A Detailed QM/MM study of the Electron Paramagnetic Resonance Parameters of Nitrosyl Myoglobin

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Supporting Information

Table S1. Computed g-tensors at the QM/MM level.

Models		BLYP	BP86	BPW91	OLYP	PBE	PBE0	B3LYP	TPSSh	O3LYP	Experiment[60]
	g_1	1.977	1.979	1.979	1.983	1.979	1.945	1.951	1.972	1.968	1.987
(**1**)	g_2	1.999	1.999	1.999	2.001	1.999	1.991	1.992	1.996	1.999	2.008
	g_3	2.026	2.026	2.026	2.031	2.026	2.024	2.025	2.021	2.032	2.075
	g_{iso}	2.001	2.001	2.001	2.005	2.002	1.987	1.989	1.996	2.000	
	g_1	1.983	1.985	1.984	1.988	1.984	1.963	1.970	1.981	1.981	1.987
(**2**)	g_2	2.002	2.003	2.003	2.005	2.003	1.994	1.998	1.999	2.004	2.008
	g_3	2.029	2.029	2.029	2.034	2.030	2.026	2.028	2.023	2.036	2.075
	g_{iso}	2.005	2.005	2.005	2.009	2.006	1.994	1.999	2.001	2.007	
	g_1	1.988	1.990	1.990	1.995	1.990	1.981	1.981	1.989	1.992	1.987
(**3**)	g_2	2.003	2.003	2.003	2.006	2.003	2.015	2.010	2.003	2.012	2.008
	g_3	2.045	2.046	2.046	2.053	2.047	2.048	2.049	2.037	2.060	2.075
	g_{iso}	2.012	2.013	2.013	2.018	2.013	2.015	2.013	2.010	2.021	
	g_1	2.017	2.019	2.018	2.023	2.019	2.034	2.025	2.024	2.032	1.987
(**4**)	g_2	2.062	2.061	2.061	2.064	2.062	2.144	2.128	2.064	2.102	2.008
	g_3	2.115	2.120	2.122	2.141	2.127	2.214	2.187	2.088	2.222	2.075
	g_{iso}	2.064	2.067	2.067	2.076	2.069	2.130	2.114	2.059	2.119	
	g_1	1.976	1.977	1.977	1.979	1.977	1.947	1.955	1.971	1.964	1.987
(**5**)	g_2	2.004	2.003	2.003	2.005	2.003	1.990	1.994	1.998	1.999	2.008
	g_3	2.009	2.009	2.009	2.012	2.009	2.001	2.006	2.007	2.011	2.075
	g_{iso}	1.996	1.996	1.996	1.998	1.997	1.979	1.985	1.992	1.991	
	g_1	1.978	1.979	1.979	1.982	1.979	1.964	1.964	1.977	1.973	1.987
(**6**)	g_2	2.001	2.000	2.000	2.002	2.000	2.000	1.999	1.999	2.003	2.008
	g_3	2.031	2.031	2.031	2.036	2.032	2.032	2.032	2.025	2.038	2.075
	g_{iso}	2.003	2.004	2.003	2.006	2.004	1.999	1.998	2.000	2.004	
	g_1	1.986	1.987	1.986	1.991	1.987	1.983	1.983	1.990	1.989	1.987
(**7**)	g_2	2.003	2.003	2.003	2.005	2.003	2.037	2.022	2.006	2.014	2.008
	g_3	2.042	2.043	2.043	2.048	2.043	2.054	2.051	2.037	2.057	2.075
	g_{iso}	2.010	2.011	2.011	2.015	2.011	2.025	2.019	2.011	2.020	

Table S2. Computed HCCs at the QM/MM level.

Models		BLYP	BP86	BPW91	OLYP	PBE	PBE0	B3LYP	TPSSh	O3LYP	Experiment[60]
(**1**)	$^{14NO}A_{iso}$	53.1	51.3	51.6	55.5	53.1	43.2	44.5	44.3	48.2	38
	$^{14NHis93}A_{iso}$	20.8	20.8	20.8	22.3	21.3	9.6	10.9	13.6	16.7	18
	$^{1HHis93}A_{iso}$	-	-	-	-	-	-	-	-	-	9
(**2**)	$^{14NO}A_{iso}$	35.7	33.9	34.3	37.7	35.5	28.9	28.7	28.8	30.7	38
	$^{14NHis93}A_{iso}$	17.1	17.1	17.1	18.6	17.5	6.7	7.8	10.3	13.2	18
	$^{1HHis93}A_{3}$	12.9	13.1	13.1	11.5	13.2	14.9	13.9	14.2	12.6	9
(**3**)	$^{14NO}A_{iso}$	22.5	20.8	21.1	22.7	21.9	15.3	16.0	16.7	17.2	38
	$^{14NHis93}A_{iso}$	16.1	15.9	15.9	17.5	16.3	4.4	6.3	8.9	12.5	18
	$^{1HHis93}A_{iso}$	24.4	24.5	24.6	21.7	24.4	24.5	23.8	24.9	20.8	9
(**4**)	$^{14NO}A_{iso}$	-7.4	-7.3	-7.1	-11.6	-7.8	-11.6	-10.1	-8.7	-13.5	38
	$^{14NHis93}A_{iso}$	-0.2	-0.6	-0.6	0.6	-0.5	-4.9	-3.5	-2.3	-0.8	18
	$^{1HNO}A_{iso}$	14.4	14.3	14.3	-13.2	14.0	10.2	11.3	11.9	-15.7	9
(**5**)	$^{14NO}A_{iso}$	49.7	47.5	47.8	52.9	49.7	45.8	44.7	42.9	46.5	38
	$^{14NHis93}A_{iso}$	16.2	16.3	16.3	17.8	16.7	6.9	7.2	9.2	11.8	18
	$^{1HHis93}A_{iso}$	-	-	-	-	-	-	-	-	-	9
(**6**)	$^{14NO}A_{iso}$	27.5	25.3	25.7	28.9	26.9	22.7	23.5	22.7	23.6	38
	$^{14NHis93}A_{iso}$	16.6	16.4	16.5	18.4	16.9	5.8	7.4	9.6	12.3	18
	$^{1HHis93}A_{iso}$	16.2	16.5	16.4	14.8	16.5	16.5	16.2	16.8	15.6	9
(**7**)	$^{14NO}A_{iso}$	15.5	13.6	13.8	15.2	14.8	10.6	11.2	11.6	11.1	38
	$^{14NHis93}A_{iso}$	14.9	14.4	14.5	16.3	14.9	2.2	4.6	7.3	10.4	18
	$^{1HHis93}A_{iso}$	29.1	29.3	29.5	27.1	29.3	25.1	24.8	27.6	24.4	9

Table S3. Calculated Mulliken spin populations (e^-) of MbNO at the QM/MM level.

Model	Atom	BLYP	BP86	BPW91	OLYP	PBE	PBE0	B3LYP	TPSSh	O3LYP
(**1**)	Fe	0.615	0.636	0.633	0.741	0.650	0.259	0.316	0.413	0.619
	N_{NO}	0.240	0.234	0.235	0.179	0.223	0.486	0.447	0.389	0.273
	O_{NO}	0.130	0.123	0.124	0.089	0.119	0.253	0.236	0.203	0.136
(**2**)	Fe	0.667	0.690	0.686	0.800	0.702	0.313	0.455	0.500	0.723
	N_{NO}	0.181	0.173	0.175	0.119	0.165	0.408	0.337	0.302	0.184
	O_{NO}	0.128	0.122	0.123	0.083	0.118	0.262	0.208	0.197	0.115
(**3**)	Fe	0.743	0.769	0.764	0.895	0.778	0.634	0.654	0.666	0.925
	N_{NO}	0.111	0.100	0.103	0.042	0.095	0.226	0.207	0.182	0.055
	O_{NO}	0.107	0.101	0.103	0.054	0.098	0.146	0.140	0.149	0.044
(**4**)	Fe	1.075	1.138	1.131	1.258	1.140	1.213	1.177	1.203	1.364
	N_{NO}	-0.120	-0.136	-0.132	-0.178	-0.135	-0.065	-0.070	-0.097	-0.163
	O_{NO}	-0.104	-0.114	-0.112	-0.163	-0.115	-0.071	-0.078	-0.097	-0.175
(**5**)	Fe	0.498	0.510	0.508	0.588	0.528	0.045	0.191	0.293	0.432
	N_{NO}	0.309	0.308	0.307	0.267	0.294	0.594	0.518	0.462	0.379
	O_{NO}	0.171	0.165	0.166	0.144	0.161	0.332	0.280	0.243	0.201
(**6**)	Fe	0.624	0.643	0.638	0.732	0.656	0.438	0.447	0.487	0.664
	N_{NO}	0.196	0.188	0.190	0.145	0.179	0.352	0.337	0.303	0.209
	O_{NO}	0.146	0.141	0.142	0.109	0.137	0.212	0.212	0.204	0.139
(**7**)	Fe	0.710	0.734	0.727	0.839	0.741	0.716	0.751	0.716	0.914
	N_{NO}	0.119	0.109	0.112	0.059	0.104	0.155	0.164	0.155	0.058
	O_{NO}	0.117	0.112	0.114	0.074	0.109	0.125	0.096	0.125	0.048