Ag⁺与 H₂O、NH(CH₃)₂和 CH₃COOH_c的转动系数、偶极矩、总能量、结合能、变形能、前线轨道能差、部分原子电荷布局 and 特殊键频率

Table s1 The rotational constants(A, B, and C in GHz), dipole moment(μ in 10⁻³⁰C·m), total energies(TE in amu), zero-point energies(in kcal·mol⁻¹), binding energies(BE in kJ·mol⁻¹), deforming energies(DE in kJ·mol⁻¹), $\Delta\epsilon(\epsilon_{\text{LUMO}}-\epsilon_{\text{HOMO}}$, in eV), some atoms charge population(e), and stretching vibrational frequencies(cm⁻¹) of O-H and N-H bonds for Ag and Ag⁺ with H₂O, NH(CH₃)₂, and CH₃COOH at the X3LYP/LACV3P**++ level.

Systems	A	B	C	μ	TE	ZPE	BE	DE	$\Delta\epsilon$
Ag-H ₂ O	349.463	4.122	4.091	3.35	-222.14176	14.0	-5.4	0.1	3.71
Ag-NH(CH ₃) ₂	8.615	1.664	1.455	3.72	-280.85515	58.6	-18.8	0.4	3.64
Ag-CH ₃ COOH _a	9.386	0.864	0.796	3.22	-374.78387	38.9	-3.7	0.6	3.77
Ag-CH ₃ COOH _b	9.458	0.735	0.685	1.07	-374.78244	38.9	-0.1	0.1	4.54
Ag-CH ₃ COOH _c	10.123	0.909	0.847	6.20	-374.77476	38.7	19.4	25.3	3.17
Ag					-145.70990				4.96
H ₂ O	826.318	430.165	282.895	2.16	-76.42880	13.4			8.26
NH(CH ₃) ₂	34.844	9.252	8.179	1.04	-135.13681	57.8			5.99
CH ₃ COOH	11.352	9.463	5.331	1.74	-229.07220	38.7			7.68
Ag ⁺ -H ₂ O	412.145	6.148	6.058	2.15	-221.90083	14.8	-125.5	0.5	6.16
Ag ⁺ -NH(CH ₃) ₂	8.450	2.128	1.793	1.56	-280.63840	59.8	-200.9	5.4	4.63
Ag ⁺ -CH ₃ COOH _a	9.671	0.999	0.910	0.54	-374.55120	39.2	-147.6	7.4	4.81
Ag ⁺ -CH ₃ COOH _b	9.127	1.030	0.931	3.34	-374.52980	38.8	-93.4	17.1	4.06
Ag ⁺ -CH ₃ COOH _c	11.112	1.290	1.164	3.66	-374.55376	39.2	-154.5	31.0	5.37
Ag ⁺					-145.42193				6.88
Systems	q _N	q _{O(-H)}	q _{O(=C)}	q _{H(-N)}	q _{H(-O)}	q _{Ag}	v _{O-H}	v _{O-H}	v _{N-H}
Ag-H ₂ O		-0.937			0.470	-0.003	3797	3906	
Ag-NH(CH ₃) ₂	-0.682			0.359		-0.056			3525
Ag-CH ₃ COOH _a		-0.680	-0.622		0.488	-0.007	3769		
Ag-CH ₃ COOH _b		-0.705	-0.581		0.488	-0.003	3766		
Ag-CH ₃ COOH _c		-0.670	-0.579		0.476	-0.009	3817		
H ₂ O		-0.918			0.459		3826	3931	
NH(CH ₃) ₂	-0.668			0.340					3538
CH ₃ COOH							3767	3931	
Ag ⁺ -H ₂ O		-1.017			0.522	0.973	3794		
Ag ⁺ -NH(CH ₃) ₂	-0.722			0.395		0.826			3492
Ag ⁺ -CH ₃ COOH _a		-0.615	-0.790		0.503	0.970	3736		
Ag ⁺ -CH ₃ COOH _b		-0.865	-0.468		0.520	0.946	3712		
Ag ⁺ -CH ₃ COOH _c		-0.689	-0.649		0.517	0.917	3772		