

ELECTRONIC SUPPLEMENTARY INFORMATION

Thermally Induced Hopping Model for Long-Range Triplet Excitation Energy Transfer in DNA

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Cartesian coordinates used for the electronic coupling calculations

1	-5.171000000	-0.628000000	-3.343000000
6	-4.089000000	-0.533000000	-3.383000000
6	-3.467000000	0.596000000	-2.849000000
1	-4.061000000	1.376000000	-2.381000000
6	-2.078000000	0.724000000	-2.909000000
1	-1.600000000	1.596000000	-2.474000000
6	-1.297000000	-0.284000000	-3.494000000
6	-1.932000000	-1.428000000	-4.004000000
1	-1.316000000	-2.215000000	-4.426000000
6	-3.318000000	-1.546000000	-3.961000000
1	-3.799000000	-2.430000000	-4.371000000
6	0.205000000	-0.246000000	-3.522000000
8	0.833000000	-1.299000000	-3.467000000
6	0.932000000	1.056000000	-3.614000000
6	2.260000000	1.098000000	-3.166000000
1	2.689000000	0.195000000	-2.744000000
6	3.022000000	2.259000000	-3.254000000
1	4.040000000	2.259000000	-2.884000000
6	2.461000000	3.411000000	-3.828000000
8	3.109000000	4.597000000	-3.971000000
6	4.454000000	4.695000000	-3.520000000
1	4.531000000	4.512000000	-2.441000000
1	4.765000000	5.718000000	-3.736000000
1	5.109000000	3.995000000	-4.055000000
6	1.141000000	3.377000000	-4.306000000
1	0.734000000	4.273000000	-4.765000000
6	0.388000000	2.218000000	-4.194000000
1	-0.623000000	2.206000000	-4.587000000
7	-1.284000000	4.500000000	0.000000000
6	-1.537000000	3.133000000	0.000000000
8	-2.659000000	2.661000000	0.000000000
7	-0.371000000	2.383000000	0.000000000
6	0.962000000	2.836000000	0.000000000
8	1.880000000	2.030000000	0.000000000
6	1.108000000	4.299000000	0.000000000
6	2.499000000	4.880000000	0.000000000
6	-0.019000000	5.048000000	0.000000000
1	-2.108000000	5.087000000	0.000000000
1	-0.498000000	1.377000000	0.000000000
1	0.006000000	6.134000000	0.000000000
1	3.225000000	4.064000000	0.000000000

1	2.683000000	5.499000000	-0.885000000
1	2.683000000	5.499000000	0.886000000
7	-1.291000000	-4.498000000	0.000000000
6	0.029000000	-4.903000000	0.000000000
7	0.881000000	-3.907000000	0.000000000
6	0.073000000	-2.780000000	0.000000000
6	0.360000000	-1.398000000	0.000000000
7	1.627000000	-0.925000000	0.000000000
7	-0.661000000	-0.522000000	0.000000000
6	-1.914000000	-1.006000000	0.000000000
7	-2.325000000	-2.278000000	0.000000000
6	-1.283000000	-3.120000000	0.000000000
1	-2.113000000	-5.085000000	0.000000000
1	0.296000000	-5.952000000	0.000000000
1	2.410000000	-1.560000000	0.000000000
1	1.780000000	0.072000000	0.000000000
1	-2.701000000	-0.254000000	0.000000000
7	-3.688000000	2.880000000	3.380000000
6	-2.858000000	3.984000000	3.380000000
7	-1.584000000	3.679000000	3.380000000
6	-1.575000000	2.292000000	3.380000000
6	-0.530000000	1.343000000	3.380000000
7	0.773000000	1.705000000	3.380000000
7	-0.842000000	0.034000000	3.380000000
6	-2.140000000	-0.311000000	3.380000000
7	-3.220000000	0.476000000	3.380000000
6	-2.872000000	1.770000000	3.380000000
1	-4.698000000	2.872000000	3.380000000
1	-3.259000000	4.989000000	3.380000000
1	1.033000000	2.679000000	3.380000000
1	1.482000000	0.988000000	3.380000000
1	-2.334000000	-1.382000000	3.380000000
7	1.606000000	-4.395000000	3.380000000
6	0.598000000	-3.438000000	3.380000000
8	-0.587000000	-3.716000000	3.380000000
7	1.101000000	-2.146000000	3.380000000
6	2.445000000	-1.729000000	3.380000000
8	2.714000000	-0.537000000	3.380000000
6	3.423000000	-2.827000000	3.380000000
6	4.890000000	-2.479000000	3.380000000
6	2.952000000	-4.095000000	3.380000000
1	1.285000000	-5.355000000	3.380000000
1	0.406000000	-1.407000000	3.380000000
1	3.610000000	-4.959000000	3.380000000
1	4.998000000	-1.392000000	3.380000000
1	5.403000000	-2.872000000	4.265000000
1	5.403000000	-2.872000000	2.494000000
7	-4.677000000	0.169000000	6.760000000
6	-3.455000000	-0.494000000	6.760000000
8	-3.352000000	-1.707000000	6.760000000
7	-2.381000000	0.384000000	6.760000000
6	-2.400000000	1.791000000	6.760000000
8	-1.350000000	2.415000000	6.760000000
6	-3.746000000	2.382000000	6.760000000
6	-3.869000000	3.885000000	6.760000000
6	-4.807000000	1.542000000	6.760000000
1	-5.489000000	-0.433000000	6.760000000
1	-1.463000000	-0.048000000	6.760000000
1	-5.832000000	1.901000000	6.760000000
1	-2.869000000	4.323000000	6.760000000

1	-4.401000000	4.251000000	5.875000000
1	-4.401000000	4.251000000	7.646000000
7	3.879000000	-2.618000000	6.760000000
6	4.672000000	-1.488000000	6.760000000
7	3.988000000	-0.369000000	6.760000000
6	2.666000000	-0.790000000	6.760000000
6	1.441000000	-0.090000000	6.760000000
7	1.382000000	1.262000000	6.760000000
7	0.292000000	-0.790000000	6.760000000
6	0.365000000	-2.131000000	6.760000000
7	1.448000000	-2.915000000	6.760000000
6	2.571000000	-2.184000000	6.760000000
1	4.183000000	-3.581000000	6.760000000
1	5.752000000	-1.558000000	6.760000000
1	2.228000000	1.810000000	6.760000000
1	0.482000000	1.715000000	6.760000000
1	-0.593000000	-2.647000000	6.760000000
7	-3.879000000	-2.618000000	10.140000000
6	-4.672000000	-1.488000000	10.140000000
7	-3.988000000	-0.369000000	10.140000000
6	-2.666000000	-0.790000000	10.140000000
6	-1.441000000	-0.090000000	10.140000000
7	-1.382000000	1.262000000	10.140000000
7	-0.292000000	-0.790000000	10.140000000
6	-0.365000000	-2.131000000	10.140000000
7	-1.448000000	-2.915000000	10.140000000
6	-2.571000000	-2.184000000	10.140000000
1	-4.183000000	-3.581000000	10.140000000
1	-5.752000000	-1.558000000	10.140000000
1	-2.228000000	1.810000000	10.140000000
1	-0.482000000	1.715000000	10.140000000
1	0.593000000	-2.647000000	10.140000000
7	4.677000000	0.169000000	10.140000000
6	3.455000000	-0.494000000	10.140000000
8	3.352000000	-1.707000000	10.140000000
7	2.381000000	0.384000000	10.140000000
6	2.400000000	1.791000000	10.140000000
8	1.350000000	2.415000000	10.140000000
6	3.746000000	2.382000000	10.140000000
6	3.869000000	3.885000000	10.140000000
6	4.807000000	1.542000000	10.140000000
1	5.489000000	-0.433000000	10.140000000
1	1.463000000	-0.048000000	10.140000000
1	5.832000000	1.901000000	10.140000000
1	2.869000000	4.323000000	10.140000000
1	4.401000000	4.251000000	11.025000000
1	4.401000000	4.251000000	9.254000000
7	-1.606000000	-4.395000000	13.520000000
6	-0.598000000	-3.438000000	13.520000000
8	0.587000000	-3.716000000	13.520000000
7	-1.101000000	-2.146000000	13.520000000
6	-2.445000000	-1.729000000	13.520000000
8	-2.714000000	-0.537000000	13.520000000
6	-3.423000000	-2.827000000	13.520000000
6	-4.890000000	-2.479000000	13.520000000
6	-2.952000000	-4.095000000	13.520000000
1	-1.285000000	-5.355000000	13.520000000
1	-0.406000000	-1.407000000	13.520000000
1	-3.610000000	-4.959000000	13.520000000
1	-4.998000000	-1.392000000	13.520000000

1	-5.403000000	-2.872000000	12.635000000
1	-5.403000000	-2.872000000	14.406000000
7	3.688000000	2.880000000	13.520000000
6	2.858000000	3.984000000	13.520000000
7	1.584000000	3.679000000	13.520000000
6	1.575000000	2.292000000	13.520000000
6	0.530000000	1.343000000	13.520000000
7	-0.773000000	1.705000000	13.520000000
7	0.842000000	0.034000000	13.520000000
6	2.140000000	-0.311000000	13.520000000
7	3.220000000	0.476000000	13.520000000
6	2.872000000	1.770000000	13.520000000
1	4.698000000	2.872000000	13.520000000
1	3.259000000	4.989000000	13.520000000
1	-1.033000000	2.679000000	13.520000000
1	-1.482000000	0.988000000	13.520000000
1	2.334000000	-1.382000000	13.520000000