

**Supporting Information**

**Cobalt complexes with hemilabile o-  
iminobenzoquinonate ligands: a novel example of  
redox-induced electron transfer**

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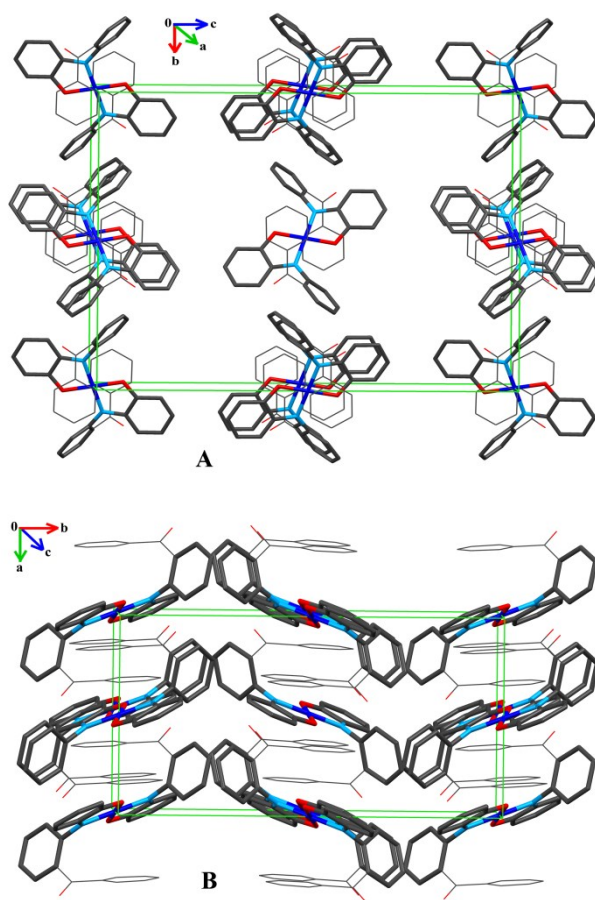
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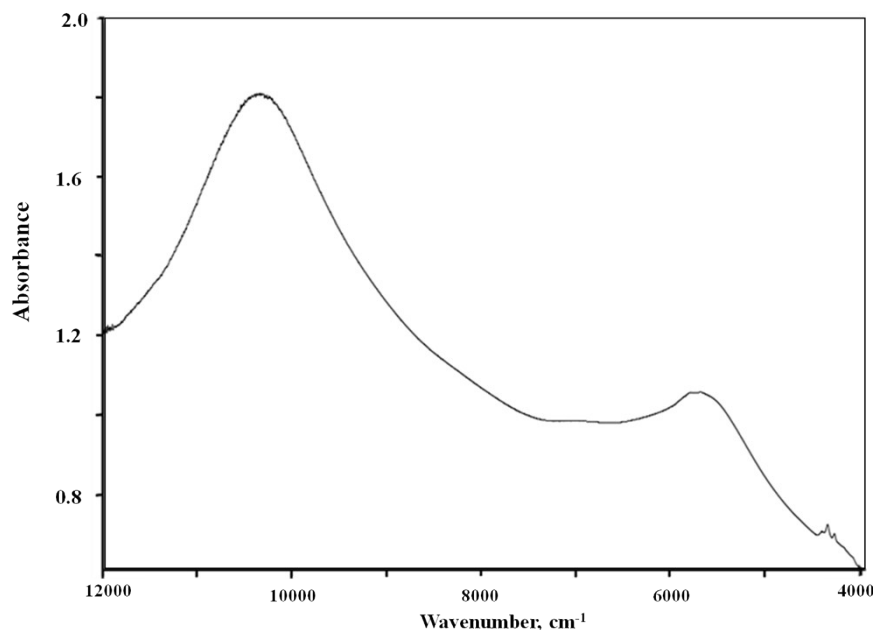
**Figure S1.** Fragment of unit cell of complex **1**. Hydrogen atoms and *tert*-butyl groups are omitted for clarity.



**Table S1.** X-Ray crystallographic data and structure refinement for **1** and **2**.

	C <sub>54</sub> H <sub>58</sub> CoN <sub>2</sub> O <sub>4</sub>	C <sub>69</sub> H <sub>74</sub> CoF <sub>3</sub> N <sub>2</sub> O <sub>7</sub> S
Formula weight	857.95	1191.29
Crystal system	Orthorhombic	Monoclinic
Space group	Pbca	P2(1)/c
Unit cell dimensions		
a (Å)	9.8173(5)	15.8911(4)
b (Å)	18.7393(10)	10.2319(3)
c (Å)	24.5585(13)	38.2603(17)
α (deg)	90	90
β (deg)	90	98.395(3)
γ (deg)	90	90
V (Å <sup>3</sup> )	4518.0(4)	6154.3(4)
Z	4	4
ρ <sub>calcd</sub> (g/cm <sup>3</sup> )	1.261	1.286
Absorption coefficient (mm <sup>-1</sup> )	0.428	0.377
F(000)	1820	2512
Crystal size (mm <sup>3</sup> )	0.380 x 0.200 x 0.090	0.430 x 0.150 x 0.120
Θ range for data collection (deg)	2.326 - 30.000	2.977 - 25.000
Reflections collected	60621	44241
Indep reflections	6590 [R <sub>int</sub> = 0.0296]	10800 [R <sub>int</sub> = 0.1152]
Completeness to Θ max	99.9 %	99.6 %
Data/ restraints/parameters	6590 / 0 / 283	10800 / 385 / 875
Final R indices [I>2σ(I)]	R1 = 0.0361 wR2 = 0.0934	R1 = 0.0847 wR2 = 0.1813
R indices (all data)	R1 = 0.0420 wR2 = 0.0964	R1 = 0.1395 wR2 = 0.2100
GOF on F <sup>2</sup>	1.038	1.063
Largest diff. peak and hole (e/Å <sup>3</sup> )	0.546/-0.209	0.861/ -0.529

**Figure S2.** The data of NIR-spectroscopy for complex **1** in Nijol.



**Table S2.** Spin states (S), total energies without ( $E_{\text{total}}$ ) and with ( $E_{\text{total}}^{\text{ZPE}}$ ) taking into account for energies of zero-point harmonic vibrations (given in a.u.), relative energies without ( $\Delta E$ ) and with ( $\Delta E^{\text{ZPE}}$ ) taking into account for energies of zero-point harmonic vibrations (given in kcal/mol), spin density at the metal center ( $q_s^{\text{Co}}$ , given in a.u.), expectation values of the spin-squared operator ( $S^2$ ) and exchange spin coupling constants (J, given in  $\text{cm}^{-1}$ ) of the isomeric forms of the complexes **1** and **2** calculated by the DFT B3LYP\*/6-311++G(d,p) method.

Structure	S	$E_{\text{total}}$	$E_{\text{total}}^{\text{ZPE}}$	$\Delta E$	$\Delta E^{\text{ZPE}}$	$q_s^{\text{Co}}$	$S^2$	$J_{\text{Co-ISQ}}$	$J_{\text{ISQ-ISQ}}$
<b>1a</b>	3/2	-3866.398281	-3865.445145	0.0	0.0	1.21	3.771	-307	–
BS $\beta\alpha^*$	1/2	-3866.406091					0.977		
<b>1b</b>	5/2	-3866.388936	-3865.436799	5.9	5.2	2.62	8.772	-260	17
BS $\beta\alpha\alpha$	3/2	-3866.396420					4.570		
BS $\alpha\beta\alpha$	1/2	-3866.404207					2.330		
<b>1c</b>	5/2	-3866.387485	-3865.435858	6.8	5.8	2.52	8.768	–	–
<b>2a</b>	4/2	-3866.220359	-3865.263792	0.0	0.0	2.58	6.014	-295	–
BS $\beta\alpha$	2/2	-3866.228807					2.870		
<b>2b</b>	4/2	-3866.210090	-3865.254864	6.4	5.6	1.73	6.036	-508	-345
BS $\beta\alpha\alpha$	2/2	-3866.224916					2.056		
BS $\alpha\beta\alpha$	0	-3866.225401					1.172		

\* $\alpha$  corresponds to the spin-up orientation,  $\beta$  corresponds to the spin-down orientation

**Table S3.** Calculated atomic coordinates of the isomeric forms of the complexes **1** and **2** (DFT B3LYP\*/6-311++G(d,p)).

<b>1a Cat-<sub>IS</sub>Co<sup>III</sup>-ISQ</b>			
27	-0.000014000	0.000021000	-0.000012000
8	-1.124252000	1.494521000	0.276146000
7	-1.636253000	-0.917484000	-0.426705000
6	-2.415629000	1.267439000	0.008514000
8	-4.334425000	-3.136049000	1.588091000
6	-2.742143000	-0.089339000	-0.404064000
6	-4.077176000	-0.439244000	-0.762875000
1	-4.289477000	-1.465683000	-1.083048000
6	-5.093606000	0.522111000	-0.702403000
6	-4.749866000	1.844745000	-0.261290000
1	-5.552140000	2.585136000	-0.206644000
6	-3.450528000	2.257357000	0.102699000
6	-6.556267000	0.128170000	-1.079062000
6	-7.520567000	1.354441000	-1.108147000
1	-7.617218000	1.833524000	-0.112913000
1	-8.533025000	1.018148000	-1.410259000
1	-7.191793000	2.124025000	-1.836390000
6	-6.580606000	-0.531964000	-2.499700000
1	-7.620446000	-0.806175000	-2.773861000
1	-5.970369000	-1.454946000	-2.540526000
1	-6.194115000	0.167454000	-3.269067000
6	-7.094954000	-0.896157000	-0.021847000
1	-7.116986000	-0.441992000	0.989857000
1	-6.463546000	-1.803937000	0.034098000
1	-8.128740000	-1.207446000	-0.281469000
6	-3.156001000	3.704179000	0.604194000
6	-4.428566000	4.607097000	0.584398000
1	-5.229685000	4.218530000	1.245672000
1	-4.842917000	4.722648000	-0.438155000
1	-4.159164000	5.618485000	0.950323000
6	-2.077977000	4.387585000	-0.303815000
1	-2.422600000	4.430648000	-1.357823000
1	-1.119284000	3.842239000	-0.265772000
1	-1.898727000	5.428003000	0.038766000
6	-2.640506000	3.637394000	2.082584000
1	-3.414282000	3.199119000	2.745964000
1	-2.409261000	4.658701000	2.451889000
1	-1.725058000	3.024421000	2.158546000
6	-1.789018000	-2.309068000	-0.755253000
6	-2.480874000	-3.223967000	0.093985000
6	-2.643901000	-4.567347000	-0.331380000
1	-3.204507000	-5.255594000	0.316067000
6	-2.103503000	-5.017013000	-1.548950000
1	-2.229254000	-6.065703000	-1.852513000
6	-1.406457000	-4.111520000	-2.377300000
1	-0.985204000	-4.448015000	-3.335218000

6	-1.254955000	-2.770391000	-1.983303000
1	-0.730742000	-2.051712000	-2.626834000
6	-3.145652000	-2.843378000	1.417733000
6	-2.346106000	-2.192756000	2.525232000
6	-0.931675000	-2.261339000	2.573007000
1	-0.376752000	-2.755469000	1.765586000
6	-0.231165000	-1.711399000	3.666440000
1	0.865203000	-1.780036000	3.701895000
6	-0.936181000	-1.075495000	4.709335000
1	-0.388645000	-0.643393000	5.559525000
6	-2.347124000	-0.997464000	4.664291000
1	-2.896834000	-0.501211000	5.476779000
6	-3.048808000	-1.561460000	3.584522000
1	-4.145512000	-1.527203000	3.541939000
8	1.124236000	-1.494473000	-0.276213000
7	1.636240000	0.917522000	0.426697000
6	2.415599000	-1.267396000	-0.008571000
8	4.334435000	3.136219000	-1.588016000
6	2.742124000	0.089378000	0.404029000
6	4.077168000	0.439262000	0.762839000
1	4.289480000	1.465689000	1.083038000
6	5.093587000	-0.522101000	0.702343000
6	4.749829000	-1.844734000	0.261227000
1	5.552096000	-2.585133000	0.206590000
6	3.450489000	-2.257328000	-0.102756000
6	6.556258000	-0.128191000	1.078991000
6	7.520482000	-1.354518000	1.108270000
1	7.617128000	-1.833747000	0.113107000
1	8.532953000	-1.018244000	1.410359000
1	7.191642000	-2.123978000	1.836614000
6	6.580605000	0.532138000	2.499538000
1	7.620455000	0.806329000	2.773679000
1	5.970422000	1.455161000	2.540225000
1	6.194062000	-0.167151000	3.268996000
6	7.095027000	0.895958000	0.021643000
1	7.117042000	0.441654000	-0.989998000
1	6.463679000	1.803771000	-0.034431000
1	8.128831000	1.207213000	0.281235000
6	3.155911000	-3.704145000	-0.604228000
6	4.428440000	-4.607114000	-0.584444000
1	5.229567000	-4.218577000	-1.245725000
1	4.842795000	-4.722682000	0.438106000
1	4.158995000	-5.618490000	-0.950368000
6	2.077876000	-4.387492000	0.303812000
1	2.422522000	-4.430562000	1.357813000
1	1.119207000	-3.842099000	0.265788000
1	1.898564000	-5.427904000	-0.038754000
6	2.640384000	-3.637358000	-2.082605000
1	3.414155000	-3.199110000	-2.746008000
1	2.409101000	-4.658661000	-2.451898000
1	1.724950000	-3.024360000	-2.158550000
6	1.788998000	2.309100000	0.755276000

6	2.480858000	3.224022000	-0.093934000
6	2.643858000	4.567396000	0.331455000
1	3.204472000	5.255658000	-0.315970000
6	2.103435000	5.017036000	1.549023000
1	2.229172000	6.065722000	1.852606000
6	1.406384000	4.111522000	2.377345000
1	0.985106000	4.447994000	3.335260000
6	1.254903000	2.770397000	1.983321000
1	0.730678000	2.051704000	2.626828000
6	3.145682000	2.843458000	-1.417668000
6	2.346213000	2.192730000	-2.525159000
6	0.931773000	2.261145000	-2.572934000
1	0.376790000	2.755208000	-1.765513000
6	0.231326000	1.711110000	-3.666360000
1	-0.865050000	1.779617000	-3.701814000
6	0.936417000	1.075279000	-4.709249000
1	0.388934000	0.643103000	-5.559434000
6	2.347369000	0.997412000	-4.664203000
1	2.897135000	0.501210000	-5.476684000
6	3.048988000	1.561502000	-3.584441000
1	4.145696000	1.527374000	-3.541860000

**1b ISQ<sub>-HS</sub>Co<sup>II</sup>-ISQ**

27	-0.526302000	0.342285000	-0.505971000
8	-2.012912000	1.679041000	-0.352558000
7	-2.101843000	-1.000790000	-0.488439000
6	-3.201959000	1.125116000	-0.261921000
8	-1.458524000	-2.207894000	2.083733000
6	-3.293878000	-0.355516000	-0.344450000
6	-4.573750000	-0.995643000	-0.233008000
1	-4.604475000	-2.091695000	-0.254307000
6	-5.737667000	-0.250955000	-0.059417000
6	-5.624496000	1.187868000	-0.006780000
1	-6.545402000	1.762719000	0.122414000
6	-4.417376000	1.895465000	-0.097892000
6	-7.110372000	-0.977820000	0.099050000
6	-8.306493000	0.013829000	0.240153000
1	-8.213448000	0.652915000	1.141468000
1	-9.250197000	-0.560162000	0.337301000
1	-8.407279000	0.672542000	-0.646433000
6	-7.375564000	-1.876649000	-1.156722000
1	-8.348549000	-2.401154000	-1.054674000
1	-6.589247000	-2.645804000	-1.286482000
1	-7.409317000	-1.264697000	-2.081190000
6	-7.072615000	-1.878434000	1.381298000
1	-6.888385000	-1.267439000	2.288148000
1	-6.273722000	-2.643230000	1.322095000
1	-8.041481000	-2.405075000	1.509912000
6	-4.365535000	3.453034000	-0.027361000
6	-5.781702000	4.083378000	0.152743000
1	-6.266526000	3.759695000	1.096527000
1	-6.459179000	3.840523000	-0.691492000



1	-5.683589000	5.187089000	0.192251000
6	-3.762796000	4.020445000	-1.358780000
1	-4.403275000	3.750470000	-2.223902000
1	-2.748245000	3.623277000	-1.539119000
1	-3.706531000	5.128225000	-1.308222000
6	-3.490330000	3.903857000	1.192577000
1	-3.925991000	3.533630000	2.143445000
1	-3.453422000	5.012369000	1.242801000
1	-2.457649000	3.521810000	1.112328000
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6	-1.331983000	-3.329166000	-0.032008000
6	-1.228021000	-4.672455000	-0.479273000
1	-0.700779000	-5.402482000	0.149572000
6	-1.815026000	-5.092698000	-1.686351000
1	-1.732889000	-6.141122000	-2.004219000
6	-2.502396000	-4.152880000	-2.483748000
1	-2.948545000	-4.459406000	-3.440795000
6	-2.611253000	-2.815508000	-2.064323000
1	-3.122270000	-2.076130000	-2.695957000
6	-0.808692000	-2.957089000	1.343686000
6	0.508704000	-3.543755000	1.819532000
6	1.555652000	-3.886577000	0.926558000
1	1.421123000	-3.753102000	-0.155020000
6	2.782692000	-4.371111000	1.423618000
1	3.594542000	-4.618429000	0.725346000
6	2.968605000	-4.534141000	2.812064000
1	3.922505000	-4.921946000	3.197556000
6	1.930689000	-4.193004000	3.708400000
1	2.075447000	-4.317454000	4.790976000
6	0.713421000	-3.689763000	3.216358000
1	-0.097079000	-3.404673000	3.900516000
8	0.862051000	-0.196130000	-1.850829000
7	1.123170000	0.636052000	0.679070000
6	2.076975000	-0.216218000	-1.350428000
8	4.006230000	3.400110000	1.713881000
6	2.266322000	0.223306000	0.053707000
6	3.569615000	0.152110000	0.654781000
1	3.670422000	0.433642000	1.707392000
6	4.668568000	-0.278696000	-0.079919000
6	4.466930000	-0.653361000	-1.464266000
1	5.348997000	-0.974983000	-2.029025000
6	3.230974000	-0.643946000	-2.118704000
6	6.100175000	-0.369513000	0.523973000
6	6.626143000	-1.841751000	0.414252000
1	6.676790000	-2.191107000	-0.636151000
1	7.647700000	-1.914454000	0.842276000
1	5.967478000	-2.536362000	0.974381000
6	6.135491000	0.050638000	2.025077000
1	7.174998000	-0.024228000	2.404508000
1	5.797779000	1.096017000	2.169704000
1	5.503489000	-0.611621000	2.651312000
6	7.057840000	0.584689000	-0.270297000

1	7.111756000	0.321280000	-1.345357000
1	6.717290000	1.636461000	-0.190701000
1	8.085808000	0.523099000	0.143994000
6	3.072351000	-1.072005000	-3.610511000
6	4.436577000	-1.472025000	-4.253694000
1	5.162237000	-0.632968000	-4.249894000
1	4.901989000	-2.340603000	-3.743793000
1	4.267830000	-1.760132000	-5.311009000
6	2.118038000	-2.311808000	-3.712413000
1	2.536718000	-3.174596000	-3.153114000
1	1.115387000	-2.082798000	-3.310084000
1	2.008573000	-2.617765000	-4.774207000
6	2.485078000	0.117816000	-4.446050000
1	3.161692000	0.996089000	-4.404200000
1	2.381581000	-0.183953000	-5.509662000
1	1.492606000	0.422733000	-4.070060000
6	1.112369000	1.274473000	1.953322000
6	1.904084000	2.424336000	2.282638000
6	1.825939000	2.959470000	3.594070000
1	2.459017000	3.823523000	3.838611000
6	0.951798000	2.424284000	4.556388000
1	0.897353000	2.869840000	5.559445000
6	0.143673000	1.317660000	4.216499000
1	-0.547273000	0.886341000	4.954900000
6	0.224779000	0.749629000	2.934129000
1	-0.380813000	-0.131977000	2.681717000
6	2.856120000	3.149440000	1.333382000
6	2.371442000	3.643642000	-0.013755000
6	0.995475000	3.804079000	-0.312718000
1	0.232845000	3.528985000	0.427652000
6	0.597330000	4.338401000	-1.555191000
1	-0.471241000	4.466901000	-1.774340000
6	1.567156000	4.704240000	-2.511543000
1	1.253932000	5.114054000	-3.482651000
6	2.941011000	4.545481000	-2.220853000
1	3.697814000	4.830410000	-2.965699000
6	3.340731000	4.026587000	-0.976977000
1	4.403578000	3.911155000	-0.727124000

**1c** ISQ<sub>-HS</sub>Co<sup>II</sup>-ISQ

27	-0.000039000	-0.000014000	-0.000031000
8	1.271982000	1.543257000	-0.198809000
7	1.784056000	-0.952748000	0.445588000
6	2.536664000	1.276022000	0.046558000
8	4.367507000	-3.101822000	-1.825902000
6	2.866072000	-0.116774000	0.415474000
6	4.217015000	-0.473280000	0.728056000
1	4.432158000	-1.510831000	1.009616000
6	5.235803000	0.479807000	0.677170000
6	4.892948000	1.825751000	0.290729000
1	5.702054000	2.559409000	0.245203000
6	3.595399000	2.258329000	-0.026486000

6	6.704976000	0.065065000	1.003733000
6	7.677114000	1.284410000	1.060093000
1	7.755740000	1.802203000	0.082859000
1	8.693631000	0.930863000	1.326711000
1	7.369013000	2.026299000	1.825174000
6	6.759444000	-0.652894000	2.395210000
1	7.804221000	-0.941960000	2.632846000
1	6.145874000	-1.574292000	2.413040000
1	6.394939000	0.016012000	3.201533000
6	7.212924000	-0.917600000	-0.107072000
1	7.209612000	-0.424432000	-1.100563000
1	6.577741000	-1.821447000	-0.181027000
1	8.252297000	-1.240610000	0.112781000
6	3.296158000	3.728631000	-0.452962000
6	4.582188000	4.612471000	-0.463070000
1	5.342343000	4.237824000	-1.178758000
1	5.049797000	4.682588000	0.540450000
1	4.311233000	5.641206000	-0.775521000
6	2.279990000	4.383947000	0.543886000
1	2.686919000	4.384652000	1.576327000
1	1.316506000	3.845330000	0.542489000
1	2.088798000	5.437725000	0.251982000
6	2.698000000	3.742211000	-1.901875000
1	3.418069000	3.307854000	-2.625810000
1	2.486395000	4.786650000	-2.213796000
1	1.757177000	3.166118000	-1.951502000
6	1.951906000	-2.352436000	0.701425000
6	2.609687000	-3.228937000	-0.215787000
6	2.771073000	-4.595406000	0.128786000
1	3.304548000	-5.250471000	-0.573807000
6	2.256133000	-5.109460000	1.331767000
1	2.377893000	-6.174638000	1.572690000
6	1.582501000	-4.246446000	2.223017000
1	1.175266000	-4.634197000	3.167681000
6	1.435575000	-2.883312000	1.910635000
1	0.928553000	-2.201418000	2.606729000
6	3.206467000	-2.783026000	-1.547525000
6	2.357101000	-2.026314000	-2.550008000
6	0.940170000	-2.074686000	-2.523450000
1	0.422946000	-2.643395000	-1.739534000
6	0.188149000	-1.419045000	-3.520917000
1	-0.909325000	-1.476666000	-3.502814000
6	0.844817000	-0.699227000	-4.541940000
1	0.258047000	-0.186242000	-5.317634000
6	2.256339000	-0.645194000	-4.571657000
1	2.768548000	-0.085728000	-5.367373000
6	3.008481000	-1.313092000	-3.587887000
1	4.106316000	-1.296770000	-3.606890000
8	-1.272075000	-1.543265000	0.198738000
7	-1.784131000	0.952755000	-0.445615000
6	-2.536760000	-1.276012000	-0.046596000
8	-4.367271000	3.101952000	1.826210000

6	-2.866158000	0.116796000	-0.415483000
6	-4.217103000	0.473325000	-0.728027000
1	-4.432239000	1.510885000	-1.009559000
6	-5.235905000	-0.479748000	-0.677130000
6	-4.893059000	-1.825702000	-0.290717000
1	-5.702173000	-2.559351000	-0.245175000
6	-3.595509000	-2.258303000	0.026458000
6	-6.705086000	-0.064976000	-1.003619000
6	-7.677231000	-1.284314000	-1.060027000
1	-7.755847000	-1.802159000	-0.082820000
1	-8.693751000	-0.930748000	-1.326610000
1	-7.369145000	-2.026164000	-1.825152000
6	-6.759606000	0.653078000	-2.395045000
1	-7.804392000	0.942167000	-2.632614000
1	-6.146034000	1.574475000	-2.412838000
1	-6.395141000	-0.015776000	-3.201430000
6	-7.212984000	0.917619000	0.107271000
1	-7.209643000	0.424384000	1.100729000
1	-6.577785000	1.821452000	0.181260000
1	-8.252360000	1.240657000	-0.112524000
6	-3.296296000	-3.728616000	0.452908000
6	-4.582345000	-4.612427000	0.462944000
1	-5.342529000	-4.237763000	1.178592000
1	-5.049902000	-4.682526000	-0.540602000
1	-4.311431000	-5.641169000	0.775405000
6	-2.280107000	-4.383926000	-0.543922000
1	-2.687002000	-4.384599000	-1.576378000
1	-1.316615000	-3.845326000	-0.542480000
1	-2.088942000	-5.437714000	-0.252039000
6	-2.698195000	-3.742244000	1.901846000
1	-3.418278000	-3.307878000	2.625762000
1	-2.486637000	-4.786697000	2.213755000
1	-1.757354000	-3.166186000	1.951520000
6	-1.951973000	2.352450000	-0.701422000
6	-2.609660000	3.228950000	0.215857000
6	-2.771028000	4.595433000	-0.128671000
1	-3.304425000	5.250499000	0.573981000
6	-2.256169000	5.109496000	-1.331682000
1	-2.377916000	6.174683000	-1.572573000
6	-1.582627000	4.246482000	-2.223000000
1	-1.175450000	4.634242000	-3.167685000
6	-1.435712000	2.883337000	-1.910657000
1	-0.928755000	2.201445000	-2.606799000
6	-3.206312000	2.783026000	1.547645000
6	-2.356861000	2.026230000	2.549992000
6	-0.939928000	2.074428000	2.523176000
1	-0.422777000	2.643054000	1.739150000
6	-0.187807000	1.418713000	3.520518000
1	0.909671000	1.476197000	3.502213000
6	-0.844378000	0.698994000	4.541672000
1	-0.257530000	0.185952000	5.317270000
6	-2.255902000	0.645130000	4.571644000

1	-2.768034000	0.085737000	5.367461000
6	-3.008141000	1.313101000	3.587998000
1	-4.105974000	1.296909000	3.607197000

**2a** IQ<sub>-HS</sub>Co<sup>II</sup>-ISQ<sup>+</sup>

27	-0.000413000	-0.000369000	0.260019000
8	0.931143000	1.702202000	-0.586554000
8	0.766176000	-1.142844000	1.937870000
8	-0.930869000	-1.702120000	-0.587364000
8	-0.764677000	1.143223000	1.937917000
7	1.828238000	-0.750527000	-0.559470000
7	-1.828468000	0.750748000	-0.559282000
6	2.116258000	1.553607000	-1.049788000
6	2.682507000	0.160236000	-1.050729000
6	4.044392000	-0.063245000	-1.480168000
1	4.454249000	-1.075308000	-1.414758000
6	4.816883000	0.992467000	-1.930733000
6	4.226169000	2.330465000	-1.969954000
1	4.866668000	3.137108000	-2.341508000
6	2.943135000	2.655993000	-1.555840000
6	6.291895000	0.828185000	-2.387754000
6	6.783232000	-0.647028000	-2.286354000
1	6.747827000	-1.025013000	-1.244467000
1	7.836160000	-0.709292000	-2.625081000
1	6.188155000	-1.327663000	-2.928471000
6	6.422165000	1.288128000	-3.882118000
1	6.137888000	2.349310000	-4.022905000
1	5.782539000	0.671417000	-4.545307000
1	7.472981000	1.177292000	-4.218191000
6	7.216760000	1.716942000	-1.484485000
1	6.958236000	2.792221000	-1.545432000
1	8.272037000	1.609086000	-1.807379000
1	7.149324000	1.408137000	-0.421776000
6	2.393813000	4.112008000	-1.599641000
6	2.008778000	4.579211000	-0.152984000
1	1.217877000	3.944402000	0.283624000
1	1.639862000	5.624967000	-0.185075000
1	2.893118000	4.552820000	0.516348000
6	3.449465000	5.116785000	-2.156129000
1	3.008791000	6.133246000	-2.167443000
1	3.749946000	4.876957000	-3.196507000
1	4.360725000	5.160010000	-1.525346000
6	1.139895000	4.167618000	-2.537677000
1	0.334354000	3.503953000	-2.178560000
1	1.410388000	3.869461000	-3.571539000
1	0.745316000	5.203647000	-2.575440000
6	2.132128000	-2.134083000	-0.504089000
6	2.537981000	-2.843263000	-1.664553000
1	2.632486000	-2.298077000	-2.612776000
6	2.763987000	-4.230176000	-1.621727000
1	3.057592000	-4.759127000	-2.539335000
6	2.594338000	-4.943106000	-0.415592000

1	2.754594000	-6.028935000	-0.383097000
6	2.206065000	-4.253906000	0.745544000
1	2.055346000	-4.811225000	1.678331000
6	1.969303000	-2.851581000	0.731269000
6	1.512913000	-2.154459000	1.979368000
6	1.929684000	-2.655415000	3.334775000
6	3.198562000	-3.252078000	3.564876000
1	3.903756000	-3.386326000	2.734383000
6	3.574332000	-3.636084000	4.866723000
1	4.564395000	-4.079279000	5.040921000
6	2.682524000	-3.450188000	5.943884000
1	2.973086000	-3.763174000	6.956507000
6	1.418893000	-2.856682000	5.723577000
1	0.725191000	-2.713169000	6.563465000
6	1.049889000	-2.445555000	4.431645000
1	0.078582000	-1.967389000	4.250037000
6	-2.116584000	-1.553431000	-1.049962000
6	-2.682762000	-0.160336000	-1.050679000
6	-2.132420000	2.134109000	-0.503614000
6	-2.539351000	2.843467000	-1.663670000
1	-2.634565000	2.298377000	-2.611875000
6	-2.765557000	4.230308000	-1.620535000
1	-3.059986000	4.759282000	-2.537872000
6	-2.595088000	4.943210000	-0.414469000
1	-2.755505000	6.029008000	-0.381766000
6	-2.205834000	4.253954000	0.746279000
1	-2.054521000	4.811202000	1.679017000
6	-1.968849000	2.851644000	0.731714000
6	-1.511730000	2.154644000	1.979548000
6	-1.928127000	2.655488000	3.335143000
6	-1.047815000	2.445961000	4.431664000
1	-0.076411000	1.968141000	4.249660000
6	-1.416434000	2.856960000	5.723745000
1	-0.722335000	2.713707000	6.563350000
6	-2.680197000	3.449999000	5.944572000
1	-2.970461000	3.762876000	6.957315000
6	-3.572507000	3.635556000	4.867774000
1	-4.562668000	4.078377000	5.042367000
6	-3.197126000	3.251676000	3.565772000
1	-3.902706000	3.385654000	2.735564000
6	-4.044685000	0.063106000	-1.479685000
1	-4.454518000	1.075170000	-1.414205000
6	-4.817492000	-0.992635000	-1.929923000
6	-4.226933000	-2.330506000	-1.969014000
1	-4.867511000	-3.137298000	-2.340096000
6	-2.943626000	-2.655829000	-1.555201000
6	-6.292661000	-0.828188000	-2.386481000
6	-6.783904000	0.647026000	-2.284649000
1	-6.748258000	1.024771000	-1.242683000
1	-7.836900000	0.709436000	-2.623152000
1	-6.188909000	1.327780000	-2.926719000
6	-6.423418000	-1.287815000	-3.880893000

1	-6.139252000	-2.348992000	-4.021938000
1	-5.783897000	-0.671047000	-4.544134000
1	-7.474312000	-1.176822000	-4.216688000
6	-7.217341000	-1.717058000	-1.483147000
1	-6.958824000	-2.792324000	-1.544347000
1	-8.272706000	-1.609134000	-1.805743000
1	-7.149613000	-1.408443000	-0.420400000
6	-2.394396000	-4.111922000	-1.598768000
6	-2.008615000	-4.578608000	-0.152149000
1	-1.217565000	-3.943551000	0.283834000
1	-1.639663000	-5.624364000	-0.184005000
1	-2.892637000	-4.551995000	0.517595000
6	-3.450344000	-5.116936000	-2.154285000
1	-3.009669000	-6.133404000	-2.165407000
1	-3.751380000	-4.877543000	-3.194601000
1	-4.361274000	-5.159892000	-1.523012000
6	-1.140994000	-4.167967000	-2.537456000
1	-0.335320000	-3.504073000	-2.179056000
1	-1.412069000	-3.870260000	-3.571297000
1	-0.746387000	-5.204002000	-2.574995000

**2b** ISQ-<sub>IS</sub>Co<sup>III</sup>-ISQ<sup>+</sup>

27	-0.001096000	0.225832000	-0.022548000
8	-1.102916000	1.379115000	-1.174966000
8	0.831828000	-1.294484000	1.160748000
8	1.078370000	1.571409000	0.919779000
8	-0.815650000	-1.471834000	-0.946643000
7	-1.498649000	0.349014000	1.198648000
7	1.501998000	0.161844000	-1.243583000
6	-2.347575000	1.450267000	-0.735649000
6	-2.621810000	0.876408000	0.584400000
6	-3.956854000	0.845252000	1.098156000
1	-4.144740000	0.341303000	2.051180000
6	-5.000248000	1.412603000	0.366193000
6	-4.687885000	2.038502000	-0.899900000
1	-5.517445000	2.497428000	-1.448271000
6	-3.415238000	2.078123000	-1.482733000
6	-1.352967000	0.183986000	2.584543000
6	-2.024220000	1.054342000	3.496437000
1	-2.639665000	1.866746000	3.093608000
6	-1.867414000	0.925013000	4.882746000
1	-2.382646000	1.629422000	5.550822000
6	-1.030956000	-0.079793000	5.419409000
1	-0.893736000	-0.172866000	6.504651000
6	-0.347478000	-0.938444000	4.546337000
1	0.338913000	-1.687607000	4.958709000
6	-0.474917000	-0.829128000	3.131927000
6	0.389893000	-1.690778000	2.275973000
6	0.812524000	-3.058878000	2.730685000
6	-0.050486000	-3.898496000	3.485131000
1	-1.046411000	-3.542345000	3.779504000
6	0.352872000	-5.204156000	3.824941000

1	-0.326023000	-5.854493000	4.393331000
6	1.624712000	-5.675028000	3.436392000
1	1.942882000	-6.689248000	3.715348000
6	2.488610000	-4.845850000	2.685907000
1	3.479777000	-5.213267000	2.386282000
6	2.080586000	-3.552119000	2.319618000
1	2.738721000	-2.904447000	1.726019000
6	2.326146000	1.579671000	0.483298000
6	2.617486000	0.789513000	-0.715638000
6	1.369208000	-0.231010000	-2.583599000
6	2.049681000	0.477323000	-3.620782000
1	2.663301000	1.344706000	-3.352261000
6	1.901331000	0.123911000	-4.968384000
1	2.421910000	0.709834000	-5.738883000
6	1.065837000	-0.953840000	-5.339734000
1	0.934655000	-1.221822000	-6.396232000
6	0.376897000	-1.659542000	-4.342787000
1	-0.305819000	-2.467478000	-4.631793000
6	0.495646000	-1.321584000	-2.964208000
6	-0.369237000	-2.038006000	-1.983886000
6	-0.784837000	-3.463259000	-2.215617000
6	-2.056338000	-3.888876000	-1.744326000
1	-2.723210000	-3.156476000	-1.271203000
6	-2.456955000	-5.226725000	-1.900880000
1	-3.450812000	-5.544835000	-1.557062000
6	-1.581933000	-6.162659000	-2.496926000
1	-1.893938000	-7.210139000	-2.611487000
6	-0.306732000	-5.755197000	-2.942194000
1	0.380443000	-6.486078000	-3.390034000
6	0.089132000	-4.409859000	-2.814543000
1	1.086952000	-4.101058000	-3.152701000
6	3.958983000	0.673503000	-1.199860000
1	4.159540000	0.013373000	-2.049481000
6	4.992489000	1.359164000	-0.561085000
6	4.661405000	2.199607000	0.568630000
1	5.483252000	2.751600000	1.036779000
6	3.380596000	2.339670000	1.117175000
6	-3.146080000	2.747547000	-2.864223000
6	-2.082894000	3.888595000	-2.700536000
1	-2.448232000	4.668190000	-2.001122000
1	-1.121697000	3.499108000	-2.320350000
1	-1.900676000	4.372397000	-3.682080000
6	-2.624803000	1.673152000	-3.880108000
1	-1.679635000	1.215915000	-3.536880000
1	-3.376438000	0.869529000	-4.023416000
1	-2.444085000	2.148133000	-4.866258000
6	-4.438054000	3.383727000	-3.464128000
1	-4.853121000	4.180496000	-2.813770000
1	-4.192033000	3.849670000	-4.438786000
1	-5.230572000	2.630479000	-3.650872000
6	3.088878000	3.254886000	2.344545000
6	4.367861000	4.006174000	2.827292000



1	5.159628000	3.310766000	3.173531000
1	4.792132000	4.659217000	2.037552000
1	4.102755000	4.655756000	3.684748000
6	2.019080000	4.333389000	1.954189000
1	2.385542000	4.968761000	1.121949000
1	1.065232000	3.868523000	1.646699000
1	1.821420000	4.994487000	2.822857000
6	2.560685000	2.388901000	3.539913000
1	3.310917000	1.626617000	3.835189000
1	2.374536000	3.039737000	4.418868000
1	1.617186000	1.875525000	3.282528000
6	6.478928000	1.249822000	-1.005514000
6	7.008030000	2.671312000	-1.403373000
1	6.950363000	3.391094000	-0.563478000
1	8.070616000	2.605238000	-1.713766000
1	6.428149000	3.089192000	-2.251086000
6	6.662675000	0.301675000	-2.228805000
1	7.734474000	0.260273000	-2.506295000
1	6.339187000	-0.735008000	-2.003500000
1	6.104672000	0.658925000	-3.118243000
6	7.335314000	0.688576000	0.182333000
1	7.297073000	1.345923000	1.073018000
1	6.982766000	-0.318301000	0.485002000
1	8.397410000	0.603070000	-0.124953000
6	-6.478292000	1.392258000	0.850320000
6	-6.987289000	2.866203000	1.016564000
1	-6.947656000	3.431707000	0.065252000
1	-8.041090000	2.865071000	1.362029000
1	-6.380523000	3.414643000	1.765203000
6	-6.643131000	0.661749000	2.217406000
1	-7.710097000	0.673482000	2.515489000
1	-6.326209000	-0.399557000	2.161354000
1	-6.069260000	1.158293000	3.026206000
6	-7.364079000	0.650439000	-0.209565000
1	-7.334646000	1.144907000	-1.200171000
1	-7.030426000	-0.398854000	-0.341365000
1	-8.421201000	0.635006000	0.125219000