Table 1. Coordinates for the BP86 optimised geometry of $[Ni(en)_3]^{2+}$.

Atom	Coordinates (Å)		
	x	***y***	***z***
Ni	0.00	0.00	0.00
N	-1.63	-0.75	1.19
C	-2.87	-0.05	0.76
H	-3.78	-0.57	1.10
H	-2.87	0.95	1.20
H	-1.75	-1.76	1.06
H	-1.49	-0.61	2.19
N	1.46	-1.04	1.19
N	0.17	1.79	1.19
N	1.46	1.04	-1.19
N	0.17	-1.79	-1.19
N	-1.63	0.75	-1.19
C	-2.87	0.05	-0.76
C	1.48	-2.46	0.76
H	2.39	-0.64	1.06
H	1.27	-0.98	2.19
C	1.39	2.52	*0.76*
H	-0.65	2.39	1.06
H	0.22	1.59	2.19
C	1.48	2.46	-0.76
H	2.39	0.64	-1.06
H	1.27	0.98	-2.19
C	1.39	-2.52	-0.76
H	-0.65	-2.39	-1.06
H	0.22	-1.59	-2.19
H	-1.75	1.76	-1.06
H	-1.49	0.61	-2.19
H	-3.78	0.57	-1.10
H	-2.87	-0.95	-1.20
H	2.38	-2.99	1.10
H	0.61	-2.96	1.20
H	1.40	3.56	1.10
H	2.26	2.01	1.20
H	2.38	2.99	-1.10
H	0.61	2.96	-1.20
H	1.40	-3.56	-1.10
H	2.26	-2.01	-1.20

Table 2. Selected bond lengths (Å) and bond angles (°) for the BP86 optimised structure $[Ni(en)_3]^{2+}$ and a comparison with those determined crystallographically[1] for $[Ni(en)_3](NO_3)_2$

bond length	BP86	experiment	bond angle	BP86	experiment
Ni-N	2.152	2.130	N-Ni-N	81.3	81.9
N-C	1.484	1.476	Ni-N-C	108.3	108.1
C-C	1.520	1.490	N-C-C	108.7	110.0
N-H	1.02	0.82			
C-H	1.10	1.02			

[1] Korp, J. D., Bernal, I., Palmer, R. A., & Robinson, J. C. (1980). On the absolute configuration of the tris(ethylenediamine)nickel(II) cation. I. The structure and absolute configuration of (-)-[Ni(en)3](NO3)2. *Acta Crystallographica Section B, 36*(3), 560-564.