Table 1: Optimized Cartesian Coordinates for the Ni-C Form of the [NiFe] Hydrogenase in Å and g-Tensor Eigenvectors.

Atom	x	y	z
C	31.4473	40.7146	114.4278
C	30.6778	42.0427	114.4450
S	31.0220	43.0629	112.8500
H	31.2052	40.1193	115.3299
H	31.1758	40.1284	113.5333
H	32.5347	40.8979	114.4040
H	30.9603	42.6573	115.3114
H	29.5956	41.8644	114.4848
C	33.4079	46.2343	114.5440
C	32.0377	46.9170	114.5961
S	30.6756	45.6612	115.1299
H	34.1853	46.9724	114.2671
H	33.6681	45.8009	115.5251
H	33.3995	45.4212	113.7998
H	31.7403	47.3332	113.6265
H	31.9986	47.7240	115.3408
C	26.7143	45.5342	109.4580
C	27.5770	45.9774	110.6493
S	28.8181	44.5653	111.0975
H	25.9784	46.3197	109.2014
H	27.3422	45.3290	108.5731
H	26.1684	44.6083	109.7090
H	26.9547	46.1933	111.5266
H	28.1514	46.8833	110.4085
C	25.7998	42.6727	114.1090
C	26.2298	44.1425	114.0444
S	27.9341	44.3659	114.9061
H	24.7975	42.5506	113.6555
H	26.5152	42.0434	113.5558
H	25.7592	42.3211	115.1544
H	25.5281	44.8096	114.5616
H	26.3425	44.4800	113.0084
FE	28.5705	46.6515	114.8035
NI	29.6397	44.8966	113.1820
C	26.9000	47.2080	114.1015
N	25.8394	47.5369	113.6654
C	29.3067	48.3722	114.4740
N	29.7808	49.4572	114.3277
C	28.1354	47.0784	116.4186
O	27.8261	47.3544	117.5511
H	28.9277	46.3353	113.1460
g-tensor	g_x	g_y	g_z
eigenvectors	-0.34741	-0.63260	-0.69218
	+0.93771	-0.23640	-0.25459
	-0.00258	-0.73751	+0.67533

Table 2: Optimized Cartesian Coordinates for the Ni-C Form of the [NiFeSe] Hydrogenase in Å and g-Tensor Eigenvectors.

Atom	x	y	z
C	31.672984	40.744162	114.401625
C	30.891326	42.061632	114.503268
S	30.994634	43.034454	112.845633
Fe	28.532744	46.630498	114.779894
C	28.142130	47.115917	116.388678
O	27.866952	47.440001	117.517671
S	30.648677	45.657951	115.129247
C	31.998003	46.847178	114.431783
C	33.363189	46.152292	114.422639
S	27.878803	44.339849	114.925826
C	26.214099	44.140392	113.978859
C	25.757388	42.678378	114.001653
C	26.846857	47.183694	114.113072
N	25.776243	47.509313	113.701342
C	29.263169	48.325946	114.330294
N	29.735001	49.390491	114.072111
Se	28.777299	44.537673	111.017493
C	27.637226	46.165506	110.573413
C	26.742524	45.876724	109.357892
H	31.584567	40.165788	115.341172
H	31.282064	40.133126	113.570912
H	32.740047	40.943189	114.207280
H	31.287988	42.704245	115.301062
H	29.828159	41.874203	114.701570
H	34.132352	46.837543	114.017442
H	33.659482	45.855264	115.443257
H	33.320977	45.247410	113.794226
H	31.676869	47.141841	113.425573
H	31.979042	47.738481	115.073244
H	26.115916	46.759254	109.127737
H	27.347124	45.630524	108.466592
H	26.076423	45.022281	109.566170
H	27.032032	46.412343	111.455291
H	28.313104	47.009745	110.375716
H	24.789902	42.580233	113.472978
H	26.499625	42.039793	113.496030
H	25.631382	42.320372	115.037817
H	25.495223	44.814009	114.462526
H	26.390386	44.484788	112.953979
H	28.861939	46.253598	113.131338
Ni	29.594338	44.829504	113.219678
g-tensor	g_x	g_y	g_z
eigenvectors	-0.38535	+0.63102	+0.67329
	+0.92246	+0.28246	+0.26323
	-0.02408	+0.72251	-0.69094