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10 Anexos

10.1 Artigos publicados

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 105 (2013) 88–101

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Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy

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Molecular structure of tetraaqua adenosine 5′-triphosphate aluminium(III) complex: A study involving Raman spectroscopy, theoretical DFT and potentiometry

Thaís Tenório [a,*], Andréa M. Silva [a,b], Joanna Maria Ramos [c], Camilla D. Buarque [a], Judith Felcman [a,1]

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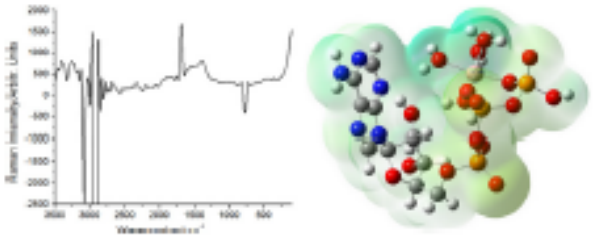
HIGHLIGHTS

- AlATP complex participates in the pathogenic process of Alzheimer's disease.
- Raman and potentiometry show that ATP acts as a bidentate ligand in $[Al(ATP)(H_2O)_4]$.
- The ATP's donor atoms are one oxygen of the phosphate β and one of the phosphate γ.
- Molecular modeling of the complex suggested a distorted octahedral structure.
- Complete analysis of vibrational spectra and DFT investigations confirm the result.

GRAPHICAL ABSTRACT



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ABSTRACT

The Alzheimer's disease is one of the most common neurodegenerative diseases that affect elderly population, due to the formation of β-amyloid protein aggregate and several symptoms, especially progressive cognitive decline. The result is a decrease in capture of glucose by cells leading to obliteration, meddling in the Krebs cycle, the principal biochemical route to the energy production leading to a decline in the levels of adenosine 5′-triphosphate.

Aluminium(III) is connected to Alzheimer's and its ion provides raise fluidity of the plasma membrane, decrease cell viability and aggregation of amyloid plaques. Studies reveal that AlATP complex promotes the formation of reactive fibrils of β-amyloid protein and independent amyloidogenic peptides, suggesting the action of the complex as a chaperone in the role pathogenic process. In this research, one of complexes formed by Al(III) and adenosine 5′-triphosphate in aqueous solution is analyzed by potentiometry, Raman spectroscopy and *ab initio* calculations. The value of the log K_{AlATP} found was 9.2 1 ± 0.0 1 and adenosine 5′-triphosphate should act as a bidentate ligand in the complex. Raman spectroscopy and potentiometry indicate that donor atoms are the oxygen of the phosphate β and the oxygen of the phosphate γ, the terminal phosphates. Computational calculations using Density Functional Theory, with hybrid functions B3LYP and 6-311++G(d,p) basis set regarding water solvent effects, have confirmed the results. Frontier molecular orbitals, electrostatic potential contour surface, electrostatic potential mapped and Mulliken charges of the title molecule were also investigated.

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Experimental and theoretical investigation of $[Al(PCr)(H_2O)]$ complex in aqueous solution

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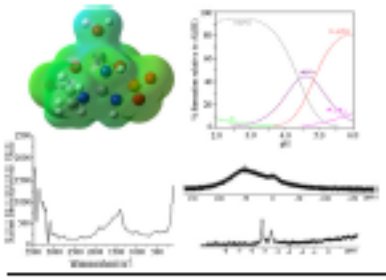
HIGHLIGHTS

- The AlPCr species formed in aqueous solution in an Al:PCr system ratio of 1:1.
- Potentiometry, ^{31}P and ^{27}Al NMR, Raman spectroscopy and DFT calculations were used.
- ^{27}Al NMR and molecular modeling of the complex suggested a tetrahedral structure.
- PCr behaves as a tridentate ligand in $[Al(PCr)(H_2O)]$.
- The phosphate oxygen, carboxylate oxygen and guanidine nitrogen are the donor atoms.

GRAPHICAL ABSTRACT



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ABSTRACT

Phosphocreatine is a phosphorylated creatine molecule synthesized in the liver and transported to muscle cells where it is used for the temporary storage of energy. In Alzheimer's disease, the capture of glucose by cells is impaired, which negatively affects the Krebs cycle, leading to problems with the generation of phosphocreatine. Furthermore, the creatine–phosphocreatine system, regulated by creatine kinase, is affected in the brains of Alzheimer's disease patients. Aluminum ions are associated with Alzheimer's disease. Al(III) decreases cell viability and increases the fluidity of the plasma membrane, profoundly altering cell morphology. In this study, one of the complexes formed by Al(III) and phosphocreatine in aqueous solution was investigated by potentiometry, ^{31}P and ^{27}Al NMR, Raman spectroscopy and density functional theory (DFT) calculations. The $\log K_{AlPCr}$ value was 11.37 ± 0.03. Phosphocreatine should act as a tridentate ligand in this complex. The ^{27}Al NMR peak at 48.92 ppm indicated a tetrahedral molecule. The fourth position in the arrangement was occupied by a coordinated water molecule. Raman spectroscopy, ^{31}P NMR and DFT calculations (DFT:B3LYP/6-311++G**) indicated that the donor atoms are oxygen in the phosphate group, the nitrogen of the guanidine group and the oxygen of the carboxylate group. Mulliken charges, NBO charges, frontier molecular orbitals, electrostatic potential contour surfaces and mapped electrostatic potential were also examined.

Introduction

Alzheimer's disease is a neurodegenerative disease with a high incidence in the older population [1]. It is characterized by progressive cognitive decline driven by the proliferation of neurofibrillary

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- Figura 2.8

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- Figura 2.9

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- Figura 2.10

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- Tabela 2.1

A tabela foi adaptada do artigo de Machado, Vanderlei Gageiro; Nome, Faruk. Química Nova - Compostos fosfatados ricos em energia 1999, vol. 22, Iss. 3, p. 351-357, que está sob a licença da http://creativecommons.org/licenses/by-nc/3.0/deed.pt_BR. É permitido remixar a figura, sem fins lucrativos, portanto que haja a citação adequada.

10.3 Tabelas

Tabela A.1 - Valores das constantes de formação empregados nos cálculos das espécies ternárias e dos adutos moleculares.

Espécies	**log β**
Espécies hidrolisadas do metal	
AlOH	-5,33
$Al(OH)_2$	-10,91
$Al(OH)_3$	-17,3
$Al_3(OH)_4$	-13,13
$Al_{13}(OH)_{32}$	-107,47
Espécies protonadas dos aminoácidos	
MetH	9,12
$MetH_2$	11,25
CisH	10,78
$CisH_2$	19,17
$CisH_3$	20,69
HcisH	10,49
$HcisH_2$	19,37
$HcisH_3$	21,94
PenH	10,85
$PenH_2$	18,70
$PenH_3$	20,17
Espécies protonadas dos ligantes fosfatados	
PCrH	11,04
$PCrH_2$	15,29
$PCrH_3$	17,99
ATPH	6,81
$ATPH_2$	11,05
Espécies formadas nos sistemas binários Al^{3+}:aminoácidos 1:1	
AlMet	6,65
AlMetOH	1,86
$AlMet(OH)_2$	-3,12
$AlMet(OH)_3$	-7,42
AlCisH	13,50
AlCis	7,06
AlCisOH	4,48
$AlCis(OH)_2$	-0,74
AlHcisH	12,81

Espécies	**log β**
AlHcis	6,90
AlHcisOH	4,92
$AlHcis(OH)_2$	-2,30
$AlHcis(OH)_3$	-4,66
AlPen	11,46
AlPenOH	8,06
$AlPen(OH)_2$	1,77
$AlPen(OH)_3$	-0,94
Espécies formadas nos sistemas binários Al^{3+}:ligantes fosfatados 1:1	
AlPCrH	15,77
AlPCr	11,37
AlPCrOH	6,53
$AlPCrOH_2$	-1,62
$AlPCrOH_3$	-11,15
$AlATPH_2$	15,68
AlATPH	13,04
AlATP	9,21
AlATPOH	2,80
Al_2ATP_2OH	16,16

Tabela A.2 - Espectro Raman experimental e calculado para o complexo [Al(ATP)(H_2O)$_4$].

Nos. modos	Números de onda observados (cm^{-1})	Deconvolução (cm^{-1})	Ajuste não linear (cm^{-1})	2nd derivada (cm^{-1})	Números de onda B3LYP escalonados (cm^{-1})	S_{Ra} [a]	Atribuições aproximadas
1					3686	41,98	ν_{as}(OH)(H_2O)
2					3663	114,31	ν(OH)(H_2O)
3					3661	87,27	ν_{as}(OH)(H_2O)
4					3641	139,97	ν_{as}(NH)
5				3468	3624	146,52	ν_s(OH)(H_2O)
6				3429	3613	152,86	ν(OH)(P_γ)
7		3495		3397	3564	93,72	ν(OH)(ribose)
8	3458	3417		3280	3548	460,77	ν_s(NH)
9	3260	3315		3217	3443	432,14	ν_s(OH)(H_2O)
10	3174	3289		3186	3338	198,85	ν(OH)(H_2O)
11	3122	3242		3125	3249	504,75	ν(CH)(adenina)
12		3205		3057	3136	160,13	ν(OH)(ribose)
13	3019	3157		2993	3121	150,74	ν(CH)(adenina)
14		3118		2942	3039	239,94	ν(OH)(H_2O)
15		3080		2885	2976	176,12	ν_{as}(CH)(CH_2)
16	2960	3007		2850	2965	175,64	ν(CH)(ribose)
17	2880	2970		2793	2954	218,64	ν(CH)(ribose)
18	2831	2941		2740	2948	411,31	ν(CH)(ribose)
19	2790			2691	2924	209,36	ν(CH)(ribose)
20	2670			2625	2907	304,74	ν_s(CH)(CH_2)
21	2335			2546	2430	159,41	ν(OH)(H_2O)
22	1754	1765		1750	1631	0,85	δ(HOH)sciss
23	1682	1733			1590	7,82	δ(HOH)sciss
24	1610	1700			1585	5,95	δ(HOH)sciss
25		1671		1671	1574	24,91	δ(HNH)sciss + ν(C-NH_2)
26	1566	1556		1585	1566	1,92	δ(HOH)sciss
27					1542	18,44	δ(HNH) + ν(CC)(adenina) + ν(CN)(adenina)
28	1510	1512	1510	1524	1527	140,79	ν(CC)(adenina) + ν(CN)(adenina)
29		1480		1490	1457	149,60	ν(CN) + ν(CC)(adenina) + ν(CN)(adenina)
30				1440	1436	85,20	δ(HCH)sciss
31					1432	16,70	δ(CH)(adenina)
32					1406	10,64	δ(OH)(ribose)
33	1386	1379	1399		1383	49,54	δ(CH)(ribose)
34					1380	13,31	δ(CH)(ribose)
35					1368	2,64	δ(CH)(ribose) +

				δ(CH)(adenina)
36	1354	1345	38,78	ω(HCH)
37		1342	2,10	δ(adenina) + δ(CH)(adenina)
38		1334	34,40	δ(CH)(ribose)
39	1310	1317	138,24	ν(CN)(adenina) + δ(CH)(ribose)
40		1300	9,49	δ(CH)(ribose)
41		1296	19,85	δ(OH)(ribose) + δ(CH)(ribose)
42	1286	1289	45,53	δ(OH)(ribose) + δ(CH)(ribose)
43		1278	33,21	δ(HCH)twist+ δ(OH)(ribose)+ δ(CH)(ribose)
44		1262	46,35	δ(CH)(ribose) + ν(CN)(adenina)
45		1257	89,77	δ(CH)(ribose)
46	1235 1243	1239	16,10	δ(adenina) + ρ(NH_2)
47		1222	17,34	δ(HCH)twist + δ(CH)(ribose)
48		1209	67,33	δ(adenina)
49	1191 1187 1202	1204	42,69	δ(OH)(ribose) + δ(CH)(ribose)
50		1181	9,66	δ(adenina) + ρ(NH_2)
51		1171	29,63	ν(CO)(ribose) + δ(adenina)
52		1171	6,38	ρ(OH)(H_2O)
53	1147	1144	31,14	δ(ribose) + ρ(OH)(H_2O)
54	1112 1116	1128	12,09	δ(ribose) + ω(HOH)
55		1083	3,88	δ(adenina) + δ(ribose)
56		1080	7,98	ρ(CH_2) + δ(OH)(P_γ)
57		1072	11,26	δ(OH)(P_γ)
58	1054 1068	1052	3,58	ν(CC)(ribose) + ν(OP_β)
59		1042	6,26	δ(ribose)
60		1038	18,90	ρ(OH)(H_2O) + ν(OP_α)+ δ(ribose)
61	1028	1030	14,16	ρ(OH)(H_2O) + ν(CC)(ribose)
62		1023	10,43	ν(OP_α) + ω(HOH)
63		1006	18,14	ρ(CH_2) + ν(CO)(ribose) +

					ω(HOH)
64				998	7,58	$\rho(NH_2)$ + δ(adenina)
65		978		983	4,75	$\nu(OP_\gamma)$ + $\rho(OH)(H_2O)$
66				970	12,29	ν(CC)(ribose) + ν(P-O-C) + $\rho(CH_2)$
67				957	5,73	δ(CH)(adenina)
68				947	10,58	$\nu(P_\alpha OP_\beta)$ + $\delta(OH)(P_\gamma)$ + $\rho(OH)(H_2O)$
69				947	2,46	$\nu(OP_\alpha)$ + $\rho(OH)(H_2O)$
70				925	2,09	$\nu(P_\beta O)$ + $\nu(P_\gamma O)$ + $\rho(OH)(H_2O)$
71		917	927	924	3,29	δ(ribose)
72				892	9,45	δ(adenina)
73				887	14,12	$\nu(P_\alpha OP_\beta)$ + $\nu(P_\beta OP_\gamma)$ + $\rho(OH)(H_2O)$
74				881	11,88	$\nu(P\alpha{=}O)$ + $\nu(P_\beta{=}O)$ + $\nu(P_\gamma{=}O)$
75	859	859	873	873	3,52	δ(CH)(adenina)
76				846	14,30	ν(fosfatos) + $\delta(OH)(P_\gamma)$ + $\rho(OH)(H_2O)$
77				839	11,97	$\rho(OH)(H_2O)$+ δ(CH)(adenina)+ δ(OH)(ribose)
78				833	4,87	ν(fosfatos)+ δ(CH)(adenina) +$\rho(OH)(H_2O)$
79				819	4,75	δ(HCH)twist + ν(CO)(ribose)
80	815	815	820	815	5,55	δ(adenina) + δ(HOH)twist
81				774	5,35	$\rho(OH)(H_2O)$ + δ(OH)(ribose)
82		768	783	766	4,32	δ(HOH)twist + $\rho(OH)(H_2O)$
83				746	23,01	ω(HOH)
84	721	721	740	710	42,06	δ(ribose) + ω(HOH)
85				703	14,58	$\nu(P_\gamma OH)$+ $\nu(P_\beta OP_\gamma)$+ $\rho(OH)(H_2O)$
86				687	10,09	$\nu(P_\beta OP_\gamma)$ +

					ρ(OH)(H_2O)
87				683	8,34	ν(adenina)
88				681	1,58	ω(HOH) + ρ(OH)(H_2O) + ν(P_γOH)
89	660		675	673	4,13	δ(adenina)
90				657	0,50	δ(adenina) + δ(ribose)
91				655	4,00	δ(adenina)
92				652	13,62	modos acoplados
93				648	8,24	ω(HOH)
94	631		628	628	1,17	δ(adenina) + δ(ribose) + δ(CHC)
95				607	7,79	modos acoplados
96				597	10,80	ν(H_2O-Al) + δ(Al-OH_2) + ω(HNH)
97	584		577	585	7,69	ν(Al-O)(P_γ) + δ(adenina) + ω(HNH)
98				559	0,38	ν(Al-O)(P_β) + ω(HNH) + ω(HOH)
99				555	0,50	δ(HNH)twist
100	552			552	2,16	δ(HNH)twist
101				543	9,69	ρ(NH_2)+ δ(Al-OH_2)
102				537	1,59	ω(HNH)
103				521	7,26	ν(H_2O-Al-O)(P_γ) + δ(H_2O-Al-OH_2) + ω(HOH)
104				516	1,11	ν(adenina)
105				514	4,60	δ(Al-OH_2) + ν(ribose)
106	505	505	515	503	2,31	δ(H_2O-Al-O)(P_γ)+ δ(H_2O-Al-O)(P_β) +δ(H_2O-Al-OH_2)
107				482	2,58	δ(Al-O)(P_γ) + δ(Al-O)(P_β) + δ($P_\beta OP_\gamma$)
108	472	473	461	465	2,90	δ(HOH)twist + ω(HOH)
109				454	3,70	δ(anel)
110	444	433	459	446	3,37	ν(H_2O-Al-O)(P_γ)+ ν(H_2O-Al-O)(P_β) +ν(H_2O-Al)+ ω(HOH)
111				432	5,22	δ(anel) +

				δ(fosfatos) + δ(ribose)
112	427	431	7,06	modos acoplados
113		415	2,69	ν(Al-OH_2)+ δ(Al-OH_2) + δ(HOH)twist
114	407 400	408	0,73	δ(HOH)twist
115		396	1,74	δ(Al-O)(P_γ)+ δ(OP_γ)+δ(OP_α)+ δ(O=P_α)
116		384	4,29	δ($P_\alpha OP_\beta$) + δ(OH)(ribose)
117	375 371	376	2,86	ν(Al-OH_2)+ δ(Al-O)(P_β) + δ(Al-O)(P_γ)
118		367	1,17	ν(Al-OH_2) + δ(anel)
119	360 360 350	357	2,88	δ(OP_α) + δ(OP_β) + δ(OP_γ) + δ($P_\beta OP_\gamma$)
120		346	2,98	δ(Al-OH_2) + δ(anel)+δ(H_2C-O)
121		341	4,76	δ(H_2C-O) + δ(HOH)twist
122		331	1,36	modos acoplados
123		320	1,10	δ(HOH)twist
124		314	1,22	ν(Al-O)(P_γ)+ δ(Al-O)(P_β) + δ(Al-OH_2)
125		310	2,34	δ(H_2O-Al-OH_2) + ρ(CH_2)
126		308	1,00	modos acoplados
127		301	3,37	δ(H_2O-Al) + δ(Al-O)(P_β)
128		290	4,38	δ(C-NH_2)
129		289	2,77	δ(adenina) + δ(H_2O-Al-OH_2) + δ(H_2O-Al-O)(P_β)+ δ(H_2O-Al-O)(Pγ)
130	282	284	2,05	δ(OH)(P_γ) + δ(H_2O-Al) + δ(anel)
131		271	0,98	δ(OH)(P_γ) + δ(H_2O-Al)
132		263	3,10	modos acoplados
133		251	1,29	modos acoplados
134		245	2,14	modos acoplados
135		244	2,36	modos acoplados
136		243	2,09	distorção angular

				(anel)
137		235	0,24	$\delta(OH)(P_\gamma)$ + $\delta(OH)$(ribose)
138		226	1,38	modos acoplados
139		224	0,82	$\delta(Al\text{-}OH_2)$ + $\delta(OH)$(ribose)
140		217	1,41	δ(adenina)
141		214	0,52	distorção angular (anel)
142		207	1,51	τ
143		198	3,00	$\delta(OH)(P_\gamma)$ + $\delta(OH)$(ribose)
144		191	0,38	$\delta(P_\gamma\text{-}OH)$ + $\delta(OH)(P_\gamma)$
145		186	5,01	modos acoplados
146		177	1,49	modos acoplados
147		173	1,56	distorção angular (anel)
148		162	0,23	distorção angular (anel)
149		148	0,21	modos acoplados
150		145	0,36	$\tau(H_2O)$
151		140	0,40	τ
152		133	0,16	$\tau(H_2O)$
153		124	0,59	τ
154		118	0,74	modos acoplados
155		116	0,59	modos acoplados
156		92	0,31	τ
157		80	0,13	τ
158		75	1,94	τ
159		65	1,09	τ
160		60	4,43	τ
161		58	5,28	δ(adenina)
162		45	5,04	δ(adenina)
163		36	5,75	τ
164		25	1,07	τ
165		15	3,71	τ

[a] Atividades Raman são calculadas em A^4 amu.

Tabela A.3 - Espectro Raman experimental e calculado para o complexo [Al(PCr)(H_2O)].

Nos. modos	**Números de onda observados (cm^{-1})**	**Deconvolução (cm^{-1})**	**Ajuste não linear (cm^{-1})**	**2nd derivada (cm^{-1})**	**Números de onda B3LYP escalonados (cm^{-1})**	**S_{Ra} [a]**	**Atribuições aproximadas**
1					3641	49,19	$\nu_{as}(OH)(H_2O)$
2				3370	3580	152,90	$\nu_{s}(OH)(H_2O)$
3	3430	3450		3315	3422	184,11	ν(NH)
4	3320	3360		3204	3296	179,44	ν(NH)
5	3150	3165		3098	3034	112,22	$\nu(CH)(CH_3)$
6	3103	3099		3030	3015	124,76	$\nu_{as}(CH)(CH_2)$
7	3034	3026		2973	2977	186,55	$\nu(CH)(CH_3)$
8	2980	2955		2906	2966	232,85	$\nu_{s}(CH)(CH_2)$
9	2900	2895		2848	2910	353,93	$\nu(CH)(CH_3)$
10	1881	1776		1720	1671	33,54	ν(C=O)
11	1812	1635		1627	1591	0,15	δ(HOH)sciss
12	1550	1535		1552	1498	3,60	ν(CN)+δ(CH) (CH_3)+ δ(NH)
13		1509	1457	1491	1439	13,98	$\delta(CH)(CH_3)$
14		1466	1409	1450	1416	17,80	$\delta(CH)(CH_3)$
15	1395	1400	1403		1408	6,05	ν(C=N)+δ(NH) +δ(CH)
16			1386		1399	0,82	δ(HCH)sciss
17		1361	1364	1391	1381	7,05	ν(CN)+δ(NH)+ δ(CH)
18		1314	1330	1309	1306	6,49	δ(CN)+δ(NH)+ δ(HCH)twist
19			1300		1284	6,69	ω(HCH)
20	1236	1238	1240	1240	1263	6,61	δ(NH)
21			1236		1202	2,86	δ(NH) + δ(HCH)twist
22					1201	7,67	ν(CO)+δ(CC)
23		1176	1179	1182	1189	23,71	ν(P=O)+ν(PO)+ δ(NH)
24		1144	1138	1121	1152	6,08	δ(CN)+δ(CH)
25			1114		1099	1,87	$\delta(CH)(CH_3)$
26		1061	1056		1078	8,76	modos acoplados
27	1042	1028	1031		1019	81,50	ν(PO)+δ(NH)
28		985	998	990	1004	17,58	$\delta(CH)(CH_3)$
29			972	940	932	9,42	$\rho(CH_2)$ + δ(CN)
30	900	923	943		909	10,41	ν(CC) + δ(OC=O) + ν(Al-O) (carboxilato)
31					894	0,99	δ(NH)
32	865	848	869	863	844	5,08	ν(Al-O)(fosfato)

							+ δ(P=O) + δ(PN)
33			802	806	811	23,58	δ(CN) + δ(NH) + ν(CN)
34	757	801	750	755	780	16,18	δ(CN) + δ(NH)
35		693	689		703	1,62	δ(NH) + ρ(OH)(H_2O)
36			670	670	668	4,56	δ(NH) + ρ(OH)(H_2O)
37					655	0,81	δ(CN) + δ(CC) + ρ(OH)(H_2O)
38			645		636	10,21	ρ(OH)(H_2O)
39		616	612		615	1,52	δ(NH) + ρ(OH)(H_2O)
40			589		604	7,38	ν(CCO) + δ(NH)
41			566	587	589	3,01	ν(Al-OH_2) + δ(NH)
42		563	543		545	2,26	modos acoplados
43			505		514	3,03	ν(N-Al-O)(fosfato) + ω(HOH)
44	506	490	485		487	6,42	ν(O-Al-O) + δ(NH) + ω(HOH)
45			477	452	468	9,89	ρ(CH_2)+δ(CO)+ ν(N-Al)
46			459		433	7,28	distorção angular(anel)
47	424	440	443		425	11,23	ω(HCH) + δ(PN) + ν(O-Al-O)
48					416	5,31	δ(Al-O) (carboxilato) + δ(CH)(CH_3)
49	386	396	394	391	396	1,14	ρ(CH_2) + δ(PO)
50			379		353	4,69	δ(N-Al) + δ(NH) + δ(CH)(CH_3)
51	333	317	333	328	327	1,94	δ(Al-O)(carboxilato) + δ(CN) +δ(CH)(CH_3)
52	288	288	329		302	2,40	δ(Al-O)(fosfato) +δ(Al-OH_2)
53					275	4,86	distorção angular(anel)
54					258	2,29	distorção

						angular(anel)
55		252	243	241	251	0,65	ω(HOH)
56					217	0,95	$\delta(Al\text{-}OH_2)$+ δ(N-Al) + δ(Al-O) (carboxilato)
57			210		204	2,65	$\delta(Al\text{-}OH_2)$+ δ(Al-O)(fosfato) + δ(Al-O) (carboxilato)
58		194			192	0,11	$\tau(CH_3)$
59					185	0,80	$\tau(CH_3)$
60		165	176	177	177	0,90	δ(HOH)twist
61			132		133	0,98	τ
62		111	95	102	103	0,74	distorção angular(anel)
63					91	1,44	distorção angular(anel)
64					72	0,52	τ
65					70	2,28	τ
66					43	2,54	τ

[a] Atividades Raman são calculadas em A^4 amu.

Tabela A.4 - Titulação potenciométrica dos ligantes Pen, Cis, Hcis e Met, todos com a adição de 1,00 mL de ácido 0,1000 mol L^{-1}.

Volume (mL) de base	pH-Penicilamina	pH-Cisteína	pH-Homocisteína	pH-Metionina
0,00	3,072	3,013	3,116	3,034
0,10	3,114	3,059	3,158	3,086
0,20	3,166	3,119	3,211	3,146
0,30	3,226	3,18	3,268	3,209
0,40	3,296	3,25	3,336	3,28
0,50	3,382	3,332	3,416	3,364
0,60	3,487	3,431	3,516	3,465
0,70	3,624	3,555	3,645	3,596
0,80	3,832	3,735	3,835	3,787
0,90	4,193	4,023	4,155	4,106
1,00	5,382	4,79	5,419	5,381
1,10	6,48	6,7	7,44	7,586
1,20	7,208	7,532	8,07	8,301
1,30	7,542	7,889	8,349	8,588
1,40	7,762	8,153	8,559	8,801
1,50	7,948	8,382	8,735	8,978
1,60	8,122	8,594	8,891	9,138
1,70	8,298	8,798	9,038	9,291
1,80	8,488	9,004	9,18	9,442
1,90	8,7	9,216	9,322	9,594
2,00	8,973	9,439	9,461	9,749
2,10	9,314	9,667	9,6	9,903
2,20	9,649	9,89	9,733	10,051
2,30	9,898	10,083	9,858	10,187
2,40	10,081	10,246	9,976	10,302
2,50	10,228	10,381	10,085	10,402
2,60	10,346	10,491	10,186	10,491
2,70	10,444	10,583	10,279	10,564
2,80	10,529	10,662	10,364	10,628
2,90	10,602	10,731	10,444	10,686
3,00	10,667	10,791	10,516	10,738

Tabela A.5 - Titulação potenciométrica dos sistemas Al:aa na proporção 1:1.

Volume (mL) de base	pH-Al:Pen	pH-Al:Cis	pH-Al:Hcis	pH-Al:Met
0,00	4,210	4,159	4,279	4,19
0,10	4,293	4,232	4,321	4,274
0,20	4,400	4,315	4,389	4,37
0,30	4,483	4,395	4,453	4,45
0,40	4,561	4,464	4,512	4,507
0,50	4,611	4,517	4,563	4,548
0,60	4,648	4,561	4,608	4,577
0,70	4,672	4,588	4,641	4,598
0,80	4,692	4,607	4,67	4,615
0,90	4,707	4,629	4,692	4,629
1,00	4,724	4,643	4,713	4,643
1,10	4,735	4,659	4,733	4,657
1,20	4,751	4,672	4,748	4,671
1,30	4,768	4,689	4,767	4,686
1,40	4,782	4,705	4,784	4,702
1,50	4,800	4,725	4,802	4,72
1,60	4,817	4,741	4,822	4,74
1,70	4,836	4,764	4,84	4,759
1,80	4,856	4,794	4,863	4,78
1,90	4,877	4,813	4,889	4,803
2,00	4,901	4,838	4,911	4,83
2,10	4,930	4,866	4,942	4,861
2,20	4,962	4,903	4,973	4,894
2,30	4,996	4,948	5,013	4,933
2,40	5,047	4,989	5,055	4,983
2,50	5,100	5,05	5,122	5,043
2,60	5,162	5,119	5,193	5,124
2,70	5,259	5,271	5,306	5,25
2,80	5,417	5,469	5,471	5,44
2,90	5,632	5,919	5,691	5,681
3,00	5,918	6,214	5,933	6,008
3,10	6,281	6,518	6,308	8,149
3,20	6,744	7,032	6,817	8,333
3,30	7,181	7,439	7,3	8,508
3,40	7,526	7,794	7,759	8,64
3,50	7,773	8,07	8,125	8,752

Tabela A.6 - Titulação potenciométrica dos ligantes PCr com 1,00 mL de ácido 0,1000 mol L^{-1} e ATP.

Volume (mL) de base	pH-PCr	pH-ATP
0,00	3,653	3,677
0,10	3,751	3,77
0,20	3,876	3,878
0,30	4,009	3,99
0,40	4,156	4,114
0,50	4,317	4,254
0,60	4,495	4,427
0,70	4,697	4,636
0,80	4,957	4,899
0,90	5,341	5,325
1,00	6,135	5,67
1,10	9,094	5,979
1,20	9,949	6,222
1,30	10,232	6,406
1,40	10,415	6,624
1,50	10,548	6,779
1,60	10,652	7,01
1,70	10,737	7,25
1,80	10,807	7,537
1,90	10,87	8,442
2,00	10,924	9,685
2,10	10,972	10,098
2,20	11,016	10,327
2,30	11,056	10,488
2,40	11,093	10,608
2,50	11,126	10,705
2,60	11,158	10,784
2,70	11,187	10,853
2,80	11,215	10,911
2,90	11,24	10,963
3,00	11,264	11,011

Tabela A.7 - Titulação potenciométrica dos sistemas Al:ATP e Al:PCr na proporção 1:1.

Volume (mL) de base	pH-Al:Pcr	pH-Al:ATP
0,00	3,653	3,677
0,10	3,751	3,77
0,20	3,876	3,878
0,30	4,009	3,99
0,40	4,156	4,114
0,50	4,317	4,254
0,60	4,495	4,427
0,70	4,697	4,636
0,80	4,957	4,899
0,90	5,341	5,325
1,00	6,135	5,67
1,10	9,094	5,979
1,20	9,949	6,222
1,30	10,232	6,406
1,40	10,415	6,624
1,50	10,548	6,779
1,60	10,652	7,01
1,70	10,737	7,25
1,80	10,807	7,537
1,90	10,87	8,442
2,00	10,924	9,685
2,10	10,972	10,098
2,20	11,016	10,327
2,30	11,056	10,488
2,40	11,093	10,608
2,50	11,126	10,705
2,60	11,158	10,784
2,70	11,187	10,853
2,80	11,215	10,911
2,90	11,24	10,963
3,00	11,264	11,011

Tabela A.8 - Titulação potenciométrica dos sistemas Al:ATP:aa na proporção 1:1:1.

Volume (mL) de base	pH Al:ATP:Pen	pH Al:ATP:Cis	pH Al:ATP:Hcis	pH Al:ATP:Met
0,00	3,112	3,116	3,198	3,158
0,10	3,137	3,147	3,211	3,188
0,20	3,174	3,184	3,245	3,228
0,30	3,212	3,222	3,282	3,273
0,40	3,256	3,264	3,325	3,314
0,50	3,302	3,31	3,373	3,361
0,60	3,351	3,358	3,426	3,414
0,70	3,404	3,411	3,479	3,47
0,80	3,462	3,469	3,542	3,535
0,90	3,522	3,529	3,618	3,599
1,00	3,585	3,591	3,677	3,666
1,10	3,653	3,658	3,746	3,741
1,20	3,724	3,73	3,823	3,815
1,30	3,802	3,807	3,912	3,896
1,40	3,883	3,889	4,005	3,985
1,50	3,97	3,978	4,181	4,167
1,60	4,064	4,074	4,205	4,235
1,70	4,168	4,178	4,348	4,312
1,80	4,277	4,295	4,453	4,455
1,90	4,404	4,424	4,658	4,6
2,00	4,544	4,573	4,872	4,888
2,10	4,719	4,744	5,045	5,223
2,20	4,887	4,936	5,324	5,398
2,30	5,092	5,141	5,526	5,594
2,40	5,278	5,35	5,682	5,844
2,50	5,532	5,569	5,946	6,081
2,60	6,033	5,825	6,202	6,303
2,70	6,248	6,116	6,496	6,646
2,80	6,516	6,413	6,692	6,765
2,90	6,761	6,678	6,888	6,98
3,00	6,907	6,887	7,03	7,111
3,10	7,04	7,053	7,191	7,25
3,20	7,17	7,171	7,298	7,341
3,30	7,246	7,262	7,395	7,427
3,40	7,308	7,338	7,455	7,559
3,50	7,361	7,404	7,547	7,58

Tabela A.9 - Titulação potenciométrica dos sistemas Al:PCr:aa na proporção 1:1:1.

Volume (mL) de base	pH Al:PCr:Pen	pH Al:PCr:Cis	pH Al:PCr:Hcis	pH Al:PCr:Met
0,00	3,938	3,939	3,98	3,92
0,10	4,011	3,988	4,032	3,882
0,20	4,086	4,045	4,102	3,926
0,30	4,154	4,108	4,171	3,984
0,40	4,225	4,176	4,258	4,047
0,50	4,3	4,251	4,35	4,119
0,60	4,381	4,325	4,431	4,193
0,70	4,463	4,407	4,522	4,28
0,80	4,564	4,489	4,637	4,373
0,90	4,656	4,573	4,756	4,463
1,00	4,748	4,663	4,86	4,562
1,10	4,84	4,752	4,96	4,657
1,20	4,933	4,846	5,04	4,759
1,30	5,004	4,934	5,11	4,857
1,40	5,07	5,008	5,193	4,939
1,50	5,136	5,071	5,283	5,006
1,60	5,196	5,138	5,334	5,076
1,70	5,267	5,206	5,421	5,135
1,80	5,346	5,277	5,495	5,199
1,90	5,491	5,352	5,597	5,266
2,00	5,546	5,443	5,703	5,35
2,10	5,704	5,547	5,841	5,417
2,20	5,902	5,682	5,995	5,518
2,30	6,292	5,896	6,199	5,654
2,40	6,64	6,154	6,49	5,887
2,50	6,923	6,457	6,793	6,143
2,60	7,109	6,794	7,099	6,482
2,70	7,334	7,159	7,427	6,812
2,80	7,507	7,475	7,724	7,242
2,90	7,636	7,747	7,969	7,601
3,00	7,749	7,923	8,168	7,884
3,10	7,873	8,08	8,308	8,149
3,20	7,98	8,213	8,432	8,333
3,30	8,08	8,341	8,556	8,508
3,40	8,19	8,458	8,652	8,64
3,50	8,289	8,58	8,727	8,752

Tabela A.10 - Parâmetros geométricos calculados pelo DFT:B3LYP/6-311++G(d,p) para o complexo $[AlMetATP(H_2O)_3]^{1-}$ (comprimentos de ligação em Å e ângulos em graus).

Comprimentos de ligação (Å)	**$[AlMetATP(H_2O)_3]^{1-}$**
C(4)-H(1)	1,091
C(4)-H(2)	1,090
C(4)-H(3)	1,090
C(4)-S(5)	1,827
C(6)-S(5)	1,839
C(6)-H(7)	1,090
C(6)-H(8)	1,092
C(6)-C(9)	1,529
C(9)-H(10)	1,095
C(9)-H(11)	1,094
C(9)-C(12)	1,540
C(12)-H(13)	1,088
C(12)-N(14)	1,512
N(14)-H(15)	1,028
N(14)-H(16)	1,023
N(14)-H(17)	1,022
C(12)-C(18)	1,536
C(18)-O(19)	1,233
C(18)-O(20)	1,286
Al-O(20)	1,923
Al-O(22)	1,931
Al-O(25)	1,977
Al-O(28)	1,986
Al-O(31)	1,837
Al-O(38)	1,872
O(22)-H(23)	0,964
O(22)-H(24)	1,030
O(25)-H(26)	0,965
O(25)-H(27)	0,992
O(28)-H(29)	1,037
O(28)-H(30)	0,964
O(31)-P(32)	1,576
O(33)-P(32)	1,539
O(34)-P(32)	1,498
O(35)-P(32)	1,700
O(35)-P(36)	1,616
O(37)-P(36)	1,490
O(38)-P(36)	1,544
O(39)-P(36)	1,628

O(39)-P(40)	1,648
O(41)-P(40)	1,519
O(42)-P(40)	1,496
O(43)-P(40)	1,642
O(43)-C(44)	1,437
C(44)-H(45)	1,093
C(44)-H(46)	1,095
C(44)-C(47)	1,517
C(47)-H(48)	1,093
C(47)-C(49)	1,532
C(47)-O(57)	1,451
C(49)-H(50)	1,094
C(49)-O(51)	1,425
O(51)-H(52)	0,969
C(49)-C(53)	1,539
C(53)-H(54)	1,090
C(53)-O(55)	1,421
O(55)-H(56)	0,964
C(53)-C(58)	1,538
C(58)-H(59)	1,093
C(58)-O(57)	1,421
C(58)-N(60)	1,451
N(60)-C(61)	1,384
N(60)-C(65)	1,382
C(61)-H(62)	1,080
C(61)-N(63)	1,311
C(64)-N(63)	1,384
C(64)-C(65)	1,395
C(64)-C(70)	1,410
C(65)-N(66)	1,339
C(67)-N(66)	1,334
C(67)-H(68)	1,086
C(67)-N(69)	1,341
C(70)-N(69)	1,348
C(70)-N(71)	1,351
N(71)-H(72)	1,008
N(71)-H(73)	1,007
Ângulos (graus)	**$[AlMetATP(H_2O)_3]^{1-}$**
H(1)-H(2)-H(3)	60,42
C(4)-S(5)-C(6)	99,52
H(7)-C(6)-H(8)	108,60
S(5)-C(6)-C(9)	109,23
C(6)-C(9)-C(12)	113,01

H(10)-C(9)-H(11)	107,49
C(9)-C(12)-C(18)	112,36
C(9)-C(12)-N(14)	109,05
H(15)-H(16)-H(17)	60,91
O(19)-C(18)-O(20)	126,98
O(20)-Al-O(22)	89,99
O(20)-Al-O(25)	87,31
O(20)-Al-O(28)	88,25
O(20)-Al-O(31)	174,78
O(20)-Al-O(38)	89,98
O(22)-Al-O(25)	88,45
O(22)-Al-O(28)	176,50
O(22)-Al-O(31)	92,06
O(22)-Al-O(38)	91,47
O(25)-Al-O(28)	88,45
O(25)-Al-O(31)	87,95
O(25)-Al-O(38)	177,29
O(31)-Al-O(38)	94,76
H(23)-O(22)-H(24)	108,29
H(26)-O(25)-H(27)	110,35
H(29)-O(28)-H(30)	108,08
O(31)-P(32)-O(33)	108,39
O(31)-P(32)-O(34)	114,47
O(31)-P(32)-O(35)	102,08
P(32)-O(35)-P(36)	127,18
O(38)-P(36)-O(37)	117,05
O(38)-P(36)-O(39)	108,13
P(36)-O(39)-P(40)	136,37
O(41)-P(40)-O(42)	118,71
O(41)-P(40)-O(43)	109,48
O(39)-P(40)-O(43)	95,90
O(43)-C(44)-C(47)	109,11
H(45)-C(44)-H(46)	108,93
C(47)-C(49)-C(53)	102,93
C(47)-C(49)-O(51)	108,73
C(49)-C(53)-O(55)	113,05
C(53)-C(58)-O(57)	106,18
C(53)-C(58)-N(60)	114,70
N(60)-C(61)-N(63)	113,32
N(60)-C(65)-C(64)	105,27
C(65)-N(66)-C(67)	111,79

N(66)-C(67)-N(69)	128,41
C(67)-N(69)-C(70)	118,74
C(65)-C(64)-C(70)	116,45
N(69)-C(70)-N(71)	118,95
H(72)-N(71)-H(73)	118,43

Tabela A.11 - Espectro Raman experimental e calculado para o complexo $[AlMetATP(H_2O)_3]^{1-}$.

Nos. Modos	Número de onda experimental (cm^{-1})				Número de onda B3LYP escalonado (cm^{-1})	S_{Ra} [a]	Atribuição aproximada
	Observados	Deconvolução	2nd derivada	Ajuste não linear			
1					3787	151,26	$\nu(OH)(H_2O)$
2					3781	144,08	$\nu(OH)(H_2O)$
3					3778	82,55	$\nu_{as}(OH)(H_2O)$
4					3777	159,74	$\nu(OH)_{ribose}$
5					3679	143,92	$\nu(OH)_{ribose}$
6					3653	97,67	$\nu_{as}(NH)(NH_2)_{adenina}$
7					3532	444,11	$\nu_{s}(NH)(NH_2)_{adenina}$
8	3458	3458	3461		3448	73,74	$\nu(NH)_{Met}$
9	3402	3402	3398		3410	110,16	$\nu(NH)_{Met}$
10	3318	3318	3316		3316	151,11	$\nu(NH)_{Met}$
11		3205	3210		3232	192,09	$\nu_{s}(OH)(H_2O)$
12		3180	3181		3189	235,17	$\nu(CH)_{adenina}$
13	3169	3163	3164		3109	278,87	$\nu(CH)_{adenina}$
14		3148	3147		3083	174,00	$\nu(CH)(CH_3)_{Met}$
15		3136	3135		3077	138,82	$\nu(CH)_{Met}$
16	3111	3112	3109		3071	95,97	$\nu(CH)(CH_3)_{Met}$
17		3094	3093		3062	167,69	$\nu_{as}(CH)(CH_2)_{Met}$
18	3083	3084	3077		3054	106,90	$\nu(CH)_{ribose}$
19	3072	3066	3068		3036	150,10	$\nu_{as}(CH)(CH_2)_{ATP}$
20	3045	3043	3038		3022	189,41	$\nu_{as}(CH)(CH_2)_{Met}$
21	3025	3023	3021		3018	350,89	$\nu(CH)_{ribose}$
22					3013	299,55	$\nu(CH)_{ribose}$
23	3009	3006	3004		3004	162,73	$\nu_{s}(CH)(CH_2)_{Met}$
24					3000	277,49	$\nu(CH)_{ribose}$
25	2974		2976		2989	407,75	$\nu(CH)(CH_3)_{Met}$
26	2964	2959	2961		2982	337,20	$\nu_{s}(CH)(CH_2)_{Met}$
27		2928	2933		2978	229,35	$\nu_{s}(CH)(CH_2)_{ATP}$
28			2502		2530	223,80	$\nu(OH)(H_2O)$
29	2420	2420	2423		2430	147,66	$\nu(OH)(H_2O)$
30	1664	1663		1660	1658	18,64	$\nu(C=O)$
31	1642			1642	1642	6,25	$\delta(NH)(NH_3)$
32				1634	1633	4,01	$\delta(HOH)sciss$
33		1625		1624	1631	3,96	$\delta(HOH)sciss$
34				1604	1610	30,23	$\nu(C\text{-}NH_2)_{ATP}$
35				1601	1609	10,01	$\delta(NH)(NH_3)$
36	1580	1578		1580	1580	17,09	$\delta(HNH)sciss_{ATP}$
37				1570	1575	157,38	$\nu(CN)_{adenina}+\delta(CN)_{adenina}$

38	1559	1556	1558	1565	7,43	δ(HOH)sciss
39	1510	1512	1506	1494	206,42	$\delta(NH)(NH_3)$
40	1485		1484	1486	4,82	$\nu(CN)_{adenina}$
41			1483	1476	1,77	$\delta(HCH)sciss_{Met}$
42	1470		1471	1470	14,64	$\delta(HCH)sciss_{ATP}$
43			1460	1466	40,56	$\nu(CN)_{adenina}$
44	1457		1455	1460	30,11	$\delta(HCH)sciss_{Met}$
45			1440	1447	13,40	$\delta(CH)(CH_3)$
46			1426	1434	21,50	$\delta(CH)(CH_3)$
47			1415	1433	29,00	$\nu(CC)_{ribose}$ + $\delta(CH)_{ribose}$
48	1413		1412	1412	50,74	$\nu(CN)_{adenina}$
49				1406	36,30	$\delta(CH)_{ribose}$
50			1401	1399	4,17	$\omega(HCH)_{Met}$
51	1389		1388	1389	15,88	$\omega(HCH)_{ATP}$
52			1379	1375	7,67	$\nu(CC)_{ATP}$
53			1377	1362	97,82	$\nu(CC)_{adenina}$+ $\delta(CH)_{adenina}$
54	1358		1365	1356	20,84	$\delta(CH)_{Met}$
55			1357	1351	5,25	$\omega(HCH)_{Met}$
56			1347	1342	37,72	$\delta(CH)_{ribose}$
57	1339		1338	1339	8,85	$\delta(CH_2)twist_{Met}$
58				1336	86,44	$\nu(CO)_{ribose}$ + $\delta(CH)_{ribose}$
59				1332	1,30	$\delta(CH)(CH_3)$
60			1326	1332	63,15	$\delta(CH)_{ribose}$
61				1318	35,13	$\delta(CO)_{ribose}$
62			1313	1313	7,86	$\delta(CO)_{ribose}$ + $\delta(CH)_{ribose}$
63			1304	1307	63,34	$\nu(CC)_{ribose}$
64			1295	1299	88,68	$\nu(CN)_{adenina}$+ $\delta(CH)_{ribose}$
65			1284	1287	8,07	$\delta(CH_2)twist_{Met}$
66			1276	1281	32,94	$\delta(CC)_{ribose}$
67				1256	2,07	$\delta(NH)(NH_3)$
68			1235	1245	32,77	$\nu(CN)_{ATP}$
69	1242		1232	1242	13,89	$\delta(CH_2)twist_{ATP}$
70	1225	1225	1224	1230	16,30	$\delta(CN)_{ATP}$
71			1214	1209	13,96	$\nu(P_\beta O)$
72	1205	1205	1206	1208	85,14	$\delta(C\text{-}NH_2)_{ATP}$
73			1194	1191	9,29	$\delta(OH)_{ribose}$
74				1188	4,48	$\nu(P_\alpha O)$
75	1187	1182	1184	1183	12,34	$\nu(P_\gamma O)$
76				1179	5,61	$\nu(CC)_{Met}$
77	1159		1160	1153	10,69	$\nu(CN)_{adenina}$
78			1122	1122	7,96	$\delta(NH)(NH_3)$
79				1112	4,41	$\delta(CO)_{ribose}$
80			1095	1103	2,55	$\delta(H_2O)twist$
81		1093	1088	1088	9,21	$\delta(CO)_{ribose}$

82				1087	1080	7,21	$\nu(CO)_{Met}$
83	1075	1075	1075	1077	1074	8,00	$\nu(CO)_{ribose}$
84				1072	1069	6,92	$\delta(H_2O)$twist
85		1063		1064	1064	5,69	$\delta(CC)_{ribose}$
86				1058	1061	5,44	$\nu(CO)_{ribose}$
87					1050	9,05	$\nu(CC)_{Met}$
88				1044	1043	63,72	$\nu(CO)_{ribose}$
89				1042	1026	13,19	$\nu(CC)_{ribose}$
90				1038	1013	3,56	$\nu(P_\beta O)$ + $\nu(P_\alpha O)$+ $\nu(P_\alpha O\text{-}C)$
91					1005	25,97	$\delta(CC)_{ribose}$
92					998	12,23	$\nu(CC)_{Met}$
93					995	6,87	$\nu(CN)_{Met}$
94					985	10,02	$\rho(NH_2)_{ATP}$
95					980	5,19	$\delta(CN)_{adenina}$
96				976	977	5,28	$\delta(CS)_{Met}$ + $\delta(CH)(CH_3)$
97					965	3,45	$\delta(CH)(CH_3)$
98				957	957	0,62	$\delta(CH)_{adenina}$
99				953	952	8,76	$\nu(P_\alpha\text{-}O\text{-}P_\beta)$ + $\nu(P_\beta\text{-}O\text{-}P_\gamma)$
100				939	946	15,14	$\nu(P_\gamma O)$
101				933	940	7,88	$\delta(NH)(NH_3)$
102				919	934	3,00	$\rho(CH_2)_{ATP}$
103				904	909	24,33	$\delta(H_2O)$twist
104				898	903	6,62	ω(HOH)
105					895	10,56	$\delta(CH)_{adenina}$
106					894	1,95	$\delta(CC)_{ribose}$
107				881	883	5,97	$\delta(CN)_{adenina}$
108				862	873	23,40	$\delta(CN)_{adenina}$
109				853	842	5,79	ω(HOH)
110				840	836	13,83	$\delta(CN)_{adenina}$
111		820		823	824	33,18	$\delta(CN)_{Met}$
112		810		809	798	2,74	$\rho(CH_2)_{Met}$
113					796	2,29	$\delta(CC)_{adenina}$ + $\delta(CN)_{adenina}$
114				792	795	34,52	$\delta(OH)_{ribose}$
115				780	771	3,07	$\rho(H_2O)$
116				764	755	0,97	$\rho(H_2O)$
117	736	750	750	750	746	3,89	$\delta(C{=}O)_{Met}$
118			736		736	24,08	$\nu(CS)$ + $\rho(CH_2)_{Met}$
119	727		730	730	725	20,52	$\nu(CN)_{adenina}$
120					710	30,94	$\delta(CN)_{adenina}$
121				692	690	24,69	$\nu(CS)$ +$\delta(CC)_{Met}$
122				688	682	6,45	$\delta(P_\alpha\text{-}O\text{-}P_\beta)$ + ω(HOH)

123					678	2,95	$\delta(CC)_{adenina}$
124					677	17,62	$\delta(CC)_{Met}$+ $\delta(CO)_{Met}$
125				667	672	6,42	modos acoplados
126				656	665	8,46	$\delta(P_\beta\text{-}O\text{-}P_\gamma)$
127				653	655	1,53	$\delta(CH)_{adenina}$
128				636	647	3,19	$\rho(H_2O)$
129				627	629	7,62	$\delta(CO)_{ATP}$
130					620	15,04	$\delta(CH)_{ribose}$
131					599	5,57	$\nu(Al\text{-}OP_\gamma)$ + $\delta(Al\text{-}OH_2)$
132					571	4,23	δ(anel)
133					568	2,22	$\delta(CN)_{adenina}$
134					562	4,89	$\nu(Al\text{-}OP_\beta)$
135					556	1,90	$\nu(H_2O\text{-}Al\text{-}OP_\beta)$ +$\delta(H_2O\text{-}Al\text{-}OH_2)$+ $\delta(CO\text{-}Al\text{-}OP_\gamma)$
136				541	543	4,65	$\delta(OH)_{ribose}$
137					536	0,97	$\nu(H_2O\text{-}Al\text{-}OH_2)$ + $\delta(CO\text{-}Al\text{-}OP_\gamma)$ + $\delta(H_2O\text{-}Al\text{-}OP_\beta)$
138				529	530	5,67	$\nu(H_2O\text{-}Al\text{-}OH_2)$ + $\delta(CO\text{-}Al\text{-}OP_\gamma)$ + $\delta(H_2O\text{-}Al\text{-}OP_\beta)$
139					522	5,12	$\nu(CC)_{adenina}$
140				514	517	8,28	$\nu(CO\text{-}Al\text{-}OP_\gamma)$ + $\delta(H_2O\text{-}Al\text{-}OH_2)$ +$\delta(H_2O\text{-}Al\text{-}OP_\beta)$
141			496	496	499	1,32	$\delta(NH_2)twist_{ATP}$
142					484	2,80	$\nu(Al\text{-}OH_2)$ + $\delta(Al\text{-}OP_\gamma)$
143	479	477		483	480	4,25	$\delta(P_\alpha O)$ + $\delta(P_\beta O)$ + $\delta(P_\gamma O)$
144				468	469	3,34	$\nu(Al\text{-}OH_2)$ + $\delta(Al\text{-}OP_\beta)$ + $\delta(Al\text{-}OP_\gamma)$
145				455	458	0,75	$\nu(Al\text{-}OH_2)$ + ν(Al-OC)
146	449	450	449	445	453	1,65	δ(anel)
147					434	3,99	δ(anel)
148				428	427	1,51	$\delta(OH)_{ribose}$
149				420	420	0,90	modos acoplados
150		409		410	409	0,43	$\nu(Al\text{-}OH_2)$ +

							ν(Al-OC)
151					403	4,99	δ(CS)
152			400	400	401	4,96	$\delta(CH)_{Met}$
153				386	387	1,32	δ(anel)
154			379	384	372	0,86	$\nu(Al\text{-}OH_2)$
155				373	363	8,48	δ(anel)
156				361	355	1,26	$\delta(Al\text{-}OH_2)$
157	350	360	350	352	351	1,07	modos acoplados
158					349	5,07	modos acoplados
159				348	348	1,65	$\delta(H_2O\text{-}Al\text{-}OH_2)$ + $\delta(H_2O\text{-}Al\text{-}OP_\beta)$
160				337	339	1,52	$\delta(CO\text{-}Al\text{-}OP_\gamma)$ + $\delta(H_2O\text{-}Al\text{-}OH_2)$
161				328	334	0,59	modos acoplados
162	314	315	312	314	325	2,34	$\delta(CC)_{Met}$
163				309	305	0,70	$\delta(Al\text{-}OH_2)$ + $\delta(Al\text{-}OP_\beta)$ + $\delta(Al\text{-}OP_\gamma)$
164				301	299	3,24	modos acoplados
165				291	293	4,91	$\tau(NH_2)_{ATP}$
166	287	292	287	287	289	1,73	$\tau(H_2O)$
167				283	278	0,61	modos acoplados
168				278	276	0,33	$\tau(H_2O)$
169					266	3,52	τ
170					264	2,08	τ
171					263	0,86	τ
172	261	264	262	262	261	2,64	$\tau(H_2O)$
173	248	248	247	249	244	2,49	τ
174					244	1,25	τ
175				240	239	5,00	τ
176					239	1,98	τ
177	232	230	231	231	226	0,35	$\tau(NH_3)$
178					225	3,82	τ
179	219	220	219	221	216	4,42	τ
180				218	208	1,91	τ
181				208	206	2,29	τ
182				194	199	1,35	τ
183					184	1,64	τ
184				183	183	8,90	$\omega(HNH)_{ATP}$
185					180	1,37	τ
186					176	0,81	τ
187				172	172	0,45	$\delta(CH)(CH_3)$
188				163	170	0,46	τ

189			155	149	0,34	τ
190			145	146	0,32	τ
191				138	0,28	τ
192			134	132	0,36	τ
193				129	0,85	τ
194			122	127	0,27	τ
195			111	112	0,82	τ
196	106	106	105	96	0,33	τ
197				90	0,06	τ
198				88	0,48	τ
199				78	0,15	τ
200				76	0,58	τ
201				66	0,63	τ
202				58	4,84	τ
203				55	0,35	τ
204				45	2,58	τ
205				42	2,24	τ
206				36	0,48	τ(CH_3)
207				33	3,96	τ
208				31	2,65	τ
209				26	3,95	τ(adenina)
210				21	1,26	τ
211				17	1,02	τ
212				14	1,77	τ
213				2	2,46	τ

[a] Atividades Raman foram calculadas em A^4amu.

Tabela A.12 - Valores de R^2 do ajuste não linear para regiões espectrais de 1700 a 100 cm^{-1}.

Regiões do ajuste não linear	Valores de R^2 obtidos
1700-1550	0,9946
1550-1400	0,9999
1400-1300	0,9999
1300-1200	0,9999
1200-1100	0,9969
1100-1000	0,9998
1000-900	0,9819
900-800	0,9999
800-700	0,9996
700-600	0,9966
600-500	0,9998
500-400	0,9999
400-300	0,9999
300-200	0,9999
200-100	0,9999

Tabela A.13 - Números de onda referentes à subtração manual dos espectros da água e da solução de nitrato.

Espectro	**Números de onda da água ou nitrato**
Experimental	3485, 3445, 3410, 3380, 3355, 3335, 3300, 3270, 3250, 3235, 1400, 1050, 970, 605 e 500
Deconvoluído	3485, 3445, 3410, 3380, 3355, 3335, 3300, 3270, 3250, 3235, 1050, 795, 605 e 500
Segunda derivada	3485, 3445, 3410, 3380, 3355, 3335, 3300, 3270, 3250, 3235 e 1050
Ajuste não linear	1400, 1050, 970, 795, 605, 490 e 435

Tabela A. 14 - Parâmetros geométricos calculados pelo DFT:B3LYP/6-311++G(d,p) para o complexo $[AlCisATP(H_2O)_2]^{2-}$ (comprimentos de ligação em Å e ângulos em graus).

Comprimentos de ligação (Å)	**$[AlCisATP(H_2O)_2]^{2-}$**
S(2)-H(1)	1,348
C(3)-S(2)	1,850
C(3)-H(4)	1,091
C(3)-H(5)	1,088
C(3)-C(6)	1,530
C(6)-H(7)	1,093
C(6)-N(8)	1,489
N(8)-H(9)	1,017
N(8)-H(10)	1,019
C(6)-C(11)	1,544
C(11)-O(12)	1,223
C(11)-O(13)	1,301
Al-N(8)	2,063
Al-O(13)	1,870
Al-O(15)	1,972
Al-O(18)	2,027
Al-O(21)	1,850
Al-O(28)	1,860
O(15)-H(16)	1,034
O(15)-H(17)	0,965
O(18)-H(19)	0,967
O(18)-H(20)	0,967
O(21)-P(22)	1,575
O(23)-P(22)	1,533
O(24)-P(22)	1,508
O(25)-P(22)	1,682
O(25)-P(26)	1,623
O(27)-P(26)	1,491
O(28)-P(26)	1,545
O(29)-P(26)	1,614
O(29)-P(30)	1,670
O(31)-P(30)	1,503
O(32)-P(30)	1,503
O(33)-P(30)	1,650
O(33)-C(34)	1,433
C(34)-H(35)	1,095
C(34)-H(36)	1,095
C(34)-C(37)	1,519
C(37)-H(38)	1,094

C(37)-C(39)	1,533
C(37)-O(47)	1,455
C(39)-H(40)	1,093
C(39)-O(41)	1,428
O(41)-H(42)	0,970
C(39)-C(43)	1,538
C(43)-H(44)	1,089
C(43)-O(45)	1,412
O(45)-H(46)	0,989
C(43)-C(48)	1,533
C(48)-H(49)	1,093
C(48)-O(47)	1,426
C(48)-N(50)	1,449
N(50)-C(51)	1,385
N(50)-C(55)	1,382
C(51)-H(52)	1,082
C(51)-N(53)	1,312
C(54)-N(53)	1,384
C(54)-C(55)	1,395
C(54)-C(60)	1,409
C(55)-N(56)	1,339
C(57)-N(56)	1,334
C(57)-H(58)	1,086
C(57)-N(59)	1,341
C(60)-N(59)	1,348
C(60)-N(61)	1,352
N(61)-H(62)	1,008
N(61)-H(63)	1,008
Ângulos (graus)	**$[AlCisATP(H_2O)_2]^{2-}$**
H(1)-S(2)-C(3)	96,32
H(4)-C(3)-H(5)	108,56
S(2)-C(3)-C(6)	112,79
C(3)-C(6)-C(11)	114,00
O(12)-C(11)-O(13)	124,90
N(8)-C(6)-C(11)	107,31
H(9)-N(8)-H(10)	106,28
C(11)-O(13)-Al	120,76
C(6)-N(8)-Al	108,56
N(8)-Al-O(13)	82,12
N(8)-Al-O(15)	88,21
N(8)-Al-O(18)	86,77
N(8)-Al-O(21)	90,65
N(8)-Al-O(28)	174,18

O(13)-Al-O(15)	94,03
O(13)-Al-O(18)	88,24
O(13)-Al-O(21)	171,08
O(13)-Al-O(28)	92,15
O(15)-Al-O(18)	174,16
O(15)-Al-O(21)	90,95
O(15)-Al-O(28)	93,21
O(21)-Al-O(28)	94,96
H(16)-O(15)-H(17)	108,66
H(19)-O(18)-H(20)	107,75
O(21)-P(22)-O(23)	108,98
O(21)-P(22)-O(24)	114,25
O(21)-P(22)-O(25)	102,18
P(22)-O(25)-P(26)	129,37
O(28)-P(26)-O(27)	117,89
O(28)-P(26)-O(29)	104,01
P(26)-O(29)-P(30)	135,29
O(31)-P(30)-O(32)	120,51
O(31)-P(30)-O(33)	110,35
O(29)-P(30)-O(33)	97,29
O(33)-C(34)-C(37)	109,61
H(35)-C(34)-H(36)	108,75
C(37)-C(39)-C(43)	102,88
C(37)-C(39)-O(41)	109,58
C(39)-C(43)-O(45)	113,26
C(43)-C(48)-O(47)	104,97
C(43)-C(48)-N(50)	115,43
N(50)-C(51)-N(53)	113,26
N(50)-C(55)-C(54)	105,40
C(55)-N(56)-C(57)	111,86
N(56)-C(57)-N(59)	128,39
C(57)-N(59)-C(60)	118,69
C(55)-C(54)-C(60)	116,49
N(59)-C(60)-N(61)	118,93
H(62)-N(61)-H(63)	118,16

Tabela A.15 - Espectro Raman experimental e calculado para o complexo $[AlCisATP(H_2O)_2]^{2-}$.

Nos. Modos	Número de onda experimental (cm^{-1}) Observados	Deconvolução	2nd derivada	Ajuste não linear	Número de onda B3LYP escalonado (cm^{-1})	S_{Ra} [a]	Atribuição aproximada
1					3791	49,30	$\nu_{as}(OH)(H_2O)$
2					3773	121,84	$\nu(OH)(H_2O)$
3					3709	179,10	$\nu_s(OH)(H_2O)$
4					3661	136,94	$\nu(OH)_{ribose}$
5					3649	99,91	$\nu_{as}(NH)_{adenina}$
6	3468	3470	3468		3529	454,81	$\nu_s(NH)_{adenina}$
7	3438	3438	3398		3488	88,98	$\nu_{as}(NH)_{Cis}$
8		3418	3365		3419	196,98	$\nu_s(NH)_{Cis}$
9	3263	3268	3260		3263	384,04	$\nu(OH)_{ribose}$
10		3178	3176		3165	315,93	$\nu(CH)_{adenina}$
11	3162	3162	3163		3108	278,77	$\nu(CH)_{adenina}$
12		3140	3138		3082	124,52	$\nu_{as}(CH)(CH_2)_{Cis}$
13	3113	3114	3113		3079	158,40	$\nu(CH)_{ribose}$
14	3088	3087	3100		3026	20,01	$\nu(CH)_{Cis}$
15	3076	3077	3087		3017	204,37	$\nu_{as}(CH)(CH_2)_{ATP}$
16		3062	3077		3015	380,30	$\nu_s(CH)(CH_2)_{Cis}$
17	3050	3050	3059		3013	264,78	$\nu(CH)_{ribose}$
18		3040	3041		3006	257,35	$\nu(CH)_{ribose}$
19	3027	3028	3029		3000	379,34	$\nu(CH)_{ribose}$
20					2971	230,86	$\nu_s(CH)(CH_2)_{ATP}$
21	2680	2678	2681		2617	423,15	$\nu(SH)$
22					2484	160,67	$\nu(OH)(H_2O)$
23	1660	1658		1659	1677	32,81	$\nu(C=O)$
24		1627		1634	1616	6,47	$\delta(HOH)sciss$
25				1616	1614	7,52	$\delta(HNH)sciss_{Cis}$
26	1611	1609		1610	1609	32,78	$\nu(C\text{-}NH_2)_{ATP}$
27	1587	1585		1589	1590	2,06	$\delta(HOH)sciss$
28	1573	1573	1585	1586	1580	13,01	$\delta(HNH)sciss_{ATP}$
29	1552	1552	1572	1582	1575	165,15	$\nu(CN)_{adenina}+\delta(CC)_{adenina}$
30	1490	1539	1551	1506	1490	177,61	$\nu(CN)_{adenina}+\delta(CN)_{adenina}$
31				1487	1479	16,23	$\delta(OH)_{ribose}$
32				1467	1467	15,72	$\delta(HCH)sciss_{ATP}$
33				1447	1464	56,34	$\nu(CN)_{adenina}$
34				1430	1444	15,58	$\delta(HCH)sciss_{Cis}$
35	1409		1412	1417	1428	64,29	$\delta(CH)_{ribose}$
36				1407	1410	39,65	$\nu(CN)_{adenina}+\delta(CN)_{adenina}$

37	1388	1389	1389	1389	1393	4,61	$\delta(CH)_{ribose}$
38				1382	1379	5,45	$\omega(HCH)_{ATP}$
39				1379	1375	15,89	$\delta(HNH)twist_{Cis}$
40				1370	1365	138,76	$\delta(CH)_{ribose}$
41				1359	1361	35,88	$\delta(OH)_{ribose}$
42				1345	1343	82,10	$\delta(HCH)twist_{ATP}$
43				1344	1338	13,20	$\delta(HCH)twist_{Cis}$
44					1335	8,50	$\delta(CH)_{ribose}$
45					1333	62,27	$\delta(HNH)twist_{adenina}$
46				1328	1324	11,38	$\delta(CH)_{ribose}$
47					1314	66,72	$\nu(CN)_{adenina}$ + $\nu(CC)_{adenina}$
48					1302	43,56	$\delta(CH)_{ribose}$
49				1300	1300	52,85	$\delta(CH)_{ribose}$
50					1299	18,14	$\omega(HCH)_{Cis}$
51				1266	1273	38,35	$\delta(CH)_{ribose}$
52				1259	1266	3,17	$\delta(CH)_{Cis}$
53				1241	1248	25,92	$\delta(CH)_{adenina}$
54				1228	1242	12,33	$\delta(CH)_{ribose}$
55	1215	1210		1215	1215	60,56	$\delta(CH)_{adenina}$
56					1201	22,90	$\delta(OH)_{ribose}$
57					1200	41,35	$\delta(OH)_{ribose}$
58				1197	1199	4,98	$\delta(CH)_{Cis}$
59	1194	1192		1181	1196	12,89	$\nu(P_{\alpha}O)$
60				1177	1157	10,96	$\omega(HOH)$
61					1152	6,77	$\delta(P_{\alpha}O)$
62				1149	1150	1,75	$\delta(CC)_{Cis}$
63					1133	6,48	$\omega(HNH)_{Cis}$
64					1118	1,71	$\nu(CC)_{ribose}$
65				1107	1103	8,79	$\nu(CO)_{ribose}$
66				1095	1079	3,62	$\omega(HOH)$
67				1075	1076	12,11	$\delta(CH)_{ribose}$
68				1070	1069	12,27	$\nu(CC)_{ribose}$
69					1067	14,59	$\nu(CN)_{Cis}$
70	1065	1064	1063	1065	1065	3,66	$\nu(CC)$
71					1052	72,15	$\nu(P_{\alpha}O)$
72				1030	1033	8,42	$\nu(CC)_{ribose}$ + $\delta(CN)_{adenina}$
73				1026	1028	4,36	$\nu(CC)_{Cis}$
74				1019	1018	9,77	$\nu(P_{\beta}O)$ + $\nu(P_{\alpha}\text{-}O\text{-}C)$
75					1004	13,99	$\nu(P_{\gamma}O) + \delta(SH)$
76					1003	31,63	$\nu(CO)_{ribose}$
77					986	8,11	$\delta(CN)_{adenina}$
78				977	982	5,58	$\omega(HNH)_{adenina}$
79					959	18,70	$\nu(CC)_{Cis}$
80				958	956	0,79	$\delta(CH)_{adenina}$
81				940	939	5,78	$\nu(P_{\gamma}\text{-}O\text{-}P_{\beta})$

82	922	934	2,45	$\delta(CC) + \rho(CH_2)$
83	911	911	21,37	$\nu(P_\beta\text{-}O\text{-}P_\alpha)$
84	907	900	7,24	Modos acoplados
85		900	8,52	$\delta(C{=}O)_{Cis}$
86	892	896	6,66	$\delta(CN)_{adenina}$
87	881	888	11,72	$\delta(CC)_{ribose}$
88	860	871	20,91	$\nu(CO)_{ribose}$
89		839	15,43	$\delta(CC)_{ribose}$
90	838	836	13,87	$\nu(CO)_{Cis}+ \delta(SH)$
91		832	7,11	$\rho(CH_2)_{Cis}$
92		797	1,88	$\delta(CC)_{adenina} + \delta(CN)_{adenina}$
93	780	779	32,14	$\nu(CO)$
94		762	0,70	$\delta(CO)_{Cis}$
95		760	11,03	$\nu(CS) + \delta(CC)_{Cis}$
96	750	751	6,56	$\rho(H_2O)$
97		728	23,67	$\delta(CS)$
98		723	34,53	$\nu(CN)_{adenina}$
99		706	25,49	$\delta(CC)_{ribose}$
100		701	2,91	$\delta(P_\gamma\text{-}O\text{-}P_\beta) + \delta(P_\beta\text{-}O\text{-}P_\alpha)$
101	692	680	1,29	$\nu(CC)_{adenina} + \nu(CN)_{adenina}$
102	674	671	3,06	$\rho(NH_2)_{Cis}$
103	662	662	6,26	$\delta(CN)$
104		658	9,95	$\rho(H_2O)$
105	652	651	0,42	$\delta(CN)_{adenina}$
106	643	642	8,86	$\delta(H_2O)$twist
107	622	623	9,19	$\nu(CN)_{adenina}$
108	612	610	13,79	$\delta(CO)_{ribose}$
109		606	3,40	$\delta(H_2O)$twist
110	598	594	7,55	Modos acoplados
111		572	10,96	$\nu(_2HN\text{-}Al\text{-}OP_\beta)+ \delta(H_2O\text{-}Al\text{-}OH_2) + \delta(CO\text{-}Al\text{-}OP_\gamma)$
112		571	4,15	$\delta(H_2O\text{-}Al\text{-}OH_2)+ \delta(CO\text{-}Al\text{-}OP_\gamma)$
113		568	4,16	$\nu(Al\text{-}OP_\gamma) + \delta(_2HN\text{-}Al\text{-}OP_\beta)$
114		559	3,56	$\delta(CN)_{adenina}$
115		550	22,92	$\delta(_2HN\text{-}Al) + \nu(CO\text{-}Al\text{-}OP_\gamma)$
116		547	4,01	$\delta(CO)_{ribose}$
117	520	522	5,09	$\delta(CO)$
118	511 516	514	6,41	Modos acoplados
119	509	508	3,59	$\nu(H_2O\text{-}Al\text{-}OH_2) + \delta(_2HN\text{-}Al\text{-}OP_\beta) + \delta(CO\text{-}Al\text{-}OP_\gamma)$
120	496	496	1,10	$\nu(Al\text{-}NH_2)$

121					491	1,63	$\rho(NH_2)_{adenina}$
122	475	476	472	476	476	1,62	$\delta(P_\gamma\text{-}O) + \delta(P_\beta\text{-}O) + \delta(P_\alpha\text{-}O)$
123				466	469	0,65	$\delta(P_\gamma\text{-}O) + \delta(P_\beta\text{-}O) + \delta(P_\alpha\text{-}O)$
124					460	0,65	$\nu(CO\text{-}Al\text{-}OP_\gamma) + \delta(H_2O\text{-}Al\text{-}OH_2)$
125				459	458	3,36	δ(anel) (6 membros)
126				451	451	2,08	$\delta(Al\text{-}OP_\gamma) + \delta(A\text{-}OP_\beta)$
127				440	438	1,69	$\nu(CO)_{ribose}$
128	430	427	429	431	430	3,00	$\delta(CO)_{ribose}$
129				422	424	2,83	$\nu(H_2O\text{-}Al\text{-}OH_2)$
130					417	0,91	$\nu(Al\text{-}OC) + \nu(Al\text{-}OH_2) + \delta(_2HN\text{-}Al\text{-}OP_\beta)$
131				408	413	4,51	$\nu(H_2O\text{-}Al\text{-}OH_2)$
132				405	400	1,45	$\delta(CO\text{-}Al\text{-}OP_\gamma) + \delta(H_2O\text{-}Al\text{-}OH_2) + \delta(_2HN\text{-}Al\text{-}OP_\beta)$
133				381	368	5,12	$\delta(Al\text{-}OP_\gamma) + \delta(_2HN\text{-}Al)$
134					361	1,82	$\delta(Al\text{-}OP_\beta) + \delta(Al\text{-}OP_\gamma)$
135				350	352	1,19	$\delta(CO)_{ribose}$
136				345	343	4,44	$\delta(Al\text{-}OP_\beta) + \delta(Al\text{-}OP_\gamma) + \delta(Al\text{-}OH_2)$
137				327	319	1,42	modos acoplados
138				321	317	2,29	$\nu(H_2O\text{-}Al\text{-}OH_2)$
139		310		313	312	3,01	$\nu(Al\text{-}OH_2)$
140				302	301	1,16	δ(anel) (5 membros)
141				299	299	4,31	δ(anel) (6 membros)
142				293	294	6,51	$\delta(CN)_{Cis}$
143				288	290	2,60	modos acoplados
144	283		280	284	282	1,32	modos acoplados
145				276	273	2,17	modos acoplados
146				269	268	0,95	modos acoplados
147				261	259	2,79	τ
148				253	251	0,73	$\tau(H_2O)$
149					247	0,44	$\tau(H_2O)$
150		238		243	244	0,46	τ
151				233	231	0,97	τ
152				223	223	4,38	τ
153					216	6,41	τ
154					213	5,71	τ
155					211	2,55	τ

156	204	205	204	208	203	2,55	τ
157					196	1,67	τ
158	188	190		188	185	0,80	τ
159				179	178	0,85	τ(SH)
160					174	0,62	τ
161					159	0,77	τ
162				157	157	0,59	τ
163					154	2,53	τ
164				140	142	0,39	τ
165					135	0,15	τ
166				124	130	0,63	τ
167					115	0,56	τ
168					109	0,35	τ
169		100		106	105	0,07	τ
170					93	0,13	τ
171					82	0,61	τ
172					73	0,14	τ
173					67	1,35	τ
174					59	0,91	τ
175					55	2,07	τ
176					47	5,55	τ
177					39	0,68	τ
178					34	0,79	τ
179					31	2,73	τ(adenina)
180					27	0,67	τ
181					24	8,19	τ(adenina)
182					17	2,40	τ
183					8	1,73	τ

[a] Atividades Raman foram calculadas em A^4amu.

Tabela A. 16 - Valores de coeficientes de correlação do ajuste não linear obtidos para regiões do espectro experimental entre 1700 e 100 cm^{-1}.

Regiões do ajuste não linear	Valores de coeficientes de correlação (R^2)
1700-1560	0,9995
1560-1400	0,9994
1400-1300	0,9992
1300-1200	0,9985
1200-1100	0,9999
1100-1000	0,9999
1000-900	0,9969
900-800	0,9999
800-700	0,9999
700-600	0,9999
600-500	0,9999
500-400	0,9999
400-300	0,9993
300-200	0,9999
200-100	0,9997

Tabela A.17 - Números de onda referentes à subtração manual dos espectros da água e da solução de nitrato.

Espectro	**Números de onda da água ou do nitrato (cm^{-1})**
Experimental	3410, 3380, 3355, 3335, 3300, 3250, 3235, 1050, 795, 605 e 490
Deconvoluído	3410, 3380, 3355, 3335, 3300, 3270, 3250, 3235, 1400, 1050, 795, 605 e 500
Segunda derivada	3445, 3410, 3380, 3355, 3335, 3300, 3235 e 490
Ajuste não linear	1050, 970, 795, 720, 605 e 490

Tabela A.18 - Parâmetros geométricos calculados pelo DFT:B3LYP/6-311++G(d,p) para o complexo $[AlMetPCr(H_2O)]^{1-}$ (comprimentos de ligação em Å e ângulos em graus).

Comprimentos de ligação (Å)	**$[AlMetPCr(H_2O)]^{1-}$**
C(1)-H(2)	1,089
C(1)-H(3)	1,090
C(1)-H(4)	1,095
C(1)-N(5)	1,465
N(5)-C(6)	1,356
C(6)-N(7)	1,360
C(6)-N(19)	1,332
N(19)-H(20)	1,013
N(7)-H(8)	1,012
N(7)-P(9)	1,815
P(9)-O(10)	1,576
P(9)-O(11)	1,503
P(9)-O(12)	1,535
N(5)-C(16)	1,472
C(16)-H(17)	1,087
C(16)-H(18)	1,097
C(16)-C(15)	1,566
C(15)-O(14)	1,229
C(15)-O(13)	1,295
Al-O(10)	1,856
Al-O(13)	1,909
Al-N(19)	2,053
Al-O(21)	2,047
Al-O(25)	1,884
Al-N(28)	2,066
O(21)-H(22)	1,003
O(21)-H(23)	0,962
N(28)-H(29)	1,017
N(28)-H(30)	1,019
N(28)-C(31)	1,488
C(26)-O(25)	1,294
C(26)-O(27)	1,227
C(26)-C(31)	1,544
C(31)-H(32)	1,094
C(31)-C(33)	1,534
C(33)-H(34)	1,094
C(33)-H(35)	1,092
C(33)-C(38)	1,530
C(38)-H(36)	1,092

C(38)-H(37)	1,093
C(38)-S(39)	1,839
C(40)-S(39)	1,827
C(40)-H(41)	1,090
C(40)-H(42)	1,091
C(40)-H(43)	1,091
Ângulos (graus)	**$[AlMetPCr(H_2O)]^{1-}$**
H(2)-H(3)-H(4)	60,15
C(1)-N(5)-C(6)	122,35
N(5)-C(6)-N(7)	120,66
C(6)-N(7)-P(9)	123,86
O(11)-P(9)-O(12)	119,14
O(11)-P(9)-O(10)	113,80
C(6)-N(19)-H(20)	110,17
C(6)-N(5)-C(16)	118,91
H(17)-C(16)-H(18)	105,71
N(5)-C(16)-C(15)	121,33
O(14)-C(15)-O(13)	123,17
C(15)-O(13)-Al	141,81
P(9)-O(10)-Al	124,55
O(10)-Al-O(13)	158,86
O(10)-Al-N(19)	84,10
O(10)-Al-O(21)	83,51
O(10)-Al-O(25)	99,53
O(10)-Al-N(28)	98,71
O(13)-Al-N(19)	84,98
O(13)-Al-O(21)	82,65
O(13)-Al-O(25)	95,34
O(13)-Al-N(28)	98,47
N(19)-Al-O(21)	107,70
N(19)-Al-O(25)	166,28
N(19)-Al-N(28)	85,74
O(21)-Al-O(25)	85,90
O(21)-Al-N(28)	166,55
H(22)-O(21)-H(23)	111,16
Al-O(25)-C(26)	121,55
O(25)-C(26)-O(27)	125,05
Al-N(28)-C(31)	109,59
H(29)-N(28)-H(30)	106,15
C(26)-C(31)-C(33)	114,51
H(34)-C(33)-H(35)	107,15
C(31)-C(33)-C(38)	114,55

H(36)-C(38)-H(37)	108,64
C(33)-C(38)-S(39)	109,67
C(38)-S(39)-C(40)	99,92

Tabela A.19 - Espectro vibracional Raman experimental e calculado DFT:B3LYP/6-311++G(d,p) para o complexo $[AlMetPCr(H_2O)]^{1-}$.

Nos. Modos	Número de onda experimental (cm^{-1})				Número de onda B3LYP escalonado (cm^{-1})	S_{Ra} [a]	Atribuição aproximada
	Observados	Deconvolução	2nd derivada	Ajuste não linear			
1					3804	142,80	$\nu(OH)(H_2O)$
2	3457	3457	3460		3528	129,33	$\nu(NH)_{PCr}$
3	3423	3422	3424		3496	137,50	$\nu(NH)_{PCr}$
4	3200	3200	3203		3489	88,96	$\nu_{as}(NH)(NH_2)_{Met}$
5		3189	3191		3419	214,47	$\nu_{s}(NH)(NH_2)_{Met}$
6	3167	3168	3167		3094	236,44	$\nu_{as}(CH)(CH_2)_{PCr}$
7		3160	3161		3081	179,93	$\nu(CH)(CH_3)_{Met}$
8	3146	3147	3148		3080	80,16	$\nu(CH)(CH_3)_{PCr}$
9	3128	3131	3135		3067	152,43	$\nu(CH)(CH_3)_{Met}$
10	3106	3103	3107		3049	166,91	$\nu(CH)(CH_3)_{PCr}$
11	3081	3086	3082		3047	22,35	$\nu_{as}(CH)(CH_2)_{Met}$
12	3065	3060	3063		3031	282,04	$\nu_{as}(CH)(CH_2)_{Met}$
13	3048	3044	3051		3008	93,13	$\nu(OH)(H_2O)$
14	3035	3034	3036		3008	386,29	$\nu(CH)_{Met}$
15	3022	3022	3023		2993	111,52	$\nu_{s}(CH)(CH_2)_{Met}$
16		3003	3002		2988	158,22	$\nu(CH)(CH_3)_{Met}$
17		2970	2974		2984	565,17	$\nu_{s}(CH)(CH_2)_{Met}$
18			2958		2972	540,11	$\nu(CH)(CH_3)_{PCr}$
19		2921	2923		2966	140,12	$\nu_{s}(CH)(CH_2)_{PCr}$
20	1643	1644		1669	1664	26,01	$\nu(C=O)_{Met}$
21		1611		1643	1626	25,39	$\nu(C=O)_{PCr}$
22		1596		1616	1621	7,52	$\delta(HNH)sciss_{Met}$
23		1578		1591	1603	4,38	$\delta(HOH)sciss$
24		1553		1550	1547	11,71	$\delta(CH)(CH_3)_{PCr} + \delta(NH)_{PCr}$
25				1508	1510	21,32	$\nu(C=N)_{PCr} + \delta(CH)(CH_3)_{PCr}$
26				1499	1480	8,80	$\nu(CN)_{PCr} + \delta(CH)(CH_3)_{PCr}$
27				1476	1473	22,36	$\delta(CH)(CH_3)_{PCr}$
28				1461	1459	0,89	$\delta(HCH)sciss_{Met}$
29					1450	8,13	$\delta(HCH)sciss_{PCr}$
30					1448	33,86	$\delta(CH)(CH_3)_{Met}$
31				1441	1446	12,73	$\delta(HCH)sciss_{Met}$
32	1425			1427	1437	12,44	$\delta(CH)(CH_3)_{PCr}$
33				1413	1433	22,19	$\delta(CH)(CH_3)_{Met}$
34				1394	1385	7,68	$\delta(CH)_{Met}$
35				1373	1371	6,64	$\omega(HCH)_{Met}$
36					1364	5,94	$\omega(HCH)_{PCr}$
37				1350	1335	17,43	$\delta(CH)(CH_3)_{PCr}$

38					1329	11,87	$\delta(CH)(CH_3)_{Met}$
39					1324	5,26	$\nu(CC)_{PCr}$
40					1310	8,74	$\nu(CO)_{PCr}$
41					1300	24,02	$\nu(CO)_{Met}$
42					1293	7,97	$\delta(CH_2)twist_{PCr}$
43					1279	5,25	$\omega(HCH)_{Met}$ + $\delta(CH)_{Met}$
44				1234	1266	9,42	$\nu(CN)_{PCr}$
45		1233		1223	1246	2,77	$\nu(CC)_{Met}$
46	1200	1208		1204	1196	4,77	$\nu(CN)_{PCr}$
47		1195		1191	1193	4,11	$\delta(CH_2)twist_{Met}$
48		1164		1170	1166	3,41	$\delta(NH_2)twist_{Met}$
49				1154	1163	11,60	$\nu(PO)_{PCr}$ + $\delta(CH_2)twist_{Met}$
50				1144	1130	9,64	$\delta(NH)_{PCr}$
51				1135	1119	2,29	$\delta(CH)(CH_3)_{Met}$
52		1090		1098	1117	3,79	$\omega(HNH)_{Met}$
53		1080		1087	1086	10,73	$\nu(CN)_{Met}$
54	1065	1065	1065	1064	1040	16,73	$\nu(CN)_{PCr}$
55					1029	7,07	$\nu(CC)_{Met}$
56				1037	1007	37,71	$\nu(PO)_{PCr}$
57				1010	1000	4,11	$\delta(CC)_{Met}$ + $\delta(CH)(CH_3)_{Met}$
58					963	3,35	$\delta(CS)_{Met}$
59					960	0,42	$\rho(CH_2)_{PCr}$ + $\nu(PO)_{PCr}$
60					956	6,48	$\nu(CC)_{Met}$
61				938	934	1,82	$\delta(H_2O)twist$
62					922	4,29	$\delta(CC)_{Met}$
63					903	20,02	$\delta(C=O)_{PCr}$
64				899	897	20,11	$\delta(CC)_{Met}$ + $\delta(CO)_{PCr}$
65					876	38,60	$\delta(NH)_{PCr}$
66				863	851	3,88	$\delta(C=O)_{Met}$
67				835	841	10,13	$\nu(PN)_{PCr}$ +$\delta(NH)_{PCr}$
68		814		803	817	5,40	$\delta(CO)_{Met}$
69			784	786	782	1,35	$\delta(CN)_{PCr}$
70				767	763	17,71	$\rho(CH_2)_{Met}$
71				748	743	1,13	$\delta(CN)_{PCr}$
72					732	20,40	$\rho(CH_2)_{Met}$+ $\nu(CS)_{Met}$
73				707	706	2,11	$\delta(CO)_{PCr}$
74				698	692	1,79	$\omega(HOH)$
75				672	692	35,58	$\nu(CS)_{Met}$
76				646	648	1,83	$\rho(NH_2)_{Met}$
77				628	627	7,21	$\delta(PN)_{PCr}$ +$\delta(PO)_{PCr}$
78					622	4,22	$\delta(CN)_{Met}$

79					604	0,87	$\delta(PO)_{PCr}$
80				592	588	8,28	$\nu(Al\text{-}OP) + \delta(Al\text{-}N_{PCr})$
81					566	9,17	$\nu(Al\text{-}N_{Met}) + \delta(Al\text{-}OC_{Met})$
82	562	551	560	548	560	3,12	$\delta(CC)_{PCr}$
83					529	5,48	$\nu(_{PCr}CO\text{-}Al\text{-}OP_{PCr})$
84				503	514	3,10	$\nu(H_2O\text{-}Al\text{-}N_{Met})$
85					498	5,74	$\delta(anel)_{PCr}$
86	475	476	472	475	474	4,54	$\nu(_{Met}CO\text{-}Al\text{-}N_{PCr}) + \delta(_{PCr}CO\text{-}Al\text{-}OP_{PCr}) + \delta(H_2O\text{-}Al\text{-}N_{Met})$
87			448	448	457	2,39	$\nu(Al\text{-}OC_{Met}) + \delta(Al\text{-}N_{PCr}) + \delta(Al\text{-}N_{Met})$
88	430		431	430	440	5,39	$\nu(Al\text{-}N_{PCr}) + \delta(Al\text{-}OC_{Met}) + \delta(Al\text{-}N_{Met})$
89				413	403	2,02	$\delta(anel)_{PCr}$
90		395	390	393	398	2,92	$\nu(Al\text{-}OH_2) + \delta(Al\text{-}N_{Met})$
91				383	389	8,27	$\nu(Al\text{-}OC_{PCr}) + \delta(Al\text{-}OP)$
92		364	356	366	370	2,52	$\delta(CN)_{PCr}$
93					359	2,42	$\delta(anel)_{Met}$
94				342	351	2,14	modos acoplados
95	322	323	318	321	341	1,43	$\delta(Al\text{-}N_{PCr}) + \delta(Al\text{-}OC_{PCr})$
96		303		301	306	2,65	$\delta(Al\text{-}OH_2)$
97					291	2,02	$\rho(H_2O)$
98					289	3,45	$\delta(CH)(CH_3)_{Met}$
99					284	3,39	modos acoplados
100		275		273	279	6,73	modos acoplados
101					267	1,60	modos acoplados
102	246	248	245	256	255	2,02	$\delta(CN)_{PCr}$
103	228	230	227	245	237	0,16	τ
104		216		216	218	1,07	τ
105	207	208	207	215	212	1,79	τ
106					201	1,15	τ
107					191	1,77	τ
108				187	182	1,29	τ
109				171	171	0,36	$\tau(CH_3)$

110				154	2,11	$\tau(CH_3)$
111			139	143	0,78	τ
112			126	130	0,66	τ
113				128	0,75	τ
114	109	107	108	112	0,36	τ
115				99	0,57	τ
116				91	2,06	τ
117				76	0,75	τ
118				67	2,31	τ
119				53	2,90	τ
120				44	1,95	τ
121				37	0,57	τ
122				27	0,03	τ
123				15	0,46	τ

[a] Atividades Raman foram calculadas em A^4amu.

Tabela A.20 - Valores de R^2 do ajuste não linear obtidos para regiões do espectro experimental abaixo de 1700 cm^{-1}.

Regiões do ajuste não linear	Valores de R^2 obtidos
1700-1500	0,9811
1500-1300	0,9944
1300-1100	0,9993
1100-900	0,9983
900-700	0,9997
700-500	0,9996
500-300	0,9996
300-100	0,9993

Tabela A.21 - Números de onda referentes à subtração manual dos espectros da água e da solução de nitrato.

Espectro	**Números de onda da água ou nitrato**
Experimental	3485, 3445, 3410, 3380, 3355, 3335, 3300, 3270, 3250, 3235, 1050, 795, 605 e 500
Deconvoluído	3485, 3445, 3410, 3380, 3355, 3335, 3300, 3270, 3250, 3235, 1050, 795, 605, 500 e 435
Segunda derivada	3485, 3445, 3410, 3380, 3355, 3335, 3300, 3270, 3250, 3235, 1050, 605 e 490
Ajuste não linear	1050, 970, 605 e 490

Tabela A.22 - Parâmetros geométricos calculados pelo DFT:B3LYP/6-311++G(d,p) para o complexo $[AlCisPCr(H_2O)]^{2-}$ (comprimentos de ligação em Å e ângulos em graus).

Comprimentos de ligação (Å)	**$[AlCisPCr(H_2O)]^{2-}$**
S(1)-C(2)	1,852
C(2)-H(3)	1,093
C(2)-H(4)	1,093
C(2)-C(5)	1,541
C(5)-H(6)	1,094
C(5)-N(7)	1,495
N(7)-H(8)	1,017
N(7)-H(9)	1,021
C(5)-C(10)	1,544
C(10)-O(11)	1,226
C(10)-O(12)	1,300
Al-N(7)	2,053
Al-O(12)	1,877
Al-O(14)	1,860
Al-N(21)	2,052
Al-O(29)	1,914
Al-O(32)	2,056
O(32)-H(33)	1,002
O(32)-H(34)	0,962
O(14)-P(15)	1,575
P(15)-O(16)	1,504
P(15)-O(17)	1,535
P(15)-N(18)	1,81
N(18)-H(19)	1,012
N(18)-C(20)	1,360
N(21)-C(20)	1,331
N(21)-H(22)	1,013
N(23)-C(20)	1,356
N(23)-C(24)	1,465
C(24)-H(25)	1,089
C(24)-H(26)	1,090
C(24)-H(27)	1,096
N(23)-C(28)	1,472
C(28)-H(35)	1,087
C(28)-H(36)	1,097
C(28)-C(31)	1,566
C(31)-O(29)	1,293
C(31)-O(30)	1,230
Ângulos (graus)	**$[AlCisPCr(H_2O)]^{2-}$**

S(1)-C(2)-C(5)	115,31
H(3)-C(2)-H(4)	107,12
C(2)-C(5)-C(10)	115,55
O(11)-C(10)-O(12)	123,93
N(7)-C(5)-C(10)	106,13
H(8)-N(7)-H(9)	105,32
C(5)-N(7)-Al	111,10
C(10)-O(12)-Al	122,29
N(7)-Al-O(12)	80,44
N(7)-Al-O(14)	97,93
N(7)-Al-N(21)	86,54
N(7)-Al-O(29)	100,06
N(7)-Al-O(32)	166,20
O(12)-Al-O(14)	99,50
O(12)-Al-N(21)	166,87
O(12)-Al-O(29)	95,66
O(12)-Al-O(32)	85,81
O(14)-Al-N(21)	83,97
O(14)-Al-O(29)	158,13
O(14)-Al-O(32)	83,13
N(21)-Al-O(29)	84,81
N(21)-Al-O(32)	107,23
O(29)-Al-O(32)	82,36
H(33)-O(32)-H(34)	111,22
Al-O(14)-P(15)	124,92
Al-N(21)-C(20)	102,19
Al-O(29)-C(31)	142,07
O(16)-P(15)-O(17)	118,97
P(15)-N(18)-C(20)	123,83
N(18)-C(20)-N(21)	118,27
N(18)-C(20)-N(23)	120,58
C(20)-N(23)-C(24)	122,37
H(25)-H(26)-H(27)	60,77
C(20)-N(23)-C(28)	118,98
H(35)-C(28)-H(36)	105,73
C(28)-C(31)-O(30)	114,05
O(29)-C(31)-O(30)	123,23

Tabela A.23 - Espectro vibracional Raman experimental e calculado DFT:B3LYP/6-311++G(d,p) para o complexo $[AlCisPCr(H_2O)]^{2-}$.

Nos. Modos	Número de onda experimental (cm^{-1})				Número de onda B3LYP escalonado (cm^{-1})	S_{Ra} [a]	Atribuição aproximada
	Observados	Deconvolução	2nd derivada	Ajuste não linear			
1					3809	141,96	$\nu(OH)(H_2O)$
2	3470	3471	3472		3527	126,09	$\nu(NH)_{PCr}$
3	3454	3403	3402		3497	136,12	$\nu(NH)_{PCr}$
4	3285	3321	3319		3483	110,02	$\nu_{as}(NH)(NH_2)_{Cis}$
5	3207	3217	3219		3405	214,29	$\nu_{s}(NH)(NH_2)_{Cis}$
6	3185	3179	3186		3093	237,26	$\nu_{as}(CH)(CH_2)_{PCr}$
7	3155	3155	3154		3078	81,00	$\nu(CH)(CH_3)_{PCr}$
8	3110	3110	3113		3048	170,22	$\nu(CH)(CH_3)_{PCr}$
9	3093	3092			3028	148,58	$\nu(OH)(H_2O)$
10	3019	3079			3013	69,13	$\nu(CH)_{Cis}$
11	3019	3020	3021		3002	248,38	$\nu_{as}(CH)(CH_2)_{Cis}$
12		2987	2986		2971	546,84	$\nu(CH)(CH_3)_{PCr}$
13					2970	327,08	$\nu_{s}(CH)(CH_2)_{Cis}$
14	2949	2949	2949		2964	149,60	$\nu_{s}(CH)(CH_2)_{PCr}$
15	1680	1643	1677	1679	1661	25,96	$\nu(C{=}O)_{Cis}$
16			1622	1621	1623	23,33	$\nu(C{=}O)_{PCr}$
17	1618	1618		1617	1612	7,94	$\delta(HNH)sciss_{Cis}$
18	1587	1585	1583	1584	1599	4,31	$\delta(HOH)sciss$
19	1552	1553	1555	1554	1548	12,27	$\nu(CN)_{PCr}$ + $\delta(CH)_{PCr}$
20	1530			1530	1509	21,99	$\nu(C{=}N)_{PCr}$+ $\delta(NH)_{PCr}$
21	1503			1503	1478	8,63	$\delta(CH)(CH_3)_{PCr}$
22					1472	23,11	$\delta(CH)(CH_3)_{PCr}$
23	1450			1449	1447	8,31	$\delta(HCH)sciss_{PCr}$
24					1443	24,40	$\delta(HCH)sciss_{Cis}$
25					1434	12,13	$\delta(CH)(CH_3)_{PCr}$
26				1395	1370	19,14	$\delta(CH)_{Cis}$ + $\delta(NH_2)twist_{Cis}$
27	1362			1361	1362	7,57	$\nu(CN)_{PCr}$
28				1336	1325	9,22	$\nu(CC)_{PCr}$ + $\nu(CO)_{PCr}$
29					1315	30,57	$\nu(CO)_{Cis}$ + $\delta(CH)_{Cis}$
30					1307	9,39	$\omega(HCH)_{PCr}$
31					1293	8,54	$\delta(CH_2)twist_{PCr}$
32					1280	9,18	$\nu(CC)_{Cis}$
33				1238	1263	9,39	$\nu(CN)_{PCr}$
34	1230	1231	1229	1230	1255	9,95	$\omega(HCH)_{Cis}$
35	1207	1203	1207	1205	1193	4,69	$\nu(CN)_{PCr}$+

							$\nu(PO)_{PCr}$
36				1187	1174	11,96	$\delta(CH_2)twist_{Cis}$
37	1176	1174	1176	1173	1162	14,40	$\nu(PO)_{PCr}$+ $\delta(H_2O)twist$
38	1150		1147	1151	1141	0,89	$\omega(HNH)_{Cis}$
39					1134	7,20	$\nu(CN)_{Cis}$
40				1122	1122	10,46	$\delta(CN)_{PCr}$
41					1117	2,11	$\delta(CH)(CH_3)_{PCr}$
42	1074	1067	1069	1074	1050	10,23	$\delta(CN)_{Cis}$
43					1039	17,53	$\delta(CN)_{PCr}$ + $\delta(CH)(CH_3)_{PCr}$
44					1008	34,08	$\nu(PO)_{PCr}$
45					986	5,73	$\nu(CC)_{Cis}$
46					957	0,42	$\rho(CH_2)_{PCr}$ + $\delta(CC)_{PCr}$
47				917	923	5,86	$\omega(HOH)$
48					908	43,70	$\delta(CC)_{Cis}$ + $\delta(CO)_{Cis}$
49					899	3,41	$\delta(C=O)_{PCr}$
50				880	895	11,54	$\delta(CO)_{PCr}$
51					868	36,63	$\nu(PN)_{PCr}$
52				847	849	0,99	$\rho(CH_2)_{Cis}$ + $\delta(C=O)_{Cis}$
53	818	817	816	812	824	1,74	$\delta(NH)_{PCr}$
54					779	1,62	$\delta(PN)_{PCr}$
55					772	4,20	$\nu(CS)_{Cis}$
56	751		776	745	743	1,46	$\delta(CN)_{PCr}$
57					716	20,56	$\delta(CC)_{Cis}$
58					705	2,30	$\delta(CN)_{PCr}$
59					686	1,73	$\rho(H_2O)$
60				651	660	1,95	$\rho(NH_2)_{Cis}$
61					628	6,28	$\delta(NH)_{PCr}$ + $\delta(PO)_{PCr}$
62				609	609	13,13	$\delta(CS)_{Cis}$
63					604	0,52	$\delta(CN)_{PCr}$ +$\delta(NH)_{PCr}$
64					586	17,62	ν(Al-OP) + $\delta(Al\text{-}N_{PCr})$
65					562	0,69	$\nu(PO\text{-}Al\text{-}OC_{PCr})$
66				543	550	3,19	$\delta(anel)_{Cis}$
67					528	5,72	$\delta(anel)_{PCr}$
68				517	515	2,44	$\nu(Al\text{-}N_{Cis})$ + $\delta(Al\text{-}OH_2)$
69				492	495	4,15	$\nu(Al\text{-}OC_{Cis})$ + $\delta(_{PCr}CO\text{-}Al\text{-}OP_{PCr})$
70	472	475	470	474	474	4,66	$\nu(Al\text{-}N_{PCr})$ + $\delta(_{PCr}CO\text{-}Al\text{-}OP_{PCr})$

71				454	448	1,37	$\nu(_{Cis}CO\text{-}Al\text{-}N_{PCr}) + \delta(_{Cis}N\text{-}Al\text{-}OH_2)$
72		425		436	422	2,34	$\delta(anel)_{PCr}$
73		406	415	413	405	9,70	$\delta(CH)(CH_3)_{PCr}$
74				390	384	4,82	$\nu(Al\text{-}OC_{PCr}) + \delta(Al\text{-}OP)$
75		379	371	378	370	2,95	$\delta(Al\text{-}OC_{Cis}) + \delta(Al\text{-}OC_{PCr})$
76				364	364	2,62	$\nu(Al\text{-}OH_2) + \delta(Al\text{-}N_{PCr})$
77				354	347	0,62	$\delta(Al\text{-}OH_2) + \delta(Al\text{-}OP)$
78	335	334	333	341	333	2,23	$\delta(Al\text{-}N_{PCr}) + \delta(Al\text{-}OC_{PCr})$
79		306		305	325	3,87	$\nu(_{Cis}N\text{-}Al\text{-}OH_2) + \delta(_{PCr}CO\text{-}Al\text{-}OP_{PCr}) + \delta(_{Cis}CO\text{-}Al\text{-}N_{PCr})$
80					289	2,00	$\delta(Al\text{-}OH_2) + \delta(Al\text{-}OC_{PCr})$
81	283	286	285	283	282	5,04	modos acoplados
82					277	1,49	modos acoplados
83					274	3,61	modos acoplados
84	263	263	262	265	263	0,82	modos acoplados
85		241		249	240	1,67	$\tau(H_2O)$
86				228	228	0,72	τ
87	210	211	208	210	211	0,43	τ
88				207	206	1,26	τ
89					198	0,89	τ
90	192			183	186	1,76	τ
91					177	0,78	τ
92				145	157	2,06	$\tau(CH_3)$
93				122	139	0,91	τ
94				114	128	1,23	τ
95	105		108	109	109	0,54	τ
96				102	98	1,41	τ
97					84	1,78	τ
98					66	1,65	τ
99					50	2,74	τ
100					44	1,32	τ
101					36	0,73	τ
102					27	1,95	τ

[a] Atividades Raman foram calculadas em A^4amu.

Tabela A.24 - Valores de R^2 do ajuste não linear para regiões do espectro experimental abaixo de 1700 cm^{-1}.

Regiões do ajuste não linear	Valores de R^2 obtidos
1700-1400	0,9963
1400-1200	0,9996
1200-1000	0,9925
1000-800	0,9983
800-600	0,9981
600-400	0,9999
400-200	0,9999
200-100	0,9934

Tabela A.25 - Números de onda referentes à subtração manual dos espectros da água e da solução de nitrato.

Espectro	**Números de onda da água ou nitrato**
Experimental	3445, 3410, 3380, 3335, 3300, 3270, 3250, 1640, 1400, 1050, 795, 605 e 500
Deconvoluído	3445, 3380, 3355, 3335, 3300, 3270, 3250, 3235, 1050, 795, 605 e 500
Segunda derivada	3445, 3380, 3335, 3270, 3250, 3235, 1050, 605, 490 e 435
Ajuste não linear	1050, 795, 605 e 500