Energy levels and radiative rates for transitions in Cr-like Co IV and Ni V

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Importance

Emission lines of Co IV and Ni V ions are listed in the CHIANTI Database at
`http://www.chiantidatabase.org`

Atomic Line List (v2.04) of Peter van Hoof at
`http://www.pa.uky.edu/~peter/atomic`

Emission lines of Ni V have been observed in several stars, such as Eta Carinae (η Car) and White Dwarf G191-B2B

Earlier Theoretical Works

Co IV
Stancalie: Phys. Scr. **83** (2011) 025301
136 *LS* terms, CIV3 code, limited CI, significant differences (up to 25%) with NIST energies, focus on collisional data

Ni V
Ong et al: Phys. Rev. **A 88** (2013) 052517
131 levels of ($3d^5$) 4s and 4p configurations, CI+MBPT, agreement with NIST energies within 2%, but lowest 34 levels of $3d^6$ ground configuration neglected

no A-values are reported

Earlier Experimental Works

Co IV and Ni V

Poppe et al: Physica **77** (1974) 165
Identified $3d^6\ ^5D - 3d^5(^6S)4p\ ^5P^o$ lines from laboratory spectrograph and deduced energies for other levels by some analytical expressions, which are in NIST

van het Hof et al: Phys. Scr. **44** (1991) 343
Uylings and Raassen: Phys. Scr. **54** (1996) 505

predicted energies for a few levels of $(3d^5)$ 4s and 4p, based on least square fitting of Slater-Condon parameters

GRASP Model

GRASP0: PH Norrington

`http://web.am.qub.ac.uk/DARC/`

21configurations

$3d^6$, $3d^5 4\ell$, $3d^5 5\ell$, $3d^4 4\ell^2$, $3d^4 4\ell 4\ell'$, and $3p^5 3d^7$

total 14 732 levels

Comparison of GRASP/NIST Energies (cm^{-1}) for Co IV.

Index	Configuration/Level	NIST	GRASP	ΔE	% Differences
1	$3d^6\ {}^5_4D_4$	0.0	0	0	0
2	$3d^6\ {}^5_4D_3$	639.1	562	77.1	12.1
3	$3d^6\ {}^5_4D_2$	1077.7	956	121.7	11.3
4	$3d^6\ {}^5_4D_1$	1357.3	1209	148.3	10.9
5	$3d^6\ {}^5_4D_0$	1493.6	1333	160.6	10.8
6	$3d^6\ {}^3_4P_2$	22883.3	29081	-6197.7	-27.1
7	$3d^6\ {}^3_4H_6$	23679.5	26414	-2734.5	-11.5
8	$3d^6\ {}^3_4H_5$	24031.8	26753	-2721.2	-11.3
9	$3d^6\ {}^3_4H_4$	24272.0	27008	-2736.0	-11.3
10	$3d^6\ {}^3_4P_1$	24729.2	30715	-5985.8	-24.2
11	$3d^6\ {}^3_4P_0$	25448.7	31378	-5929.3	-23.3
12	$3d^6\ {}^3_4F_4$	25396.0	30270	-4874.0	-19.2
13	$3d^6\ {}^3_4F_3$	25735.9	30592	-4856.1	-18.9
14	$3d^6\ {}^3_4F_2$	25969.0	30819	-4850.0	-18.7
15	$3d^6\ {}^3_4G_5$	29021.8	33282	-4260.2	-14.7
16	$3d^6\ {}^3_4G_4$	29592.2	33813	-4220.8	-14.3
17	$3d^6\ {}^3_4G_3$	29867.5	34080	-4212.5	-14.1
18	$3d^6\ {}^1_4I_6$	35942.7	39747	-3804.3	-10.6
19	$3d^6\ {}^3_4D_2$	36348.0	42787	-6439.0	-17.7
20	$3d^6\ {}^3_4D_1$	36382.0	42778	-6396.0	-17.6
21	$3d^6\ {}^3_4D_3$	36554.5	42939	-6384.5	-17.5

Comparison of GRASP/NIST Energies ... cont.

Index	Configuration/Level	NIST	GRASP	ΔE	% Differences
22	$3d^6\ {}^1_4G_4$	36683.3	42130	-5446.7	-14.8
23	$3d^6\ {}^1_4S_0$	41441.9	48782	-7340.1	-17.7
24	$3d^6\ {}^1_4D_2$	42341.8	52248	-9906.2	-23.4
25	$3d^6\ {}^1_4F_3$	50630.1	60097	-9466.9	-18.7
26	$3d^6\ {}^3_2P_0$	58320.6	69566	-11245.4	-19.3
27	$3d^6\ {}^3_2P_1$	58919.8	70113	-11193.2	-19.0
28	$3d^6\ {}^3_2F_2$	59748.9	69869	-10120.1	-16.9
29	$3d^6\ {}^3_2F_4$	59838.2	69966	-10127.8	-16.9
30	$3d^6\ {}^3_2F_3$	59902.8	69996	-10093.2	-16.8
31	$3d^6\ {}^3_2P_2$	60098.4	71167	-11068.6	-18.4
32	$3d^6\ {}^1_2G_4$	67907.0	79426	-11519.0	-17.0
33	$3d^5({}^6_5S)4s\ {}^7S_3$	90554.4	71035	19519.4	21.6

NIST/GRASP differences are up to 27%
and they are not systematic

FAC Models

FAC: MF Gu: Can. J. Phys. **86** (2008) 675

https://www-amdis.iaea.org/FAC/

FAC1: 1334 levels

$3d^6$, $3d^5 4\ell$, $3p^5 3d^7$, $3p^4 3d^8$, $3p^3 3d^9$, and $3p^2 3d^{10}$

FAC2: 21 992 levels

$3d^6$, $3d^5 4\ell$, $3d^5 5\ell$, $3p^6 3d^4 4\ell 4\ell'$, $3p^5 3d^7$, and $3p^4 3d^7 4\ell$

FAC3: 59 190 levels

(FAC2 $+$) $3p^4 3d^8$, $3p^3 3d^9$, $3p^2 3d^{10}$, $3p^6 3d^4 5\ell 5\ell'$, and $3p^4 3d^7 5\ell$

FAC4: 71 528 levels

(FAC3 $+$) $3p^5 3d^6 4\ell$ and $3p^5 3d^6 5\ell$

FAC5: 76 138 levels

(FAC4 $+$) $3p^3 3d^8 4\ell$, $3p^2 3d^9 4\ell$ and $3p 3d^{10} 4\ell$

Comparison of FAC/NIST Energies (cm^{-1}) for Co IV.

Index	Configuration/Level	NIST	FAC	ΔE	% Differences
1	$3d^6\ {}^5_4D_4$	0.0	0	0	0
2	$3d^6\ {}^5_4D_3$	639.1	606	77.1	5.2
3	$3d^6\ {}^5_4D_2$	1077.7	1022	121.7	5.2
4	$3d^6\ {}^5_4D_1$	1357.3	1287	148.3	5.2
5	$3d^6\ {}^5_4D_0$	1493.6	1416	160.6	5.2
6	$3d^6\ {}^3_4P_2$	22883.3	24427	-6197.7	-6.7
7	$3d^6\ {}^3_4H_6$	23679.5	27126	-2734.5	-14.6
8	$3d^6\ {}^3_4H_5$	24031.8	27457	-2721.2	-14.3
9	$3d^6\ {}^3_4H_4$	24272.0	27468	-2736.0	-13.2
10	$3d^6\ {}^3_4P_1$	24729.2	26197	-5985.8	-5.9
11	$3d^6\ {}^3_4P_0$	25448.7	26863	-5929.3	-5.6
12	$3d^6\ {}^3_4F_4$	25396.0	27890	-4874.0	-9.8
13	$3d^6\ {}^3_4F_3$	25735.9	27999	-4856.1	-8.8
14	$3d^6\ {}^3_4F_2$	25969.0	28231	-4850.0	-8.7
15	$3d^6\ {}^3_4G_5$	29021.8	32378	-4260.2	-11.6
16	$3d^6\ {}^3_4G_4$	29592.2	32891	-4220.8	-11.1
17	$3d^6\ {}^3_4G_3$	29867.5	33160	-4212.5	-11.0
18	$3d^6\ {}^1_4I_6$	35942.7	40844	-3804.3	-13.6
19	$3d^6\ {}^3_4D_2$	36348.0	39600	-6439.0	-8.9
20	$3d^6\ {}^3_4D_1$	36382.0	39612	-6396.0	-8.9
21	$3d^6\ {}^3_4D_3$	36554.5	39791	-6384.5	-8.9

Comparison of FAC/NIST Energies ... cont.

Index	Configuration/Level	NIST	FAC	ΔE	% Differences
22	$3d^6\ {}^1_4G_4$	36683.3	38839	-5446.7	-5.9
23	$3d^6\ {}^1_4S_0$	41441.9	41549	-7340.1	-0.3
24	$3d^6\ {}^1_4D_2$	42341.8	47274	-9906.2	-11.6
25	$3d^6\ {}^1_4F_3$	50630.1	56308	-9466.9	-11.2
26	$3d^6\ {}^3_2P_0$	58320.6	63400	-11245.4	-8.7
27	$3d^6\ {}^3_2P_1$	58919.8	64000	-11193.2	-8.6
28	$3d^6\ {}^3_2F_2$	59748.9	65151	-10120.1	-9.0
29	$3d^6\ {}^3_2F_4$	59838.2	64712	-10127.8	-8.1
30	$3d^6\ {}^3_2F_3$	59902.8	64725	-10093.2	-8.1
31	$3d^6\ {}^3_2P_2$	60098.4	64545	-11068.6	-7.4
32	$3d^6\ {}^1_2G_4$	67907.0	74469	-11519.0	-9.7
33	$3d^5({}^6_5S)4s\ {}^7S_3$	90554.4	59639	19519.4	34.1

NIST/FAC differences are up to 34%
– see particularly level 33
and they are not systematic

QRHF Model

QRHF: Bogdanovich and Rancova: Phys. Rev. **A 74** (2006) 052501 + **A 76** (2007) 012507

All orbitals up to $n = 8$ and one and two electron excitations from $3\ell^N$

Over 1000 configurations and levels (CSFs) exceed 10^9

568 even and 310 odd configurations selected leading to

656 832 even and 907 014 odd CSFs

Comparison of QRHF/NIST Energies (cm^{-1}) for Co IV.

Index	Configuration/Level	NIST	QRHF	ΔE	% Differences
1	$3d^6\ {}^5_4D_4$	0.0	0	0	0
2	$3d^6\ {}^5_4D_3$	639.1	636	3.1	0.5
3	$3d^6\ {}^5_4D_2$	1077.7	1076	1.7	0.2
4	$3d^6\ {}^5_4D_1$	1357.3	1358	-0.7	-0.1
5	$3d^6\ {}^5_4D_0$	1493.6	1496	-2.4	-0.2
6	$3d^6\ {}^3_4P_2$	22883.3	23613	-729.7	-3.2
7	$3d^6\ {}^3_4H_6$	23679.5	24357	-677.5	-2.9
8	$3d^6\ {}^3_4H_5$	24031.8	24717	-685.2	-2.9
9	$3d^6\ {}^3_4H_4$	24272.0	24975	-703.0	-2.9
10	$3d^6\ {}^3_4P_1$	24729.2	25379	-649.8	-2.6
11	$3d^6\ {}^3_4P_0$	25448.7	26151	-702.3	-2.8
12	$3d^6\ {}^3_4F_4$	25396.0	26081	-685.0	-2.7
13	$3d^6\ {}^3_4F_3$	25735.9	26490	-754.1	-2.9
14	$3d^6\ {}^3_4F_2$	25969.0	26721	-752.0	-2.9
15	$3d^6\ {}^3_4G_5$	29021.8	29830	-808.2	-2.8
16	$3d^6\ {}^3_4G_4$	29592.2	30399	-806.8	-2.7
17	$3d^6\ {}^3_4G_3$	29867.5	30687	-819.5	-2.7
18	$3d^6\ {}^1_4I_6$	35942.7	36999	-1056.3	-2.9
19	$3d^6\ {}^3_4D_2$	36348.0	37435	-1087.0	-3.0
20	$3d^6\ {}^3_4D_1$	36382.0	37467	-1085.0	-3.0
21	$3d^6\ {}^3_4D_3$	36554.5	37613	-1058.5	-2.9
22	$3d^6\ {}^1_4G_4$	36683.3	37727	-1043.7	-2.8

Comparison of QRHF/NIST Energies ... cont.

Index	Configuration/Level	NIST	QRHF	ΔE	% Differences
22	$3d^6\ {}^1_4G_4$	36683.3	37727	-1043.7	-2.8
23	$3d^6\ {}^1_4S_0$	41441.9	42693	-1251.1	-3.0
24	$3d^6\ {}^1_4D_2$	42341.8	43577	-1235.2	-2.9
25	$3d^6\ {}^1_4F_3$	50630.1	52124	-1493.9	-3.0
26	$3d^6\ {}^3_2P_0$	58320.6	60380	-2059.4	-3.5
27	$3d^6\ {}^3_2P_1$	58919.8	60930	-2010.2	-3.4
28	$3d^6\ {}^3_2F_2$	59748.9	61734	-1985.1	-3.3
29	$3d^6\ {}^3_2F_4$	59838.2	61739	-1900.8	-3.2
30	$3d^6\ {}^3_2F_3$	59902.8	61834	-1931.2	-3.2
31	$3d^6\ {}^3_2P_2$	60098.4	62006	-1907.6	-3.2
32	$3d^6\ {}^1_2G_4$	67907.0	70057	-2150.0	-3.2
33	$3d^5({}^6_5S)4s\ {}^7S_3$	90554.4	88117	2437.4	2.7

NIST/QRHF differences are up to 3.5% for the lowest 34 levels of $3d^6$ configuration

– but are within 1% for the remaining 288 levels of the $3d^5$ 4s and 4p configurations

Comparison of Energies for the $3d^5$ 4s and 4p levels of Co IV (cm^{-1}).

Index	Configuration/Level	Present	Earlier[a]
55	$3d^5(^4_3P)4s\ ^3P_0$	140554	141238
64	$3d^5(^2_5D)4s\ ^3D_1$	150602	151202
70	$3d^5(^4_3F)4s\ ^5F_1$	152090	152844
87	$3d^5(^4_3F)4s\ ^3F_3$	160219	160433
91	$3d^5(^2_5F)4s\ ^3F_2$	163283	163789
98	$3d^5(^2_5S)4s\ ^1S_0$	173942	173968
99	$3d^5(^2_3D)4s\ ^3D_1$	178332	178380
117	$3d^5(^4_3P)4p\ ^5D^o_0$	195340	195562.2
271	$3d^5(^2_5S)4p\ ^3P^o_0$	233747	232730.5
301	$3d^5(^2_3P)4p\ ^3P^o_0$	268904	267271.7
304	$3d^5(^2_3P)4p\ ^1S^o_0$	272355	270879.8
319	$3d^5(^2_1D)4p\ ^3P^o_1$	289735	287698.9
320	$3d^5(^2_1D)4p\ ^3P^o_0$	290083	288081.3
322	$3d^5(^2_1D)4p\ ^1P^o_1$	295845	292881.3

a: energies for the $3d^5$4s levels are of van het Hof *et al* (1991) and for $3d^5$4p are of Uylings *et al* (1996)
– no significant differences

Comparison of Energies for the $3d^5$ 4s and 4p levels of Ni V (cm^{-1}).

Index	Configuration/Level	Present	Earlier[a]
55	$3d^5(^4_3P)4s\ ^3P_0$	221924	221693
98	$3d^5(^2_5S)4s\ ^1S_0$	259591	258454
153	$3d^5(^2_3P)4s\ ^3P_2$	297781	296114
154	$3d^5(^2_3P)4s\ ^3P_1$	297821	296157
155	$3d^5(^2_3P)4s\ ^3P_0$	297848	296187
168	$3d^5(^2_3P)4s\ ^1P_0$	302675	300587
116	$3d^5(^4_3P)4p\ ^5D^o_0$	287705	287776.7
304	$3d^5(^2_3P)4p\ ^1S^o_0$	374539	373086.6
319	$3d^5(^2_1D)4p\ ^3P^o_1$	394868	393054.9
321	$3d^5(^2_1D)4p\ ^3P^o_0$	395370	393602.5
322	$3d^5(^2_1D)4p\ ^1P^o_1$	401752	399195.4

a: energies for the $3d^5$4s levels are of van het Hof *et al* (1991) and for $3d^5$4p are of Uylings *et al* (1996)
– no significant differences

Comparison of Energies for the $3d^5$ 4s levels of Ni V (cm^{-1}).

Index	Configuration	Level	NIST	QRHF	CI+MBPT	δE	τ (s)
...							
35	$3d^5(^6_5S)4s$	$^7S_3$	164525.9	163527	161376	-0.61	2.883−01
36	$3d^5(^6_5S)4s$	$^5S_2$	178019.8	177804	175638	-0.12	3.751−05
37	$3d^5(^4_5G)4s$	$^5G_6$	208046.4	207923	206960	-0.06	1.086−04
38	$3d^5(^4_5G)4s$	$^5G_5$	208131.0	208005	206965	-0.06	1.101−04
39	$3d^5(^4_5G)4s$	$^5G_4$	208163.7	208043	206930	-0.06	1.113−04
40	$3d^5(^4_5G)4s$	$^5G_2$	208151.5	208053	206820	-0.05	1.130−04
41	$3d^5(^4_5G)4s$	$^5G_3$	208164.6	208055	206873	-0.05	1.123−04
42	$3d^5(^4_3P)4s$	$^5P_3$	212095.8	212052	212267	-0.02	9.852−05
43	$3d^5(^4_3P)4s$	$^5P_2$	212253.4	212184	212451	-0.03	9.939−05
44	$3d^5(^4_3P)4s$	$^5P_1$	212455.7	212346	212727	-0.05	9.991−05
45	$3d^5(^4_5D)4s$	$^5D_4$	216189.9	216154	215975	-0.02	9.248−05
46	$3d^5(^4_5D)4s$	$^5D_0$	216305.7	216290		-0.01	9.314−05
47	$3d^5(^4_5D)4s$	$^5D_1$	216434.7	216382	216201	-0.02	9.320−05
48	$3d^5(^4_5D)4s$	$^5D_3$	216596.0	216481	216518	-0.05	9.330−05
49	$3d^5(^4_5D)4s$	$^5D_2$	216590.5	216491	216469	-0.05	9.334−05
50	$3d^5(^4_5G)4s$	$^3G_5$	217048.7	217525	216442	0.22	3.674−05
51	$3d^5(^4_5G)4s$	$^3G_4$	217129.1	217613	216431	0.22	3.673−05
52	$3d^5(^4_5G)4s$	$^3G_3$	217101.0	217615	216298	0.24	3.668−05
53	$3d^5(^4_3P)4s$	$^3P_2$	221087.6	221648	221778	0.25	3.475−05
54	$3d^5(^4_3P)4s$	$^3P_1$	221429.0	221924	222149	0.22	3.470−05
...							

CI+MBPT: energies of Ong et al (2013)
– no significant differences

Conclusions

- Energies for the $3d^6$ levels of Co IV and Ni V are accurate to $\sim$3%, but better than 1% for the remaining 288 levels of the ($3d^5$) 4s and 4p configurations. Therefore, scope remains for improvement.
- Energies for 26 levels of Co IV and 12 of Ni V are predicted, which are not in the NIST database.
- Measurements of energies for Cr-like ions has been useful in improving theoretical results. Measurements for a few more levels will be further helpful in improving theory.
- For some ions such as Cr-like, large calculations from QRHF (or other similar codes) are necessary.

Conclusions ... cont.

- If differences between theoretical results and/or with measurements are significant, do not ignore.
- Detailed results will be available in ADNDT **107** (2016) 000 also see – http://arxiv.org/abs/1509.07648
- Further calculations for Ω and Υ will be welcome.