Electronic Supplementary Information

Forward Molecular Design for Highly Efficient OLED Emitters: A Theoretical Analysis of Photophysical Properties of Platinum(II) Complexes with *N*-Heterocyclic Carbene Ligands

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Table S1. The optimized S_0 geometric parameters of **5** obtained by different functionals.

	GGA				meta-GGA	Expt.
	BP86	PBE	mPBE	PW91	TPSS	
Pt-C:$_1$	2.052	2.049	2.052	2.048	2.055	2.024
Pt-C:$_2$	2.052	2.049	2.052	2.048	2.055	2.028
Pt-C:$_3$	2.052	2.049	2.052	2.048	2.055	2.028
Pt-C:$_4$	2.052	2.049	2.052	2.048	2.055	2.025
C:$_1$-Pt-C:$_4$	180.0	180.0	180.0	180.0	180.0	180.0
C:$_2$-Pt-C:$_3$	180.0	180.0	180.0	180.0	180.0	180.0
C:$_1$-Pt-C:$_3$	95.6	96.5	96.6	96.5	96.7	95.8
C:$_2$-Pt-C:$_4$	96.6	96.5	96.6	96.5	96.7	95.8
N_1-C_5-N_2	109.5	109.6	109.6	109.6	109.3	108.7
N_3-C_6-N_4	109.5	109.6	109.6	109.6	109.3	108.7

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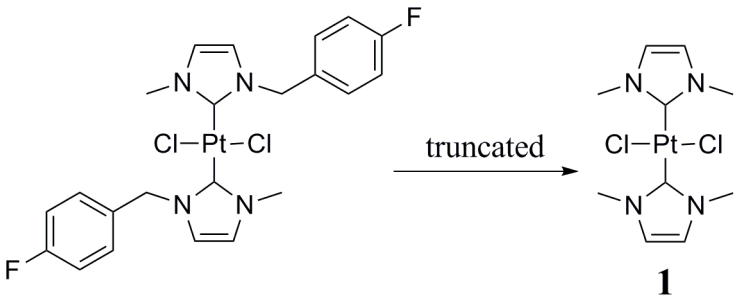
Figure S1. The truncated models, and the frontier molecular orbitals of non-truncated model **7**.



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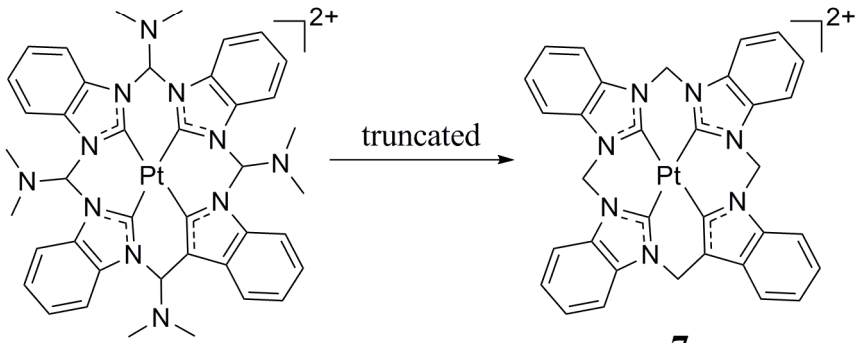

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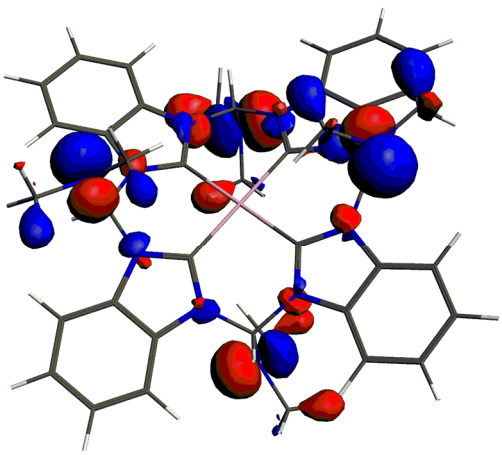
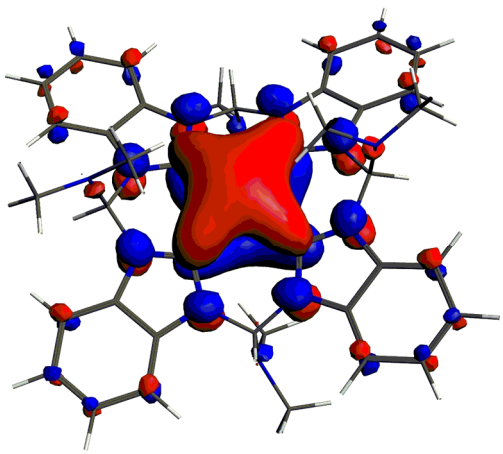


HOMO



LUMO

Figure S2. The optimized geometry of **1-8**.

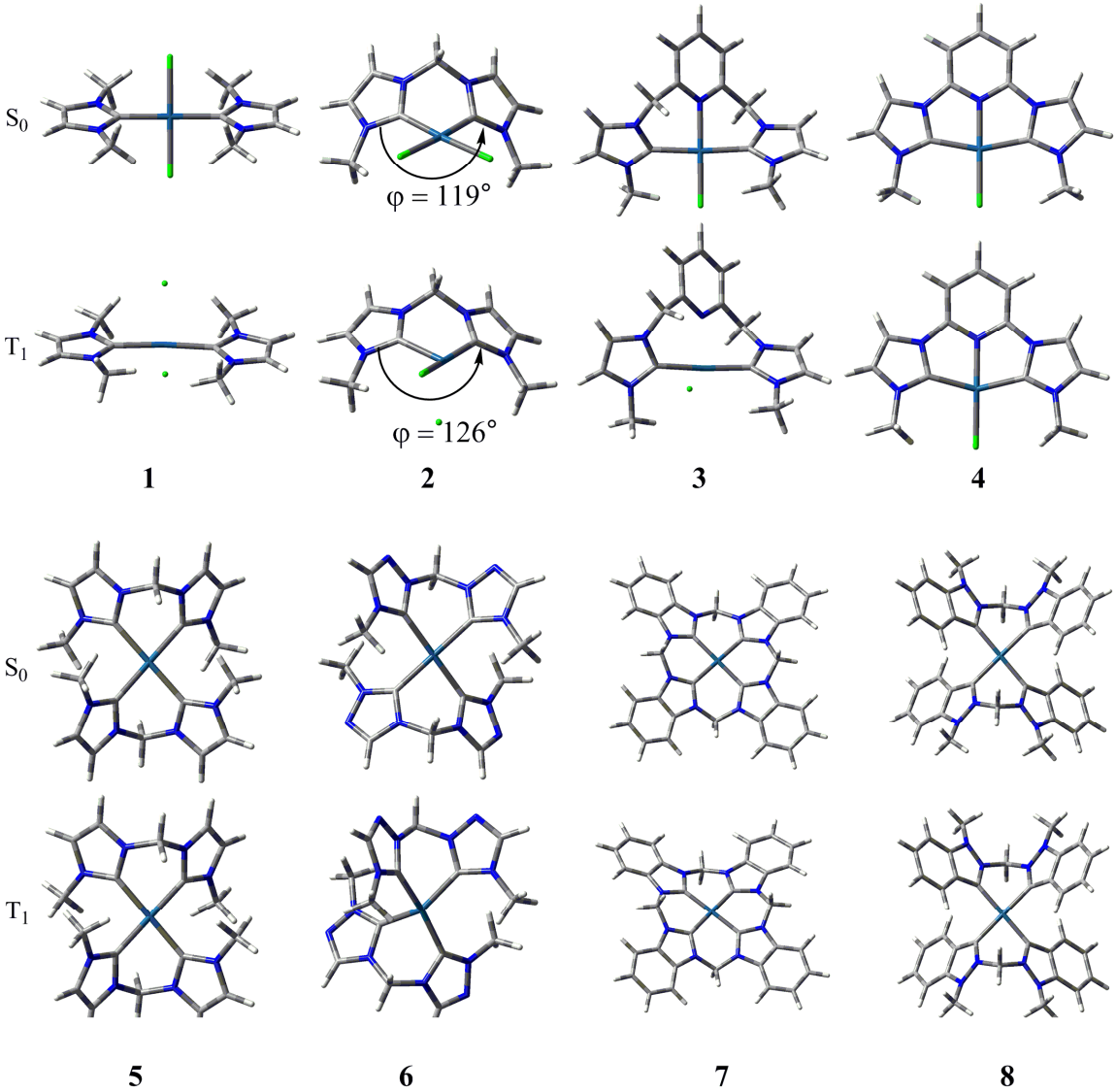


Table S2. The optimized S_0 geometrical parameters of **7** and the non-truncated model, together with the experimental values.

	7	non-truncated	Expt.
Pt-C:$_1$	1.996	2.000	1.980
Pt-C:$_2$	1.996	2.000	1.969
Pt-C:$_3$	1.996	2.000	1.978
Pt-C:$_4$	1.996	2.000	1.973
C:$_1$-Pt-C:$_4$	180.0	179.5	179.0
C:$_2$-Pt-C:$_3$	180.0	179.5	178.8
C:$_1$-Pt-C:$_3$	90.0	90.0	90.2
C:$_2$-Pt-C:$_4$	90.0	90.0	90.6
N_1-C_5-N_2	114.6	110.7	110.9
N_3-C_6-N_4	114.6	110.7	110.3
N_5-C_7-N_6	114.6	110.7	110.7
N_7-C_8-N_8	114.6	110.7	110.9
$D_{NHC1-NHC2}$	180.0	175.5	178.1
$D_{NHC2-NHC3}$	180.0	175.4	175.8
$D_{NHC3-NHC4}$	180.0	175.4	176.0
$D_{NHC4-NHC1}$	180.0	175.5	178.0

Table S3. The lowest unoccupied molecular orbital (LUMO) compositions (%) in the ground state for tetracarbene complexes **5**-**8**.

	5	**6**	**7**	**8**
$6p_z$(Pt)	12.63	10.51	12.72	6.13
p(C:$_{NHC}$)	25.16	31.40	32.67	16.29

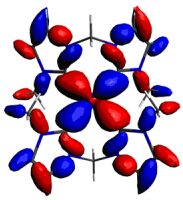
Table S4. The topological properties involving platinum at the BCP of the S_0 and T_1 of **1-8**.

		(3, -1)	$\rho(r_c)$	λ_1	λ_2	λ_3	$\nabla^2\rho_c$	ε	$H(r_c)$	$H(r_c)/\rho(r_c)$	$G(r_c)$	$G(r_c)/\rho(r_c)$	$V(r_c)$	$V(r_c)/\rho(r_c)$	$\Delta H(r_c)/\rho(r_c)$
1	S_0	Pt-C:$_1$	0.137	-0.145	-0.134	0.689	0.410	0.086	-0.060	-0.439	0.163	1.188	-0.223	-1.627	
		Pt-C:$_2$	0.137	-0.145	-0.134	0.689	0.410	0.087	-0.060	-0.439	0.163	1.189	-0.223	-1.627	
		Pt-Cl$_1$	0.091	-0.077	-0.072	0.485	0.336	0.072	-0.025	-0.271	0.109	1.195	-0.133	-1.466	
		Pt-Cl$_2$	0.091	-0.077	-0.072	0.485	0.336	0.072	-0.025	-0.271	0.109	1.195	-0.133	-1.466	
	T_1	Pt-C:$_1$	0.130	-0.138	-0.130	0.718	0.449	0.059	-0.055	-0.418	0.167	1.281	-0.221	-1.699	-4.60%
		Pt-C:$_2$	0.130	-0.138	-0.130	0.718	0.450	0.057	-0.055	-0.418	0.167	1.282	-0.222	-1.700	-4.72%
		Pt-Cl$_1$	0.071	-0.060	-0.059	0.329	0.210	0.011	-0.016	-0.221	0.068	0.963	-0.084	-1.185	-18.58%
		Pt-Cl$_2$	0.071	-0.060	-0.060	0.331	0.211	0.006	-0.016	-0.225	0.069	0.970	-0.085	-1.196	-16.63%
2	S_0	Pt-C:$_1$	0.154	-0.172	-0.159	0.813	0.483	0.085	-0.069	-0.447	0.190	1.231	-0.258	-1.678	
		Pt-C:$_2$	0.154	-0.169	-0.160	1.383	0.484	0.056	-0.068	-0.444	0.189	1.231	-0.258	-1.674	
		Pt-Cl$_1$	0.089	-0.078	-0.073	0.481	0.330	0.069	-0.023	-0.262	0.106	1.190	-0.129	-1.453	
		Pt-Cl$_2$	0.089	-0.078	-0.074	0.481	0.329	0.048	-0.024	-0.266	0.106	1.191	-0.129	-1.457	
	T_1	Pt-C:$_1$	0.127	-0.140	-0.123	0.658	0.395	0.135	-0.048	-0.375	0.147	1.150	-0.194	-1.525	-16.16%
		Pt-C:$_2$	0.145	-0.162	-0.147	0.796	0.487	0.100	-0.061	0.420	0.183	1.258	-0.244	-1.678	-5.26%
		Pt-Cl$_1$	0.091	-0.083	-0.080	0.508	0.344	0.035	-0.024	-0.266	0.110	1.211	-0.135	-1.477	1.98%
		Pt-Cl$_2$	0.073	-0.064	-0.062	0.330	0.205	0.032	-0.017	-0.234	0.068	0.938	-0.085	-1.172	-12.12%
3	S_0	Pt-C:$_1$	0.136	-0.137	-0.108	0.664	0.419	0.267	-0.054	-0.398	0.159	1.170	-0.213	-1.569	
		Pt-C:$_2$	0.136	-0.138	-0.104	0.661	0.419	0.326	-0.054	-0.398	0.159	1.170	-0.213	-1.567	
		Pt-Cl	0.103	-0.092	-0.088	0.556	0.376	0.043	-0.031	-0.303	0.125	1.217	-0.156	-1.520	
		Pt-N	0.115	-0.113	-0.112	0.761	0.536	0.015	-0.032	-0.279	0.166	1.444	-0.198	-1.723	
	T_1	Pt-C:$_1$	0.135	-0.139	-0.101	0.699	0.460	0.376	-0.054	-0.399	0.169	1.252	-0.222	-1.650	0.16%
		Pt-C:$_2$	0.134	-0.140	-0.107	0.706	0.459	0.310	-0.053	-0.392	0.167	1.247	-0.220	-1.639	-1.43%
		Pt-Cl	0.078	-0.067	-0.051	0.344	0.225	0.311	-0.018	-0.237	0.075	0.964	-0.093	-1.201	-21.35%
		Pt-N	0.084	-0.078	-0.074	0.472	0.320	0.060	-0.019	-0.222	0.099	1.177	-0.117	-1.399	-20.68%
4	S_0	Pt-C:$_1$	0.139	-0.159	-0.148	0.744	0.437	0.072	-0.057	-0.408	0.166	1.195	-0.223	-1.603	
		Pt-C:$_2$	0.139	-0.153	-0.139	0.728	0.436	0.103	-0.057	-0.410	0.166	1.195	-0.223	-1.605	
		Pt-Cl	0.103	-0.096	-0.084	0.591	0.411	0.140	-0.031	-0.302	0.134	1.295	-0.165	-1.597	
		Pt-N	0.141	-0.152	-0.148	0.938	0.639	0.028	-0.049	-0.345	0.208	1.481	-0.257	-1.826	
	T_1	Pt-C:$_1$	0.144	-0.184	-0.159	0.742	0.399	0.159	-0.061	-0.426	0.161	1.121	-0.222	-1.547	4.36%
		Pt-C:$_2$	0.144	-0.171	-0.166	0.737	0.400	0.028	-0.061	-0.425	0.161	1.120	-0.222	-1.546	3.57%
		Pt-Cl	0.107	-0.098	-0.088	0.598	0.412	0.115	-0.034	-0.314	0.137	1.278	-0.170	-1.592	4.25%
		Pt-N	0.128	-0.149	-0.138	0.813	0.526	0.074	-0.042	-0.326	0.173	1.352	-0.215	-1.678	-5.55%
5	S_0	Pt-C:$_1$	0.132	-0.142	-0.133	0.666	0.390	0.071	-0.055	-0.414	0.152	1.157	-0.207	-1.571	
		Pt-C:$_2$	0.132	-0.138	-0.134	0.679	0.408	0.033	-0.050	-0.383	0.152	1.157	-0.203	-1.540	
		Pt-C:$_3$	0.132	-0.138	-0.134	0.679	0.408	0.033	-0.050	-0.383	0.152	1.157	-0.203	-1.540	
		Pt-C:$_4$	0.132	-0.142	-0.133	0.666	0.390	0.071	-0.055	-0.414	0.152	1.157	-0.207	-1.571	
	T_1	Pt-C:$_1$	0.139	-0.156	-0.149	0.702	0.397	0.049	-0.060	-0.435	0.159	1.151	-0.220	-1.586	4.83%
		Pt-C:$_2$	0.138	-0.150	-0.149	0.714	0.415	0.009	-0.056	-0.401	0.159	1.150	-0.215	-1.551	4.69%
		Pt-C:$_3$	0.138	-0.150	-0.149	0.714	0.415	0.009	-0.056	-0.401	0.159	1.150	-0.215	-1.551	4.69%
		Pt-C:$_4$	0.139	-0.156	-0.149	0.701	0.397	0.049	-0.060	-0.435	0.159	1.151	-0.220	-1.586	4.83%
6	S_0	Pt-C:$_1$	0.131	-0.142	-0.131	0.679	0.407	0.081	-0.051	-0.387	0.153	1.161	-0.203	-1.548	
		Pt-C:$_2$	0.131	-0.138	-0.137	0.683	0.409	0.010	-0.050	-0.383	0.152	1.162	-0.203	-1.544	
		Pt-C:$_3$	0.132	-0.139	-0.137	0.690	0.414	0.012	-0.051	-0.385	0.154	1.168	-0.205	-1.553	
		Pt-C:$_4$	0.132	-0.142	-0.131	0.685	0.412	0.086	-0.051	-0.388	0.154	1.167	-0.205	-1.555	
	T_1	Pt-C:$_1$	0.132	-0.145	-0.131	0.691	0.414	0.103	-0.051	-0.390	0.155	1.178	-0.206	-1.568	0.86%
		Pt-C:$_2$	0.117	-0.136	-0.124	0.565	0.305	0.095	-0.041	-0.354	0.118	1.009	-0.159	-1.364	-7.31%
		Pt-C:$_3$	0.122	-0.140	-0.088	0.550	0.322	0.598	-0.044	-0.362	0.125	1.025	-0.169	-1.387	-5.83%
		Pt-C:$_4$	0.118	-0.123	-0.118	0.632	0.392	0.045	-0.042	-0.351	0.139	1.179	-0.181	-1.530	-9.43%
7	S_0	Pt-C:$_1$	0.148	-0.162	-0.111	0.736	0.463	0.451	-0.065	-0.437	0.180	1.221	-0.245	-1.659	
		Pt-C:$_2$	0.148	-0.161	-0.113	0.738	0.464	0.433	-0.064	-0.436	0.180	1.221	-0.245	-1.657	
		Pt-C:$_3$	0.148	-0.161	-0.114	0.738	0.464	0.417	-0.065	-0.437	0.180	1.221	-0.245	-1.659	
		Pt-C:$_4$	0.148	-0.161	-0.113	0.736	0.463	0.428	-0.065	-0.439	0.180	1.221	-0.245	-1.660	
	T_1	Pt-C:$_1$	0.153	-0.171	-0.120	0.762	0.470	0.425	-0.070	-0.453	0.187	1.220	-0.257	-1.673	3.58%
		Pt-C:$_2$	0.153	-0.171	-0.122	0.764	0.471	0.406	-0.069	-0.452	0.187	1.221	-0.256	-1.673	3.72%
		Pt-C:$_3$	0.153	-0.171	-0.121	0763	0.470	0.409	-0.070	-0.453	0.187	1.221	-0.257	-1.674	3.81%
		Pt-C:$_4$	0.153	-0.171	-0.121	0.761	0.469	0.418	-0.070	-0.455	0.187	1.220	-0.257	-1.674	3.64%
8	S_0	Pt-C:$_1$	0.134	-0.142	-0.092	0.630	0.395	0.539	-0.053	-0.399	0.152	1.139	-0.205	-1.539	
		Pt-C:$_2$	0.134	-0.142	-0.092	0.630	0.395	0.539	-0.053	-0.399	0.152	1.139	-0.205	-1.539	
		Pt-C:$_3$	0.134	-0.142	-0.092	0.630	0.396	0.540	-0.053	-0.399	0.152	1.140	-0.206	-1.539	
		Pt-C:$_4$	0.134	-0.142	-0.092	0.630	0.395	0.539	-0.053	-0.399	0.152	1.139	-0.205	-1.539	
	T_1	Pt-C:$_1$	0.137	-0.149	-0.099	0.646	0.398	0.501	-0.056	-0.410	0.156	1.135	-0.212	-1.545	2.79%
		Pt-C:$_2$	0.137	-0.149	-0.099	0.646	0.398	0.501	-0.056	-0.410	0.156	1.136	-0.212	-1.546	2.92%
		Pt-C:$_3$	0.137	-0.149	-0.099	0.646	0.398	0.501	-0.056	-0.410	0.156	1.136	-0.212	-1.546	2.84%
		Pt-C:$_4$	0.137	-0.149	-0.099	0.646	0.398	0.501	-0.056	-0.410	0.156	1.135	-0.212	-1.545	2.83%

$\nabla^2\rho_c$ = Laplacian of charge denity at the BCP. λ_1, λ_2, λ_3 =eigenvalues of $\nabla^2\rho_c$ ($\nabla^2\rho_c = \lambda_1 + \lambda_2 + \lambda_3$). ε = bond ellipticity. $G(r_c)$ = electronic kinetic energy density at the BCP. $V(r_c)$ = electronic potential energy density at the BCP. $H(r_c)$ = the total electronic energy density ($H(r_c) = G(r_c) + V(r_c)$) . $\Delta H(r_c)/\rho(r_c) = (T_1\text{-}S_0)/S_0 \times 100\%$.

Figure S3. The localization and delocalization of sigma Pt-C: in occupied orbitals of S_0 state for tetracarbene complexes **5-8**.

5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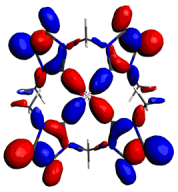
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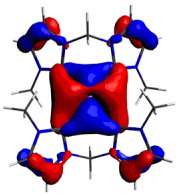
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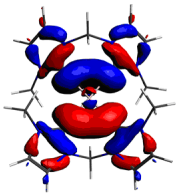
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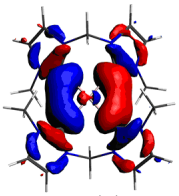
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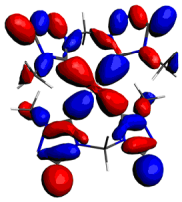
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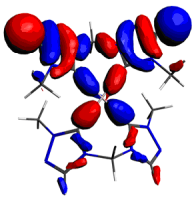
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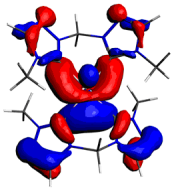
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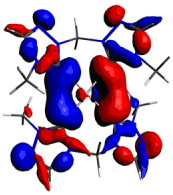
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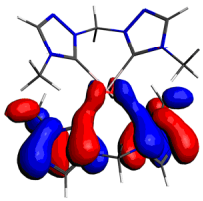
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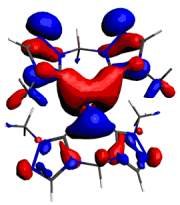
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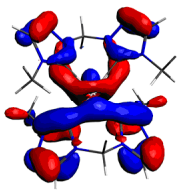
H-5

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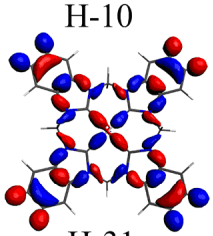
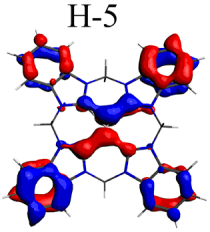

H-31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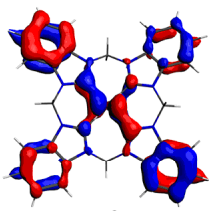
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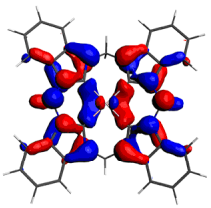
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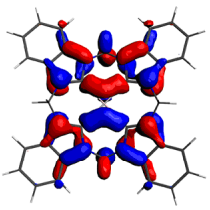
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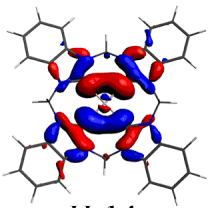
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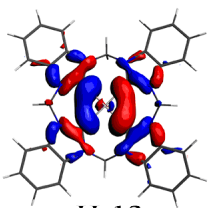
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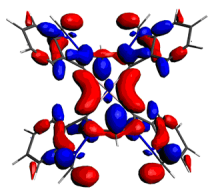
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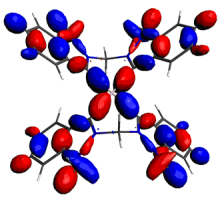
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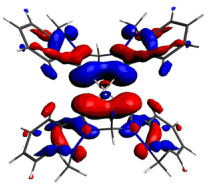
H-13

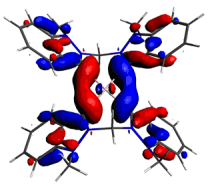
H-12

Table S5. Transition energies calculated at the optimized S_0 geometry of **1** in the gas phase.

State	E/nm(eV)	*f*	Config. (CI coeff.)	Assignment
S_1	331(3.74)	0.0015	H→L+1(0.997)	MLCT/XLCT
S_4	309(4.01)	0.0269	H-1→L+1(0.967)	MLCT/XLCT
S_9	282(4.40)	0.0033	H-2→L+1(0.994)	MLCT
S_{12}	272(4.56)	0.0118	H-4→L(0.968)	XMCT
S_{15}	262(4.73)	0.0122	H-5→L(0.948)	LMCT
S_{16}	261(4.75)	0.2422	H-3→L+1(0.904)	MLCT/XLCT
S_{33}	233(5.33)	0.0157	H-7→L+1(0.908)	XLCT
S_{47}	213(5.81)	0.0166	H-2→L+6(0.967)	MLCT
S_{50}	207(5.98)	0.0210	H-3→L+7(0.914)	MLCT/XLCT

Table S6. Transition energies calculated at the optimized S_0 geometry of **2** in the gas phase.

State	E/nm(eV)	*f*	Config. (CI coeff.)	Assignment
S_1	360(3.44)	0.0130	H→L(0.784)	XLCT/MLCT
			H-2→L(0.195)	XLCT/MLCT
S_2	356(3.48)	0.0106	H-2→L(0.802)	XLCT/MLCT
			H→L(0.186)	XLCT/MLCT
S_4	329(3.77)	0.0381	H-3→L(0.815)	XLCT/XMCT
S_9	308(4.03)	0.0135	H→L+2(0.875)	XLCT/MLCT/MC
S_{14}	300(4.14)	0.0232	H-1→L+2(0.834)	XLCT/MC
S_{15}	293(4.24)	0.0227	H-3→L+2(0.813)	XLCT/XMCT
S_{17}	291(4.26)	0.0109	H-4→L(0.950)	MLCT
S_{21}	269(4.62)	0.0109	H-2→L+4(0.946)	XLCT/MLCT/MC
S_{26}	259(4.78)	0.0249	H-3→L+4(0.572)	XLCT/XMCT
			H-4→L+2(0.268)	MLCT/MXCT/MC
S_{28}	258(4.80)	0.0326	H-4→L+2(0.494)	MLCT/MXCT/MC
			H-5→L(0.298)	XLCT/MLCT/ILCT
S_{29}	254(4.87)	0.0186	H-6→L(0.788)	XLCT/ILCT
S_{32}	239(5.18)	0.0125	H-5→L+1(0.678)	XLCT/MLCT/ILCT
			H-6→L+3(0.290)	XLCT/MLCT/ILCT
S_{41}	230(5.38)	0.0121	H-2→L+7(0.911)	XLCT/MLCT
S_{42}	229(5.43)	0.0528	H-5→L+2(0.383)	XLCT/MC
			H-4→L+5(0.364)	MLCT
S_{44}	226(5.48)	0.0385	H-4→L+5(0.602)	MLCT
			H-5→L+2(0.184)	XLCT/MC
S_{46}	225(5.50)	0.0099	H-6→L+2(0.712)	XLCT/MC
S_{48}	223(5.57)	0.0158	H-8→L+1(0.413)	XLCT/MLCT
			H-5→L+3(0.295)	XLCT/MLCT/ILCT

Table S7. Transition energies calculated at the optimized S_0 geometry of **3** in the gas phase.

State	E/nm(eV)	*f*	Config. (CI coeff.)	Assignment
S_1	501(2.48)	0.0008	H→L(0.593)	$ML_{py}CT/XL_{py}CT$
			H-1→L(0.406)	$ML_{py}CT/XL_{py}CT$
S_2	459(2.70)	0.0563	H-1→L(0.582)	$ML_{py}CT/XL_{py}CT$
			H→L(0.394)	$ML_{py}CT/XL_{py}CT$
S_{17}	283(4.39)	0.0142	H-10→L(0.710)	$ML_{py}CT/L_{NHC}L_{py}CT/XL_{py}CT$
			H-5→L(0.247)	$ML_{py}CT/L_{NHC}L_{py}CT$
S_{19}	276(4.49)	0.0316	H-5→L(0.585)	$ML_{py}CT/L_{NHC}L_{py}CT$
			H-10→L(0.235)	$ML_{py}CT/L_{NHC}L_{py}CT/XL_{py}CT$
S_{21}	266(4.66)	0.0525	H-2→L+3(0.660)	$ML_{NHC}CT$
			H→L+4(0.259)	$ML_{NHC}CT/XL_{NHC}CT$
S_{23}	260(4.77)	0.0101	H-3→L+2(0.544)	MC/MXCT/MLCT
			H→L+4(0.156)	$ML_{NHC}CT/XL_{NHC}CT$
S_{24}	259(4.79)	0.0221	H→L+4(0.362)	$ML_{NHC}CT/XL_{NHC}CT$
			H-3→L+2(0.194)	MC/MXCT/MLCT
			H-1→L+4(0.163)	$ML_{NHC}CT/XL_{NHC}CT$
S_{26}	256(4.84)	0.0598	H-5→L+1(0.401)	$ML_{py}CT/L_{NHC}L_{py}CT$
			H-9→L(0.316)	$IL_{py}CT/L_{py}MCT$
S_{31}	250(4.95)	0.0128	H-4→L+3(0.921)	$XL_{NHC}CT/IL_{NHC}CT/ML_{NHC}CT$
S_{36}	246(5.05)	0.0141	H-2→L(0.594)	$ML_{py}CT/L_{NHC}L_{py}CT$
			H-4→L+2(0.210)	$L_{NHC}MCT/L_{NHC}XCT/L_{NHC}L_{py}CT$
S_{39}	235(5.28)	0.0594	H-5→L+1(0.420)	$ML_{py}CT/L_{NHC}L_{py}CT$
			H-9→L(0.339)	$IL_{py}CT$/LMCT
S_{49}	219(5.67)	0.2115	H-3→L+4(0.700)	$ML_{NHC}CT$
S_{50}	215(5.78)	0.0911	H-12→L+1(0.748)	$ML_{py}CT/XL_{py}CT/L_{NHC}L_{py}CT$

Table S8. Transition energies calculated at the optimized S_0 geometry of **4** in the gas phase.

State	E/nm(eV)	*f*	Config. (CI coeff.)	Assignment
S_2	438(2.83)	0.0073	H-2→L(0.993)	$ML_{py}CT/L_{NHC}L_{py}CT$
S_3	436(2.84)	0.0654	H-1→L(0.950)	MLCT/XLCT
S_7	347(3.57)	0.0164	H-4→L(0.647)	$L_{NHC}MCT/L_{NHC}L_{py}CT$
			H-2→L+1(0.299)	$ML_{py}CT/L_{NHC}L_{py}CT$
S_8	332(3.74)	0.0455	H-2→L+1(0.586)	$ML_{py}CT/L_{NHC}L_{py}CT$
			H-4→L(0.331)	$L_{NHC}MCT/L_{NHC}L_{py}CT$
S_{11}	311(3.98)	0.0499	H-5→L(0.807)	$L_{NHC}MCT/L_{NHC}L_{py}CT$
S_{14}	285(4.36)	0.0203	H-4→L+1(0.585)	$L_{NHC}L_{py}CT$
			H→L+3(0.255)	$XMCT/XL_{py}CT$
S_{21}	267(4.65)	0.1883	H-2→L+2(0.657)	$ML_{py}CT$
			H-6→L+1(0.222)	MLCT/XLCT
S_{26}	255(4.87)	0.0370	H-5→L+1(0.600)	$L_{NHC}L_{py}CT$
			H-10→L(0.305)	$L_{NHC}L_{py}CT$
S_{28}	247(5.02)	0.1968	H-6→L+1(0.609)	MLCT/XLCT
S_{30}	238(5.20)	0.1130	H-3→L+3(0.520)	MC/MXCT/MLCT
			H-10→L(0.278)	$L_{NHC}L_{py}CT$
S_{31}	238(5.21)	0.0899	H-2→L+4(0.733)	$ML_{NHC}CT/L_{py}L_{NHC}CT/IL_{NHC}CT$
S_{33}	237(5.23)	0.0998	H-10→L(0.328)	$L_{NHC}L_{py}CT$
			H-3→L+3(0.324)	MC/MXCT/MLCT
S_{39}	227(5.45)	0.0204	H-4→L+2(0.345)	$L_{NHC}L_{py}CT$
			H-9→L+1(0.326)	MLCT/XLCT
S_{41}	226(5.47)	0.0167	H-9→L+1(0.498)	MLCT/XLCT
			H-2→L+5(0.224)	$ML_{NHC}CT/L_{py}L_{NHC}CT$
			H-4→L+4(0.155)	$IL_{NHC}CT$
S_{45}	220(5.64)	0.1197	H-10→L+1(0.687)	$L_{NHC}L_{py}CT$
			H-13→L(0.178)	$L_{NHC}MCT/L_{NHC}L_{py}CT$
S_{49}	205(6.03)	0.0330	H-5→L+4(0.881)	$L_{py}L_{NHC}CT$

Table S9. Transition energies calculated at the optimized S_0 geometry of **5** in the gas phase, and together with the available experimental values.

State	E/nm(eV)	*f*	Config. (CI coeff.)	Assignment	Expt.(nm)
S_1	334(3.71)	0.0834	H-1→L(0.976)	MLCT/ILCT	
S_2	332(3.73)	0.1725	H→L(0.972)	MLCT/ILCT	315
S_5	287(4.31)	0.0130	H-3→L(0.989)	LMCT	280
S_8	250(4.96)	0.0550	H→L+2(0.796)	MLCT/ILCT	
			H-2→L+1(0.183)	MLCT	
S_9	246(5.03)	0.1004	H-1→L+2(0.878)	MLCT/ILCT	
S_{10}	244(5.09)	0.0122	H-5→L(0.985)	MLCT	
S_{11}	240(5.16)	0.0417	H-6→L(0.776)	MLCT/ILCT	
			H-2→L+1(0.153)	MLCT	
S_{17}	235(5.27)	0.0225	H-2→L+1(0.506)	MLCT	
			H-6→L(0.178)	MLCT/ILCT	
S_{20}	230(5.39)	0.0101	H→L+6(0.437)	MLCT/ILCT	
			H-2→L+3(0.361)	MLCT	
S_{24}	228(5.43)	0.0355	H-8→L(0.885)	LMCT/ILCT	
S_{29}	226(5.50)	0.0160	H-1→L+6(0.266)	MLCT/ILCT	
			H-9→L(0.262)	LMCT/ILCT	
			H-2→L+7(0.161)	MLCT	
S_{33}	218(5.70)	0.0928	H-2→L+5(0.326)	MLCT	
			H-4→L+3(0.284)	ILCT	220
			H-2→L+7(0.234)	MLCT	
S_{36}	216(5.73)	0.0425	H-2→L+3(0.342)	MLCT	
			H-4→L+7(0.319)	ILCT	
S_{40}	214(5.79)	0.1406	H-2→L+5(0.240)	MLCT	
			H-4→L+3(0.199)	ILCT	
			H-2→L+7(0.184)	MLCT	
S_{45}	206(6.03)	0.0215	H-4→L+5(0.612)	LMCT/ILCT	
			H-1→L+9(0.181)	MLCT/ILCT	

Table S10. Transition energies calculated at the optimized S_0 geometry of **6** in the gas phase, and together with the available experimental values.

State	E/nm(eV)	*f*	Config. (CI coeff.)	Assignment	Expt.(nm)
S_1	300(4.14)	0.1444	H→L(0.962)	MLCT/ILCT	
S_2	299(4.14)	0.0734	H-1→L(0.969)	MLCT/ILCT	
S_3	289(4.29)	0.0127	H-2→L(0.988)	MLCT	
S_4	275(4.50)	0.0047	H-3→L(0.965)	LMCT	
S_5	267(4.65)	0.0032	H-4→L(0.934)	MLCT/ILCT	
S_{13}	233(5.32)	0.0254	H-9→L(0.398)	MLCT/ILCT	
			H-1→L+1(0.315)	MLCT	
S_{16}	231(5.38)	0.0295	H→L+2(0.580)	MLCT/ILCT	
S_{19}	228(5.44)	0.0205	H-12→L(0.771)	MLCT/LLCT	
S_{21}	227(5.46)	0.0645	H-1→L+2(0.677)	MLCT/ILCT	
S_{28}	219(5.66)	0.0178	H-14→L(0.705)	LMCT/LLCT	216

Table S11. Transition energies calculated at the optimized S_0 geometry of **7** in the gas phase.

State	E/nm(eV)	*f*	Config. (CI coeff.)	Assignment
S_1	405(3.06)	0.2546	H→L(0.857)	MLCT/ILCT
S_2	405(3.06)	0.2546	H-1→L(0.857)	MLCT/ILCT
S_5	378(3.28)	0.0117	H-4→L(0.728)	LMCT/LLCT
			H-5→L(0.247)	LMCT/ILCT
S_6	378(3.28)	0.0117	H-5→L(0.728)	LMCT/ILCT
			H-4→L(0.247)	LMCT/LLCT
S_9	311(3.98)	0.2123	H→L+1(0.901)	MLCT/LLCT
S_{10}	311(3.98)	0.2123	H-1→L+1(0.901)	MLCT/LLCT
S_{11}	311(3.98)	0.0140	H-8→L(0.993)	MLCT
S_{24}	274(4.53)	0.0499	H-2→L+2(0.772)	LMCT/ILCT
			H-7→L+3(0.168)	ILCT
S_{25}	274(4.53)	0.0499	H-2→L+3(0.771)	LMCT/ILCT
			H-7→L+2(0.168)	LLCT
S_{32}	260(4.76)	0.0804	H-7→L+2(0.331)	LLCT
			H→L+4(0.272)	MLCT/LLCT
S_{33}	260(4.76)	0.0802	H-7→L+3(0.330)	ILCT
			H-1→L+4(0.272)	MLCT/LLCT
S_{35}	259(4.80)	0.0750	H-9→L(0.583)	MLCT/ILCT
			H-1→L+4(0.227)	MLCT/LLCT
S_{36}	258(4.80)	0.0751	H-10→L(0.583)	MLCT/ILCT
			H→L+4(0.228)	MLCT/LLCT
S_{37}	253(4.90)	0.0272	H-1→L+5(0.397)	MLCT/LLCT
			H→L+5(0.141)	MLCT/LLCT
S_{38}	253(4.90)	0.0273	H→L+5(0.393)	MLCT/LLCT
			H-1→L+5(0.139)	MLCT/LLCT

Table S12. Transition energies calculated at the optimized S_0 geometry of **8** in the gas phase.

State	E/nm(eV)	*f*	Config. (CI coeff.)	Assignment
S_1	477(2.60)	0.0296	H-1→L(0.955)	MLCT/ILCT
S_2	474(2.61)	0.1048	H→L(0.949)	MLCT/ILCT
S_8	384(3.23)	0.0180	H-4→L(0.984)	MLCT
S_9	377(3.29)	0.0249	H-1→L+2(0.760)	MLCT/ILCT
S_{11}	369(3.36)	0.0884	H-5→L(0.829)	MLCT/ILCT
S_{12}	365(3.39)	0.0786	H→L+2(0.386)	MLCT/ILCT
			H-2→L+1(0.289)	LMCT/ILCT
			H-3→L+3(0.203)	ILCT
S_{16}	353(3.51)	0.0436	H-8→L(0.934)	ILCT
S_{21}	325(3.82)	0.1866	H-2→L+3(0.408)	ILCT
			H-3→L+1(0.270)	LMCT/ILCT
			H-1→L+2(0.176)	MLCT/ILCT
S_{22}	322(3.85)	0.0201	H-3→L+3(0.629)	ILCT
S_{26}	314(3.95)	0.0439	H-11→L(0.753)	MLCT
			H-12→L(0.174)	ILCT
S_{29}	307(4.04)	0.0630	H-12→L(0.806)	ILCT
S_{31}	306(4.06)	0.0580	H-6→L+1(0.720)	LMCT/ILCT
			H-8→L+2(0.181)	ILCT
S_{36}	293(4.23)	0.0268	H-8→L+2(0.545)	ILCT
			H-7→L+3(0.399)	MLCT
S_{39}	282(4.40)	0.0406	H-9→L+2(0.826)	MLCT
S_{41}	273(4.53)	0.1380	H-11→L+2(0.269)	MLCT
			H-7→L+3(0.263)	MLCT
S_{43}	273(4.55)	0.0115	H-10→L+1(0.860)	MLCT
S_{47}	268(4.63)	0.0925	H-1→L+4(0.523)	MLCT/ILCT

Table S13. Excitation energies E(T_m), zero-filed-splitting (ZFS) parameters and radiative decay rate constants k_r of the $T_m \rightarrow S_0$ transitions of **1-8** at their respective T_1 optimized geometries obtained by DFT/TDDFT calculations. [a,b]

Complexes		E(T_m)	ΔE_{1-2}	ΔE_{1-3}	k_r^1	k_r^2	k_r^3	k_r
		nm	cm^{-1}		s^{-1}			
1	T_1	1328	14.2	320.5	0.17	2020.61	2076.84	1365.88
	T_2	737	1358.1	1439.4	1.35E+5	41.77	1457.73	4.56E+4
2	T_1	4001	37.5	371.3	41.53	44.86	775.19	287.20
	T_2	855	5023.1	5045.1	4.13E+4	9132.42	2939.45	1.78E+4
3	T_1	2309	24.0	315.6	18.64	23.13	257.93	99.90
	T_2	859	1382.1	1548.4	4.39E+4	4655.49	2.09E+4	2.32E+4
	T_3	811	260.0	1557.0	2.02E+4	1.54E+5	4597.70	5.97E+4
4	T_1	814	2.1	169.7	60.75	8190.01	9.81E+4	3.55E+4
5	T_1	409	15.5	209.9	243.07	1.71E+4	8.55E+5	2.91E+5
	T_2	406	245.0	304.5	1.63E+6	3.03E+2	2.06E+5	6.13E+5
6	T_1	867	11.7	83.2	6.99E+3	4.30E+3	6.46E+3	5.92E+3
	T_2	438	6014.6	6071.4	1.14E+5	2.73E+4	1.99E+5	1.13E+5
	T_3	406	824.1	2618.7	7.42E+5	2.09E+6	9.79E+3	9.49E+5
7	T_1	478	1.4	133.2	0.06	255.89	5.76E+5	1.92E+5
	T_2	477	150.7	216.8	6.14E+5	0.00	8.09E+4	2.32E+5
8	T_1	559	4.2	97.4	8.50	3995.21	1.49E+5	5.12E+4
	T_2	556	105.3	112.6	3.32E+5	0.22	1.53E+4	1.16E+5
	T_3	541	0.8	830.8	5.22	358.68	8.40E+6	2.80E+6

[a] $k_r^i \equiv \frac{1}{\tau_i} = \frac{2}{t_0}\alpha_0^3 \left(\Delta E^i\right)^2 f^i$ where $t_0 = (4\pi\varepsilon_0)^2\hbar^3/m_e e$, α_0 is the fine structure constant. Excitation energies ΔE^i and oscillator strengths f^i can be calculated with inclusion of SOC effects.

[b] $k_r^i = \frac{1}{3}\left(k_r^1 + k_r^2 + k_r^3\right)$

Table S14. Molecular orbital compositions at the optimized geometry for **6**.

Orbits	Energy (eV)	d_{Pt} (%)	π (%)	
			p_{pt}	π_{NHC}
HOMO−1	-12.58	43.70		36.29
HOMO	-11.32	22.81	46.86	12.34
LUMO	-9.85	16.54	21.01	42.86

Table S15. Cartesian coordinates of **1** at the S_0 optimized geometry.

Pt	0.000000	0.000000	0.001851
Cl	1.820525	-1.489054	0.002391
Cl	-1.820525	1.489054	0.002391
C	0.000000	0.000000	2.031201
N	0.268139	1.043297	2.868573
C	0.656257	2.375955	2.417947
H	0.027865	2.651923	1.565056
H	1.711784	2.385159	2.119889
H	0.500341	3.084206	3.238344
C	0.172487	0.658434	4.196284
H	0.356322	1.342219	5.013791
C	-0.172487	-0.658434	4.196284
H	-0.356322	-1.342219	5.013791
N	-0.268139	-1.043297	2.868573
C	-0.656257	-2.375955	2.417947
H	-0.500341	-3.084206	3.238344
H	-0.027865	-2.651923	1.565056
C	0.000000	0.000000	-2.027680
N	-0.267173	-1.043573	-2.865188
C	-0.656978	-2.375930	-2.415476
H	-1.720634	-2.392552	-2.147761
H	-0.050346	-2.638974	-1.543125
H	-0.470829	-3.089724	-3.224781
C	-0.172061	-0.658510	-4.192921
H	-0.355636	-1.342376	-5.010447
C	0.172061	0.658510	-4.192921
H	0.355636	1.342376	-5.010447
N	0.267173	1.043573	-2.865188
C	0.656978	2.375930	-2.415476
H	0.050346	2.638974	-1.543125
H	0.470829	3.089724	-3.224781
H	1.720634	2.392552	-2.147761
H	-1.711784	-2.385159	2.119889

Table S16. Cartesian coordinates of **1** at the T_1 optimized geometry.

Pt	-0.060704	-0.106733	0.001849
Cl	2.421449	0.237078	0.020569
Cl	-1.351791	2.039937	-0.019351
C	-0.106004	-0.233707	2.051780
N	0.305916	0.684190	2.973735
C	0.908370	1.978689	2.648270
H	0.263648	2.499749	1.932452
H	1.893618	1.819859	2.196570
H	0.996217	2.558103	3.572414
C	0.119817	0.219525	4.262688
H	0.390925	0.802777	5.132428
C	-0.426132	-1.023797	4.162222

H	-0.726984	-1.729980	4.924127
N	-0.553771	-1.284965	2.808228
C	-1.128647	-2.507087	2.266628
H	-0.746530	-3.372315	2.820578
H	-0.828757	-2.577538	1.215955
C	-0.114563	-0.228501	-2.048308
N	-0.629513	-1.250057	-2.803207
C	-1.263182	-2.440159	-2.256539
H	-2.286525	-2.536017	-2.639915
H	-1.287619	-2.318011	-1.167619
H	-0.685934	-3.336718	-2.515238
C	-0.481005	-1.001631	-4.157414
H	-0.828333	-1.686379	-4.919390
C	0.142744	0.204415	-4.259394
H	0.445007	0.770689	-5.130133
N	0.354318	0.660347	-2.971286
C	1.007243	1.930497	-2.647660
H	0.380777	2.478290	-1.935506
H	1.118843	2.504078	-3.572900
H	1.983954	1.735803	-2.192067
H	-2.224335	-2.483949	2.330308

Table S17. Cartesian coordinates of **2** at the S_0 optimized geometry.

Pt	0.082938	0.108674	0.063815
Cl	-1.708388	0.035737	-1.475672
Cl	-1.480590	-0.063629	1.827222
N	1.629368	-0.242518	-2.586537
C	1.406292	0.353220	-1.379173
N	2.439538	1.251658	-1.257708
N	2.603256	1.182295	1.113236
C	1.593056	0.273930	1.323088
N	1.977770	-0.390023	2.451606
C	2.582746	2.049191	-0.052119
H	1.730051	2.733844	0.026790
H	3.518211	2.613120	-0.100150
C	0.856570	-1.354495	-3.137923
H	-0.129212	-1.352174	-2.660618
H	1.379020	-2.301034	-2.949457
H	0.738514	-1.205697	-4.216641
C	2.769066	0.273423	-3.191462
H	3.105719	-0.064932	-4.162142
C	3.287789	1.211389	-2.355729
H	4.151511	1.854168	-2.457618
C	1.283794	-1.535195	3.038721
H	0.242471	-1.510857	2.700175
H	1.313139	-1.448078	4.130181
H	1.773479	-2.466927	2.728113
C	3.594343	1.081684	2.079863
H	4.466436	1.720977	2.099138
C	3.191820	0.094629	2.923046

H	3.657442	-0.298163	3.816853

Table S18. Cartesian coordinates of **2** at the T_1 optimized geometry.

Pt	0.096949	-0.060433	0.156256
Cl	-2.052212	-0.029375	-0.805814
Cl	0.642885	-2.492053	0.151455
N	1.531735	-0.208260	-2.636542
C	1.362058	0.373489	-1.422243
N	2.461246	1.171983	-1.268970
N	2.643740	1.166087	1.126964
C	1.589071	0.334099	1.431149
N	1.956322	-0.234004	2.617960
C	2.640637	1.980905	-0.072517
H	1.813216	2.698988	-0.012556
H	3.590382	2.517355	-0.143704
C	0.607027	-1.184604	-3.212015
H	-0.359688	-1.073360	-2.710826
H	0.983308	-2.199606	-3.042293
H	0.500710	-0.988485	-4.284542
C	2.718609	0.210451	-3.226638
H	3.036564	-0.136509	-4.201066
C	3.311145	1.081831	-2.365335
H	4.232263	1.643360	-2.446764
C	1.153847	-1.221354	3.331902
H	0.102478	-1.054415	3.076095
H	1.306098	-1.095102	4.409529
H	1.426742	-2.234051	3.015881
C	3.637436	1.109829	2.097742
H	4.542935	1.699485	2.049251
C	3.197808	0.227792	3.034530
H	3.658899	-0.101445	3.956105

Table S19. Cartesian coordinates of **3** at the S_0 optimized geometry.

Pt	2.017362	4.733120	7.697408
Cl	-0.267518	4.675956	7.956606
N	4.069355	4.784471	7.463502
C	4.776822	3.632362	7.304331
N	3.208065	2.161031	8.496043
C	4.002945	2.334506	7.284059
C	2.277507	3.084733	8.866381
N	1.785882	2.623987	10.044779
C	0.794233	3.294086	10.888272
C	2.399529	1.428831	10.397107

C	3.302492	1.134552	9.423144
C	6.160504	3.643755	7.149500
C	6.848015	4.853916	7.145870
C	4.736772	5.970918	7.465602
N	2.868999	7.356939	6.667424
C	3.924561	7.229163	7.667559
C	1.925964	6.386233	6.510177
N	1.158627	6.816690	5.476497
C	0.034121	6.096241	4.876310
C	1.616201	8.039876	5.003676
C	2.700154	8.383054	5.750559
C	6.118549	6.028636	7.304276
H	3.329774	2.323689	6.415618
H	4.693173	1.491128	7.198607
H	2.142332	0.894558	11.302059
H	3.974391	0.294872	9.308039
H	6.690940	2.700981	7.029312
H	7.928623	4.880944	7.022321
H	3.465288	7.211685	8.665675
H	4.573978	8.105906	7.599795
H	1.134973	8.556758	4.184052
H	3.338452	9.255508	5.716618
H	6.615196	6.997103	7.307161
H	-0.106533	5.158192	5.415508
H	-0.877404	6.696939	4.964424
H	0.249825	5.902589	3.819455
H	1.243854	3.532269	11.858972
H	0.467307	4.205215	10.384680
H	-0.070116	2.637074	11.031899

Table S20. Cartesian coordinates of **3** at the T_1 optimized geometry.

Pt	1.939417	4.871619	7.887412
Cl	0.975580	3.471827	6.103764
N	4.100917	4.664205	7.340571
C	4.663168	3.437295	7.285073
N	3.073511	2.280290	8.821476
C	3.789254	2.230575	7.545012
C	2.185529	3.267188	9.124182
N	1.684103	2.922183	10.338472
C	0.684274	3.692601	11.073892
C	2.247293	1.735437	10.785212
C	3.126556	1.328667	9.828366
C	6.008447	3.284794	6.945085
C	6.773046	4.408412	6.646125
C	4.835623	5.767091	7.085427
N	2.953331	7.354435	6.587522
C	4.202338	7.125952	7.305009
C	1.842690	6.583386	6.776988
N	0.890646	7.157374	5.996189

C	-0.496017	6.702070	5.891538
C	1.394427	8.271106	5.341238
C	2.698072	8.398429	5.709770
C	6.177698	5.664932	6.720360
H	3.038364	2.163431	6.741493
H	4.402298	1.326058	7.537146
H	1.980328	1.285314	11.732097
H	3.763755	0.455982	9.779712
H	6.444483	2.287920	6.910947
H	7.820129	4.307758	6.367242
H	4.008432	7.242438	8.382121
H	4.909218	7.904448	7.005899
H	0.791534	8.871126	4.672743
H	3.445534	9.128297	5.429956
H	6.748253	6.566670	6.504895
H	-0.539776	5.651612	6.190227
H	-1.140912	7.311584	6.535545
H	-0.825218	6.790100	4.851560
H	1.075723	3.971123	12.058700
H	0.464300	4.596754	10.498486
H	-0.231422	3.102840	11.193573

Table S21. Cartesian coordinates of **4** at the S_0 optimized geometry.

Pt	9.876229	0.033372	19.214321
N	8.188781	-1.436671	21.521495
N	8.387305	0.718702	21.549034
N	9.557918	1.835952	19.963306
N	10.802577	2.535264	18.204105
N	11.626761	1.149024	16.760207
C	8.750259	-0.425183	20.832530
C	7.493843	-0.962613	22.634483
C	7.614932	0.388241	22.656682
C	8.820402	1.964421	21.087845
C	8.574811	3.214484	21.644424
C	9.117385	4.329960	20.999698
C	9.880585	4.196657	19.836038
C	10.082447	2.913668	19.340027
C	11.497191	3.307922	17.280430
C	12.010998	2.434722	16.378492
C	10.881333	1.177660	17.881140
C	11.994863	-0.065176	16.025892
C	8.285618	-2.854605	21.162290
H	6.974872	-1.627942	23.312101
H	7.225104	1.117955	23.351003
H	7.982475	3.321334	22.548140
H	8.942291	5.321233	21.411614
H	10.300666	5.065149	19.337667
H	11.568396	4.384197	17.336714
H	12.616024	2.614613	15.499447

H	8.885805	-2.937710	20.251749
H	7.280832	-3.254122	20.986851
H	8.765693	-3.404097	21.979313
H	11.561535	-0.924805	16.544996
H	13.086192	-0.155477	15.997334
H	11.600917	-0.005625	15.005498
Cl	10.246024	-2.060002	18.344590

Table S22. Cartesian coordinates of **4** at the T_1 optimized geometry.

Pt	9.779626	0.017973	19.135887
N	8.518759	-1.427402	21.679864
N	8.401944	0.754678	21.561353
N	9.358426	1.876169	19.841005
N	10.807252	2.560222	18.239410
N	11.894916	1.106584	17.017313
C	8.926890	-0.369510	20.919343
C	7.740519	-0.985127	22.732624
C	7.665810	0.376521	22.672028
C	8.740915	2.004688	21.055308
C	8.579770	3.238779	21.659454
C	9.129104	4.365528	21.027955
C	9.886221	4.219501	19.855161
C	10.007535	2.955487	19.306004
C	11.542530	3.286495	17.317278
C	12.211337	2.370608	16.557433
C	11.005069	1.190438	18.049507
C	12.452059	-0.140004	16.495709
C	8.879854	-2.821970	21.432210
H	7.286770	-1.670309	23.437218
H	7.137110	1.077067	23.301803
H	8.068543	3.327668	22.614197
H	9.022248	5.346192	21.483593
H	10.390960	5.070979	19.406838
H	11.516639	4.364444	17.252274
H	12.875964	2.524936	15.717053
H	8.858006	-3.012125	20.354424
H	8.158270	-3.468576	21.938337
H	9.888688	-3.021923	21.811965
H	11.660785	-0.895015	16.448076
H	13.251403	-0.498650	17.154639
H	12.851111	0.043812	15.494821
Cl	9.891926	-2.016420	18.110211；q

Table S23. Cartesian coordinates of **5** at the S_0 optimized geometry.

Pt	-0.031372	0.070633	0.106224
C	1.721211	0.732779	-3.690608
H	2.612843	1.039180	-4.221788
C	0.396804	0.302753	-1.886908
N	2.367566	-1.881171	0.721129
N	-0.279028	0.047004	-3.037288
N	2.892633	-0.195807	-0.511133
N	1.628759	0.725099	-2.305736
C	0.513592	0.310886	-4.148667
H	0.156255	0.167875	-5.160411
C	3.711388	-2.019245	0.392320
H	4.306740	-2.856430	0.733523
C	4.044738	-0.960504	-0.391326
H	4.984697	-0.689641	-0.854065
C	1.846555	-0.753154	0.171887
C	2.707248	0.975331	-1.358209
H	3.630547	1.174399	-1.906303
H	2.458232	1.842703	-0.737668
C	1.630775	-2.890383	1.483469
H	0.601780	-2.549417	1.610506
H	2.100380	-3.036821	2.462093
H	1.633214	-3.838930	0.935010
C	-1.624565	-0.519779	-3.140680
H	-2.037494	-0.624798	-2.135851
H	-1.572157	-1.505721	-3.615805
H	-2.262436	0.137884	-3.740888
C	-1.784591	-0.591125	3.902891
H	-2.676345	-0.897390	4.433912
C	-0.459821	-0.161510	2.099370
N	-2.430348	2.022283	-0.509087
N	0.215743	0.094620	3.249825
N	-2.955465	0.337055	0.723304
N	-1.691887	-0.583645	2.518055
C	-0.577067	-0.169140	4.361089
H	-0.219910	-0.025990	5.372867
C	-3.774344	2.160064	-0.180847
H	-4.369794	2.997029	-0.522414
C	-4.107694	1.101468	0.602980
H	-5.047717	0.830575	1.065571
C	-1.909296	0.894458	0.040503
C	-2.770216	-0.834048	1.570457
H	-3.693579	-1.033070	2.118456
H	-2.521108	-1.701466	0.950049
C	-1.693335	3.031932	-1.270596
H	-0.664559	2.690634	-1.398434
H	-2.163272	3.179724	-2.248851
H	-1.695099	3.979848	-0.721034
C	1.561259	0.661439	3.353405
H	1.974915	0.765051	2.348723
H	1.508667	1.648011	3.827208
H	2.198625	0.004480	3.954908

Table S24. Cartesian coordinates of **5** at the T_1 optimized geometry.

Pt	-0.031467	0.070588	0.106209
C	1.715770	0.711271	-3.687376
H	2.609759	0.964131	-4.242936
C	0.395951	0.353976	-1.856429
N	2.361953	-1.840899	0.781170
N	-0.311532	0.107764	-3.018280
N	2.905197	-0.187137	-0.523575
N	1.646833	0.731722	-2.309930
C	0.477062	0.328251	-4.127523
H	0.114073	0.184523	-5.137425
C	3.683339	-2.009675	0.429889
H	4.275080	-2.848070	0.775296
C	4.028710	-0.976218	-0.400790
H	4.967619	-0.757295	-0.893075
C	1.840360	-0.700017	0.197101
C	2.721440	0.979493	-1.366780
H	3.645752	1.202155	-1.903379
H	2.434297	1.829130	-0.727243
C	1.599429	-2.811962	1.561575
H	0.605598	-2.921217	1.114930
H	1.494310	-2.486565	2.603536
H	2.122290	-3.772276	1.539716
C	-1.667445	-0.431896	-3.082231
H	-1.794429	-1.161834	-2.276075
H	-1.808082	-0.921860	-4.049896
H	-2.415120	0.362949	-2.973000
C	-1.778568	-0.569246	3.899941
H	-2.672560	-0.821895	4.455595
C	-0.458769	-0.212439	2.068881
N	-2.425039	1.981916	-0.569111
N	0.248763	0.033983	3.230675
N	-2.968136	0.328355	0.735915
N	-1.709676	-0.589998	2.522503
C	-0.539813	-0.186222	4.339978
H	-0.176788	-0.042294	5.349841
C	-3.746514	2.150547	-0.217991
H	-4.338353	2.988763	-0.563641
C	-4.091786	1.117236	0.612880
H	-5.030723	0.898239	1.105121
C	-1.903340	0.841224	0.015199
C	-2.784289	-0.838049	1.579423
H	-3.708586	-1.060611	2.116096
H	-2.497117	-1.687845	0.940105
C	-1.662667	2.953009	-1.349652
H	-0.668500	3.061677	-0.903638
H	-1.558412	2.628020	-2.391830
H	-2.185114	3.913535	-1.327024
C	1.604761	0.573451	3.294537
H	1.732269	1.302157	2.487361
H	1.745009	1.064827	4.261550

H	2.352339	-0.221713	3.186861

Table S25. Cartesian coordinates of **6** at the S_0 optimized geometry.

Pt	-0.053643	-0.003983	-0.031401
N	-2.802148	0.333177	-1.165299
N	-1.628758	1.864602	-2.052124
N	-3.663552	0.966878	-2.019251
C	-1.549975	0.843319	-1.149839
N	1.499713	-1.855440	1.989759
N	-2.231064	-1.925032	-0.755260
N	-0.414431	-2.939474	-1.178215
C	-2.919110	1.905178	-2.542431
N	2.708753	-0.343003	1.109715
C	-3.209067	-0.882637	-0.473406
H	-4.178079	-1.199161	-0.865647
H	-3.272819	-0.702957	0.605128
N	2.744395	-2.006339	2.554172
N	0.297109	2.905450	1.122626
C	1.432363	-0.854378	1.093449
N	2.136146	1.926125	0.695268
N	1.279936	3.790760	1.497986
C	-0.890913	-1.762806	-0.676533
C	0.989228	-3.314224	-1.384229
H	1.578969	-2.407877	-1.536573
H	1.058815	-3.940330	-2.278639
H	1.370150	-3.873229	-0.522575
C	3.463669	-1.066073	2.007785
C	0.774134	1.753522	0.617126
C	0.428454	-2.712695	2.492103
H	-0.484844	-2.496366	1.934539
H	0.274965	-2.500939	3.555723
H	0.721223	-3.760699	2.374958
C	-1.086732	3.284481	1.399670
H	-1.746213	2.494691	1.035174
H	-1.304726	4.236734	0.906340
H	-1.212367	3.405489	2.480891
C	2.394620	3.167141	1.236083
C	-0.544127	2.752349	-2.486964
H	0.408842	2.235248	-2.357478
H	-0.551846	3.682144	-1.907777
H	-0.681825	2.987072	-3.546753
C	3.078505	0.860132	0.371341
H	3.052590	0.657076	-0.704524
H	4.087400	1.167413	0.658464
N	-2.628560	-3.126576	-1.275746
C	-1.494632	-3.729804	-1.518138
H	3.385671	3.573714	1.405147
H	-1.407426	-4.723595	-1.944723
H	-3.263547	2.621254	-3.280245

H	4.512620	-0.888790	2.217137

Table S26. Cartesian coordinates of **6** at the T_1 optimized geometry.

Pt	0.138699	-0.082430	-0.240991
N	-2.587436	0.677405	-1.278932
N	-1.175266	1.599068	-2.572868
N	-3.351990	1.357182	-2.185483
C	-1.253816	0.787403	-1.477151
N	2.091525	-1.845126	1.660807
N	-2.592129	-1.467426	-0.284437
N	-1.118930	-2.972306	-0.638116
C	-2.459019	1.919596	-2.960897
N	2.877993	0.016328	0.998439
C	-3.204852	-0.158820	-0.250824
H	-4.268714	-0.258685	-0.477159
H	-3.057054	0.293051	0.734539
N	3.298785	-1.701063	2.308978
N	-0.337152	2.443632	1.735343
C	1.795791	-0.826544	0.824495
N	1.675993	2.056772	1.132999
N	0.398494	3.515216	2.184293
C	-1.254167	-1.681484	-0.189385
C	0.119300	-3.707670	-0.922129
H	0.968120	-3.030546	-0.805097
H	0.090638	-4.062180	-1.958065
H	0.216576	-4.564447	-0.248506
C	3.749013	-0.549443	1.905101
C	0.401868	1.533267	1.075045
C	1.285381	-2.994612	2.058650
H	0.255321	-2.833584	1.735106
H	1.322634	-3.066839	3.149854
H	1.701284	-3.911704	1.629322
C	-1.760077	2.409259	2.061296
H	-2.028076	1.401226	2.391623
H	-2.357257	2.716413	1.195305
H	-1.922172	3.116772	2.878208
C	1.621389	3.253986	1.807003
C	0.051005	2.036532	-3.248057
H	0.847322	1.325854	-3.009321
H	0.330015	3.042507	-2.915627
H	-0.116285	2.042698	-4.329481
C	2.840817	1.389110	0.539688
H	2.749132	1.406835	-0.553621
H	3.751033	1.911407	0.844984
N	-3.297256	-2.536305	-0.783514
C	-2.375149	-3.440352	-0.969819
H	2.474349	3.896306	1.995852
H	-2.564030	-4.439648	-1.347248
H	-2.696551	2.549049	-3.811542

H	4.687009	-0.105561	2.219908

Table S27. Cartesian coordinates of **7** at the S_0 optimized geometry.

Pt	-0.031513	0.127925	0.117245
C	-0.221089	1.497051	-1.322371
C	-0.175480	3.470928	-2.444016
C	-0.677223	2.485878	-3.314968
C	-1.063850	2.793705	-4.618755
H	-1.469498	2.047923	-5.299062
C	-0.910437	4.118432	-5.025260
H	-1.197569	4.399144	-6.036069
C	-0.393288	5.098523	-4.161052
H	-0.286241	6.119929	-4.519179
C	-0.014359	4.793680	-2.854468
H	0.388087	5.563474	-2.199451
C	-1.297217	0.047333	-3.055554
H	-1.173366	0.010552	-4.141644
N	0.077611	2.818018	-1.224798
N	-0.673440	1.284318	-2.584788
C	-0.267786	-1.323410	-1.232099
C	-0.758488	-2.421919	-3.157939
C	-0.289048	-3.365426	-2.225170
C	-0.172690	-4.716395	-2.549918
H	0.204348	-5.455737	-1.846485
C	-0.562787	-5.091380	-3.834795
H	-0.490353	-6.136636	-4.126681
C	-1.047590	-4.151840	-4.760603
H	-1.344764	-4.486858	-5.751773
C	-1.156365	-2.799443	-4.439835
H	-1.537540	-2.085606	-5.166957
C	0.677194	-3.214068	0.107652
H	0.378211	-4.263360	0.184117
N	-0.714120	-1.176929	-2.506050
N	-0.012964	-2.644610	-1.049998
C	0.157760	-1.241176	1.556921
C	0.450775	-3.222429	2.627041
C	0.272434	-2.222684	3.601374
C	0.277579	-2.522249	4.963114
H	0.124151	-1.764340	5.728369
C	0.488461	-3.854880	5.314236
H	0.502758	-4.129710	6.366491
C	0.683600	-4.850414	4.341739
H	0.848593	-5.877757	4.658464
C	0.670137	-4.553463	2.979635
H	0.826894	-5.335391	2.239633
C	-0.292917	0.241435	3.522264
H	0.149523	0.265988	4.522227
N	0.357954	-2.572923	1.383505
N	0.110004	-1.017694	2.895330

C	0.204999	1.579253	1.466550
C	0.355331	2.685066	3.444159
C	0.565693	3.613950	2.408037
C	0.829919	4.956735	2.674931
H	1.011653	5.684082	1.886562
C	0.855160	5.339563	4.015266
H	1.054810	6.378971	4.265798
C	0.628189	4.415348	5.049269
H	0.653035	4.756296	6.081802
C	0.372442	3.070768	4.783948
H	0.194875	2.368918	5.596014
C	0.788080	3.437008	-0.105478
H	0.524246	4.498399	-0.096400
N	0.151655	1.443510	2.816484
N	0.449589	2.889696	1.208534
H	-1.387781	0.262980	3.616528
H	1.762419	-3.164147	-0.059239
H	-2.370522	0.072618	-2.820071
H	1.870792	3.340452	-0.268147

Table S28. Cartesian coordinates of **7** at the T_1 optimized geometry.

Pt	0.028319	0.126355	0.108374
C	-0.177142	1.484685	-1.313458
C	-0.165933	3.470888	-2.426338
C	-0.670795	2.474910	-3.304224
C	-1.076237	2.787420	-4.601608
H	-1.481976	2.040474	-5.280217
C	-0.937473	4.114714	-5.004744
H	-1.238360	4.399068	-6.010508
C	-0.412384	5.098525	-4.141304
H	-0.316080	6.120808	-4.500047
C	-0.015418	4.793473	-2.839263
H	0.388553	5.564570	-2.187148
C	-1.324097	0.049604	-2.997010
H	-1.340339	0.014911	-4.089059
N	0.101813	2.826166	-1.217412
N	-0.641475	1.275827	-2.591924
C	-0.224145	-1.312477	-1.223816
C	-0.752946	-2.410880	-3.147693
C	-0.281271	-3.365155	-2.207243
C	-0.176127	-4.715798	-2.534546
H	0.202003	-5.456860	-1.833925
C	-0.584383	-5.089893	-3.814912
H	-0.523225	-6.135688	-4.107391
C	-1.076486	-4.146112	-4.740228
H	-1.387613	-4.483831	-5.726169
C	-1.169848	-2.791831	-4.422963
H	-1.550596	-2.076519	-5.148496
C	0.765030	-3.179432	0.093202

H	0.581452	-4.254896	0.152978
N	-0.682483	-1.170380	-2.513578
N	0.009468	-2.653768	-1.041801
C	0.197517	-1.231180	1.535736
C	0.454654	-3.223224	2.607825
C	0.276326	-2.212362	3.589623
C	0.262002	-2.515680	4.950901
H	0.108485	-1.756542	5.714584
C	0.457830	-3.850226	5.303211
H	0.457790	-4.127992	6.354785
C	0.660136	-4.849896	4.329135
H	0.815108	-5.877629	4.649710
C	0.664705	-4.553649	2.965981
H	0.823387	-5.337047	2.228311
C	-0.335509	0.240330	3.474809
H	-0.024885	0.268696	4.522070
N	0.378130	-2.582656	1.369786
N	0.143384	-1.011045	2.893046
C	0.244282	1.566021	1.446075
C	0.357660	2.673614	3.432993
C	0.568752	3.612991	2.388690
C	0.823374	4.955892	2.661112
H	1.007487	5.684671	1.874966
C	0.829740	5.338918	4.002450
H	1.019075	6.379354	4.256678
C	0.595007	4.411024	5.038320
H	0.605014	4.755477	6.069917
C	0.354566	3.063896	4.772002
H	0.176433	2.360816	5.582558
C	0.875490	3.397881	-0.117418
H	0.727972	4.480492	-0.126863
N	0.184275	1.435235	2.814668
N	0.469826	2.897339	1.194172
H	-1.436686	0.257065	3.422797
H	1.839296	-3.002197	-0.076243
H	-2.359698	0.079027	-2.619871
H	1.943097	3.174407	-0.273756

Table S29. Cartesian coordinates of non-truncated **7** at the S_0 optimized geometry.

Pt	7.852893	10.804151	1.706477
C	6.070329	11.710816	1.746874
C	4.262449	12.873911	2.472734
C	4.162586	12.742773	1.078106
C	3.101259	13.317799	0.374915
H	3.010132	13.241816	-0.705192
C	2.146018	14.011346	1.114885
H	1.308492	14.473922	0.597767
C	2.243661	14.130767	2.511383
H	1.479042	14.681855	3.054140

C	3.307807	13.570558	3.213961
H	3.389037	13.692830	4.290936
C	5.437321	11.482215	-0.736381
H	5.059522	12.296722	-1.365183
C	4.940393	9.115261	-0.246960
H	6.011625	8.991541	-0.047247
H	4.596666	8.239202	-0.810808
H	4.401687	9.142410	0.717817
C	3.319833	10.478937	-1.491754
H	2.610316	10.625497	-0.659486
H	3.019443	9.580595	-2.044845
H	3.241660	11.331757	-2.178493
N	5.441422	12.209547	2.846101
N	5.297221	12.014339	0.669963
N	4.707545	10.311307	-1.056177
C	7.911383	11.007588	-0.282563
C	7.259032	11.262767	-2.440649
C	8.622171	10.925185	-2.436533
C	9.327213	10.761980	-3.631457
H	10.378312	10.487331	-3.653788
C	8.626066	10.960213	-4.818955
H	9.144473	10.837676	-5.767154
C	7.265017	11.308876	-4.818547
H	6.751341	11.453289	-5.766271
C	6.555726	11.458793	-3.629321
H	5.496204	11.700972	-3.640438
C	10.428727	10.632801	-0.659675
H	10.857253	9.961325	-1.412696
C	10.756125	12.919921	0.206737
H	9.953447	13.510918	-0.270932
H	11.606488	13.585069	0.401664
H	10.390152	12.545503	1.170382
C	11.852166	12.227996	-1.880285
H	12.263255	11.354141	-2.402242
H	12.690512	12.892029	-1.636566
H	11.173744	12.765219	-2.564905
N	6.864785	11.320442	-1.094520
N	8.986762	10.780437	-1.083507
N	11.213841	11.811155	-0.630340
C	9.643468	9.913393	1.668019
C	11.720464	9.282565	1.007522
C	11.539774	8.858982	2.334209
C	12.563266	8.209168	3.028325
H	12.452033	7.884932	4.059449
C	13.758308	7.989905	2.346503
H	14.576683	7.489524	2.859057
C	13.931095	8.405249	1.015463
H	14.879617	8.217862	0.517326
C	12.917716	9.065783	0.325124
H	13.071421	9.408153	-0.694950
C	9.597645	8.799596	3.986843
H	10.410271	8.845370	4.721094
C	9.991804	6.393011	4.323931
H	10.613537	6.073334	3.470223
H	9.402866	5.531393	4.661460

H	10.650384	6.688054	5.151119
C	8.058947	7.139614	3.004038
H	7.338167	7.958482	2.891513
H	7.514049	6.252962	3.351116
H	8.496237	6.914818	2.014090
N	10.523510	9.911332	0.629711
N	10.242082	9.264879	2.702743
N	9.071088	7.484920	4.002006
C	7.785860	10.583865	3.693439
C	8.167586	9.794282	5.786021
C	7.084992	10.686533	5.849800
C	6.417012	10.923372	7.053664
H	5.568337	11.598196	7.125022
C	6.877409	10.249556	8.182861
H	6.377399	10.408820	9.135484
C	7.968047	9.366263	8.117042
H	8.297094	8.857183	9.020090
C	8.627508	9.117396	6.915777
H	9.452144	8.410823	6.870002
C	5.946750	12.299695	4.234722
H	5.082962	12.110436	4.882456
C	7.655551	14.040031	3.860487
H	8.559279	13.646072	4.360300
H	7.697058	15.136039	3.883847
H	7.668251	13.722235	2.810926
C	6.248554	14.112152	5.873053
H	5.256801	13.837399	6.255129
H	6.300364	15.207456	5.845456
H	7.015347	13.747712	6.577894
N	8.580609	9.773391	4.444462
N	6.884436	11.155093	4.536503
N	6.418361	13.606678	4.509461

Table S30. Cartesian coordinates of **8** at the S_0 optimized geometry.

Pt	0.006207	-0.003012	-0.000278
N	-0.773229	2.597110	1.203399
C	0.815924	1.815916	2.515415
N	-0.446313	3.651681	2.069312
C	0.004091	1.502439	1.387280
C	-0.802968	-1.824465	-2.514417
N	-0.775167	2.597242	-1.202546
C	0.813888	1.817404	-2.515647
C	0.493078	3.136620	2.935094
N	0.788076	-2.602710	-1.202689
C	-1.573535	2.793278	0.001113
H	-2.018539	3.789028	0.001556
H	-2.370326	2.042266	0.001676
C	-0.479642	-3.145444	-2.932486
C	-0.804821	-1.823442	2.513464
C	0.009385	-1.509060	-1.387071

N	0.787373	-2.602400	1.203500
C	-0.482123	-3.144348	2.932250
C	0.002666	1.503023	-1.387225
N	0.460394	-3.659477	-2.066326
C	0.008706	-1.508615	1.386793
N	0.458695	-3.658769	2.067174
C	1.587097	-2.797995	0.000675
H	2.383407	-2.046452	0.000786
H	2.032677	-3.793455	0.000860
N	-0.448176	3.653098	-2.067335
C	0.490744	3.138327	-2.934143
C	1.806952	1.093325	-3.207616
C	2.415599	1.684670	-4.297781
C	2.054674	2.988702	-4.715282
C	1.092727	3.734820	-4.052059
C	-1.797105	-1.101270	-3.205728
C	-2.406548	-1.693525	-4.294968
C	-2.045340	-2.997557	-4.712195
C	-1.082359	-3.742824	-4.049487
C	1.809502	1.091407	3.206227
C	2.419038	1.682057	4.296226
C	2.058564	2.985914	4.714793
C	1.096125	3.732460	4.052874
C	-1.799679	-1.099926	3.203425
C	-2.410439	-1.691782	4.292142
C	-2.049869	-2.995747	4.710118
C	-1.086177	-3.741307	4.048770
H	2.079021	0.092136	-2.881819
H	3.183069	1.148167	-4.851501
H	2.551772	3.422036	-5.581281
H	0.839004	4.739297	-4.384204
H	-2.069317	-0.100029	-2.880239
H	-3.174862	-1.157699	-4.848175
H	-2.543004	-3.431567	-5.577540
H	-0.828346	-4.747334	-4.381328
H	2.081310	0.090420	2.879596
H	3.186937	1.145189	4.848998
H	2.556493	3.418704	5.580586
H	0.842770	4.736776	4.385805
H	-2.071446	-0.098753	2.877328
H	-3.179300	-1.155692	4.844331
H	-2.548656	-3.429498	5.574935
H	-0.832679	-4.745735	4.381243
C	1.436159	-4.691346	-2.397792
H	1.713406	-5.269223	-1.509378
H	0.952953	-5.382674	-3.093027
H	2.332659	-4.270741	-2.874922
C	1.433916	-4.690810	2.399704
H	0.949834	-5.382048	3.094401
H	1.711997	-5.268619	1.511535
H	2.329957	-4.270298	2.877783
C	-1.418030	4.688669	2.395602
H	-0.937806	5.372296	3.100399
H	-1.681280	5.273604	1.507481
H	-2.322601	4.271871	2.860678

C	-1.422858	4.686578	-2.396613
H	-1.695348	5.266540	-1.508078
H	-0.940926	5.375604	-3.094977
H	-2.322137	4.267182	-2.869571

Table S31. Cartesian coordinates of **8** at the T_1 optimized geometry.

Pt	0.005800	-0.003467	0.000207
N	-0.852250	2.588131	1.211197
C	0.809120	1.834707	2.474302
N	-0.460948	3.663518	2.034720
C	-0.044001	1.493433	1.375810
C	-0.797025	-1.841890	-2.474101
N	-0.852145	2.587904	-1.210945
C	0.808615	1.834027	-2.474745
C	0.509652	3.168149	2.873570
N	0.864362	-2.594812	-1.210816
C	-1.642582	2.763424	0.000052
H	-2.139269	3.734847	-0.000086
H	-2.395972	1.966530	0.000082
C	-0.497038	-3.175183	-2.873427
C	-0.797803	-1.841296	2.474577
C	0.055856	-1.500407	-1.375506
N	0.863456	-2.594782	1.211185
C	-0.498087	-3.174716	2.873978
C	-0.043997	1.492966	-1.375718
N	0.473561	-3.670422	-2.034370
C	0.055054	-1.499955	1.375829
N	0.472769	-3.669508	2.035441
C	1.654437	-2.770008	0.000513
H	2.407646	-1.972935	0.000791
H	2.151323	-3.741339	0.000715
N	-0.461280	3.662765	-2.035129
C	0.509104	3.167491	-2.874098
C	1.817719	1.130013	-3.148966
C	2.468105	1.747676	-4.214618
C	2.137768	3.059882	-4.609585
C	1.158085	3.794058	-3.949319
C	-1.806779	-1.138212	-3.147868
C	-2.457093	-1.755993	-4.213282
C	-2.125939	-3.067967	-4.608605
C	-1.145725	-3.801743	-3.948779
C	1.818750	1.130828	3.147960
C	2.469549	1.748585	4.213129
C	2.138929	3.060676	4.608370
C	1.158786	3.794664	3.948685
C	-1.807322	-1.137633	3.148454
C	-2.458086	-1.755637	4.213716
C	-2.127570	-3.067754	4.608725
C	-1.147335	-3.801570	3.948882

H	2.078068	0.120285	-2.840349
H	3.247762	1.213978	-4.754086
H	2.665643	3.513751	-5.445805
H	0.923827	4.811473	-4.255756
H	-2.067535	-0.128685	-2.838935
H	-3.237288	-1.222744	-4.752415
H	-2.653677	-3.521923	-5.444875
H	-0.910839	-4.818883	-4.255635
H	2.079116	0.121169	2.839142
H	3.249738	1.215186	4.752065
H	2.666989	3.514579	5.444435
H	0.924288	4.811898	4.255496
H	-2.067761	-0.127926	2.839863
H	-3.238192	-1.222259	4.752801
H	-2.655704	-3.521844	5.444655
H	-0.912828	-4.818889	4.255431
C	1.400259	-4.750352	-2.336407
H	1.640400	-5.325077	-1.434638
H	0.902628	-5.428471	-3.034177
H	2.322922	-4.372229	-2.800413
C	1.395385	-4.754133	2.332017
H	0.899828	-5.427716	3.035597
H	1.624747	-5.332170	1.429501
H	2.323917	-4.380229	2.787645
C	-1.386298	4.744817	2.335669
H	-0.888369	5.422304	3.033824
H	-1.624726	5.319739	1.433569
H	-2.309942	4.368105	2.798850
C	-1.384943	4.746191	-2.333230
H	-1.617212	5.323333	-1.430897
H	-0.888747	5.421002	-3.035201
H	-2.311898	4.371171	-2.791152