Supplementary Information for ***Acta Phys. -Chim. Sin.*** **2014**, *30* (6), 1071-1085
doi: 10.3866/PKU.WHXB201404151

脯氨酸与 $Zn^{2+/1+/0}$ 相互作用及性质

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Interaction and Properties of Proline-$Zn^{2+/1+/0}$ Complexes

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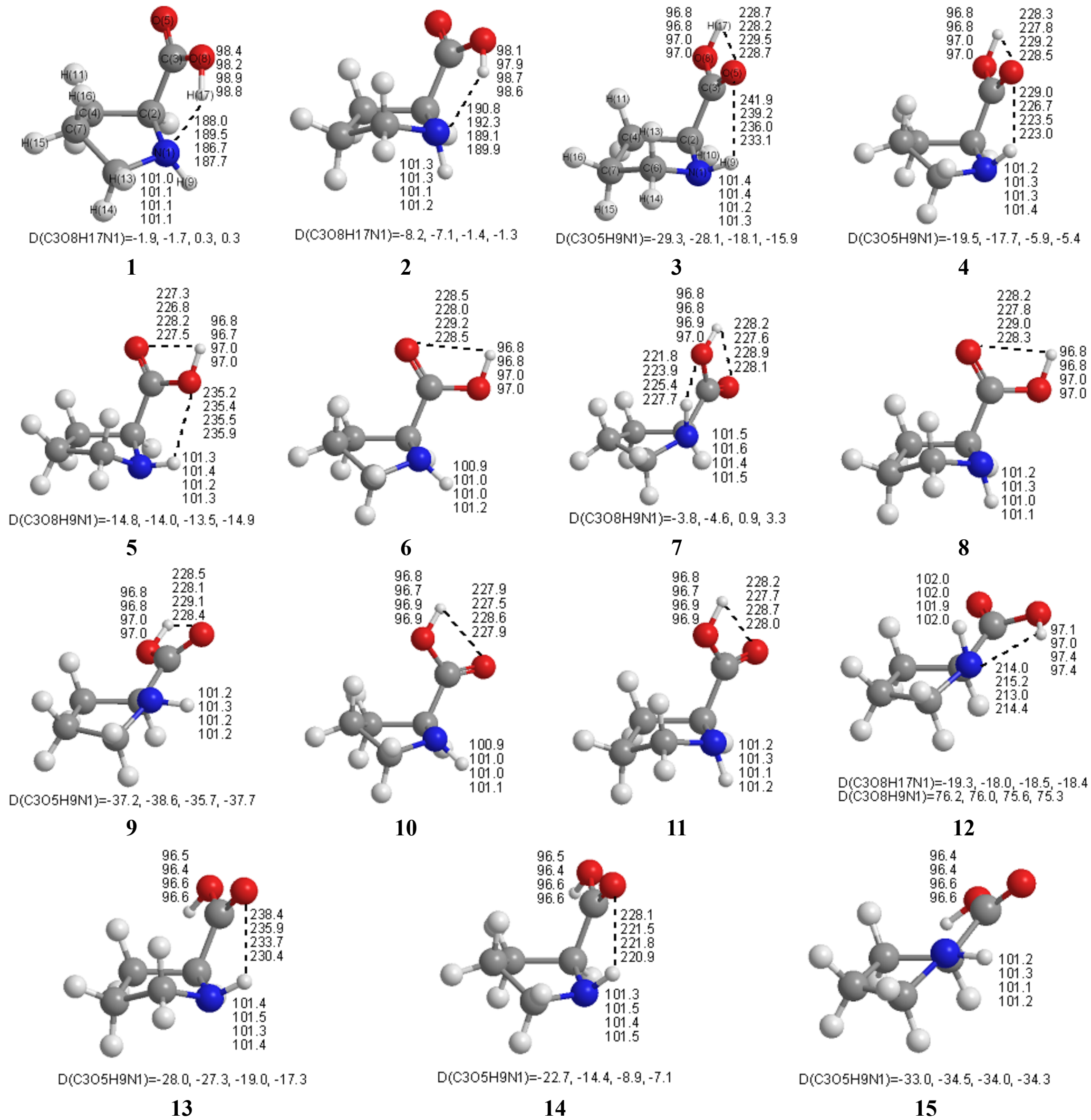

图 S1　15 种 Pro 构象的几何结构

Fig.S1　Geometrical structures of fifteen proline conformers

Bonds distance in pm and dihedral angles (D) in degree, from top to bottom and from left to right corresponding to the results of M062X/TZVP, M062X/6-311++G(2*d*, *p*)+(LANL2DZ), X3LYP/TZVP, X3LYP/6-311++G(2*d*, *p*)+(LANL2DZ), respectively

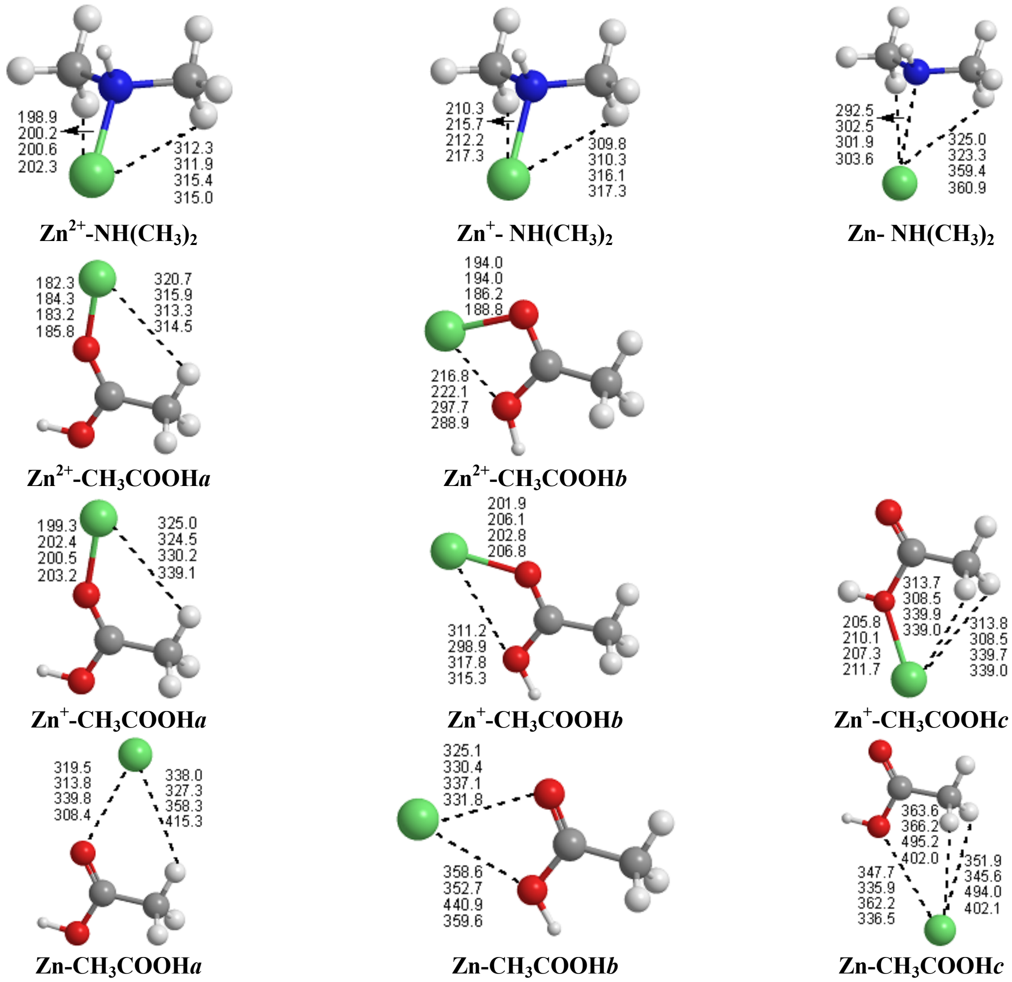

图 S2 $Zn^{+2/+1/0}$-$(CH_3)_2NH$ 和 $Zn^{+2/+1/0}$-CH_3COOH 体系几何结构

Fig.S2 Geometrical structures of $Zn^{+2/+1/0}$-$(CH_3)_2NH$ and $Zn^{+2/+1/0}$-CH_3COOH complexes

Bonds distance in pm, from top to bottom and from left to right corresponding to the results of M062X/TZVP, M062X/6-311++G(*2d*, *p*)+(LANL2DZ), X3LYP/TZVP, X3LYP/6-311++G(*2d*, *p*)+(LANL2DZ), respectively. Symbol *a*, *b* and *c* represent the modes of $Zn^{+2/+1/0}$ combined to CH_3COOH.

表 S1　15 种 Pro 构象的相对能(E_{R1}, kJ·mol^{-1})、相对吉布斯自由能($\Delta\Delta G$, kJ·mol^{-1})、前线轨道能差(Δε, eV)、偶极矩(μ, 10^{-30} C•m)、转动系数(A, B, C, GHz)和 O－H 和 N－H 的伸缩振动频率(ν, cm^{-1})

Table S1　Relative energies (E_{R1}, kJ·mol^{-1}), relative Gibbs free energies ($\Delta\Delta G$, kJ·mol^{-1}), Δε (ε_{LUMO}-ε_{HOMO}, eV), dipole moment (μ, 10^{-30} C•m), rotational constants (A, B, C, GHz), and stretching vibrational frequencies (ν, cm^{-1}) of O－H and N－H bonds for proline conformers

	Complex		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
E_{R1}	M062X	BS1	0.00	2.92	5.54	6.39	11.41	12.89	16.75	16.07	16.03	16.34	16.72	23.10	26.03	26.74	37.69
		BS2	0.00	2.94	3.90	4.20	10.42	11.98	15.06	14.73	13.94	15.04	15.11	21.23	23.25	23.20	34.48
	X3LYP	BS1	0.00	1.92	6.46	7.38	13.18	12.95	15.63	15.44	15.22	16.86	17.39	22.56	26.60	27.54	36.79
		BS2	0.00	1.74	4.67	5.58	12.23	12.29	14.10	14.52	13.64	15.78	15.94	21.41	24.23	24.86	34.55
$\Delta\Delta G$	M062X	BS1	0.00	1.14	2.42	4.75	9.02	11.42	14.73	14.53	12.15	14.11	15.04	22.46	24.05	24.72	35.02
		BS2	0.00	0.29	0.75	2.60	8.47	10.31	12.49	12.53	10.70	12.70	12.86	20.70	20.74	21.12	31.97
	X3LYP	BS1	0.00	0.17	4.19	4.63	10.25	9.59	12.16	12.81	12.43	14.37	14.99	21.08	24.51	24.76	34.50
		BS2	0.00	0.34	2.18	2.32	9.09	7.66	8.92	11.75	10.99	11.92	12.70	20.37	21.89	22.03	32.14
$\Delta\varepsilon$	M062X	BS1	9.57	9.69	9.17	8.96	9.05	9.16	9.45	9.29	9.23	9.30	9.43	9.92	9.09	9.01	9.21
		BS2	8.20	8.41	7.96	7.89	7.95	7.81	8.17	8.08	8.00	7.84	8.06	8.78	7.84	7.84	7.95
	X3LYP	BS1	6.93	7.04	6.18	6.15	6.18	6.37	6.52	6.44	6.39	6.41	6.59	7.21	6.25	6.27	6.48
		BS2	6.29	6.38	5.95	6.02	5.96	6.06	6.28	6.09	6.05	6.03	6.15	6.82	5.78	5.92	5.99
μ	M062X	BS1	5.88	5.80	1.56	1.82	1.35	2.26	2.68	2.24	2.28	2.46	2.78	4.78	3.80	3.76	5.12
		BS2	5.67	5.65	1.60	1.83	1.33	2.24	2.68	2.18	2.28	2.46	2.74	4.61	3.73	3.83	4.98
	X3LYP	BS1	5.87	5.98	1.75	1.94	1.40	2.26	2.58	2.39	2.17	2.36	2.66	4.75	3.97	3.95	4.96
		BS2	5.75	5.86	1.83	1.96	1.41	2.29	2.61	2.41	2.24	2.42	2.70	4.65	3.96	3.94	4.90
A	M062X	BS1	3.692	3.747	3.871	3.779	3.528	3.923	4.215	4.070	4.347	4.034	4.084	4.243	3.870	3.752	4.304
		BS2	3.686	3.800	3.915	3.810	3.514	3.912	4.222	4.059	4.346	4.052	4.088	4.241	3.889	3.859	4.303
	X3LYP	BS1	3.739	4.036	4.080	3.943	3.633	4.046	4.208	4.140	4.324	4.029	4.108	4.226	4.046	3.910	4.287
		BS2	3.742	4.036	4.124	3.959	3.613	4.126	4.235	4.147	4.325	4.051	4.114	4.221	4.094	3.955	4.287
B	M062X	BS1	1.705	1.693	1.637	1.650	1.770	1.601	1.443	1.500	1.480	1.537	1.490	1.516	1.631	1.654	1.485
		BS2	1.704	1.670	1.621	1.635	1.775	1.605	1.437	1.505	1.479	1.520	1.497	1.516	1.624	1.606	1.485
	X3LYP	BS1	1.651	1.561	1.536	1.549	1.684	1.529	1.422	1.443	1.464	1.507	1.440	1.498	1.539	1.553	1.466
		BS2	1.648	1.560	1.522	1.542	1.693	1.508	1.412	1.441	1.462	1.490	1.447	1.498	1.523	1.533	1.466
C	M062X	BS1	1.426	1.340	1.338	1.421	1.433	1.342	1.336	1.390	1.174	1.415	1.432	1.176	1.326	1.430	1.169
		BS2	1.418	1.322	1.326	1.413	1.439	1.349	1.338	1.395	1.175	1.424	1.414	1.176	1.322	1.393	1.169
	X3LYP	BS1	1.378	1.253	1.251	1.334	1.353	1.253	1.295	1.318	1.160	1.372	1.386	1.162	1.252	1.341	1.156
		BS2	1.373	1.252	1.244	1.332	1.361	1.220	1.285	1.314	1.161	1.376	1.369	1.163	1.245	1.333	1.156
ν_{O-H}	M062X	BS1	3469	3535	3810	3819	3808	3828	3825	3815	3814	3822	3820	3760	3854	3861	3867
		BS2	3506	3564	3820	3830	3822	3834	3833	3826	3826	3830	3831	3777	3868	3869	3878
	X3LYP	BS1	3567	3561	3551	3531	3561	3571	3526	3562	3562	3581	3556	3453	3546	3525	3569
		BS2	3402	3433	3759	3759	3757	3760	3761	3755	3759	3764	3765	3668	3800	3801	3805
ν_{N-H}	M062X	BS1	3608	3574	3565	3578	3583	3625	3552	3583	3582	3623	3581	3471	3563	3575	3592
		BS2	3602	3573	3565	3568	3580	3614	3553	3568	3577	3616	3576	3470	3558	3554	3585
	X3LYP	BS1	3369	3403	3745	3748	3746	3746	3750	3743	3746	3750	3752	3644	3784	3785	3791
		BS2	3563	3558	3545	3523	3557	3558	3520	3559	3558	3575	3555	3451	3539	3514	3564

Note: the results optimized at M062X/TZVP(BS1), M062X/6-311++G(*2d*, *p*)+(LANL2DZ)(BS2), X3LYP/TZVP(BS1), X3LYP/6-311++G(*2d*, *p*)+(LANL2DZ)(BS2) levels, respectively.

表 S2　19 种 Pro-Zn^{2+}结构的相对能(E_{R1}, E_{R2}, kJ·mol^{-1})、结合能(E_{R1}, E_{R2}, kJ·mol^{-1})、变形能(E_D, kJ·mol^{-1})、相对吉布斯自由能($\Delta\Delta G$, kJ·mol^{-1})、前线轨道能差($\Delta\varepsilon$, eV)

Table S2　Relative energies (E_{R1}, E_{R2}, kJ·mol^{-1}), binding energies (E_{R1}, E_{R2}, kJ·mol^{-1}), deformation energies (E_D, kJ·mol^{-1}), relative Gibbs free energies ($\Delta\Delta G$, kJ·mol^{-1}), and Δε ($\varepsilon_{LUMO}-\varepsilon_{HOMO}$, eV) of Pro-$Zn^{2+}$ complexes

Complex	E_{R1}				E_{R2}				E_B			
	M062X		X3LYP		M062X		X3LYP		M062X		X3LYP	
	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2
CII1	0.0	0.0	0.0	0.0	-897.6	-865.6	-928.4	-871.7	-900.5	-868.5	-930.4	-873.4
CII2	0.9	12.1	9.4	24.1	-896.7	-853.5	-919.0	-847.6	-913.4	-868.6	-936.4	-863.5
CII3	2.6	2.7	3.0	3.1	-895.0	-862.8	-925.4	-868.6	-895.0	-862.8	-925.4	-868.6
CII4	4.2	14.6	13.3	28.1	-893.4	-850.9	-915.1	-843.6	-909.7	-866.0	-932.0	-859.4
CII5	28.1	36.7	36.5	49.1	-869.5	-828.9	-891.9	-822.6	-895.5	-852.1	-918.5	-846.9
CII6	31.0	39.8	40.5	53.0	-866.6	-825.8	-887.9	-818.7	-904.3	-849.0	-915.5	-843.6
CII7	39.9	49.5	49.3	62.2	-857.6	-816.1	-879.1	-809.5	-874.4	-831.1	-894.7	-823.6
CII8	65.7	73.3	75.7	86.4	-831.8	-792.3	-852.8	-785.3	-858.6	-815.5	-880.3	-810.2
CII9	84.5	101.8	91.5	111.9	-813.0	-763.7	-837.0	-759.8	-829.1	-778.5	-852.4	-774.3
CII10	86.7	104.3	96.0	116.2	-810.8	-761.3	-832.4	-755.5	-823.7	-773.3	-845.4	-767.8
CII11	87.9	105.8	98.3	118.5	-809.7	-759.7	-830.2	-753.2	-826.1	-774.8	-847.0	-767.3
CII12	104.7	120.8	112.9	131.5	-792.9	-744.7	-815.6	-740.2	-816.0	-766.0	-838.1	-761.6
CII13	199.6	201.7	206.5	211.7	-698.0	-663.8	-721.9	-659.9	-700.9	-666.8	-723.8	-661.7
CII14	212.4	219.0	201.8	216.9	-685.1	-646.6	-726.6	-654.8	-696.5	-657.0	-739.8	-667.0
CII15	217.1	225.9	162.6	177.7	-680.5	-639.6	-765.9	-694.0	-707.2	-662.8	-793.4	-718.9
CII16	225.7	226.6	233.6	237.7	-671.9	-639.0	-694.8	-634.0	-695.0	-660.2	-717.4	-655.4
CII17	234.9	247.5	167.4	187.4	-662.6	-618.0	-761.1	-684.3	-675.5	-630.0	-774.0	-696.6
CII18	240.3	254.0	169.8	189.4	-657.3	-611.6	-758.6	-682.3	-673.4	-626.3	-774.1	-696.8
CII19	246.1	259.0	182.6	201.2	-651.5	-606.6	-745.8	-670.4	-667.5	-620.5	-761.1	-684.1

Complex	E_D				$\Delta\Delta G$				Δε			
	M062X		X3LYP		M062X		X3LYP		M062X		X3LYP	
	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2
CII1	133.5	129.8	122.3	115.5	0.0	0.0	0.0	0.0	6.21	6.44	3.67	3.99
CII2	43.4	38.6	42.5	37.6	4.2	15.4	12.4	27.1	6.54	6.70	4.07	4.28
CII3	129.1	125.8	120.5	113.8	3.3	3.4	2.0	2.2	6.15	6.37	3.58	3.90
CII4	43.5	38.7	43.4	38.2	7.7	21.7	15.4	29.6	6.58	6.76	4.06	4.27
CII5	61.9	56.6	61.0	55.9	31.2	39.6	39.5	51.8	6.78	6.91	4.28	4.48
CII6	61.3	56.3	60.6	55.5	34.0	41.9	42.4	55.1	6.78	6.93	4.24	4.44
CII7	63.5	58.1	63.9	58.4	43.5	52.8	52.6	65.2	6.06	6.23	3.62	3.83
CII8	79.2	73.6	78.4	72.8	69.1	76.4	78.8	89.2	6.36	6.50	3.90	4.09
CII9	58.8	48.3	62.6	52.2	86.3	103.5	91.7	112.0	6.07	6.14	3.69	3.74
CII10	60.0	50.5	65.5	54.9	89.1	106.4	97.3	117.0	6.11	6.21	3.69	3.75
CII11	55.2	46.1	60.8	50.1	89.4	106.8	98.7	119.3	6.24	6.24	3.68	3.72
CII12	64.3	54.9	67.8	56.0	106.4	122.4	114.5	132.6	5.74	5.87	3.38	3.53
CII13	52.4	46.4	51.1	43.2	202.6	204.7	207.3	213.1	4.01	4.06	1.44	1.57
CII14	35.5	30.9	31.2	27.8	213.8	219.3	199.7	214.5	3.79	3.94	1.71	1.75
CII15	54.7	52.7	49.1	47.3	212.5	220.9	157.4	172.9	2.16	2.20	1.09	1.06
CII16	55.1	51.0	54.6	48.2	227.8	229.2	233.7	238.6	3.89	4.00	1.26	1.40
CII17	49.6	49.1	45.8	44.0	231.4	243.1	161.5	181.9	2.01	2.05	1.07	1.05
CII18	46.2	46.3	41.5	40.6	236.3	249.9	166.3	185.4	1.91	1.93	1.00	0.97
CII19	42.5	42.9	44.1	41.9	242.0	254.8	177.8	196.5	2.05	2.07	1.07	1.03

Note: the results optimized at M062X/TZVP(BS1), M062X/6-311++G(*2d*, *p*)+(LANL2DZ)(BS2), X3LYP/TZVP(BS1), X3LYP/6-311++G(*2d*, *p*)+(LANL2DZ)(BS2) levels, respectively.

表 S3　21 种 Pro-Zn^+结构的相对能(E_{R1}, E_{R2}, kJ·mol^{-1})、结合能(E_{R1}, E_{R2}, kJ·mol^{-1})、变形能(E_D, kJ·mol^{-1})、相对吉布斯自由能($\Delta\Delta G$, kJ·mol^{-1})、前线轨道能差($\Delta\varepsilon$, eV)

Table S3　Relative energies (E_{R1}, E_{R2}, kJ·mol^{-1}), binding energies (E_{R1}, E_{R2}, kJ·mol^{-1}), deformation energies (E_D, kJ·mol^{-1}), relative Gibbs free energies ($\Delta\Delta G$, kJ·mol^{-1}), and Δε ($\varepsilon_{LUMO}-\varepsilon_{HOMO}$, eV) of Pro-$Zn^+$ complexes

Complex	E_{R1}				E_{R2}				E_B			
	M062X		X3LYP		M062X		X3LYP		M062X		X3LYP	
	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2
CI1	0.0	0.0	4.0	9.7	-301.2	-310.7	-283.2	-292.1	-317.5	-325.8	-300.1	-307.9
CI2	0.5	0.8	2.4	8.2	-300.6	-309.9	-284.8	-293.6	-317.4	-325.1	-302.2	-309.5
CI3	9.7	5.5	0.0	0.0	-291.5	-305.2	-287.2	-301.8	-291.5	-305.2	-287.2	-301.8
CI4	12.6	8.0	1.6	1.4	-288.6	-302.7	-285.6	-300.4	-291.5	-305.7	-287.5	-302.2
CI5	26.4	24.0	30.1	33.5	-274.8	-286.7	-257.1	-268.3	-301.5	-309.9	-284.7	-293.1
CI6	27.2	25.4	28.8	32.6	-274.0	-285.3	-258.5	-269.2	-300.0	-308.6	-285.1	-293.5
CI7	30.9	29.4	30.2	34.4	-270.2	-281.3	-257.0	-267.5	-287.0	-296.4	-272.6	-281.6
CI8	42.5	46.1	44.4	52.6	-258.6	-264.7	-242.9	-249.3	-274.7	-279.4	-258.3	-263.8
CI9	42.8	46.1	46.2	54.8	-258.3	-264.6	-241.0	-247.1	-271.2	-276.6	-254.0	-259.3
CI10	43.5	46.3	47.7	55.8	-257.7	-264.5	-239.5	-246.0	-274.4	-279.5	-255.2	-260.1
CI11	50.1	50.8	39.6	44.0	-251.0	-259.9	-247.7	-257.8	-253.9	-262.8	-249.6	-259.6
CI12	56.1	52.6	55.9	57.9	-245.0	-258.1	-231.4	-244.0	-271.8	-281.4	-258.9	-268.8
CI13	57.1	58.3	56.9	64.0	-244.0	-252.4	-230.3	-237.8	-267.1	-273.6	-252.9	-259.2
CI14	78.6	77.8	72.6	81.5	-222.6	-232.9	-214.6	-220.3	-234.0	-243.3	-227.8	-232.6
CI15	97.4	92.5	87.5	87.1	-203.8	-218.2	-199.7	-214.7	-226.9	-239.5	-222.3	-236.2
CI16	106.5	100.2	95.6	94.3	-194.7	-210.5	-191.7	-207.5	-221.4	-233.7	-219.2	-232.4
CI17	110.7	105.6	98.1	100.9	-190.5	-205.1	-189.2	-201.0	-201.9	-215.5	-202.3	-213.2
CI18	111.0	104.5	99.6	98.2	-190.1	-206.2	-187.6	-203.6	-216.2	-229.4	-214.2	-227.8
CI19	111.1	105.8	97.6	99.4	-190.0	-205.0	-189.7	-202.4	-206.1	-219.7	-205.1	-217.0
CI20	111.3	105.2	101.3	100.5	-189.9	-205.5	-186.0	-201.4	-216.6	-228.7	-213.5	-226.2
CI21	172.7	167.4	165.5	167.0	-128.5	-143.4	-121.7	-134.9	-145.2	-158.5	-139.1	-150.8

Complex	E_D				$\Delta\Delta G$				Δε			
	M062X		X3LYP		M062X		X3LYP		M062X		X3LYP	
	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2
CI1	17.2	14.7	16.7	14.2	0.0	0.0	7.6	11.9	6.63	6.45	4.51	4.41
CI2	18.3	15.4	16.6	14.5	-2.5	-0.4	5.8	11.0	6.65	6.41	4.56	4.41
CI3	89.6	87.1	76.8	74.7	7.4	4.7	0.0	0.0	7.00	6.23	5.57	4.73
CI4	95.5	92.2	82.8	79.1	9.0	6.2	0.9	1.1	6.98	6.18	5.29	4.73
CI5	32.4	30.1	31.2	29.2	26.0	24.3	33.5	35.2	6.60	6.41	4.48	4.38
CI6	33.8	31.1	32.2	30.4	26.5	26.0	32.0	35.3	6.59	6.33	4.52	4.37
CI7	32.6	28.3	31.3	28.2	30.4	29.8	33.3	36.4	6.56	6.32	4.59	4.41
CI8	18.3	14.8	18.6	15.8	40.1	44.6	44.5	57.4	7.28	6.75	5.40	5.08
CI9	21.5	17.2	21.8	18.8	39.6	48.4	47.8	55.3	7.30	6.74	5.28	5.05
CI10	18.8	15.2	18.3	14.6	41.3	49.3	49.2	56.4	7.47	6.85	5.44	5.21
CI11	23.7	18.5	20.6	15.5	45.9	47.3	40.3	43.9	7.71	7.24	5.66	5.35
CI12	45.5	41.5	42.8	40.1	55.7	52.9	59.0	59.8	6.49	6.27	4.52	4.36
CI13	18.9	16.1	16.5	13.3	54.8	55.9	58.1	64.0	7.33	6.73	5.43	5.08
CI14	8.9	7.6	11.1	9.2	73.2	74.7	71.3	79.4	7.83	7.14	6.09	5.47
CI15	14.0	13.4	13.9	11.7	92.9	88.5	87.4	86.3	7.45	7.11	5.43	5.19
CI16	29.0	27.5	27.2	26.1	99.4	94.6	91.4	90.3	7.31	7.13	4.56	4.60
CI17	17.8	15.3	20.1	14.6	103.8	102.9	94.4	97.7	7.17	7.00	4.90	4.73
CI18	14.5	12.8	15.9	13.6	104.4	98.7	96.5	94.6	7.20	7.05	4.45	4.45
CI19	22.1	19.0	18.2	15.5	105.2	101.5	95.1	96.6	7.44	7.11	4.91	4.81
CI20	15.0	14.6	18.6	16.8	104.5	99.2	98.0	96.8	7.02	6.93	4.34	4.35
CI21	25.7	19.6	29.6	24.4	167.9	164.7	162.1	161.3	7.71	7.30	5.03	4.68

Note: the results optimized at M062X/TZVP(BS1), M062X/6-311++G(*2d*, *p*)+(LANL2DZ)(BS2), X3LYP/TZVP(BS1), X3LYP/6-311++G(*2d*, *p*)+(LANL2DZ)(BS2) levels, respectively.

表 S4　19 种 Pro-Zn^{2+}结构的转动系数(*A*, *B*, *C*, GHz)、偶极矩(*μ*, 10^{-30} C•m)、O－H 和 N－H 的伸缩振动频率(*ν*, cm^{-1})

Table S4　Rotational constants (*A*, *B*, *C*, GHz), dipole moment (*μ*, 10^{-30} C•m), and stretching vibrational frequencies (*ν*, cm^{-1}) of O－H and N－H bonds of Pro-Zn^{2+} complexes

Complex	*A*				*B*				*C*			
	M062X		X3LYP		M062X		X3LYP		M062X		X3LYP	
	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2
CII1	3.888	3.882	3.899	3.885	0.563	0.563	0.553	0.553	0.522	0.522	0.513	0.513
CII2	1.595	1.593	1.577	1.570	1.233	1.218	1.229	1.209	0.743	0.737	0.737	0.728
CII3	3.386	3.396	3.483	3.481	0.603	0.602	0.580	0.579	0.574	0.572	0.551	0.550
CII4	1.545	1.518	1.519	1.503	1.331	1.333	1.322	1.306	0.809	0.805	0.794	0.786
CII5	1.599	1.595	1.575	1.567	1.223	1.208	1.224	1.203	0.740	0.734	0.734	0.725
CII6	1.518	1.488	1.486	1.476	1.349	1.354	1.345	1.323	0.811	0.807	0.797	0.788
CII7	1.633	1.632	1.616	1.612	1.144	1.132	1.143	1.124	0.694	0.689	0.690	0.682
CII8	1.629	1.627	1.612	1.607	1.139	1.127	1.139	1.119	0.691	0.686	0.688	0.680
CII9	1.628	1.660	1.578	1.586	1.176	1.143	1.191	1.159	0.729	0.725	0.721	0.712
CII10	1.728	1.733	1.668	1.680	1.170	1.150	1.178	1.146	0.789	0.779	0.774	0.762
CII11	1.533	1.493	1.424	1.397	1.364	1.363	1.381	1.377	0.856	0.843	0.806	0.800
CII12	1.619	1.615	1.597	1.589	1.136	1.126	1.132	1.115	0.690	0.686	0.684	0.677
CII13	1.851	1.857	1.868	1.873	1.017	0.997	0.973	0.954	0.701	0.690	0.686	0.672
CII14	2.508	2.487	1.964	2.011	0.768	0.763	0.748	0.739	0.699	0.695	0.640	0.638
CII15	2.490	2.674	2.408	2.420	0.585	0.582	0.563	0.563	0.539	0.546	0.518	0.518
CII16	1.731	1.735	1.701	1.713	1.033	1.013	1.004	0.990	0.667	0.659	0.651	0.646
CII17	3.532	3.607	3.078	2.987	0.470	0.464	0.478	0.483	0.455	0.453	0.440	0.443
CII18	3.146	3.136	3.163	3.078	0.479	0.478	0.465	0.467	0.428	0.427	0.416	0.416
CII19	2.029	2.036	2.062	2.057	0.610	0.608	0.573	0.573	0.531	0.531	0.507	0.506

Complex	*μ*				ν_{O-H}				ν_{N-H}			
	M062X		X3LYP		M062X		X3LYP		M062X		X3LYP	
	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2
CII1	3.17	3.42	2.89	3.19					3405 3470	3410 3473	3408 3467	3409 3469
CII2	3.52	3.95	3.02	3.63	3647	3674	3621	3642	3467	3467	3464	3463
CII3	3.08	3.30	2.85	3.11					3396 3480	3398 3477	3393 3462	3394 3464
CII4	3.42	3.74	2.99	3.52	3658	3686	3622	3643	3456	3454	3463	3459
CII5	3.91	4.02	3.68	3.80	3739	3754	3695	3716	3474	3472	3463	3463
CII6	4.12	4.08	3.92	3.93	3745	3749	3692	3712	3455	3459	3460	3457
CII7	3.48	3.95	2.91	3.62	3641	3653	3606	3627	3389	3387	3378	3376
CII8	3.15	3.37	2.90	3.15	3728	3748	3691	3712	3389	3388	3378	3376
CII9	6.55	7.12	5.85	6.61	3650	3659	3627	3638	3466	3432	3449	3442
CII10	6.65	7.15	6.01	6.74	3665	3668	3630	3642	3465	3463	3463	3459
CII11	5.52	6.06	5.37	6.01	3666	3663	3628	3639	3454	3449	3439	3436
CII12	6.30	6.85	5.60	6.38	3675	3688	3632	3642	3380	3379	3384	3381
CII13	5.95	6.17	5.49	5.82	3379	3415	3132	3226	3568	3557	3534	3535
CII14	9.01	9.47	7.37	8.30	3732	3735	3651	3667	3411	3416	3353	3368
CII15	4.18	5.57	2.61	3.24	3697	3701	3679	3696	3597	3612	3566	3576
CII16	5.38	5.71	4.14	5.12	3599	3627	3615	3608	3483	3478	3484	3471
CII17	4.67	5.52	2.77	3.60	3691	3709	3659	3684	3594	3583	3548	3560
CII18	4.88	5.62	2.92	3.80	3724	3746	3669	3691	3573	3583	3551	3563
CII19	4.80	5.60	2.86	3.88	3701	3728	3652	3680	3576	3591	3549	3559

Note: the results optimized at M062X/TZVP(BS1), M062X/6-311++G(*2d*, *p*)+(LANL2DZ)(BS2), X3LYP/TZVP(BS1), X3LYP/6-311++G(*2d*, *p*)+(LANL2DZ)(BS2) levels, respectively.

表 S5　21 种 Pro-Zn+结构的转动系数(*A*, *B*, *C*, GHz)、偶极矩(*μ*, 10^{-30} C•m)、O－H 和 N－H 的伸缩振动频率(*ν*, cm^{-1})

Table S5　Rotational constants (*A*, *B*, *C*, GHz), dipole moment (*μ*, 10^{-30} C•m), and stretching vibrational frequencies (*ν*, cm^{-1}) of O－H and N－H bonds of Pro-Zn^+ complexes

Complex	*A*				*B*				*C*			
	M062X		X3LYP		M062X		X3LYP		M062X		X3LYP	
	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2
CI1	1.544	1.521	1.508	1.492	1.215	1.202	1.189	1.166	0.771	0.762	0.745	0.734
CI2	1.569	1.567	1.538	1.542	1.126	1.101	1.116	1.083	0.701	0.691	0.688	0.677
CI3	3.200	3.168	3.434	3.262	0.593	0.594	0.526	0.567	0.565	0.565	0.500	0.539
CI4	3.661	3.608	3.786	3.733	0.549	0.552	0.524	0.531	0.512	0.514	0.488	0.494
CI5	1.540	1.514	1.500	1.481	1.213	1.201	1.189	1.168	0.770	0.760	0.744	0.733
CI6	1.597	1.590	1.548	1.553	1.105	1.083	1.103	1.070	0.698	0.688	0.685	0.674
CI7	1.575	1.573	1.546	1.552	1.056	1.036	1.050	1.021	0.652	0.644	0.644	0.634
CI8	1.716	1.718	1.563	1.596	1.033	1.007	1.076	1.028	0.702	0.691	0.676	0.664
CI9	1.799	1.818	1.711	1.713	1.033	0.996	1.040	1.009	0.740	0.725	0.721	0.705
CI10	1.465	1.447	1.422	1.403	1.265	1.240	1.237	1.212	0.787	0.776	0.754	0.744
CI11	3.751	3.780	3.750	2.723	0.491	0.490	0.479	0.529	0.459	0.458	0.447	0.439
CI12	1.584	1.581	1.556	1.561	1.047	1.027	1.040	1.012	0.650	0.642	0.642	0.632
CI13	1.531	1.528	1.500	1.503	1.070	1.047	1.055	1.028	0.651	0.642	0.639	0.630
CI14	2.167	2.208	1.879	1.917	0.726	0.710	0.736	0.717	0.650	0.644	0.622	0.612
CI15	3.945	3.975	3.871	3.869	0.469	0.469	0.460	0.458	0.427	0.428	0.419	0.417
CI16	2.501	2.585	2.468	2.455	0.545	0.562	0.552	0.549	0.525	0.523	0.509	0.506
CI17	2.142	2.091	2.134	2.243	0.702	0.726	0.631	0.602	0.569	0.579	0.542	0.527
CI18	2.725	2.848	2.668	2.723	0.551	0.542	0.536	0.529	0.505	0.499	0.491	0.485
CI19	2.075	2.037	2.073	2.039	0.707	0.726	0.628	0.631	0.559	0.569	0.536	0.534
CI20	2.454	2.512	2.420	2.409	0.601	0.595	0.577	0.576	0.552	0.548	0.528	0.527
CI21	1.921	1.939	1.869	1.874	0.772	0.771	0.711	0.714	0.587	0.596	0.537	0.544

Complex	*μ*				ν_{O-H}				ν_{N-H}			
	M062X		X3LYP		M062X		X3LYP		M062X		X3LYP	
	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2
CI1	2.35	2.09	2.21	1.87	3748	3765	3703	3717	3537	3527	3511	3505
CI2	2.24	1.97	2.11	1.76	3741	3755	3702	3716	3523	3525	3513	3510
CI3	6.98	6.86	5.73	6.42					3278 3499	3290 3501	3151 3501	3213 3501
CI4	7.10	6.97	6.55	6.56					3313 3497	3320 3495	3239 3496	3326 3497
CI5	5.22	4.78	5.04	4.56	3807	3825	3756	3772	3536	3524	3512	3505
CI6	5.15	4.73	4.99	4.50	3812	3832	3759	3775	3513	3515	3514	3511
CI7	1.74	1.44	1.55	1.15	3750	3761	3693	3707	3419	3423	3418	3416
CI8	2.62	2.77	2.84	3.04	3738	3744	3694	3479	3492	3487	3491	3703
CI9	2.66	2.82	2.85	3.06	3741	3747	3696	3705	3520	3522	3510	3504
CI10	2.48	2.57	2.69	2.86	3738	3765	3695	3705	3503	3492	3483	3476
CI11	0.82	0.68	0.75	0.90	2469	2682	2474	2707	3575	3578	3551	3550
CI12	4.60	4.15	4.42	3.91	3811	3829	3757	3773	3420	3424	3420	3419
CI13	2.45	2.64	2.75	2.97	3757	3764	3699	3709	3429	3429	3427	3425
CI14	4.14	4.36	4.19	4.56	3787	3797	3724	3734	3459	3462	3451	3458
CI15	1.81	2.10	1.84	2.31	3507	3546	3361	3422	3447	3446	3432	3432
CI16	2.92	3.03	2.88	2.96	3791	3800	3730	3748	3630	3619	3595	3588
CI17	3.30	3.23	1.64	2.83	3728	3745	3694	3711	3611	3600	3634	3603
CI18	3.56	3.75	3.30	3.69	3781	3786	3730	3748	3611	3594	3600	3587
CI19	2.82	2.82	1.89	2.57	3753	3769	3694	3710	3616	3591	3622	3609
CI20	3.47	3.69	3.11	3.55	3782	3803	3729	3746	3630	3619	3624	3606
CI21	5.20	5.55	4.84	5.66	3737	3748	3675	3689	3600	3592	3617	3600

Note: the results optimized at M062X/TZVP(BS1), M062X/6-311++G(*2d*, *p*)+(LANL2DZ)(BS2), X3LYP/TZVP(BS1), X3LYP/6-311++G(*2d*, *p*)+(LANL2DZ)(BS2) levels, respectively.

表 S6　24 种 Pro-Zn 结构的转动系数(A, B, C, GHz)、偶极矩(μ, 10^{-30} C•m)、O－H 和 N－H 的伸缩振动频率(ν, cm^{-1})

Table S6　Rotational constants (A, B, C, GHz), dipole moment (μ, 10^{-30} C•m), and stretching vibrational frequencies (ν, cm^{-1}) of O－H and N－H bonds of Pro-Zn complexes

Complex	*A*				*B*				*C*			
	M062X		X3LYP		M062X		X3LYP		M062X		X3LYP	
	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2
A1	1.789	1.739	1.981	2.172	0.619	0.651	0.478	0.464	0.539	0.563	0.420	0.421
A2	1.929	1.907	2.065	2.128	0.532	0.537	0.455	0.472	0.462	0.466	0.417	0.426
A3	1.882	1.827	1.568	1.484	0.560	0.560	0.570	0.608	0.514	0.509	0.485	0.501
A4	1.452	1.455	1.336	1.381	0.745	0.762	0.638	0.640	0.615	0.627	0.525	0.531
A5	1.844	1.842	1.769	1.956	0.548	0.552	0.501	0.492	0.458	0.464	0.425	0.423
A6	1.758	1.660	1.573	1.520	0.568	0.582	0.572	0.597	0.506	0.509	0.490	0.503
A7	1.525	1.512	1.444	1.422	0.680	0.688	0.601	0.647	0.534	0.537	0.477	0.501
A8	3.263	3.333	3.760	3.402	0.403	0.379	0.336	0.350	0.385	0.363	0.319	0.330
A9	1.623	1.614	1.467	1.446	0.638	0.666	0.575	0.612	0.537	0.557	0.478	0.503
A10	2.201	2.299	1.923	1.960	0.534	0.515	0.518	0.527	0.509	0.495	0.476	0.487
A11	1.397	1.426	1.309	1.314	0.855	0.850	0.753	0.791	0.651	0.656	0.571	0.594
A12	1.999	1.923	1.815	1.741	0.546	0.549	0.540	0.566	0.515	0.513	0.489	0.505
A13	1.631	1.596	1.662	1.543	0.589	0.605	0.457	0.568	0.462	0.469	0.372	0.439
A14	3.378	3.430	3.632	3.129	0.362	0.372	0.304	0.352	0.340	0.349	0.293	0.339
A15	1.313	1.278	1.282	1.282	0.845	0.868	0.755	0.809	0.616	0.621	0.562	0.578
A16	1.467	1.482	1.423	1.443	0.736	0.751	0.603	0.649	0.605	0.620	0.499	0.542
A17	1.403	1.406	1.380	1.380	0.833	0.826	0.735	0.778	0.626	0.623	0.561	0.585
A18	1.528	1.532	1.485	1.439	0.761	0.750	0.697	0.754	0.570	0.564	0.525	0.548
A19	1.606	1.636	1.449	1.519	0.728	0.727	0.664	0.685	0.573	0.578	0.513	0.531
A20	1.842	1.849	1.802	1.999	0.546	0.554	0.484	0.480	0.461	0.467	0.421	0.418
A21	1.517	1.541	1.454	1.477	0.735	0.721	0.675	0.694	0.556	0.550	0.510	0.520
A22	1.620	1.612	1.513	1.726	0.548	0.557	0.500	0.485	0.447	0.453	0.412	0.408
A23	1.858	1.784	1.552	1.468	0.563	0.565	0.570	0.612	0.513	0.507	0.485	0.503
A24	1.758	1.658	1.561	1.482	0.565	0.581	0.570	0.609	0.506	0.510	0.491	0.510

Complex	μ				ν_{O-H}				ν_{N-H}			
	M062X		X3LYP		M062X		X3LYP		M062X		X3LYP	
	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2
A1	5.93	5.63	6.08	6.46	3470	3480	3353	3371	3613	3597	3567	3565
A2	5.80	5.46	5.77	5.85	3474	3509	3358	3383	3608	3601	3566	3562
A3	2.38	2.14	2.71	2.90	3805	3822	3747	3760	3576	3568	3532	3519
A4	5.47	5.18	5.67	5.53	3528	3557 3567	3392	3409	3570	3557 3567	3555	3554
A5	5.77	5.43	5.77	5.87	3498	3536	3394	3415	3575	3564	3560	3553
A6	2.69	2.50	2.66	2.79	3809	3820	3745	3759	3556	3568	3543	3535
A7	2.15	2.17	1.97	2.22	3811	3822	3747	3759	3573	3543	3527	3515
A8	6.22	6.82	6.80	7.02	3496	3553 3565	3388	3412	3580	3553 3565	3560	3556
A9	1.69	1.58	1.89	1.60	3815	3821	3748	3757	3580	3550	3528	3514
A10	2.09	1.95	1.88	1.99	3815	3827	3747	3758	3579	3566	3555	3547
A11	3.00	2.92	2.77	2.99	3799	3810	3744	3756	3616	3618	3571	3563
A12	2.51	2.49	2.16	2.37	3813	3823	3746	3759	3611	3603	3588	3582
A13	2.11	2.20	2.06	2.39	3803	3813	3745	3756	3541	3534	3545	3525
A14	1.39	1.36	1.63	1.54	3773	3771	3654	3682	3560	3558	3549	3546
A15	3.40	3.31	3.00	3.49	3815	3821	3746	3760	3575	3570	3556	3548
A16	1.31	1.29	1.29	1.18	3814	3820	3746	3756	3580	3576	3561	3555
A17	2.98	2.91	2.67	2.89	3802	3818	3746	3755	3608	3604	3576	3569
A18	3.99	3.96	3.64	4.09	3808	3821	3747	3760	3617	3611	3592	3568
A19	3.08	3.03	2.99	3.21	3792	3805	3740	3750	3571	3572	3565	3556
A20	2.01	2.02	1.76	2.28	3816	3819	3744	3755	3589	3583	3565	3559
A21	3.53	3.46	3.16	3.38	3805	3816	3748	3758	3580	3578	3561	3556
A22	2.88	2.84	2.67	2.96	3806	3815	3749	3758	3537	3533	3522	3525
A23	2.94	2.91	3.65	3.70	3854	3861	3784	3799	3565	3563	3524	3511
A24	3.64	3.59	3.81	3.79	3851	3868	3785	3799	3549	3561	3538	3529

Note: the results optimized at M062X/TZVP(BS1), M062X/6-311++G(*2d*, *p*)+(LANL2DZ)(BS2), X3LYP/TZVP(BS1), X3LYP/6-311++G(*2d*, *p*)+(LANL2DZ)(BS2) levels, respectively.

表 S7　19 种 Pro-Zn^{2+}结构的原子自然电荷数(q, e)

Table S7　Natural atom charge (q, e) of Pro-Zn^{2+} complexes

Complex	q_N				$q_{O(-H)}$				$q_{O(=C)}$			
	M062X		X3LYP		M062X		X3LYP		M062X		X3LYP	
	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2
CII1	-0.507	-0.577	-0.495	-0.562					-0.708 -0.758	-0.764 -0.811	-0.662 -0.709	-0.728 -0.775
CII2	-0.786	-0.858	-0.751	-0.824	-0.546	-0.590	-0.527	-0.571	-0.732	-0.785	-0.696	-0.759
CII3	-0.507	-0.578	-0.494	-0.561					-0.710 -0.763	-0.767 -0.814	-0.664 -0.713	-0.731 -0.777
CII4	-0.781	-0.852	-0.745	-0.818	-0.549	-0.592	-0.529	-0.573	-0.730	-0.784	-0.695	-0.758
CII5	-0.781	-0.854	-0.748	-0.822	-0.530	-0.575	-0.512	-0.557	-0.706	-0.763	-0.670	-0.736
CII6	-0.775	-0.847	-0.740	-0.814	-0.531	-0.577	-0.513	-0.559	-0.704	-0.762	-0.669	-0.735
CII7	-0.777	-0.847	-0.742	-0.814	-0.535	-0.577	-0.516	-0.559	-0.733	-0.787	-0.698	-0.760
CII8	-0.772	-0.843	-0.739	-0.812	-0.519	-0.564	-0.502	-0.547	-0.708	-0.766	-0.673	-0.740
CII9	-0.799	-0.868	-0.768	-0.839	-0.893	-0.923	-0.874	-0.907	-0.361	-0.412	-0.341	-0.395
CII10	-0.806	-0.878	-0.773	-0.844	-0.892	-0.923	-0.874	-0.907	-0.363	-0.414	-0.344	-0.398
CII11	-0.770	-0.848	-0.750	-0.821	-0.895	-0.926	-0.874	-0.909	-0.351	-0.402	-0.338	-0.390
CII12	-0.786	-0.857	-0.748	-0.820	-0.902	-0.930	-0.882	-0.914	-0.337	-0.389	-0.318	-0.372
CII13	-0.623	-0.709	-0.603	-0.686	-0.502	-0.553	-0.481	-0.534	-0.743	-0.808	-0.700	-0.772
CII14	-0.736	-0.803	-0.685	-0.748	-0.691	-0.725	-0.662	-0.699	-0.450	-0.496	-0.361	-0.421
CII15	-0.433	-0.543	-0.358	-0.452	-0.613	-0.676	-0.577	-0.621	-0.713	-0.752	-0.671	-0.736
CII16	-0.578	-0.665	-0.533	-0.640	-0.509	-0.556	-0.496	-0.540	-0.729	-0.793	-0.694	-0.767
CII17	-0.374	-0.462	-0.306	-0.395	-0.566	-0.601	-0.558	-0.592	-0.778	-0.824	-0.700	-0.772
CII18	-0.369	-0.458	-0.307	-0.396	-0.565	-0.600	-0.562	-0.597	-0.779	-0.829	-0.704	-0.778
CII19	-0.389	-0.487	-0.319	-0.414	-0.558	-0.595	-0.547	-0.585	-0.796	-0.842	-0.714	-0.784

Complex	q_{Zn}				$q_{H(-O)}$				$q_{H(-N)}$			
	M062X		X3LYP		M062X		X3LYP		M062X		X3LYP	
	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2
CII1	1.664	1.714	1.581	1.658					0.453 0.462	0.452 0.462	0.448 0.455	0.446 0.455
CII2	1.656	1.713	1.583	1.664	0.553	0.550	0.547	0.544	0.445	0.442	0.441	0.436
CII3	1.665	1.716	1.582	1.660					0.458 0.459	0.457 0.459	0.452 0.451	0.450 0.452
CII4	1.647	1.704	1.573	1.654	0.553	0.550	0.547	0.545	0.450	0.446	0.445	0.440
CII5	1.662	1.719	1.591	1.671	0.538	0.539	0.534	0.535	0.445	0.441	0.441	0.436
CII6	1.651	1.708	1.578	1.660	0.538	0.539	0.533	0.535	0.450	0.446	0.445	0.439
CII7	1.668	1.722	1.595	1.672	0.554	0.551	0.548	0.546	0.424	0.419	0.422	0.415
CII8	1.674	1.729	1.604	1.682	0.540	0.542	0.536	0.538	0.423	0.418	0.421	0.415
CII9	1.682	1.733	1.612	1.683	0.583	0.578	0.576	0.571	0.445	0.440	0.441	0.435
CII10	1.683	1.734	1.614	1.685	0.583	0.578	0.576	0.571	0.449	0.445	0.445	0.439
CII11	1.653	1.710	1.593	1.666	0.583	0.578	0.577	0.571	0.454	0.450	0.448	0.442
CII12	1.681	1.729	1.605	1.673	0.580	0.576	0.573	0.568	0.430	0.426	0.427	0.422
CII13	1.691	1.762	1.596	1.693	0.557	0.560	0.543	0.548	0.419	0.417	0.419	0.417
CII14	1.573	1.631	1.356	1.446	0.546	0.544	0.548	0.546	0.485	0.478	0.473	0.463
CII15	1.329	1.425	1.188	1.279	0.555	0.561	0.544	0.547	0.436	0.430	0.432	0.426
CII16	1.688	1.765	1.578	1.705	0.555	0.556	0.547	0.549	0.382	0.380	0.387	0.379
CII17	1.256	1.308	1.103	1.193	0.532	0.526	0.528	0.524	0.441	0.436	0.439	0.434
CII18	1.257	1.311	1.113	1.203	0.534	0.530	0.530	0.527	0.441	0.437	0.439	0.434
CII19	1.287	1.352	1.121	1.220	0.533	0.527	0.527	0.522	0.435	0.430	0.434	0.427

Note: the results optimized at M062X/TZVP(BS1), M062X/6-311++G(*2d*, *p*)+(LANL2DZ)(BS2), X3LYP/TZVP(BS1), X3LYP/6-311++G(*2d*, *p*)+(LANL2DZ)(BS2) levels, respectively.

表 S8　21 种 Pro-Zn^+结构的原子自然电荷数(*q*, *e*)

Table S8　Natural atom charge (*q*, *e*) of Pro-Zn^+ complexes

Complex	q_N				$q_{O(-H)}$				$q_{O(=C)}$			
	M062X		X3LYP		M062X		X3LYP		M062X		X3LYP	
	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2
CI1	-0.716	-0.785	-0.689	-0.763	-0.609	-0.649	-0.593	-0.634	-0.679	-0.722	-0.655	-0.679
CI2	-0.716	-0.784	-0.691	-0.764	-0.609	-0.649	-0.593	-0.633	-0.676	-0.718	-0.651	-0.676
CI3	-0.518	-0.589	-0.509	-0.575					-0.727 -0.760	-0.755 -0.806	-0.774 -0.655	-0.727 -0.760
CI4	-0.513	-0.583	-0.504	-0.572					-0.727 -0.758	-0.754 -0.805	-0.719 -0.704	-0.727 -0.758
CI5	-0.710	-0.780	-0.683	-0.758	-0.590	-0.632	-0.575	-0.618	-0.649	-0.697	-0.626	-0.649
CI6	-0.708	-0.777	-0.684	-0.758	-0.590	-0.631	-0.575	-0.617	-0.647	-0.692	-0.623	-0.647
CI7	-0.705	-0.772	-0.681	-0.754	-0.601	-0.640	-0.587	-0.626	-0.664	-0.705	-0.639	-0.664
CI8	-0.725	-0.791	-0.704	-0.774	-0.786	-0.814	-0.762	-0.796	-0.475	-0.518	-0.471	-0.475
CI9	-0.734	-0.799	-0.709	-0.781	-0.786	-0.811	-0.761	-0.795	-0.475	-0.518	-0.471	-0.475
CI10	-0.723	-0.792	-0.697	-0.769	-0.792	-0.822	-0.766	-0.802	-0.468	-0.511	-0.465	-0.468
CI11	-0.641	-0.733	-0.629	-0.718	-0.628	-0.682	-0.599	-0.653	-0.754	-0.778	-0.727	-0.754
CI12	-0.696	-0.765	-0.674	-0.748	-0.582	-0.623	-0.569	-0.610	-0.638	-0.682	-0.614	-0.638
CI13	-0.723	-0.786	-0.696	-0.765	-0.776	-0.804	-0.748	-0.783	-0.463	-0.506	-0.461	-0.463
CI14	-0.735	-0.781	-0.702	-0.761	-0.699	-0.731	-0.685	-0.719	-0.511	-0.552	-0.499	-0.511
CI15	-0.621	-0.706	-0.613	-0.696	-0.632	-0.678	-0.603	-0.652	-0.727	-0.752	-0.707	-0.727
CI16	-0.611	-0.696	-0.596	-0.682	-0.639	-0.682	-0.614	-0.656	-0.724	-0.749	-0.700	-0.724
CI17	-0.599	-0.680	-0.545	-0.648	-0.592	-0.632	-0.582	-0.622	-0.780	-0.809	-0.704	-0.780
CI18	-0.597	-0.680	-0.585	-0.667	-0.641	-0.685	-0.616	-0.659	-0.737	-0.760	-0.709	-0.737
CI19	-0.593	-0.677	-0.553	-0.647	-0.560	-0.602	-0.564	-0.602	-0.799	-0.827	-0.722	-0.799
CI20	-0.602	-0.683	-0.587	-0.668	-0.641	-0.684	-0.617	-0.659	-0.733	-0.757	-0.702	-0.733
CI21	-0.581	-0.663	-0.576	-0.665	-0.877	-0.896	-0.863	-0.895	-0.430	-0.478	-0.417	-0.430

Complex	q_{Zn}				$q_{H(-O)}$				$q_{H(-N)}$			
	M062X		X3LYP		M062X		X3LYP		M062X		X3LYP	
	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2
CI1	0.828	0.846	0.796	0.833	0.523	0.521	0.517	0.516	0.416	0.412	0.410	0.405
CI2	0.832	0.849	0.802	0.837	0.523	0.521	0.517	0.516	0.411	0.407	0.406	0.401
CI3	0.837	0.844	0.818	0.833					0.439 0.474	0.437 0.474	0.432 0.462	0.431 0.465
CI4	0.836	0.843	0.806	0.832					0.434 0.476	0.433 0.476	0.430 0.466	0.428 0.467
CI5	0.831	0.848	0.800	0.836	0.505	0.507	0.500	0.503	0.416	0.412	0.410	0.404
CI6	0.836	0.852	0.805	0.841	0.505	0.507	0.500	0.503	0.410	0.406	0.405	0.400
CI7	0.842	0.857	0.814	0.847	0.524	0.522	0.517	0.517	0.391	0.386	0.389	0.382
CI8	0.848	0.861	0.819	0.849	0.544	0.538	0.536	0.532	0.409	0.403	0.405	0.398
CI9	0.848	0.861	0.819	0.848	0.544	0.538	0.536	0.532	0.414	0.408	0.409	0.403
CI10	0.837	0.852	0.808	0.840	0.545	0.539	0.536	0.532	0.418	0.413	0.412	0.406
CI11	0.879	0.883	0.855	0.881	0.525	0.540	0.509	0.526	0.404	0.402	0.399	0.396
CI12	0.843	0.860	0.817	0.850	0.508	0.511	0.503	0.506	0.391	0.386	0.388	0.381
CI13	0.854	0.862	0.824	0.850	0.540	0.535	0.530	0.528	0.399	0.394	0.395	0.389
CI14	0.833	0.832	0.787	0.814	0.522	0.521	0.518	0.518	0.441	0.432	0.437	0.426
CI15	0.888	0.890	0.865	0.887	0.546	0.548	0.533	0.536	0.357	0.356	0.355	0.355
CI16	0.887	0.890	0.860	0.887	0.518	0.520	0.511	0.513	0.389	0.387	0.384	0.382
CI17	0.896	0.907	0.764	0.851	0.523	0.522	0.516	0.515	0.392	0.389	0.400	0.387
CI18	0.887	0.890	0.852	0.882	0.522	0.525	0.515	0.517	0.387	0.382	0.385	0.379
CI19	0.900	0.913	0.783	0.841	0.518	0.517	0.514	0.513	0.383	0.382	0.393	0.387
CII20	0.884	0.887	0.840	0.874	0.522	0.524	0.514	0.517	0.388	0.383	0.388	0.381
CII21	0.909	0.922	0.858	0.906	0.546	0.542	0.533	0.532	0.384	0.381	0.389	0.384

Note: the results optimized at M062X/TZVP(BS1), M062X/6-311++G(2*d*, *p*)+(LANL2DZ)(BS2), X3LYP/TZVP(BS1), X3LYP/6-311++G(2*d*, *p*)+(LANL2DZ)(BS2) levels, respectively.

表 S9 24 种 Pro-Zn 结构的原子自然电荷数(q, e)

Table S9 Natural atom charge (q, e) of Pro-Zn complexes

Complex	q_N				$q_{O(-H)}$				$q_{O(=C)}$			
	M062X		X3LYP		M062X		X3LYP		M062X		X3LYP	
	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2
A1	-0.661	-0.744	-0.646	-0.730	-0.669	-0.712	-0.648	-0.689	-0.591	-0.623	-0.582	-0.636
A2	-0.661	-0.744	-0.647	-0.729	-0.665	-0.707	-0.648	-0.690	-0.595	-0.633	-0.580	-0.635
A3	-0.649	-0.723	-0.632	-0.713	-0.675	-0.712	-0.657	-0.694	-0.590	-0.627	-0.581	-0.621
A4	-0.646	-0.726	-0.641	-0.723	-0.670	-0.710	-0.654	-0.703	-0.577	-0.615	-0.563	-0.602
A5	-0.648	-0.728	-0.643	-0.722	-0.664	-0.705	-0.647	-0.689	-0.593	-0.630	-0.578	-0.633
A6	-0.653	-0.731	-0.636	-0.719	-0.673	-0.710	-0.657	-0.695	-0.589	-0.626	-0.580	-0.621
A7	-0.617	-0.703	-0.603	-0.687	-0.673	-0.710	-0.657	-0.694	-0.609	-0.644	-0.589	-0.638
A8	-0.647	-0.728	-0.642	-0.723	-0.671	-0.712	-0.647	-0.688	-0.583	-0.623	-0.580	-0.634
A9	-0.612	-0.697	-0.600	-0.681	-0.677	-0.711	-0.658	-0.691	-0.597	-0.633	-0.584	-0.638
A10	-0.636	-0.714	-0.623	-0.705	-0.690	-0.726	-0.674	-0.712	-0.577	-0.617	-0.570	-0.611
A11	-0.635	-0.717	-0.618	-0.705	-0.677	-0.712	-0.664	-0.703	-0.588	-0.625	-0.571	-0.609
A12	-0.651	-0.727	-0.637	-0.719	-0.688	-0.723	-0.673	-0.711	-0.581	-0.621	-0.571	-0.612
A13	-0.610	-0.696	-0.606	-0.691	-0.676	-0.712	-0.660	-0.697	-0.607	-0.645	-0.590	-0.641
A14	-0.609	-0.695	-0.606	-0.693	-0.678	-0.715	-0.664	-0.699	-0.604	-0.642	-0.585	-0.636
A15	-0.630	-0.709	-0.611	-0.697	-0.678	-0.715	-0.662	-0.701	-0.572	-0.610	-0.564	-0.606
A16	-0.605	-0.690	-0.598	-0.681	-0.688	-0.722	-0.673	-0.708	-0.592	-0.628	-0.578	-0.621
A17	-0.637	-0.719	-0.617	-0.703	-0.694	-0.727	-0.669	-0.709	-0.576	-0.612	-0.570	-0.608
A18	-0.630	-0.710	-0.613	-0.695	-0.682	-0.718	-0.669	-0.705	-0.591	-0.627	-0.572	-0.618
A19	-0.614	-0.694	-0.604	-0.696	-0.673	-0.708	-0.659	-0.697	-0.591	-0.626	-0.576	-0.613
A20	-0.606	-0.691	-0.600	-0.683	-0.686	-0.720	-0.671	-0.705	-0.599	-0.635	-0.585	-0.637
A21	-0.624	-0.702	-0.608	-0.693	-0.696	-0.730	-0.669	-0.707	-0.571	-0.607	-0.568	-0.608
A22	-0.594	-0.680	-0.585	-0.672	-0.690	-0.724	-0.674	-0.709	-0.587	-0.625	-0.571	-0.623
A23	-0.645	-0.721	-0.628	-0.711	-0.659	-0.696	-0.643	-0.681	-0.556	-0.595	-0.547	-0.588
A24	-0.649	-0.729	-0.632	-0.717	-0.658	-0.695	-0.644	-0.682	-0.554	-0.594	-0.546	-0.588

Complex	q_{Zn}				$q_{H(-O)}$				$q_{H(-N)}$			
	M062X		X3LYP		M062X		X3LYP		M062X		X3LYP	
	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2	BS1	BS2
A1	0.004	0.003	0.004	0.004	0.509	0.515	0.494	0.503	0.381	0.380	0.376	0.376
A2	0.005	0.006	0.004	0.006	0.508	0.514	0.494	0.503	0.381	0.380	0.376	0.376
A3	0.005	0.005	0.001	0.001	0.493	0.494	0.487	0.490	0.391	0.388	0.385	0.386
A4	0.007	0.006	0.003	0.002	0.511	0.515	0.497	0.505	0.371	0.371	0.370	0.371
A5	0.007	0.009	0.004	0.006	0.510	0.515	0.497	0.505	0.372	0.371	0.372	0.371
A6	0.003	0.004	-0.001	-0.001	0.493	0.493	0.487	0.490	0.394	0.393	0.387	0.388
A7	0.008	0.009	0.004	0.006	0.493	0.493	0.486	0.489	0.379	0.378	0.374	0.371
A8	-0.001	-0.004	0.001	0.002	0.512	0.517	0.497	0.505	0.372	0.372	0.372	0.372
A9	0.003	0.004	0.003	0.004	0.493	0.493	0.486	0.489	0.379	0.380	0.374	0.374
A10	0.003	0.002	-0.001	-0.003	0.495	0.495	0.489	0.492	0.384	0.379	0.380	0.378
A11	0.001	-0.003	0.000	-0.005	0.491	0.492	0.485	0.489	0.378	0.375	0.372	0.371
A12	0.004	0.005	0.001	0.002	0.495	0.496	0.489	0.493	0.387	0.384	0.384	0.383
A13	0.005	0.006	0.002	0.006	0.492	0.493	0.485	0.489	0.376	0.372	0.376	0.371
A14	0.003	0.009	0.010	0.012	0.491	0.487	0.481	0.481	0.378	0.378	0.377	0.379
A15	0.002	-0.002	-0.002	-0.001	0.493	0.493	0.486	0.489	0.381	0.374	0.376	0.370
A16	0.004	0.003	0.003	0.001	0.495	0.496	0.487	0.491	0.375	0.373	0.372	0.370
A17	0.002	-0.001	0.000	-0.004	0.496	0.495	0.486	0.490	0.378	0.376	0.371	0.370
A18	0.005	0.002	0.002	-0.002	0.491	0.492	0.484	0.489	0.376	0.373	0.369	0.368
A19	0.000	-0.004	0.000	-0.002	0.491	0.492	0.484	0.488	0.364	0.363	0.362	0.363
A20	0.005	0.005	0.004	0.005	0.495	0.496	0.488	0.492	0.375	0.373	0.373	0.371
A21	0.001	-0.003	0.000	-0.004	0.496	0.495	0.487	0.490	0.367	0.365	0.362	0.363
A22	0.004	0.005	0.003	0.002	0.497	0.497	0.490	0.494	0.364	0.364	0.361	0.363
A23	0.005	0.006	0.002	0.003	0.477	0.480	0.473	0.478	0.393	0.392	0.388	0.389
A24	0.003	0.005	0.001	0.001	0.477	0.481	0.473	0.478	0.398	0.397	0.391	0.392

Note: the results optimized at M062X/TZVP(BS1), M062X/6-311++G(*2d*, *p*)+(LANL2DZ)(BS2), X3LYP/TZVP(BS1), X3LYP/6-311++G(*2d*, *p*)+(LANL2DZ)(BS2) levels, respectively.