

Supplementary material

N-methyl-2,6-di-*tert*-butyl-4,4'-pyrylogen. A dialkyl example of a new class of electron transfer sensitizers.

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Dedicated to Prof. Nicolò Vivona on the occasion of his 70th birthday

Computational Details

N-Methyl-2,6-di-*tert*-butyl-4,4'-pyrylogen dication, 4^{2+}

C	0.025819	0.004375	0.002894	C	0.976770	-1.014835	-0.162066
C	2.162497	-0.978996	0.553888	C	1.518149	1.017632	1.609562
C	0.322587	1.033706	0.911694	C	-1.252858	-0.003579	-0.762067
C	-1.760962	1.185597	-1.307152	C	-2.948000	1.162244	-2.023884
C	-3.152406	-1.192333	-1.658458	C	-1.962063	-1.200455	-0.946663
H	0.823901	-1.827500	-0.863641	H	2.927216	-1.739638	0.447792
H	1.783684	1.785704	2.327098	H	-0.375069	1.841464	1.103618
H	-1.231534	2.123956	-1.207964	H	-1.617298	-2.132843	-0.519716
C	3.683595	0.023820	2.214836	H	3.481233	-0.387995	3.206750
H	4.424007	-0.587154	1.699508	H	4.048902	1.047889	2.298206
N	2.419337	0.023863	1.424923	O	-3.578474	-0.018468	-2.158849
C	-3.648230	2.312018	-2.704271	C	-4.068440	-2.353354	-1.955542
C	-2.891655	3.631704	-2.462365	H	-2.841157	3.889624	-1.398365
H	-1.877856	3.610655	-2.877728	H	-3.426957	4.441637	-2.964745
C	-5.090630	2.420994	-2.137194	H	-5.596853	3.253358	-2.634197
H	-5.671904	1.514144	-2.324734	H	-5.087890	2.623793	-1.061082
C	-3.704420	2.011405	-4.229303	H	-4.258712	1.093266	-4.442901
H	-4.218647	2.838987	-4.726280	H	-2.702165	1.929199	-4.662731
C	-3.506237	-3.658678	-1.361987	H	-2.531718	-3.920582	-1.789406
H	-3.422780	-3.615893	-0.270193	H	-4.191036	-4.476905	-1.599613
C	-5.460401	-2.049904	-1.332752	H	-5.907091	-1.145373	-1.754736
H	-6.127879	-2.888431	-1.551211	H	-5.401490	-1.941492	-0.244668
C	-4.202303	-2.493464	-3.497701	H	-4.874264	-3.329332	-3.712098
H	-4.627064	-1.595045	-3.953698	H	-3.237494	-2.708210	-3.969091

Zero-point correction=	0.424725 (Hartree/Particle)
Thermal correction to Energy=	0.447000
Thermal correction to Enthalpy=	0.447945
Thermal correction to Gibbs Free Energy=	0.372688
Sum of electronic and zero-point Energies=	-869.296220

N-Methyl-2,6-di-*tert*-butyl-4,4'-pyrylogen radical cation, 4⁺

C	.018019	.005090	.009218	C	.808762	-1.170262	.213227
C	1.981446	-1.133989	.914406	C	1.739628	1.179252	1.285695
C	.561089	1.193319	.593912	C	-1.214798	-.006573	-.721690
C	-2.016391	1.167029	-.892277	C	-3.187602	1.138367	-1.588149
C	-2.907286	-1.186889	-2.024044	C	-1.732436	-1.192432	-1.333914
H	.503127	-2.130466	-.181263	H	2.585569	-2.018485	1.077033
H	2.159796	2.073208	1.730845	H	.059241	2.147529	.500141
S1							
H	-1.715753	2.112956	-.467131	H	-1.200103	-2.129794	-1.269532
C	3.692377	.029538	2.259622	H	3.456908	-.140353	3.315116
H	4.357694	-.759039	1.904571	H	4.196226	.991308	2.149805
N	2.463600	.028902	1.452860	O	-3.620109	-.030131	-2.142874
C	-3.585349	-2.350024	-2.723322	C	-4.143024	2.285906	-1.856955
C	-3.635711	3.590184	-1.216336	H	-3.554415	3.507216	-.126633
H	-2.663801	3.894257	-1.621079	H	-4.345130	4.395028	-1.430630
C	-5.530190	1.931913	-1.264434	H	-6.230795	2.749052	-1.464499
H	-5.938395	1.020497	-1.710311	H	-5.475012	1.791277	-.179286
C	-4.976049	-2.577219	-2.078557	H	-5.611896	-1.692010	-2.169299
H	-5.479690	-3.408385	-2.582664	H	-4.885364	-2.830442	-1.016492
C	-2.749895	-3.636147	-2.593742	H	-1.760987	-3.529959	-3.054033
H	-2.622159	-3.938830	-1.548275	H	-3.264861	-4.452167	-3.109391
C	-4.266850	2.483528	-3.388706	H	-4.964661	3.301556	-3.594604
H	-3.300598	2.741854	-3.835881	H	-4.645946	1.583763	-3.881393
C	-3.757327	-2.002128	-4.223095	H	-4.256259	-2.831740	-4.734240
H	-4.367011	-1.104771	-4.360538	H	-2.788156	-1.839781	-4.707452

Zero-point correction=	.423884 (Hartree/Particle)
Thermal correction to Energy=	.446241
Thermal correction to Enthalpy=	.447185
Thermal correction to Gibbs Free Energy=	.371548
Sum of electronic and zero-point Energies=	-869.624817

Neutral N-Methyl-2,6-di-*tert*-butyl-4,4'-pyrylogen dication, 4⁰

C	.021279	.015150	-.038671	C	.863717	-1.161366	.151900
C	2.029722	-1.120736	.835187	C	1.755941	1.194468	1.260740
C	.583428	1.207727	.587613	C	-1.174735	.001221	-.734354
C	-2.014092	1.177674	-.920403	C	-3.180306	1.143098	-1.593047
C	-2.901247	-1.188081	-2.026147	C	-1.730269	-1.191243	-1.361034
H	.572263	-2.117546	-.266601	H	2.649709	-2.000448	.973563
H	2.166725	2.085537	1.724096	H	.067157	2.158118	.518624
H	-1.705106	2.128409	-.508270	H	-1.194400	-2.128679	-1.301147
C	3.627894	.004003	2.341222	H	3.289498	-.225862	3.363499
H	4.349145	-.760238	2.035935	H	4.142615	.969559	2.356539
N	2.535486	.050380	1.387813	O	-3.656665	-.031963	-2.155158
C	-3.587053	-2.356877	-2.714557	C	-4.140272	2.291643	-1.857547
C	-3.630177	3.604091	-1.238160	H	-3.526306	3.524537	-.150248
H	-2.661267	3.898290	-1.656747	H	-4.342661	4.409953	-1.447166
C	-5.521286	1.952757	-1.245651	H	-6.235532	2.759178	-1.451638
H	-5.923162	1.025359	-1.663576	H	-5.447429	1.831619	-.158753
C	-4.967293	-2.596227	-2.055462	H	-5.597385	-1.704576	-2.119991
H	-5.488689	-3.421234	-2.555887	H	-4.853693	-2.856308	-.996791
C	-2.751752	-3.643641	-2.601175	H	-1.768601	-3.529567	-3.071485
S2							
H	-2.601948	-3.938494	-1.556551	H	-3.271502	-4.464465	-3.107953
C	-4.293262	2.485644	-3.385627	H	-5.003061	3.294932	-3.595417
H	-3.332338	2.746882	-3.843625	H	-4.661666	1.574661	-3.865701
C	-3.787893	-2.021476	-4.212155	H	-4.302817	-2.846369	-4.719271
H	-4.387282	-1.115460	-4.337714	H	-2.823960	-1.863521	-4.709320

Zero-point correction= .421708 (Hartree/Particle)
 Thermal correction to Energy= .444234
 Thermal correction to Enthalpy= .445178
 Thermal correction to Gibbs Free Energy= .370817
 Sum of electronic and zero-point Energies= -869.800536

Electrospray Ionization for 4^{2+}

Calculated for $C_{19}H_{27}NO = 285.2$; Observed = 285.2

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