The program used for deriving the susceptibility equation is based on the Irreducible Tensor Operators Method, which does not make use of a ready-to-fit equation. It is a general program applicable to any kind of Hamiltonian form where the only input is the form of the Heisenberg Hamiltonian (number of J's and the corresponding S_iS_j's). The program is based on Fortran routines (3-j, 6-j, 9-j symbols) and after finding the eigenvalues diagonalizes the respective matrices for a given set of starting J's. In the case of a fitting procedure the latter procedure is repeated until the global minimum is reached.

Table SI1. Experimental (χ_M(exp)) and calculated (χ_M(calc)) magnetic susceptibility data for complex **1**.

T(K)	χ_M(exp)	χ_M(calc)
2.74	0.01210	0.01597
2.43	0.01279	0.01801
2.38	0.01305	0.01843
2.04	0.01371	0.02144
2.51	0.01260	0.01743
2.90	0.01176	0.01511
3.17	0.01122	0.01382
3.68	0.01034	0.01189
4.21	0.00960	0.01041
4.70	0.00899	0.00932
5.16	0.00852	0.00849
6.15	0.00761	0.00712
7.11	0.00697	0.00618
8.12	0.00645	0.00544
9.12	0.00606	0.00490
10.13	0.00578	0.00453

12.07	0.00551	0.00419
13.99	0.00553	0.00423
15.90	0.00578	0.00455
17.87	0.00619	0.00507
19.83	0.00669	0.00567
22.79	0.00753	0.00661
23.81	0.00780	0.00692
28.84	0.00906	0.00826
31.83	0.00966	0.00888
35.82	0.01026	0.00954
39.49	0.01073	0.01000
44.43	0.01119	0.01049
49.36	0.01156	0.01087
54.29	0.01182	0.01118
59.51	0.01205	0.01145
64.44	0.01224	0.01168
69.39	0.01240	0.01187
79.32	0.01267	0.01222
89.31	0.01288	0.01251
99.45	0.01306	0.01276
109.33	0.01321	0.01298
119.46	0.01337	0.01318
129.35	0.01348	0.01336
139.39	0.01361	0.01352
149.35	0.01373	0.01367
159.57	0.01385	0.01381
169.45	0.01394	0.01393
179.63	0.01405	0.01405
189.65	0.01415	0.01416
199.52	0.01425	0.01426

209.69	0.01433	0.01435
219.48	0.01440	0.01444
229.73	0.01448	0.01452
239.74	0.01455	0.01459
249.76	0.01462	0.01466
259.76	0.01468	0.01472
269.82	0.01474	0.01477
279.56	0.01477	0.01482
289.61	0.01480	0.01487
299.63	0.01480	0.01490